



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 18, 2021 – 07:14 PM EST

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 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 : 2.16
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) : 2.16

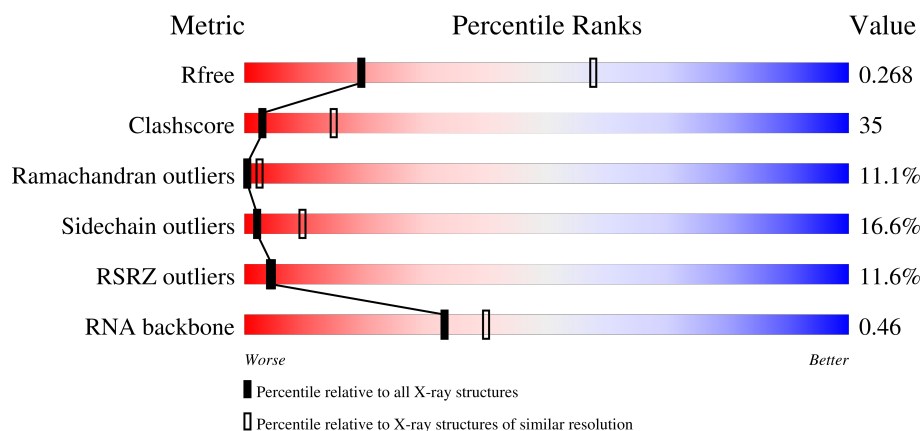
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	

Continued on next page...

Continued from previous page...

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	




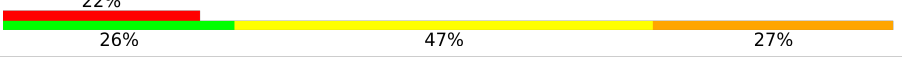
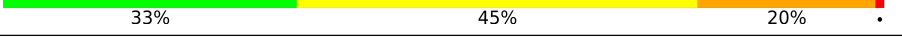
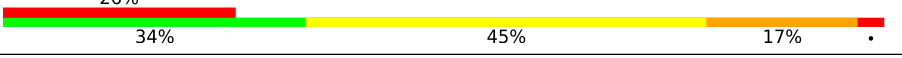
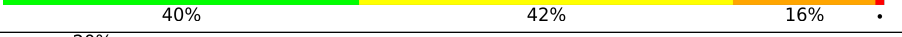
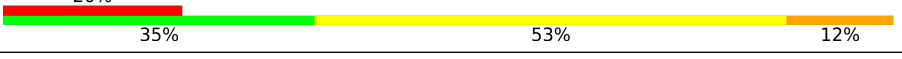
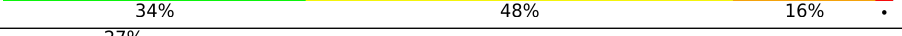
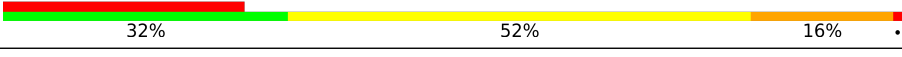
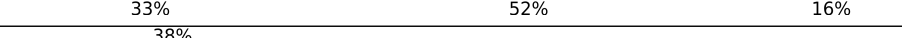
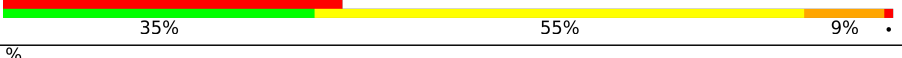
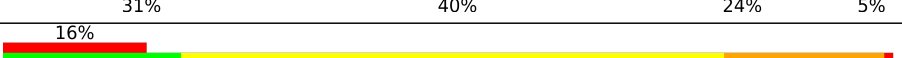
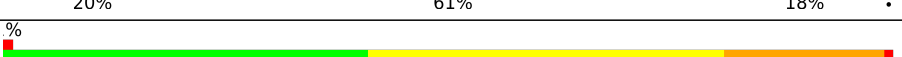
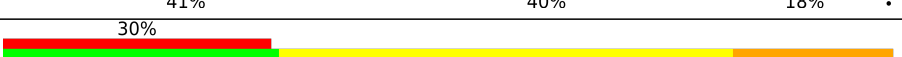
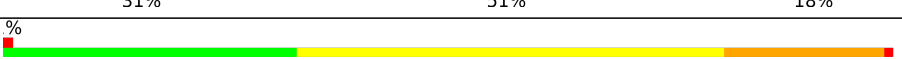
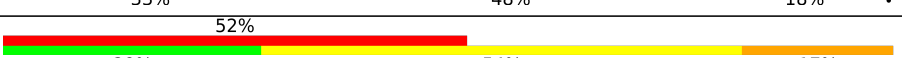
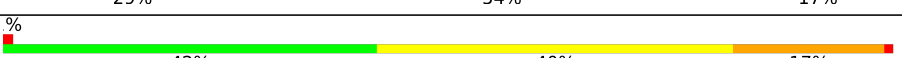
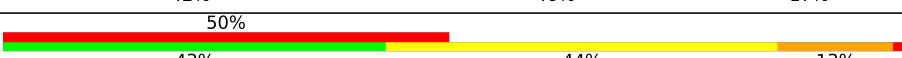
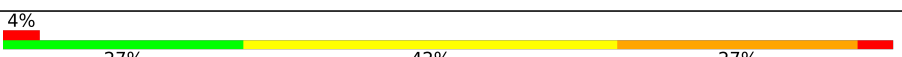
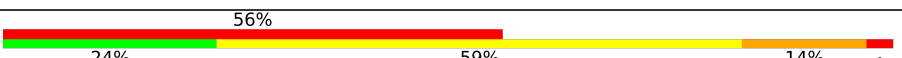
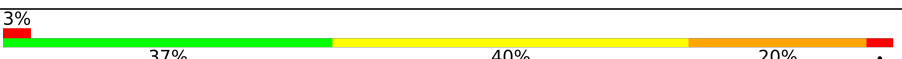
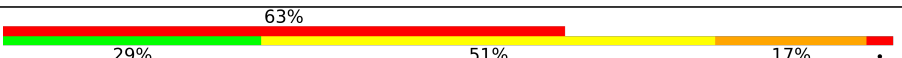
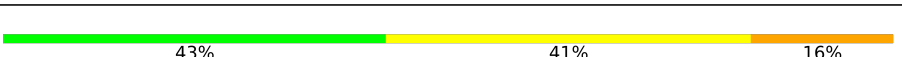

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

- 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			

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- # TEL



Continued from previous page...

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

Continued on next page...

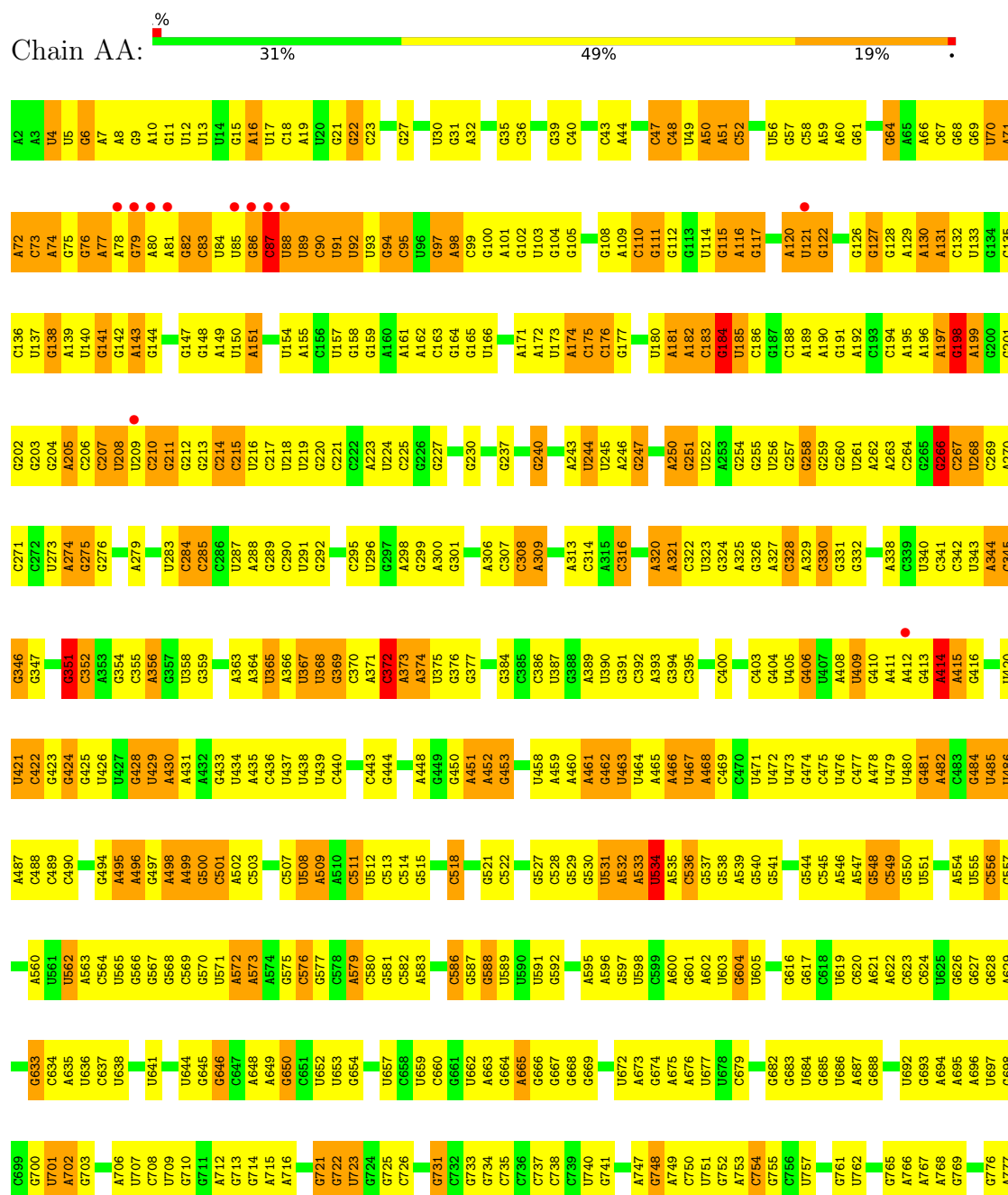
Continued from previous page...

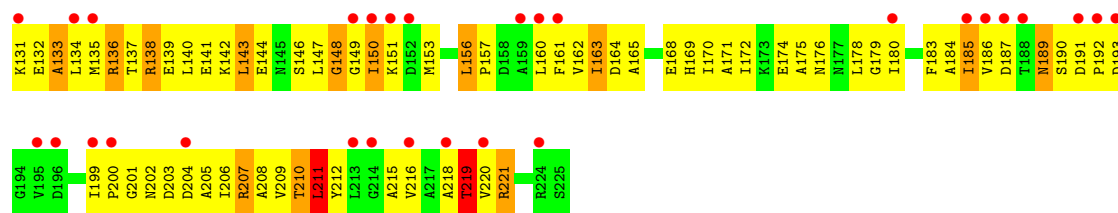
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	DC	13	Total 13	O 13	0	0
62	DD	3	Total 3	O 3	0	0
62	DE	3	Total 3	O 3	0	0
62	DJ	6	Total 6	O 6	0	0
62	DL	6	Total 6	O 6	0	0
62	DN	2	Total 2	O 2	0	0
62	DT	3	Total 3	O 3	0	0
62	DU	2	Total 2	O 2	0	0
62	DV	1	Total 1	O 1	0	0
62	D2	1	Total 1	O 1	0	0
62	D3	1	Total 1	O 1	0	0
62	D4	3	Total 3	O 3	0	0

3 Residue-property plots

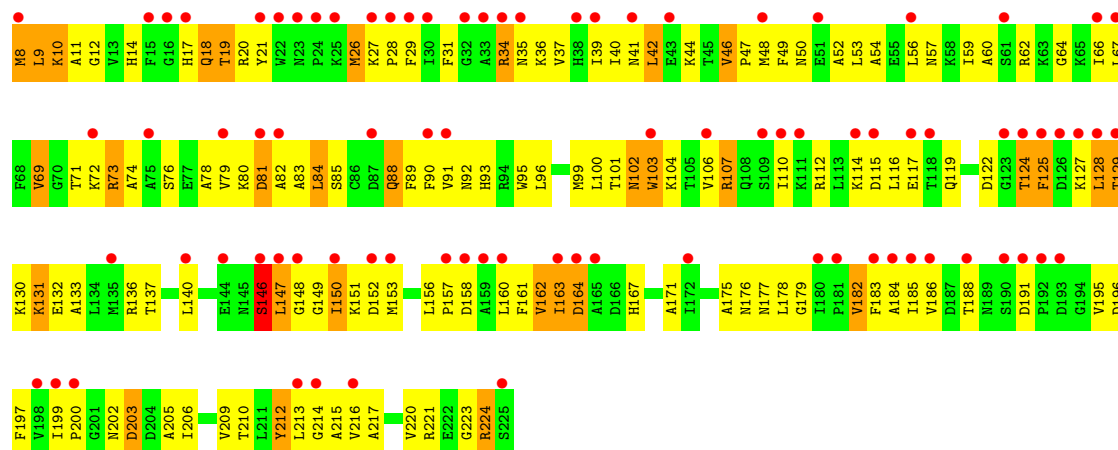
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

