



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 07:26 PM EDT

PDB ID : 4V7U / pdb_00004v7u
Title : Crystal structure of the E. coli ribosome bound to erythromycin.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-15
Resolution : 3.10 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

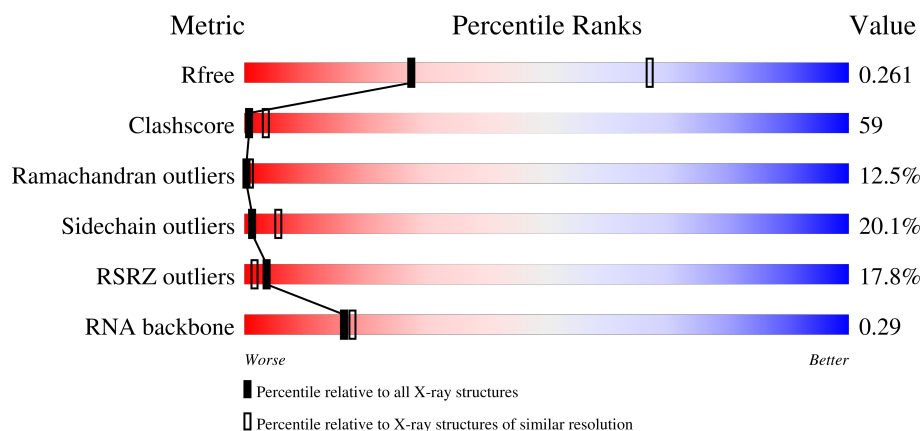
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	1533	2% 15% 50% 24% 11%
1	CA	1533	10% 12% 50% 29% 9%
2	AB	218	5% 19% 57% 21% .
2	CB	218	18% 22% 63% 14% .

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Mol	Chain	Length	Quality of chain
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	
15	AO	88	

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Mol	Chain	Length	Quality of chain
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	2904	
22	DA	2904	
23	BB	118	
23	DB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	178	
27	DF	178	

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Mol	Chain	Length	Quality of chain
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	
40	BS	110	

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	79	
44	DW	79	
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	
52	D4	38	

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
53	MG	DA	3026	-	-	-	X
53	MG	DA	3028	-	-	-	X
53	MG	DA	3057	-	-	-	X
53	MG	DA	3063	-	-	-	X
53	MG	DA	3074	-	-	-	X
53	MG	DA	3108	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284525 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	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- 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	150	Total	C	N	O	S	0	0	0
			1175	730	226	215	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	1
			877	541	178	155	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	95	Total	C	N	O	S	0	0	0
			769	480	159	127	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
			714	439	144	130	1			
15	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	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	81	Total	C	N	O	S	0	0	1
			639	400	127	111	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	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
22	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
23	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- 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	178	Total	C	N	O	S	0	0	1
			1411	899	250	256	6			
27	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	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
			1111	699	197	214	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	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			
			780	492	146	142	0	0	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BW	79	Total	C	N	O	S		
			596	367	120	108	1	0	0
44	DW	79	Total	C	N	O	S		
			596	367	120	108	1	0	0

- 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		
			625	388	129	106	2	0	0
45	DX	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

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

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

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

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

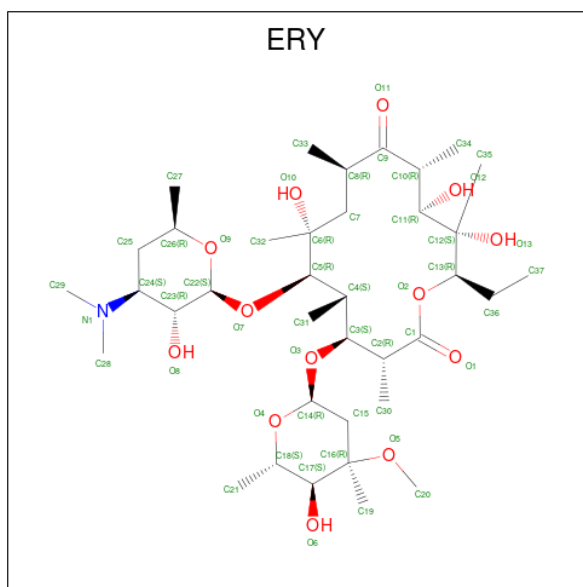
- Molecule 52 is a protein called 50S ribosomal protein L36.

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	AA	41	Total	Mg	0	0
			41	41		
53	AN	2	Total	Mg	0	0
			2	2		
53	BA	135	Total	Mg	0	0
			135	135		
53	BB	4	Total	Mg	0	0
			4	4		
53	CA	42	Total	Mg	0	0
			42	42		
53	DA	133	Total	Mg	0	0
			133	133		
53	DB	1	Total	Mg	0	0
			1	1		
53	DC	2	Total	Mg	0	0
			2	2		
53	DJ	1	Total	Mg	0	0
			1	1		

- Molecule 54 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	BA	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	197	Total O 197 197	0	0
56	AE	1	Total O 1 1	0	0
56	AL	1	Total O 1 1	0	0
56	AN	7	Total O 7 7	0	0
56	AT	1	Total O 1 1	0	0
56	AU	1	Total O 1 1	0	0
56	BA	605	Total O 605 605	0	0
56	BB	19	Total O 19 19	0	0
56	BC	7	Total O 7 7	0	0
56	BD	3	Total O 3 3	0	0
56	BE	1	Total O 1 1	0	0
56	BL	4	Total O 4 4	0	0
56	BN	2	Total O 2 2	0	0
56	BR	1	Total O 1 1	0	0
56	BT	2	Total O 2 2	0	0
56	BV	1	Total O 1 1	0	0
56	B3	3	Total O 3 3	0	0
56	B4	2	Total O 2 2	0	0

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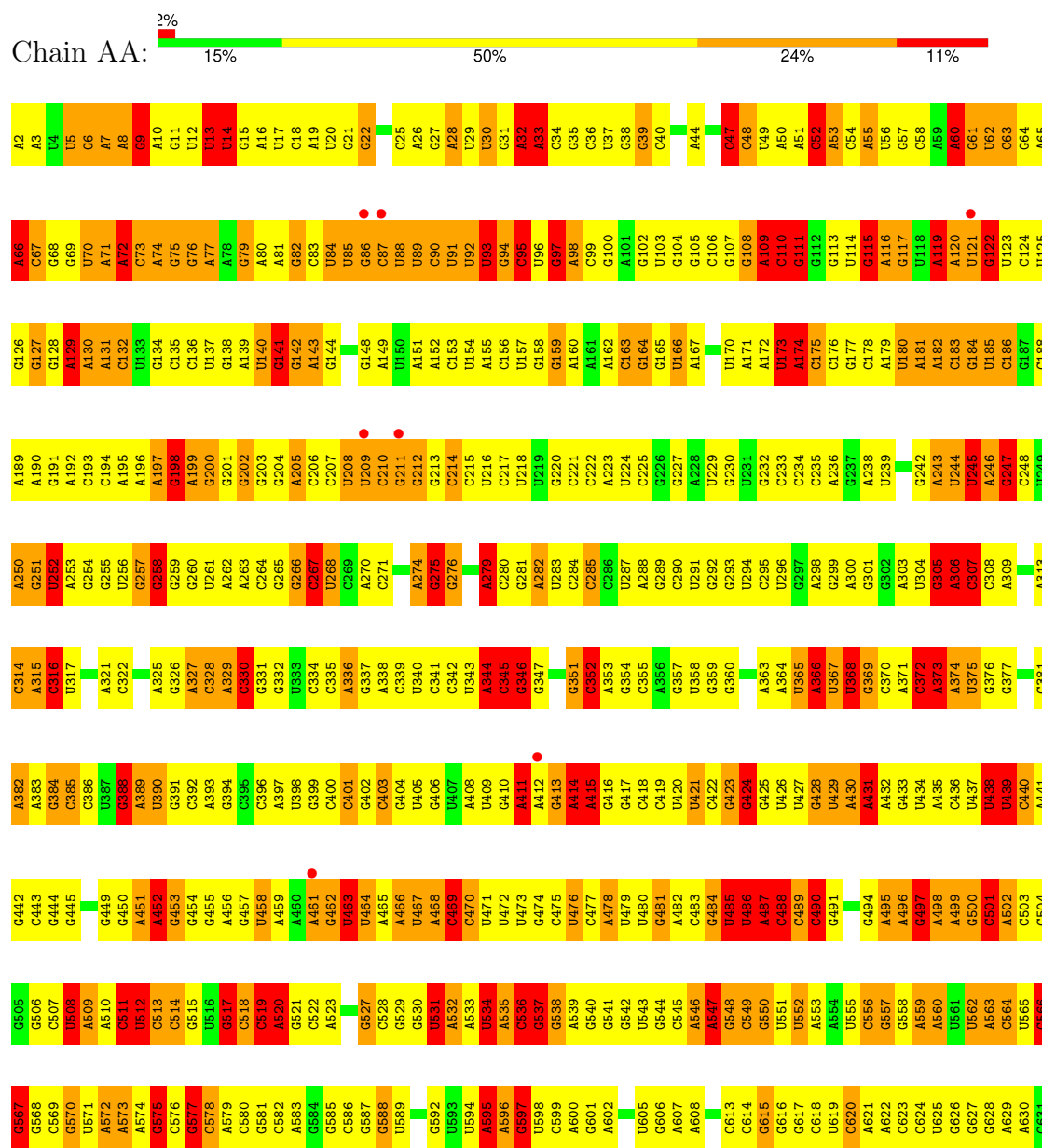
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CA	195	Total 195	O 195	0	0
56	CE	3	Total 3	O 3	0	0
56	CL	1	Total 1	O 1	0	0
56	CN	3	Total 3	O 3	0	0
56	CT	4	Total 4	O 4	0	0
56	CU	1	Total 1	O 1	0	0
56	DA	600	Total 600	O 600	0	0
56	DB	3	Total 3	O 3	0	0
56	DC	13	Total 13	O 13	0	0
56	DD	2	Total 2	O 2	0	0
56	DE	4	Total 4	O 4	0	0
56	DJ	3	Total 3	O 3	0	0
56	DL	4	Total 4	O 4	0	0
56	DN	2	Total 2	O 2	0	0
56	DT	2	Total 2	O 2	0	0
56	DU	2	Total 2	O 2	0	0
56	DV	2	Total 2	O 2	0	0
56	D2	1	Total 1	O 1	0	0
56	D3	1	Total 1	O 1	0	0
56	D4	4	Total 4	O 4	0	0

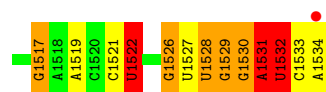
3 Residue-property plots

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.

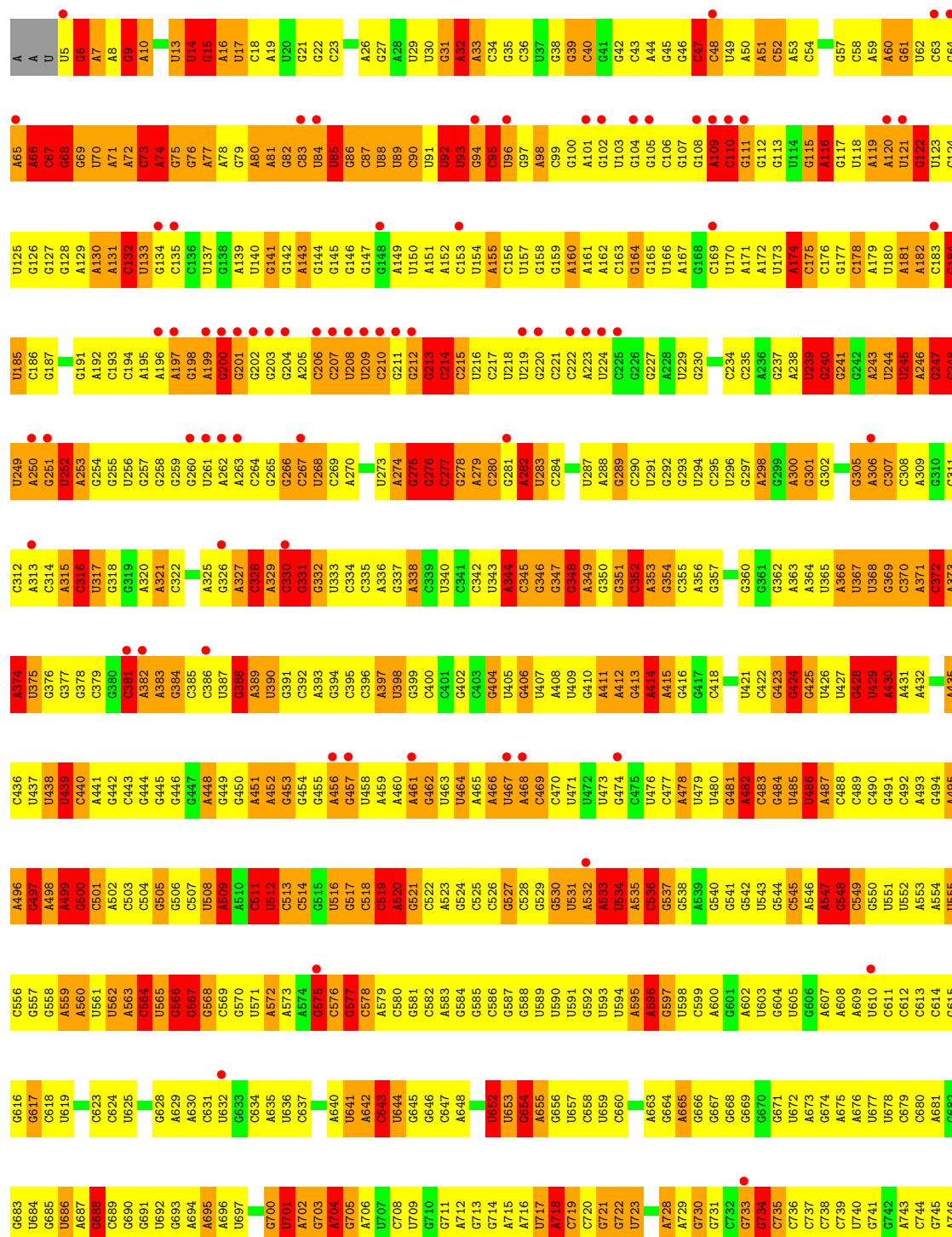
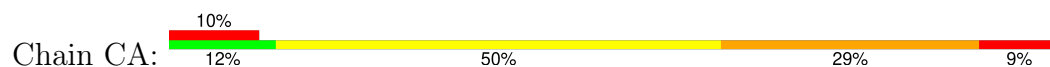
• Molecule 1: 16S rRNA

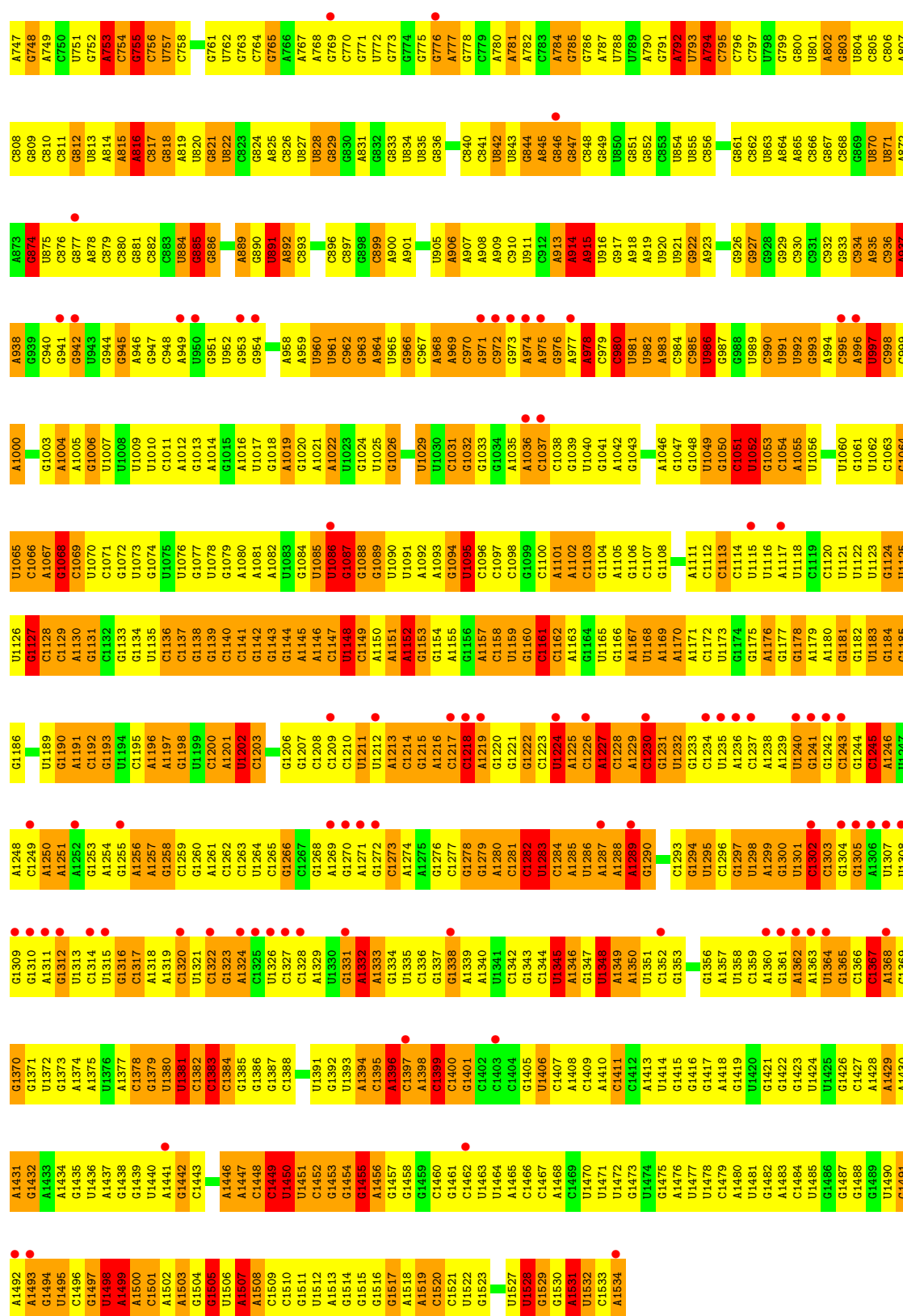


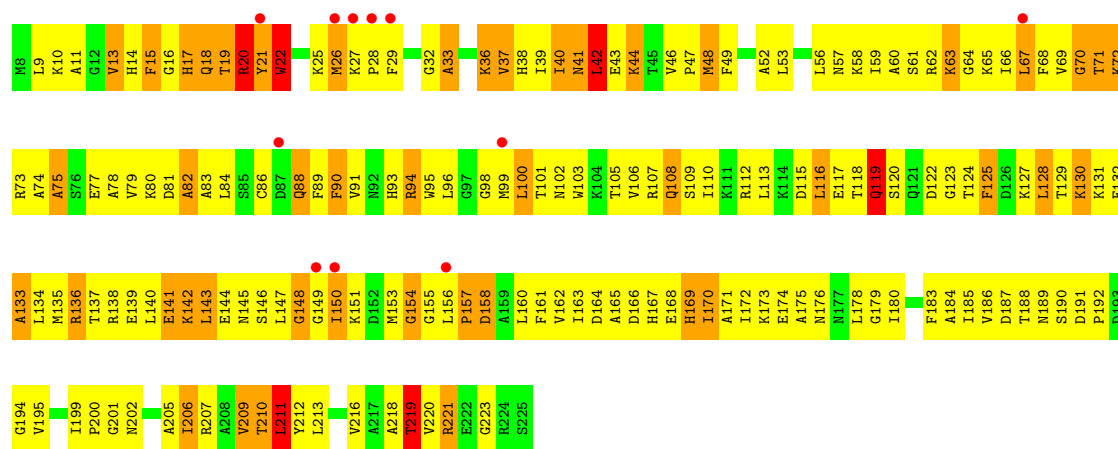
G1454	G1455	G1391	G1392	G1328	U1264	G1138	U1076	G1011	G948	U884	G818	C756	G632
G1456	G1457	U1329	G1393	G1329	C1287	G1139	G1077	A1012	A949	G885	A819	U757	G633
A1458	U1330	U1330	G1394	G1330	G1288	C1140	U1078	G1013	U950	G886	U820	C758	G634
G1459	G1331	G1331	G1395	G1331	A1269	C1141	U1079	A1014	G951	G887	G821	G759	A635
C1460	A1332	A1332	G1396	A1332	G1270	G1142	A1080	G1015	U952	G888	G824	G760	U636
G1461	A1333	A1333	C1397	A1333	G1271	G1143	A1081	G1016	G953	G889	G825	G761	C637
C1462	G1334	G1334	A1398	G1334	G1272	G1144	A1082	U1017	G954	G890	A826	U762	U638
G1399	U1335	U1335	G1399	U1335	G1273	A1145	U1083	G1018	U957	U891	U827	G763	G639
U1463	C1336	C1336	G1400	C1336	A1274	A1146	U1085	A1021	U958	G895	U828	C764	A640
U1464	G1337	G1337	G1401	G1337	A1275	C1147	U1086	A1022	A959	G896	U829	G765	U641
A1465	G1338	G1338	C1402	G1338	G1276	C1149	G1087	U1023	U960	G897	G830	A767	A642
	A1339	A1339	C1403	A1339	C1277	C1150	G1088	G1024	U961	U962	A831	A768	A643
A1468			G1404		G1278	A1151	G1089	U1025	C962		G832	G769	U644
C1469	G1343	G1343	G1405	G1343	G1279	A1152	U1090	U1026		A900	G833	G770	G645
U1470	C1344	C1344		C1344	A1280	G1153	U1091	C1027	U965	G902	G834	C771	G646
U1471	U1345	U1345	A1409	U1345	C1281	G1154	U1092	G1028	G966	G903	G772	C770	C647
U1472	A1346	A1346	A1410	A1346	G1282	G1155	A1093	U1029	G967	U904	U773	G771	U709
G1473	G1347	G1347	C1411	G1347	U1283	C1156	G1094	U1030	A968	U905	G774	G772	A648
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G1475	A1349	A1349	A1413	A1349	C1285	C1158	C1096	G1032	C970	A908	C841	A777	G710
A1476	U1350	U1350	G1414	U1350	U1286	U1159	G1097	G1033	G971	A909	U842	A778	G711
U1477	U1351	U1351	G1415	U1351	A1287	G1160	C1098	G1034	C972	G910	U843	C779	G651
U1478	C1352	C1352	G1416	C1352	A1288	C1161	G1099	G1037	G973	U911	C844	C779	G650
G1479	G1353	G1353	G1417	G1353	A1289	C1162	C1100	U1037	A974	C912	A845	C780	C651
A1480	U1354	U1354	A1418			A1163	A1101	G1038	A975	A913	G846	A781	U652
U1481	G1355	G1355		G1355	G1292	U1164	A1102	C1039	G976	A914	G847	A782	U653
G1482	C1356	C1356	G1421	G1482	U1293	U1165	C1103	U1040	A977	A915	C848	C783	U654
A1483	U1357	U1357	G1422	U1357	G1294	G1166	G1104	G1045	A978	U916	U849	C784	C660
G1484	C1358	C1358	G1423	C1358	U1295	A1167	G1108	C1051	G979	G917	U850	C785	G661
U1485	C1359	C1359	U1424	C1359	U1296	U1168	C1109	C1052	C980	A918	U855	A787	U662
G1486	A1360	A1360	U1425	A1360	G1297	A1169	G1110	G1047	U981	A919	U856	C788	A663
U1487	G1361	G1361	G1426	G1361	U1298	A1170	A1110	U1048	U982	U920	C856	U788	G664
G1488	A1362	A1362	G1427	A1362	A1299	A1171	C1111	U1049	U983	U921	C857	U789	A665
A1489	C1363	C1363	G1428	C1363	G1300	C1172	C1112	G1050	C984	G922	G858	C790	G666
G1490	U1364	U1364	U1429	U1364	U1232	U1173	C1113	C1051	C985	A923	G859	A791	G667
G1491	G1365	G1365	A1430	G1365	A1239	G1174	C1114	U1052	U986	C924	A860	A792	G668
A1492	C1366	C1366		C1366	U1240	G1175	U1115	G1053	G987	G925	C861	U793	G669
G1493	C1367	C1367	G1431	C1367	G1241	A1176	U1116	C1054	U988	G926	C862	A794	G670
A1494	A1368	A1368	G1432	A1368	G1242	G1177	A1117	A1055	U989	G927	U863	C795	G671
U1495	C1369	C1369	A1433	C1369	C1243	G1178	U1118	U1056	C990	G928	A864	C796	U672
G1496	G1370	G1370	G1434	G1370	U1307	A1179	C1119	G1057	U991	G929	A865	C797	A673
U1497	U1371	U1371	U1435	U1371	U1308	G1180	U1120	G1058	U992	C930	C866	U798	G674
A1498	G1372	G1372	G1436	G1372	G1309	A1181	U1121	C1059	G993	C931	C867	G799	A675
U1499	G1373	G1373	G1437	G1373	G1310	G1182	U1122	U1060	A994	C932	C868	G800	G676
A1500	A1374	A1374	G1438	A1374	A1247	U1183	U1123	G1061	C995	G933	G869	U804	U677
C1501	G1375	G1375	G1439	C1501	A1248	G1184	G1124	U1062	A996	C934	U871	C805	U678
A1502	U1376	U1376	U1440	U1376	C1249	G1185	U1125	C1063	C999	A935	G872	C806	C679
A1503	C1377	C1377	G1442	C1377	A1252	U1186	U1126	G1064	C999	C936	A873	C807	G682
G1504	G1378	G1378	G1443	G1378	G1253	G1187	G1127	U1065	A1000	A937	G874	A807	G683
U1505	G1379	G1379	U1444	G1379	A1254	G1188	C1128	C1066	C1001	A938	U875	C808	U684
U1506	U1380	U1380	U1445	U1380	G1255	A1191	C1129	G1067	G1002	G939	G876	C809	G685
A1507	A1381	A1381	A1446	A1381	A1256	C1192	A1130	G1068	U1003	C940	C877	C810	U686
U1508	C1382	C1382	A1447	C1382	U1257	C1193	G1131	C1069	A1004	G941	G878	C811	G687
C1509	G1383	G1383	G1448	C1509	G1258	A1196	C1132	U1070	A1005	U943	G879	C812	A687
U1449	U1321	U1321	C1449	U1449	G1259	A1197	G1133	C1071	G1006	U944	C880	U813	G688
G1510	C1322	C1322	G1450	G1510	G1260	A1198	G1134	G1072	U1007	G945	A814	G750	C689
G1511	G1386	G1386	U1451	G1511	A1261	G1199	U1135	U1073	U1008	G946	A815	C751	G690
U1512	C1387	C1387	U1452	U1512	A1324	U1199	C1136	G1074	U1009	A946	C882	C752	G691
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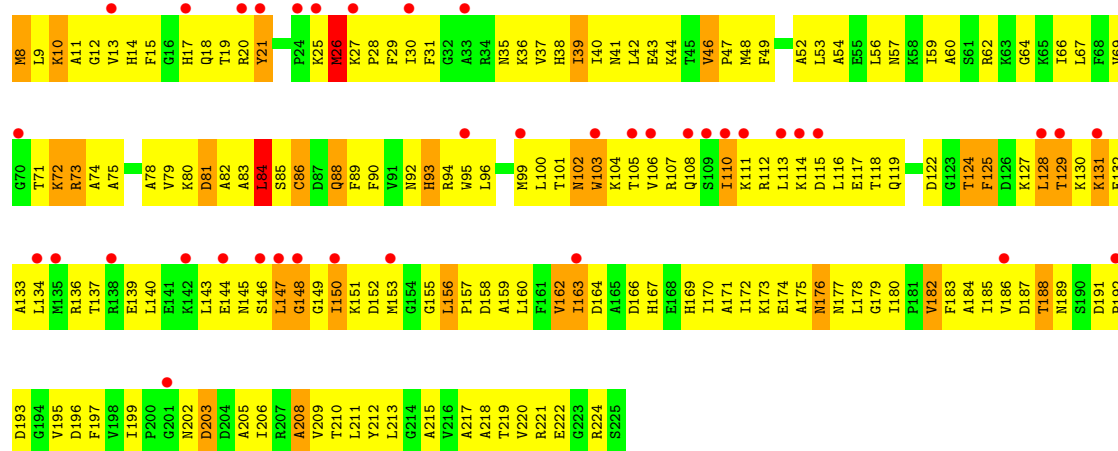
● Molecule 1: 16S rRNA



