



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2023 – 03:15 AM EDT

PDB ID : 4V7S
Title : Crystal structure of the E. coli ribosome bound to telithromycin.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-05
Resolution : 3.25 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

<https://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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

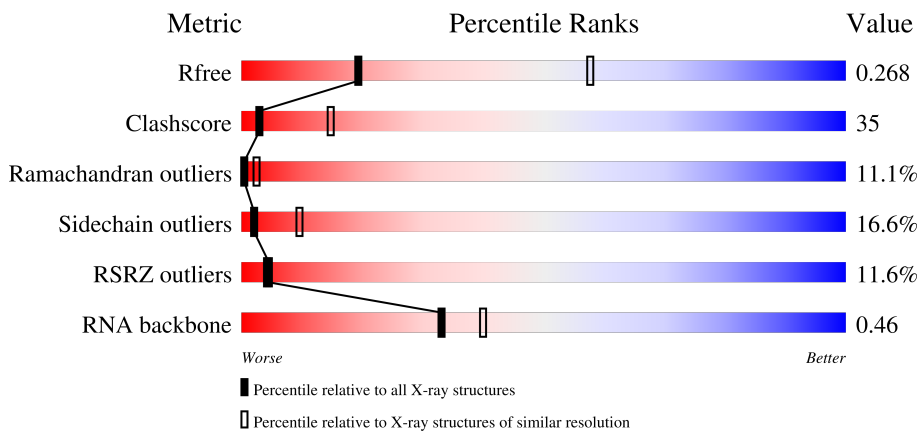
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)
RNA backbone	3102	1072 (3.62-2.90)

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	AB	218	
2	CB	218	
3	AC	206	

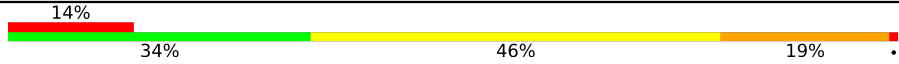
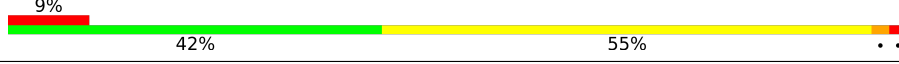

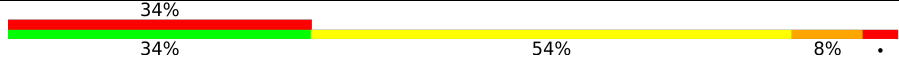

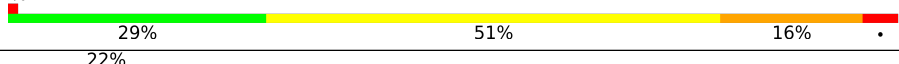

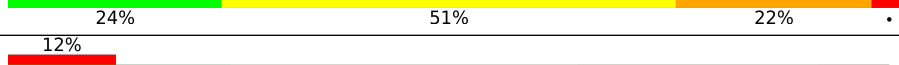
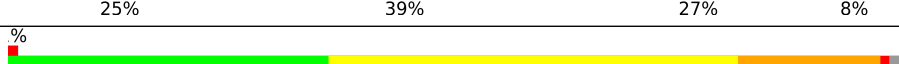
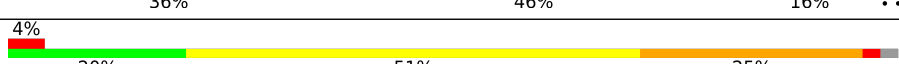
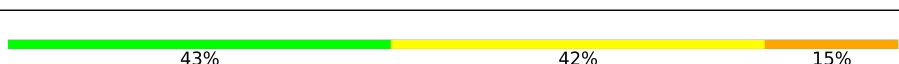
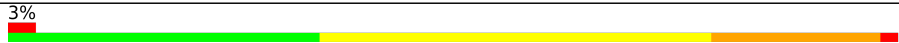
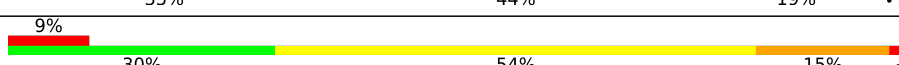
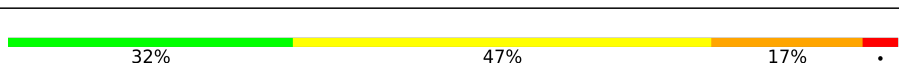

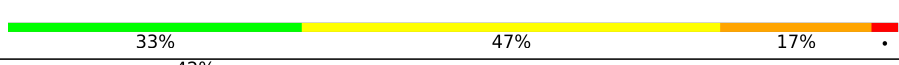
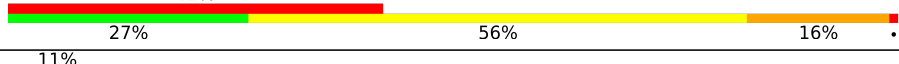



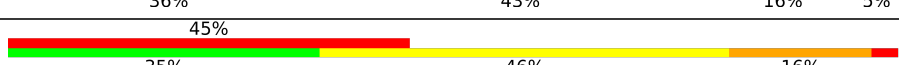




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Mol	Chain	Length	Quality of chain
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
14	AN	100	
14	CN	100	
15	AO	88	
15	CO	88	
16	AP	82	
17	AQ	80	




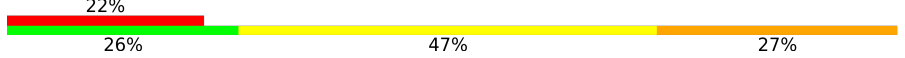




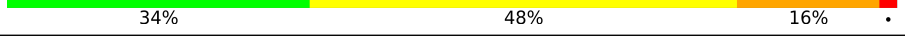

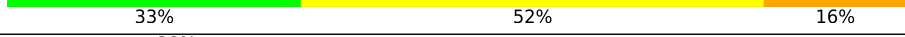

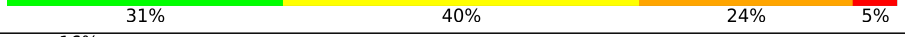
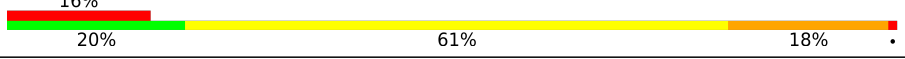



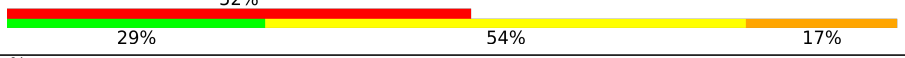


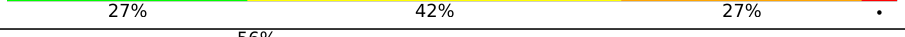
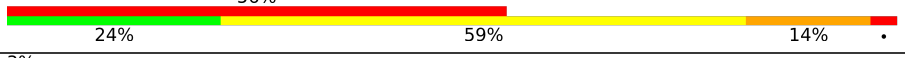

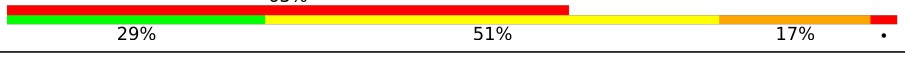

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Mol	Chain	Length	Quality of chain
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	

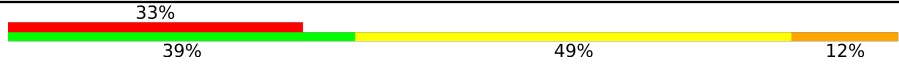

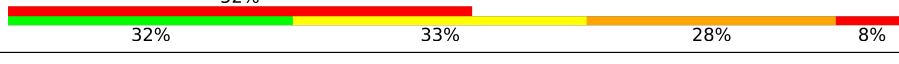
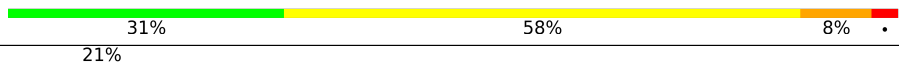
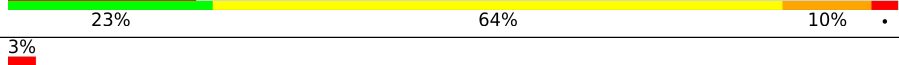
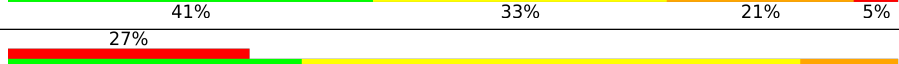
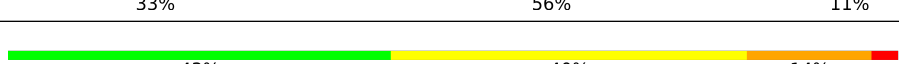
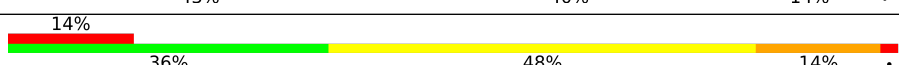
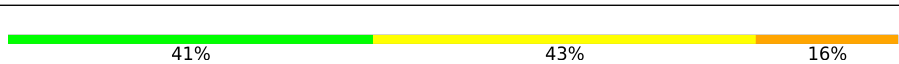
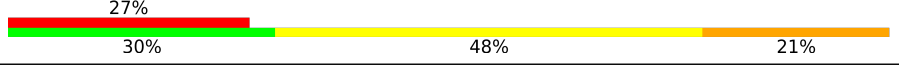
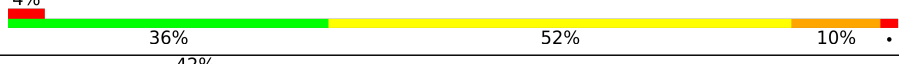
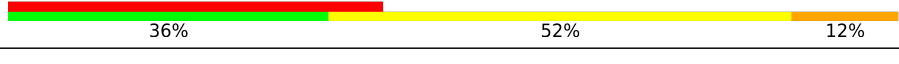
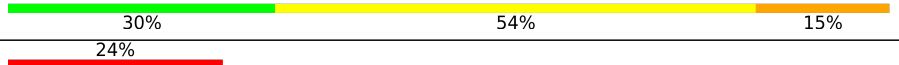

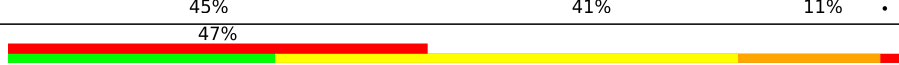
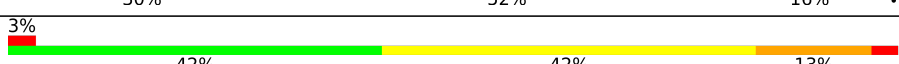

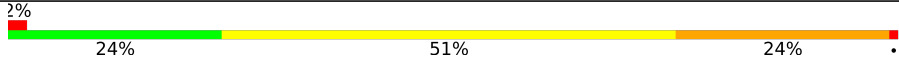
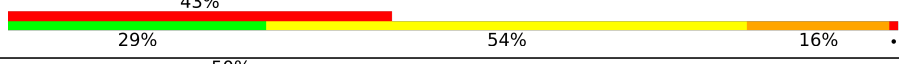


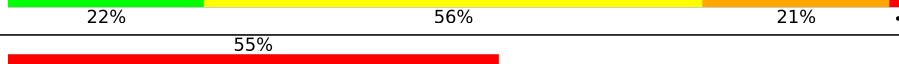



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Mol	Chain	Length	Quality of chain
31	BJ	142	 32% 51% 14% .
31	DJ	142	 23% 35% 48% 15% .
32	BK	122	 20% 52% 28%
32	DK	122	 22% 26% 47% 27%
33	BL	143	 33% 45% 20% .
33	DL	143	 26% 34% 45% 17% .
34	BM	136	 40% 42% 16% .
34	DM	136	 20% 35% 53% 12%
35	BN	120	 34% 48% 16% .
35	DN	120	 27% 32% 52% 16% .
36	BO	116	 33% 52% 16%
36	DO	116	 38% 35% 55% 9% .
37	BP	114	 % 31% 40% 24% 5%
37	DP	114	 16% 20% 61% 18% .
38	BQ	117	 % 41% 40% 18% .
38	DQ	117	 30% 31% 51% 18%
39	BR	103	 % 33% 48% 18% .
39	DR	103	 52% 29% 54% 17%
40	BS	110	 % 42% 40% 17% .
40	DS	110	 50% 43% 44% 13% .
41	BT	93	 4% 27% 42% 27% .
41	DT	93	 56% 24% 59% 14% .
42	BU	102	 3% 37% 40% 20% .
42	DU	102	 63% 29% 51% 17% .
43	BV	94	 43% 41% 16%

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Mol	Chain	Length	Quality of chain
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	
53	CA	1530	
54	CG	150	
55	CM	113	
56	CP	80	
57	DB	117	
58	DF	178	

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
59	MG	AA	1619	-	-	-	X
59	MG	DA	3002	-	-	-	X
59	MG	DA	3003	-	-	-	X
59	MG	DA	3005	-	-	-	X
59	MG	DA	3007	-	-	-	X
59	MG	DA	3010	-	-	-	X
59	MG	DA	3015	-	-	-	X
59	MG	DA	3016	-	-	-	X
59	MG	DA	3020	-	-	-	X
59	MG	DA	3026	-	-	-	X
59	MG	DA	3028	-	-	-	X
59	MG	DA	3036	-	-	-	X
59	MG	DA	3049	-	-	-	X
59	MG	DA	3060	-	-	-	X
59	MG	DA	3062	-	-	-	X
59	MG	DA	3063	-	-	-	X
59	MG	DA	3064	-	-	-	X
59	MG	DA	3074	-	-	-	X
59	MG	DA	3079	-	-	-	X
59	MG	DA	3106	-	-	-	X
59	MG	DA	3109	-	-	-	X
59	MG	DA	3127	-	-	-	X
59	MG	DA	3129	-	-	-	X
59	MG	DA	3130	-	-	-	X
59	MG	DA	3132	-	-	-	X
59	MG	DJ	201	-	-	-	X
60	TEL	BA	3135	X	-	-	-

2 Entry composition [i](#)

There are 62 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
			Total	C	N	O	P			
1	AA	1533	32895	14671	6036	10655	1533	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			

- 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			

- 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	S	0	0	0
			456	288	86	82				
18	CR	55	Total	C	N	O	S	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	DA	2841	60995	27210	11229	19715	2841	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	BB	118	2529	1126	464	821	118	0	0	0

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

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

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

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

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

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

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

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

- 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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			449	281	87	79	2			
47	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- 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			

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
53	CA	1530	32831	14642	6024	10635	1530	0	0	0

- Molecule 54 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	CG	150	1175	730	226	215	4	0	0	0

- Molecule 55 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	CM	113	877	541	177	156	3	0	0	0

- Molecule 56 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	CP	80	639	400	126	112	1	0	0	0

- Molecule 57 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
57	DB	117	2507	1116	459	815	117	0	0	0

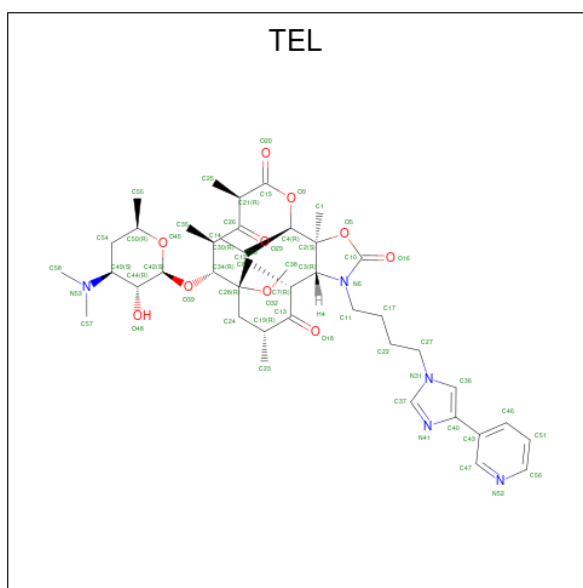
- Molecule 58 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
58	DF	178	1420	905	251	258	6	0	0	0

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	43	Total 43	Mg 43	0	0
59	BA	134	Total 134	Mg 134	0	0
59	BB	4	Total 4	Mg 4	0	0
59	CA	41	Total 41	Mg 41	0	0
59	CE	1	Total 1	Mg 1	0	0
59	DA	133	Total 133	Mg 133	0	0
59	DB	1	Total 1	Mg 1	0	0
59	DC	2	Total 2	Mg 2	0	0
59	DJ	1	Total 1	Mg 1	0	0

- Molecule 60 is TELITHROMYCIN (three-letter code: TEL) (formula: C₄₃H₆₅N₅O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
60	BA	1	58	43	5	10	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
62	AA	198	198	198	0	0
62	AL	1	1	1	0	0
62	AN	6	6	6	0	0
62	AT	2	2	2	0	0
62	AU	1	1	1	0	0
62	BA	598	598	598	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	BB	20	Total O 20 20	0	0
62	BC	10	Total O 10 10	0	0
62	BD	2	Total O 2 2	0	0
62	BE	1	Total O 1 1	0	0
62	BL	2	Total O 2 2	0	0
62	BN	3	Total O 3 3	0	0
62	BQ	1	Total O 1 1	0	0
62	BR	1	Total O 1 1	0	0
62	BT	1	Total O 1 1	0	0
62	B2	1	Total O 1 1	0	0
62	B3	3	Total O 3 3	0	0
62	B4	1	Total O 1 1	0	0
62	CA	192	Total O 192 192	0	0
62	CE	5	Total O 5 5	0	0
62	CI	1	Total O 1 1	0	0
62	CL	1	Total O 1 1	0	0
62	CN	3	Total O 3 3	0	0
62	CT	3	Total O 3 3	0	0
62	CU	2	Total O 2 2	0	0
62	DA	595	Total O 595 595	0	0
62	DB	4	Total O 4 4	0	0

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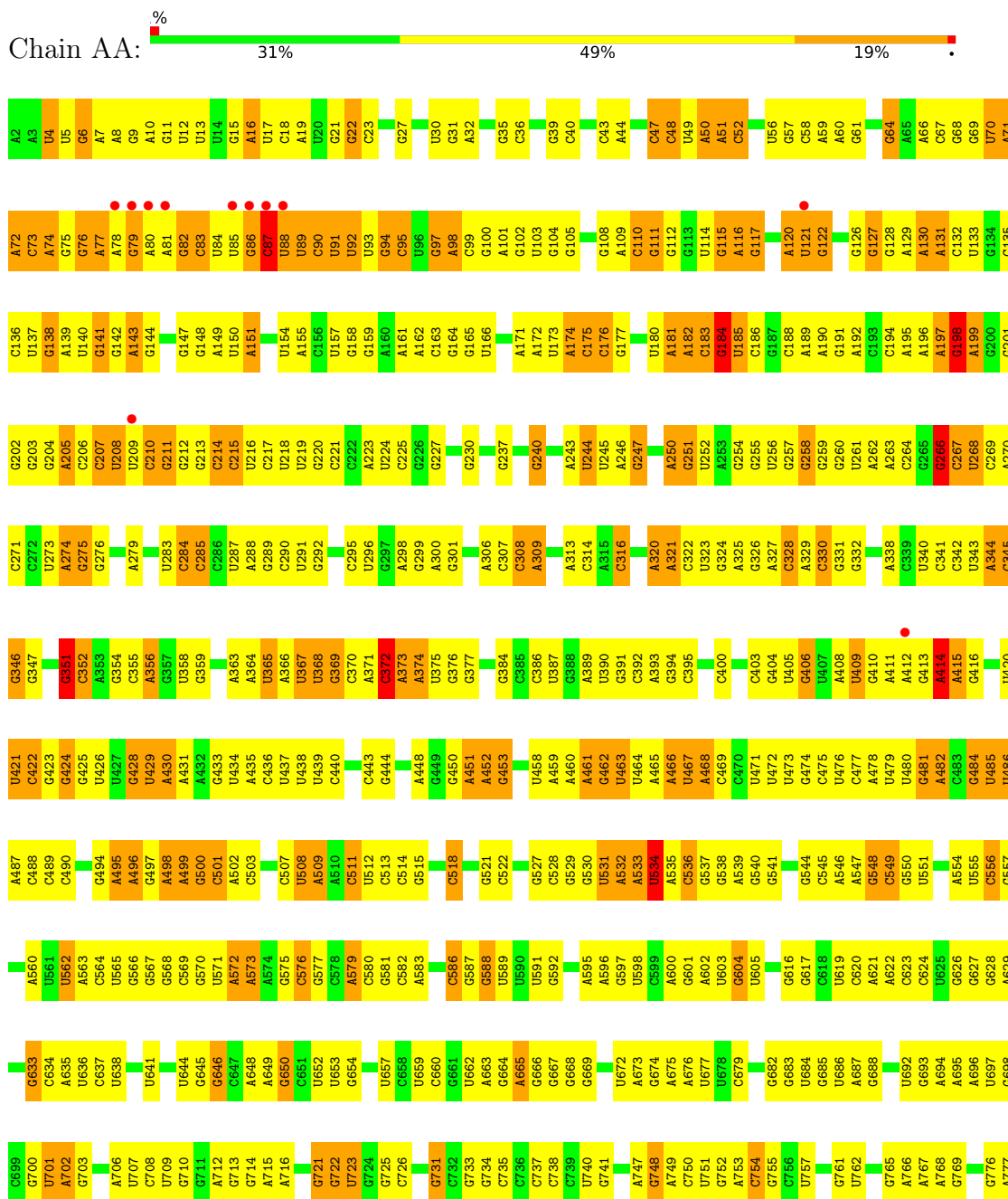
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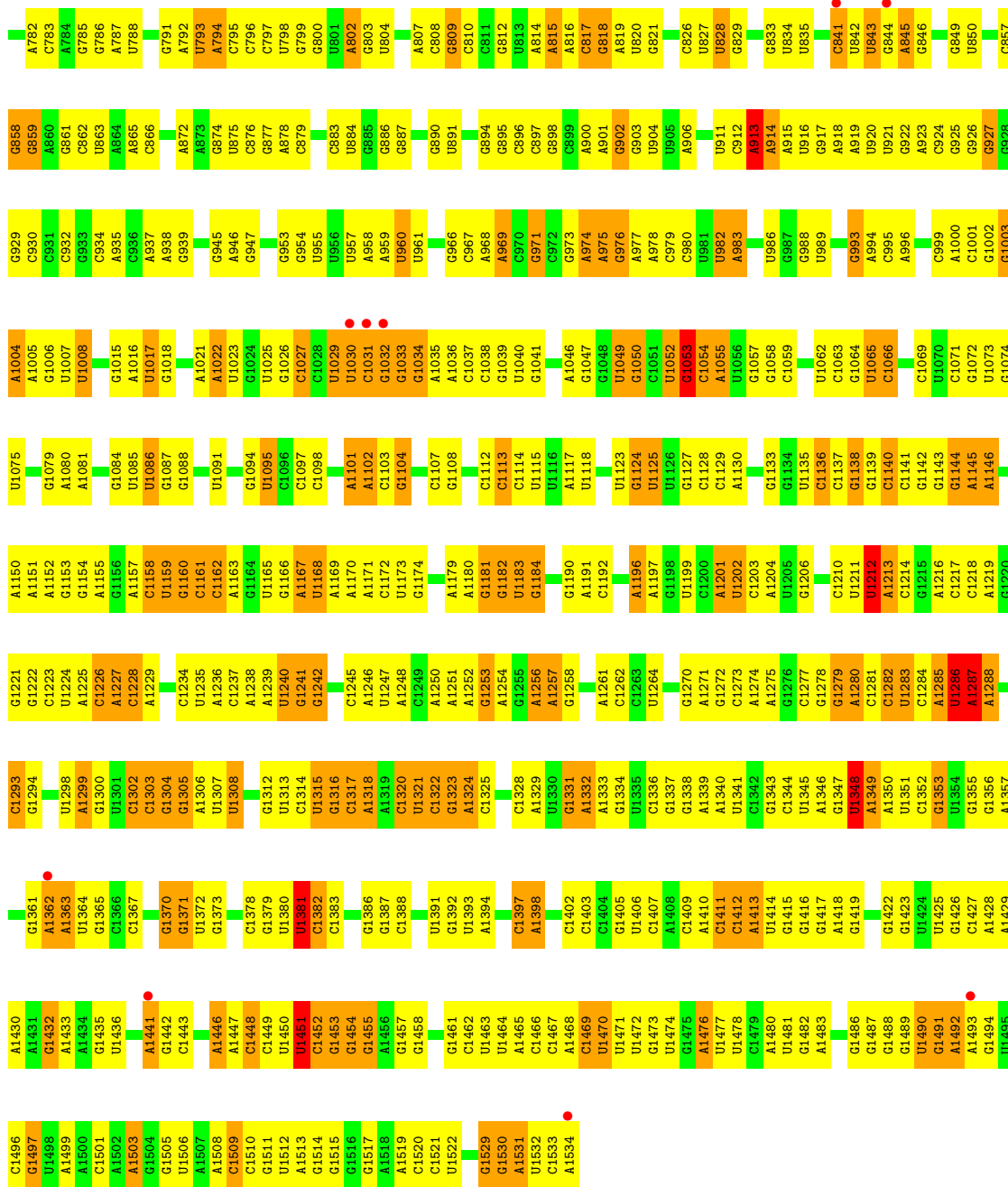
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62	DD	3	Total 3	O 3	0	0
62	DE	3	Total 3	O 3	0	0
62	DJ	6	Total 6	O 6	0	0
62	DL	6	Total 6	O 6	0	0
62	DN	2	Total 2	O 2	0	0
62	DT	3	Total 3	O 3	0	0
62	DU	2	Total 2	O 2	0	0
62	DV	1	Total 1	O 1	0	0
62	D2	1	Total 1	O 1	0	0
62	D3	1	Total 1	O 1	0	0
62	D4	3	Total 3	O 3	0	0