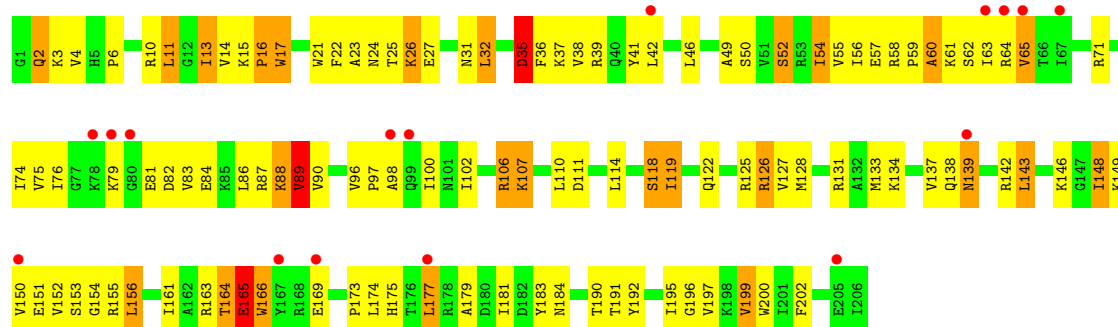




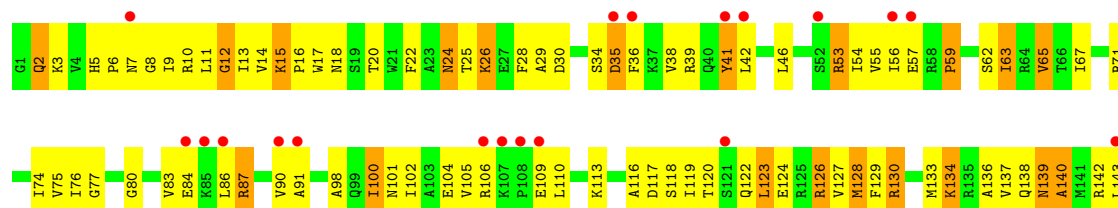
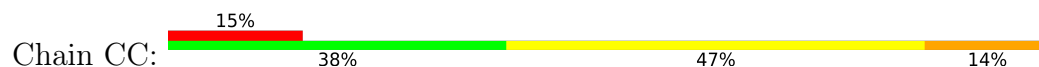
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3

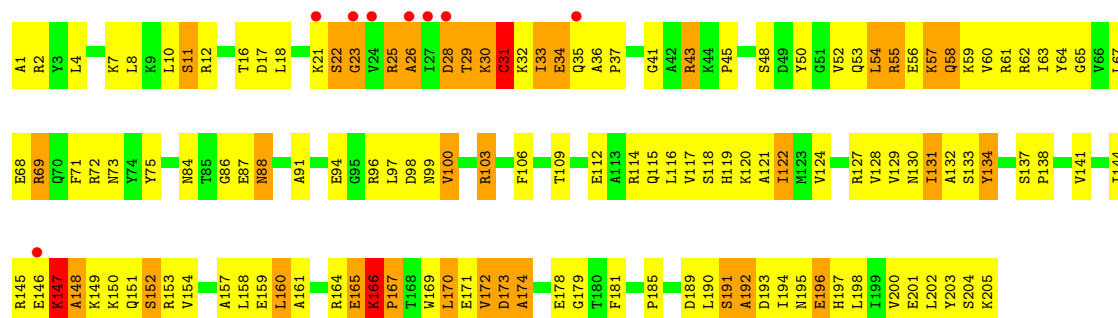


• Molecule 3: 30S ribosomal protein S3

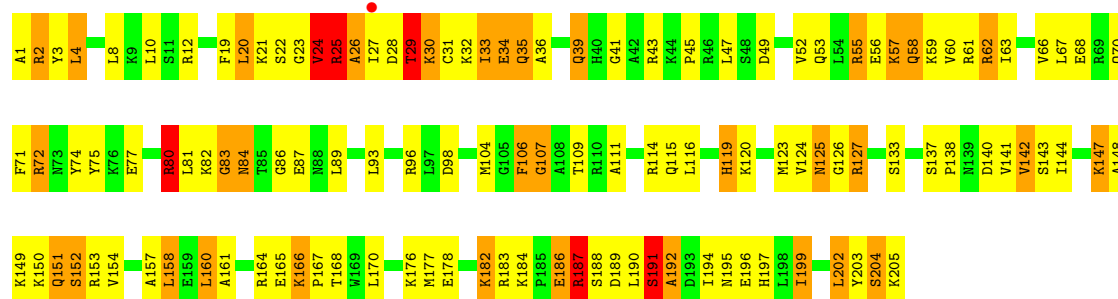




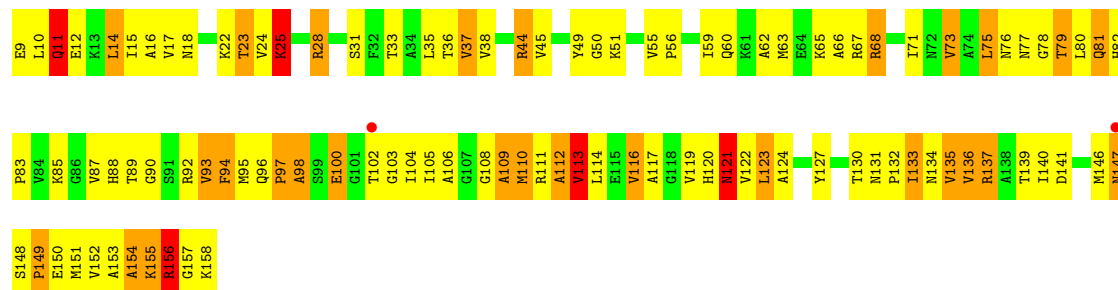
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

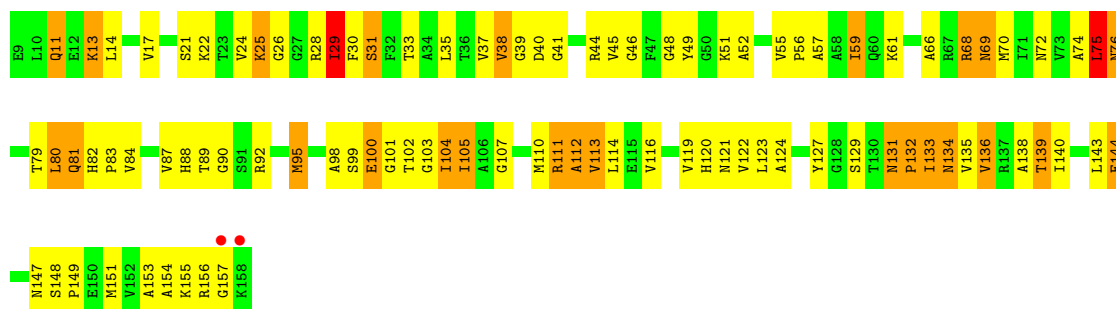


• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

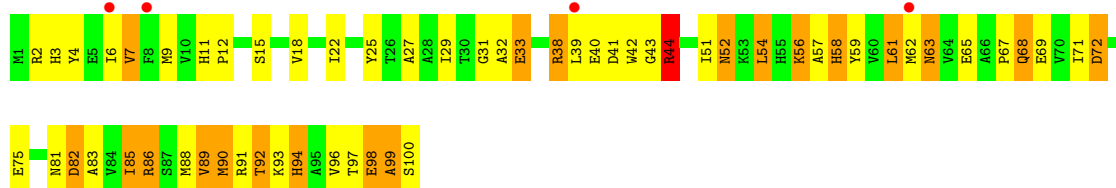
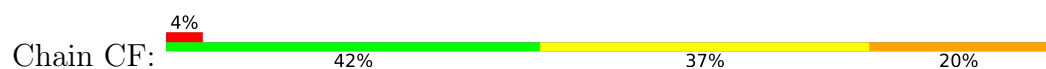




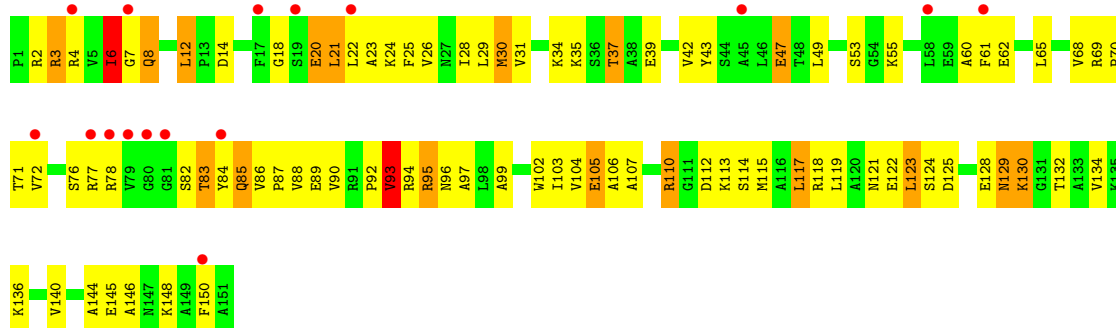
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