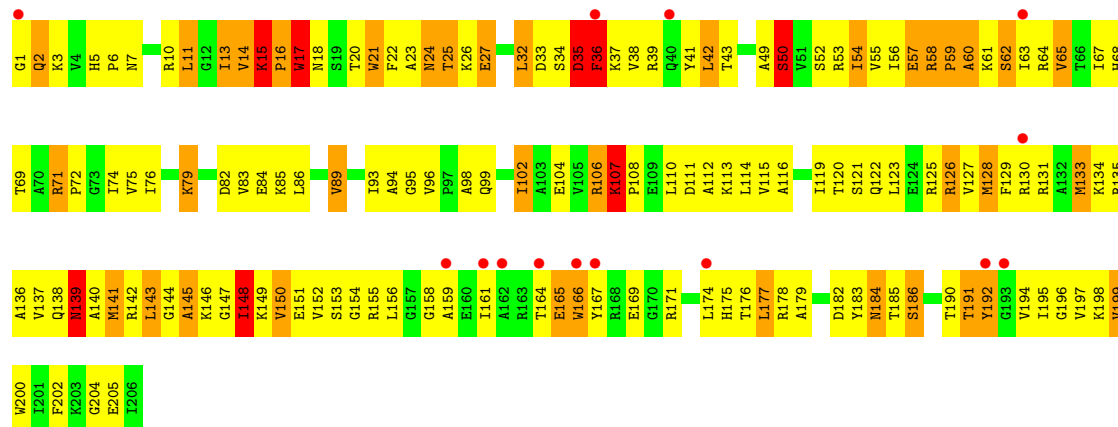




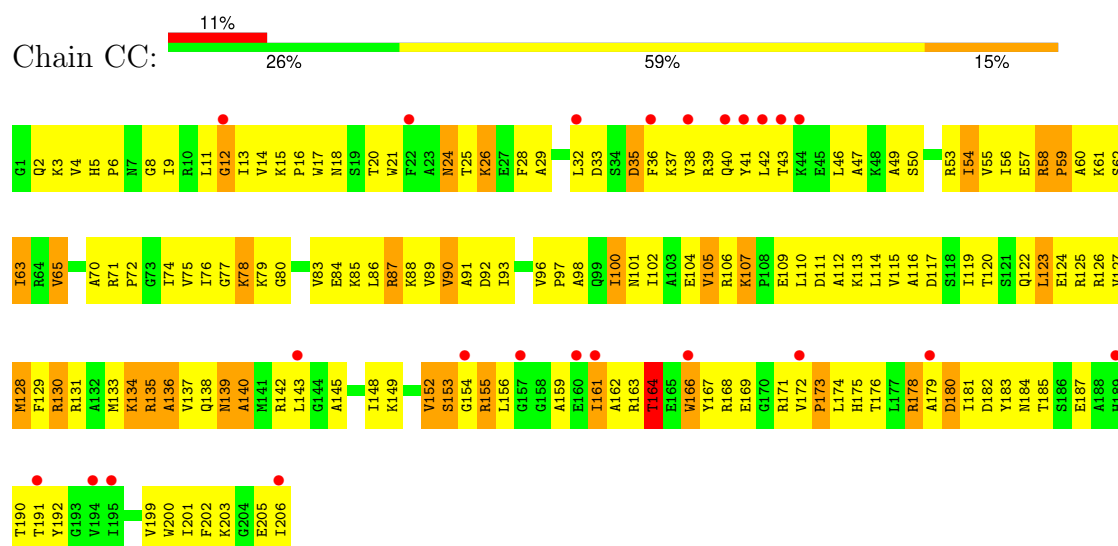
• Molecule 2: 30S ribosomal protein S2



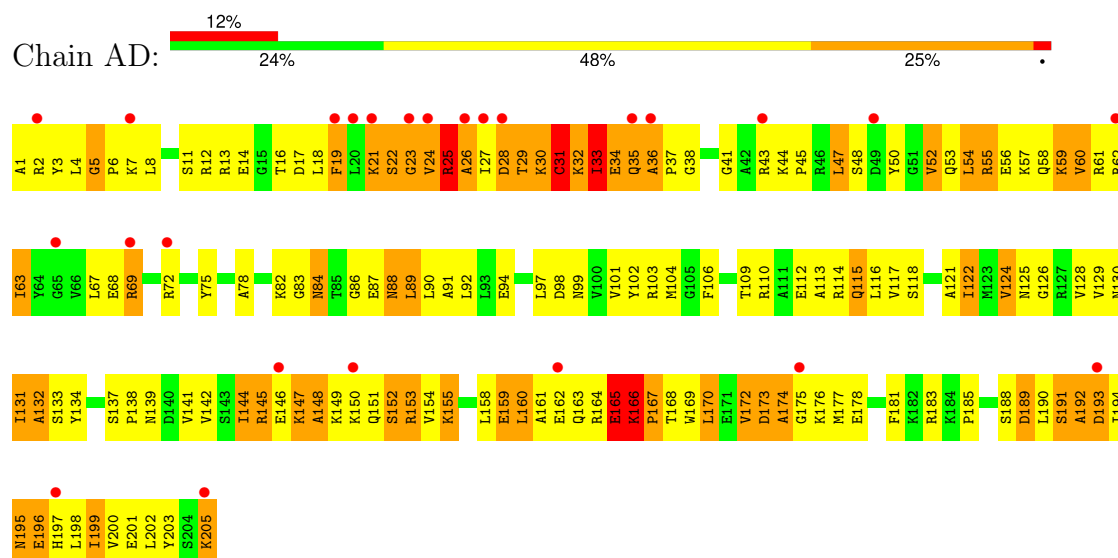
• Molecule 3: 30S ribosomal protein S3



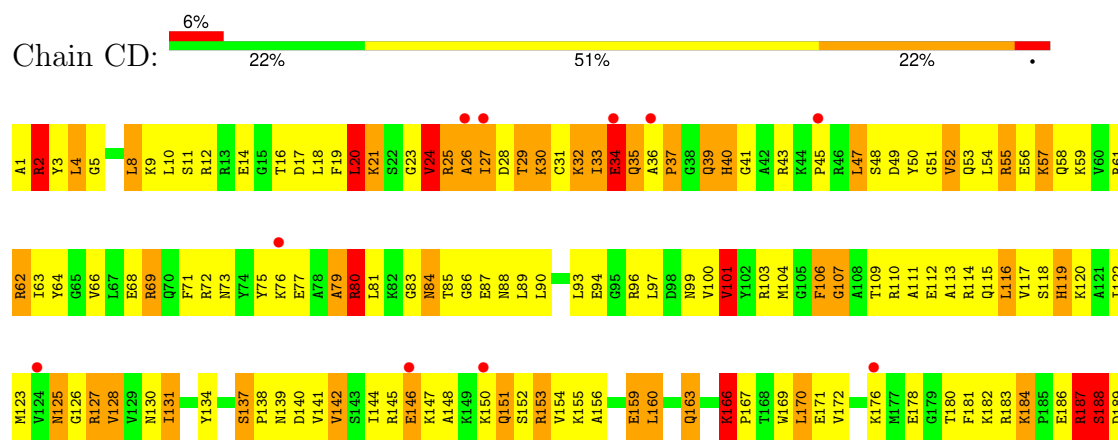
• Molecule 3: 30S ribosomal protein S3

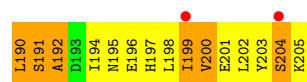


• Molecule 4: 30S ribosomal protein S4

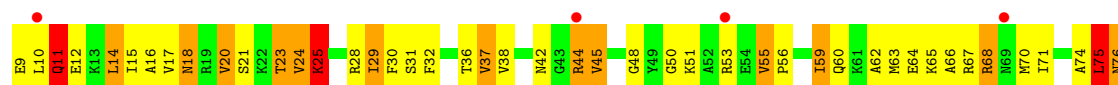


• Molecule 4: 30S ribosomal protein S4





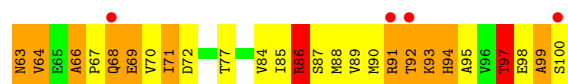
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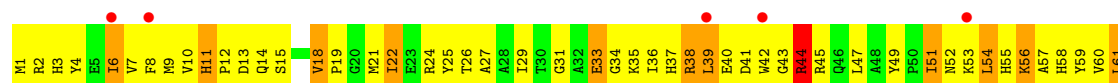
• Molecule 5: 30S ribosomal protein S5

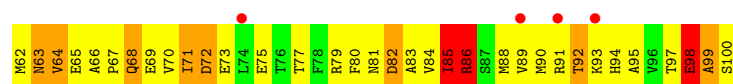


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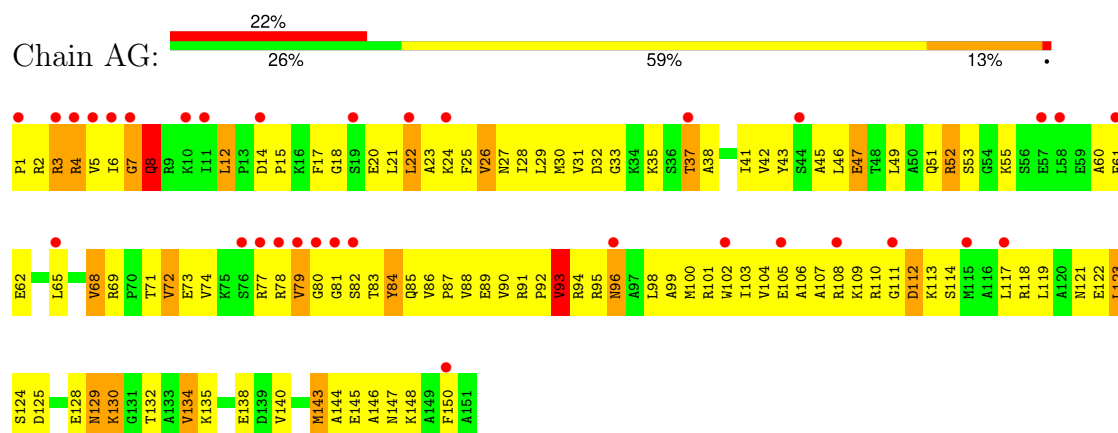


• Molecule 6: 30S ribosomal protein S6

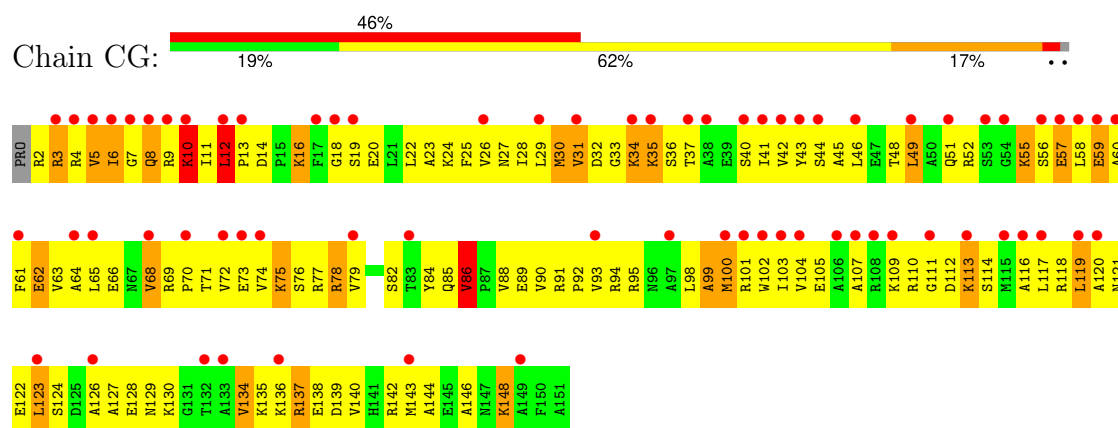




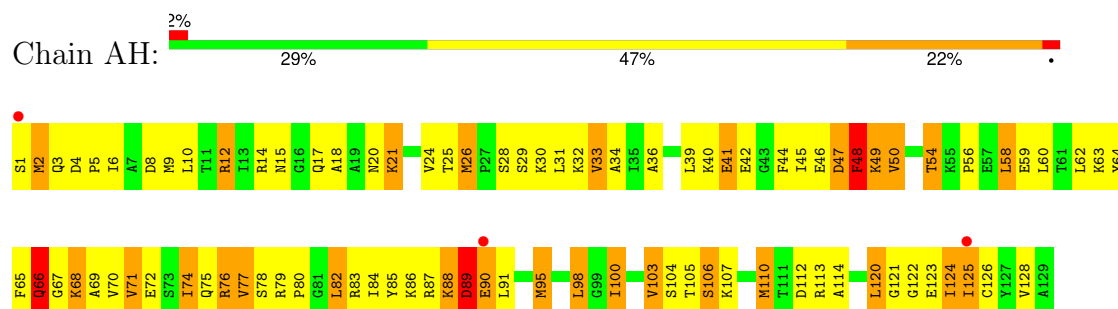
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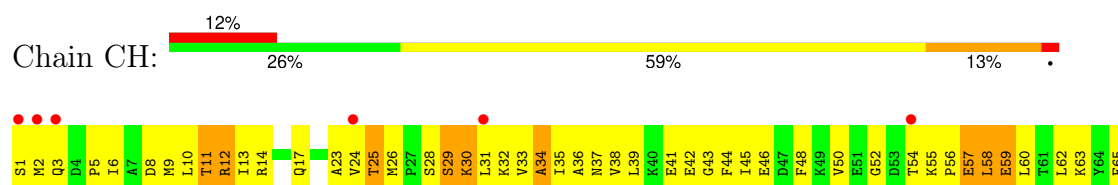
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

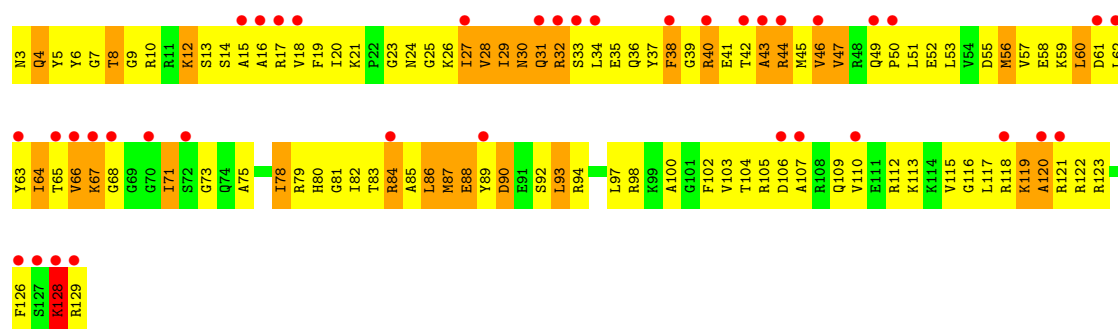


• Molecule 8: 30S ribosomal protein S8

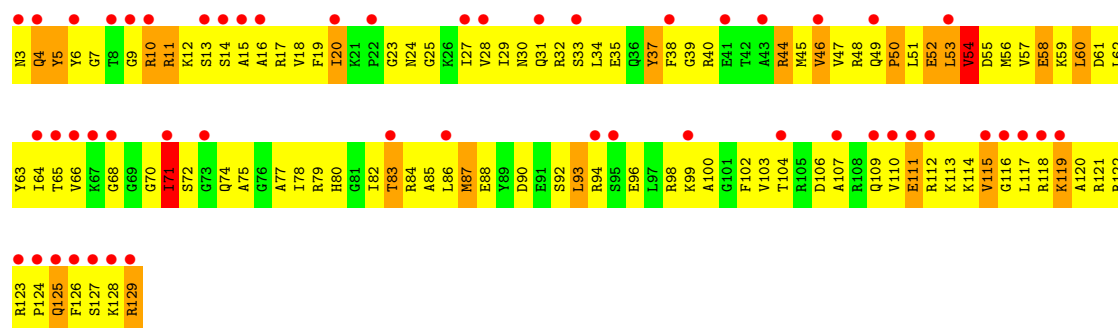




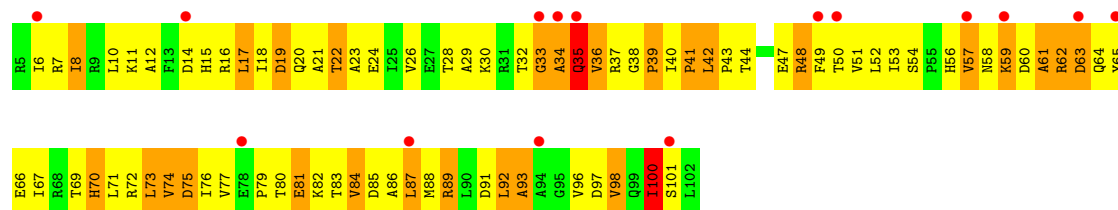
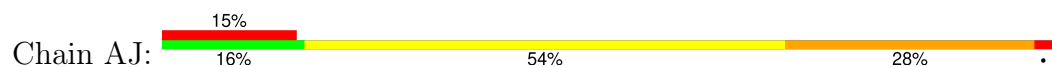
• Molecule 9: 30S ribosomal protein S9



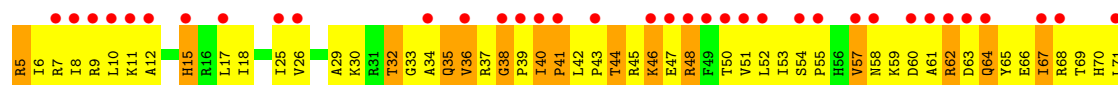
• Molecule 9: 30S ribosomal protein S9

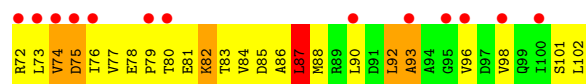


• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10





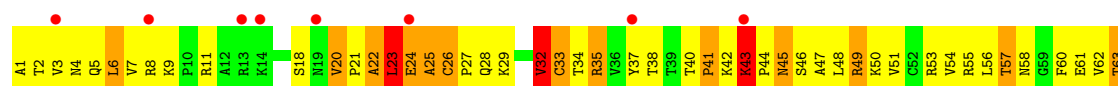
• Molecule 11: 30S ribosomal protein S11



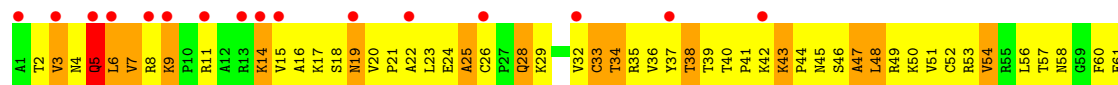
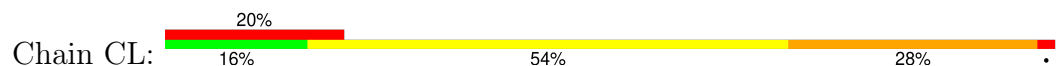
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12

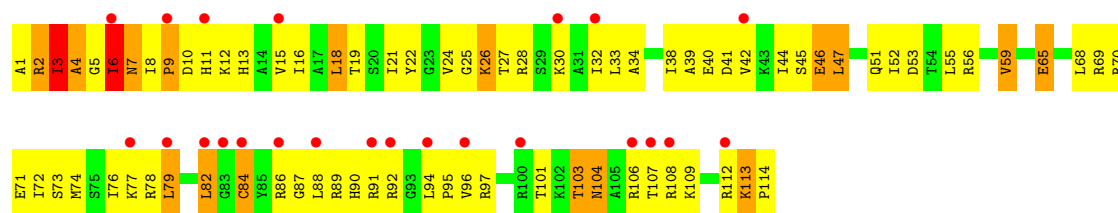


• Molecule 12: 30S ribosomal protein S12

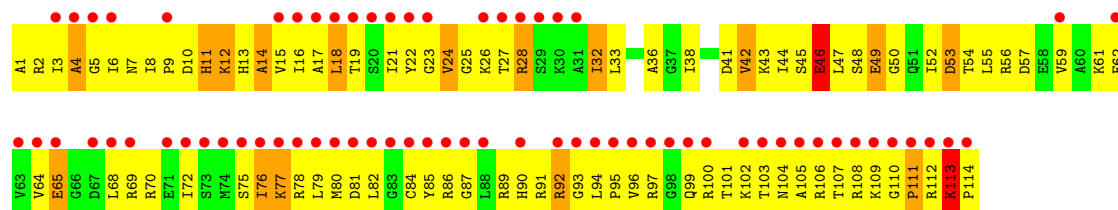


• Molecule 13: 30S ribosomal protein S13

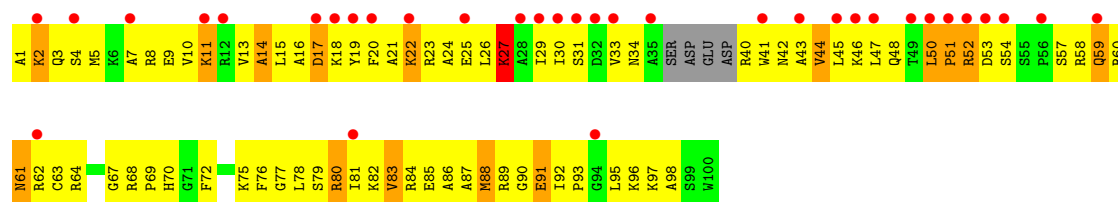




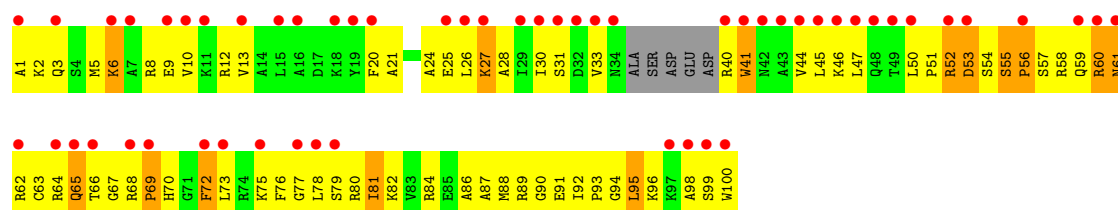
• Molecule 13: 30S ribosomal protein S13



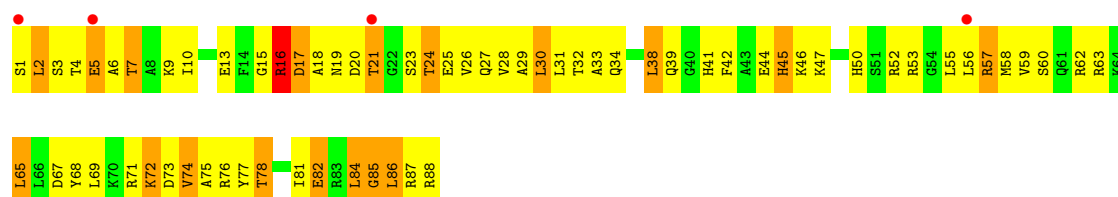
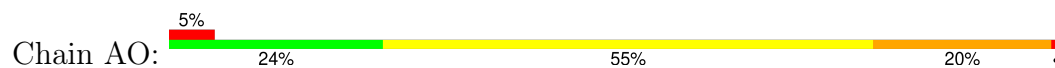
• Molecule 14: 30S ribosomal protein S14



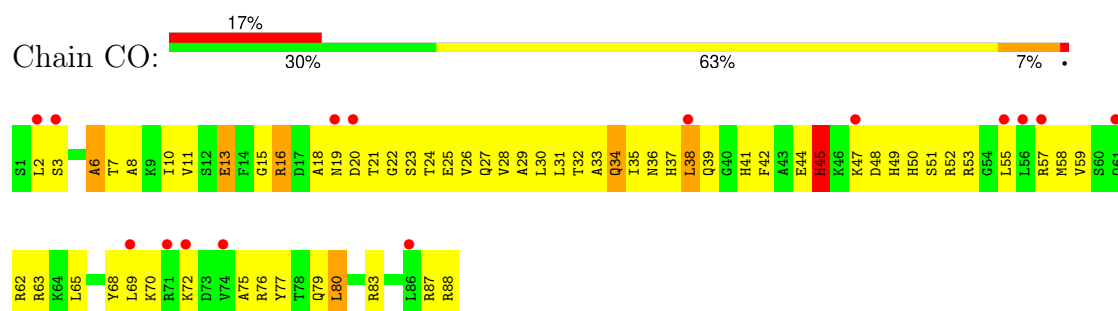
• Molecule 14: 30S ribosomal protein S14