3 Residue-property plots [i](#)

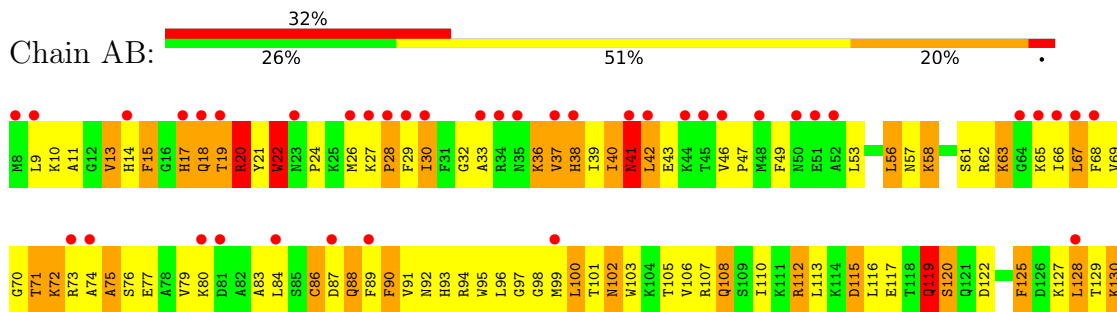
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

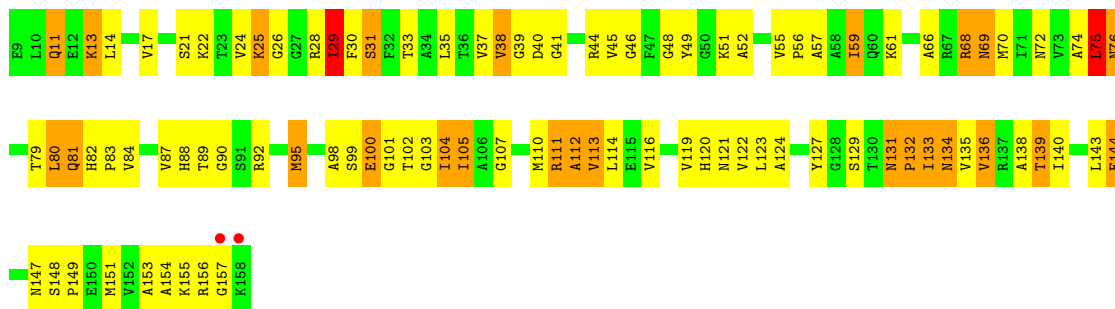
- Molecule 1: 16S rRNA



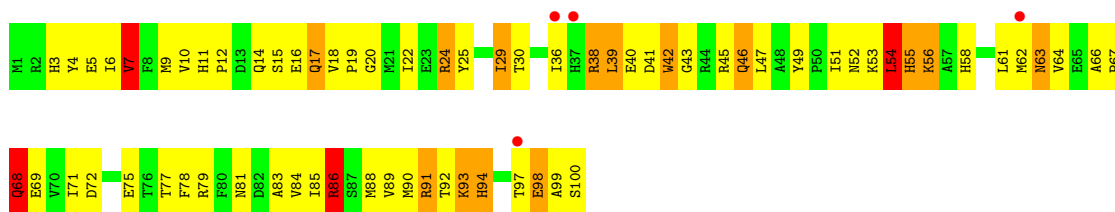


• Molecule 2: 30S ribosomal protein S2

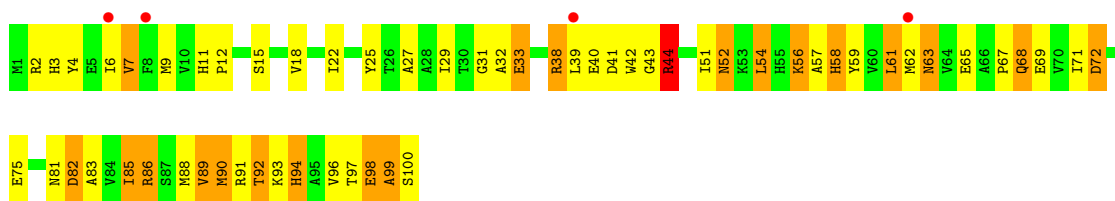




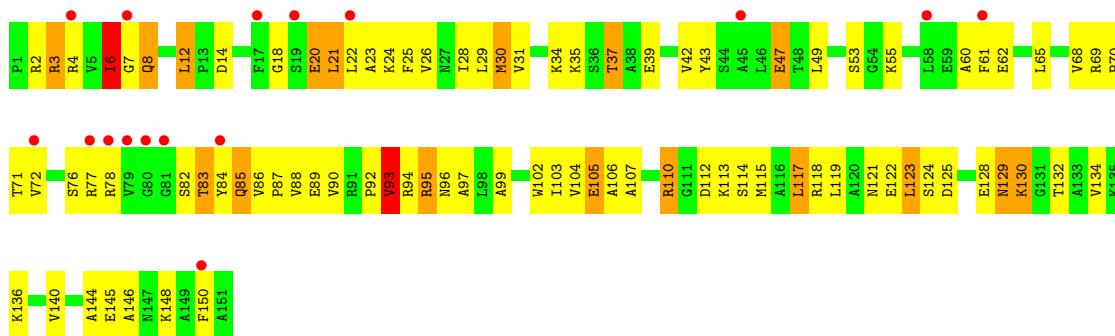
• Molecule 6: 30S ribosomal protein S6



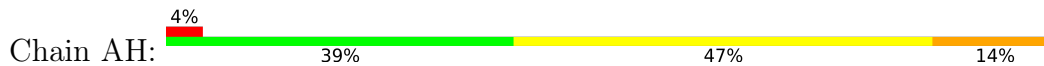
• Molecule 6: 30S ribosomal protein S6

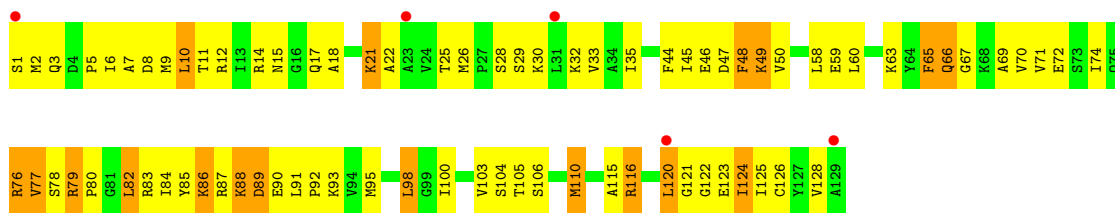


• Molecule 7: 30S ribosomal protein S7

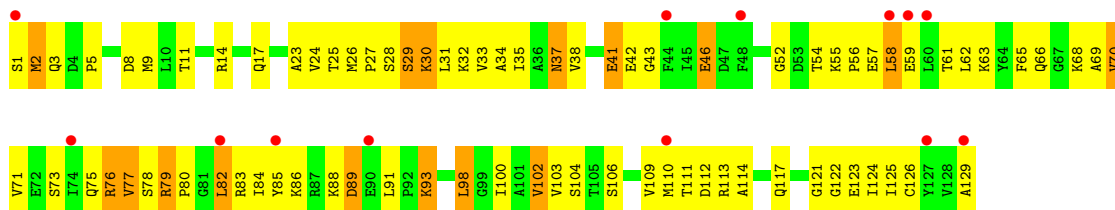


• Molecule 8: 30S ribosomal protein S8

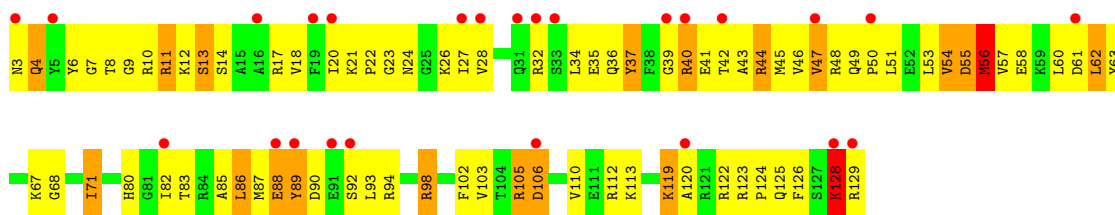




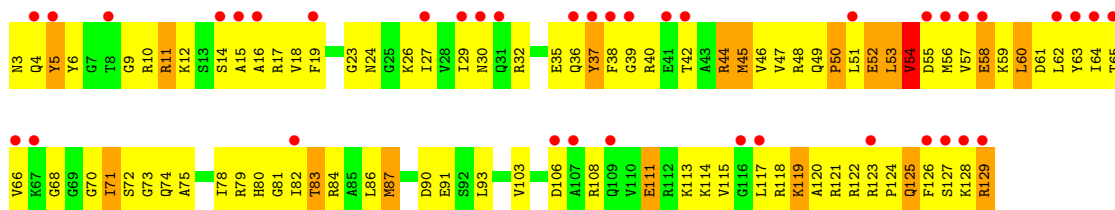
• Molecule 8: 30S ribosomal protein S8



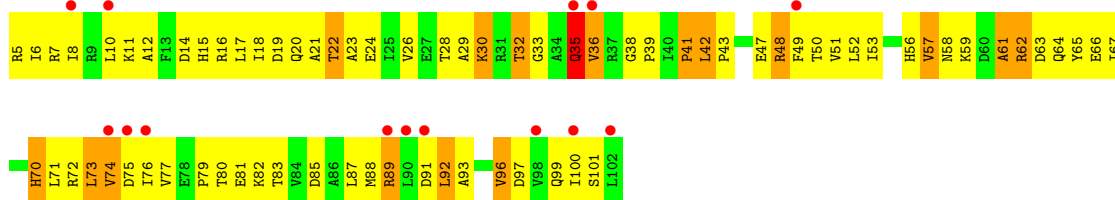
• Molecule 9: 30S ribosomal protein S9



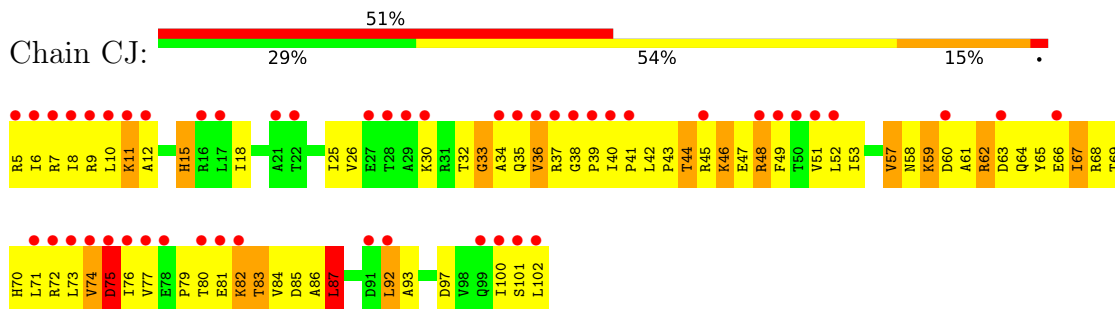
• Molecule 9: 30S ribosomal protein S9



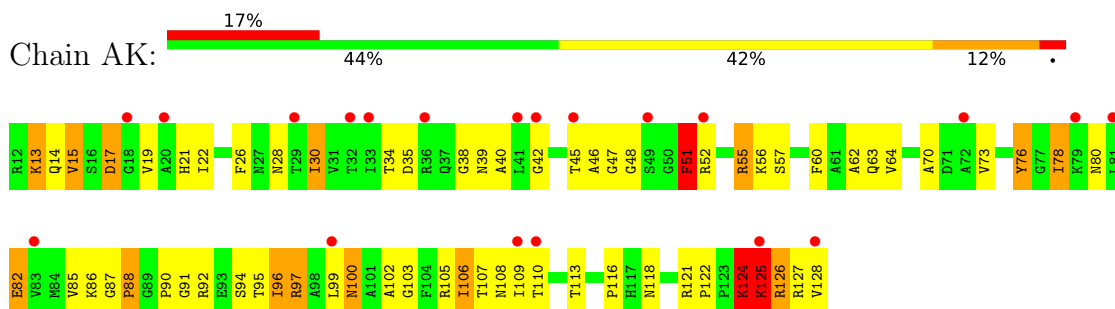
• Molecule 10: 30S ribosomal protein S10



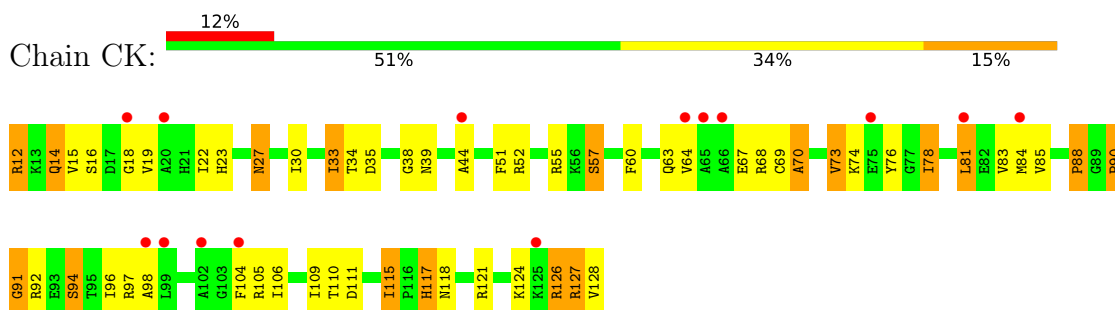
- Molecule 10: 30S ribosomal protein S10



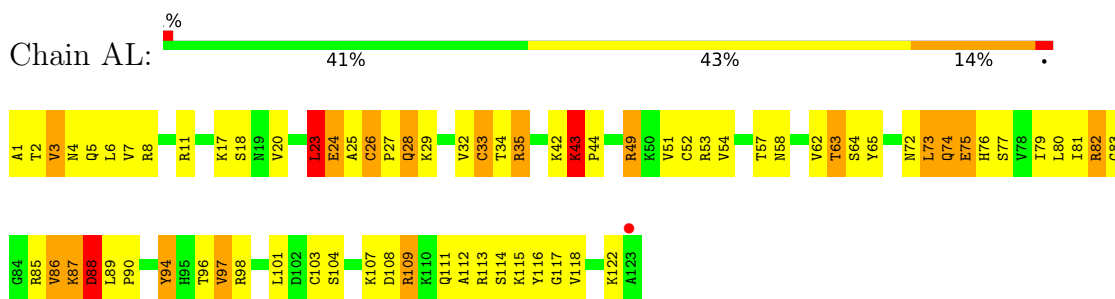
- Molecule 11: 30S ribosomal protein S11



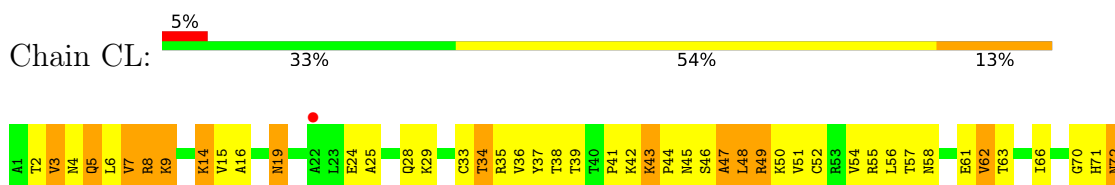
- Molecule 11: 30S ribosomal protein S11

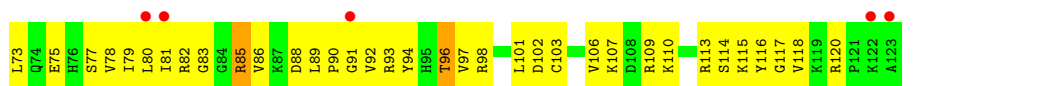


- Molecule 12: 30S ribosomal protein S12

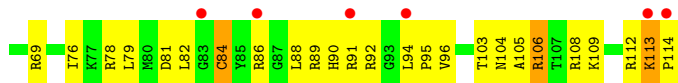
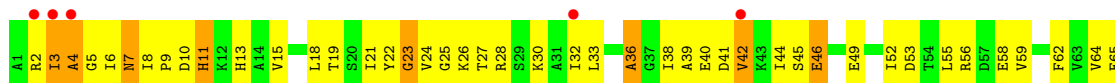


- Molecule 12: 30S ribosomal protein S12

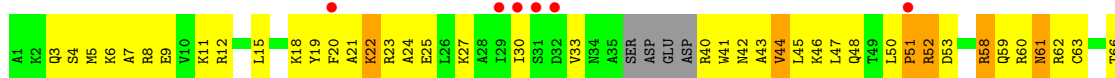




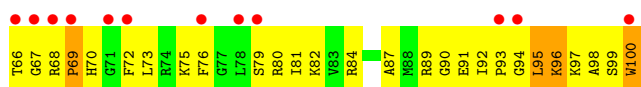
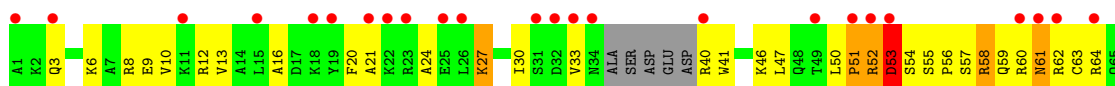
- Molecule 13: 30S ribosomal protein S13



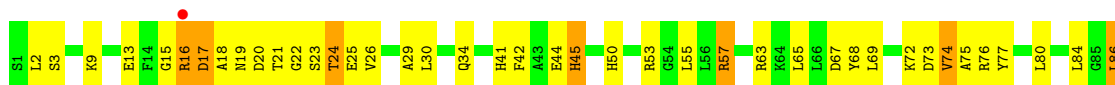
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

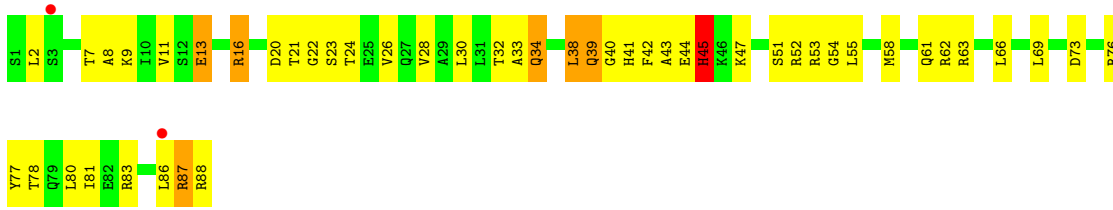


- Molecule 15: 30S ribosomal protein S15

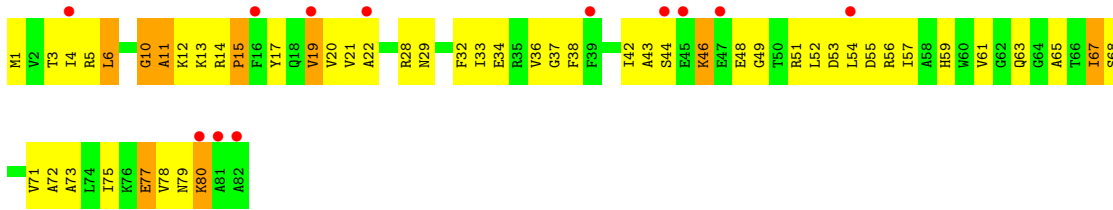


- Molecule 15: 30S ribosomal protein S15

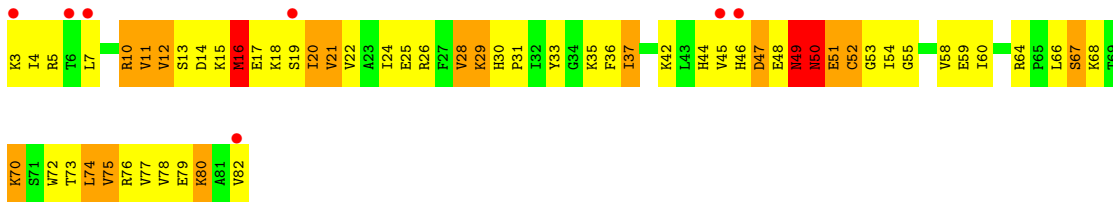




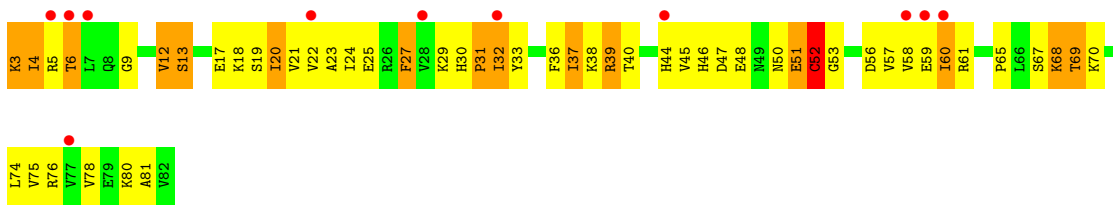
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

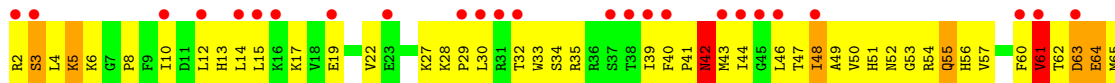


- Molecule 18: 30S ribosomal protein S18

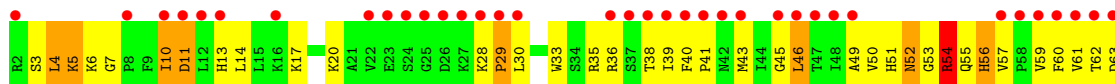




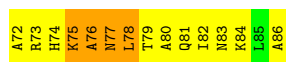
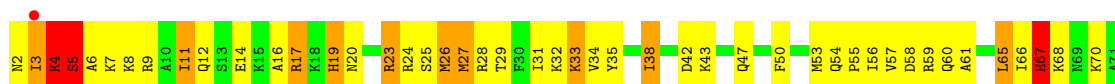
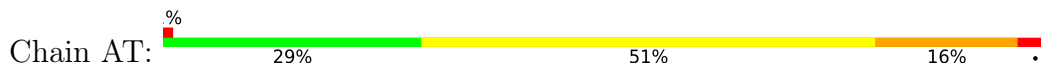
- Molecule 19: 30S ribosomal protein S19



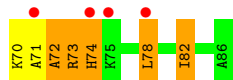
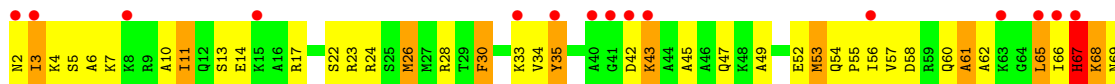
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

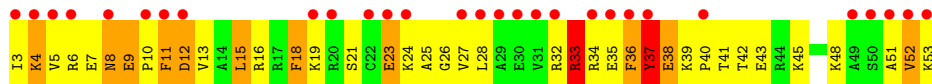


- Molecule 20: 30S ribosomal protein S20

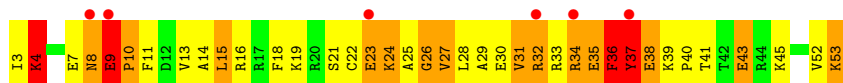
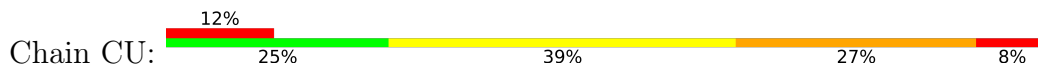