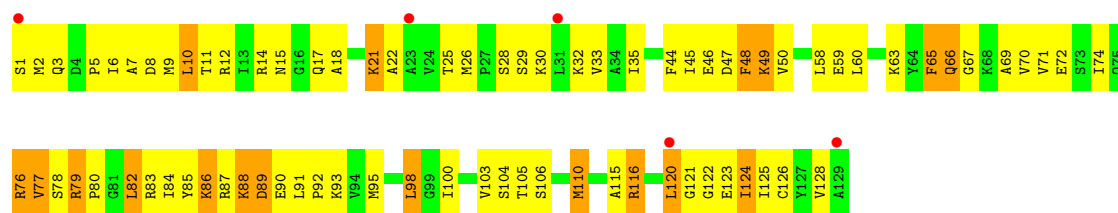


• Molecule 7: 30S ribosomal protein S7

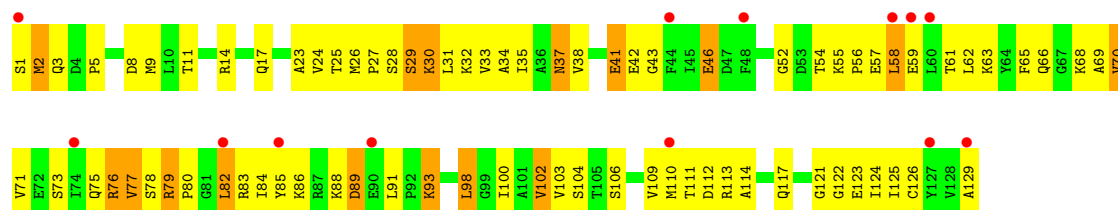


• Molecule 8: 30S ribosomal protein S8

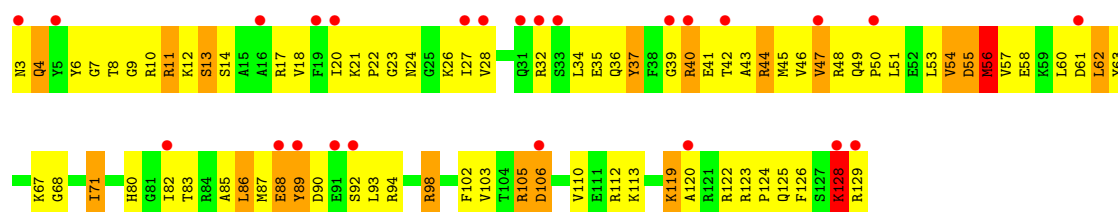




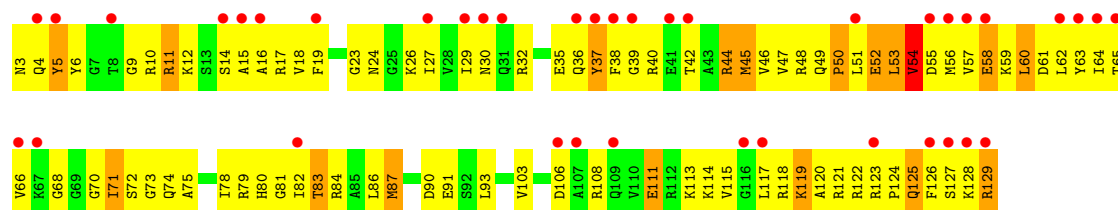
• Molecule 8: 30S ribosomal protein S8



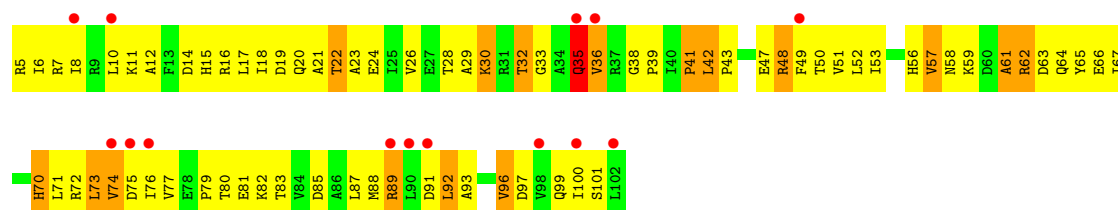
• Molecule 9: 30S ribosomal protein S9



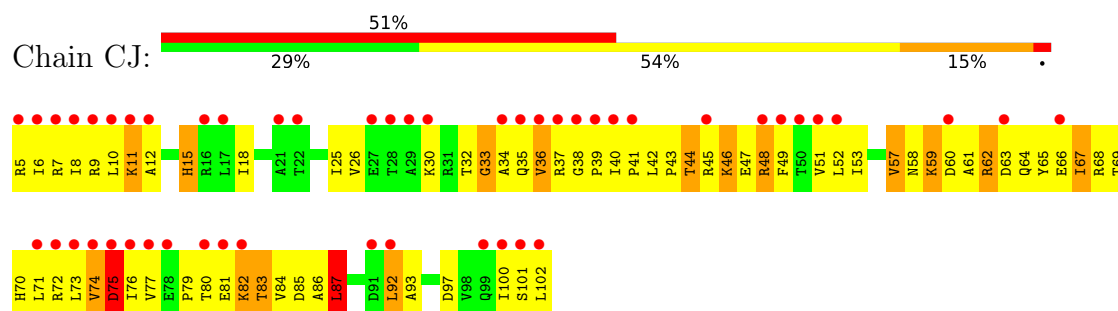
• Molecule 9: 30S ribosomal protein S9



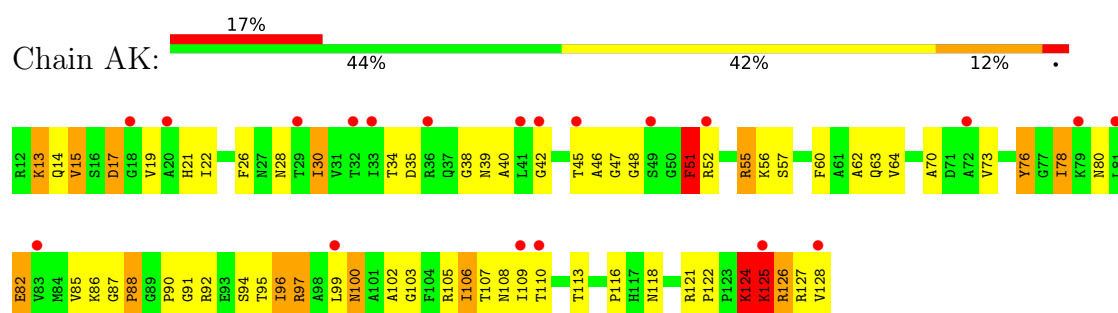
• Molecule 10: 30S ribosomal protein S10



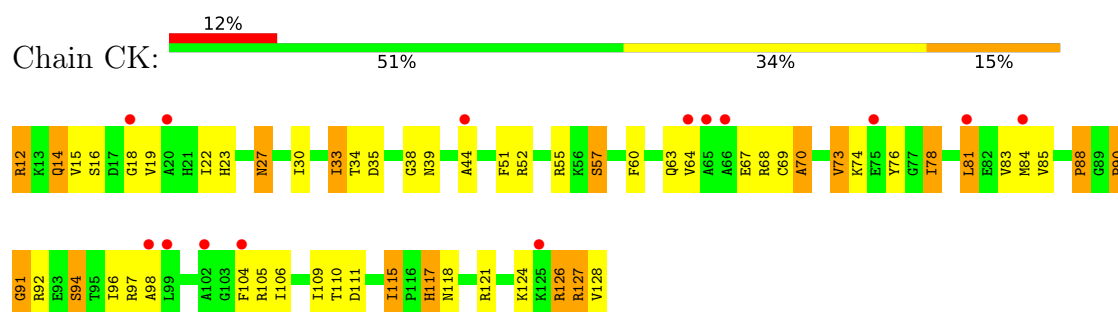
- Molecule 10: 30S ribosomal protein S10



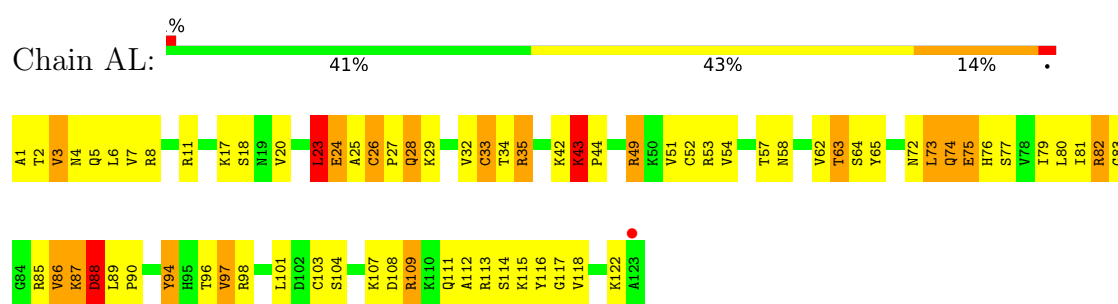
- Molecule 11: 30S ribosomal protein S11



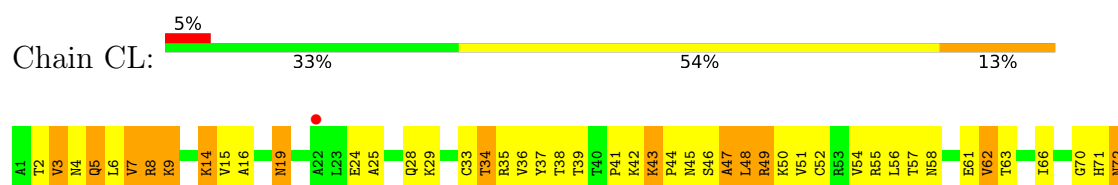
- Molecule 11: 30S ribosomal protein S11

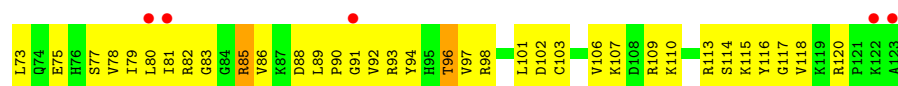


- Molecule 12: 30S ribosomal protein S12

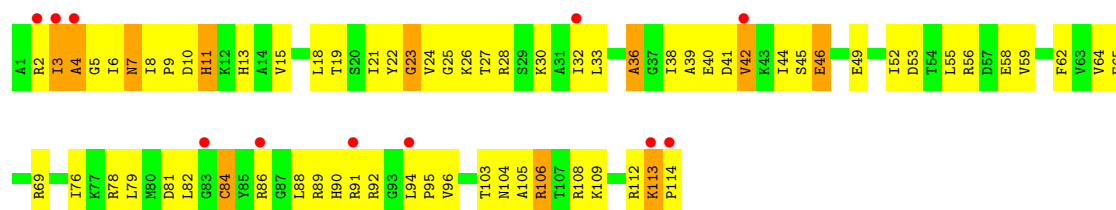


- Molecule 12: 30S ribosomal protein S12

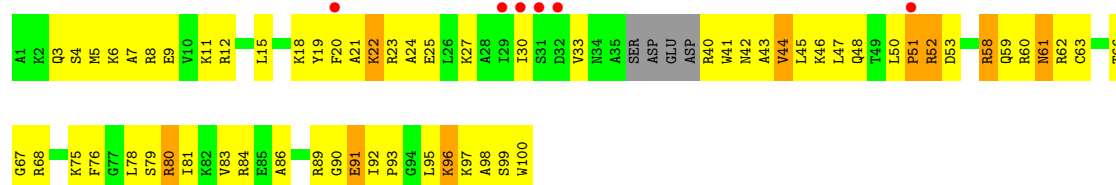




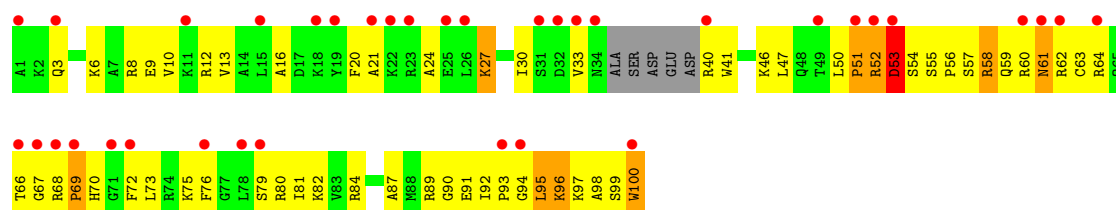
- Molecule 13: 30S ribosomal protein S13



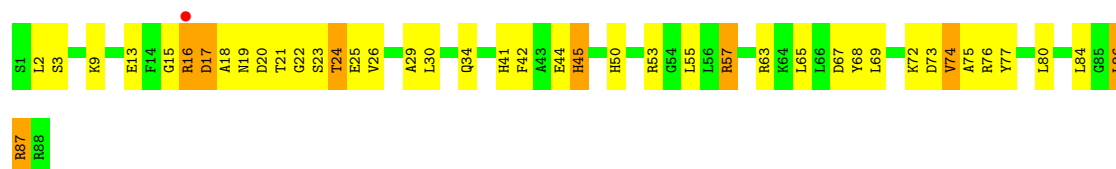
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

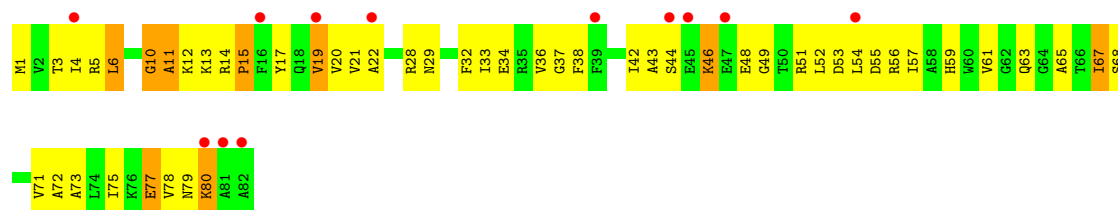


- Molecule 15: 30S ribosomal protein S15

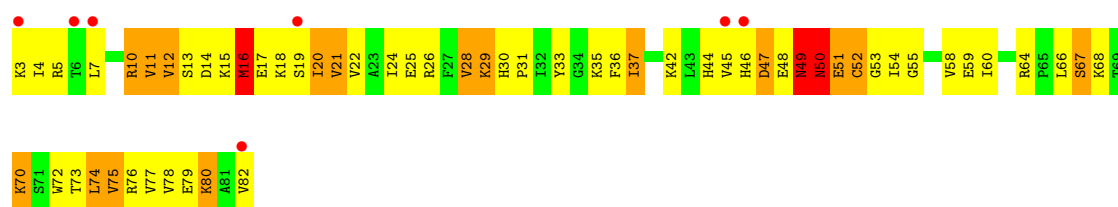




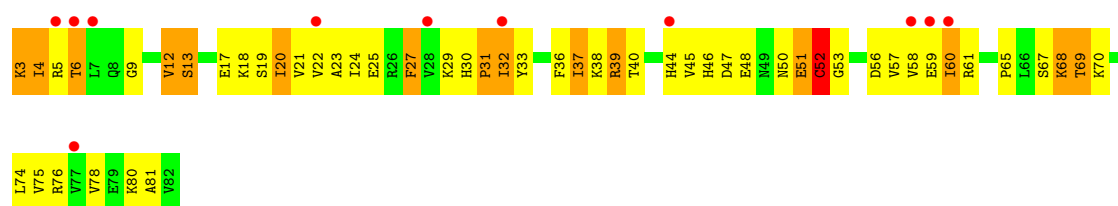
• Molecule 16: 30S ribosomal protein S16



• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

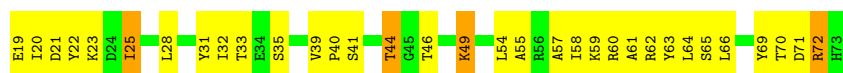


• Molecule 18: 30S ribosomal protein S18

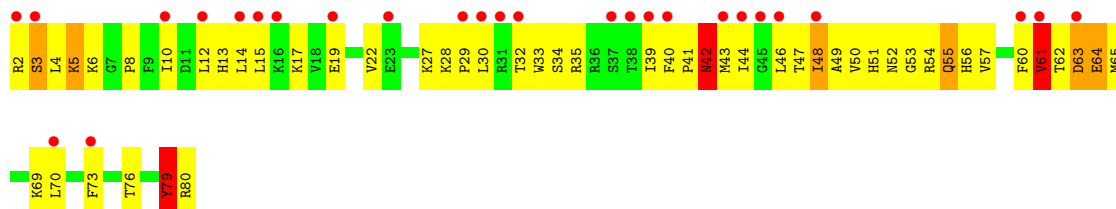


• Molecule 18: 30S ribosomal protein S18

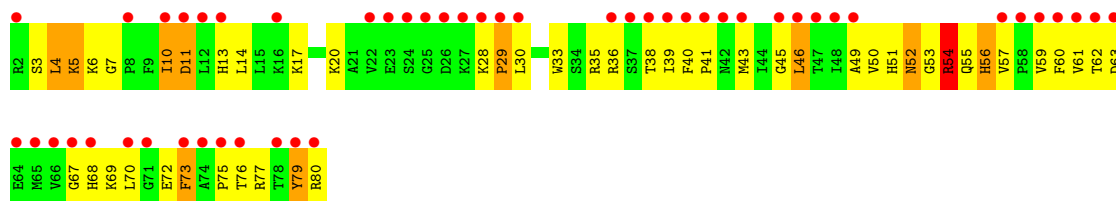




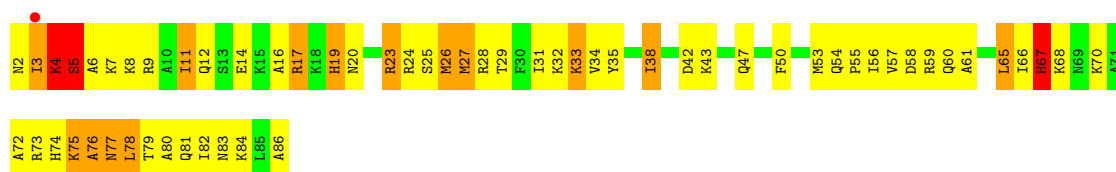
• Molecule 19: 30S ribosomal protein S19



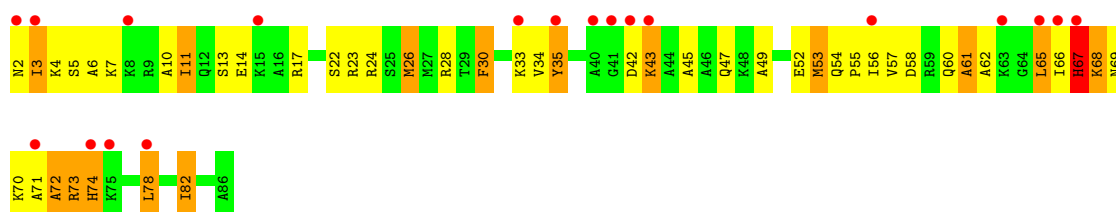
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20

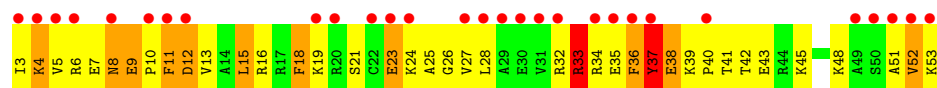


• Molecule 20: 30S ribosomal protein S20

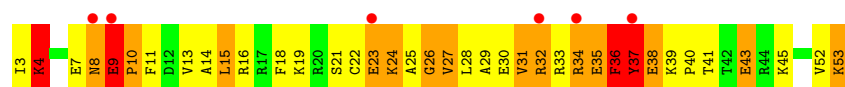
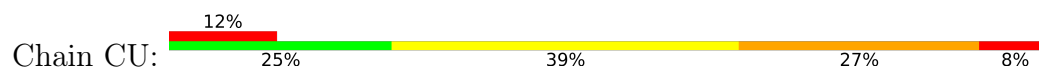