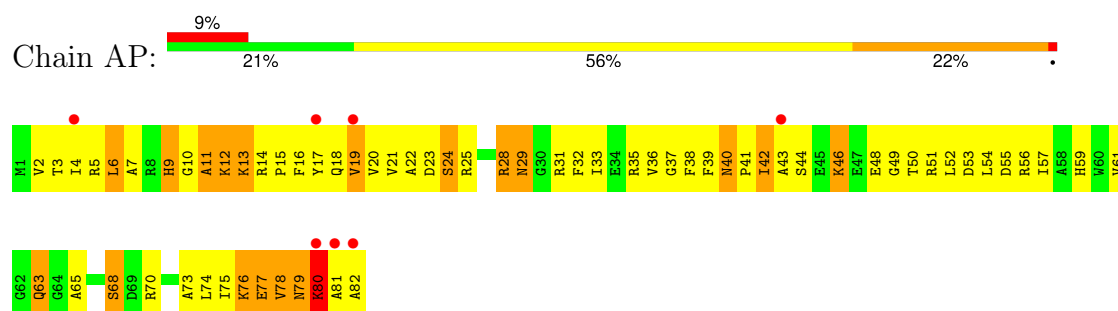
• Molecule 15: 30S ribosomal protein S15



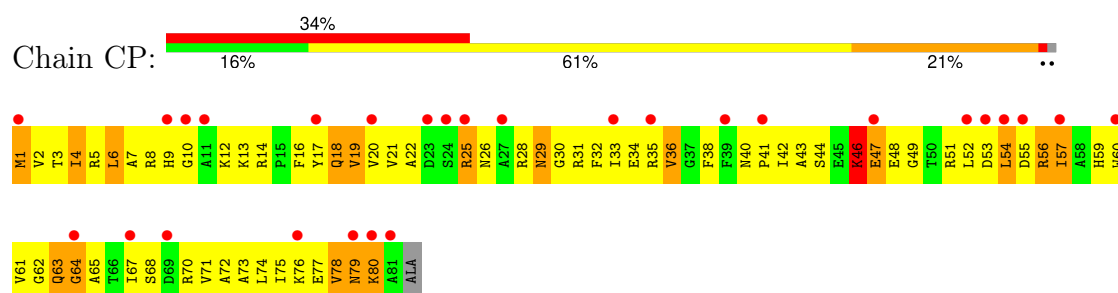
- Molecule 15: 30S ribosomal protein S15



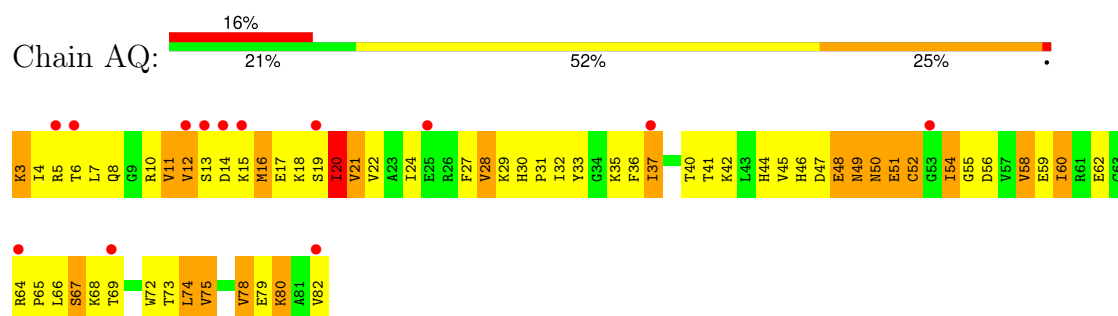
- Molecule 16: 30S ribosomal protein S16



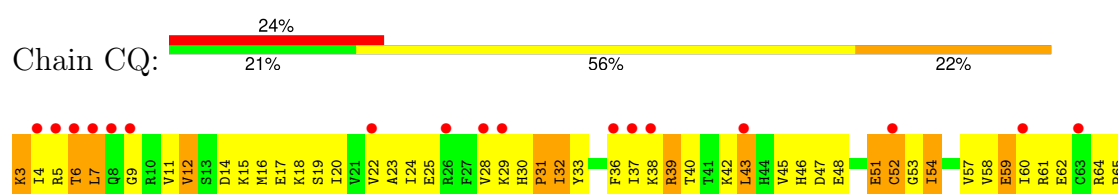
- Molecule 16: 30S ribosomal protein S16

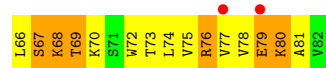


- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

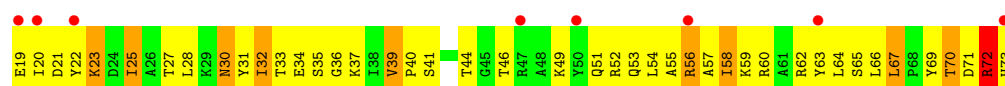




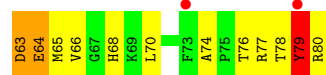
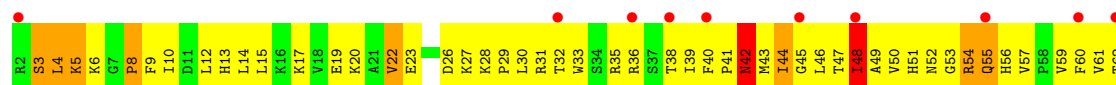
- Molecule 18: 30S ribosomal protein S18



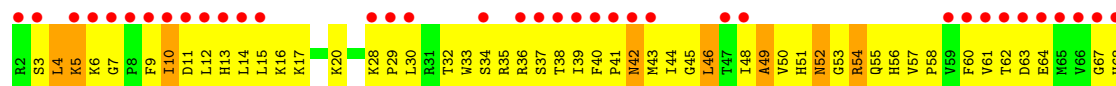
- Molecule 18: 30S ribosomal protein S18



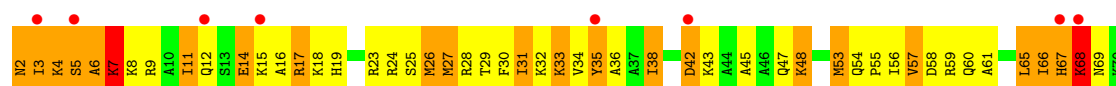
- Molecule 19: 30S ribosomal protein S19



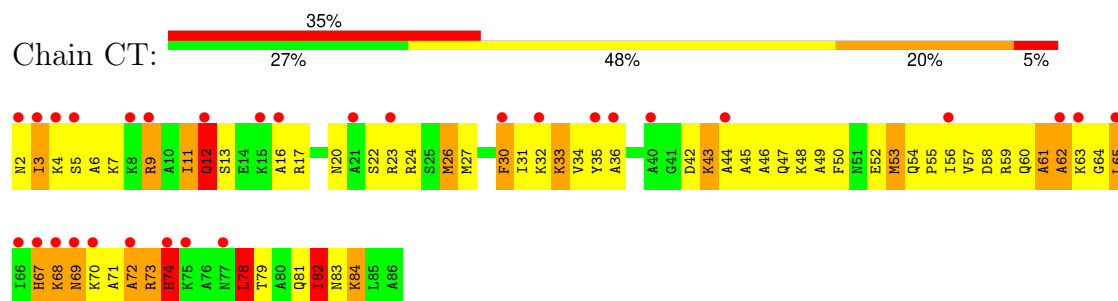
- Molecule 19: 30S ribosomal protein S19



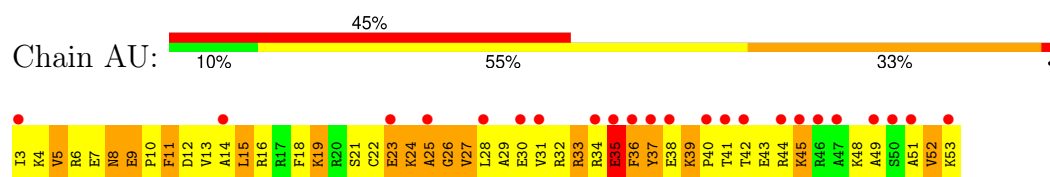
- Molecule 20: 30S ribosomal protein S20



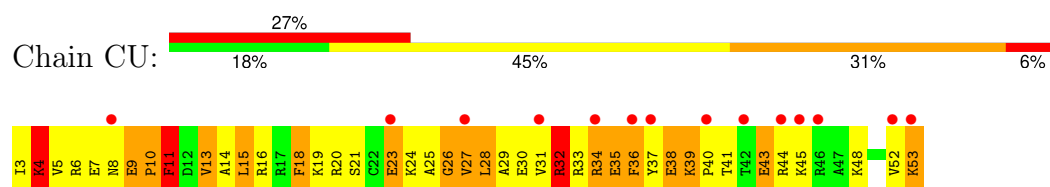
- Molecule 20: 30S ribosomal protein S20



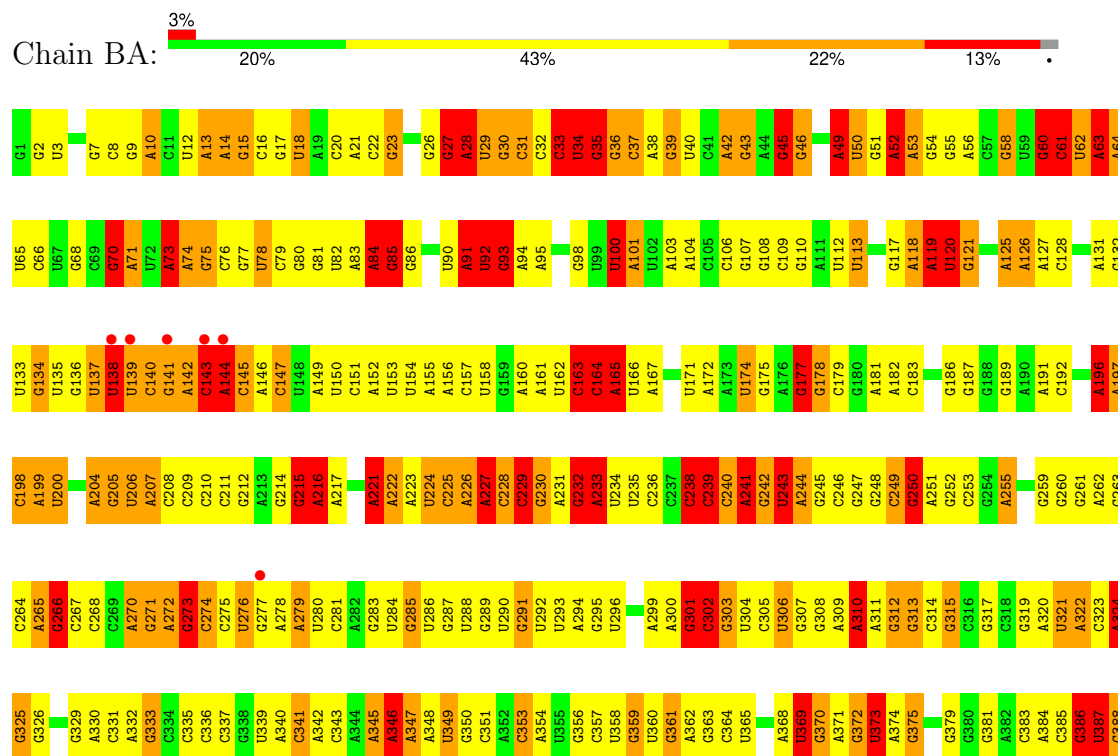
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

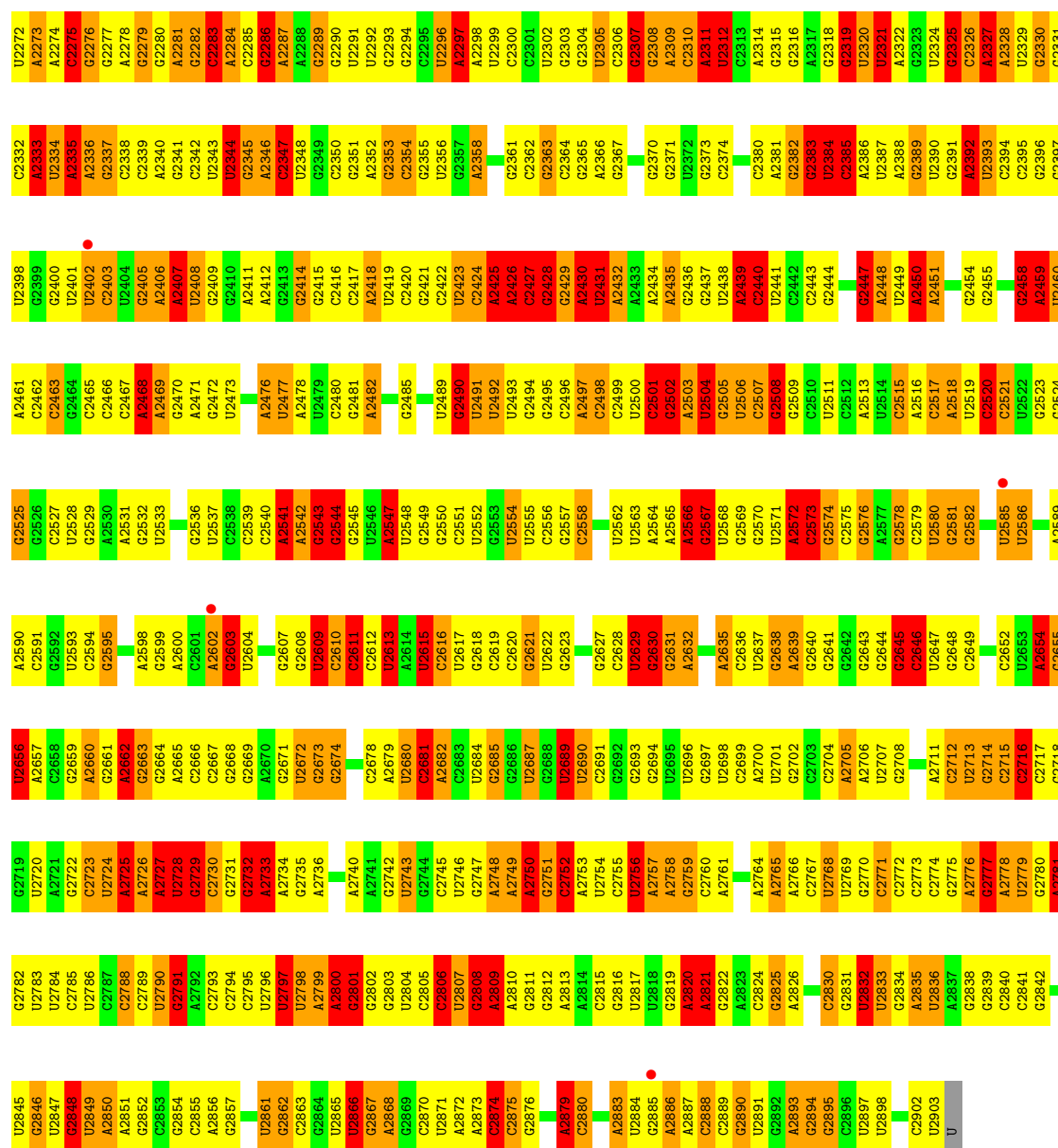


- Molecule 22: 23S rRNA

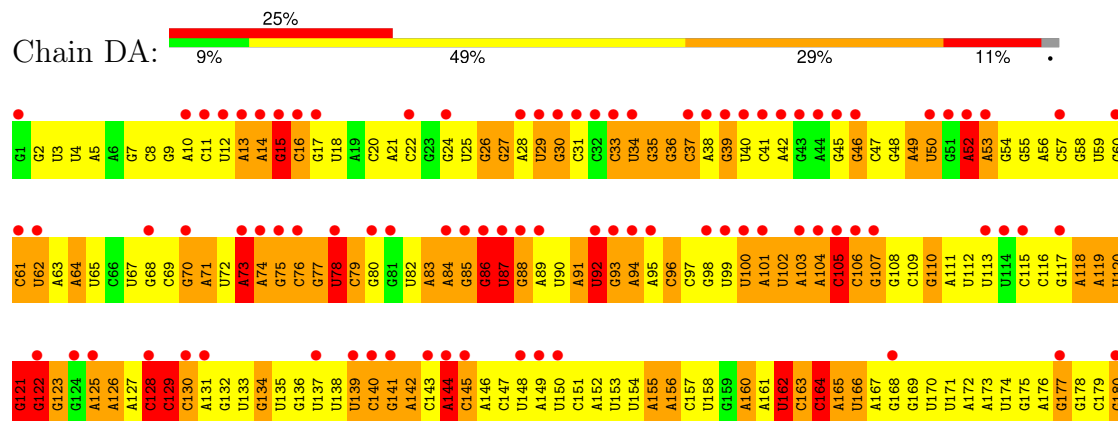




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			U2079	A2013	C1947	C1817	U1748	U1683	A1544	A1477	C1417	
			C2080	A2014	U1882	G1818	A1749	U1687	A1545	G1478	G1418	
			U2081	A2015	U1883	U1819		G1687	G1546	U1481	A1419	
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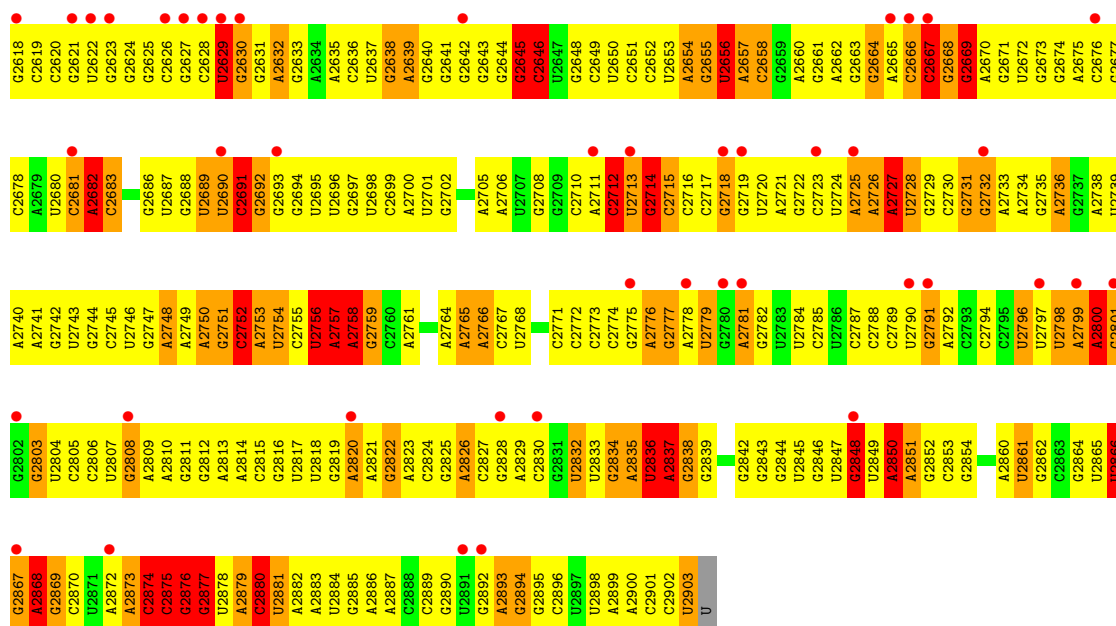
• Molecule 22: 23S rRNA



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G976	C183	U243	G303	C363	A423	A453	U547	U607	A667	A730	C791	U852	C915	G976
G977	C184	A244	U304	G364	A424	A454	A547	U608	A668	G731	A792	C853	C916	G977
A978	G185	G245	C305	U365	G425	C485	G548	C609	G669	G732	A793	C854	A917	A978
A980	G186	C246	U306	C366	G426	C486	G549	C610	A670	G733	A794	C855	A918	A980
A981	G187	G247	G307	G367	U427	C487	G550	C611	C671	G734	C795	G856	U919	A981
C982	G188	G248	G308	A368	A428	G488	G551	G612	C672	A735	C796	G857	A920	C982
A983	G189	C249	A309	U369	A429	G489	U552	A613	C673	G736	G797	G858	C921	A983
A984	A190	C250	A310	G370	A430	C490	U553	U614	G674	C737	G798	C859	C922	A984
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C986	C192	G252	G312	G372	A432	A492	G555	A616	A676	A739	A800	A861	G924	C986
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C991	C197	C257	G317	G377	U438	U499	U561	A621	G675	U744	G805	A866	U929	C991
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A995	U201	C261	U321	C381	U441	A502	C565	G625	A685	G748	G809	U870	U933	A995
A996	U202	A262	A322	A382	G442	A503	U566	A626	U686	A749	U810	U871	U934	A996
C997	A203	G263	C323	C383	A443	A504	U567	A627	U687	A750	U811	U872	U935	C997
C998	A204	C264	A324	A384	C444	A505	U568	G628	U688	A751	C812	C873	A936	C998
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A1008	G214	C274	C334	C394	A454	A515	U578	G638	G701	A761	G822	U	U	A1008
A1010	G215	C275	C335	U395	C455	C516	A579	U639	U702	G762	A825	C	C	A1010
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G1012	A217	G277	C337	U397	A457	G518	C581	U641	U704	A764	U827	U	U	G1012
U1018	A218	A278	G338	C398	C458	U519	A582	U642	G705	G765	U828	C	C	U1018
A1019	G219	U279	U339	U399	U459	C523	G583	A643	A706	U766	U829	U	U	A1019
A1020	G220	U280	A340	G400	A460	G524	C584	A644	G707	G770	U830	C	C	A1020
A1021	A221	C281	C341	A401	C461	G525	A585	C645	G708	U771	C831	G	G	A1021
G1022	A222	A282	A342	A402	C462	U526	A586	U646	U709	G772	U832	A	A	G1022
U1023	U223	G283	C343	U403	G463	A527	C587	G647	U710	C773	A833	U	U	U1023
G1024	C225	U284	A344	A404	U464	A528	U588	G648	G711	U774	G834	C	C	G1024
C1025	A226	G285	A345	U405	C465	A529	U589	G649	G712	G775	C835	U	U	C1025
A1026	G227	U286	A346	G406	A466	G530	A590	C650	G713	G776	C836	A	A	A1026
A1027	C228	U287	A347	G407	C467	G531	U591	G651	G714	G777	C837	C	C	A1027
A1028	G229	G288	U348	G408	G468	A532	A592	U652	A715	G778	C838	U	U	A1028
G1029	C230	U289	U349	G409	C469	A533	U593	U653	A716	G779	U839	C	C	G1029
C1030	A231	U290	C350	G410	A470	G534	U594	A654	C717	U780	C840	U	U	C1030
A1031	G232	C291	C351	G411	A471	U534	C595	A655	G718	G781	G841	C	C	A1031
A1032	A233	U292	A352	A412	A472	G535	U596	G656	A719	U782	U842	U	U	A1032
U1033	U234	G293	C353	C413	G473	G536	U597	U657	C720	A783	C843	U	U	U1033
	A235	U294	A354	C414	G474	G537	U598	U658	A721	G784	A844	G	G	
	C236	G295	U355	A415	C475	A538	A599	G659	U724	G785	A845	U	U	
	C237	U296	U356	U416	G476	G539	G600	C660	G725	G786	U846	U	U	
	C238	G297	C357	C417	A477	C540	G601	C661	U726	G787	U847	U	U	
	C239	U298	U358	C418	A478	A541	A602	G662	G727	C788	C848	U	U	
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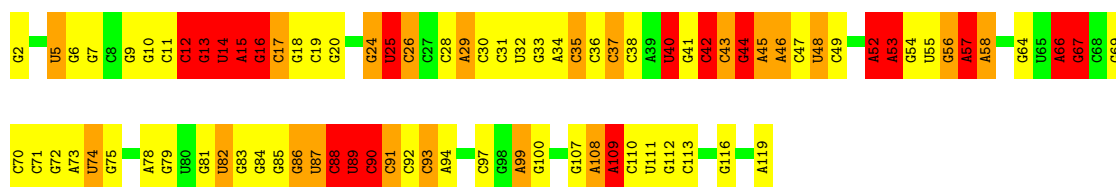