- Molecule 21: 30S ribosomal protein S21

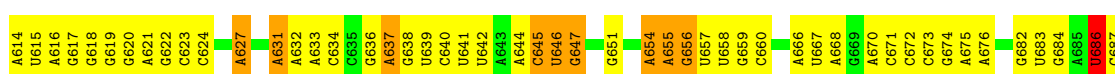
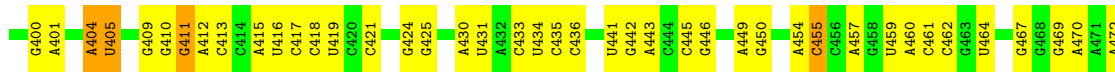
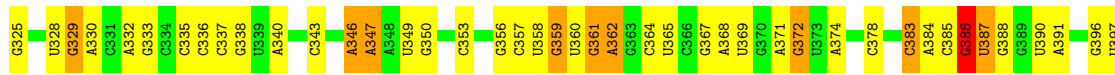


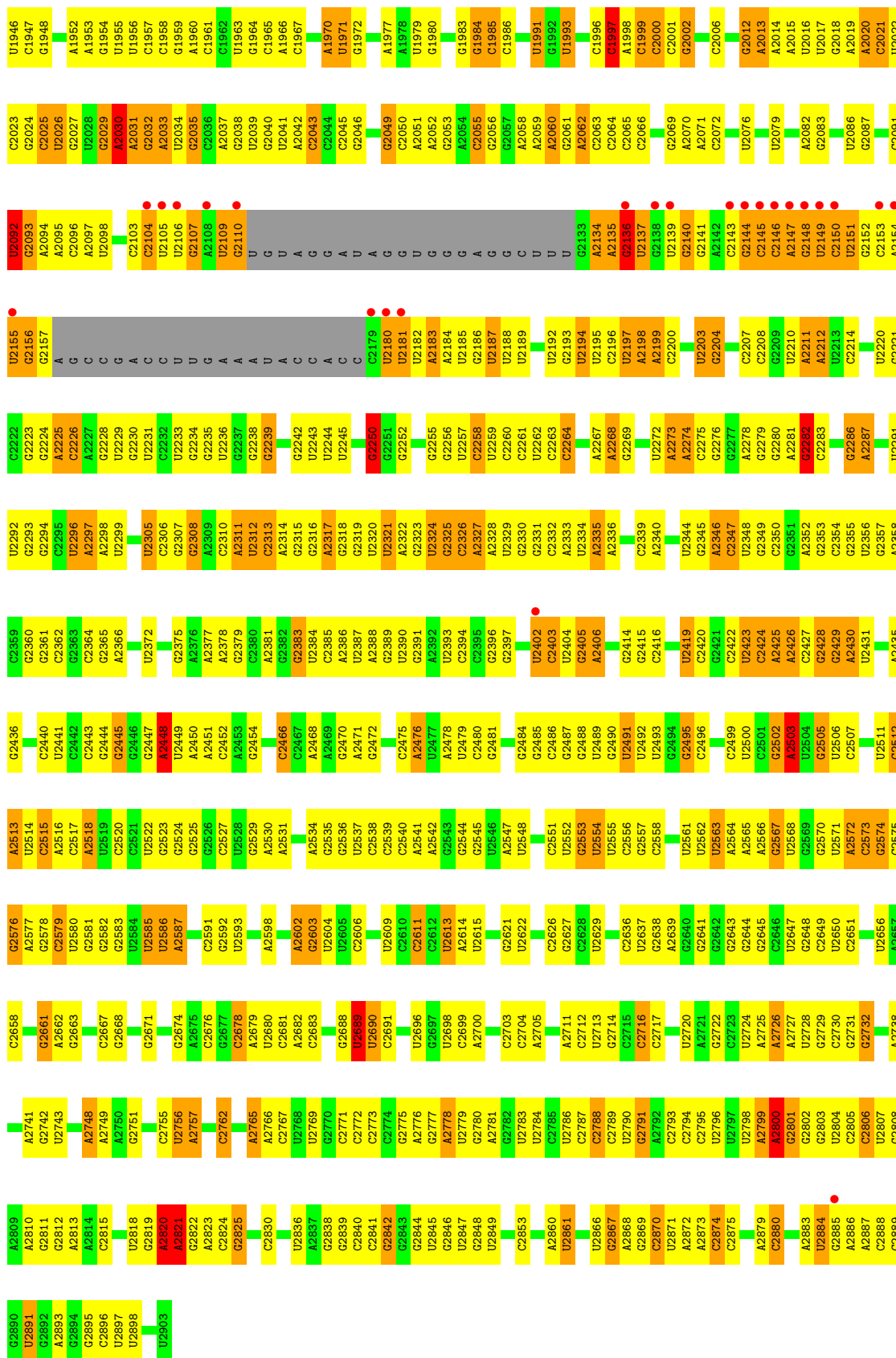


• Molecule 21: 30S ribosomal protein S21

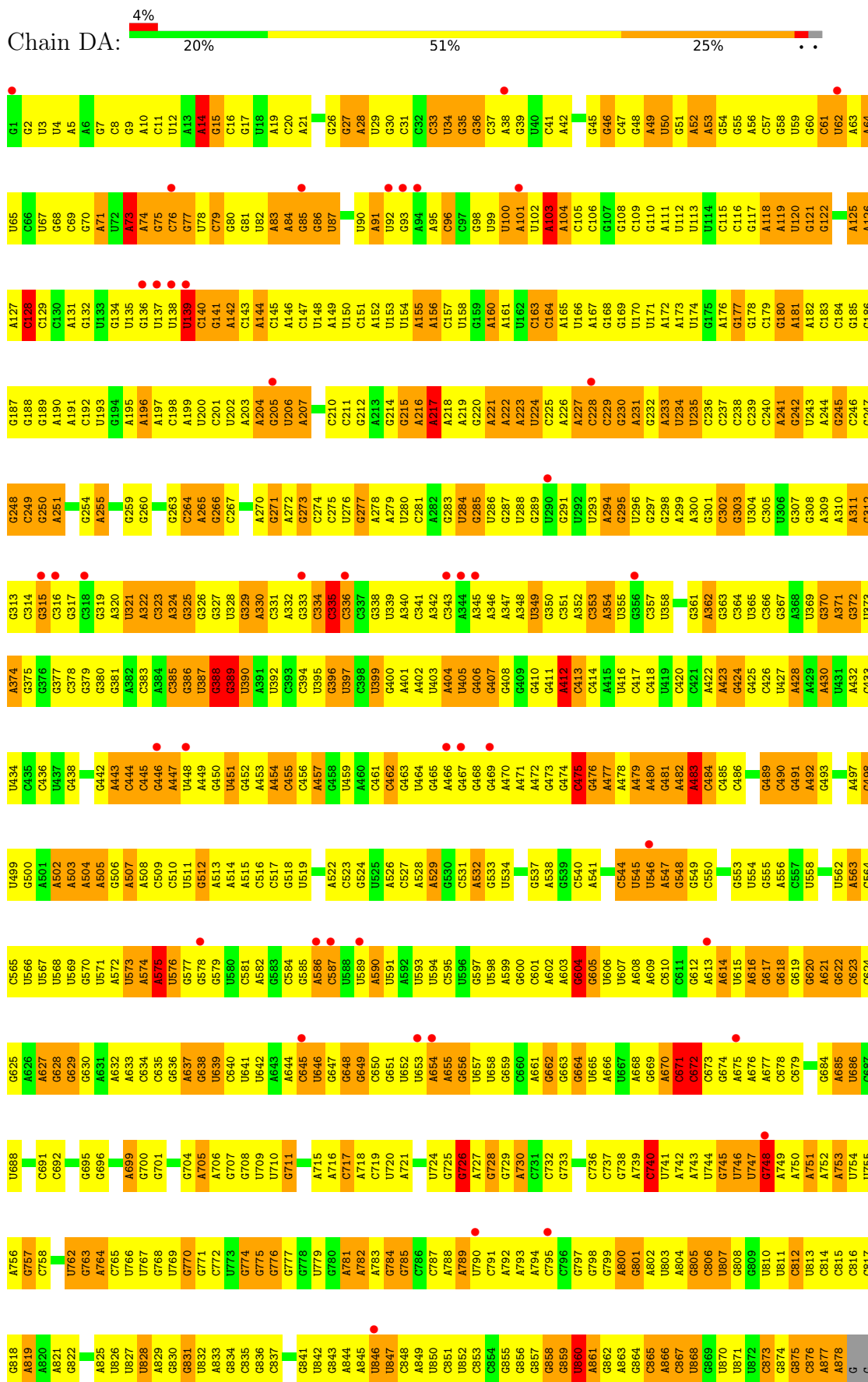


• Molecule 22: 23S rRNA

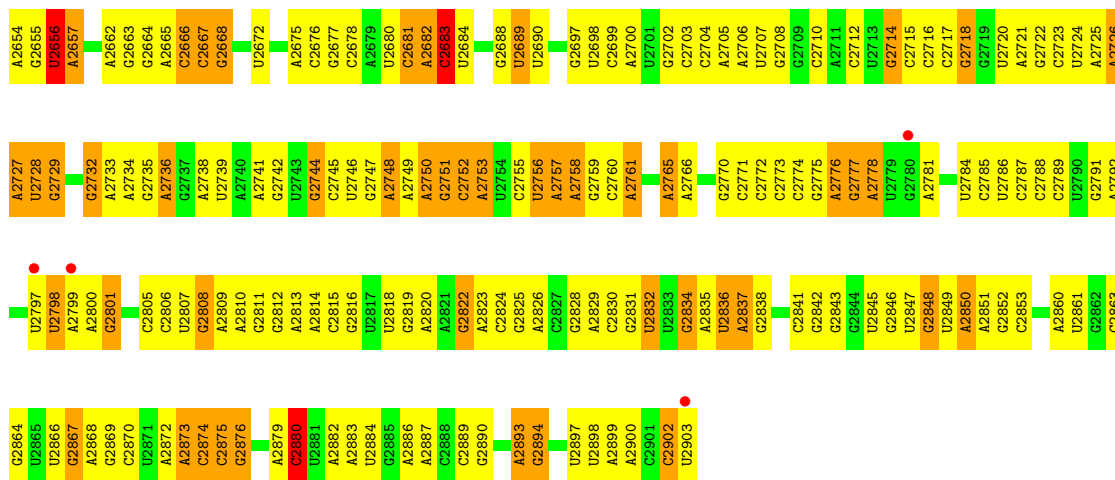




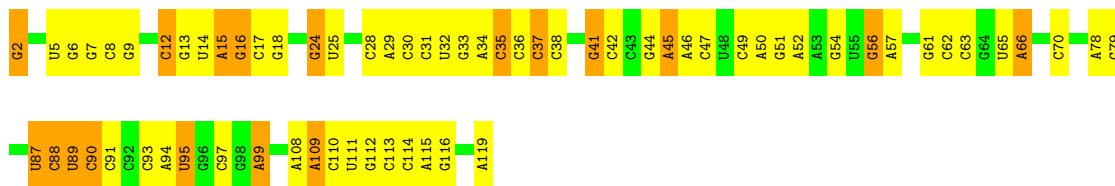
• Molecule 22: 23S rRNA



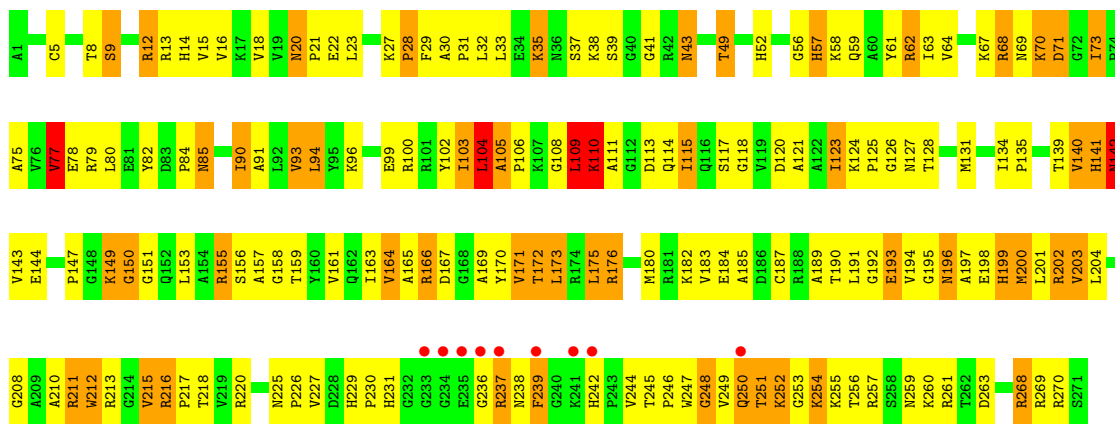
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C	G952	G1016	U1083	A1147	G1212	G1278	G1341	U1411	U1471	U1537	U1602	C1609	G1710
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U	U955	A1020	A1086	G1153	U1222	G1282	U1345	U1409	U1476	G1540	C1606	C1607	U1715
C	G956	A1021	G1087	C1154	U1223	G1283	G1346	U1410	U1477	U1541	C1608	C1609	G1716
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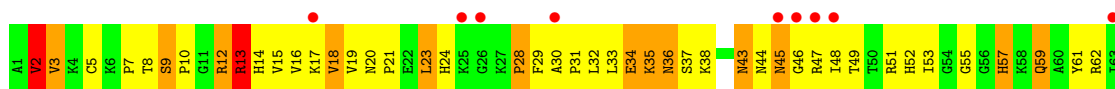
• Molecule 23: 5S rRNA

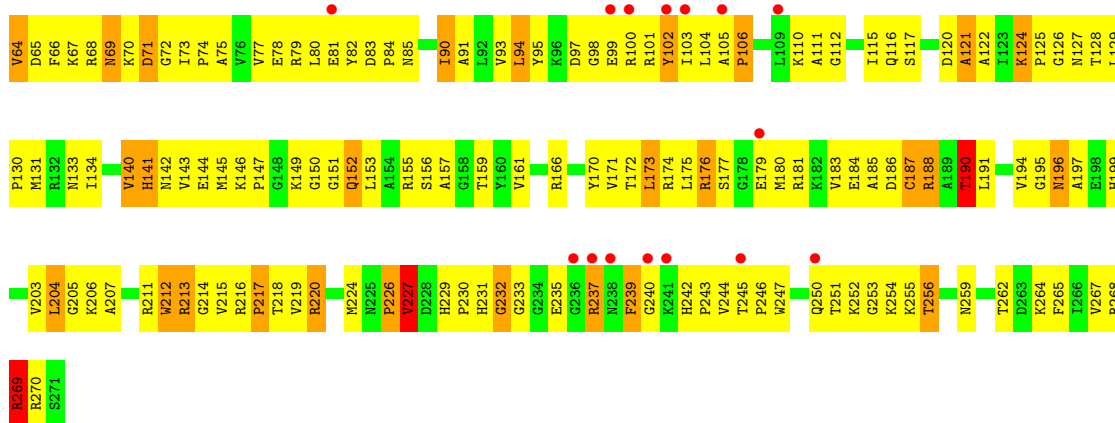


• Molecule 24: 50S ribosomal protein L2

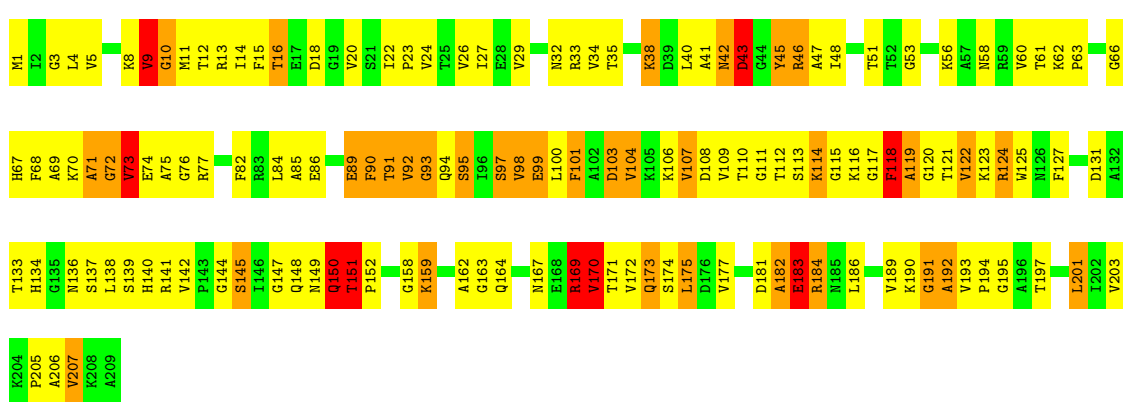


• Molecule 24: 50S ribosomal protein L2

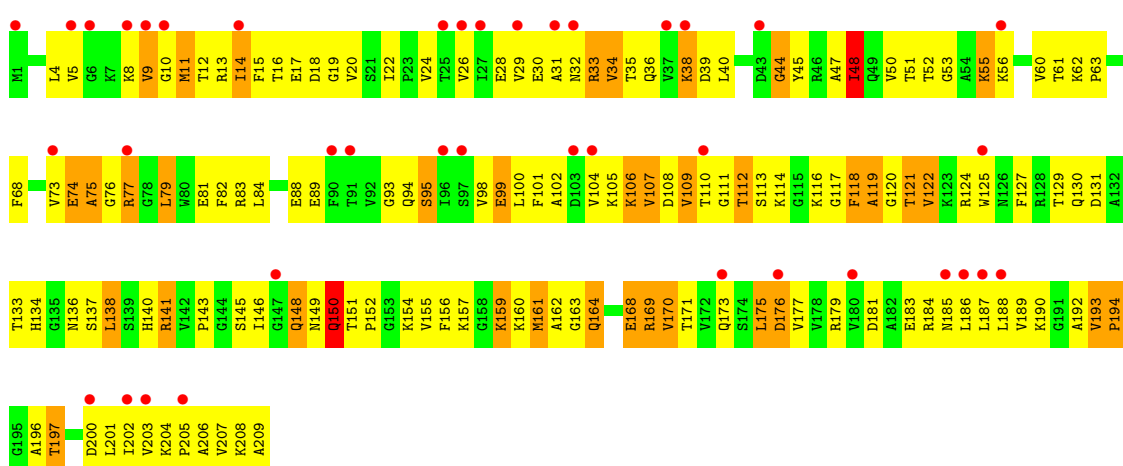
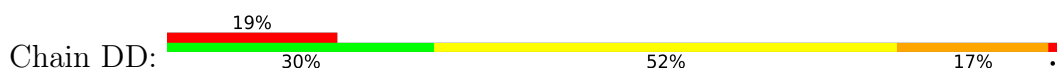




• Molecule 25: 50S ribosomal protein L3

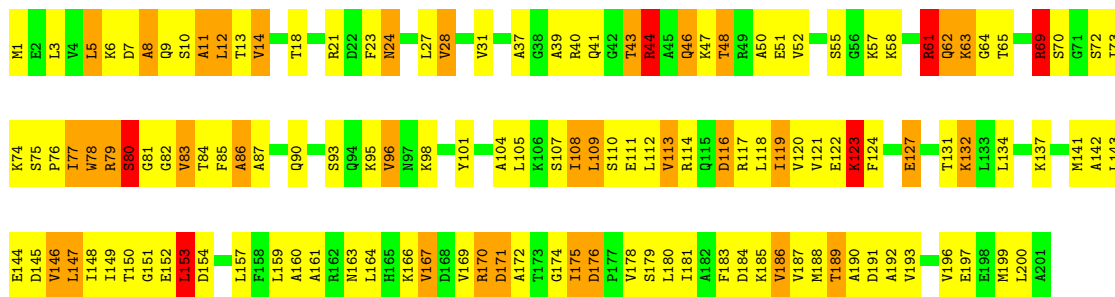


• Molecule 25: 50S ribosomal protein L3

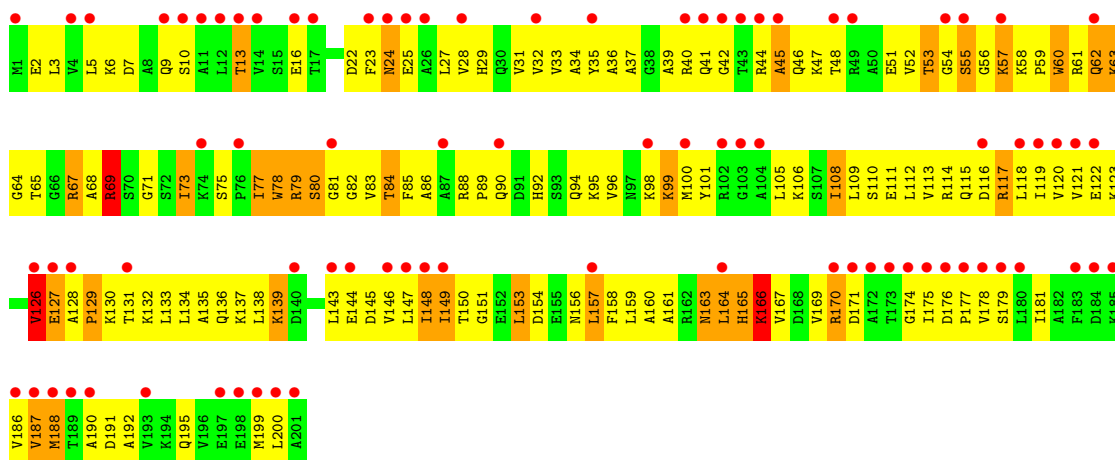
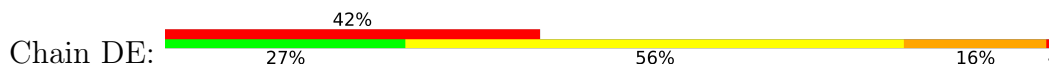