• Molecule 21: 30S ribosomal protein S21

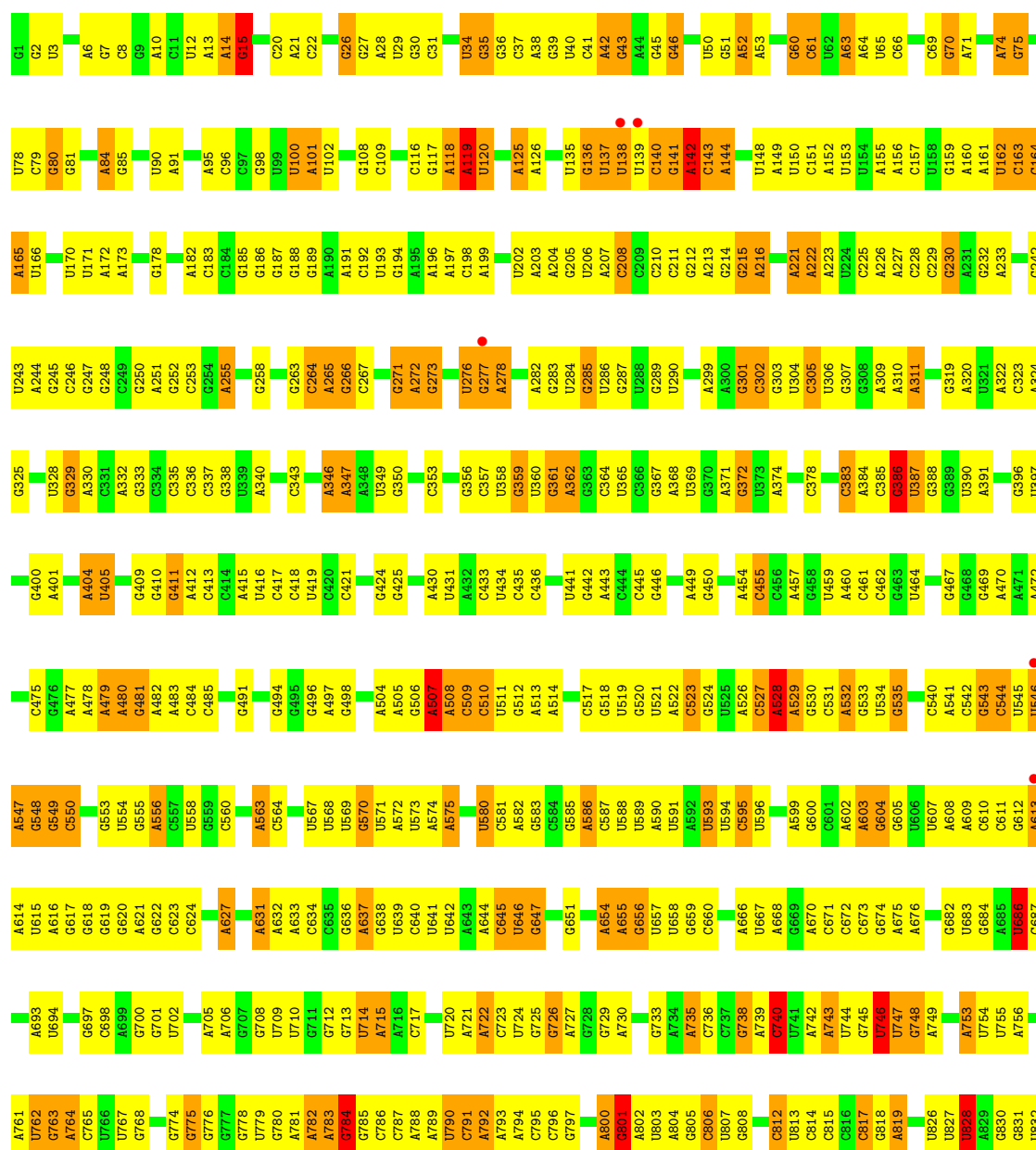




- Molecule 21: 30S ribosomal protein S21



- Molecule 22: 23S rRNA





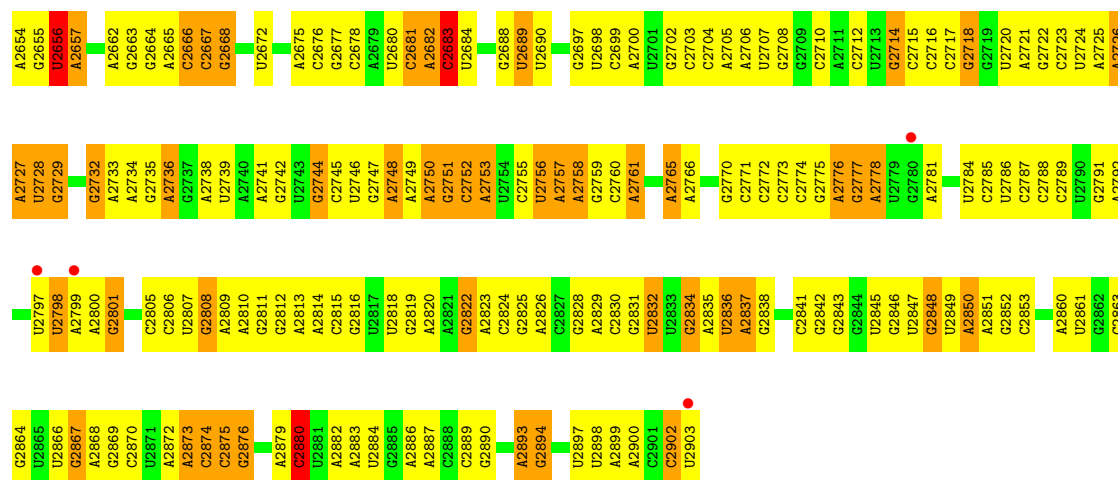
G2890	A2809	A2741	G2576	A2513	G2436	G2359	U2292	G2232	U2155	U2082	G2023	U1946
U2891	G2810	G2742	A2577	U2514	C2440	G2360	G2293	G2223	G2156	G2093	G2024	C1947
A2892	G2811	U2743	G2578	G2515	C2441	G2361	G2294	A2224	A	A2094	U2025	G1948
A2893	A2662	A2663	G2579	A2516	U2440	G2362	G2295	A2225	G	A2095	U2026	
G2894	A2663	G2663	U2580	G2517	C2442	G2363	G2296	G2226	C	C2096	G2027	A1952
G2895	A2814	A2748	G2581	A2518	C2443	G2364	U2297	A2227	C	C2097	U2028	A1953
G2896	G2815	A2749	G2582	U2519	G2444	G2365	A2298	G2228	C	U2098	G2029	G1954
U2897	U2750	A2750	G2583	G2520	G2445	A2366	U2299	U2229	G		A2030	U1955
U2898	U2818	G2751	U2584	G2521	G2446	U2372	U2305	G2230	A	C2103	A2031	U1956
U2903	G2819	C2755	U2585	U2522	G2447	G2375	U2306	U2231	C	C2104	G2032	C1957
	A2820	U2756	U2586	G2523	A2448	G2376	C2306	G2232	C	U2105	A2033	C1958
	A2821	A2757	A2587	G2524	U2449	A2377	G2307	U2233	U	U2106	U2034	C1959
	A2823	G2676	C2591	G2525	A2451	A2378	G2308	G2234	U	G2107	G2035	A1960
	G2824	G2677	U2593	G2526	C2452	A2379	A2309	G2235	G	A2108	C2036	C1961
	G2825	A2679	U2594	G2527	A2453	G2380	U2310	U2236	A	U2109	A2037	C1962
	G2830	A2681	A2598	G2528	G2454	G2381	U2311	G2237	A	G2110	U2038	U1963
	U2836	A2682	A2602	A2530	C2456	G2382	U2312	G2238	U	G	U2039	G1964
A2837	A2837	A2683	U2603	A2531	C2467	G2383	A2314	G2239	A	U	U2040	C1965
G2838	G2838	G2770	U2604	A2534	A2468	U2384	G2315	G2242	C	A	A2042	A1966
G2839	G2771	G2772	U2605	G2535	A2469	U2385	G2316	U2243	C	A	G2043	C1967
G2840	C2772	G2773	G2606	G2536	A2470	A2386	G2317	U2244	A	A	C2044	U1970
C2841	C2773	U2689	C2606	U2537	A2471	U2387	G2318	U2245	A	A	C2045	U1971
G2842	G2774	U2690	U2615	G2538	A2472	U2388	G2319	G2246	C	U	G2046	G1972
G2843	G2775	C2691	U2616	G2539		G2389	U2320	G2250	C2179	A		
G2844	A2776	U2696	G2610	G2540	C2475	U2390	U2321	G2251	U2180	G	G2049	A1977
G2845	G2777	G2697	A2611	A2541	A2476	U2391	A2322	G2252	U2181	G	C2050	A1978
G2846	G2778	U2698	U2612	G2542	A2477	U2392	U2323	G2253	U2182	U	A2051	U1979
U2847	U2779	U2699	A2614	G2543	U2478	U2393	U2324	G2254	A2183	G	A2052	G1980
U2848	G2780	A2700	U2615	G2544	U2479	G2394	G2325	G2255	A2184	G	G2053	
U2849	A2781	A2700	U2616	G2545	C2480	G2395	G2326	G2256	U2185	G	A2054	G1983
	G2782	C2703	U2617	U2546	G2481	G2396	A2327	G2257	U2186	A	G2055	G1984
	U2783	G2704	U2622	G2547		G2397	U2328	G2258	U2187	G	G2056	G1985
	U2784	A2705	U2622	U2548	G2484	U2402	A2329	G2259	U2188	C	C2057	C1986
	U2785	C2626	C2626	G2551	C2485	U2403	G2330	G2260	U2189	U	A2058	U1991
	U2786	G2627	U2627	G2552	G2486	U2404	G2331	G2261	U2192	U	A2059	G1992
	G2787	U2628	U2629	G2553	U2487	G2405	G2332	G2262	G2193	U	A2060	U1993
	G2788	G2629	U2630	G2554	G2488	A2406	A2333	G2263	U2194	G2193	A2061	
	G2789	U2631	U2632	G2555	U2489	G2406	U2334	A2267	U2195	A2134	A2062	C1996
	U2790	C2636	U2633	G2556	G2490	G2406	A2335	A2268	U2196	A2135	C2063	C1997
	G2791	U2637	G2638	G2557	U2491	G2414	U2336	G2269	U2197	G2136	C2064	A1998
	U2792	A2639	U2639	G2558	U2492	G2415	A2337	G2270	A2198	U2137	C2065	C1999
	G2793	G2640	U2640	U2561	G2494	C2416	U2338	U2272	C2199	G2138	C2066	C2000
	G2794	G2641	U2641	G2562	G2495	U2419	A2340	A2273	C2200	U2139	G2069	C2001
	U2795	G2642	U2642	U2563	C2496	G2420	U2341	A2274	U2203	G2140	A2070	G2002
	U2796	G2643	G2643	G2564	G2497	G2421	A2342	G2275	G2204	A2142	A2071	
	U2797	G2644	G2644	G2565	C2499	G2422	A2343	G2276	C2143	C2143	C2072	C2006
	U2798	G2645	G2645	A2566	U2500	U2423	U2344	G2277	C2144	G2144	U2076	
	A2800	G2646	G2646	G2567	G2501	G2424	U2345	A2278	C2145	G2145	U2076	G2012
	G2801	U2647	U2647	U2568	C2502	A2425	G2346	G2279	C2208	C2146	A2014	A2013
	G2802	U2648	U2648	G2569	A2503	A2426	U2347	G2280	G2209	A2147	A2015	A2016
	G2803	G2649	G2649	G2570	U2504	G2427	G2351	A2281	U2210	G2148	U2017	U2018
	G2804	U2650	U2650	G2571	G2505	G2428	A2352	G2282	A2211	A2149	G2082	U2019
	G2805	G2651	G2651	A2572	G2506	G2429	G2353	G2283	U2212	U2150	G2083	G2018
	G2806	U2656	U2656	G2573	C2507	A2430	G2354	G2286	U2213	C2151	U2086	A2019
	U2807	U2657	U2657	G2574	U2511	U2431	U2355	A2287	C2214	G2152	G2087	A2020
	G2808	A2657	A2657	G2575	C2512	A2435	A2358	U2291	U2220	C2153	C2091	U2022

• Molecule 22: 23S rRNA

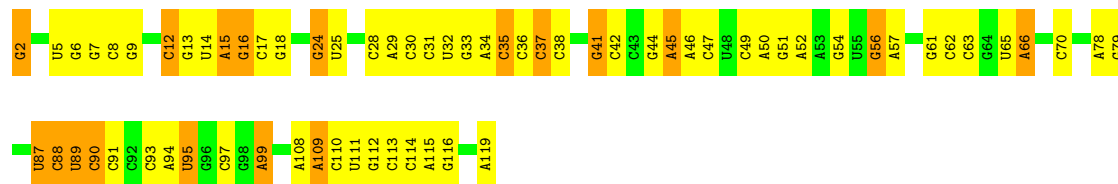


C1663	A1598	C1533	U1467	G1337	A1274	C1208	U1141	U1078	U1012	C948	G
A1664	U1599	U1534	U1468	G1336	A1275	U1209	A1142	C1079	C1013	G949	G
A1665	A1535	A1402	A1470	G1339	A1276	G1210	A1143	U1210	A1014	G950	G
G1666	C1536	A1403	A1470	U1340	G1277	G1211	A1144	U1082	U1015	C951	U
G1667	G1537	C1404	U1405	A1342	G1278	G1212	A1147	U1083	G1016	G952	C
A1668	U1538	G1475	U1476	G1343	G1280	A1213	U1148	A1084	U1019	G953	A
C1669	G1539	U1477	U1477	U1344	G1281	G1218	U1149	A1085	U1019	G954	U
C1670	G1540	U1478	U1478	U1345	U1282	U1222	G1153	A1086	A1021	G955	C
A1671	U1541	G1479	U1479	G1346	U1283	U1223	C1154	G1087	A1020	U956	C
G1674	G1542	G1480	U1480	G1347	A1284	U1224	A1155	U1088	U1023	U958	G
C1675	U1543	A1411	U1411	C1348	A1285	U1225	A1156	A1089	G1024	A959	A
A1676	C1480	U1412	U1412	C1349	A1286	A1226	U1157	A1090	G1025	A960	C
A1677	A1413	C1414	U1414	C1350	A1287	G1227	G1158	G1091	G1026	C961	U
C1680	G1482	U1415	U1415	C1351	G1288	G1228	U1159	C1092	A1027	G962	U
U1681	G1483	G1416	U1416	U1352	C1289	U1229	U1160	U1093	U1032	U963	U
C1682	C1489	C1417	U1417	G1355	C1290	A1230	C1161	U1094	C964	C965	A
U1683	G1491	U1418	U1418	G1356	C1291	A1231	G1162	U1095	U1033	G966	C
C1686	G1492	A1420	U1420	C1357	G1292	C1232	G1166	U1097	G1036	U967	C
G1687	C1493	G1421	U1421	G1358	G1296	U1234	C1167	U1098	G1037	C968	C
U1688	A1494	G1422	U1422	C1359	G1297	G1235	G1168	G1099	G1038	G969	C
A1689	A1495	U1423	U1423	G1360	A1301	G1236	A1169	C1100	A1039	U970	A
C1690	U1496	G1425	U1425	C1361	A1302	A1237	C1170	U1101	A1040	G971	C
U1691	C1497	A1426	U1426	C1362	G1300	G1238	G1171	C1102	G1043	A972	C
C1692	C1498	A1427	U1427	C1363	A1301	G1239	C1172	A1103	C1044	A973	A
U1693	G1499	C1428	U1428	G1364	A1302	U1240	U1173	U1107	C1045	A974	C
G1694	C1500	G1429	U1429	A1365	G1303	A1241	U1174	U1108	C1046	A975	C
C1695	G1501	A1430	U1430	A1366	A1304	U1242	A1175	C1109	G1047	G976	C
U1696	A1502	A1431	U1431	C1367	C1305	C1243	U1176	G1110	G1048	G977	C
G1697	C1503	G1432	U1432	G1368	G1306	U1244	C1177	G1111	C1049	A980	C
C1698	A1504	A1433	U1433	U1372	A1307	G1245	C1178	G1112	A981	A981	C
A1699	U1505	C1437	U1437	A1373	A1308	U1246	G1179	G1113	C982	A982	C
U1700	C1506	U1507	U1507	G1374	G1309	A1247	U1180	C1114	A983	U919	C
A1701	A1507	A1438	U1438	U1375	G1310	U1249	U1181	G1115	A984	A920	C
C1706	C1508	U1440	U1440	C1376	G1311	C1250	U1183	G1116	C921	G921	C
G1707	G1510	G1441	U1441	G1377	U1312	C1251	U1184	C1117	G1055	C922	C
C1708	G1511	U1442	U1442	A1378	C1314	G1252	G1185	G1118	G1056	A988	C
U1709	U1512	G1444	U1444	U1379	C1315	A1253	U1119	U1119	G1057	G923	C
G1710	G1513	G1444	U1444	G1380	U1316	A1254	U1186	G1120	U1058	G924	C
A1713	U1514	U1447	U1447	G1381	G1317	U1255	G1187	G1121	A990	A925	C
U1714	A1515	G1448	U1448	G1382	U1318	G1256	U1188	G1122	G991	G926	C
C1715	G1516	G1449	U1449	A1383	C1319	C1257	U1189	U1061	C992	A927	C
U1716	U1517	G1452	U1452	A1384	C1320	U1258	G1190	G1062	G993	A928	C
A1717	G1518	U1453	U1453	A1385	A1321	G1259	G1191	G1063	C994	U929	C
G1718	U1519	C1454	U1454	C1386	G1324	A1260	A1194	C1064	U930	G930	C
C1721	U1520	G1455	U1455	A1387	U1325	C1261	G1195	U1065	U931	U931	C
A1722	G1521	C1456	U1456	G1388	U1326	U1262	U1196	C997	A932	A932	C
G1723	U1522	G1457	U1457	U1389	A1327	A1263	G1197	U1067	U933	U934	C
U1724	U1523	U1458	U1458	U1390	U1328	A1264	U1198	G1068	C935	U934	C
C1728	G1524	C1459	U1459	A1391	A1328	U1265	U1199	A1000	A936	A936	C
U1729	U1525	U1460	U1460	A1392	U1329	G1266	A1133	C1006	A941	A941	C
C1730	C1526	G1461	U1461	A1393	C1330	U1267	C1200	G1071	G942	G942	C
G1731	G1527	C1462	U1462	U1394	G1331	A1268	U1203	A1072	A943	A943	C
U1732	A1528	C1463	U1463	A1395	G1332	A1269	A1204	G1073	C944	C944	C
C1732	U1529	G1465	U1465	U1396	G1333	C1270	A1205	G1074	A1008	A1008	C
	G1530	U1466	U1466	U1397	G1334	G1271	G1206	G1075	A1009	A945	C
	A1531			C1398	C1335	A1272	C1207	C1076	C946	A946	C
	A1532			C1399	A1336	U1273		A1077	A947	A947	C