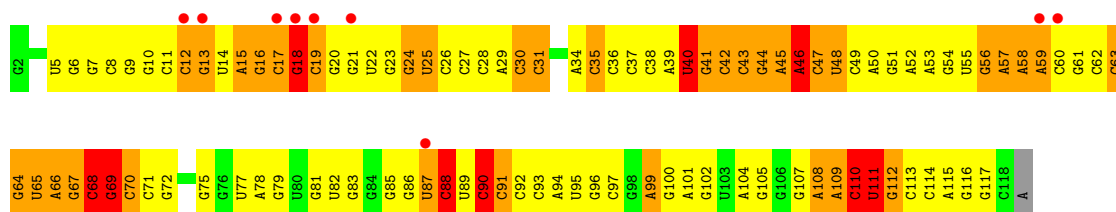
• Molecule 23: 5S rRNA

Chain BB: 28% 39% 18% 15%



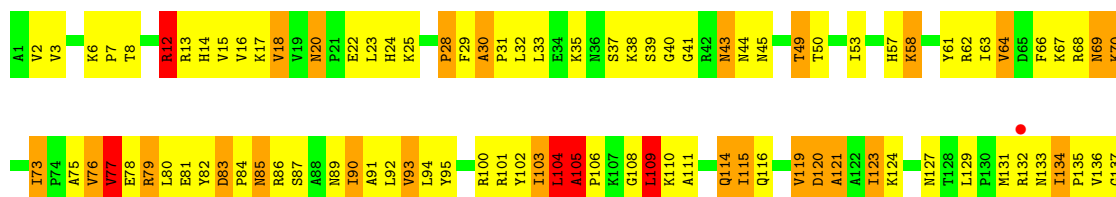
• Molecule 23: 5S rRNA

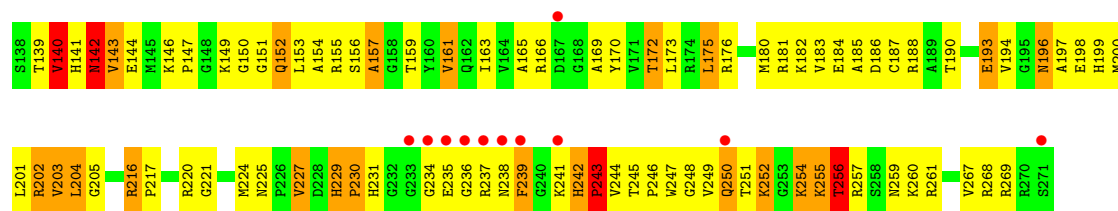
Chain DB: 8% 12% 51% 29% 8%



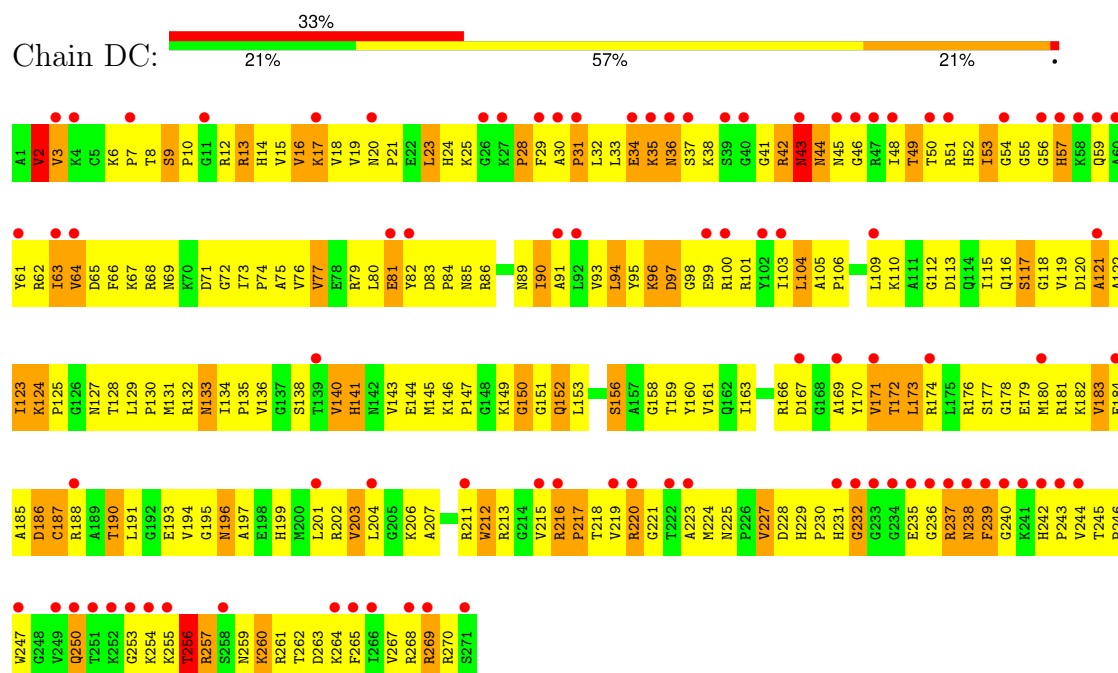
• Molecule 24: 50S ribosomal protein L2

Chain BC: 4% 32% 47% 17%

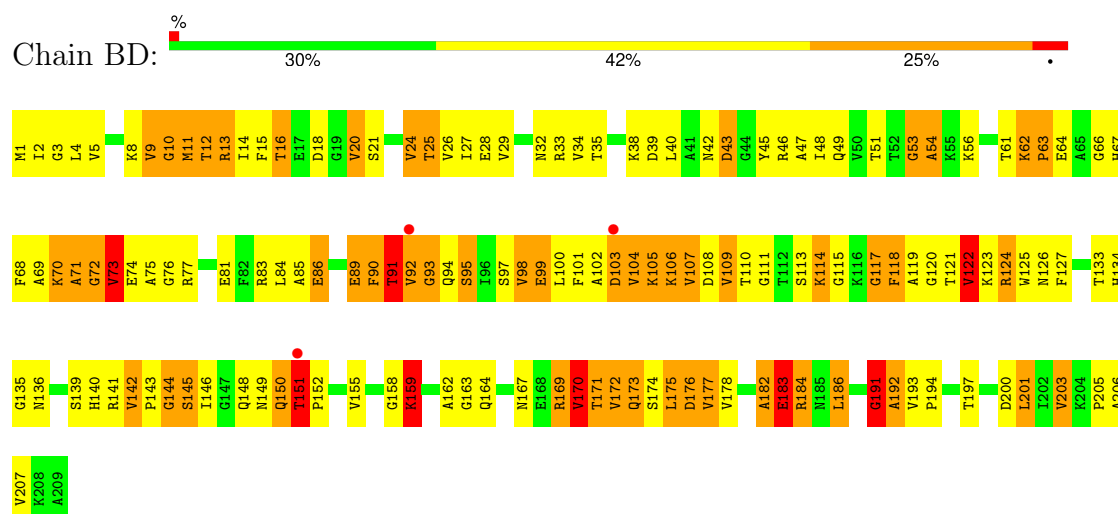




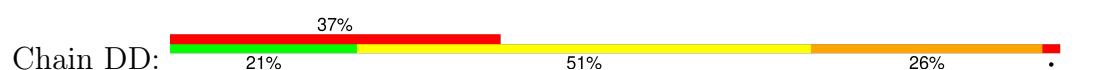
• Molecule 24: 50S ribosomal protein L2

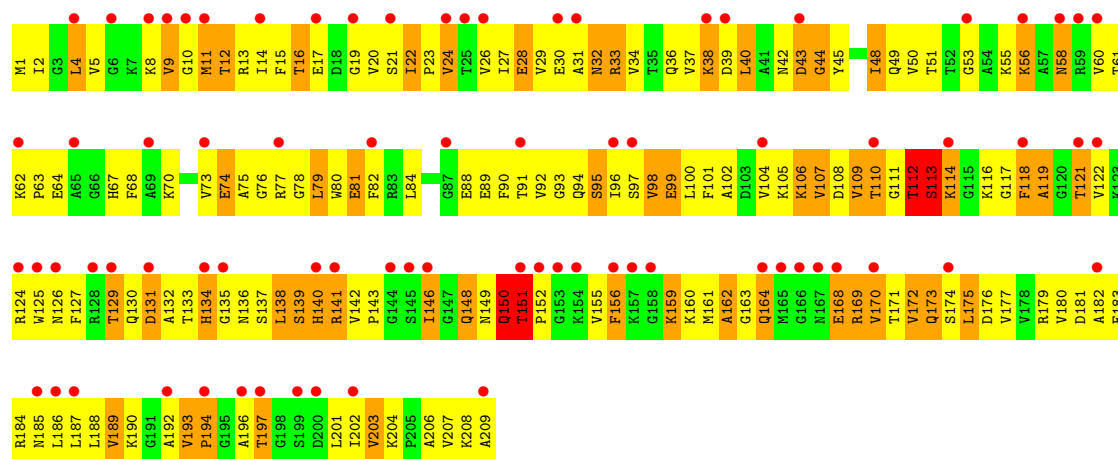


• Molecule 25: 50S ribosomal protein L3

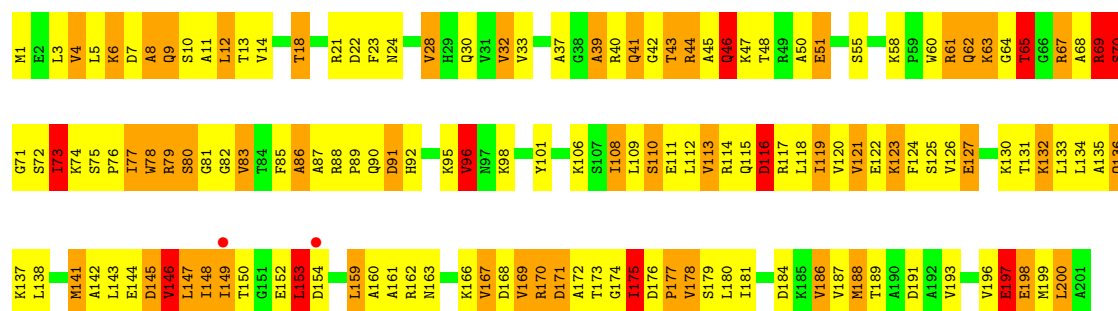


• Molecule 25: 50S ribosomal protein L3

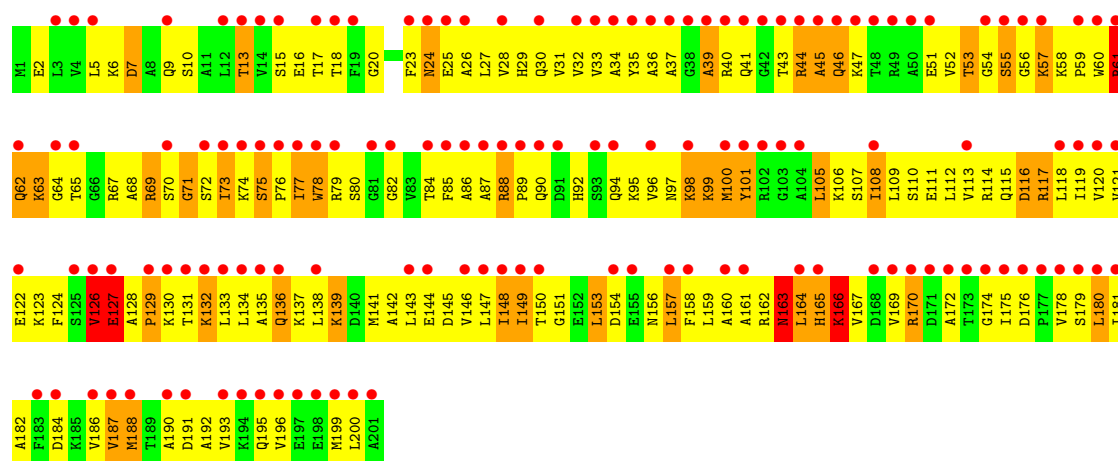
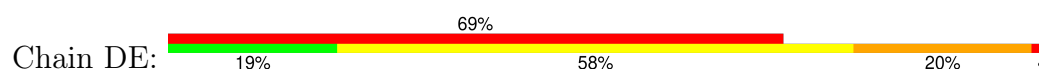




• Molecule 26: 50S ribosomal protein L4

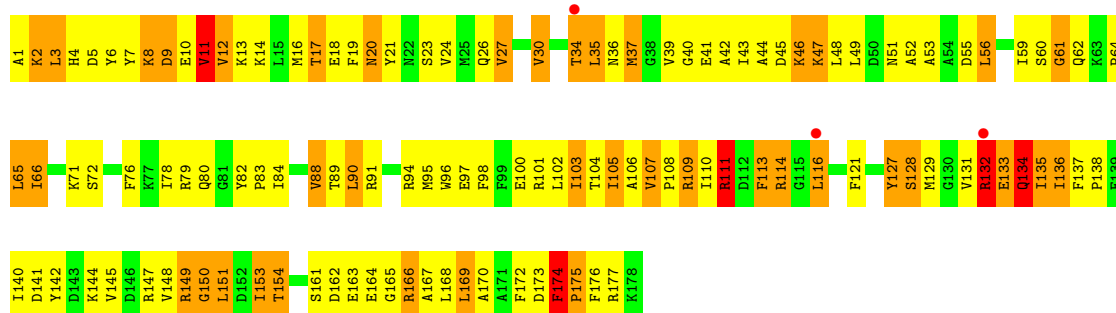


• Molecule 26: 50S ribosomal protein L4

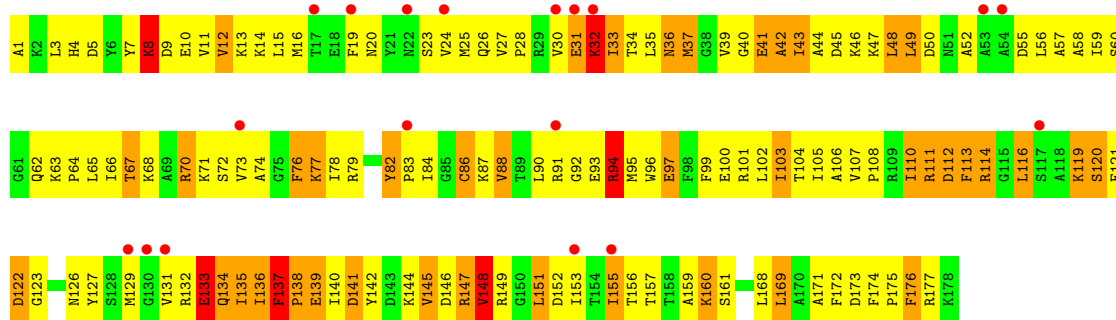


• Molecule 27: 50S ribosomal protein L5

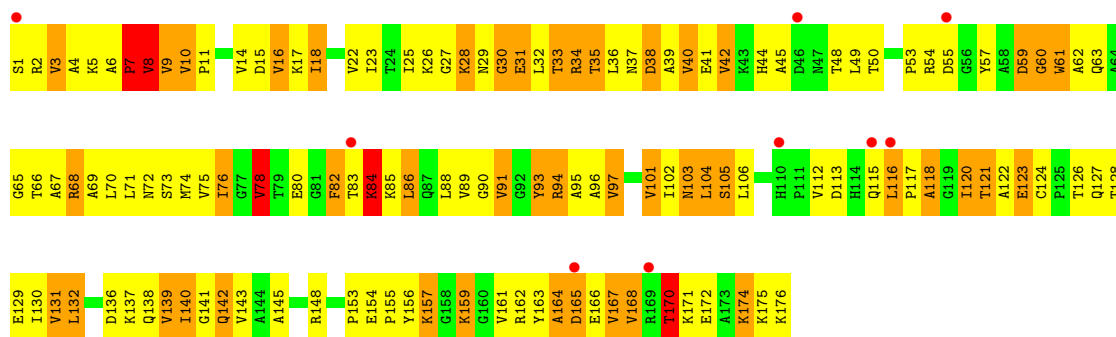




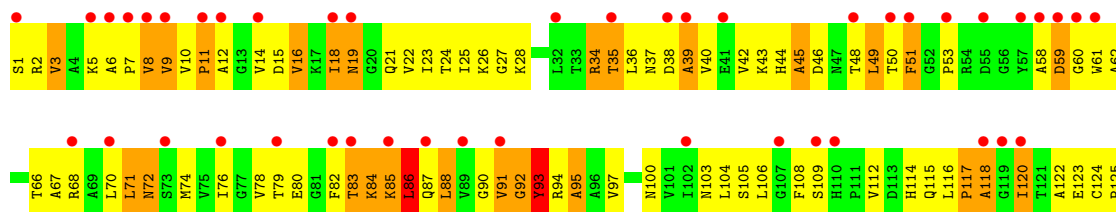
• Molecule 27: 50S ribosomal protein L5

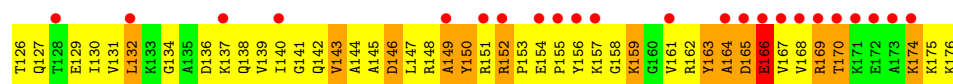


• Molecule 28: 50S ribosomal protein L6

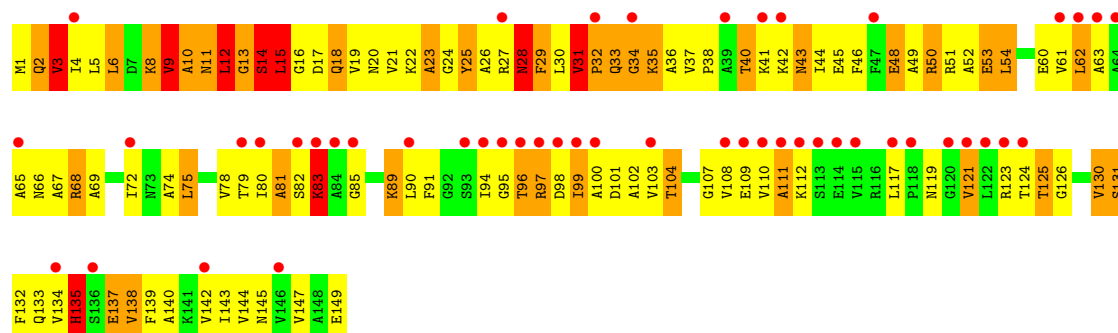


• Molecule 28: 50S ribosomal protein L6

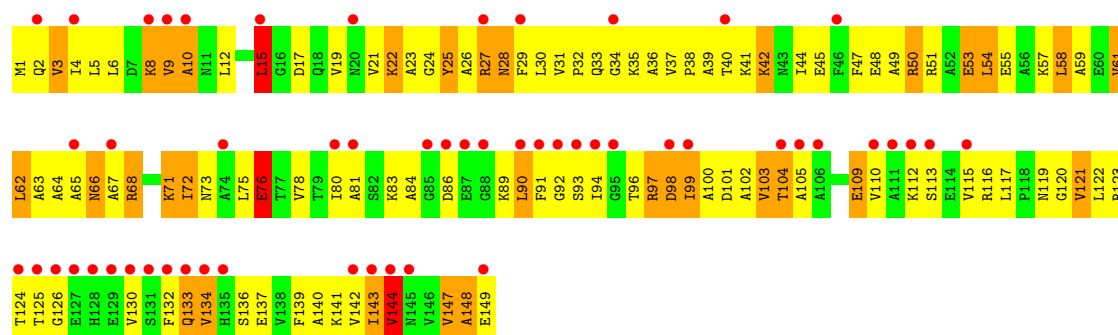




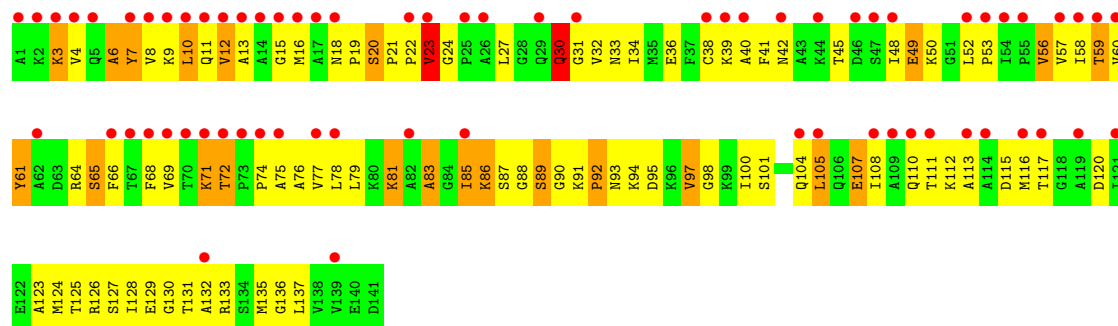
• Molecule 29: 50S ribosomal protein L9



• Molecule 29: 50S ribosomal protein L9

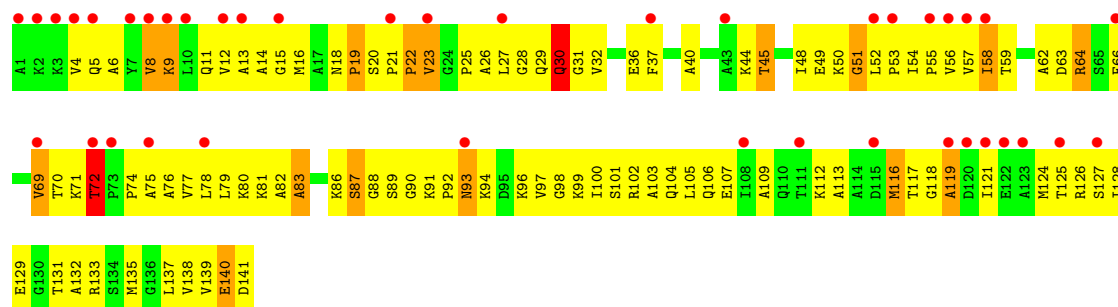


• Molecule 30: 50S ribosomal protein L11

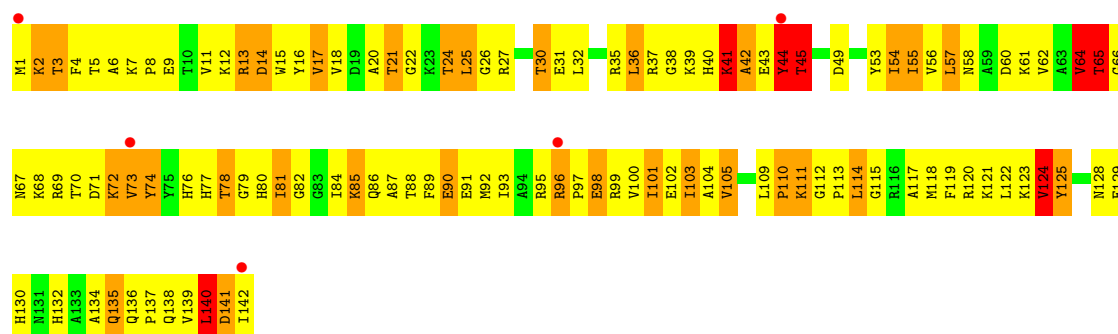
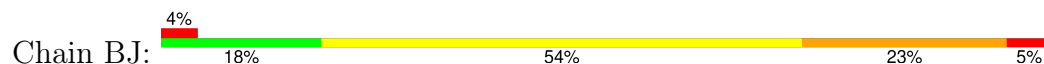


• Molecule 30: 50S ribosomal protein L11

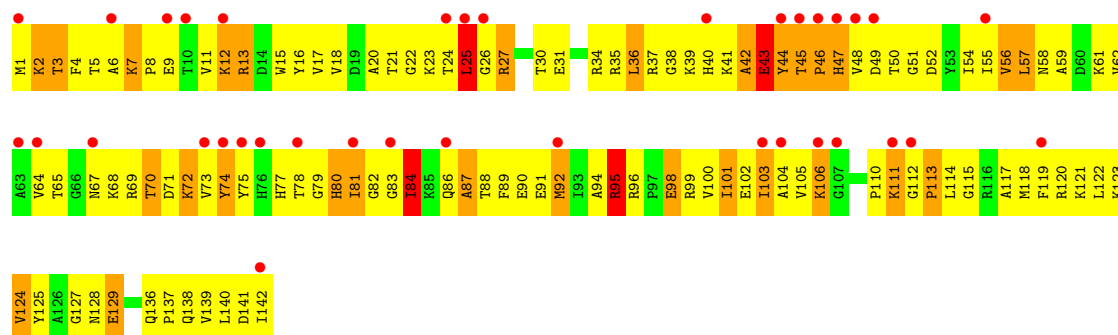




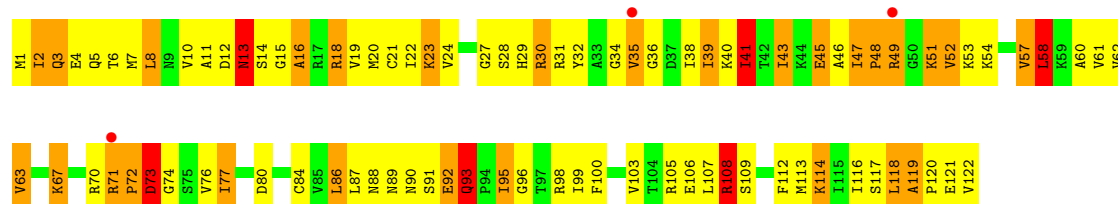
• Molecule 31: 50S ribosomal protein L13



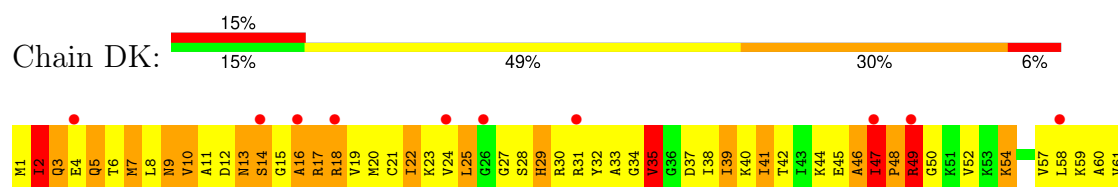
• Molecule 31: 50S ribosomal protein L13



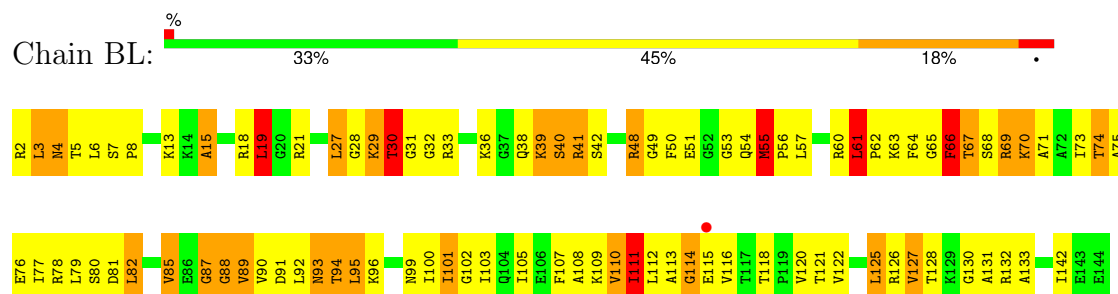
• Molecule 32: 50S ribosomal protein L14



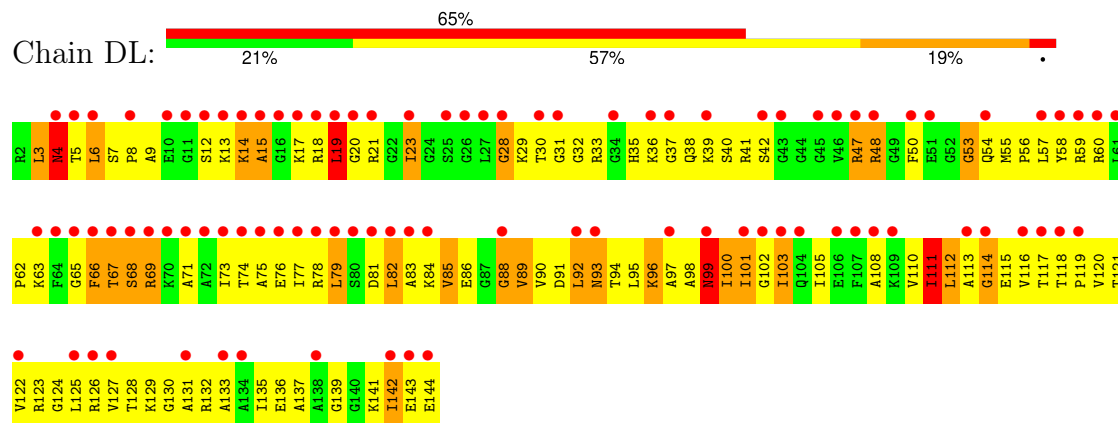
• Molecule 32: 50S ribosomal protein L14