• Molecule 26: 50S ribosomal protein L4

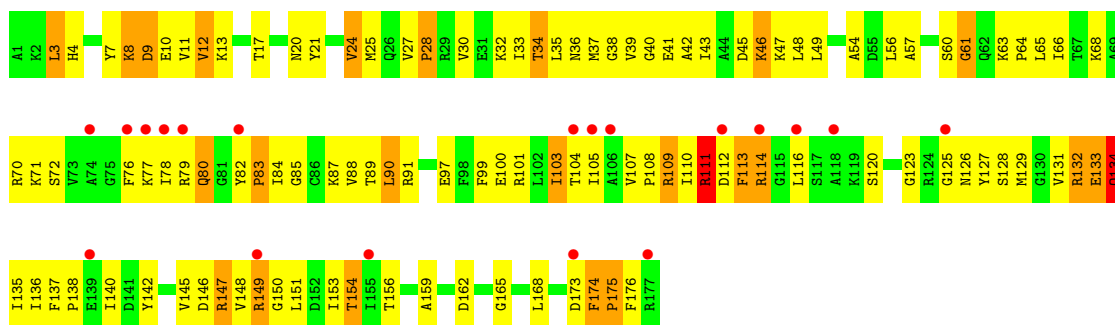




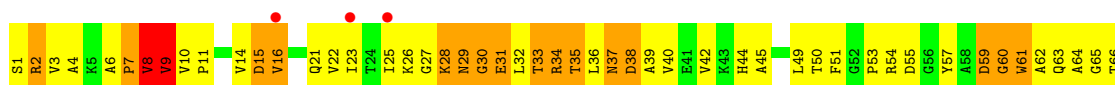
- Molecule 26: 50S ribosomal protein L4

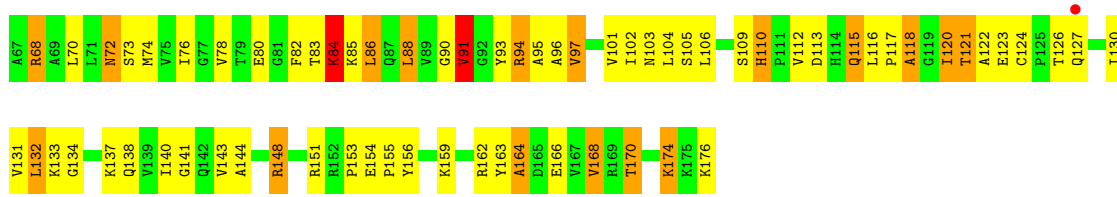


- Molecule 27: 50S ribosomal protein L5

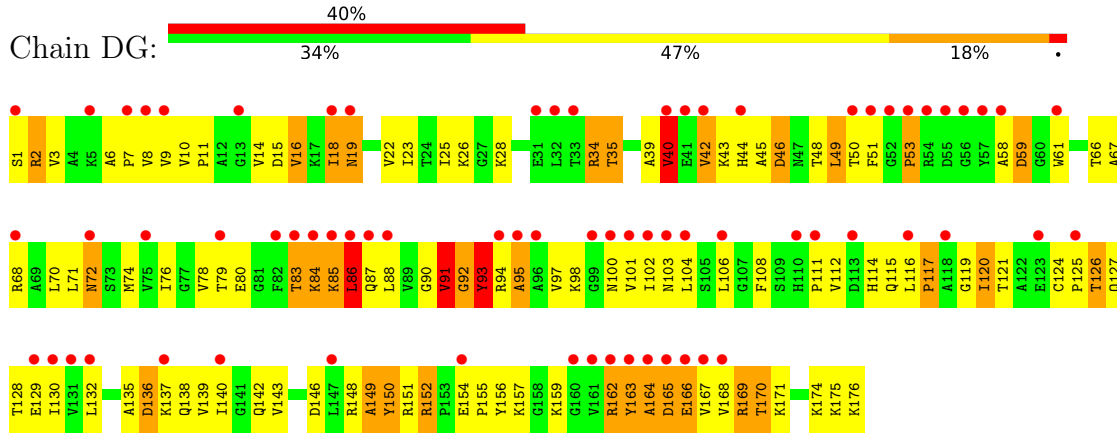


- Molecule 28: 50S ribosomal protein L6

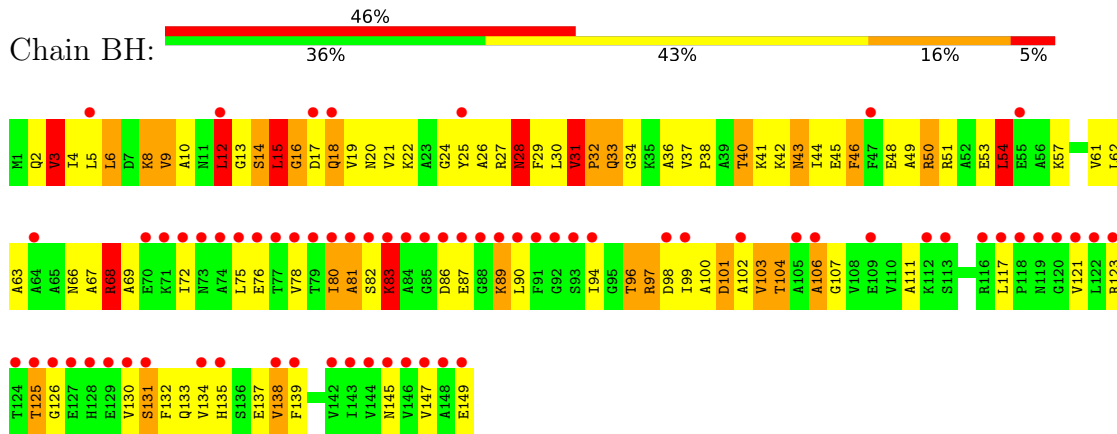




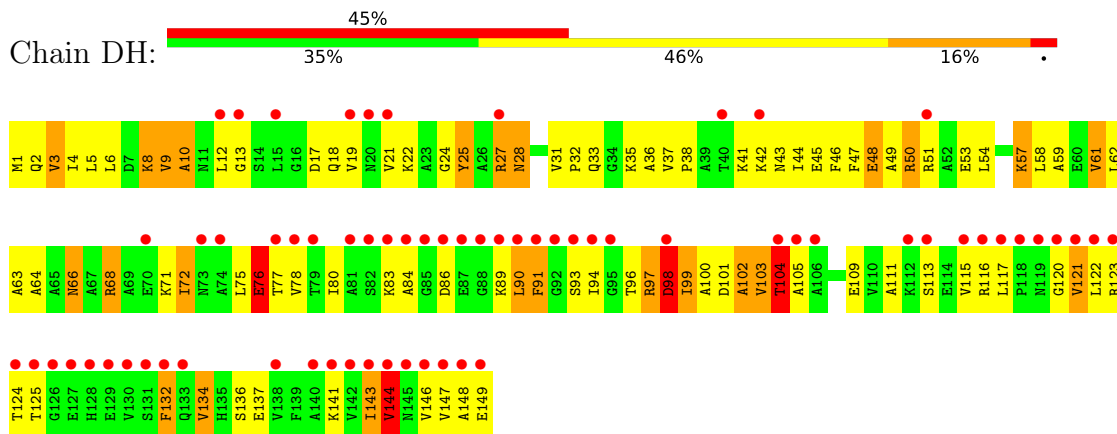
• Molecule 28: 50S ribosomal protein L6



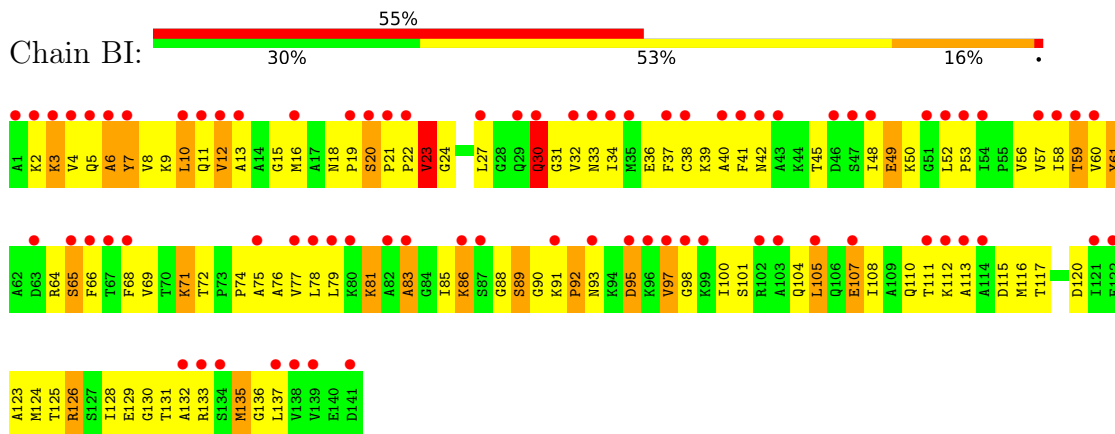
• Molecule 29: 50S ribosomal protein L9



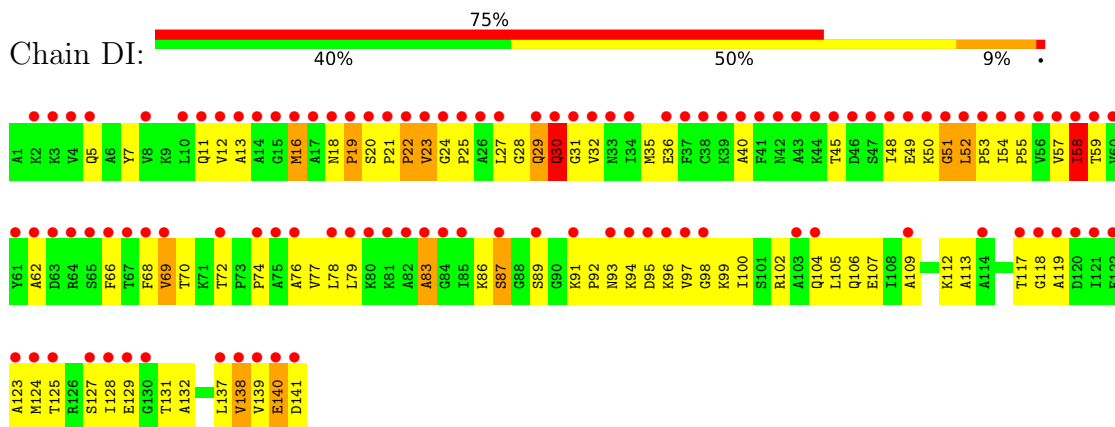
• Molecule 29: 50S ribosomal protein L9



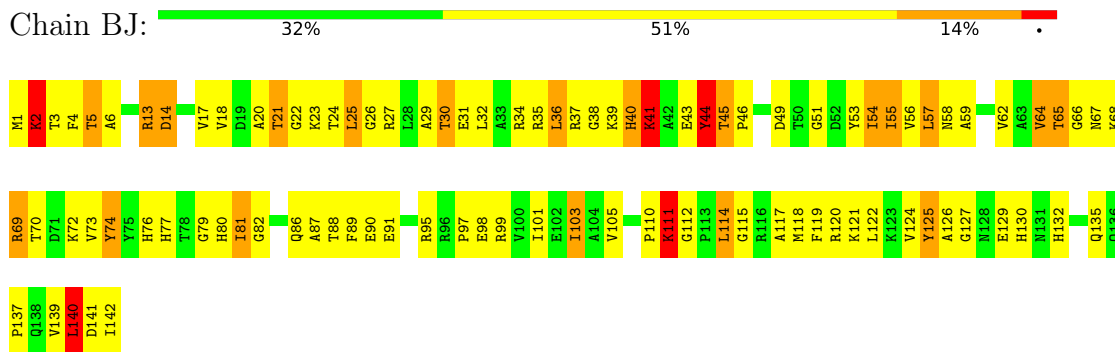
- Molecule 30: 50S ribosomal protein L11



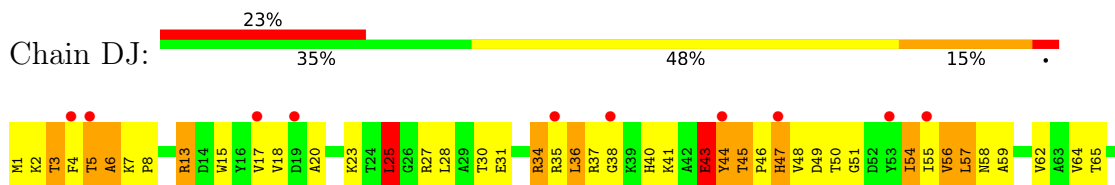
- Molecule 30: 50S ribosomal protein L11

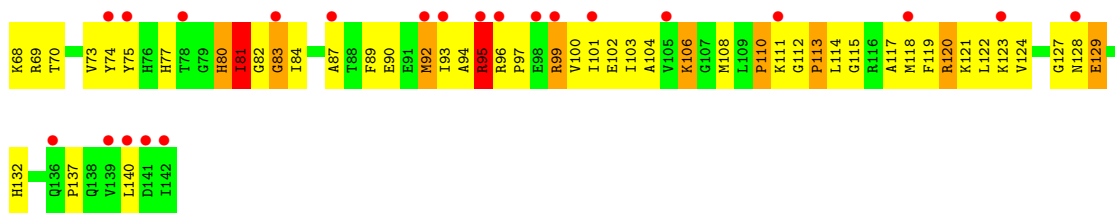


- Molecule 31: 50S ribosomal protein L13

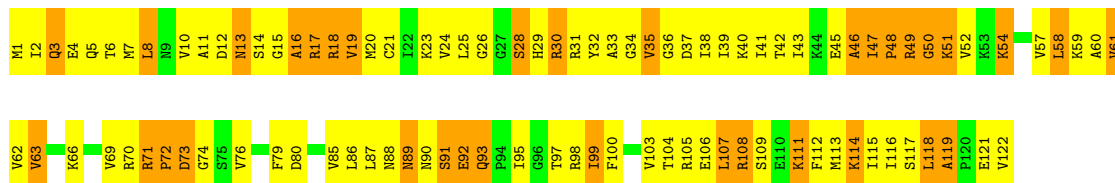


- Molecule 31: 50S ribosomal protein L13

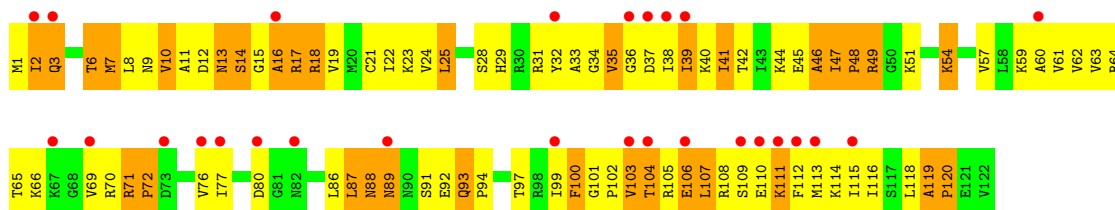




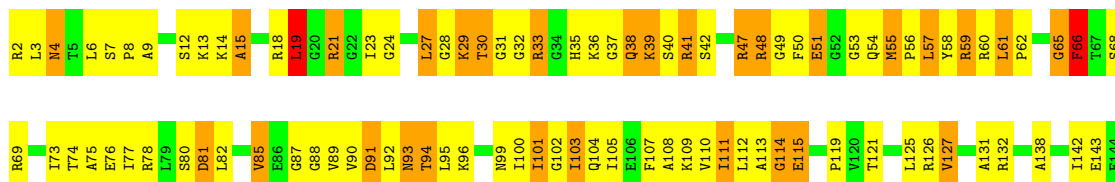
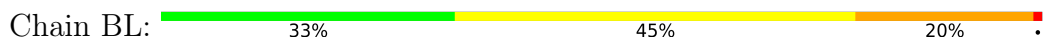
- Molecule 32: 50S ribosomal protein L14



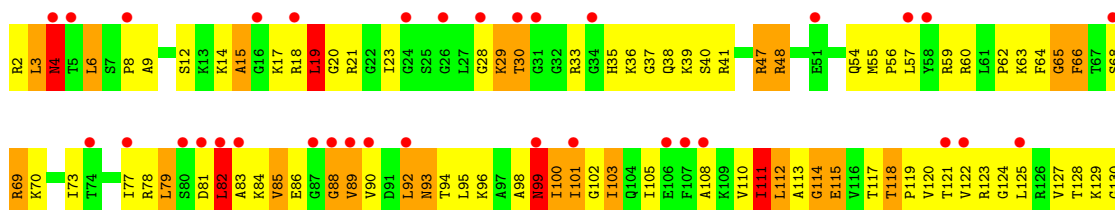
- Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15



- Molecule 33: 50S ribosomal protein L15

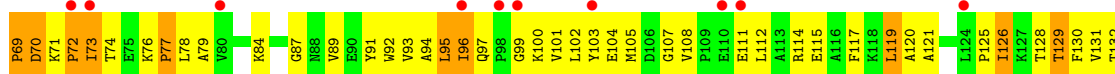
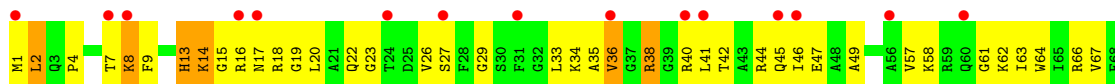




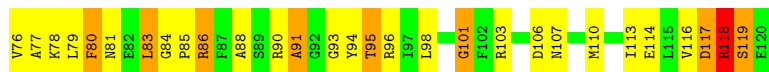
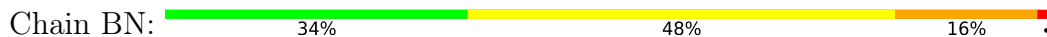
- Molecule 34: 50S ribosomal protein L16



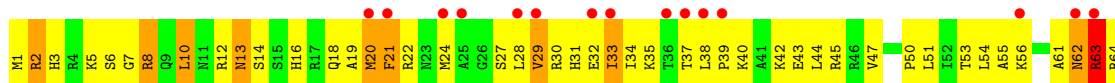
- Molecule 34: 50S ribosomal protein L16



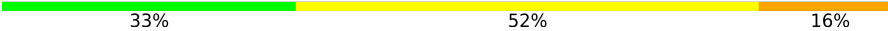
- Molecule 35: 50S ribosomal protein L17

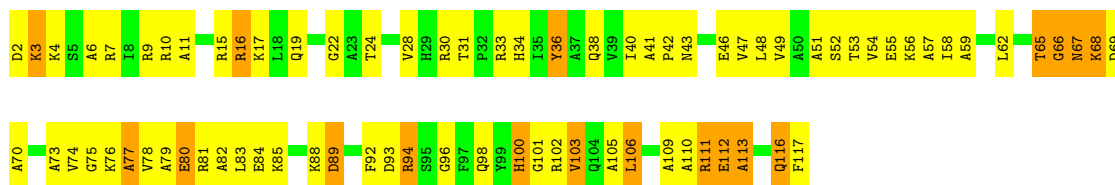


- Molecule 35: 50S ribosomal protein L17



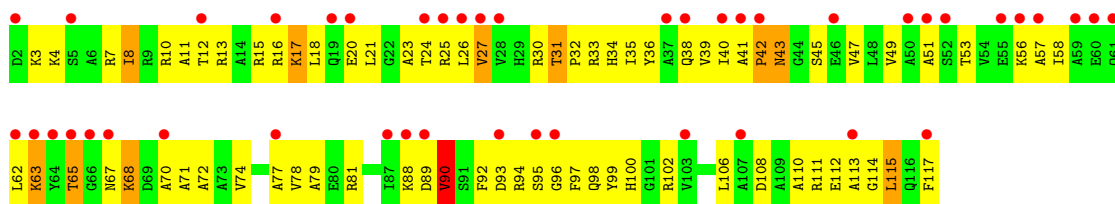
- Molecule 36: 50S ribosomal protein L18

Chain BO:  33% 52% 16%



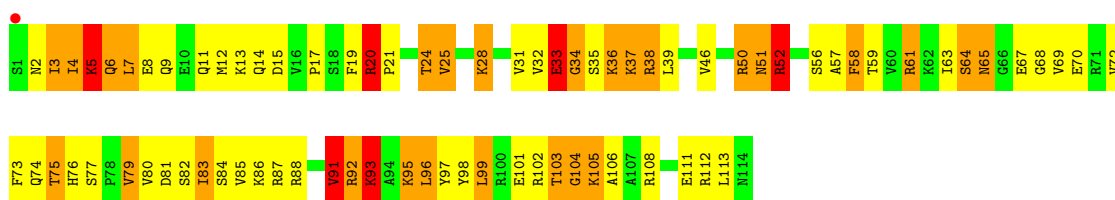
- Molecule 36: 50S ribosomal protein L18

Chain DO:  35% 55% 9%



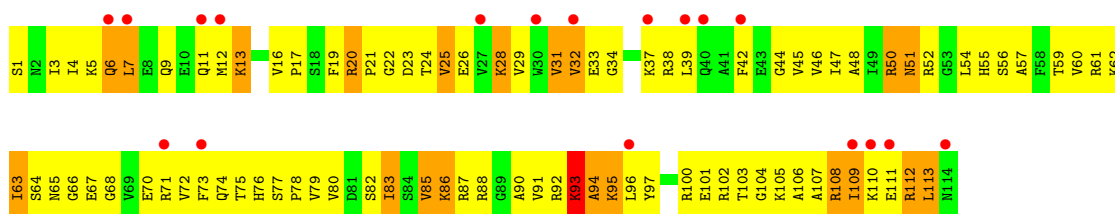
- Molecule 37: 50S ribosomal protein L19

Chain BP:  31% 40% 24% 5%




- Molecule 37: 50S ribosomal protein L19

Chain DP:  20% 61% 18%



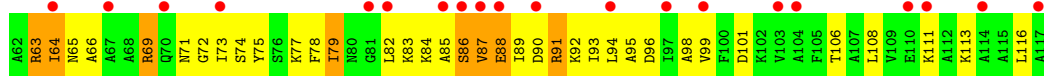
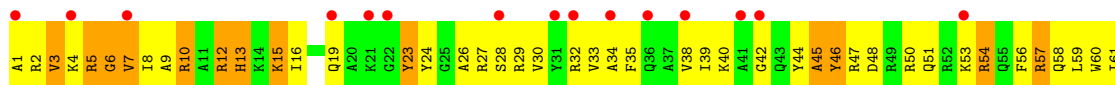
- Molecule 38: 50S ribosomal protein L20

Chain BQ:  41% 40% 18%

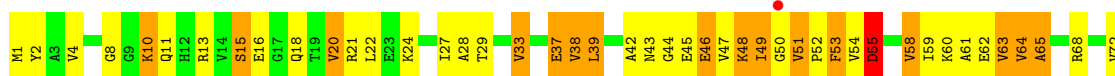




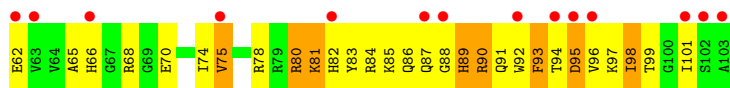
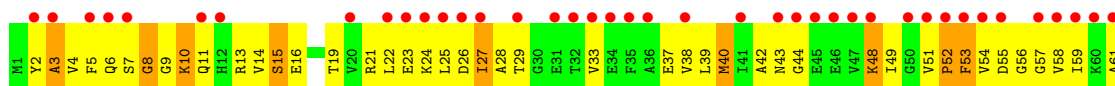
• Molecule 38: 50S ribosomal protein L20



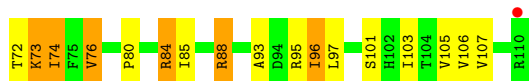
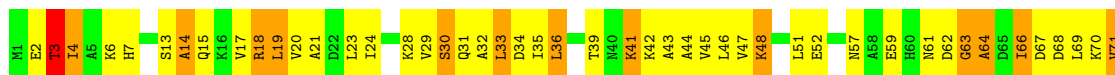
• Molecule 39: 50S ribosomal protein L21



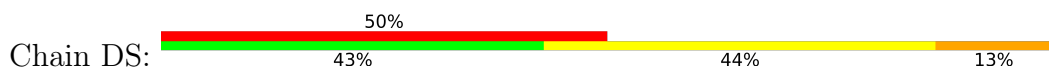
• Molecule 39: 50S ribosomal protein L21

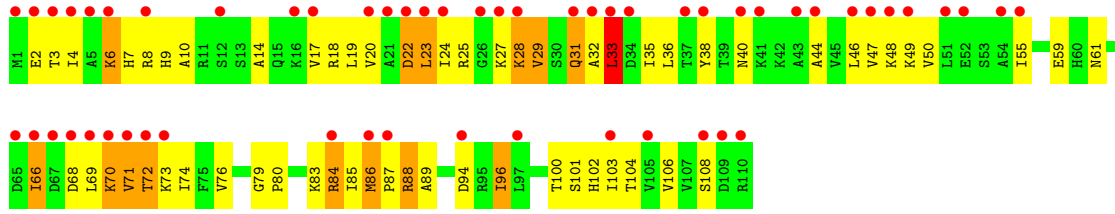


• Molecule 40: 50S ribosomal protein L22

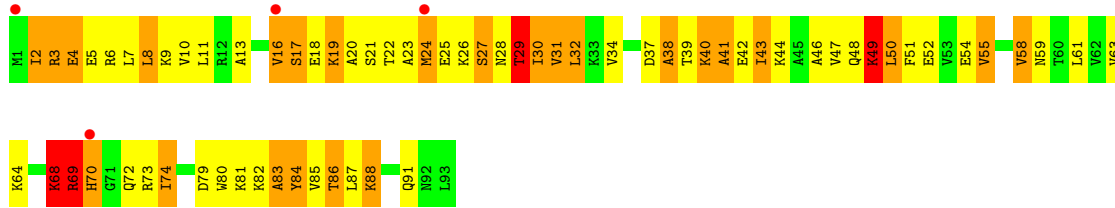


• Molecule 40: 50S ribosomal protein L22

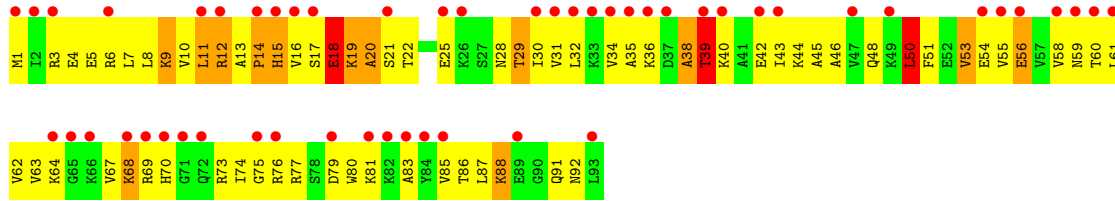




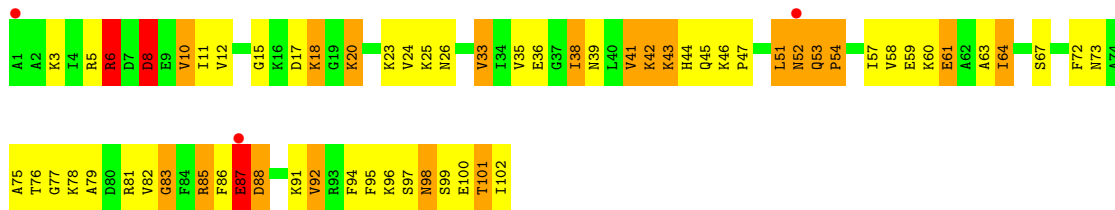
• Molecule 41: 50S ribosomal protein L23



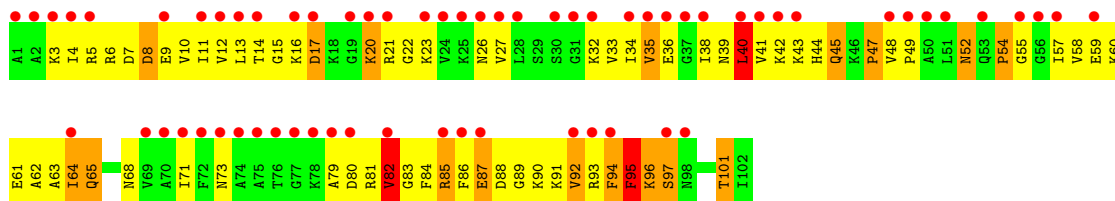
• Molecule 41: 50S ribosomal protein L23