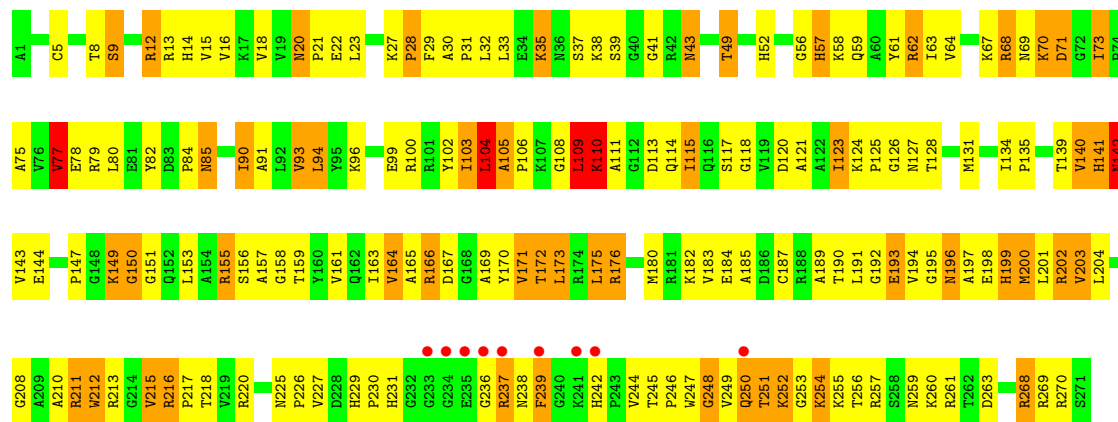




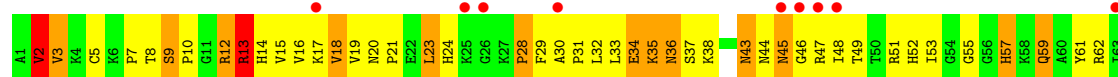
• Molecule 23: 5S rRNA

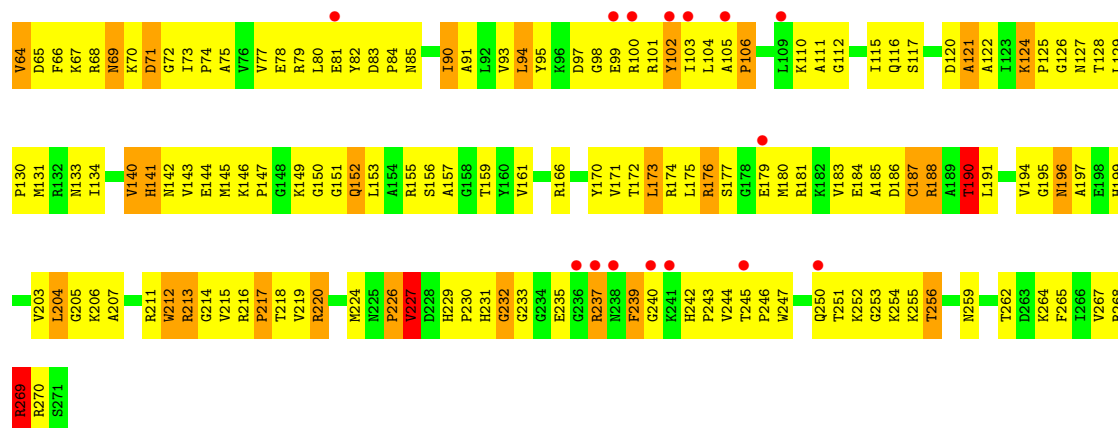


• Molecule 24: 50S ribosomal protein L2



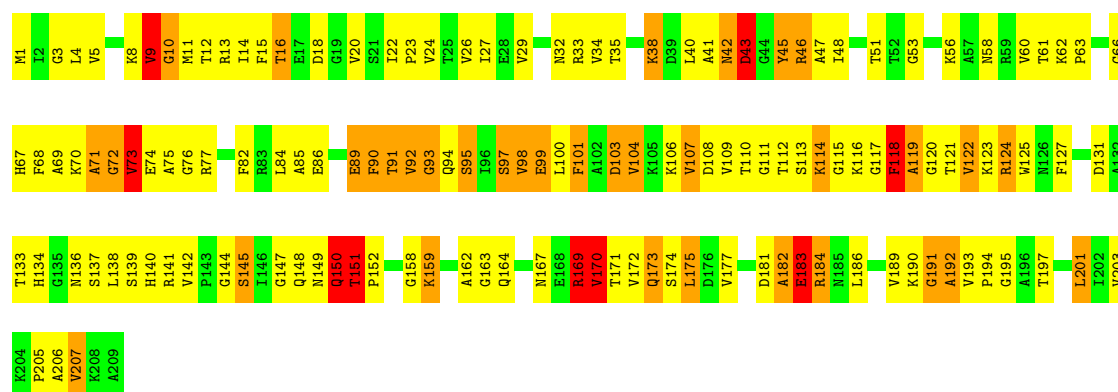
• Molecule 24: 50S ribosomal protein L2





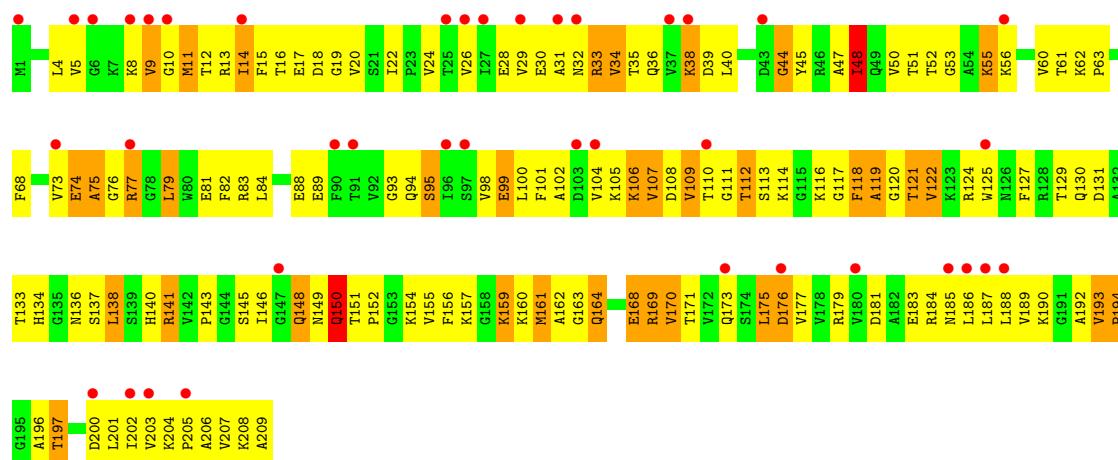
• Molecule 25: 50S ribosomal protein L3

Chain BD: 32% 47% 17% .



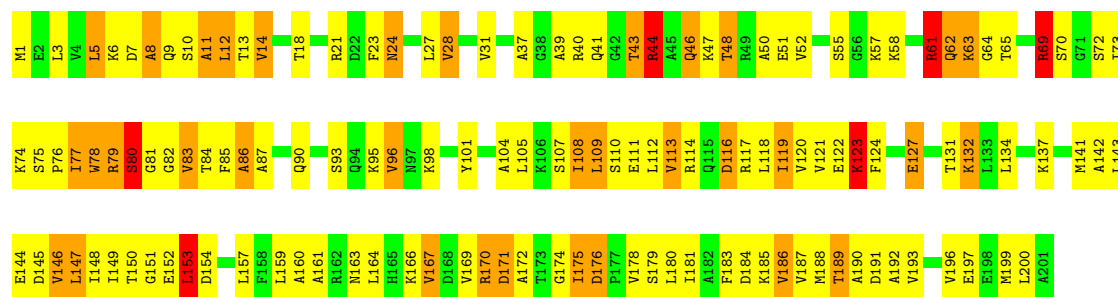
• Molecule 25: 50S ribosomal protein L3

Chain DD: 19% 30% 52% 17% .

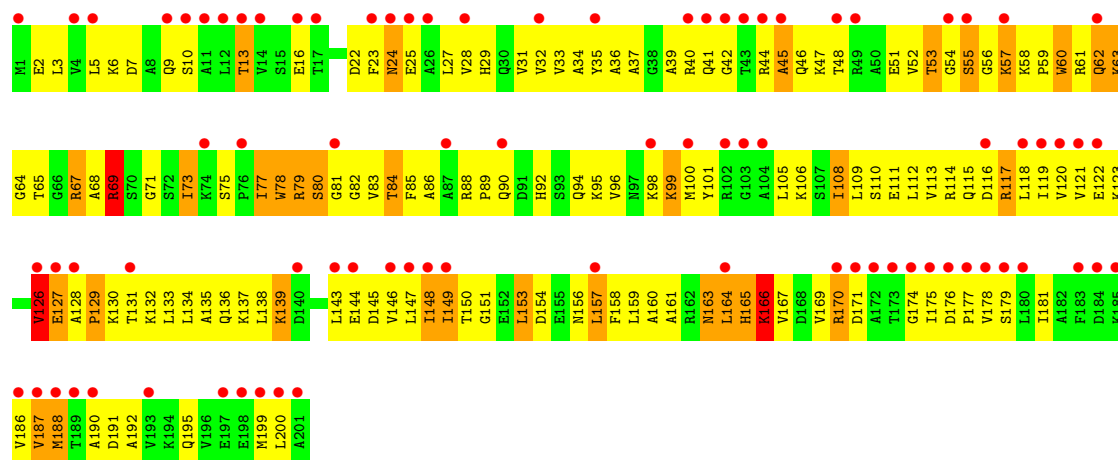


• Molecule 26: 50S ribosomal protein L4

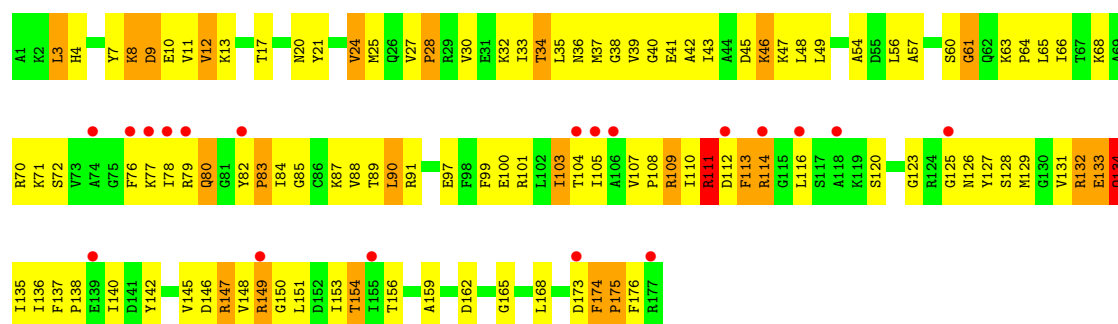
Chain BE: 33% 47% 17% .