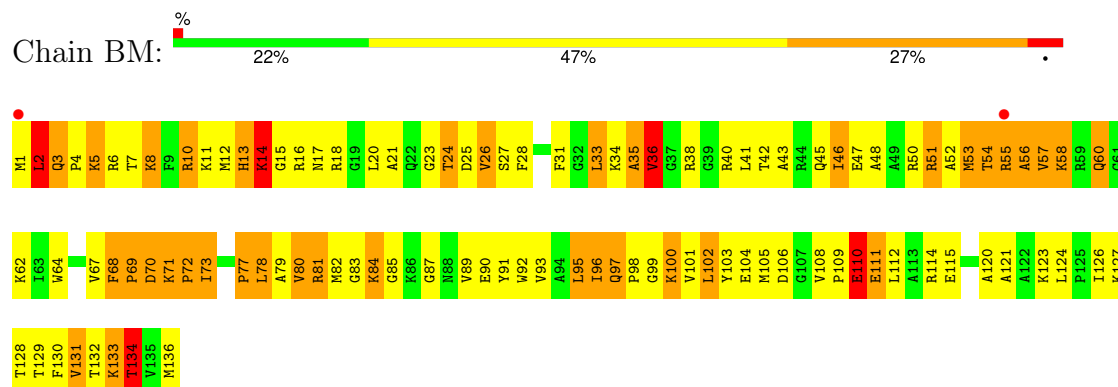
• Molecule 33: 50S ribosomal protein L15



• Molecule 33: 50S ribosomal protein L15

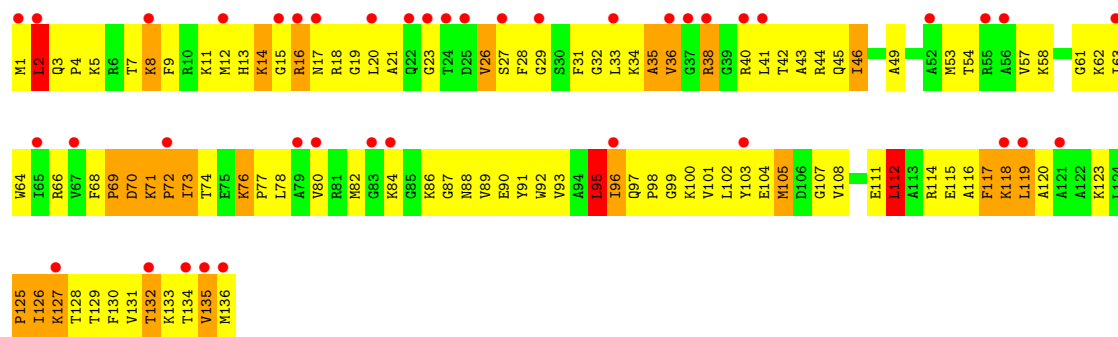


• Molecule 34: 50S ribosomal protein L16

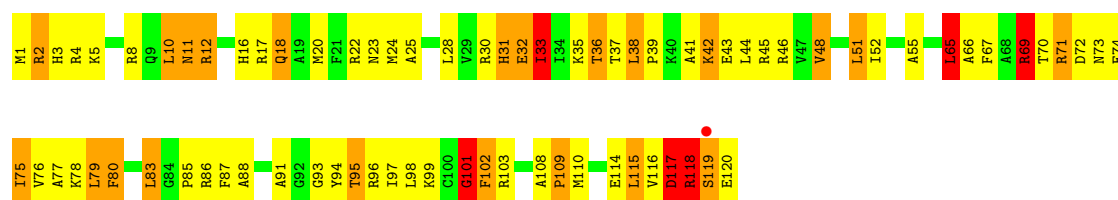


• Molecule 34: 50S ribosomal protein L16

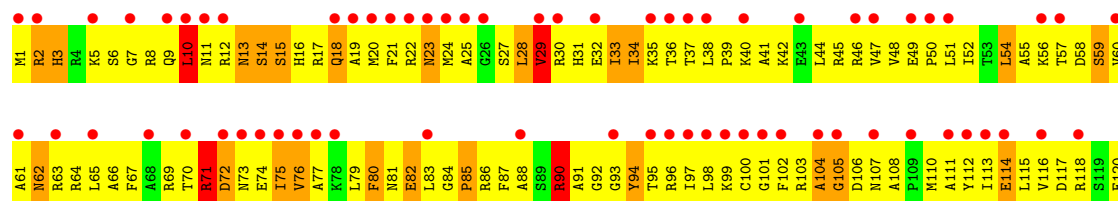
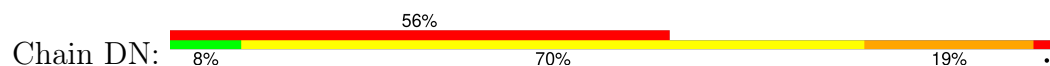




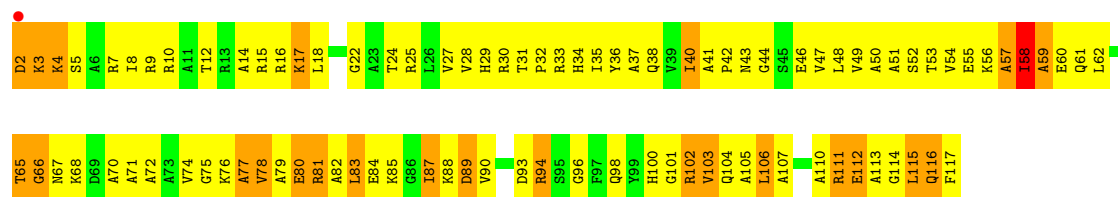
• Molecule 35: 50S ribosomal protein L17



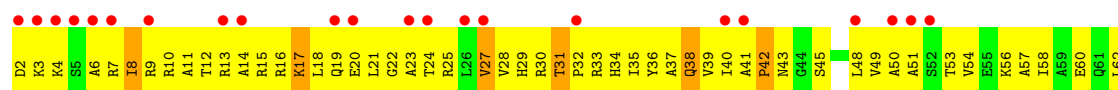
• Molecule 35: 50S ribosomal protein L17

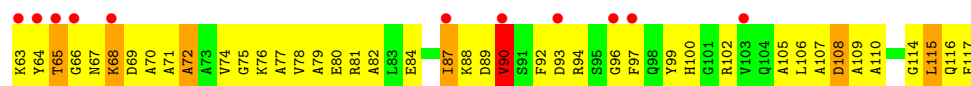


• Molecule 36: 50S ribosomal protein L18

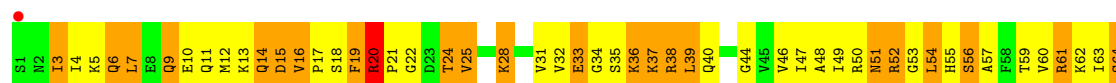
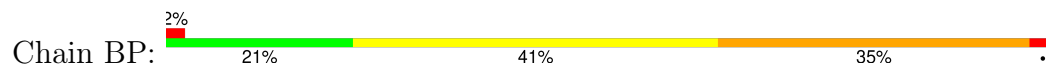


• Molecule 36: 50S ribosomal protein L18

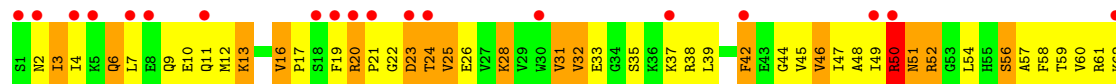




• Molecule 37: 50S ribosomal protein L19



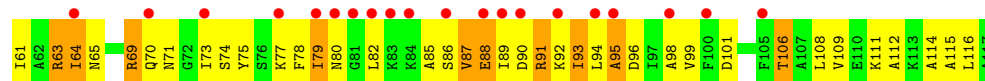
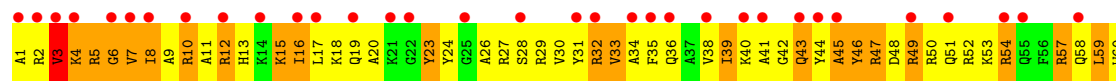
• Molecule 37: 50S ribosomal protein L19



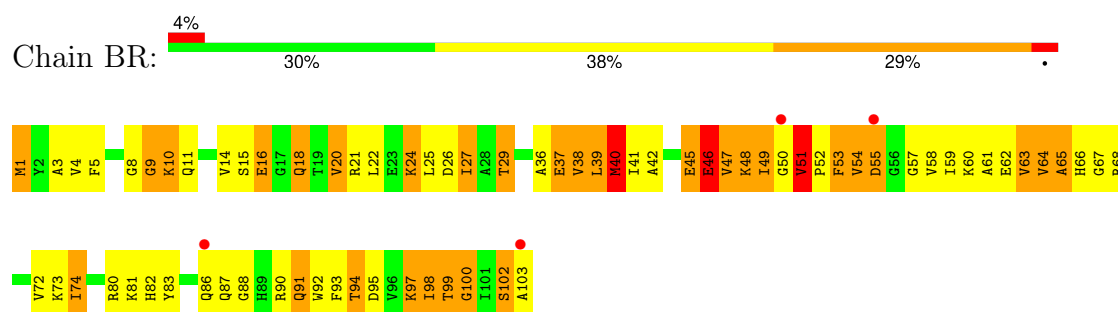
• Molecule 38: 50S ribosomal protein L20



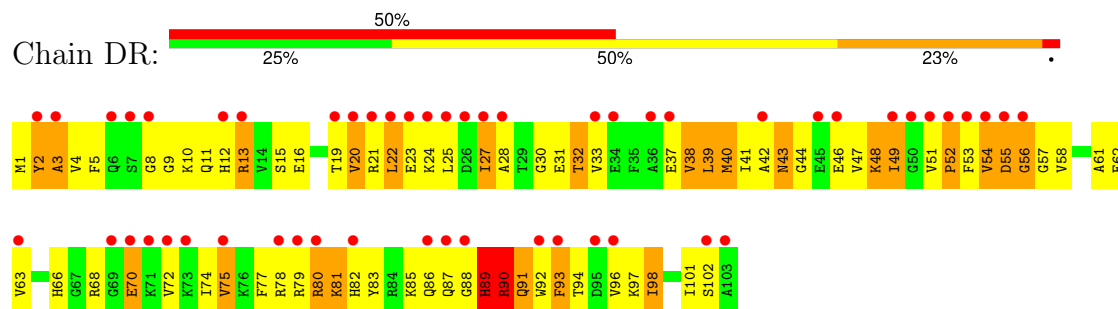
• Molecule 38: 50S ribosomal protein L20



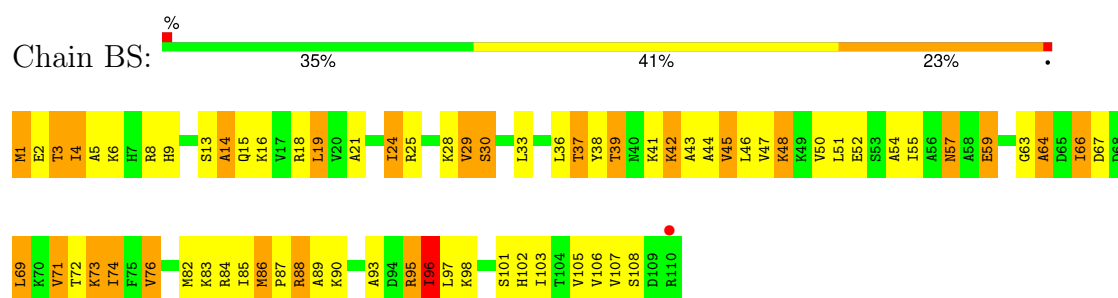
• Molecule 39: 50S ribosomal protein L21



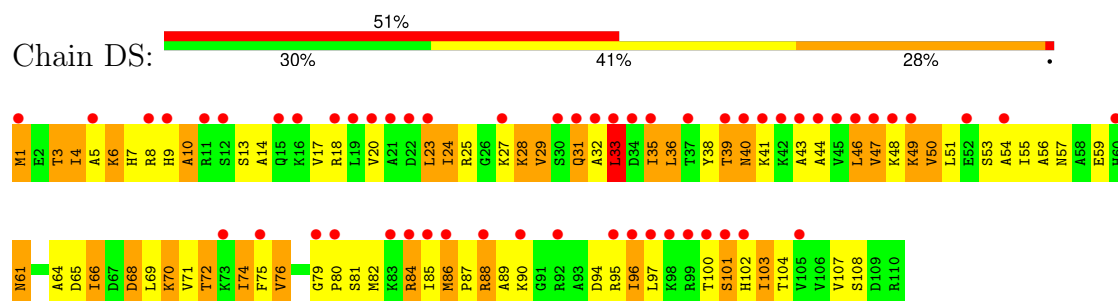
• Molecule 39: 50S ribosomal protein L21



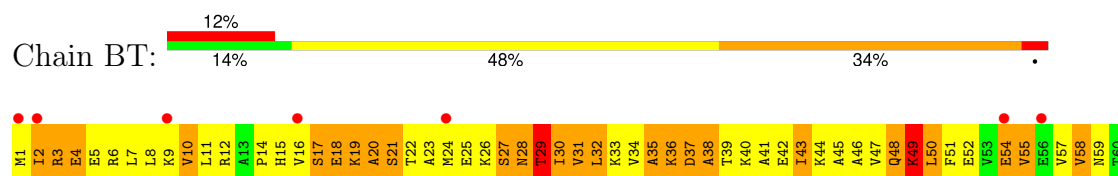
• Molecule 40: 50S ribosomal protein L22



• Molecule 40: 50S ribosomal protein L22

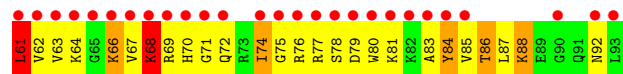
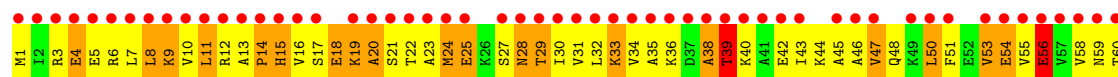
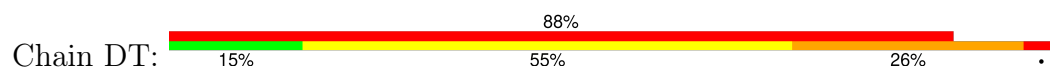


• Molecule 41: 50S ribosomal protein L23

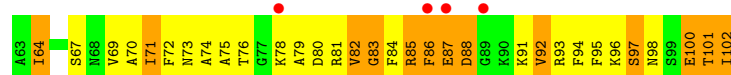




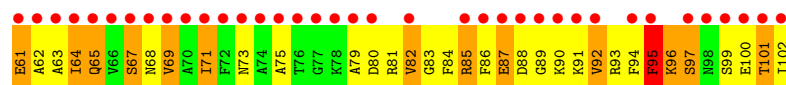
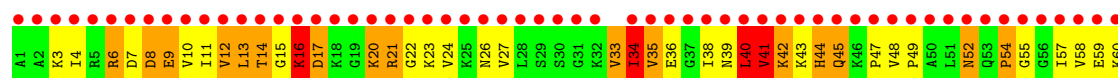
- Molecule 41: 50S ribosomal protein L23



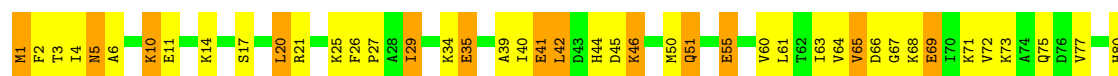
- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24

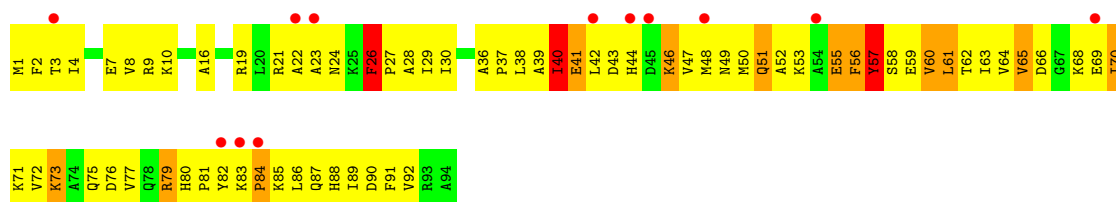


- Molecule 43: 50S ribosomal protein L25

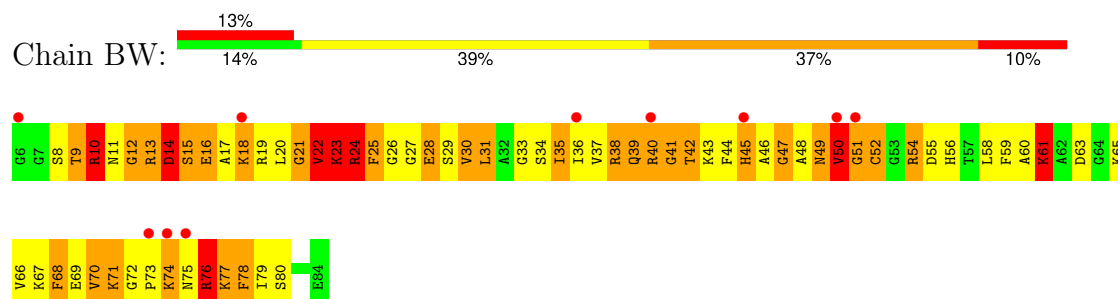


- Molecule 43: 50S ribosomal protein L25

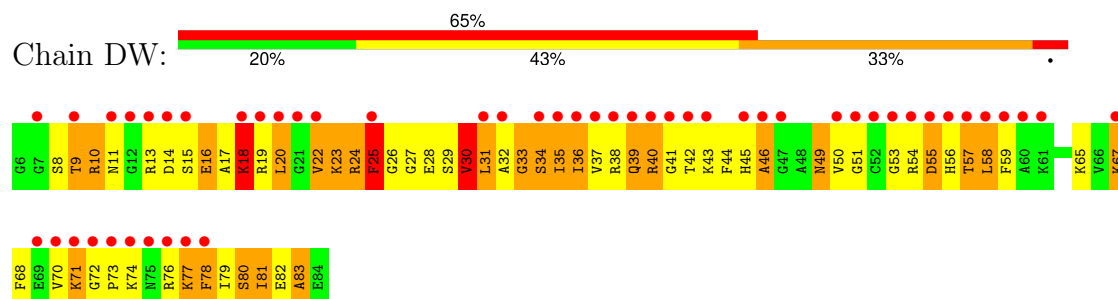




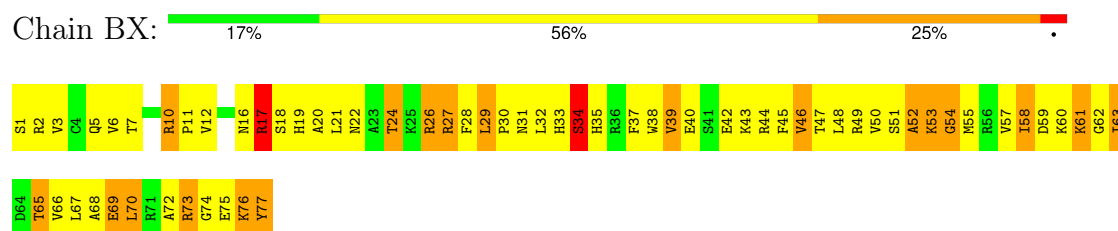
• Molecule 44: 50S ribosomal protein L27



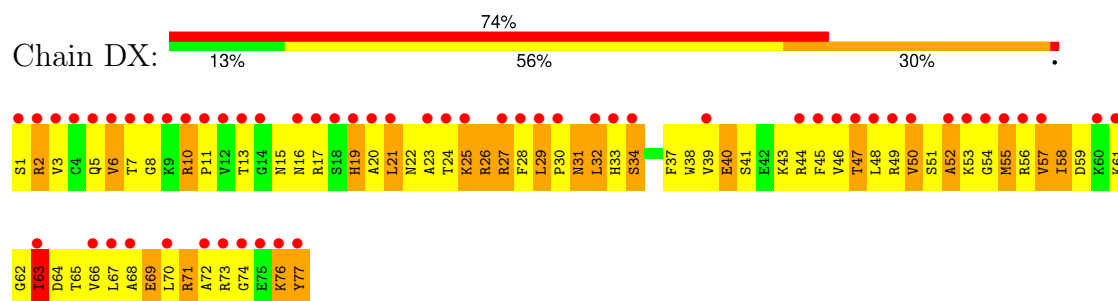
• Molecule 44: 50S ribosomal protein L27



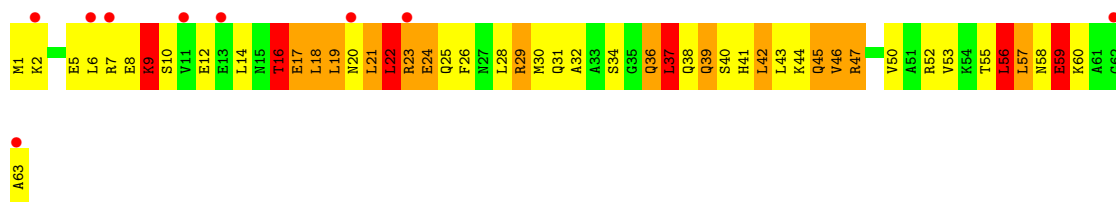
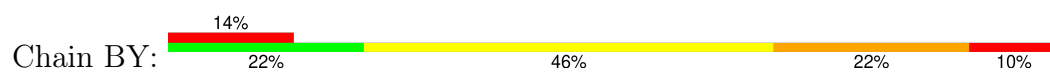
• Molecule 45: 50S ribosomal protein L28



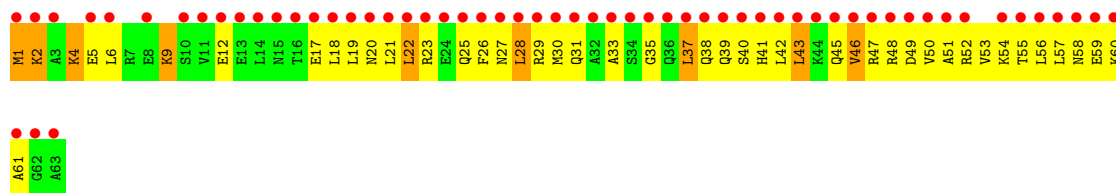
• Molecule 45: 50S ribosomal protein L28



• Molecule 46: 50S ribosomal protein L29



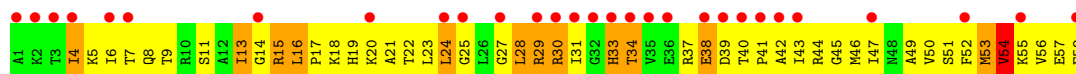
- Molecule 46: 50S ribosomal protein L29



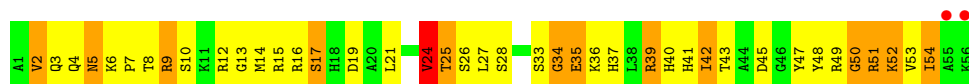
- Molecule 47: 50S ribosomal protein L30



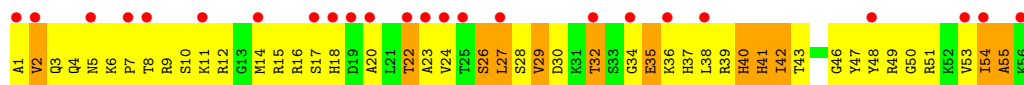
- Molecule 47: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L32



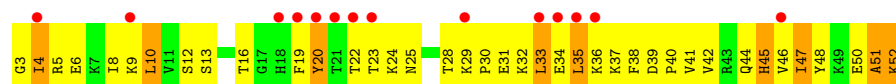
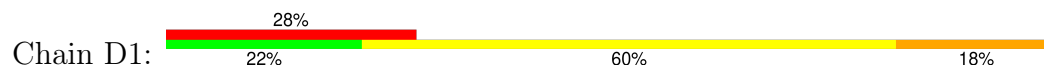
- Molecule 48: 50S ribosomal protein L32



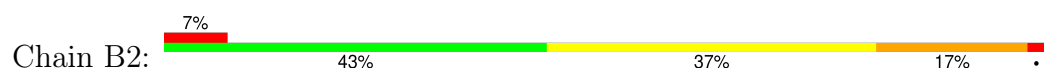
- Molecule 49: 50S ribosomal protein L33



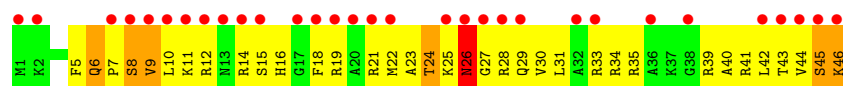
- Molecule 49: 50S ribosomal protein L33



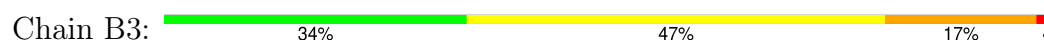
- Molecule 50: 50S ribosomal protein L34



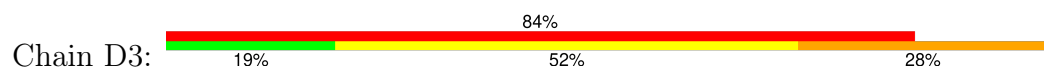
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35

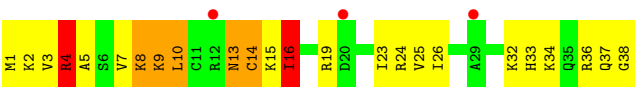


- Molecule 51: 50S ribosomal protein L35

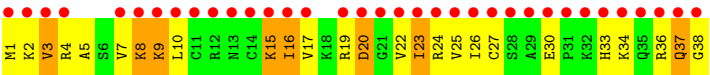
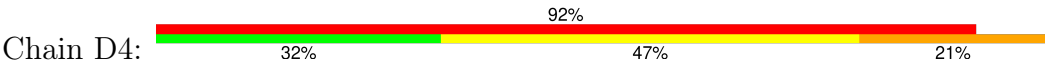