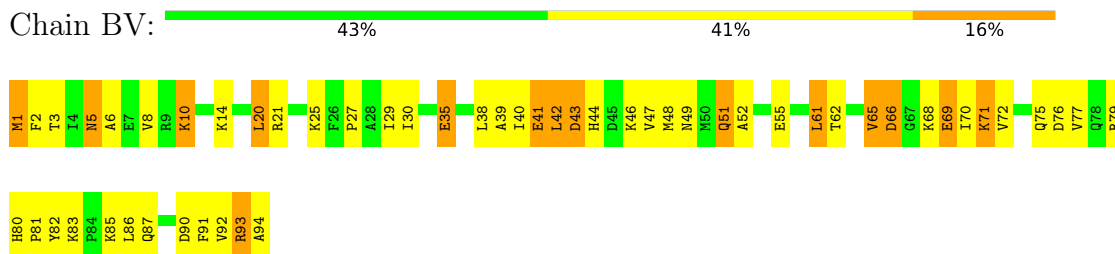
• Molecule 42: 50S ribosomal protein L24



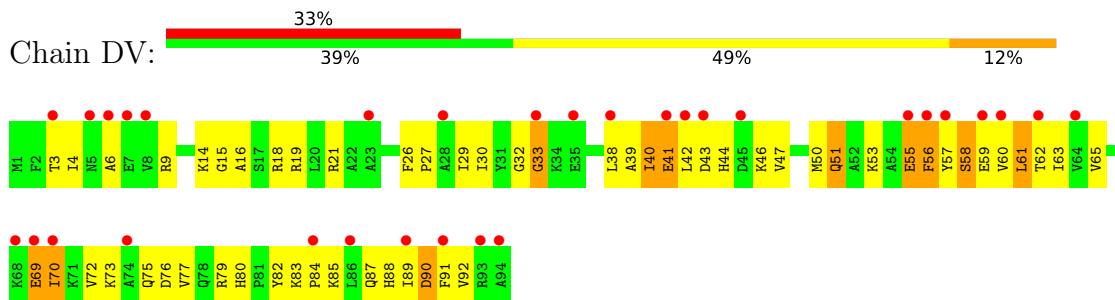
• Molecule 42: 50S ribosomal protein L24



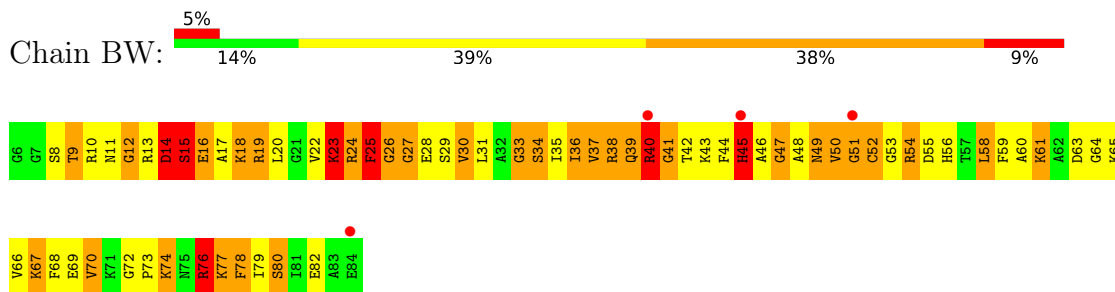
- Molecule 43: 50S ribosomal protein L25



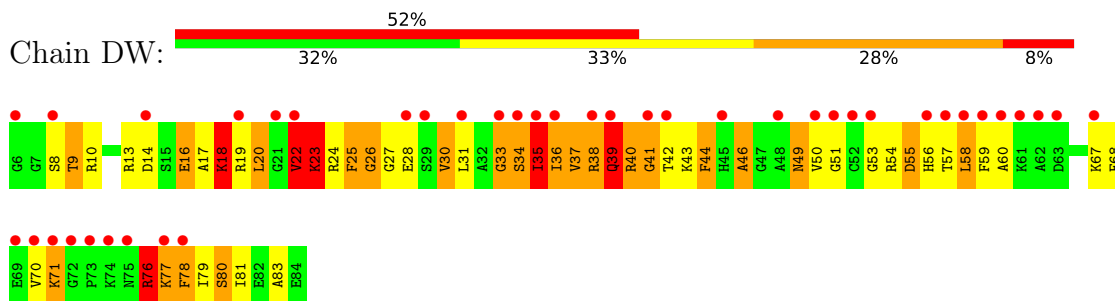
- Molecule 43: 50S ribosomal protein L25



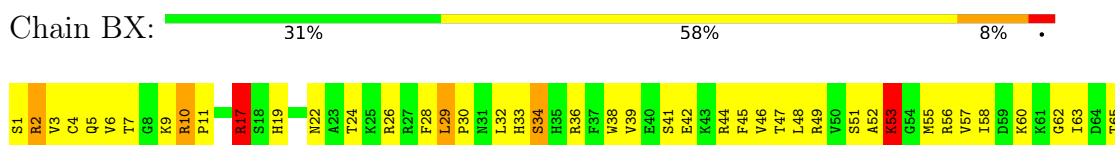
- Molecule 44: 50S ribosomal protein L27



- Molecule 44: 50S ribosomal protein L27

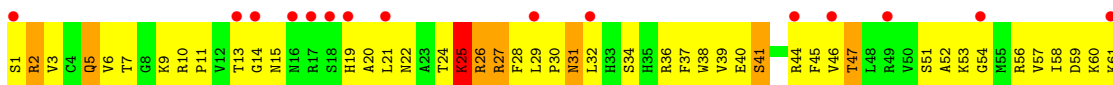


- Molecule 45: 50S ribosomal protein L28

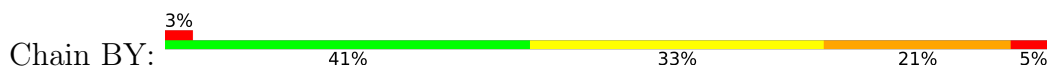




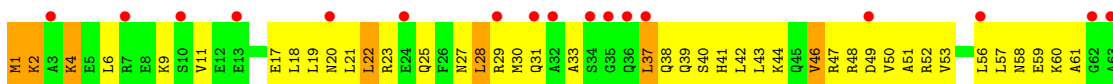
- Molecule 45: 50S ribosomal protein L28



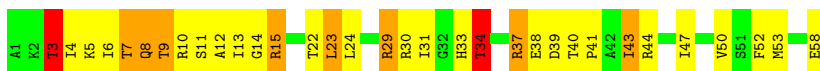
- Molecule 46: 50S ribosomal protein L29



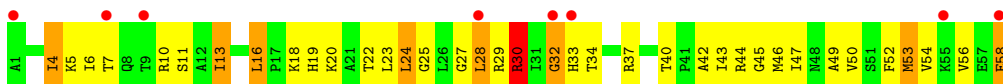
- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30



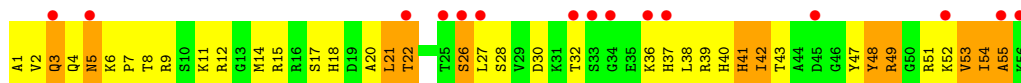
- Molecule 47: 50S ribosomal protein L30



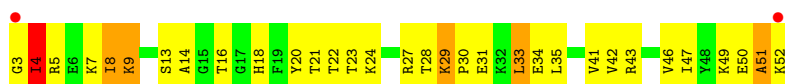
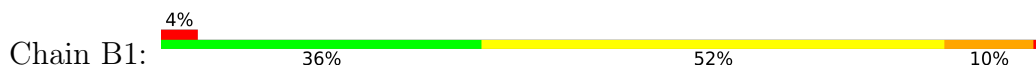
- Molecule 48: 50S ribosomal protein L32



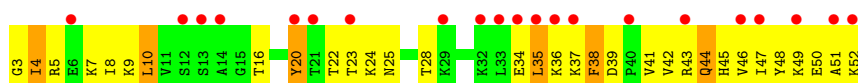
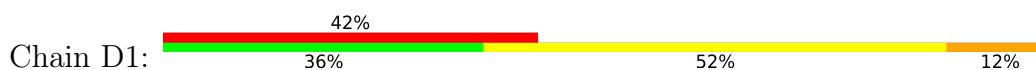
- Molecule 48: 50S ribosomal protein L32



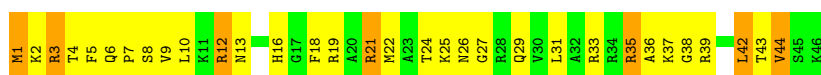
- Molecule 49: 50S ribosomal protein L33



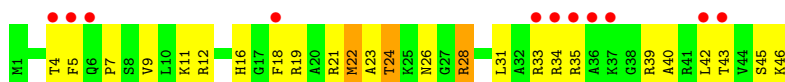
- Molecule 49: 50S ribosomal protein L33



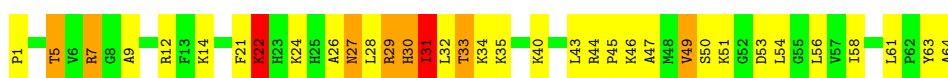
- Molecule 50: 50S ribosomal protein L34



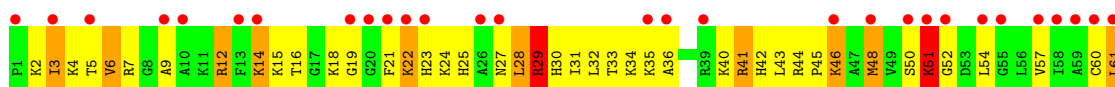
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35

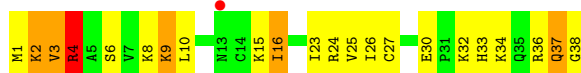


- Molecule 51: 50S ribosomal protein L35

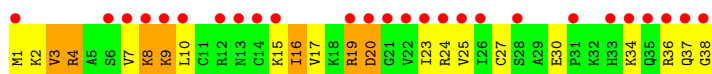




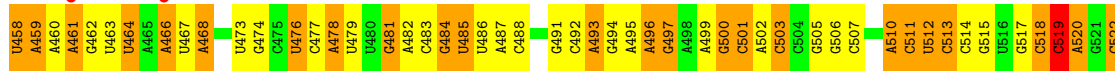
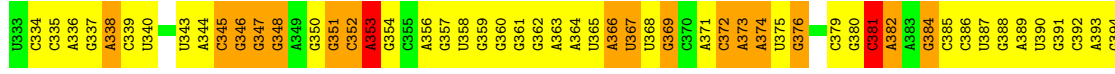
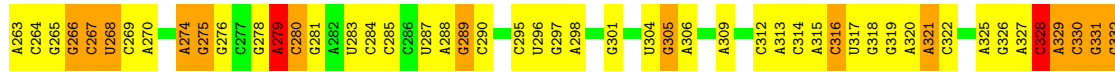
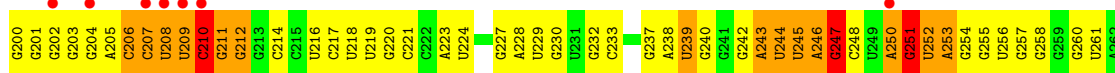
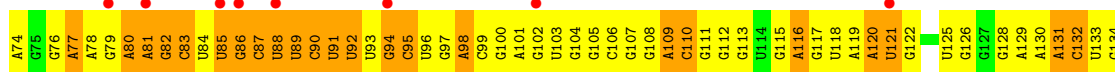
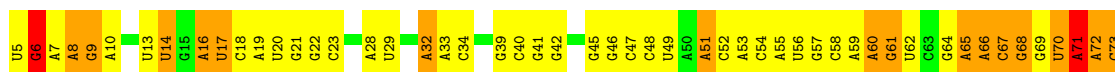
● Molecule 52: 50S ribosomal protein L36



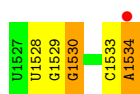
● Molecule 52: 50S ribosomal protein L36



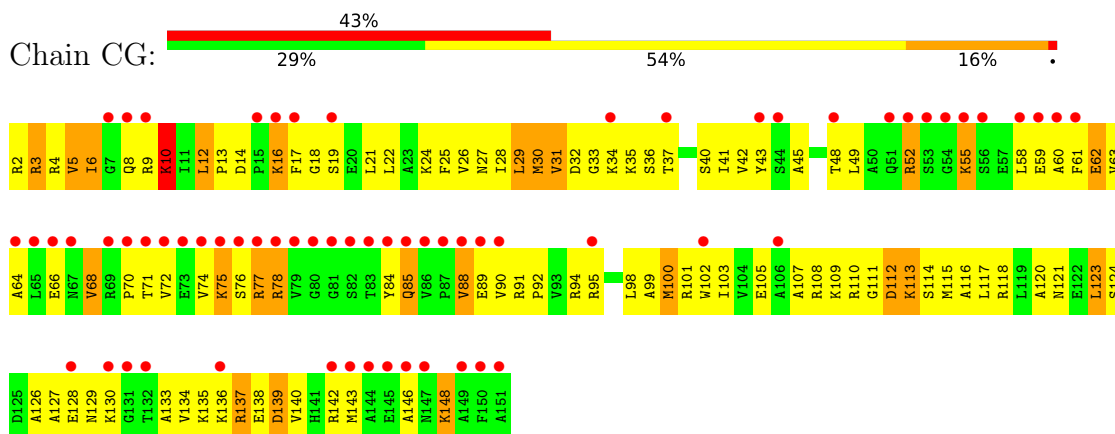
● Molecule 53: 16S rRNA



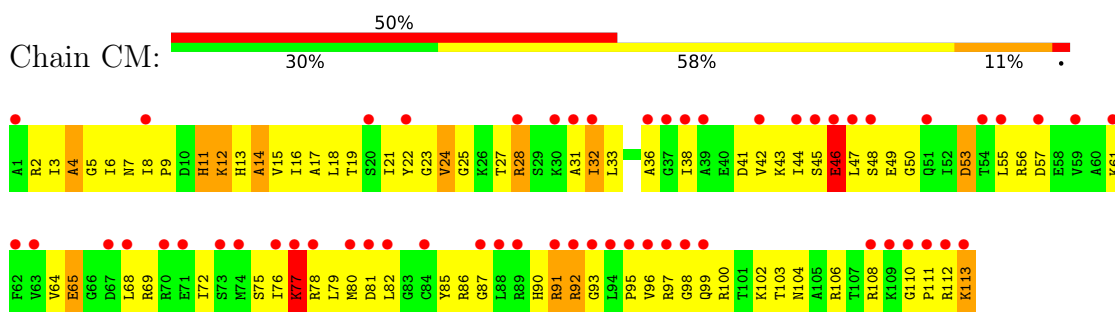
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U1394	C1395	A1396	C1397	A1398	C1399	C1400	G1401	C1402	C1403	C1404	A1405	U1406	C1407	A1408	C1409	A1410	G1411	C1412	A1413	G1414	G1415	G1416	G1417	G1422	G1423	U1424	A1429	A1430	A1431	A1432	A1433	G1434	A1435	U1436	A1437	G1438	G1439	U1440	A1441	G1442	C1443	A1446	C1447	C1448	C1449	U1450	U1451	C1452	G1453	G1454	G1455	C1456	G1457	G1458	C1459	C1460																																										
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G1267	G1268	A1269	G1270	A1271	G1272	C1273	A1274	A1275	G1276	C1277	G1278	A1280	C1281	C1282	U1283	G1284	A1285	U1286	A1287	A1288	A1289	G1293	G1294	U1295	C1296	U1297	U1298	A1299	C1300	U1301	C1302	G1303	C1304	G1305	U1308	G1309	G1310	A1311	U1312	U1313	C1314	U1315	G1316	C1317	A1318	A1319	C1320	U1321	G1386	C1322	G1323	A1324	C1388	C1395	U1326	C1327	C1328	A1329																																								
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G1068	C1069	U1070	C1071	U1072	G1073	U1074	U1075	U1076	U1077	U1078	U1079	A1080	A1081	A1082	U1083	G1084	U1085	U1086	G1087	U1088	U1089	U1090	U1091	A1092	A1093	U1094	U1095	C1096	U1097	C1098	U1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1113	C1114	U1118	C1119	U1123	U1124	U1125	U1126	C1127	C1128	C1129	U1130	C1131	C1132	C1133	C1134																																										
A1005	G1006	U1007	U1008	U1009	U1010	C1011	A1012	G1013	U1014	G1015	C881	G882	G885	G886	G887	U960	U961	U962	C962	G963	G966	C967	G898	A968	A969	C970	C972	G973	U974	A975	G976	A977	A978	C979	C980	U981	U982	A983	C984	U985	U986	G987	G988	U989	C990	U991	U992	G993	U994	U995	U996	U997	C998	C999	A1000	C1001	G1002	C1003	A1004																																							
C726	G727	A728	A729	G730	G731	C732	G733	G734	C735	G736	G737	C738	C739	U740	G741	G745	A746	A747	G748	A749	U750	C751	G752	C613	C614	G615	G616	G617	G618	G619	G620	G621	G622	G623	C624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U636	C637	U638	U639	A640	U641	A642	C643	U644	G645	G646	C647	A648	A649	G650	C651	U652	U653																																				
U871	A872	A873	U874	U875	C876	G877	A878	C879	C880	C881	C882	G885	G886	G887	A816	U888	G889	G890	U891	A892	C893	G898	A900	A901	A902	U826	U827	U828	U829	G833	U834	A909	U835	C910	C841	U842	U843	G844	A845	G846	G847	U921	G922	A923	G926	G927	G928	C929	C930	C931	C932	G933	C934	A935	C936	A937	C940																																									
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G654	A655	C658	U659	U690	U691	G663	G664	A665	G666	G667	G668	G669	U672	A673	G674	A675	A676	U677	C678	C679	U684	G685	U686	G688	C689	G690	G691	G692	G693	A694	A695	A696	G700	U701	A702	G703	A704	G705	U706	U707	U708	U709	A712	G713	U717	A718	C719	A720	A721	G722	U723	U724	U725	U726																																												
A583	G584	G587	U590	U591	G592	A595	A596	G597	U598	C599	G604	U605	G606	A607	A608	A609	U610	C611	C612	C613	C614	G615	G616	G617	G618	U619	C623	C624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U636	C637	U638	U639	A640	U641	A642	C643	U644	G645	G646	C647	A648	A649	G650	C651	U652	U653																																											



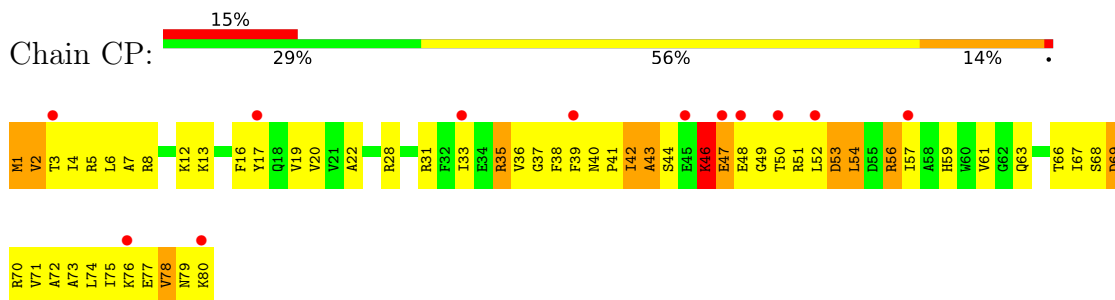
- Molecule 54: 30S ribosomal protein S7



- Molecule 55: 30S ribosomal protein S13



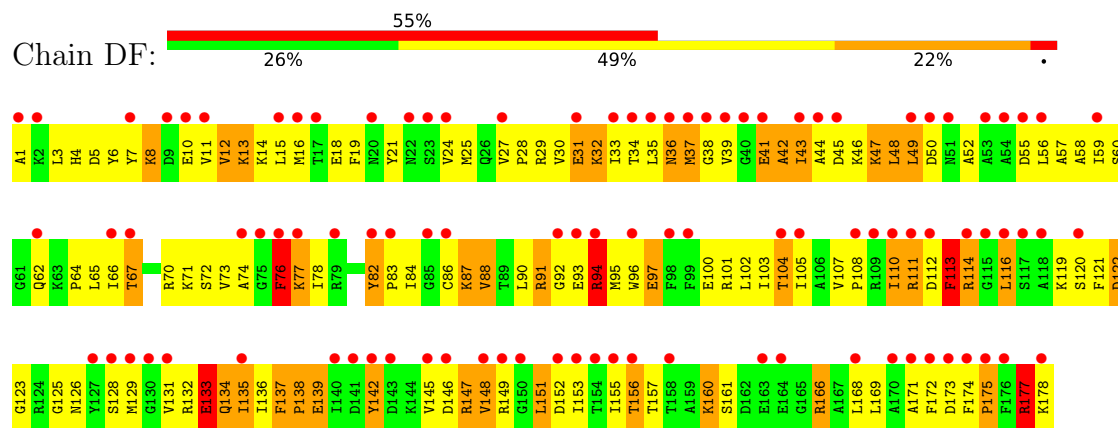
- Molecule 56: 30S ribosomal protein S16



- Molecule 57: 5S rRNA



- Molecule 58: 50S ribosomal protein L5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.76Å 433.27Å 618.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.22 – 3.25 85.13 – 3.25	Depositor EDS
% Data completeness (in resolution range)	85.8 (85.22-3.25) 85.6 (85.13-3.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.26Å)	Xtrriage
Refinement program	PHENIX 1.6.1_357, PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.193 , 0.245 0.224 , 0.268	Depositor DCC
R_{free} test set	16191 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtrriage
Anisotropy	0.387	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	284525	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TEL, 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	0.45	2/36834 (0.0%)	0.87	33/57462 (0.1%)
2	AB	0.34	1/1736 (0.1%)	0.52	1/2338 (0.0%)
2	CB	0.30	1/1736 (0.1%)	0.58	4/2338 (0.2%)
3	AC	0.28	0/1652	0.50	0/2225
3	CC	0.25	0/1652	0.44	0/2225
4	AD	0.32	0/1665	0.53	0/2227
4	CD	0.39	0/1665	0.61	0/2227
5	AE	0.45	1/1119 (0.1%)	0.66	2/1504 (0.1%)
5	CE	0.36	0/1119	0.58	0/1504
6	AF	0.31	0/836	0.49	0/1128
6	CF	0.30	0/836	0.50	0/1128
7	AG	0.25	0/1196	0.45	0/1602
8	AH	0.33	0/989	0.55	0/1326
8	CH	0.30	0/989	0.52	0/1326
9	AI	0.26	0/1034	0.48	0/1375
9	CI	0.23	0/1034	0.43	0/1375
10	AJ	0.28	0/797	0.48	0/1077
10	CJ	0.24	0/797	0.47	0/1077
11	AK	0.30	0/893	0.53	0/1205
11	CK	0.28	0/893	0.52	0/1205
12	AL	0.38	0/969	0.69	1/1300 (0.1%)
12	CL	0.36	0/969	0.58	0/1300
13	AM	0.25	0/893	0.47	0/1193
14	AN	0.28	0/785	0.50	0/1043
14	CN	0.23	0/780	0.39	0/1036
15	AO	0.29	0/722	0.48	0/964
15	CO	0.39	1/722 (0.1%)	0.48	0/964
16	AP	0.31	0/659	0.51	0/884
17	AQ	0.40	0/658	0.62	0/881
17	CQ	0.34	0/658	0.52	0/881
18	AR	0.31	0/463	0.50	0/621
18	CR	0.31	0/463	0.47	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AS	0.25	0/653	0.45	0/877
19	CS	0.21	0/653	0.42	0/877
20	AT	0.37	0/671	0.56	0/888
20	CT	0.28	0/671	0.50	0/888
21	AU	0.29	0/431	0.46	0/570
21	CU	0.34	0/431	0.59	0/570
22	BA	0.77	9/68626 (0.0%)	1.12	282/107056 (0.3%)
22	DA	0.39	1/68314 (0.0%)	0.86	83/106569 (0.1%)
23	BB	0.68	0/2828	1.04	4/4410 (0.1%)
24	BC	0.48	0/2122	0.73	1/2852 (0.0%)
24	DC	0.31	0/2122	0.54	0/2852
25	BD	0.55	0/1586	0.78	1/2134 (0.0%)
25	DD	0.31	0/1586	0.58	0/2134
26	BE	0.45	0/1571	0.68	1/2113 (0.0%)
26	DE	0.26	0/1571	0.48	0/2113
27	BF	0.34	0/1435	0.53	0/1926
28	BG	0.39	0/1343	0.62	0/1816
28	DG	0.24	0/1343	0.47	0/1816
29	BH	0.33	0/1122	0.52	0/1515
29	DH	0.38	1/1122 (0.1%)	0.52	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.21	0/1046	0.42	0/1410
31	BJ	0.58	0/1152	0.84	1/1551 (0.1%)
31	DJ	0.29	0/1152	0.57	1/1551 (0.1%)
32	BK	0.55	0/948	0.80	0/1268
32	DK	0.35	0/948	0.57	0/1268
33	BL	0.46	0/1054	0.79	1/1403 (0.1%)
33	DL	0.27	0/1054	0.53	0/1403
34	BM	0.54	0/1093	0.73	0/1460
34	DM	0.30	0/1093	0.50	0/1460
35	BN	0.51	0/974	0.75	0/1301
35	DN	0.28	0/974	0.51	0/1301
36	BO	0.43	0/902	0.66	0/1209
36	DO	0.24	0/902	0.43	0/1209
37	BP	0.51	0/929	0.74	0/1242
37	DP	0.32	0/929	0.50	0/1242
38	BQ	0.61	0/960	0.78	0/1278
38	DQ	0.29	0/960	0.47	0/1278
39	BR	0.63	1/829 (0.1%)	0.79	0/1107
39	DR	0.29	0/829	0.51	0/1107
40	BS	0.57	0/864	0.78	0/1156
40	DS	0.28	0/864	0.52	0/1156
41	BT	0.45	0/745	0.70	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	DT	0.24	0/745	0.48	0/994
42	BU	0.43	0/788	0.70	0/1051
42	DU	0.24	0/788	0.46	0/1051
43	BV	0.44	0/766	0.61	0/1025
43	DV	0.25	0/766	0.43	0/1025
44	BW	0.61	0/603	0.89	0/797
44	DW	0.29	0/603	0.51	0/797
45	BX	0.41	0/635	0.70	0/848
45	DX	0.29	0/635	0.56	0/848
46	BY	0.37	0/510	0.64	0/677
46	DY	0.23	0/510	0.44	0/677
47	BZ	0.52	0/453	0.83	0/605
47	DZ	0.28	0/453	0.51	0/605
48	B0	0.48	0/450	0.73	0/599
48	D0	0.29	0/450	0.50	0/599
49	B1	0.38	0/417	0.62	0/554
49	D1	0.27	0/417	0.46	0/554
50	B2	0.53	0/380	0.78	0/498
50	D2	0.27	0/380	0.49	0/498
51	B3	0.49	0/513	0.70	0/676
51	D3	0.29	0/513	0.53	0/676
52	B4	0.53	0/303	0.70	0/397
52	D4	0.45	0/303	0.50	0/397
53	CA	0.41	2/36762 (0.0%)	0.83	32/57350 (0.1%)
54	CG	0.23	0/1188	0.44	0/1591
55	CM	0.20	0/885	0.40	0/1181
56	CP	0.29	0/649	0.53	0/870
57	DB	0.36	1/2803 (0.0%)	0.81	2/4371 (0.0%)
58	DF	0.23	0/1444	0.53	3/1937 (0.2%)
All	All	0.51	21/306773 (0.0%)	0.86	453/458565 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	BD	0	1
35	BN	0	1
51	B3	0	1
All	All	0	3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2092	U	O3'-P	-13.97	1.44	1.61
22	DA	2197	U	O3'-P	-13.44	1.45	1.61
53	CA	1396	A	O3'-P	-13.34	1.45	1.61
22	BA	1142	A	N9-C4	-9.96	1.31	1.37
57	DB	107	G	O3'-P	-9.89	1.49	1.61