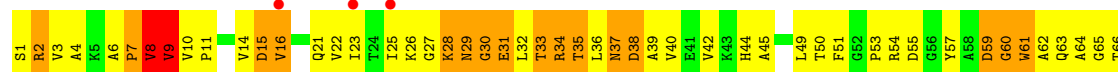
• Molecule 26: 50S ribosomal protein L4

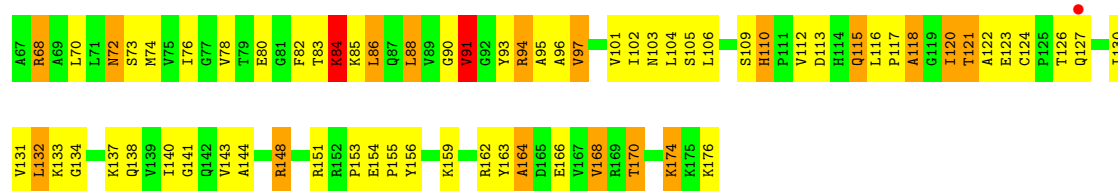


• Molecule 27: 50S ribosomal protein L5

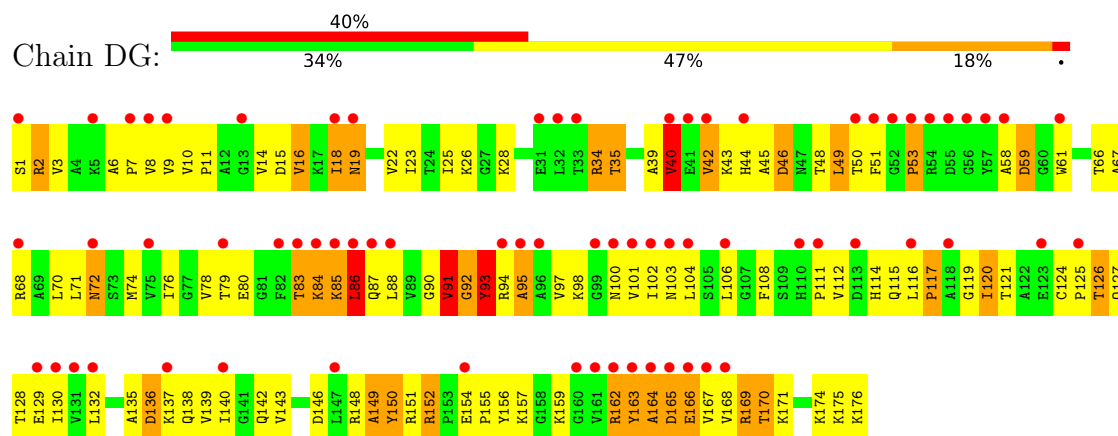


• Molecule 28: 50S ribosomal protein L6

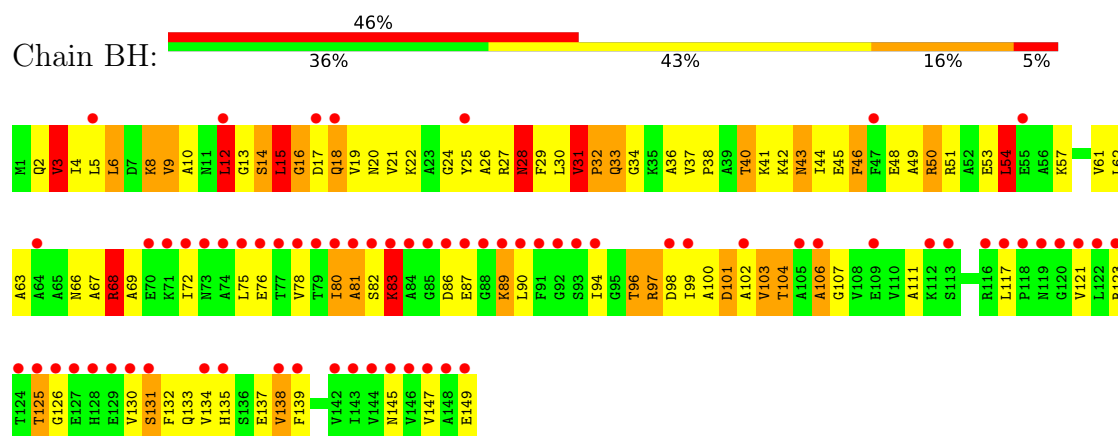




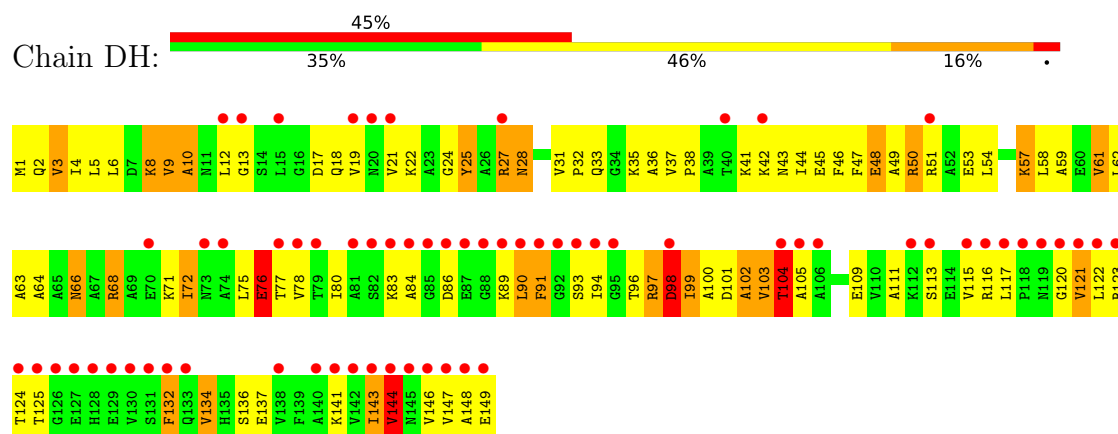
• Molecule 28: 50S ribosomal protein L6



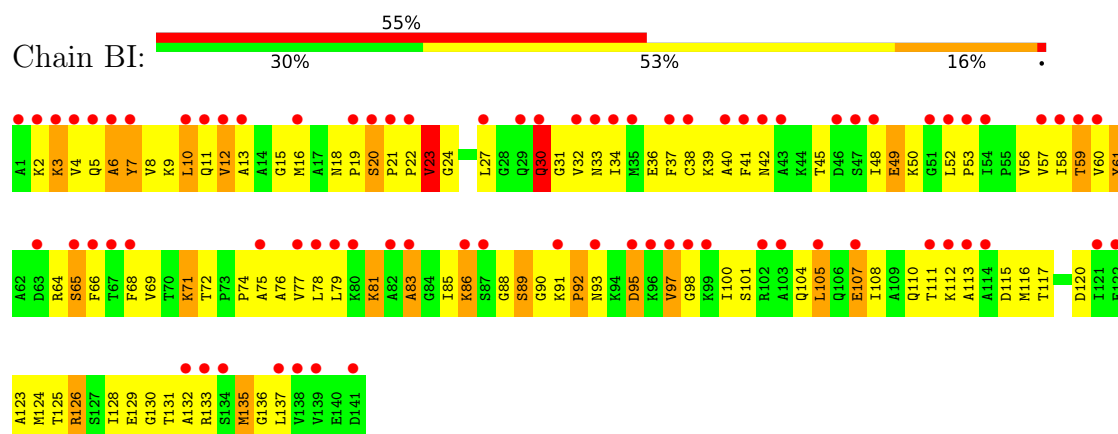
• Molecule 29: 50S ribosomal protein L9



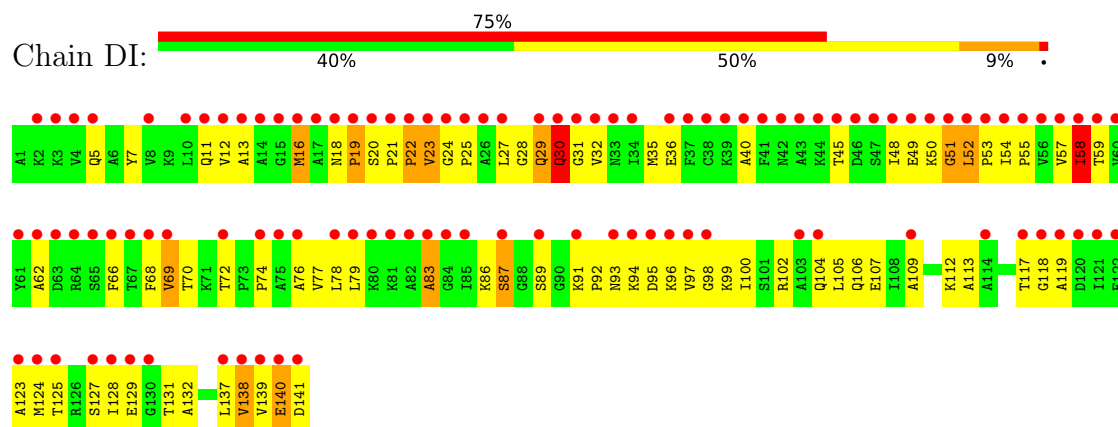
• Molecule 29: 50S ribosomal protein L9



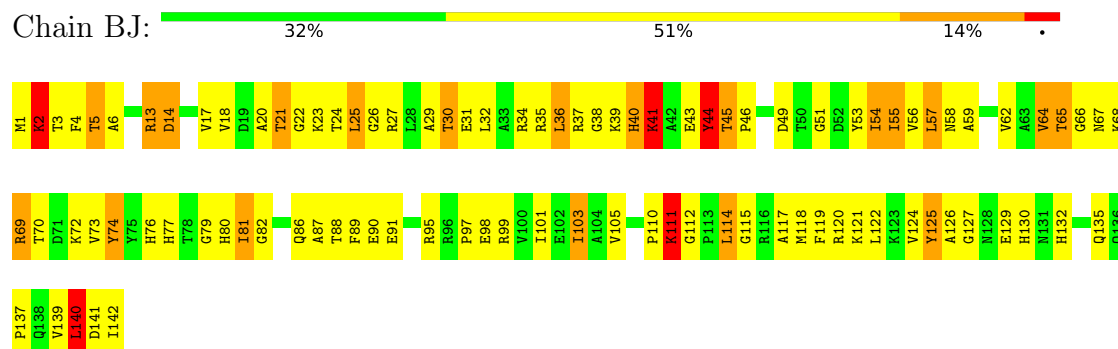
- Molecule 30: 50S ribosomal protein L11



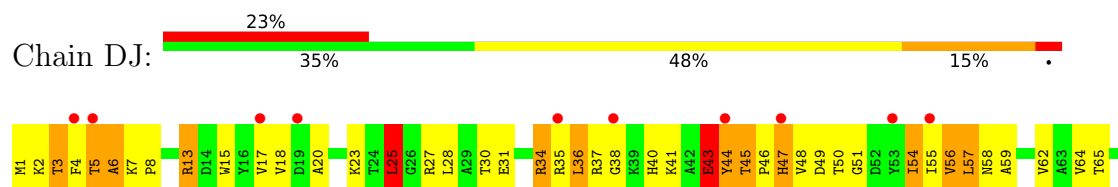
- Molecule 30: 50S ribosomal protein L11

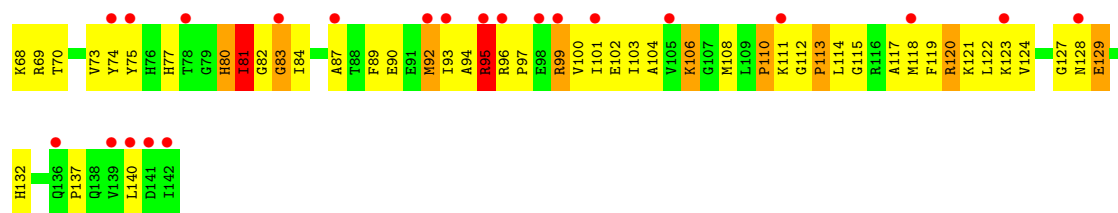


- Molecule 31: 50S ribosomal protein L13

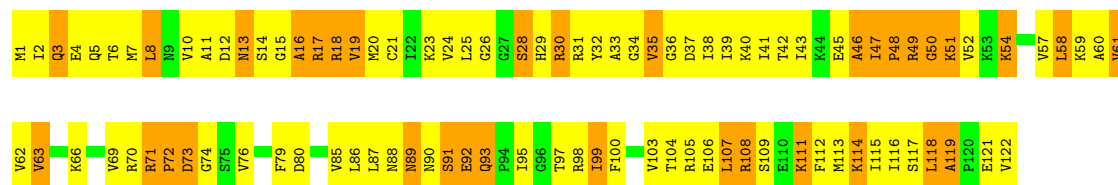


- Molecule 31: 50S ribosomal protein L13

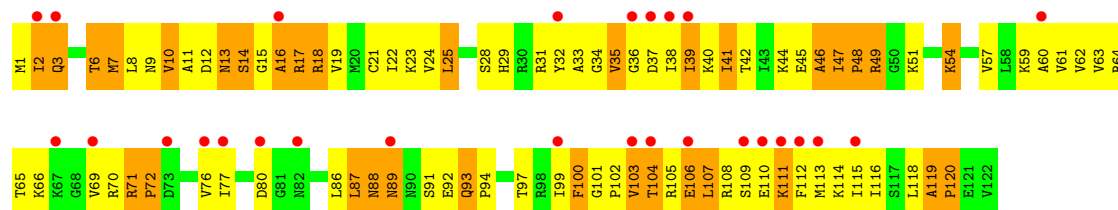




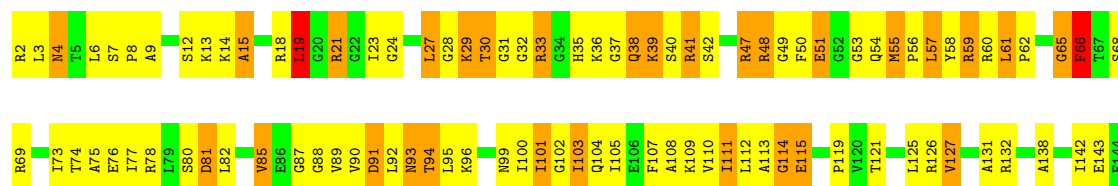
• Molecule 32: 50S ribosomal protein L14



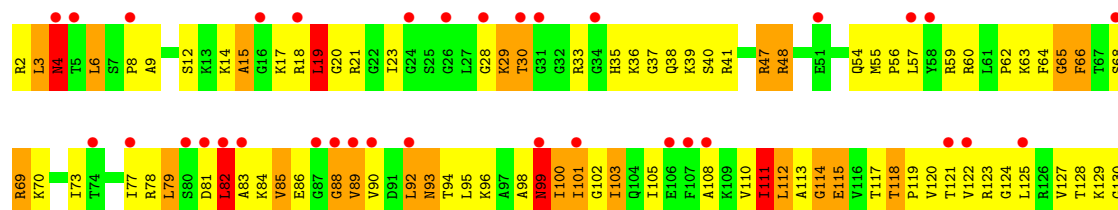
• Molecule 32: 50S ribosomal protein L14

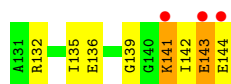


• Molecule 33: 50S ribosomal protein L15



• Molecule 33: 50S ribosomal protein L15





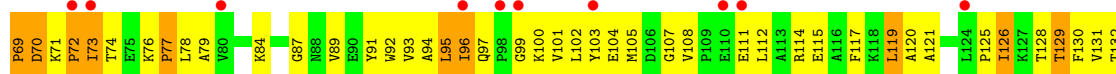
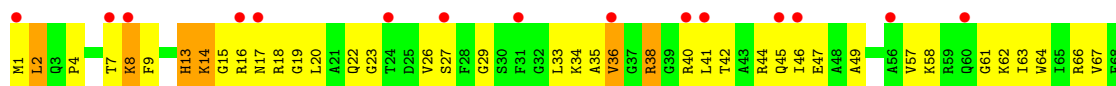
- Molecule 34: 50S ribosomal protein L16