- Molecule 52: 50S ribosomal protein L36





● Molecule 52: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.96Å 434.53Å 623.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.40 – 3.10 82.40 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (82.40-3.10) 83.9 (82.40-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.205 , 0.254 0.215 , 0.261	Depositor DCC
R_{free} test set	18659 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284525	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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: ERY, MG, ZN

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	0.33	0/36834	1.01	264/57462 (0.5%)
1	CA	0.30	0/36762	0.93	184/57350 (0.3%)
2	AB	0.31	0/1736	0.80	3/2338 (0.1%)
2	CB	0.29	0/1736	0.87	5/2338 (0.2%)
3	AC	0.33	0/1652	0.88	7/2225 (0.3%)
3	CC	0.31	0/1652	0.77	2/2225 (0.1%)
4	AD	0.36	0/1665	0.85	4/2227 (0.2%)
4	CD	0.47	0/1665	0.91	3/2227 (0.1%)
5	AE	0.42	0/1119	0.95	2/1504 (0.1%)
5	CE	0.39	0/1119	0.92	3/1504 (0.2%)
6	AF	0.39	0/836	0.86	6/1128 (0.5%)
6	CF	0.36	0/836	0.82	2/1128 (0.2%)
7	AG	0.30	0/1196	0.78	0/1602
7	CG	0.29	0/1188	0.86	4/1591 (0.3%)
8	AH	0.42	0/989	0.93	2/1326 (0.2%)
8	CH	0.35	0/989	0.83	1/1326 (0.1%)
9	AI	0.29	0/1034	0.75	0/1375
9	CI	0.28	0/1034	0.72	0/1375
10	AJ	0.32	0/797	0.81	2/1077 (0.2%)
10	CJ	0.30	0/797	0.83	5/1077 (0.5%)
11	AK	0.34	0/893	0.93	2/1205 (0.2%)
11	CK	0.34	0/893	0.88	2/1205 (0.2%)
12	AL	0.49	0/969	1.03	5/1300 (0.4%)
12	CL	0.41	0/969	0.97	4/1300 (0.3%)
13	AM	0.32	0/893	0.84	1/1193 (0.1%)
13	CM	0.33	1/885 (0.1%)	0.69	0/1183
14	AN	0.32	0/785	0.82	2/1043 (0.2%)
14	CN	0.26	0/780	0.76	0/1036
15	AO	0.39	0/722	0.79	1/964 (0.1%)
15	CO	0.31	0/722	0.72	0/964
16	AP	0.42	0/659	0.88	4/884 (0.5%)
16	CP	0.46	1/649 (0.2%)	0.83	2/872 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.45	0/658	0.94	2/881 (0.2%)
17	CQ	0.34	0/658	0.79	0/881
18	AR	0.38	0/463	0.81	2/621 (0.3%)
18	CR	0.35	0/463	0.79	2/621 (0.3%)
19	AS	0.29	0/653	0.78	0/877
19	CS	0.24	0/653	0.80	0/877
20	AT	0.44	0/671	0.94	3/888 (0.3%)
20	CT	0.33	0/671	0.93	6/888 (0.7%)
21	AU	0.30	0/431	0.80	0/570
21	CU	0.38	0/431	0.84	0/570
22	BA	0.49	1/68626 (0.0%)	1.21	825/107056 (0.8%)
22	DA	0.31	0/68314	0.96	422/106569 (0.4%)
23	BB	0.45	0/2828	1.15	32/4410 (0.7%)
23	DB	0.28	0/2803	0.82	12/4371 (0.3%)
24	BC	0.63	0/2122	1.17	13/2852 (0.5%)
24	DC	0.38	0/2122	0.93	7/2852 (0.2%)
25	BD	0.79	1/1586 (0.1%)	1.15	8/2134 (0.4%)
25	DD	0.35	0/1586	0.87	2/2134 (0.1%)
26	BE	0.65	0/1571	1.05	5/2113 (0.2%)
26	DE	0.33	0/1571	0.86	4/2113 (0.2%)
27	BF	0.46	1/1435 (0.1%)	0.91	3/1928 (0.2%)
27	DF	0.28	0/1444	0.79	3/1937 (0.2%)
28	BG	0.50	0/1343	0.92	2/1816 (0.1%)
28	DG	0.29	0/1343	0.81	3/1816 (0.2%)
29	BH	0.37	0/1122	0.85	7/1515 (0.5%)
29	DH	0.35	0/1122	0.76	0/1515
30	BI	0.35	0/1046	0.88	4/1410 (0.3%)
30	DI	0.30	0/1046	0.82	2/1410 (0.1%)
31	BJ	0.79	0/1152	1.30	14/1551 (0.9%)
31	DJ	0.35	0/1152	0.90	4/1551 (0.3%)
32	BK	0.73	0/948	1.19	5/1268 (0.4%)
32	DK	0.37	0/948	0.88	2/1268 (0.2%)
33	BL	0.69	1/1054 (0.1%)	1.23	7/1403 (0.5%)
33	DL	0.32	0/1054	0.81	1/1403 (0.1%)
34	BM	0.73	0/1093	1.16	5/1460 (0.3%)
34	DM	0.35	0/1093	0.93	6/1460 (0.4%)
35	BN	0.77	0/974	1.17	7/1301 (0.5%)
35	DN	0.36	0/974	0.89	3/1301 (0.2%)
36	BO	0.57	0/902	1.01	4/1209 (0.3%)
36	DO	0.29	0/902	0.73	0/1209
37	BP	0.66	0/929	1.08	3/1242 (0.2%)
37	DP	0.34	0/929	0.84	3/1242 (0.2%)
38	BQ	0.88	0/960	1.20	7/1278 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.34	0/960	0.79	2/1278 (0.2%)
39	BR	0.78	1/829 (0.1%)	1.17	5/1107 (0.5%)
39	DR	0.31	0/829	0.72	1/1107 (0.1%)
40	BS	0.85	0/864	1.14	2/1156 (0.2%)
40	DS	0.37	0/864	0.84	1/1156 (0.1%)
41	BT	0.65	0/745	1.09	1/994 (0.1%)
41	DT	0.29	0/745	0.75	0/994
42	BU	0.58	0/788	1.09	3/1051 (0.3%)
42	DU	0.31	0/788	0.81	1/1051 (0.1%)
43	BV	0.61	0/766	0.94	1/1025 (0.1%)
43	DV	0.30	0/766	0.84	3/1025 (0.3%)
44	BW	0.85	1/603 (0.2%)	1.21	4/797 (0.5%)
44	DW	0.31	0/603	0.76	0/797
45	BX	0.58	0/635	1.04	2/848 (0.2%)
45	DX	0.36	0/635	0.91	6/848 (0.7%)
46	BY	0.48	0/510	0.90	4/677 (0.6%)
46	DY	0.27	0/510	0.73	0/677
47	BZ	0.80	0/453	1.30	5/605 (0.8%)
47	DZ	0.33	0/453	0.82	1/605 (0.2%)
48	B0	0.70	0/450	1.10	4/599 (0.7%)
48	D0	0.33	0/450	0.77	0/599
49	B1	0.46	0/417	1.03	4/554 (0.7%)
49	D1	0.30	0/417	0.78	0/554
50	B2	0.74	0/380	1.06	2/498 (0.4%)
50	D2	0.35	0/380	1.09	3/498 (0.6%)
51	B3	0.65	0/513	1.08	1/676 (0.1%)
51	D3	0.36	0/513	0.81	0/676
52	B4	0.54	0/303	0.97	0/397
52	D4	0.31	0/303	0.64	0/397
All	All	0.41	8/306773 (0.0%)	1.02	2018/458571 (0.4%)

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
12	AL	0	1
20	AT	0	1
25	BD	0	1
31	BJ	0	1
35	BN	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BF	177	ARG	C-N	-7.00	1.23	1.33
16	CP	80	LYS	C-N	-7.00	1.23	1.33
13	CM	113	LYS	C-N	-6.87	1.23	1.34
44	BW	50	VAL	CA-CB	6.70	1.63	1.54
33	BL	30	THR	CA-CB	6.63	1.62	1.54

The worst 5 of 2018 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2848	G	P-O3'-C3'	13.26	140.09	120.20
22	BA	1603	A	P-O3'-C3'	-13.01	100.69	120.20
22	BA	627	A	P-O3'-C3'	12.66	139.19	120.20
24	BC	105	ALA	CA-C-N	12.48	133.28	119.92
24	BC	105	ALA	C-N-CA	12.48	133.28	119.92

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	AL	22	ALA	Peptide
20	AT	6	ALA	Peptide
25	BD	191	GLY	Peptide
31	BJ	110	PRO	Peptide
35	BN	101	GLY	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	32895	0	16553	2311	0
1	CA	32831	0	16521	2691	0
2	AB	1705	0	1732	297	0
2	CB	1705	0	1732	271	0
3	AC	1625	0	1699	200	0
3	CC	1625	0	1699	242	0
4	AD	1643	0	1710	296	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CD	1643	0	1710	278	0
5	AE	1106	0	1148	217	0
5	CE	1106	0	1148	190	0
6	AF	818	0	808	120	0
6	CF	818	0	808	142	0
7	AG	1182	0	1240	157	0
7	CG	1175	0	1230	211	0
8	AH	979	0	1034	164	0
8	CH	979	0	1034	147	0
9	AI	1022	0	1070	173	0
9	CI	1022	0	1070	182	0
10	AJ	787	0	828	172	0
10	CJ	787	0	828	144	0
11	AK	877	0	887	175	0
11	CK	877	0	887	142	0
12	AL	955	0	1019	137	0
12	CL	955	0	1019	177	0
13	AM	884	0	944	125	0
13	CM	877	0	937	185	0
14	AN	774	0	827	140	0
14	CN	769	0	822	152	0
15	AO	714	0	737	99	0
15	CO	714	0	737	77	0
16	AP	649	0	666	105	0
16	CP	639	0	656	140	0
17	AQ	649	0	691	140	0
17	CQ	649	0	691	101	0
18	AR	456	0	478	58	0
18	CR	456	0	478	98	0
19	AS	638	0	665	97	0
19	CS	638	0	665	122	0
20	AT	665	0	714	121	0
20	CT	665	0	714	106	0
21	AU	426	0	449	141	0
21	CU	426	0	449	128	0
22	BA	61274	0	30819	3105	1
22	DA	60995	0	30679	5714	1
23	BB	2529	0	1281	106	0
23	DB	2507	0	1270	239	0
24	BC	2083	0	2157	325	0
24	DC	2083	0	2157	356	0
25	BD	1565	0	1616	284	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DD	1565	0	1616	328	0
26	BE	1552	0	1619	208	0
26	DE	1552	0	1619	327	0
27	BF	1411	0	1447	218	0
27	DF	1420	0	1460	301	0
28	BG	1323	0	1374	230	0
28	DG	1323	0	1374	234	0
29	BH	1111	0	1148	192	0
29	DH	1111	0	1148	212	0
30	BI	1032	0	1088	140	0
30	DI	1032	0	1088	153	0
31	BJ	1129	0	1162	223	0
31	DJ	1129	0	1162	215	0
32	BK	939	0	1012	159	0
32	DK	939	0	1012	193	0
33	BL	1045	0	1117	176	0
33	DL	1045	0	1117	229	0
34	BM	1074	0	1157	159	0
34	DM	1074	0	1157	162	0
35	BN	961	0	1000	133	0
35	DN	961	0	1000	228	0
36	BO	892	0	923	128	0
36	DO	892	0	923	123	0
37	BP	917	0	965	197	0
37	DP	917	0	965	186	0
38	BQ	947	0	1022	200	0
38	DQ	947	0	1022	205	0
39	BR	816	0	839	149	0
39	DR	816	0	839	152	0
40	BS	857	0	922	96	0
40	DS	857	0	922	129	0
41	BT	739	0	807	164	0
41	DT	739	0	807	177	0
42	BU	780	0	834	105	0
42	DU	780	0	834	151	0
43	BV	753	0	780	65	0
43	DV	753	0	780	125	0
44	BW	596	0	610	286	0
44	DW	596	0	610	182	0
45	BX	625	0	655	117	0
45	DX	625	0	655	134	0
46	BY	509	0	543	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DY	509	0	543	119	0
47	BZ	449	0	491	49	0
47	DZ	449	0	491	76	0
48	B0	444	0	461	55	0
48	D0	444	0	461	97	0
49	B1	410	0	440	73	0
49	D1	410	0	440	55	0
50	B2	377	0	418	32	0
50	D2	377	0	418	65	0
51	B3	504	0	574	71	0
51	D3	504	0	574	104	0
52	B4	302	0	340	47	0
52	D4	302	0	343	50	0
53	AA	41	0	0	0	0
53	AN	2	0	0	0	0
53	BA	135	0	0	0	0
53	BB	4	0	0	0	0
53	CA	42	0	0	0	0
53	DA	133	0	0	0	0
53	DB	1	0	0	0	0
53	DC	2	0	0	0	0
53	DJ	1	0	0	0	0
54	BA	51	0	67	4	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	197	0	0	12	0
56	AE	1	0	0	0	0
56	AL	1	0	0	0	0
56	AN	7	0	0	0	0
56	AT	1	0	0	0	0
56	AU	1	0	0	0	0
56	B3	3	0	0	0	0
56	B4	2	0	0	0	0
56	BA	605	0	0	46	0
56	BB	19	0	0	0	0
56	BC	7	0	0	0	0
56	BD	3	0	0	2	0
56	BE	1	0	0	1	0
56	BL	4	0	0	1	0
56	BN	2	0	0	0	0
56	BR	1	0	0	0	0
56	BT	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BV	1	0	0	1	0
56	CA	195	0	0	3	0
56	CE	3	0	0	1	0
56	CL	1	0	0	0	0
56	CN	3	0	0	0	0
56	CT	4	0	0	0	0
56	CU	1	0	0	0	0
56	D2	1	0	0	1	0
56	D3	1	0	0	0	0
56	D4	4	0	0	0	0
56	DA	600	0	0	30	0
56	DB	3	0	0	0	0
56	DC	13	0	0	2	0
56	DD	2	0	0	0	0
56	DE	4	0	0	0	0
56	DJ	3	0	0	0	0
56	DL	4	0	0	1	0
56	DN	2	0	0	0	0
56	DT	2	0	0	0	0
56	DU	2	0	0	0	0
56	DV	2	0	0	0	0
All	All	284525	0	190908	27707	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 59.

The worst 5 of 27707 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)
37:BP:50:ARG:CG	37:BP:57:ALA:H	1.24	1.44
37:BP:50:ARG:HD2	37:BP:51:ASN:N	1.27	1.42
37:BP:50:ARG:HG2	37:BP:57:ALA:N	1.13	1.41
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.37	1.34
1:CA:238:A:C2'	1:CA:239:U:H5''	1.57	1.34

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)
22:BA:138:U:O4	22:DA:305:C:OP1[3_545]	2.02	0.18

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%)	133 (62%)	51 (24%)	32 (15%)	0	0
2	CB	216/218 (99%)	158 (73%)	38 (18%)	20 (9%)	0	3
3	AC	204/206 (99%)	144 (71%)	36 (18%)	24 (12%)	0	1
3	CC	204/206 (99%)	138 (68%)	47 (23%)	19 (9%)	0	3
4	AD	203/205 (99%)	127 (63%)	43 (21%)	33 (16%)	0	0
4	CD	203/205 (99%)	138 (68%)	40 (20%)	25 (12%)	0	1
5	AE	148/150 (99%)	97 (66%)	28 (19%)	23 (16%)	0	0
5	CE	148/150 (99%)	111 (75%)	21 (14%)	16 (11%)	0	2
6	AF	98/100 (98%)	71 (72%)	15 (15%)	12 (12%)	0	1
6	CF	98/100 (98%)	66 (67%)	19 (19%)	13 (13%)	0	1
7	AG	149/151 (99%)	100 (67%)	37 (25%)	12 (8%)	1	4
7	CG	148/151 (98%)	96 (65%)	38 (26%)	14 (10%)	0	3
8	AH	127/129 (98%)	101 (80%)	15 (12%)	11 (9%)	0	4
8	CH	127/129 (98%)	96 (76%)	23 (18%)	8 (6%)	1	6
9	AI	125/127 (98%)	81 (65%)	28 (22%)	16 (13%)	0	1
9	CI	125/127 (98%)	84 (67%)	32 (26%)	9 (7%)	1	5
10	AJ	96/98 (98%)	69 (72%)	10 (10%)	17 (18%)	0	0
10	CJ	96/98 (98%)	61 (64%)	21 (22%)	14 (15%)	0	0
11	AK	115/117 (98%)	80 (70%)	20 (17%)	15 (13%)	0	1
11	CK	115/117 (98%)	87 (76%)	16 (14%)	12 (10%)	0	2
12	AL	121/123 (98%)	88 (73%)	21 (17%)	12 (10%)	0	3
12	CL	121/123 (98%)	84 (69%)	24 (20%)	13 (11%)	0	2
13	AM	112/114 (98%)	83 (74%)	19 (17%)	10 (9%)	0	3
13	CM	112/114 (98%)	62 (55%)	37 (33%)	13 (12%)	0	1
14	AN	92/100 (92%)	60 (65%)	18 (20%)	14 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	91/100 (91%)	57 (63%)	26 (29%)	8 (9%)	0	3
15	AO	86/88 (98%)	59 (69%)	19 (22%)	8 (9%)	0	3
15	CO	86/88 (98%)	53 (62%)	30 (35%)	3 (4%)	3	16
16	AP	80/82 (98%)	59 (74%)	12 (15%)	9 (11%)	0	2
16	CP	79/82 (96%)	48 (61%)	23 (29%)	8 (10%)	0	3
17	AQ	78/80 (98%)	48 (62%)	24 (31%)	6 (8%)	1	4
17	CQ	78/80 (98%)	59 (76%)	11 (14%)	8 (10%)	0	2
18	AR	53/55 (96%)	40 (76%)	10 (19%)	3 (6%)	1	8
18	CR	53/55 (96%)	33 (62%)	17 (32%)	3 (6%)	1	8
19	AS	77/79 (98%)	51 (66%)	15 (20%)	11 (14%)	0	1
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	0	3
20	AT	83/85 (98%)	57 (69%)	21 (25%)	5 (6%)	1	7
20	CT	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	0	1
21	AU	49/51 (96%)	25 (51%)	12 (24%)	12 (24%)	0	0
21	CU	49/51 (96%)	20 (41%)	13 (26%)	16 (33%)	0	0
24	BC	269/271 (99%)	197 (73%)	46 (17%)	26 (10%)	0	3
24	DC	269/271 (99%)	174 (65%)	64 (24%)	31 (12%)	0	1
25	BD	207/209 (99%)	141 (68%)	32 (16%)	34 (16%)	0	0
25	DD	207/209 (99%)	131 (63%)	41 (20%)	35 (17%)	0	0
26	BE	199/201 (99%)	144 (72%)	35 (18%)	20 (10%)	0	3
26	DE	199/201 (99%)	115 (58%)	54 (27%)	30 (15%)	0	0
27	BF	176/178 (99%)	124 (70%)	36 (20%)	16 (9%)	0	3
27	DF	176/178 (99%)	87 (49%)	58 (33%)	31 (18%)	0	0
28	BG	174/176 (99%)	111 (64%)	38 (22%)	25 (14%)	0	0
28	DG	174/176 (99%)	99 (57%)	40 (23%)	35 (20%)	0	0
29	BH	147/149 (99%)	62 (42%)	50 (34%)	35 (24%)	0	0
29	DH	147/149 (99%)	70 (48%)	54 (37%)	23 (16%)	0	0
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	0	3
30	DI	139/141 (99%)	75 (54%)	48 (34%)	16 (12%)	0	1
31	BJ	140/142 (99%)	104 (74%)	24 (17%)	12 (9%)	0	4
31	DJ	140/142 (99%)	92 (66%)	28 (20%)	20 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BK	120/122 (98%)	89 (74%)	17 (14%)	14 (12%)	0	1
32	DK	120/122 (98%)	76 (63%)	17 (14%)	27 (22%)	0	0
33	BL	141/143 (99%)	100 (71%)	30 (21%)	11 (8%)	1	4
33	DL	141/143 (99%)	77 (55%)	44 (31%)	20 (14%)	0	1
34	BM	134/136 (98%)	96 (72%)	18 (13%)	20 (15%)	0	0
34	DM	134/136 (98%)	90 (67%)	26 (19%)	18 (13%)	0	1
35	BN	118/120 (98%)	91 (77%)	16 (14%)	11 (9%)	0	3
35	DN	118/120 (98%)	74 (63%)	25 (21%)	19 (16%)	0	0
36	BO	114/116 (98%)	85 (75%)	18 (16%)	11 (10%)	0	3
36	DO	114/116 (98%)	74 (65%)	30 (26%)	10 (9%)	0	3
37	BP	112/114 (98%)	78 (70%)	20 (18%)	14 (12%)	0	1
37	DP	112/114 (98%)	60 (54%)	31 (28%)	21 (19%)	0	0
38	BQ	115/117 (98%)	100 (87%)	7 (6%)	8 (7%)	1	5
38	DQ	115/117 (98%)	75 (65%)	27 (24%)	13 (11%)	0	2
39	BR	101/103 (98%)	76 (75%)	14 (14%)	11 (11%)	0	2
39	DR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	1
40	BS	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	2	12
40	DS	108/110 (98%)	72 (67%)	25 (23%)	11 (10%)	0	3
41	BT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	0
41	DT	91/93 (98%)	41 (45%)	26 (29%)	24 (26%)	0	0
42	BU	100/102 (98%)	66 (66%)	16 (16%)	18 (18%)	0	0
42	DU	100/102 (98%)	52 (52%)	22 (22%)	26 (26%)	0	0
43	BV	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	5	24
43	DV	92/94 (98%)	60 (65%)	24 (26%)	8 (9%)	0	4
44	BW	77/79 (98%)	31 (40%)	22 (29%)	24 (31%)	0	0
44	DW	77/79 (98%)	30 (39%)	25 (32%)	22 (29%)	0	0
45	BX	75/77 (97%)	58 (77%)	10 (13%)	7 (9%)	0	3
45	DX	75/77 (97%)	44 (59%)	20 (27%)	11 (15%)	0	0
46	BY	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	1
46	DY	61/63 (97%)	40 (66%)	16 (26%)	5 (8%)	0	4
47	BZ	56/58 (97%)	47 (84%)	5 (9%)	4 (7%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DZ	56/58 (97%)	31 (55%)	20 (36%)	5 (9%)	0	3
48	B0	54/56 (96%)	41 (76%)	9 (17%)	4 (7%)	1	5
48	D0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	0	3
49	B1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	0	2
49	D1	48/50 (96%)	35 (73%)	8 (17%)	5 (10%)	0	2
50	B2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
50	D2	44/46 (96%)	29 (66%)	10 (23%)	5 (11%)	0	1
51	B3	62/64 (97%)	53 (86%)	5 (8%)	4 (6%)	1	6
51	D3	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0	1
52	B4	36/38 (95%)	24 (67%)	9 (25%)	3 (8%)	0	4
52	D4	36/38 (95%)	21 (58%)	9 (25%)	6 (17%)	0	0
All	All	11241/11452 (98%)	7412 (66%)	2420 (22%)	1409 (12%)	0	1