The worst 5 of 453 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	783	A	C5-N7-C8	-11.37	98.22	103.90
22	BA	974	G	C5-N7-C8	-11.01	98.79	104.30
22	BA	974	G	C4-C5-N7	10.99	115.20	110.80
2	CB	146	SER	O-C-N	-10.79	105.44	122.70
22	BA	2499	C	N1-C2-O2	-10.28	112.73	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	B3	29	ARG	Peptide
25	BD	9	VAL	Peptide
35	BN	101	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32895	0	16553	1232	1
2	AB	1705	0	1732	183	0
2	CB	1705	0	1732	151	0
3	AC	1625	0	1699	109	0
3	CC	1625	0	1699	128	0
4	AD	1643	0	1710	145	0
4	CD	1643	0	1710	157	0
5	AE	1106	0	1148	148	0
5	CE	1106	0	1148	101	0
6	AF	818	0	808	87	0
6	CF	818	0	808	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AG	1182	0	1240	86	0
8	AH	979	0	1034	99	0
8	CH	979	0	1034	92	0
9	AI	1022	0	1070	84	0
9	CI	1022	0	1070	107	0
10	AJ	787	0	828	78	0
10	CJ	787	0	828	91	0
11	AK	877	0	887	91	0
11	CK	877	0	887	71	0
12	AL	955	0	1019	90	0
12	CL	955	0	1019	100	0
13	AM	884	0	944	73	0
14	AN	774	0	827	69	0
14	CN	769	0	822	77	0
15	AO	714	0	737	46	0
15	CO	714	0	737	52	0
16	AP	649	0	666	50	0
17	AQ	649	0	691	71	0
17	CQ	649	0	691	66	0
18	AR	456	0	478	30	0
18	CR	456	0	478	39	0
19	AS	638	0	665	59	0
19	CS	638	0	665	65	0
20	AT	665	0	714	81	0
20	CT	665	0	714	45	0
21	AU	426	0	449	80	0
21	CU	426	0	449	80	0
22	BA	61274	0	30819	1937	6
22	DA	60995	0	30679	3516	8
23	BB	2529	0	1281	73	0
24	BC	2083	0	2157	217	0
24	DC	2083	0	2157	215	0
25	BD	1565	0	1616	196	1
25	DD	1565	0	1616	189	0
26	BE	1552	0	1619	151	0
26	DE	1552	0	1619	180	0
27	BF	1411	0	1447	135	0
28	BG	1323	0	1374	146	0
28	DG	1323	0	1374	126	0
29	BH	1111	0	1148	102	0
29	DH	1111	0	1148	96	0
30	BI	1032	0	1088	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	DI	1032	0	1088	65	0
31	BJ	1129	0	1162	156	0
31	DJ	1129	0	1162	140	0
32	BK	939	0	1012	121	0
32	DK	939	0	1012	109	0
33	BL	1045	0	1117	130	1
33	DL	1045	0	1117	128	0
34	BM	1074	0	1157	90	0
34	DM	1074	0	1157	94	0
35	BN	961	0	1000	89	0
35	DN	961	0	1000	122	0
36	BO	892	0	923	74	0
36	DO	892	0	923	79	0
37	BP	917	0	965	141	0
37	DP	917	0	965	121	0
38	BQ	947	0	1022	127	0
38	DQ	947	0	1022	121	0
39	BR	816	0	839	116	0
39	DR	816	0	839	93	0
40	BS	857	0	922	74	0
40	DS	857	0	922	60	0
41	BT	739	0	807	112	0
41	DT	739	0	807	99	0
42	BU	780	0	834	54	0
42	DU	780	0	834	92	0
43	BV	753	0	780	66	0
43	DV	753	0	780	60	0
44	BW	596	0	610	204	0
44	DW	596	0	610	115	0
45	BX	625	0	655	56	0
45	DX	625	0	655	75	0
46	BY	509	0	543	50	0
46	DY	509	0	543	63	0
47	BZ	449	0	491	33	0
47	DZ	449	0	491	40	1
48	B0	444	0	461	30	0
48	D0	444	0	461	57	0
49	B1	410	0	440	33	0
49	D1	410	0	440	36	0
50	B2	377	0	418	35	0
50	D2	377	0	418	42	0
51	B3	504	0	574	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	D3	504	0	574	57	0
52	B4	302	0	340	30	0
52	D4	302	0	342	27	0
53	CA	32831	0	16521	1619	0
54	CG	1175	0	1230	131	0
55	CM	877	0	937	91	0
56	CP	639	0	656	61	0
57	DB	2507	0	1270	159	0
58	DF	1420	0	1460	184	0
59	AA	43	0	0	0	0
59	BA	134	0	0	0	0
59	BB	4	0	0	0	0
59	CA	41	0	0	0	0
59	CE	1	0	0	0	0
59	DA	133	0	0	0	0
59	DB	1	0	0	0	0
59	DC	2	0	0	0	0
59	DJ	1	0	0	0	0
60	BA	58	0	64	8	0
61	B4	1	0	0	0	0
61	D4	1	0	0	0	0
62	AA	198	0	0	5	0
62	AL	1	0	0	0	0
62	AN	6	0	0	1	0
62	AT	2	0	0	0	0
62	AU	1	0	0	0	0
62	B2	1	0	0	0	0
62	B3	3	0	0	0	0
62	B4	1	0	0	0	0
62	BA	598	0	0	29	0
62	BB	20	0	0	1	0
62	BC	10	0	0	0	0
62	BD	2	0	0	0	0
62	BE	1	0	0	0	0
62	BL	2	0	0	1	0
62	BN	3	0	0	1	0
62	BQ	1	0	0	0	0
62	BR	1	0	0	0	0
62	BT	1	0	0	1	0
62	CA	192	0	0	6	0
62	CE	5	0	0	1	0
62	CI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	CL	1	0	0	0	0
62	CN	3	0	0	0	0
62	CT	3	0	0	0	0
62	CU	2	0	0	0	0
62	D2	1	0	0	1	0
62	D3	1	0	0	0	0
62	D4	3	0	0	0	0
62	DA	595	0	0	28	0
62	DB	4	0	0	0	0
62	DC	13	0	0	1	0
62	DD	3	0	0	1	0
62	DE	3	0	0	0	0
62	DJ	6	0	0	0	0
62	DL	6	0	0	1	0
62	DN	2	0	0	0	0
62	DT	3	0	0	0	0
62	DU	2	0	0	0	0
62	DV	1	0	0	0	0
All	All	284525	0	190904	16341	9

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 35.

The worst 5 of 16341 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)
53:CA:1157:A:H4'	53:CA:1158:C:O5'	1.38	1.20
22:DA:1808:A:H3'	22:DA:1809:A:H8	1.05	1.20
53:CA:120:A:C3'	53:CA:121:U:H5''	1.73	1.19
22:DA:2091:C:OP2	22:DA:2092:U:H3'	1.39	1.18
22:BA:900:A:C2'	22:BA:901:C:H5'	1.74	1.17

The worst 5 of 9 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]	1.58	0.62
22:BA:138:U:O4	22:DA:305:C:P[3_545]	1.90	0.30
1:AA:416:G:OP1	22:DA:2139:U:O4'[4_455]	1.91	0.29
25:BD:181:ASP:OD1	22:DA:2903:U:O4[2_454]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:138:U:C4	22:DA:304:U:O3'[3_545]	1.98	0.22

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	132 (61%)	52 (24%)	32 (15%)	0	1
2	CB	216/218 (99%)	155 (72%)	46 (21%)	15 (7%)	1	8
3	AC	204/206 (99%)	156 (76%)	32 (16%)	16 (8%)	1	6
3	CC	204/206 (99%)	147 (72%)	37 (18%)	20 (10%)	0	3
4	AD	203/205 (99%)	138 (68%)	37 (18%)	28 (14%)	0	1
4	CD	203/205 (99%)	140 (69%)	43 (21%)	20 (10%)	0	3
5	AE	148/150 (99%)	105 (71%)	23 (16%)	20 (14%)	0	1
5	CE	148/150 (99%)	112 (76%)	21 (14%)	15 (10%)	0	3
6	AF	98/100 (98%)	73 (74%)	13 (13%)	12 (12%)	0	2
6	CF	98/100 (98%)	65 (66%)	24 (24%)	9 (9%)	1	4
7	AG	149/151 (99%)	111 (74%)	32 (22%)	6 (4%)	3	17
8	AH	127/129 (98%)	92 (72%)	28 (22%)	7 (6%)	2	11
8	CH	127/129 (98%)	94 (74%)	22 (17%)	11 (9%)	1	5
9	AI	125/127 (98%)	89 (71%)	26 (21%)	10 (8%)	1	6
9	CI	125/127 (98%)	89 (71%)	25 (20%)	11 (9%)	1	5
10	AJ	96/98 (98%)	70 (73%)	13 (14%)	13 (14%)	0	1
10	CJ	96/98 (98%)	55 (57%)	28 (29%)	13 (14%)	0	1
11	AK	115/117 (98%)	85 (74%)	20 (17%)	10 (9%)	1	5
11	CK	115/117 (98%)	89 (77%)	19 (16%)	7 (6%)	1	10
12	AL	121/123 (98%)	88 (73%)	22 (18%)	11 (9%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	CL	121/123 (98%)	86 (71%)	27 (22%)	8 (7%)	1	9
13	AM	112/114 (98%)	88 (79%)	13 (12%)	11 (10%)	0	3
14	AN	92/100 (92%)	60 (65%)	20 (22%)	12 (13%)	0	2
14	CN	91/100 (91%)	59 (65%)	27 (30%)	5 (6%)	2	11
15	AO	86/88 (98%)	59 (69%)	23 (27%)	4 (5%)	2	14
15	CO	86/88 (98%)	67 (78%)	16 (19%)	3 (4%)	3	21
16	AP	80/82 (98%)	58 (72%)	14 (18%)	8 (10%)	0	3
17	AQ	78/80 (98%)	51 (65%)	15 (19%)	12 (15%)	0	1
17	CQ	78/80 (98%)	62 (80%)	8 (10%)	8 (10%)	0	3
18	AR	53/55 (96%)	46 (87%)	5 (9%)	2 (4%)	3	19
18	CR	53/55 (96%)	42 (79%)	11 (21%)	0	100	100
19	AS	77/79 (98%)	58 (75%)	10 (13%)	9 (12%)	0	2
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	4
20	AT	83/85 (98%)	58 (70%)	19 (23%)	6 (7%)	1	7
20	CT	83/85 (98%)	63 (76%)	12 (14%)	8 (10%)	0	4
21	AU	49/51 (96%)	25 (51%)	15 (31%)	9 (18%)	0	1
21	CU	49/51 (96%)	22 (45%)	8 (16%)	19 (39%)	0	0
24	BC	269/271 (99%)	203 (76%)	40 (15%)	26 (10%)	0	4
24	DC	269/271 (99%)	183 (68%)	54 (20%)	32 (12%)	0	2
25	BD	207/209 (99%)	148 (72%)	31 (15%)	28 (14%)	0	1
25	DD	207/209 (99%)	136 (66%)	40 (19%)	31 (15%)	0	1
26	BE	199/201 (99%)	149 (75%)	32 (16%)	18 (9%)	1	4
26	DE	199/201 (99%)	125 (63%)	46 (23%)	28 (14%)	0	1
27	BF	175/177 (99%)	130 (74%)	30 (17%)	15 (9%)	1	5
28	BG	174/176 (99%)	118 (68%)	32 (18%)	24 (14%)	0	1
28	DG	174/176 (99%)	102 (59%)	41 (24%)	31 (18%)	0	1
29	BH	147/149 (99%)	67 (46%)	52 (35%)	28 (19%)	0	1
29	DH	147/149 (99%)	76 (52%)	53 (36%)	18 (12%)	0	2
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	0	3
30	DI	139/141 (99%)	84 (60%)	38 (27%)	17 (12%)	0	2
31	BJ	140/142 (99%)	103 (74%)	26 (19%)	11 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DJ	140/142 (99%)	96 (69%)	29 (21%)	15 (11%)	0	3
32	BK	120/122 (98%)	88 (73%)	12 (10%)	20 (17%)	0	1
32	DK	120/122 (98%)	82 (68%)	18 (15%)	20 (17%)	0	1
33	BL	141/143 (99%)	103 (73%)	28 (20%)	10 (7%)	1	7
33	DL	141/143 (99%)	80 (57%)	41 (29%)	20 (14%)	0	1
34	BM	134/136 (98%)	100 (75%)	21 (16%)	13 (10%)	0	4
34	DM	134/136 (98%)	95 (71%)	27 (20%)	12 (9%)	1	4
35	BN	118/120 (98%)	92 (78%)	14 (12%)	12 (10%)	0	3
35	DN	118/120 (98%)	70 (59%)	36 (30%)	12 (10%)	0	3
36	BO	114/116 (98%)	88 (77%)	17 (15%)	9 (8%)	1	6
36	DO	114/116 (98%)	81 (71%)	26 (23%)	7 (6%)	1	10
37	BP	112/114 (98%)	74 (66%)	21 (19%)	17 (15%)	0	1
37	DP	112/114 (98%)	64 (57%)	29 (26%)	19 (17%)	0	1
38	BQ	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	1	7
38	DQ	115/117 (98%)	83 (72%)	20 (17%)	12 (10%)	0	3
39	BR	101/103 (98%)	80 (79%)	14 (14%)	7 (7%)	1	8
39	DR	101/103 (98%)	71 (70%)	18 (18%)	12 (12%)	0	2
40	BS	108/110 (98%)	84 (78%)	17 (16%)	7 (6%)	1	9
40	DS	108/110 (98%)	74 (68%)	25 (23%)	9 (8%)	1	5
41	BT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	1
41	DT	91/93 (98%)	48 (53%)	28 (31%)	15 (16%)	0	1
42	BU	100/102 (98%)	67 (67%)	17 (17%)	16 (16%)	0	1
42	DU	100/102 (98%)	51 (51%)	28 (28%)	21 (21%)	0	0
43	BV	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	14	46
43	DV	92/94 (98%)	64 (70%)	21 (23%)	7 (8%)	1	6
44	BW	77/79 (98%)	28 (36%)	22 (29%)	27 (35%)	0	0
44	DW	77/79 (98%)	33 (43%)	23 (30%)	21 (27%)	0	0
45	BX	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	2	12
45	DX	75/77 (97%)	50 (67%)	17 (23%)	8 (11%)	0	3
46	BY	61/63 (97%)	44 (72%)	11 (18%)	6 (10%)	0	3
46	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	BZ	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	3	20
47	DZ	56/58 (97%)	34 (61%)	17 (30%)	5 (9%)	1	4
48	B0	54/56 (96%)	41 (76%)	9 (17%)	4 (7%)	1	7
48	D0	54/56 (96%)	40 (74%)	8 (15%)	6 (11%)	0	2
49	B1	48/50 (96%)	39 (81%)	5 (10%)	4 (8%)	1	5
49	D1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	5
50	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	2	15
50	D2	44/46 (96%)	29 (66%)	11 (25%)	4 (9%)	1	4
51	B3	62/64 (97%)	50 (81%)	7 (11%)	5 (8%)	1	6
51	D3	62/64 (97%)	39 (63%)	18 (29%)	5 (8%)	1	6
52	B4	36/38 (95%)	29 (81%)	3 (8%)	4 (11%)	0	2
52	D4	36/38 (95%)	23 (64%)	8 (22%)	5 (14%)	0	1
54	CG	148/150 (99%)	100 (68%)	36 (24%)	12 (8%)	1	6
55	CM	111/113 (98%)	64 (58%)	35 (32%)	12 (11%)	0	3
56	CP	78/80 (98%)	50 (64%)	18 (23%)	10 (13%)	0	2
58	DF	176/178 (99%)	98 (56%)	46 (26%)	32 (18%)	0	1
All	All	11238/11447 (98%)	7713 (69%)	2283 (20%)	1242 (11%)	0	2

5 of 1242 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	18	GLN
2	AB	20	ARG
2	AB	33	ALA
2	AB	40	ILE
2	AB	72	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	141 (78%)	39 (22%)	1	4
2	CB	180/180 (100%)	152 (84%)	28 (16%)	2	11
3	AC	170/170 (100%)	142 (84%)	28 (16%)	2	10
3	CC	170/170 (100%)	151 (89%)	19 (11%)	6	23
4	AD	172/172 (100%)	145 (84%)	27 (16%)	2	11
4	CD	172/172 (100%)	135 (78%)	37 (22%)	1	4
5	AE	113/113 (100%)	86 (76%)	27 (24%)	0	2
5	CE	113/113 (100%)	90 (80%)	23 (20%)	1	4
6	AF	87/87 (100%)	73 (84%)	14 (16%)	2	10
6	CF	87/87 (100%)	74 (85%)	13 (15%)	3	12
7	AG	124/124 (100%)	106 (86%)	18 (14%)	3	14
8	AH	104/104 (100%)	89 (86%)	15 (14%)	3	14
8	CH	104/104 (100%)	91 (88%)	13 (12%)	4	19
9	AI	105/105 (100%)	83 (79%)	22 (21%)	1	4
9	CI	105/105 (100%)	91 (87%)	14 (13%)	4	16
10	AJ	86/86 (100%)	74 (86%)	12 (14%)	3	15
10	CJ	86/86 (100%)	75 (87%)	11 (13%)	4	18
11	AK	90/90 (100%)	75 (83%)	15 (17%)	2	9
11	CK	90/90 (100%)	78 (87%)	12 (13%)	4	16
12	AL	103/103 (100%)	85 (82%)	18 (18%)	2	8
12	CL	103/103 (100%)	86 (84%)	17 (16%)	2	10
13	AM	92/92 (100%)	87 (95%)	5 (5%)	22	53
14	AN	79/83 (95%)	75 (95%)	4 (5%)	24	54
14	CN	79/83 (95%)	69 (87%)	10 (13%)	4	18
15	AO	76/76 (100%)	70 (92%)	6 (8%)	12	37
15	CO	76/76 (100%)	70 (92%)	6 (8%)	12	37
16	AP	65/65 (100%)	58 (89%)	7 (11%)	6	24
17	AQ	74/74 (100%)	57 (77%)	17 (23%)	1	3
17	CQ	74/74 (100%)	60 (81%)	14 (19%)	1	6
18	AR	48/48 (100%)	45 (94%)	3 (6%)	18	47
18	CR	48/48 (100%)	43 (90%)	5 (10%)	7	25
19	AS	70/70 (100%)	62 (89%)	8 (11%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	CS	70/70 (100%)	63 (90%)	7 (10%)	7	27
20	AT	65/65 (100%)	49 (75%)	16 (25%)	0	2
20	CT	65/65 (100%)	51 (78%)	14 (22%)	1	4
21	AU	44/44 (100%)	34 (77%)	10 (23%)	1	3
21	CU	44/44 (100%)	36 (82%)	8 (18%)	1	7
24	BC	216/216 (100%)	167 (77%)	49 (23%)	1	3
24	DC	216/216 (100%)	189 (88%)	27 (12%)	4	19
25	BD	164/164 (100%)	134 (82%)	30 (18%)	1	7
25	DD	164/164 (100%)	144 (88%)	20 (12%)	5	20
26	BE	165/165 (100%)	122 (74%)	43 (26%)	0	1
26	DE	165/165 (100%)	147 (89%)	18 (11%)	6	24
27	BF	148/148 (100%)	130 (88%)	18 (12%)	5	20
28	BG	137/137 (100%)	105 (77%)	32 (23%)	1	3
28	DG	137/137 (100%)	119 (87%)	18 (13%)	4	17
29	BH	114/114 (100%)	96 (84%)	18 (16%)	2	11
29	DH	114/114 (100%)	96 (84%)	18 (16%)	2	11
30	BI	109/109 (100%)	91 (84%)	18 (16%)	2	10
30	DI	109/109 (100%)	102 (94%)	7 (6%)	17	47
31	BJ	116/116 (100%)	88 (76%)	28 (24%)	0	2
31	DJ	116/116 (100%)	100 (86%)	16 (14%)	3	16
32	BK	103/103 (100%)	81 (79%)	22 (21%)	1	4
32	DK	103/103 (100%)	83 (81%)	20 (19%)	1	5
33	BL	102/102 (100%)	76 (74%)	26 (26%)	0	1
33	DL	102/102 (100%)	85 (83%)	17 (17%)	2	9
34	BM	109/109 (100%)	87 (80%)	22 (20%)	1	5
34	DM	109/109 (100%)	96 (88%)	13 (12%)	5	20
35	BN	100/100 (100%)	82 (82%)	18 (18%)	1	7
35	DN	100/100 (100%)	85 (85%)	15 (15%)	3	12
36	BO	86/86 (100%)	69 (80%)	17 (20%)	1	5
36	DO	86/86 (100%)	77 (90%)	9 (10%)	7	25
37	BP	99/99 (100%)	73 (74%)	26 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DP	99/99 (100%)	89 (90%)	10 (10%)	7	27
38	BQ	89/89 (100%)	71 (80%)	18 (20%)	1	5
38	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	9
39	BR	84/84 (100%)	70 (83%)	14 (17%)	2	9
39	DR	84/84 (100%)	71 (84%)	13 (16%)	2	11
40	BS	93/93 (100%)	74 (80%)	19 (20%)	1	4
40	DS	93/93 (100%)	79 (85%)	14 (15%)	3	12
41	BT	80/80 (100%)	61 (76%)	19 (24%)	0	2
41	DT	80/80 (100%)	73 (91%)	7 (9%)	10	33
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	4
42	DU	83/83 (100%)	74 (89%)	9 (11%)	6	24
43	BV	78/78 (100%)	59 (76%)	19 (24%)	0	2
43	DV	78/78 (100%)	68 (87%)	10 (13%)	4	18
44	BW	59/59 (100%)	41 (70%)	18 (30%)	0	1
44	DW	59/59 (100%)	42 (71%)	17 (29%)	0	1
45	BX	67/67 (100%)	54 (81%)	13 (19%)	1	5
45	DX	67/67 (100%)	58 (87%)	9 (13%)	4	16
46	BY	55/55 (100%)	41 (74%)	14 (26%)	0	1
46	DY	55/55 (100%)	52 (94%)	3 (6%)	21	52
47	BZ	48/48 (100%)	33 (69%)	15 (31%)	0	1
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	2	9
48	B0	47/47 (100%)	39 (83%)	8 (17%)	2	9
48	D0	47/47 (100%)	39 (83%)	8 (17%)	2	9
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	7
49	D1	45/45 (100%)	41 (91%)	4 (9%)	9	32
50	B2	38/38 (100%)	29 (76%)	9 (24%)	1	2
50	D2	38/38 (100%)	33 (87%)	5 (13%)	4	17
51	B3	51/51 (100%)	44 (86%)	7 (14%)	3	16
51	D3	51/51 (100%)	40 (78%)	11 (22%)	1	4
52	B4	34/34 (100%)	28 (82%)	6 (18%)	2	8
52	D4	34/34 (100%)	29 (85%)	5 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	CG	123/123 (100%)	102 (83%)	21 (17%)	2	9
55	CM	91/91 (100%)	80 (88%)	11 (12%)	5	20
56	CP	65/65 (100%)	57 (88%)	8 (12%)	4	20
58	DF	149/149 (100%)	123 (83%)	26 (17%)	2	8
All	All	9331/9339 (100%)	7786 (83%)	1545 (17%)	2	9