5 of 1409 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	21	TYR
2	AB	33	ALA
2	AB	37	VAL
2	AB	72	LYS
2	AB	75	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%)	148 (82%)	32 (18%)	2	9
2	CB	180/180 (100%)	158 (88%)	22 (12%)	5	20
3	AC	170/170 (100%)	136 (80%)	34 (20%)	1	6
3	CC	170/170 (100%)	155 (91%)	15 (9%)	9	33
4	AD	172/172 (100%)	134 (78%)	38 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/172 (100%)	128 (74%)	44 (26%)	0	2
5	AE	113/113 (100%)	76 (67%)	37 (33%)	0	0
5	CE	113/113 (100%)	85 (75%)	28 (25%)	1	2
6	AF	87/87 (100%)	69 (79%)	18 (21%)	1	5
6	CF	87/87 (100%)	71 (82%)	16 (18%)	1	8
7	AG	124/124 (100%)	109 (88%)	15 (12%)	5	20
7	CG	123/124 (99%)	98 (80%)	25 (20%)	1	5
8	AH	104/104 (100%)	79 (76%)	25 (24%)	1	3
8	CH	104/104 (100%)	87 (84%)	17 (16%)	2	11
9	AI	105/105 (100%)	84 (80%)	21 (20%)	1	6
9	CI	105/105 (100%)	87 (83%)	18 (17%)	2	10
10	AJ	86/86 (100%)	68 (79%)	18 (21%)	1	5
10	CJ	86/86 (100%)	75 (87%)	11 (13%)	4	18
11	AK	90/90 (100%)	75 (83%)	15 (17%)	2	10
11	CK	90/90 (100%)	79 (88%)	11 (12%)	5	20
12	AL	103/103 (100%)	78 (76%)	25 (24%)	1	3
12	CL	103/103 (100%)	75 (73%)	28 (27%)	0	1
13	AM	92/92 (100%)	81 (88%)	11 (12%)	5	21
13	CM	91/92 (99%)	82 (90%)	9 (10%)	7	29
14	AN	79/83 (95%)	72 (91%)	7 (9%)	9	33
14	CN	79/83 (95%)	69 (87%)	10 (13%)	4	18
15	AO	76/76 (100%)	61 (80%)	15 (20%)	1	6
15	CO	76/76 (100%)	69 (91%)	7 (9%)	8	31
16	AP	65/65 (100%)	53 (82%)	12 (18%)	1	8
16	CP	65/65 (100%)	52 (80%)	13 (20%)	1	6
17	AQ	74/74 (100%)	57 (77%)	17 (23%)	1	4
17	CQ	74/74 (100%)	59 (80%)	15 (20%)	1	5
18	AR	48/48 (100%)	42 (88%)	6 (12%)	4	19
18	CR	48/48 (100%)	40 (83%)	8 (17%)	2	10
19	AS	70/70 (100%)	60 (86%)	10 (14%)	3	14
19	CS	70/70 (100%)	66 (94%)	4 (6%)	18	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AT	65/65 (100%)	45 (69%)	20 (31%)	0	0
20	CT	65/65 (100%)	51 (78%)	14 (22%)	1	5
21	AU	44/44 (100%)	34 (77%)	10 (23%)	1	4
21	CU	44/44 (100%)	34 (77%)	10 (23%)	1	4
24	BC	216/216 (100%)	169 (78%)	47 (22%)	1	5
24	DC	216/216 (100%)	172 (80%)	44 (20%)	1	5
25	BD	164/164 (100%)	131 (80%)	33 (20%)	1	5
25	DD	164/164 (100%)	123 (75%)	41 (25%)	0	2
26	BE	165/165 (100%)	106 (64%)	59 (36%)	0	0
26	DE	165/165 (100%)	142 (86%)	23 (14%)	3	15
27	BF	148/149 (99%)	110 (74%)	38 (26%)	0	2
27	DF	149/149 (100%)	123 (83%)	26 (17%)	2	9
28	BG	137/137 (100%)	99 (72%)	38 (28%)	0	1
28	DG	137/137 (100%)	117 (85%)	20 (15%)	3	14
29	BH	114/114 (100%)	93 (82%)	21 (18%)	1	8
29	DH	114/114 (100%)	93 (82%)	21 (18%)	1	8
30	BI	109/109 (100%)	95 (87%)	14 (13%)	4	18
30	DI	109/109 (100%)	103 (94%)	6 (6%)	19	50
31	BJ	116/116 (100%)	87 (75%)	29 (25%)	0	2
31	DJ	116/116 (100%)	95 (82%)	21 (18%)	2	8
32	BK	103/103 (100%)	77 (75%)	26 (25%)	0	2
32	DK	103/103 (100%)	76 (74%)	27 (26%)	0	2
33	BL	102/102 (100%)	76 (74%)	26 (26%)	0	2
33	DL	102/102 (100%)	84 (82%)	18 (18%)	2	9
34	BM	109/109 (100%)	78 (72%)	31 (28%)	0	1
34	DM	109/109 (100%)	95 (87%)	14 (13%)	4	18
35	BN	100/100 (100%)	79 (79%)	21 (21%)	1	5
35	DN	100/100 (100%)	84 (84%)	16 (16%)	2	12
36	BO	86/86 (100%)	67 (78%)	19 (22%)	1	4
36	DO	86/86 (100%)	77 (90%)	9 (10%)	6	26
37	BP	99/99 (100%)	64 (65%)	35 (35%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DP	99/99 (100%)	83 (84%)	16 (16%)	2	11
38	BQ	89/89 (100%)	61 (68%)	28 (32%)	0	0
38	DQ	89/89 (100%)	66 (74%)	23 (26%)	0	2
39	BR	84/84 (100%)	59 (70%)	25 (30%)	0	1
39	DR	84/84 (100%)	65 (77%)	19 (23%)	1	4
40	BS	93/93 (100%)	67 (72%)	26 (28%)	0	1
40	DS	93/93 (100%)	67 (72%)	26 (28%)	0	1
41	BT	80/80 (100%)	52 (65%)	28 (35%)	0	0
41	DT	80/80 (100%)	71 (89%)	9 (11%)	5	23
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	5
42	DU	83/83 (100%)	68 (82%)	15 (18%)	2	8
43	BV	78/78 (100%)	63 (81%)	15 (19%)	1	7
43	DV	78/78 (100%)	67 (86%)	11 (14%)	3	15
44	BW	59/59 (100%)	39 (66%)	20 (34%)	0	0
44	DW	59/59 (100%)	45 (76%)	14 (24%)	1	3
45	BX	67/67 (100%)	51 (76%)	16 (24%)	1	3
45	DX	67/67 (100%)	57 (85%)	10 (15%)	3	13
46	BY	55/55 (100%)	39 (71%)	16 (29%)	0	1
46	DY	55/55 (100%)	51 (93%)	4 (7%)	13	40
47	BZ	48/48 (100%)	34 (71%)	14 (29%)	0	1
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	5
48	B0	47/47 (100%)	36 (77%)	11 (23%)	1	4
48	D0	47/47 (100%)	40 (85%)	7 (15%)	3	13
49	B1	45/45 (100%)	36 (80%)	9 (20%)	1	6
49	D1	45/45 (100%)	38 (84%)	7 (16%)	2	12
50	B2	38/38 (100%)	29 (76%)	9 (24%)	1	3
50	D2	38/38 (100%)	34 (90%)	4 (10%)	6	26
51	B3	51/51 (100%)	42 (82%)	9 (18%)	2	9
51	D3	51/51 (100%)	37 (72%)	14 (28%)	0	1
52	B4	34/34 (100%)	28 (82%)	6 (18%)	2	9
52	D4	34/34 (100%)	30 (88%)	4 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9331/9342 (100%)	7455 (80%)	1876 (20%)	1 5

5 of 1876 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	BT	74	ILE
41	DT	56	GLU
4	CD	187	ARG
40	DS	66	ILE
32	DK	2	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 377 such sidechains are listed below:

Mol	Chain	Res	Type
5	CE	131	ASN
24	DC	89	ASN
7	CG	67	ASN
13	CM	90	HIS
28	DG	19	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	535 (34%)	236 (15%)
1	CA	1529/1533 (99%)	587 (38%)	242 (15%)
22	BA	2850/2904 (98%)	993 (34%)	429 (15%)
22	DA	2839/2904 (97%)	1144 (40%)	498 (17%)
23	BB	117/118 (99%)	37 (31%)	17 (14%)
23	DB	116/118 (98%)	45 (38%)	16 (13%)
All	All	8983/9110 (98%)	3341 (37%)	1438 (16%)

5 of 3341 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G

5 of 1438 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	DA	15	G
22	DA	1272	A
22	DA	163	C
22	DA	14	A
22	DA	621	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 364 ligands modelled in this entry, 363 are monoatomic - leaving 1 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	$\# Z > 2$
54	ERY	BA	3136	-	53,53,53	0.81	1 (1%)	82,82,82	1.69	18 (21%)

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	ERY	BA	3136	-	-	9/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	3136	ERY	C6-C5	2.44	1.59	1.55

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	3136	ERY	C25-C24-C23	-5.04	102.77	110.02
54	BA	3136	ERY	O7-C5-C6	-4.99	100.45	106.40
54	BA	3136	ERY	O2-C1-O1	-3.70	117.27	123.95
54	BA	3136	ERY	C3-C2-C1	-3.44	102.98	109.93
54	BA	3136	ERY	C27-C26-C25	-3.14	108.53	113.27

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

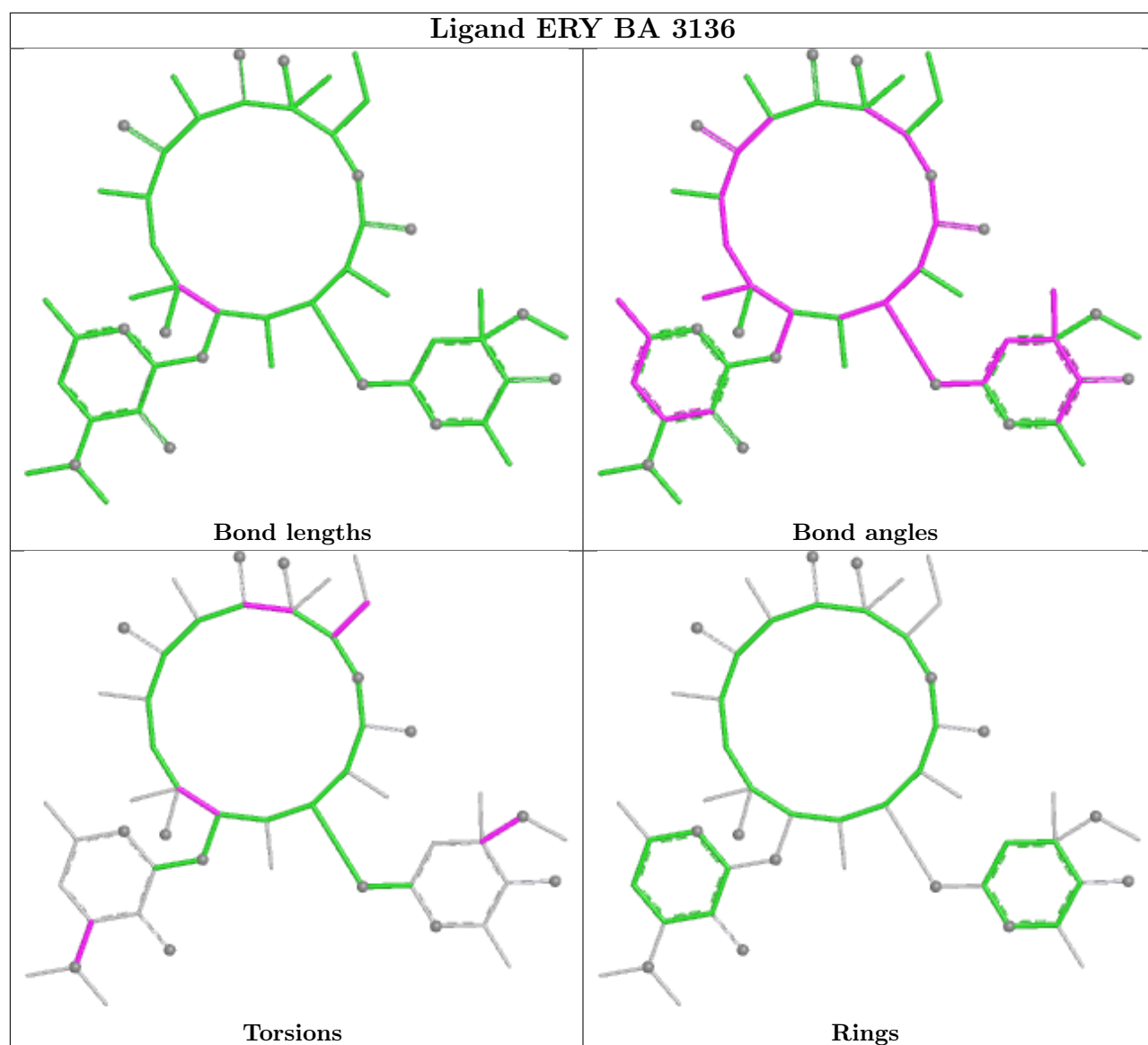
Mol	Chain	Res	Type	Atoms
54	BA	3136	ERY	C15-C16-O5-C20
54	BA	3136	ERY	C19-C16-O5-C20
54	BA	3136	ERY	C10-C11-C12-O13
54	BA	3136	ERY	C25-C24-N1-C28
54	BA	3136	ERY	C4-C5-C6-C32

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	BA	3136	ERY	4	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	1533/1533 (100%)	-0.10	29 (1%) 66 45	21, 74, 188, 404	0
1	CA	1530/1533 (99%)	0.90	155 (10%) 12 6	38, 102, 287, 422	0
2	AB	218/218 (100%)	0.77	11 (5%) 34 18	72, 142, 202, 237	0
2	CB	218/218 (100%)	1.27	39 (17%) 3 1	98, 165, 222, 272	0
3	AC	206/206 (100%)	0.42	14 (6%) 23 12	54, 101, 149, 187	0
3	CC	206/206 (100%)	0.86	23 (11%) 10 5	80, 139, 210, 243	0
4	AD	205/205 (100%)	0.68	25 (12%) 8 5	38, 80, 182, 310	0
4	CD	205/205 (100%)	0.51	12 (5%) 28 15	29, 54, 103, 236	0
5	AE	150/150 (100%)	0.51	10 (6%) 24 13	37, 70, 136, 207	0
5	CE	150/150 (100%)	1.25	30 (20%) 3 1	38, 87, 150, 253	0
6	AF	100/100 (100%)	0.48	8 (8%) 18 10	43, 85, 149, 174	0
6	CF	100/100 (100%)	0.75	9 (9%) 15 8	58, 109, 180, 202	0
7	AG	151/151 (100%)	1.31	33 (21%) 2 1	82, 155, 235, 286	0
7	CG	150/151 (99%)	1.98	70 (46%) 0 0	112, 196, 246, 272	0
8	AH	129/129 (100%)	0.26	3 (2%) 61 39	41, 69, 120, 203	0
8	CH	129/129 (100%)	1.05	15 (11%) 9 5	52, 107, 161, 197	0
9	AI	127/127 (100%)	1.54	38 (29%) 1 1	68, 153, 256, 288	0
9	CI	127/127 (100%)	1.99	52 (40%) 0 0	102, 200, 285, 325	0
10	AJ	98/98 (100%)	1.01	15 (15%) 5 3	60, 119, 200, 251	0
10	CJ	98/98 (100%)	2.19	49 (50%) 0 0	102, 192, 267, 283	0
11	AK	117/117 (100%)	0.61	4 (3%) 48 28	38, 104, 176, 222	0
11	CK	117/117 (100%)	0.76	5 (4%) 40 22	53, 102, 161, 200	0
12	AL	123/123 (100%)	0.30	9 (7%) 21 11	16, 49, 111, 187	0
12	CL	123/123 (100%)	1.14	24 (19%) 3 1	41, 81, 128, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	1.27	23 (20%) 3 1	69, 139, 213, 258	0
13	CM	114/114 (100%)	2.68	69 (60%) 0 0	190, 427, 522, 545	0
14	AN	96/100 (96%)	1.60	34 (35%) 1 0	68, 111, 199, 266	0
14	CN	95/100 (95%)	2.29	55 (57%) 0 0	112, 209, 319, 350	0
15	AO	88/88 (100%)	0.30	4 (4%) 38 20	34, 70, 111, 172	0
15	CO	88/88 (100%)	1.25	15 (17%) 4 2	68, 112, 187, 286	0
16	AP	82/82 (100%)	0.58	7 (8%) 16 9	45, 68, 174, 288	0
16	CP	81/82 (98%)	1.53	28 (34%) 1 0	46, 97, 157, 229	0
17	AQ	80/80 (100%)	1.00	13 (16%) 4 2	35, 71, 134, 209	0
17	CQ	80/80 (100%)	1.26	19 (23%) 2 1	47, 103, 151, 188	0
18	AR	55/55 (100%)	0.47	7 (12%) 8 4	50, 80, 154, 211	0
18	CR	55/55 (100%)	0.93	8 (14%) 6 3	51, 87, 157, 235	0
19	AS	79/79 (100%)	1.24	12 (15%) 5 3	81, 150, 212, 259	0
19	CS	79/79 (100%)	2.47	43 (54%) 0 0	217, 411, 508, 531	0
20	AT	85/85 (100%)	0.55	8 (9%) 14 8	35, 69, 129, 176	0
20	CT	85/85 (100%)	2.00	30 (35%) 1 0	66, 130, 204, 226	0
21	AU	51/51 (100%)	2.27	23 (45%) 0 0	90, 146, 226, 252	0
21	CU	51/51 (100%)	1.36	14 (27%) 1 1	54, 109, 189, 269	0
22	BA	2854/2904 (98%)	-0.55	75 (2%) 57 36	6, 25, 148, 390	0
22	DA	2841/2904 (97%)	1.43	734 (25%) 1 1	55, 116, 270, 526	0
23	BB	118/118 (100%)	-0.45	0 100 100	12, 40, 73, 109	0
23	DB	117/118 (99%)	0.84	9 (7%) 19 10	88, 164, 221, 243	0
24	BC	271/271 (100%)	0.12	12 (4%) 39 21	8, 35, 82, 192	0
24	DC	271/271 (100%)	1.81	89 (32%) 1 0	42, 95, 151, 215	0
25	BD	209/209 (100%)	-0.22	3 (1%) 73 53	6, 21, 69, 179	0
25	DD	209/209 (100%)	1.87	78 (37%) 1 0	55, 115, 199, 284	0
26	BE	201/201 (100%)	-0.17	2 (0%) 79 61	6, 36, 86, 150	0
26	DE	201/201 (100%)	3.00	139 (69%) 0 0	61, 235, 398, 470	0
27	BF	178/178 (100%)	0.28	3 (1%) 69 48	21, 63, 136, 167	0
27	DF	178/178 (100%)	1.10	18 (10%) 12 6	142, 219, 259, 301	0
28	BG	176/176 (100%)	0.29	9 (5%) 33 18	20, 61, 131, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	1.90	67 (38%) 1 0	88, 239, 337, 389	0
29	BH	149/149 (100%)	1.58	49 (32%) 1 0	40, 171, 260, 304	0
29	DH	149/149 (100%)	1.75	54 (36%) 1 0	68, 188, 268, 298	0
30	BI	141/141 (100%)	2.13	68 (48%) 0 0	170, 245, 289, 301	0
30	DI	141/141 (100%)	1.75	40 (28%) 1 1	178, 312, 349, 370	0
31	BJ	142/142 (100%)	-0.18	5 (3%) 47 27	7, 16, 60, 137	0
31	DJ	142/142 (100%)	1.50	36 (25%) 1 1	50, 106, 169, 198	0
32	BK	122/122 (100%)	-0.14	3 (2%) 58 37	11, 24, 69, 242	0
32	DK	122/122 (100%)	0.93	18 (14%) 5 3	59, 97, 147, 210	0
33	BL	143/143 (100%)	-0.05	1 (0%) 84 68	6, 30, 71, 123	0
33	DL	143/143 (100%)	2.76	93 (65%) 0 0	59, 164, 279, 354	0
34	BM	136/136 (100%)	-0.27	2 (1%) 72 52	7, 22, 59, 147	0
34	DM	136/136 (100%)	1.65	41 (30%) 1 1	37, 112, 192, 250	0
35	BN	120/120 (100%)	-0.25	1 (0%) 82 65	8, 17, 40, 149	0
35	DN	120/120 (100%)	2.36	67 (55%) 0 0	63, 131, 211, 305	0
36	BO	116/116 (100%)	-0.04	1 (0%) 81 63	21, 41, 72, 113	0
36	DO	116/116 (100%)	1.55	33 (28%) 1 1	106, 172, 240, 273	0
37	BP	114/114 (100%)	-0.13	2 (1%) 67 47	12, 32, 87, 176	0
37	DP	114/114 (100%)	1.69	40 (35%) 1 0	50, 110, 175, 196	0
38	BQ	117/117 (100%)	-0.33	3 (2%) 57 36	6, 15, 39, 225	0
38	DQ	117/117 (100%)	2.03	53 (45%) 0 0	65, 113, 193, 331	0
39	BR	103/103 (100%)	-0.22	4 (3%) 43 24	6, 26, 67, 184	0
39	DR	103/103 (100%)	2.30	52 (50%) 0 0	73, 144, 238, 305	0
40	BS	110/110 (100%)	-0.38	1 (0%) 81 63	7, 15, 48, 172	0
40	DS	110/110 (100%)	2.24	56 (50%) 0 0	71, 132, 214, 254	0
41	BT	93/93 (100%)	0.65	11 (11%) 9 5	13, 43, 123, 233	0
41	DT	93/93 (100%)	4.34	82 (88%) 0 0	124, 265, 379, 423	0
42	BU	102/102 (100%)	0.33	8 (7%) 19 10	21, 45, 131, 240	0
42	DU	102/102 (100%)	4.38	96 (94%) 0 0	148, 305, 420, 554	0
43	BV	94/94 (100%)	-0.16	0 100 100	14, 38, 78, 135	0
43	DV	94/94 (100%)	1.12	12 (12%) 7 4	88, 136, 193, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	79/79 (100%)	0.61	10 (12%) 8 4	13, 29, 98, 213	0
44	DW	79/79 (100%)	3.32	51 (64%) 0 0	73, 169, 279, 323	0
45	BX	77/77 (100%)	-0.05	0 100 100	13, 37, 77, 108	0
45	DX	77/77 (100%)	2.94	57 (74%) 0 0	62, 118, 214, 280	0
46	BY	63/63 (100%)	0.55	9 (14%) 6 3	27, 59, 126, 209	0
46	DY	63/63 (100%)	4.48	59 (93%) 0 0	152, 379, 492, 508	0
47	BZ	58/58 (100%)	-0.26	0 100 100	9, 16, 47, 61	0
47	DZ	58/58 (100%)	2.01	29 (50%) 0 0	68, 143, 251, 271	0
48	B0	56/56 (100%)	-0.26	2 (3%) 46 26	6, 18, 71, 138	0
48	D0	56/56 (100%)	2.01	24 (42%) 0 0	63, 144, 246, 262	0
49	B1	50/50 (100%)	0.01	1 (2%) 65 44	27, 47, 93, 115	0
49	D1	50/50 (100%)	1.69	14 (28%) 1 1	97, 154, 208, 231	0
50	B2	46/46 (100%)	-0.14	3 (6%) 25 13	10, 19, 43, 195	0
50	D2	46/46 (100%)	2.67	31 (67%) 0 0	59, 119, 184, 211	0
51	B3	64/64 (100%)	-0.23	0 100 100	8, 22, 38, 65	0
51	D3	64/64 (100%)	3.43	54 (84%) 0 0	64, 122, 197, 255	0
52	B4	38/38 (100%)	0.57	3 (7%) 18 10	25, 49, 94, 97	0
52	D4	38/38 (100%)	4.46	35 (92%) 0 0	87, 173, 235, 241	0
All	All	20434/20562 (99%)	0.82	3646 (17%) 4 2	6, 93, 274, 554	0

The worst 5 of 3646 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	DU	30	SER	15.4
13	CM	97	ARG	14.6
41	DT	15	HIS	12.3
12	AL	123	ALA	11.4
46	DY	14	LEU	10.8