5 of 1545 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CC	183	TYR
19	CS	11	ASP
4	CD	160	LEU
3	CC	182	ASP
9	CI	37	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
19	CS	51	HIS
37	DP	74	GLN
24	DC	57	HIS
28	DG	44	HIS
41	DT	15	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	363 (23%)	63 (4%)
22	BA	2850/2903 (98%)	554 (19%)	87 (3%)
22	DA	2837/2903 (97%)	869 (30%)	183 (6%)
23	BB	117/118 (99%)	19 (16%)	0
53	CA	1529/1530 (99%)	445 (29%)	81 (5%)
57	DB	116/117 (99%)	33 (28%)	7 (6%)
All	All	8981/9104 (98%)	2283 (25%)	421 (4%)

5 of 2283 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A

5 of 421 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	DA	14	A
22	DA	800	A
22	DA	2667	C
22	DA	103	A
22	DA	389	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 363 ligands modelled in this entry, 362 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	$\# Z > 2$
60	TEL	BA	3135	-	59,62,62	2.30	11 (18%)	77,92,92	3.45	30 (38%)

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
60	TEL	BA	3135	-	1/1/19/19	10/73/108/108	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3135	TEL	O16-C10	10.86	1.37	1.21
60	BA	3135	TEL	C10-N6	8.50	1.51	1.35
60	BA	3135	TEL	O5-C10	4.45	1.42	1.35
60	BA	3135	TEL	O9-C4	-4.21	1.39	1.46
60	BA	3135	TEL	O45-C50	-3.39	1.38	1.44

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	3135	TEL	C3-N6-C10	-13.95	93.00	111.69
60	BA	3135	TEL	O5-C10-N6	-10.64	101.29	109.81
60	BA	3135	TEL	O5-C10-O16	-10.15	110.75	122.46
60	BA	3135	TEL	O16-C10-N6	-7.97	117.54	128.01
60	BA	3135	TEL	O5-C2-C3	-7.40	95.68	103.16

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
60	BA	3135	TEL	C3

5 of 10 torsion outliers are listed below:

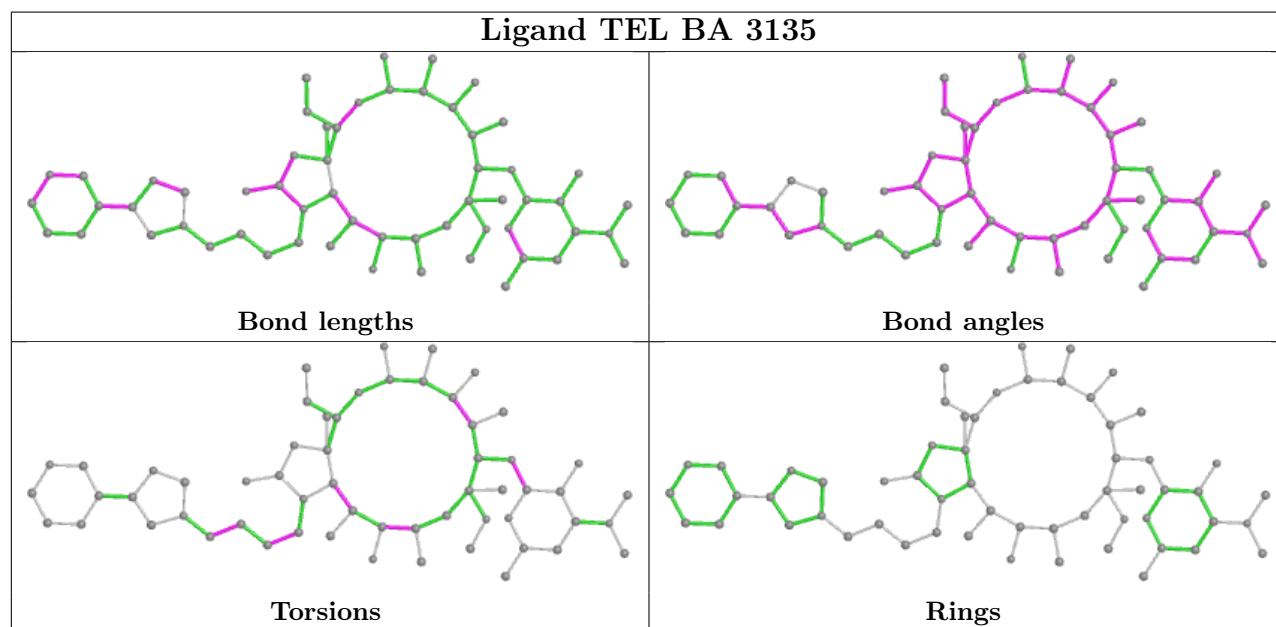
Mol	Chain	Res	Type	Atoms
60	BA	3135	TEL	C2-C3-C7-C12
60	BA	3135	TEL	C2-C3-C7-C13
60	BA	3135	TEL	O18-C13-C19-C23
60	BA	3135	TEL	N6-C11-C17-C22
60	BA	3135	TEL	C17-C22-C27-N31

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	3135	TEL	8	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.42	20 (1%) 77 75	31, 83, 185, 422	0
2	AB	218/218 (100%)	1.61	69 (31%) 0 0	67, 161, 222, 300	0
2	CB	218/218 (100%)	1.74	86 (39%) 0 0	76, 168, 231, 274	0
3	AC	206/206 (100%)	0.79	16 (7%) 13 12	53, 101, 156, 201	0
3	CC	206/206 (100%)	0.97	31 (15%) 2 2	76, 138, 202, 264	0
4	AD	205/205 (100%)	0.30	8 (3%) 39 36	48, 93, 168, 305	0
4	CD	205/205 (100%)	-0.16	1 (0%) 91 90	26, 60, 114, 257	0
5	AE	150/150 (100%)	0.14	2 (1%) 77 75	38, 76, 150, 231	0
5	CE	150/150 (100%)	0.24	2 (1%) 77 75	34, 85, 143, 282	0
6	AF	100/100 (100%)	0.20	4 (4%) 38 35	52, 100, 147, 188	0
6	CF	100/100 (100%)	0.25	4 (4%) 38 35	69, 109, 169, 214	0
7	AG	151/151 (100%)	0.67	16 (10%) 6 6	77, 131, 195, 217	0
8	AH	129/129 (100%)	0.37	5 (3%) 39 36	45, 82, 133, 191	0
8	CH	129/129 (100%)	0.66	13 (10%) 7 7	60, 101, 151, 212	0
9	AI	127/127 (100%)	1.06	25 (19%) 1 1	64, 137, 207, 266	0
9	CI	127/127 (100%)	1.51	39 (30%) 0 0	98, 168, 246, 283	0
10	AJ	98/98 (100%)	0.83	14 (14%) 2 2	65, 111, 196, 260	0
10	CJ	98/98 (100%)	2.69	50 (51%) 0 0	94, 178, 248, 272	0
11	AK	117/117 (100%)	0.91	20 (17%) 1 1	44, 108, 190, 238	0
11	CK	117/117 (100%)	0.78	14 (11%) 4 4	49, 112, 169, 192	0
12	AL	123/123 (100%)	-0.03	1 (0%) 86 86	24, 62, 106, 208	0
12	CL	123/123 (100%)	0.44	6 (4%) 29 27	37, 73, 124, 211	0
13	AM	114/114 (100%)	0.51	11 (9%) 8 8	86, 135, 206, 262	0
14	AN	96/100 (96%)	0.54	6 (6%) 20 19	58, 105, 187, 274	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	CN	95/100 (95%)	1.83	36 (37%) 0 0	95, 187, 280, 335	0
15	AO	88/88 (100%)	-0.21	1 (1%) 80 80	43, 81, 124, 170	0
15	CO	88/88 (100%)	0.16	2 (2%) 60 58	57, 107, 153, 265	0
16	AP	82/82 (100%)	0.77	12 (14%) 2 2	56, 80, 166, 241	0
17	AQ	80/80 (100%)	0.67	7 (8%) 10 10	44, 78, 145, 219	0
17	CQ	80/80 (100%)	1.01	11 (13%) 2 2	57, 106, 146, 163	0
18	AR	55/55 (100%)	0.42	5 (9%) 9 10	60, 88, 151, 212	0
18	CR	55/55 (100%)	0.05	0 100 100	55, 88, 179, 249	0
19	AS	79/79 (100%)	1.62	27 (34%) 0 0	96, 137, 193, 233	0
19	CS	79/79 (100%)	3.10	50 (63%) 0 0	183, 316, 391, 403	0
20	AT	85/85 (100%)	-0.02	1 (1%) 79 77	47, 84, 131, 157	0
20	CT	85/85 (100%)	1.30	19 (22%) 0 1	66, 115, 191, 210	0
21	AU	51/51 (100%)	2.20	29 (56%) 0 0	96, 152, 206, 217	0
21	CU	51/51 (100%)	0.78	6 (11%) 4 4	66, 117, 183, 253	0
22	BA	2854/2903 (98%)	-0.38	36 (1%) 77 75	5, 32, 160, 403	0
22	DA	2841/2903 (97%)	0.52	117 (4%) 37 34	53, 122, 250, 469	0
23	BB	118/118 (100%)	-0.41	0 100 100	13, 44, 74, 101	0
24	BC	271/271 (100%)	-0.15	9 (3%) 46 43	12, 42, 93, 209	0
24	DC	271/271 (100%)	0.72	24 (8%) 9 10	59, 93, 144, 185	0
25	BD	209/209 (100%)	-0.30	0 100 100	4, 26, 73, 178	0
25	DD	209/209 (100%)	1.17	39 (18%) 1 1	58, 109, 173, 246	0
26	BE	201/201 (100%)	-0.26	0 100 100	5, 43, 103, 156	0
26	DE	201/201 (100%)	2.12	84 (41%) 0 0	65, 192, 378, 459	0
27	BF	177/177 (100%)	0.48	19 (10%) 6 6	27, 75, 156, 242	0
28	BG	176/176 (100%)	0.15	4 (2%) 60 58	22, 62, 121, 186	0
28	DG	176/176 (100%)	1.79	70 (39%) 0 0	100, 185, 264, 328	0
29	BH	149/149 (100%)	3.03	69 (46%) 0 0	49, 179, 279, 375	0
29	DH	149/149 (100%)	2.64	67 (44%) 0 0	93, 184, 287, 326	0
30	BI	141/141 (100%)	2.93	78 (55%) 0 0	136, 253, 308, 367	0
30	DI	141/141 (100%)	3.80	106 (75%) 0 0	167, 294, 351, 377	0
31	BJ	142/142 (100%)	-0.43	0 100 100	7, 23, 64, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
31	DJ	142/142 (100%)	1.14	32 (22%) 0 1	52, 106, 159, 195	0
32	BK	122/122 (100%)	-0.26	0 100 100	10, 31, 80, 254	0
32	DK	122/122 (100%)	1.23	27 (22%) 0 1	57, 91, 150, 229	0
33	BL	143/143 (100%)	-0.24	0 100 100	7, 38, 74, 111	0
33	DL	143/143 (100%)	1.35	37 (25%) 0 0	69, 149, 262, 337	0
34	BM	136/136 (100%)	-0.34	0 100 100	6, 29, 76, 120	0
34	DM	136/136 (100%)	0.99	27 (19%) 1 1	46, 107, 161, 204	0
35	BN	120/120 (100%)	-0.49	0 100 100	9, 25, 46, 155	0
35	DN	120/120 (100%)	1.39	32 (26%) 0 0	73, 124, 194, 293	0
36	BO	116/116 (100%)	-0.02	0 100 100	24, 44, 83, 116	0
36	DO	116/116 (100%)	1.73	44 (37%) 0 0	113, 162, 224, 259	0
37	BP	114/114 (100%)	-0.13	1 (0%) 84 84	11, 41, 104, 161	0
37	DP	114/114 (100%)	0.98	18 (15%) 2 2	63, 105, 164, 195	0
38	BQ	117/117 (100%)	-0.52	1 (0%) 84 84	4, 20, 47, 206	0
38	DQ	117/117 (100%)	1.58	35 (29%) 0 0	67, 108, 191, 312	0
39	BR	103/103 (100%)	-0.35	1 (0%) 82 82	5, 30, 80, 109	0
39	DR	103/103 (100%)	2.45	54 (52%) 0 0	80, 138, 239, 291	0
40	BS	110/110 (100%)	-0.41	1 (0%) 84 84	6, 21, 61, 178	0
40	DS	110/110 (100%)	2.29	55 (50%) 0 0	70, 133, 241, 285	0
41	BT	93/93 (100%)	0.19	4 (4%) 35 33	23, 51, 121, 235	0
41	DT	93/93 (100%)	2.69	52 (55%) 0 0	110, 202, 299, 369	0
42	BU	102/102 (100%)	0.08	3 (2%) 51 50	19, 55, 136, 246	0
42	DU	102/102 (100%)	3.23	64 (62%) 0 0	122, 287, 418, 543	0
43	BV	94/94 (100%)	-0.05	0 100 100	13, 43, 85, 124	0
43	DV	94/94 (100%)	1.67	31 (32%) 0 0	100, 144, 196, 226	0
44	BW	79/79 (100%)	0.14	4 (5%) 28 26	10, 36, 110, 208	0
44	DW	79/79 (100%)	2.30	41 (51%) 0 0	87, 141, 230, 253	0
45	BX	77/77 (100%)	-0.25	0 100 100	15, 46, 88, 135	0
45	DX	77/77 (100%)	1.17	16 (20%) 1 1	67, 118, 172, 239	0
46	BY	63/63 (100%)	0.12	2 (3%) 47 45	34, 75, 134, 210	0
46	DY	63/63 (100%)	1.55	17 (26%) 0 0	130, 305, 419, 450	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	BZ	58/58 (100%)	-0.31	0 100 100	6, 24, 74, 116	0
47	DZ	58/58 (100%)	0.96	8 (13%) 2 2	86, 123, 190, 236	0
48	B0	56/56 (100%)	-0.56	0 100 100	3, 22, 75, 168	0
48	D0	56/56 (100%)	1.58	15 (26%) 0 0	66, 132, 242, 278	0
49	B1	50/50 (100%)	0.34	2 (4%) 38 35	30, 50, 98, 178	0
49	D1	50/50 (100%)	1.77	21 (42%) 0 0	98, 155, 211, 275	0
50	B2	46/46 (100%)	-0.47	0 100 100	13, 27, 51, 183	0
50	D2	46/46 (100%)	1.40	11 (23%) 0 0	78, 118, 155, 203	0
51	B3	64/64 (100%)	-0.31	0 100 100	9, 27, 46, 71	0
51	D3	64/64 (100%)	1.92	30 (46%) 0 0	90, 125, 198, 250	0
52	B4	38/38 (100%)	0.34	1 (2%) 56 52	28, 49, 87, 112	0
52	D4	38/38 (100%)	2.88	26 (68%) 0 0	78, 141, 210, 225	0
53	CA	1530/1530 (100%)	0.04	36 (2%) 59 55	38, 100, 272, 376	0
54	CG	150/150 (100%)	2.29	65 (43%) 0 0	118, 209, 283, 333	0
55	CM	113/113 (100%)	2.30	57 (50%) 0 0	196, 344, 437, 471	0
56	CP	80/80 (100%)	0.91	12 (15%) 2 2	59, 91, 145, 249	0
57	DB	117/117 (100%)	0.12	0 100 100	95, 167, 229, 249	0
58	DF	178/178 (100%)	2.30	98 (55%) 0 0	135, 220, 279, 350	0
All	All	20431/20551 (99%)	0.51	2372 (11%) 4 4	3, 97, 258, 543	0

The worst 5 of 2372 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	CS	29	PRO	18.4
29	DH	124	THR	17.9
29	DH	91	PHE	17.5
29	BH	118	PRO	15.2
29	DH	105	ALA	15.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
59	MG	DJ	201	1/1	-0.24	1.05	312,312,312,312	0
59	MG	DA	3002	1/1	-0.04	0.64	225,225,225,225	0
59	MG	DA	3005	1/1	-0.03	0.50	284,284,284,284	0
59	MG	DA	3016	1/1	0.07	1.14	214,214,214,214	0
59	MG	DA	3074	1/1	0.10	0.96	247,247,247,247	0
59	MG	DA	3018	1/1	0.16	0.17	125,125,125,125	0
59	MG	DA	3092	1/1	0.25	0.25	119,119,119,119	0
59	MG	DA	3091	1/1	0.30	0.37	154,154,154,154	0
59	MG	DA	3111	1/1	0.35	0.19	179,179,179,179	0
59	MG	DA	3004	1/1	0.35	0.17	122,122,122,122	0
59	MG	DA	3063	1/1	0.37	2.20	213,213,213,213	0
59	MG	DA	3130	1/1	0.41	3.18	280,280,280,280	0
59	MG	DA	3060	1/1	0.41	0.61	198,198,198,198	0
59	MG	DA	3133	1/1	0.43	0.38	198,198,198,198	0
59	MG	DA	3020	1/1	0.44	0.63	240,240,240,240	0
59	MG	CA	1618	1/1	0.45	0.30	146,146,146,146	0
59	MG	DA	3106	1/1	0.45	0.74	316,316,316,316	0
59	MG	DA	3039	1/1	0.45	0.17	79,79,79,79	0
59	MG	DA	3043	1/1	0.47	0.28	179,179,179,179	0
59	MG	DA	3110	1/1	0.48	0.38	146,146,146,146	0
59	MG	DA	3109	1/1	0.49	0.48	184,184,184,184	0
59	MG	DA	3045	1/1	0.50	0.25	160,160,160,160	0
59	MG	DA	3027	1/1	0.51	0.27	157,157,157,157	0
59	MG	DA	3047	1/1	0.51	0.21	142,142,142,142	0
59	MG	DA	3129	1/1	0.52	0.53	210,210,210,210	0
59	MG	CA	1619	1/1	0.53	0.34	210,210,210,210	0
59	MG	DA	3028	1/1	0.54	0.63	222,222,222,222	0
59	MG	DA	3084	1/1	0.55	0.17	201,201,201,201	0
59	MG	DA	3007	1/1	0.56	0.62	248,248,248,248	0
59	MG	DA	3090	1/1	0.56	0.11	78,78,78,78	0
59	MG	CA	1628	1/1	0.56	0.16	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	DA	3022	1/1	0.56	0.37	173,173,173,173	0
59	MG	DA	3097	1/1	0.57	0.39	137,137,137,137	0
59	MG	DA	3049	1/1	0.58	0.63	192,192,192,192	0
59	MG	DA	3127	1/1	0.58	0.87	228,228,228,228	0
59	MG	DA	3024	1/1	0.58	0.20	100,100,100,100	0
59	MG	AA	1629	1/1	0.59	0.11	84,84,84,84	0
59	MG	DA	3077	1/1	0.59	0.19	123,123,123,123	0
59	MG	DA	3120	1/1	0.60	0.20	91,91,91,91	0
59	MG	CA	1603	1/1	0.60	0.34	177,177,177,177	0
59	MG	DA	3019	1/1	0.61	0.18	192,192,192,192	0
59	MG	CA	1617	1/1	0.61	0.12	214,214,214,214	0
59	MG	DA	3026	1/1	0.62	0.91	258,258,258,258	0
59	MG	DA	3132	1/1	0.62	0.87	185,185,185,185	0
59	MG	DA	3015	1/1	0.63	0.74	176,176,176,176	0
59	MG	DA	3083	1/1	0.63	0.29	204,204,204,204	0
59	MG	DA	3010	1/1	0.63	0.57	195,195,195,195	0
59	MG	DA	3003	1/1	0.65	0.82	229,229,229,229	0
59	MG	DA	3079	1/1	0.66	0.89	200,200,200,200	0
59	MG	DA	3064	1/1	0.66	0.66	280,280,280,280	0
59	MG	DA	3014	1/1	0.66	0.37	133,133,133,133	0
59	MG	DA	3099	1/1	0.66	0.19	164,164,164,164	0
59	MG	DA	3001	1/1	0.66	0.09	149,149,149,149	0
59	MG	DA	3038	1/1	0.67	0.12	203,203,203,203	0
59	MG	DA	3082	1/1	0.67	0.19	132,132,132,132	0
59	MG	DA	3126	1/1	0.67	0.24	112,112,112,112	0
59	MG	DA	3088	1/1	0.68	0.17	170,170,170,170	0
59	MG	DA	3125	1/1	0.68	0.36	152,152,152,152	0
59	MG	AA	1616	1/1	0.68	0.14	106,106,106,106	0
59	MG	DA	3078	1/1	0.69	0.24	182,182,182,182	0
59	MG	CA	1615	1/1	0.70	0.30	170,170,170,170	0
59	MG	CA	1613	1/1	0.70	0.15	107,107,107,107	0
59	MG	DA	3006	1/1	0.70	0.10	176,176,176,176	0
59	MG	DA	3089	1/1	0.71	0.18	100,100,100,100	0
59	MG	DA	3123	1/1	0.71	0.30	183,183,183,183	0
59	MG	DA	3058	1/1	0.71	0.32	202,202,202,202	0
59	MG	BA	3117	1/1	0.71	0.26	173,173,173,173	0
59	MG	DA	3102	1/1	0.71	0.21	87,87,87,87	0
59	MG	DA	3062	1/1	0.72	0.56	213,213,213,213	0
59	MG	DA	3050	1/1	0.72	0.28	160,160,160,160	0
59	MG	CA	1610	1/1	0.72	0.06	151,151,151,151	0
59	MG	DA	3032	1/1	0.72	0.19	131,131,131,131	0
59	MG	CA	1620	1/1	0.73	0.15	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3044	1/1	0.73	0.17	92,92,92,92	0
59	MG	DA	3086	1/1	0.73	0.39	84,84,84,84	0
59	MG	DA	3098	1/1	0.73	0.33	151,151,151,151	0
59	MG	DA	3011	1/1	0.74	0.39	145,145,145,145	0
59	MG	DA	3008	1/1	0.74	0.17	112,112,112,112	0
59	MG	DA	3030	1/1	0.74	0.31	104,104,104,104	0
59	MG	DA	3071	1/1	0.75	0.18	74,74,74,74	0
59	MG	AA	1627	1/1	0.75	0.37	137,137,137,137	0
59	MG	DA	3035	1/1	0.75	0.14	79,79,79,79	0
59	MG	CA	1637	1/1	0.75	0.11	170,170,170,170	0
59	MG	DA	3041	1/1	0.76	0.15	110,110,110,110	0
59	MG	DA	3087	1/1	0.76	0.28	152,152,152,152	0
59	MG	DA	3059	1/1	0.76	0.39	197,197,197,197	0
59	MG	DA	3113	1/1	0.76	0.12	121,121,121,121	0
59	MG	DA	3116	1/1	0.76	0.12	54,54,54,54	0
59	MG	DA	3056	1/1	0.77	0.18	72,72,72,72	0
59	MG	DA	3033	1/1	0.77	0.32	132,132,132,132	0
59	MG	AA	1619	1/1	0.77	0.69	209,209,209,209	0
59	MG	DA	3036	1/1	0.77	0.58	222,222,222,222	0
59	MG	BA	3068	1/1	0.77	0.09	151,151,151,151	0
59	MG	DA	3053	1/1	0.77	0.25	98,98,98,98	0
61	ZN	D4	101	1/1	0.77	0.10	157,157,157,157	0
59	MG	DA	3040	1/1	0.78	0.15	65,65,65,65	0
59	MG	DA	3072	1/1	0.78	0.16	131,131,131,131	0
59	MG	DA	3104	1/1	0.78	0.16	33,33,33,33	0
59	MG	DA	3021	1/1	0.78	0.15	83,83,83,83	0
59	MG	AA	1626	1/1	0.79	0.10	52,52,52,52	0
59	MG	CA	1601	1/1	0.79	0.10	120,120,120,120	0
59	MG	DC	301	1/1	0.79	0.25	155,155,155,155	0
59	MG	AA	1617	1/1	0.79	0.16	147,147,147,147	0
59	MG	DA	3037	1/1	0.79	0.11	97,97,97,97	0
59	MG	DA	3115	1/1	0.80	0.21	126,126,126,126	0
59	MG	AA	1603	1/1	0.80	0.14	131,131,131,131	0
59	MG	CA	1623	1/1	0.80	0.17	121,121,121,121	0
59	MG	CA	1608	1/1	0.80	0.17	44,44,44,44	0
59	MG	BA	3007	1/1	0.80	0.15	104,104,104,104	0
59	MG	BA	3018	1/1	0.80	0.14	44,44,44,44	0
59	MG	DA	3048	1/1	0.80	0.15	95,95,95,95	0
59	MG	CA	1626	1/1	0.81	0.40	196,196,196,196	0
59	MG	CA	1607	1/1	0.81	0.23	134,134,134,134	0
59	MG	DA	3067	1/1	0.81	0.21	64,64,64,64	0
59	MG	CA	1602	1/1	0.81	0.16	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	CA	1614	1/1	0.81	0.71	245,245,245,245	0
59	MG	DA	3108	1/1	0.81	0.67	212,212,212,212	0
59	MG	DA	3017	1/1	0.82	0.13	51,51,51,51	0
59	MG	CA	1612	1/1	0.82	0.41	113,113,113,113	0
59	MG	DB	201	1/1	0.82	0.10	88,88,88,88	0
59	MG	AA	1623	1/1	0.82	0.12	89,89,89,89	0
59	MG	DA	3031	1/1	0.82	0.18	76,76,76,76	0
59	MG	CA	1616	1/1	0.82	0.39	203,203,203,203	0
59	MG	DA	3124	1/1	0.83	0.18	70,70,70,70	0
59	MG	DA	3096	1/1	0.83	0.14	93,93,93,93	0
59	MG	BA	3089	1/1	0.83	0.13	95,95,95,95	0
59	MG	DA	3013	1/1	0.83	0.38	189,189,189,189	0
59	MG	DA	3122	1/1	0.83	0.15	94,94,94,94	0
59	MG	DA	3095	1/1	0.83	0.20	122,122,122,122	0
59	MG	AA	1630	1/1	0.84	0.37	189,189,189,189	0
59	MG	DA	3094	1/1	0.84	0.26	134,134,134,134	0
59	MG	DA	3076	1/1	0.84	0.25	149,149,149,149	0
59	MG	CE	201	1/1	0.84	0.27	132,132,132,132	0
59	MG	AA	1638	1/1	0.84	0.17	47,47,47,47	0
59	MG	DA	3069	1/1	0.84	0.57	233,233,233,233	0
59	MG	BA	3021	1/1	0.84	0.34	158,158,158,158	0
59	MG	CA	1635	1/1	0.84	0.14	201,201,201,201	0
59	MG	DA	3070	1/1	0.85	0.13	60,60,60,60	0
59	MG	CA	1625	1/1	0.85	0.17	48,48,48,48	0
59	MG	DA	3118	1/1	0.85	0.10	59,59,59,59	0
59	MG	BA	3085	1/1	0.85	0.20	124,124,124,124	0
59	MG	AA	1602	1/1	0.85	0.12	152,152,152,152	0
59	MG	AA	1639	1/1	0.85	0.12	109,109,109,109	0
59	MG	DA	3055	1/1	0.85	0.11	72,72,72,72	0
59	MG	DA	3046	1/1	0.85	0.24	125,125,125,125	0
59	MG	BB	201	1/1	0.85	0.28	228,228,228,228	0
59	MG	BA	3057	1/1	0.86	0.14	147,147,147,147	0
59	MG	DA	3128	1/1	0.86	0.31	116,116,116,116	0
59	MG	CA	1636	1/1	0.87	0.30	119,119,119,119	0
59	MG	BA	3004	1/1	0.87	0.24	156,156,156,156	0
59	MG	BA	3045	1/1	0.87	0.14	30,30,30,30	0
59	MG	DA	3042	1/1	0.87	0.20	99,99,99,99	0
59	MG	AA	1625	1/1	0.87	0.08	64,64,64,64	0
59	MG	BA	3003	1/1	0.87	0.10	58,58,58,58	0
59	MG	DA	3051	1/1	0.87	0.15	91,91,91,91	0
59	MG	DA	3073	1/1	0.87	0.08	148,148,148,148	0
59	MG	BA	3059	1/1	0.88	0.33	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1637	1/1	0.88	0.12	96,96,96,96	0
59	MG	DA	3121	1/1	0.88	0.13	122,122,122,122	0
59	MG	CA	1627	1/1	0.88	1.25	237,237,237,237	0
59	MG	DA	3075	1/1	0.88	0.41	172,172,172,172	0
59	MG	DA	3100	1/1	0.88	0.33	105,105,105,105	0
59	MG	CA	1631	1/1	0.89	0.10	160,160,160,160	0
59	MG	DA	3057	1/1	0.89	0.54	185,185,185,185	0
59	MG	BA	3025	1/1	0.89	0.56	165,165,165,165	0
59	MG	BA	3090	1/1	0.89	0.14	120,120,120,120	0
59	MG	BA	3055	1/1	0.89	0.35	215,215,215,215	0
59	MG	DA	3061	1/1	0.89	0.12	131,131,131,131	0
59	MG	DA	3085	1/1	0.89	0.44	132,132,132,132	0
59	MG	BB	202	1/1	0.90	0.06	64,64,64,64	0
59	MG	DA	3012	1/1	0.90	0.21	41,41,41,41	0
59	MG	AA	1628	1/1	0.90	0.35	136,136,136,136	0
59	MG	BA	3031	1/1	0.90	0.11	26,26,26,26	0
59	MG	AA	1614	1/1	0.90	0.17	156,156,156,156	0
59	MG	DA	3117	1/1	0.90	0.20	73,73,73,73	0
59	MG	CA	1606	1/1	0.90	0.16	54,54,54,54	0
59	MG	DA	3103	1/1	0.90	0.17	76,76,76,76	0
59	MG	DA	3081	1/1	0.90	0.28	78,78,78,78	0
59	MG	CA	1638	1/1	0.90	0.09	141,141,141,141	0
59	MG	BA	3131	1/1	0.90	0.40	184,184,184,184	0
59	MG	BA	3005	1/1	0.90	0.11	75,75,75,75	0
59	MG	BA	3070	1/1	0.91	0.21	135,135,135,135	0
59	MG	AA	1607	1/1	0.91	0.07	105,105,105,105	0
59	MG	DA	3009	1/1	0.91	0.14	100,100,100,100	0
59	MG	AA	1621	1/1	0.91	0.17	143,143,143,143	0
59	MG	BA	3034	1/1	0.91	0.28	197,197,197,197	0
59	MG	CA	1611	1/1	0.91	0.19	111,111,111,111	0
59	MG	CA	1629	1/1	0.91	0.24	126,126,126,126	0
59	MG	BA	3103	1/1	0.91	0.17	21,21,21,21	0
59	MG	DA	3119	1/1	0.91	0.11	67,67,67,67	0
59	MG	AA	1641	1/1	0.91	0.23	148,148,148,148	0
59	MG	CA	1621	1/1	0.91	0.18	50,50,50,50	0
59	MG	DC	302	1/1	0.91	0.31	159,159,159,159	0
59	MG	DA	3029	1/1	0.91	0.94	142,142,142,142	0
59	MG	DA	3080	1/1	0.91	0.11	152,152,152,152	0
59	MG	BA	3023	1/1	0.92	0.10	16,16,16,16	0
59	MG	AA	1620	1/1	0.92	0.10	126,126,126,126	0
59	MG	DA	3112	1/1	0.92	0.14	80,80,80,80	0
59	MG	BA	3028	1/1	0.92	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	DA	3114	1/1	0.92	0.10	147,147,147,147	0
59	MG	BA	3108	1/1	0.92	0.09	83,83,83,83	0
59	MG	DA	3052	1/1	0.92	0.12	56,56,56,56	0
59	MG	DA	3023	1/1	0.92	0.14	111,111,111,111	0
59	MG	CA	1639	1/1	0.92	0.22	161,161,161,161	0
59	MG	DA	3068	1/1	0.92	0.16	67,67,67,67	0
59	MG	BA	3114	1/1	0.92	0.15	8,8,8,8	0
59	MG	BA	3115	1/1	0.92	0.10	7,7,7,7	0
59	MG	DA	3093	1/1	0.92	0.17	234,234,234,234	0
59	MG	BA	3010	1/1	0.92	0.07	17,17,17,17	0
59	MG	BA	3067	1/1	0.93	0.12	17,17,17,17	0
59	MG	DA	3065	1/1	0.93	0.17	77,77,77,77	0
59	MG	BB	204	1/1	0.93	0.08	23,23,23,23	0
59	MG	BA	3077	1/1	0.93	0.13	38,38,38,38	0
59	MG	CA	1633	1/1	0.93	0.14	138,138,138,138	0
59	MG	BA	3118	1/1	0.93	0.14	23,23,23,23	0
59	MG	DA	3131	1/1	0.93	0.17	91,91,91,91	0
59	MG	DA	3105	1/1	0.93	0.20	61,61,61,61	0
59	MG	CA	1622	1/1	0.93	0.13	190,190,190,190	0
59	MG	DA	3107	1/1	0.93	0.24	91,91,91,91	0
59	MG	BA	3129	1/1	0.93	1.07	243,243,243,243	0
59	MG	BA	3001	1/1	0.93	0.09	117,117,117,117	0
59	MG	BA	3134	1/1	0.93	0.36	196,196,196,196	0
59	MG	BA	3069	1/1	0.93	0.25	136,136,136,136	0
59	MG	BA	3127	1/1	0.94	0.14	2,2,2,2	0
59	MG	BA	3073	1/1	0.94	0.17	17,17,17,17	0
59	MG	BA	3074	1/1	0.94	0.17	85,85,85,85	0
59	MG	BA	3133	1/1	0.94	0.26	146,146,146,146	0
59	MG	BA	3076	1/1	0.94	0.10	119,119,119,119	0
59	MG	BA	3047	1/1	0.94	0.09	151,151,151,151	0
59	MG	BA	3078	1/1	0.94	0.20	31,31,31,31	0
59	MG	BB	203	1/1	0.94	0.11	34,34,34,34	0
59	MG	DA	3101	1/1	0.94	0.13	75,75,75,75	0
59	MG	BA	3081	1/1	0.94	0.18	92,92,92,92	0
59	MG	BA	3048	1/1	0.94	0.17	101,101,101,101	0
59	MG	BA	3088	1/1	0.94	0.10	62,62,62,62	0
59	MG	AA	1618	1/1	0.94	0.18	87,87,87,87	0
59	MG	BA	3024	1/1	0.94	0.12	18,18,18,18	0
59	MG	CA	1630	1/1	0.94	0.27	126,126,126,126	0
59	MG	AA	1624	1/1	0.94	0.15	102,102,102,102	0
59	MG	BA	3060	1/1	0.94	0.30	188,188,188,188	0
59	MG	AA	1631	1/1	0.94	0.17	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1633	1/1	0.94	0.10	62,62,62,62	0
59	MG	AA	1635	1/1	0.94	0.14	73,73,73,73	0
59	MG	AA	1636	1/1	0.94	0.32	199,199,199,199	0
59	MG	BA	3121	1/1	0.94	0.13	35,35,35,35	0
59	MG	BA	3122	1/1	0.94	0.71	155,155,155,155	0
59	MG	BA	3095	1/1	0.95	0.19	117,117,117,117	0
59	MG	CA	1634	1/1	0.95	0.09	74,74,74,74	0
59	MG	CA	1604	1/1	0.95	0.05	57,57,57,57	0
59	MG	BA	3097	1/1	0.95	0.10	33,33,33,33	0
59	MG	BA	3101	1/1	0.95	0.09	18,18,18,18	0
59	MG	BA	3063	1/1	0.95	0.13	12,12,12,12	0
59	MG	AA	1610	1/1	0.95	0.11	201,201,201,201	0
59	MG	CA	1641	1/1	0.95	0.12	82,82,82,82	0
59	MG	BA	3110	1/1	0.95	0.16	89,89,89,89	0
59	MG	BA	3033	1/1	0.95	0.21	14,14,14,14	0
59	MG	AA	1640	1/1	0.95	0.04	84,84,84,84	0
59	MG	BA	3036	1/1	0.95	0.34	187,187,187,187	0
59	MG	BA	3071	1/1	0.95	0.11	7,7,7,7	0
59	MG	DA	3034	1/1	0.95	0.17	78,78,78,78	0
59	MG	BA	3037	1/1	0.95	0.17	24,24,24,24	0
59	MG	BA	3017	1/1	0.95	0.11	33,33,33,33	0
59	MG	BA	3124	1/1	0.95	0.14	33,33,33,33	0
59	MG	BA	3046	1/1	0.95	0.08	12,12,12,12	0
59	MG	AA	1612	1/1	0.95	0.10	85,85,85,85	0
59	MG	AA	1643	1/1	0.95	0.12	43,43,43,43	0
59	MG	BA	3132	1/1	0.95	0.13	1,1,1,1	0
59	MG	AA	1613	1/1	0.95	0.08	50,50,50,50	0
59	MG	BA	3083	1/1	0.95	0.17	37,37,37,37	0
59	MG	AA	1605	1/1	0.95	0.12	52,52,52,52	0
59	MG	BA	3086	1/1	0.95	0.12	134,134,134,134	0
59	MG	AA	1604	1/1	0.95	0.09	121,121,121,121	0
59	MG	AA	1609	1/1	0.95	0.12	54,54,54,54	0
59	MG	BA	3062	1/1	0.95	0.18	5,5,5,5	0
59	MG	BA	3091	1/1	0.95	0.07	49,49,49,49	0
59	MG	BA	3011	1/1	0.96	0.21	126,126,126,126	0
59	MG	BA	3032	1/1	0.96	0.12	25,25,25,25	0
59	MG	DA	3066	1/1	0.96	0.14	61,61,61,61	0
59	MG	BA	3015	1/1	0.96	0.17	95,95,95,95	0
59	MG	BA	3016	1/1	0.96	0.09	4,4,4,4	0
59	MG	AA	1615	1/1	0.96	0.10	128,128,128,128	0
59	MG	AA	1632	1/1	0.96	0.07	90,90,90,90	0
59	MG	CA	1640	1/1	0.96	0.16	80,80,80,80	0

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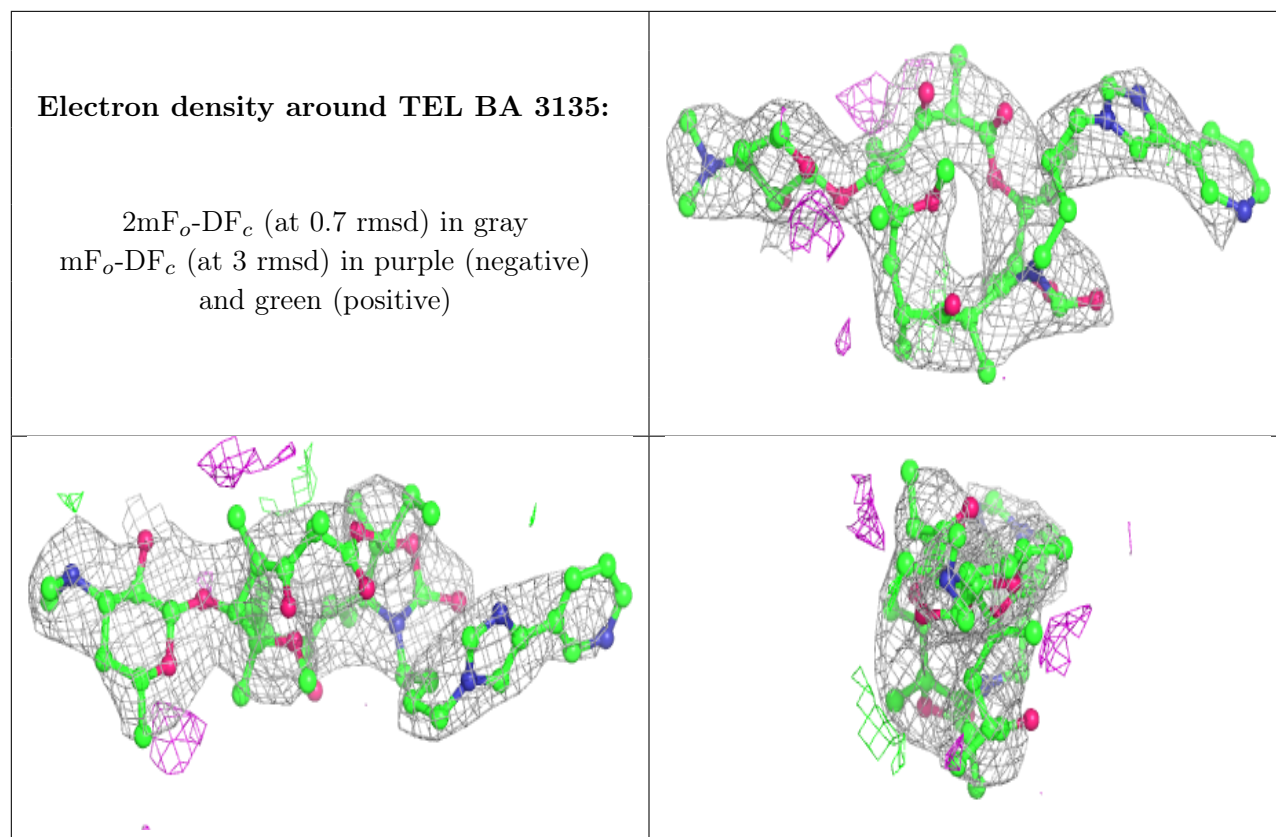
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3043	1/1	0.96	0.06	18,18,18,18	0
59	MG	BA	3092	1/1	0.96	0.07	70,70,70,70	0
59	MG	AA	1601	1/1	0.96	0.10	77,77,77,77	0
59	MG	DA	3025	1/1	0.96	0.18	104,104,104,104	0
59	MG	BA	3096	1/1	0.96	0.14	93,93,93,93	0
59	MG	BA	3022	1/1	0.96	0.16	5,5,5,5	0
59	MG	AA	1606	1/1	0.96	0.08	72,72,72,72	0
59	MG	BA	3102	1/1	0.96	0.21	9,9,9,9	0
59	MG	BA	3008	1/1	0.96	0.16	12,12,12,12	0
59	MG	BA	3106	1/1	0.96	0.22	5,5,5,5	0
59	MG	BA	3049	1/1	0.96	0.13	6,6,6,6	0
59	MG	BA	3109	1/1	0.96	0.16	112,112,112,112	0
59	MG	BA	3051	1/1	0.96	0.17	24,24,24,24	0
59	MG	BA	3113	1/1	0.96	0.09	138,138,138,138	0
59	MG	BA	3009	1/1	0.96	0.17	38,38,38,38	0
59	MG	BA	3002	1/1	0.96	0.10	85,85,85,85	0
61	ZN	B4	101	1/1	0.96	0.07	118,118,118,118	0
59	MG	BA	3116	1/1	0.96	0.14	71,71,71,71	0
59	MG	BA	3027	1/1	0.97	0.17	119,119,119,119	0
59	MG	BA	3056	1/1	0.97	0.31	219,219,219,219	0
59	MG	BA	3012	1/1	0.97	0.13	1,1,1,1	0
59	MG	BA	3111	1/1	0.97	0.15	38,38,38,38	0
59	MG	BA	3058	1/1	0.97	0.04	47,47,47,47	0
59	MG	BA	3035	1/1	0.97	0.10	5,5,5,5	0
59	MG	BA	3072	1/1	0.97	0.21	97,97,97,97	0
59	MG	CA	1624	1/1	0.97	0.26	128,128,128,128	0
59	MG	BA	3029	1/1	0.97	0.10	52,52,52,52	0
59	MG	BA	3061	1/1	0.97	0.17	11,11,11,11	0
59	MG	DA	3054	1/1	0.97	0.14	70,70,70,70	0
59	MG	BA	3075	1/1	0.97	0.06	26,26,26,26	0
59	MG	BA	3119	1/1	0.97	0.07	47,47,47,47	0
59	MG	BA	3120	1/1	0.97	0.21	3,3,3,3	0
59	MG	AA	1634	1/1	0.97	0.08	62,62,62,62	0
59	MG	CA	1609	1/1	0.97	0.12	97,97,97,97	0
59	MG	CA	1632	1/1	0.97	0.09	65,65,65,65	0
59	MG	BA	3098	1/1	0.97	0.13	26,26,26,26	0
59	MG	BA	3026	1/1	0.97	0.08	32,32,32,32	0
59	MG	BA	3064	1/1	0.97	0.13	5,5,5,5	0
59	MG	BA	3065	1/1	0.97	0.11	20,20,20,20	0
59	MG	BA	3130	1/1	0.97	0.14	108,108,108,108	0
60	TEL	BA	3135	58/58	0.97	0.22	0,23,68,74	0
59	MG	BA	3066	1/1	0.97	0.10	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3107	1/1	0.97	0.16	12,12,12,12	0
59	MG	BA	3052	1/1	0.98	0.16	46,46,46,46	0
59	MG	BA	3126	1/1	0.98	0.15	18,18,18,18	0
59	MG	BA	3100	1/1	0.98	0.13	85,85,85,85	0
59	MG	BA	3128	1/1	0.98	0.12	15,15,15,15	0
59	MG	BA	3079	1/1	0.98	0.17	11,11,11,11	0
59	MG	BA	3080	1/1	0.98	0.04	26,26,26,26	0
59	MG	BA	3053	1/1	0.98	0.15	6,6,6,6	0
59	MG	BA	3104	1/1	0.98	0.16	13,13,13,13	0
59	MG	BA	3105	1/1	0.98	0.17	27,27,27,27	0
59	MG	BA	3082	1/1	0.98	0.11	109,109,109,109	0
59	MG	BA	3054	1/1	0.98	0.09	58,58,58,58	0
59	MG	BA	3084	1/1	0.98	0.16	3,3,3,3	0
59	MG	BA	3040	1/1	0.98	0.18	13,13,13,13	0
59	MG	BA	3041	1/1	0.98	0.17	21,21,21,21	0
59	MG	BA	3087	1/1	0.98	0.12	36,36,36,36	0
59	MG	BA	3112	1/1	0.98	0.09	41,41,41,41	0
59	MG	BA	3006	1/1	0.98	0.07	31,31,31,31	0
59	MG	AA	1611	1/1	0.98	0.07	60,60,60,60	0
59	MG	CA	1605	1/1	0.98	0.14	32,32,32,32	0
59	MG	AA	1608	1/1	0.98	0.22	47,47,47,47	0
59	MG	BA	3013	1/1	0.98	0.19	1,1,1,1	0
59	MG	BA	3014	1/1	0.98	0.21	44,44,44,44	0
59	MG	BA	3093	1/1	0.98	0.07	35,35,35,35	0
59	MG	BA	3094	1/1	0.98	0.06	22,22,22,22	0
59	MG	AA	1642	1/1	0.98	0.14	36,36,36,36	0
59	MG	BA	3050	1/1	0.98	0.09	33,33,33,33	0
59	MG	BA	3030	1/1	0.98	0.17	9,9,9,9	0
59	MG	BA	3123	1/1	0.98	0.14	11,11,11,11	0
59	MG	BA	3039	1/1	0.99	0.16	8,8,8,8	0
59	MG	BA	3019	1/1	0.99	0.18	13,13,13,13	0
59	MG	AA	1622	1/1	0.99	0.19	40,40,40,40	0
59	MG	BA	3042	1/1	0.99	0.11	16,16,16,16	0
59	MG	BA	3125	1/1	0.99	0.14	16,16,16,16	0
59	MG	BA	3038	1/1	0.99	0.10	12,12,12,12	0
59	MG	BA	3044	1/1	0.99	0.06	43,43,43,43	0
59	MG	BA	3099	1/1	0.99	0.20	8,8,8,8	0
59	MG	BA	3020	1/1	1.00	0.12	11,11,11,11	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.