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
53	MG	DA	3003	1/1	0.33	0.30	268,268,268,268	0
53	MG	CA	1629	1/1	0.37	0.20	217,217,217,217	0
53	MG	DA	3078	1/1	0.39	0.33	210,210,210,210	0
53	MG	CA	1617	1/1	0.41	0.18	280,280,280,280	0
53	MG	DA	3007	1/1	0.44	0.22	253,253,253,253	0
53	MG	DJ	201	1/1	0.44	0.38	284,284,284,284	0
53	MG	BA	3069	1/1	0.45	0.16	176,176,176,176	0
53	MG	DA	3125	1/1	0.47	0.27	163,163,163,163	0
53	MG	DA	3010	1/1	0.50	0.28	171,171,171,171	0
53	MG	DA	3028	1/1	0.51	0.50	262,262,262,262	0
53	MG	DA	3006	1/1	0.51	0.18	267,267,267,267	0
53	MG	DA	3109	1/1	0.53	0.28	176,176,176,176	0
53	MG	DA	3013	1/1	0.53	0.34	185,185,185,185	0
53	MG	DA	3016	1/1	0.53	0.27	231,231,231,231	0
53	MG	DA	3020	1/1	0.59	0.26	218,218,218,218	0
53	MG	DA	3015	1/1	0.59	0.25	145,145,145,145	0
53	MG	DA	3082	1/1	0.60	0.25	189,189,189,189	0
53	MG	AA	1610	1/1	0.60	0.15	210,210,210,210	0
53	MG	DA	3074	1/1	0.62	0.47	240,240,240,240	0
53	MG	BB	201	1/1	0.63	0.16	236,236,236,236	0
53	MG	DA	3063	1/1	0.63	0.69	192,192,192,192	0
53	MG	AA	1617	1/1	0.64	0.26	203,203,203,203	0
53	MG	DA	3026	1/1	0.64	0.50	244,244,244,244	0
53	MG	DA	3045	1/1	0.65	0.25	233,233,233,233	0
53	MG	DA	3058	1/1	0.65	0.16	235,235,235,235	0
53	MG	DA	3002	1/1	0.65	0.26	160,160,160,160	0
53	MG	DA	3130	1/1	0.66	0.19	279,279,279,279	0
53	MG	DA	3059	1/1	0.67	0.17	183,183,183,183	0
53	MG	DA	3132	1/1	0.68	0.18	175,175,175,175	0
53	MG	CA	1628	1/1	0.68	0.24	236,236,236,236	0
53	MG	CA	1616	1/1	0.69	0.20	232,232,232,232	0
53	MG	DA	3099	1/1	0.70	0.17	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DA	3084	1/1	0.70	0.22	182,182,182,182	0
53	MG	DA	3018	1/1	0.71	0.19	232,232,232,232	0
53	MG	DA	3033	1/1	0.71	0.29	149,149,149,149	0
53	MG	CA	1639	1/1	0.72	0.13	226,226,226,226	0
53	MG	DA	3005	1/1	0.72	0.38	309,309,309,309	0
53	MG	DA	3110	1/1	0.72	0.15	183,183,183,183	0
53	MG	DA	3049	1/1	0.72	0.11	235,235,235,235	0
53	MG	DA	3079	1/1	0.72	0.25	150,150,150,150	0
53	MG	CA	1640	1/1	0.72	0.22	149,149,149,149	0
53	MG	CA	1622	1/1	0.72	0.11	208,208,208,208	0
53	MG	DA	3133	1/1	0.73	0.23	239,239,239,239	0
53	MG	CA	1603	1/1	0.73	0.17	165,165,165,165	0
53	MG	CA	1615	1/1	0.74	0.10	124,124,124,124	0
53	MG	DA	3011	1/1	0.74	0.16	152,152,152,152	0
53	MG	DA	3043	1/1	0.74	0.15	213,213,213,213	0
53	MG	CA	1614	1/1	0.75	0.30	231,231,231,231	0
53	MG	CA	1602	1/1	0.75	0.18	175,175,175,175	0
53	MG	DA	3036	1/1	0.75	0.14	211,211,211,211	0
53	MG	DA	3057	1/1	0.75	0.41	212,212,212,212	0
53	MG	DA	3108	1/1	0.76	0.41	172,172,172,172	0
53	MG	CA	1636	1/1	0.76	0.16	155,155,155,155	0
53	MG	DA	3097	1/1	0.77	0.19	116,116,116,116	0
53	MG	DC	301	1/1	0.77	0.20	124,124,124,124	0
53	MG	CA	1612	1/1	0.77	0.23	120,120,120,120	0
53	MG	CA	1632	1/1	0.78	0.13	163,163,163,163	0
53	MG	DA	3038	1/1	0.78	0.13	204,204,204,204	0
53	MG	DA	3029	1/1	0.78	0.28	151,151,151,151	0
53	MG	DA	3009	1/1	0.78	0.14	101,101,101,101	0
53	MG	DA	3127	1/1	0.78	0.37	199,199,199,199	0
53	MG	DA	3019	1/1	0.79	0.19	224,224,224,224	0
53	MG	CA	1620	1/1	0.79	0.12	170,170,170,170	0
53	MG	DA	3093	1/1	0.79	0.16	228,228,228,228	0
53	MG	BA	3047	1/1	0.79	0.21	152,152,152,152	0
53	MG	DA	3034	1/1	0.79	0.17	89,89,89,89	0
53	MG	CA	1627	1/1	0.80	0.19	198,198,198,198	0
53	MG	DA	3064	1/1	0.80	0.21	230,230,230,230	0
53	MG	AA	1634	1/1	0.80	0.15	199,199,199,199	0
53	MG	DA	3062	1/1	0.80	0.36	193,193,193,193	0
53	MG	DA	3076	1/1	0.81	0.17	158,158,158,158	0
53	MG	CA	1607	1/1	0.81	0.13	154,154,154,154	0
53	MG	DA	3041	1/1	0.81	0.10	122,122,122,122	0
53	MG	DA	3083	1/1	0.82	0.13	224,224,224,224	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DA	3106	1/1	0.82	0.19	205,205,205,205	0
53	MG	BA	3118	1/1	0.83	0.25	168,168,168,168	0
53	MG	AA	1625	1/1	0.83	0.18	121,121,121,121	0
53	MG	DA	3069	1/1	0.83	0.17	202,202,202,202	0
53	MG	CA	1624	1/1	0.83	0.27	179,179,179,179	0
53	MG	CA	1619	1/1	0.83	0.12	201,201,201,201	0
53	MG	DA	3022	1/1	0.83	0.15	162,162,162,162	0
53	MG	DA	3129	1/1	0.84	0.40	203,203,203,203	0
53	MG	BA	3130	1/1	0.84	0.40	205,205,205,205	0
53	MG	CA	1601	1/1	0.84	0.14	179,179,179,179	0
53	MG	DA	3092	1/1	0.85	0.14	121,121,121,121	0
53	MG	BA	3112	1/1	0.85	0.24	89,89,89,89	0
53	MG	BA	3135	1/1	0.85	0.29	196,196,196,196	0
53	MG	AA	1628	1/1	0.85	0.10	183,183,183,183	0
53	MG	BA	3132	1/1	0.86	0.20	165,165,165,165	0
53	MG	DA	3075	1/1	0.86	0.25	140,140,140,140	0
53	MG	DA	3060	1/1	0.86	0.33	161,161,161,161	0
53	MG	DA	3025	1/1	0.86	0.09	110,110,110,110	0
53	MG	CA	1610	1/1	0.86	0.12	175,175,175,175	0
53	MG	DA	3008	1/1	0.86	0.13	142,142,142,142	0
53	MG	AA	1618	1/1	0.86	0.10	164,164,164,164	0
53	MG	DA	3072	1/1	0.86	0.13	132,132,132,132	0
53	MG	DA	3123	1/1	0.87	0.20	165,165,165,165	0
53	MG	BA	3011	1/1	0.87	0.25	131,131,131,131	0
53	MG	DA	3001	1/1	0.87	0.13	130,130,130,130	0
53	MG	CA	1625	1/1	0.87	0.16	91,91,91,91	0
53	MG	DA	3087	1/1	0.87	0.09	164,164,164,164	0
53	MG	DA	3042	1/1	0.87	0.12	94,94,94,94	0
53	MG	DA	3073	1/1	0.87	0.07	162,162,162,162	0
53	MG	DA	3114	1/1	0.87	0.12	123,123,123,123	0
53	MG	DA	3115	1/1	0.87	0.17	139,139,139,139	0
53	MG	DA	3095	1/1	0.88	0.13	116,116,116,116	0
53	MG	BA	3070	1/1	0.88	0.15	134,134,134,134	0
53	MG	CA	1611	1/1	0.88	0.17	122,122,122,122	0
53	MG	BA	3086	1/1	0.88	0.14	88,88,88,88	0
53	MG	DB	201	1/1	0.88	0.10	114,114,114,114	0
53	MG	BA	3048	1/1	0.88	0.14	104,104,104,104	0
53	MG	BA	3004	1/1	0.88	0.18	147,147,147,147	0
53	MG	DA	3105	1/1	0.89	0.08	51,51,51,51	0
53	MG	DA	3050	1/1	0.89	0.09	125,125,125,125	0
53	MG	AA	1619	1/1	0.89	0.12	125,125,125,125	0
53	MG	DA	3091	1/1	0.89	0.24	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	AA	1626	1/1	0.89	0.15	106,106,106,106	0
53	MG	DA	3111	1/1	0.89	0.13	127,127,127,127	0
53	MG	BA	3036	1/1	0.90	0.26	169,169,169,169	0
53	MG	DA	3086	1/1	0.90	0.10	94,94,94,94	0
53	MG	DA	3039	1/1	0.90	0.11	99,99,99,99	0
53	MG	DA	3112	1/1	0.90	0.14	66,66,66,66	0
53	MG	DA	3100	1/1	0.90	0.16	93,93,93,93	0
53	MG	AA	1616	1/1	0.90	0.08	78,78,78,78	0
53	MG	AN	202	1/1	0.90	0.09	169,169,169,169	0
53	MG	BA	3055	1/1	0.90	0.16	191,191,191,191	0
53	MG	BA	3025	1/1	0.91	0.21	119,119,119,119	0
53	MG	CA	1613	1/1	0.91	0.08	114,114,114,114	0
53	MG	DA	3014	1/1	0.91	0.16	128,128,128,128	0
53	MG	CA	1631	1/1	0.91	0.16	88,88,88,88	0
53	MG	DA	3116	1/1	0.91	0.19	66,66,66,66	0
53	MG	DA	3118	1/1	0.91	0.07	70,70,70,70	0
53	MG	DA	3047	1/1	0.91	0.17	136,136,136,136	0
53	MG	DA	3031	1/1	0.91	0.08	79,79,79,79	0
53	MG	DA	3032	1/1	0.91	0.11	100,100,100,100	0
53	MG	DA	3053	1/1	0.91	0.11	80,80,80,80	0
53	MG	BA	3110	1/1	0.91	0.13	102,102,102,102	0
53	MG	CA	1623	1/1	0.91	0.12	120,120,120,120	0
53	MG	BA	3059	1/1	0.91	0.21	109,109,109,109	0
53	MG	BA	3082	1/1	0.91	0.13	85,85,85,85	0
53	MG	BA	3125	1/1	0.91	0.12	41,41,41,41	0
53	MG	DA	3085	1/1	0.91	0.12	148,148,148,148	0
53	MG	DA	3119	1/1	0.92	0.08	88,88,88,88	0
53	MG	CA	1634	1/1	0.92	0.14	153,153,153,153	0
53	MG	BA	3087	1/1	0.92	0.11	125,125,125,125	0
53	MG	CA	1637	1/1	0.92	0.11	63,63,63,63	0
53	MG	DA	3128	1/1	0.92	0.17	123,123,123,123	0
53	MG	DA	3077	1/1	0.92	0.11	114,114,114,114	0
53	MG	AA	1603	1/1	0.92	0.09	121,121,121,121	0
53	MG	BA	3060	1/1	0.92	0.28	174,174,174,174	0
53	MG	CA	1618	1/1	0.92	0.09	139,139,139,139	0
53	MG	DA	3051	1/1	0.92	0.12	124,124,124,124	0
53	MG	DA	3040	1/1	0.92	0.08	52,52,52,52	0
53	MG	BA	3131	1/1	0.92	0.17	140,140,140,140	0
53	MG	AA	1607	1/1	0.93	0.09	119,119,119,119	0
53	MG	BA	3061	1/1	0.93	0.23	223,223,223,223	0
53	MG	BA	3123	1/1	0.93	0.21	118,118,118,118	0
53	MG	DA	3027	1/1	0.93	0.08	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DA	3101	1/1	0.93	0.13	104,104,104,104	0
53	MG	BA	3002	1/1	0.93	0.12	77,77,77,77	0
53	MG	AA	1614	1/1	0.93	0.21	197,197,197,197	0
53	MG	DA	3107	1/1	0.93	0.17	121,121,121,121	0
53	MG	BA	3075	1/1	0.93	0.15	69,69,69,69	0
53	MG	AA	1638	1/1	0.93	0.12	102,102,102,102	0
53	MG	BA	3056	1/1	0.93	0.24	233,233,233,233	0
53	MG	BA	3057	1/1	0.93	0.24	161,161,161,161	0
53	MG	BA	3098	1/1	0.93	0.12	51,51,51,51	0
53	MG	DA	3113	1/1	0.93	0.07	96,96,96,96	0
53	MG	DC	302	1/1	0.93	0.14	121,121,121,121	0
53	MG	AA	1639	1/1	0.93	0.12	126,126,126,126	0
53	MG	DA	3035	1/1	0.94	0.13	84,84,84,84	0
53	MG	BA	3077	1/1	0.94	0.12	121,121,121,121	0
53	MG	DA	3070	1/1	0.94	0.07	56,56,56,56	0
53	MG	DA	3121	1/1	0.94	0.18	119,119,119,119	0
53	MG	DA	3104	1/1	0.94	0.08	34,34,34,34	0
53	MG	CA	1641	1/1	0.94	0.10	80,80,80,80	0
53	MG	BA	3007	1/1	0.94	0.07	69,69,69,69	0
53	MG	BA	3083	1/1	0.94	0.13	113,113,113,113	0
53	MG	DA	3088	1/1	0.94	0.08	141,141,141,141	0
53	MG	DA	3090	1/1	0.94	0.07	91,91,91,91	0
53	MG	DA	3030	1/1	0.94	0.11	111,111,111,111	0
53	MG	BA	3111	1/1	0.94	0.12	74,74,74,74	0
53	MG	BA	3028	1/1	0.94	0.07	32,32,32,32	0
53	MG	DA	3023	1/1	0.94	0.06	78,78,78,78	0
53	MG	CA	1630	1/1	0.94	0.09	123,123,123,123	0
53	MG	DA	3098	1/1	0.94	0.12	118,118,118,118	0
53	MG	BA	3134	1/1	0.95	0.14	143,143,143,143	0
53	MG	DA	3048	1/1	0.95	0.15	132,132,132,132	0
53	MG	BA	3073	1/1	0.95	0.22	135,135,135,135	0
53	MG	BA	3114	1/1	0.95	0.08	144,144,144,144	0
53	MG	DA	3126	1/1	0.95	0.08	76,76,76,76	0
53	MG	BB	203	1/1	0.95	0.07	17,17,17,17	0
53	MG	AA	1629	1/1	0.95	0.10	183,183,183,183	0
53	MG	BA	3091	1/1	0.95	0.18	113,113,113,113	0
53	MG	BA	3014	1/1	0.95	0.09	42,42,42,42	0
53	MG	DA	3131	1/1	0.95	0.11	70,70,70,70	0
53	MG	BA	3104	1/1	0.95	0.08	12,12,12,12	0
53	MG	DA	3004	1/1	0.95	0.10	80,80,80,80	0
53	MG	DA	3080	1/1	0.95	0.10	137,137,137,137	0
53	MG	BA	3018	1/1	0.95	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	AA	1622	1/1	0.95	0.09	97,97,97,97	0
53	MG	DA	3046	1/1	0.95	0.05	76,76,76,76	0
55	ZN	D4	101	1/1	0.95	0.08	151,151,151,151	0
53	MG	AA	1636	1/1	0.96	0.07	25,25,25,25	0
53	MG	DA	3061	1/1	0.96	0.13	134,134,134,134	0
53	MG	AA	1637	1/1	0.96	0.07	104,104,104,104	0
53	MG	AA	1612	1/1	0.96	0.10	104,104,104,104	0
53	MG	AA	1602	1/1	0.96	0.07	119,119,119,119	0
53	MG	AN	201	1/1	0.96	0.06	105,105,105,105	0
53	MG	CA	1609	1/1	0.96	0.08	80,80,80,80	0
53	MG	DA	3120	1/1	0.96	0.13	76,76,76,76	0
53	MG	DA	3094	1/1	0.96	0.07	96,96,96,96	0
53	MG	DA	3071	1/1	0.96	0.11	52,52,52,52	0
53	MG	DA	3024	1/1	0.96	0.08	106,106,106,106	0
53	MG	BA	3084	1/1	0.96	0.10	50,50,50,50	0
53	MG	AA	1630	1/1	0.96	0.09	87,87,87,87	0
53	MG	BA	3034	1/1	0.96	0.17	154,154,154,154	0
53	MG	BA	3090	1/1	0.96	0.08	73,73,73,73	0
53	MG	DA	3102	1/1	0.96	0.04	62,62,62,62	0
53	MG	BA	3062	1/1	0.96	0.08	15,15,15,15	0
53	MG	BA	3096	1/1	0.96	0.09	45,45,45,45	0
53	MG	CA	1633	1/1	0.96	0.07	77,77,77,77	0
53	MG	DA	3052	1/1	0.96	0.06	49,49,49,49	0
53	MG	AA	1633	1/1	0.96	0.05	75,75,75,75	0
53	MG	AA	1604	1/1	0.96	0.11	120,120,120,120	0
53	MG	BB	202	1/1	0.96	0.05	43,43,43,43	0
54	ERY	BA	3136	51/51	0.96	0.10	5,11,15,16	0
53	MG	CA	1638	1/1	0.96	0.12	139,139,139,139	0
53	MG	AA	1615	1/1	0.97	0.06	128,128,128,128	0
53	MG	BA	3103	1/1	0.97	0.12	7,7,7,7	0
53	MG	DA	3037	1/1	0.97	0.09	81,81,81,81	0
53	MG	AA	1635	1/1	0.97	0.05	88,88,88,88	0
53	MG	DA	3054	1/1	0.97	0.06	71,71,71,71	0
53	MG	DA	3055	1/1	0.97	0.08	84,84,84,84	0
53	MG	DA	3124	1/1	0.97	0.05	48,48,48,48	0
53	MG	DA	3056	1/1	0.97	0.08	112,112,112,112	0
53	MG	BA	3108	1/1	0.97	0.08	8,8,8,8	0
53	MG	DA	3103	1/1	0.97	0.09	98,98,98,98	0
53	MG	BA	3005	1/1	0.97	0.07	93,93,93,93	0
53	MG	BA	3074	1/1	0.97	0.07	18,18,18,18	0
53	MG	AA	1613	1/1	0.97	0.05	57,57,57,57	0
53	MG	BA	3089	1/1	0.97	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DA	3044	1/1	0.97	0.10	83,83,83,83	0
53	MG	AA	1608	1/1	0.97	0.07	32,32,32,32	0
53	MG	DA	3017	1/1	0.97	0.08	68,68,68,68	0
53	MG	DA	3066	1/1	0.97	0.05	48,48,48,48	0
53	MG	DA	3068	1/1	0.97	0.06	78,78,78,78	0
53	MG	BA	3120	1/1	0.97	0.10	53,53,53,53	0
53	MG	BA	3078	1/1	0.97	0.06	41,41,41,41	0
53	MG	BA	3081	1/1	0.97	0.06	39,39,39,39	0
53	MG	BA	3106	1/1	0.98	0.06	25,25,25,25	0
53	MG	BA	3046	1/1	0.98	0.09	16,16,16,16	0
53	MG	CA	1605	1/1	0.98	0.10	40,40,40,40	0
53	MG	CA	1606	1/1	0.98	0.07	63,63,63,63	0
53	MG	BA	3076	1/1	0.98	0.04	32,32,32,32	0
53	MG	CA	1608	1/1	0.98	0.07	51,51,51,51	0
53	MG	CA	1635	1/1	0.98	0.04	85,85,85,85	0
53	MG	BA	3015	1/1	0.98	0.14	38,38,38,38	0
53	MG	AA	1627	1/1	0.98	0.05	78,78,78,78	0
53	MG	BA	3050	1/1	0.98	0.07	37,37,37,37	0
53	MG	DA	3117	1/1	0.98	0.08	71,71,71,71	0
53	MG	BA	3115	1/1	0.98	0.07	10,10,10,10	0
53	MG	BA	3021	1/1	0.98	0.06	43,43,43,43	0
53	MG	AA	1631	1/1	0.98	0.08	69,69,69,69	0
53	MG	DA	3089	1/1	0.98	0.12	69,69,69,69	0
53	MG	DA	3122	1/1	0.98	0.04	72,72,72,72	0
53	MG	BA	3027	1/1	0.98	0.10	109,109,109,109	0
53	MG	AA	1621	1/1	0.98	0.08	91,91,91,91	0
53	MG	BA	3127	1/1	0.98	0.08	15,15,15,15	0
53	MG	BA	3029	1/1	0.98	0.09	66,66,66,66	0
53	MG	BA	3030	1/1	0.98	0.12	15,15,15,15	0
53	MG	BA	3031	1/1	0.98	0.04	34,34,34,34	0
53	MG	DA	3096	1/1	0.98	0.06	92,92,92,92	0
53	MG	CA	1621	1/1	0.98	0.14	55,55,55,55	0
53	MG	DA	3065	1/1	0.98	0.09	83,83,83,83	0
53	MG	BA	3033	1/1	0.98	0.08	10,10,10,10	0
53	MG	BA	3001	1/1	0.98	0.08	110,110,110,110	0
53	MG	BA	3097	1/1	0.98	0.10	80,80,80,80	0
53	MG	BA	3071	1/1	0.98	0.09	112,112,112,112	0
53	MG	DA	3012	1/1	0.98	0.04	51,51,51,51	0
53	MG	CA	1626	1/1	0.98	0.14	29,29,29,29	0
53	MG	AA	1623	1/1	0.98	0.06	72,72,72,72	0
55	ZN	B4	101	1/1	0.98	0.10	84,84,84,84	0
53	MG	BA	3043	1/1	0.98	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BA	3093	1/1	0.99	0.06	45,45,45,45	0
53	MG	BA	3094	1/1	0.99	0.12	24,24,24,24	0
53	MG	AA	1641	1/1	0.99	0.05	39,39,39,39	0
53	MG	AA	1605	1/1	0.99	0.06	35,35,35,35	0
53	MG	BA	3052	1/1	0.99	0.04	25,25,25,25	0
53	MG	BA	3099	1/1	0.99	0.04	18,18,18,18	0
53	MG	BA	3100	1/1	0.99	0.06	24,24,24,24	0
53	MG	BA	3101	1/1	0.99	0.06	64,64,64,64	0
53	MG	BA	3102	1/1	0.99	0.07	23,23,23,23	0
53	MG	BA	3054	1/1	0.99	0.04	25,25,25,25	0
53	MG	BA	3016	1/1	0.99	0.03	7,7,7,7	0
53	MG	BA	3105	1/1	0.99	0.06	9,9,9,9	0
53	MG	BA	3017	1/1	0.99	0.05	30,30,30,30	0
53	MG	BA	3107	1/1	0.99	0.10	8,8,8,8	0
53	MG	AA	1609	1/1	0.99	0.05	28,28,28,28	0
53	MG	BA	3109	1/1	0.99	0.02	57,57,57,57	0
53	MG	BA	3058	1/1	0.99	0.04	35,35,35,35	0
53	MG	BA	3019	1/1	0.99	0.19	10,10,10,10	0
53	MG	BA	3020	1/1	0.99	0.05	35,35,35,35	0
53	MG	BA	3113	1/1	0.99	0.03	21,21,21,21	0
53	MG	AA	1620	1/1	0.99	0.11	28,28,28,28	0
53	MG	BA	3024	1/1	0.99	0.05	17,17,17,17	0
53	MG	BA	3116	1/1	0.99	0.02	17,17,17,17	0
53	MG	BA	3117	1/1	0.99	0.06	83,83,83,83	0
53	MG	BA	3063	1/1	0.99	0.07	13,13,13,13	0
53	MG	BA	3119	1/1	0.99	0.03	12,12,12,12	0
53	MG	BA	3066	1/1	0.99	0.04	11,11,11,11	0
53	MG	BA	3122	1/1	0.99	0.06	21,21,21,21	0
53	MG	CA	1642	1/1	0.99	0.04	58,58,58,58	0
53	MG	BA	3067	1/1	0.99	0.05	10,10,10,10	0
53	MG	BA	3124	1/1	0.99	0.06	16,16,16,16	0
53	MG	BA	3068	1/1	0.99	0.03	20,20,20,20	0
53	MG	AA	1606	1/1	0.99	0.05	58,58,58,58	0
53	MG	BA	3003	1/1	0.99	0.05	42,42,42,42	0
53	MG	AA	1611	1/1	0.99	0.06	54,54,54,54	0
53	MG	AA	1601	1/1	0.99	0.07	78,78,78,78	0
53	MG	BA	3006	1/1	0.99	0.03	31,31,31,31	0
53	MG	AA	1624	1/1	0.99	0.14	31,31,31,31	0
53	MG	BA	3008	1/1	0.99	0.05	13,13,13,13	0
53	MG	BA	3009	1/1	0.99	0.07	13,13,13,13	0
53	MG	DA	3067	1/1	0.99	0.03	38,38,38,38	0
53	MG	BA	3010	1/1	0.99	0.04	19,19,19,19	0

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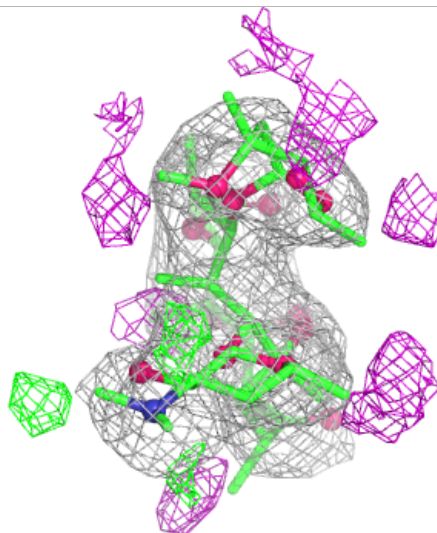
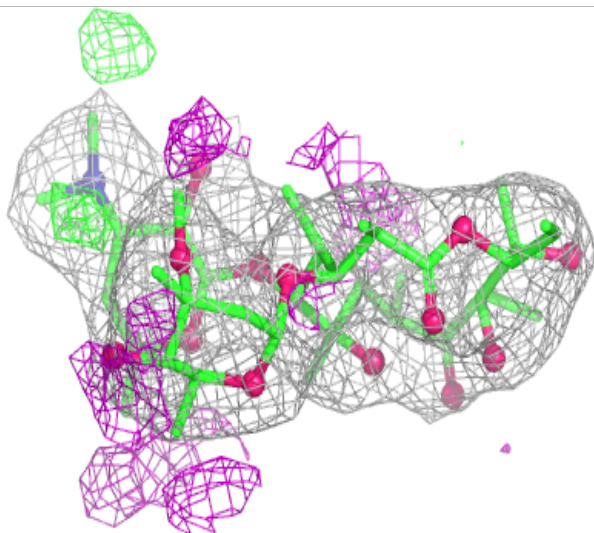
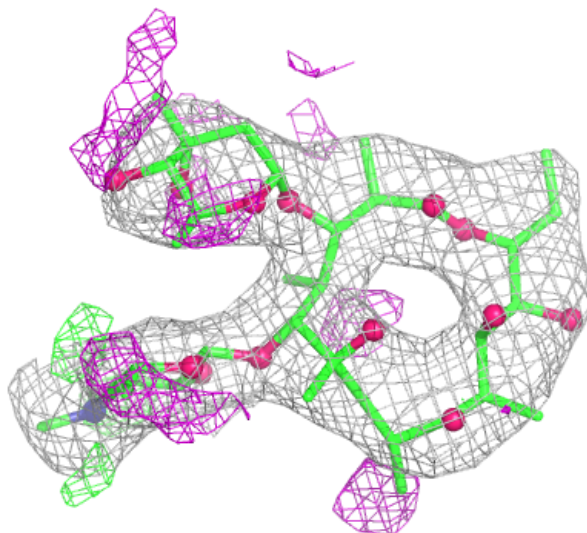
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BA	3079	1/1	0.99	0.06	30,30,30,30	0
53	MG	BA	3037	1/1	0.99	0.04	17,17,17,17	0
53	MG	BA	3038	1/1	0.99	0.03	7,7,7,7	0
53	MG	CA	1604	1/1	0.99	0.05	60,60,60,60	0
53	MG	BA	3039	1/1	0.99	0.04	20,20,20,20	0
53	MG	BA	3040	1/1	0.99	0.13	8,8,8,8	0
53	MG	BA	3085	1/1	0.99	0.06	6,6,6,6	0
53	MG	BA	3042	1/1	0.99	0.04	18,18,18,18	0
53	MG	DA	3021	1/1	0.99	0.09	41,41,41,41	0
53	MG	AA	1640	1/1	0.99	0.06	17,17,17,17	0
53	MG	BA	3045	1/1	0.99	0.07	17,17,17,17	0
53	MG	BA	3012	1/1	0.99	0.06	6,6,6,6	0
53	MG	DA	3081	1/1	0.99	0.06	92,92,92,92	0
53	MG	BA	3013	1/1	0.99	0.06	9,9,9,9	0
53	MG	BA	3092	1/1	0.99	0.05	38,38,38,38	0
53	MG	BA	3026	1/1	1.00	0.07	19,19,19,19	0
53	MG	BB	204	1/1	1.00	0.02	20,20,20,20	0
53	MG	BA	3044	1/1	1.00	0.10	14,14,14,14	0
53	MG	BA	3023	1/1	1.00	0.05	7,7,7,7	0
53	MG	BA	3032	1/1	1.00	0.02	16,16,16,16	0
53	MG	AA	1632	1/1	1.00	0.03	31,31,31,31	0
53	MG	BA	3121	1/1	1.00	0.05	10,10,10,10	0
53	MG	BA	3072	1/1	1.00	0.02	10,10,10,10	0
53	MG	BA	3088	1/1	1.00	0.05	11,11,11,11	0
53	MG	BA	3022	1/1	1.00	0.04	9,9,9,9	0
53	MG	BA	3049	1/1	1.00	0.03	11,11,11,11	0
53	MG	BA	3126	1/1	1.00	0.02	18,18,18,18	0
53	MG	BA	3041	1/1	1.00	0.08	13,13,13,13	0
53	MG	BA	3128	1/1	1.00	0.05	7,7,7,7	0
53	MG	BA	3129	1/1	1.00	0.03	14,14,14,14	0
53	MG	BA	3051	1/1	1.00	0.03	10,10,10,10	0
53	MG	BA	3035	1/1	1.00	0.05	11,11,11,11	0
53	MG	BA	3064	1/1	1.00	0.02	6,6,6,6	0
53	MG	BA	3133	1/1	1.00	0.06	10,10,10,10	0
53	MG	BA	3095	1/1	1.00	0.02	22,22,22,22	0
53	MG	BA	3065	1/1	1.00	0.03	7,7,7,7	0
53	MG	BA	3080	1/1	1.00	0.03	11,11,11,11	0
53	MG	BA	3053	1/1	1.00	0.02	9,9,9,9	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ERY BA 3136:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.