Chain BM: 40% 42% 16%



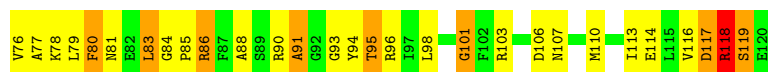
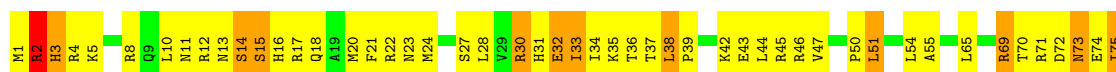
- Molecule 34: 50S ribosomal protein L16

Chain DM: 20% 35% 53% 12%



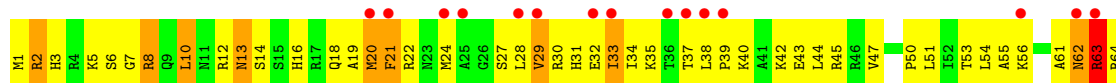
- Molecule 35: 50S ribosomal protein L17

Chain BN: 34% 48% 16%



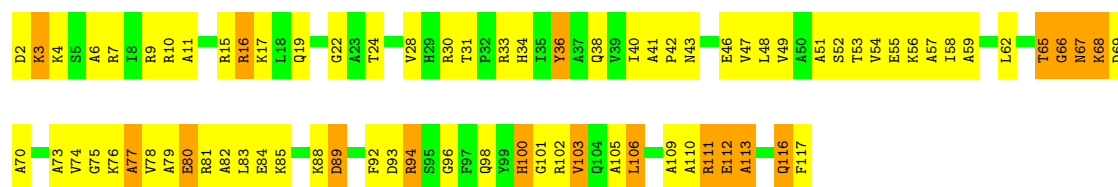
- Molecule 35: 50S ribosomal protein L17

Chain DN: 27% 32% 52% 16%



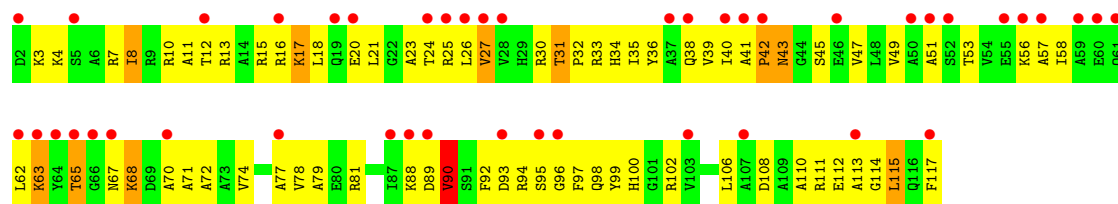
- Molecule 36: 50S ribosomal protein L18

Chain BO:  33% 52% 16%



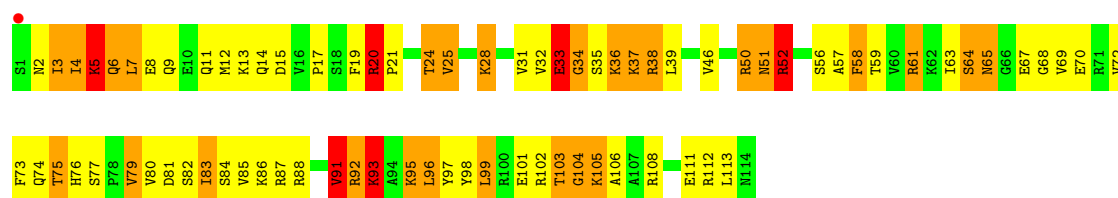
• Molecule 36: 50S ribosomal protein L18

Chain DO:  38% 35% 55% 9%



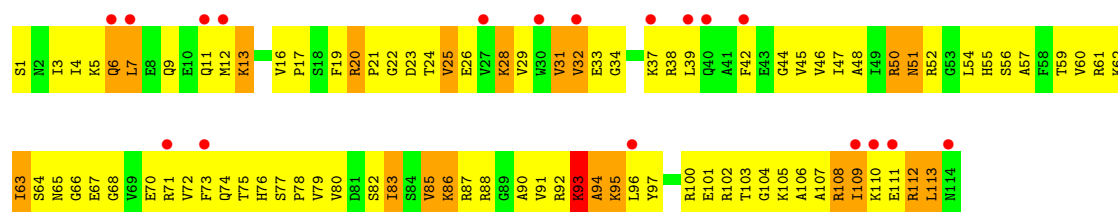
• Molecule 37: 50S ribosomal protein L19

Chain BP:  % 31% 40% 24% 5%

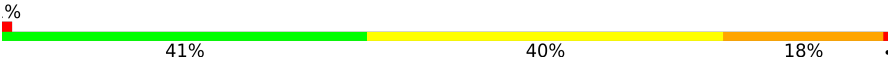


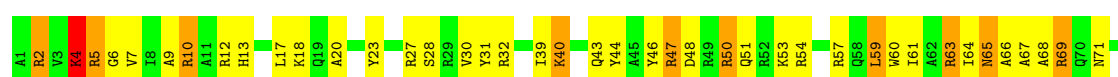
• Molecule 37: 50S ribosomal protein L19

Chain DP:  16% 20% 61% 18%



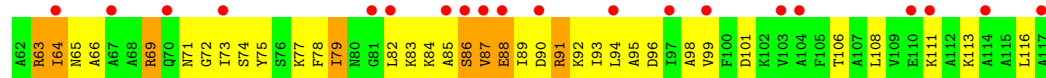
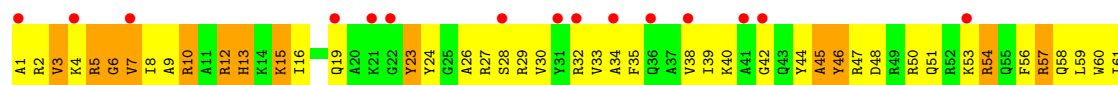
• Molecule 38: 50S ribosomal protein L20

Chain BQ:  % 41% 40% 18%





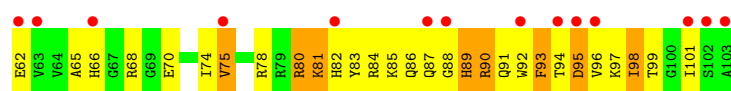
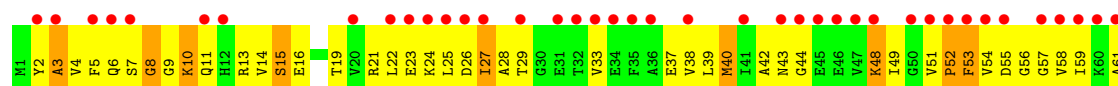
• Molecule 38: 50S ribosomal protein L20



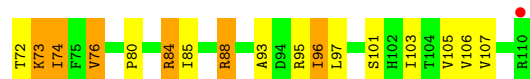
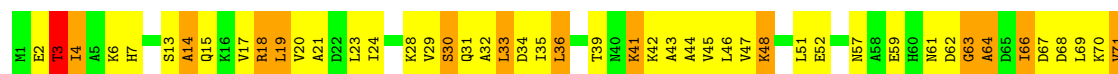
• Molecule 39: 50S ribosomal protein L21



• Molecule 39: 50S ribosomal protein L21

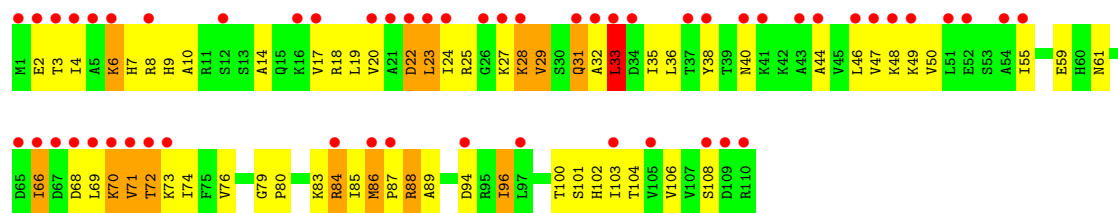


• Molecule 40: 50S ribosomal protein L22

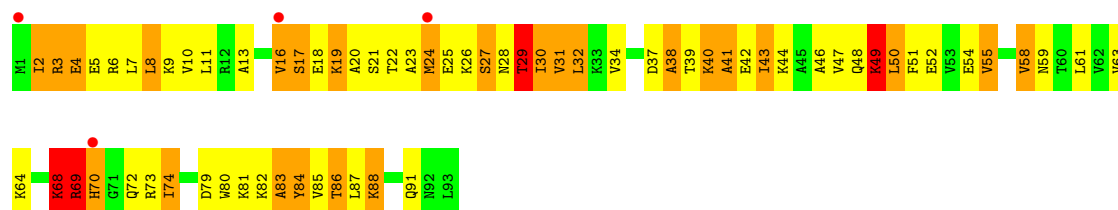


• Molecule 40: 50S ribosomal protein L22

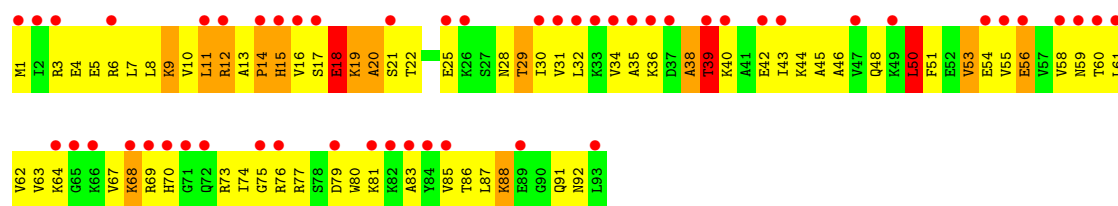




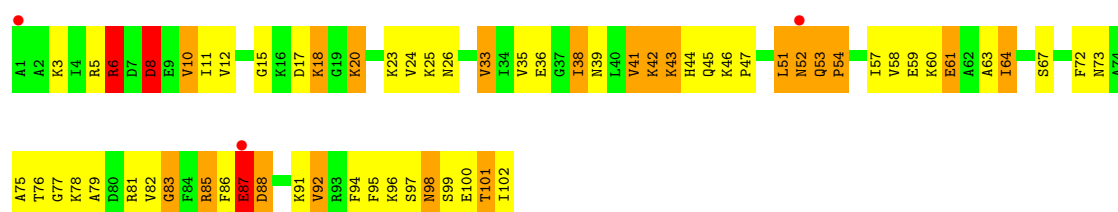
• Molecule 41: 50S ribosomal protein L23



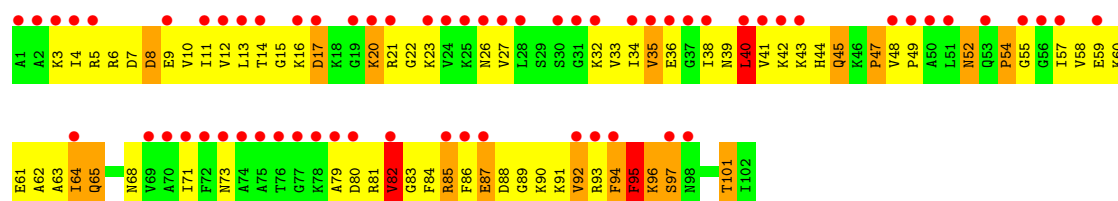
• Molecule 41: 50S ribosomal protein L23



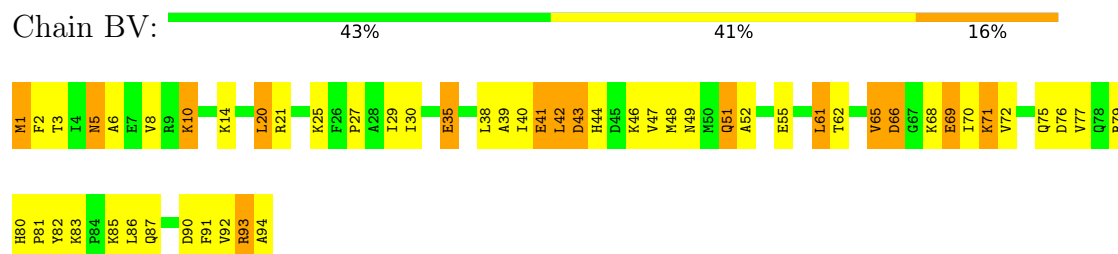
• Molecule 42: 50S ribosomal protein L24



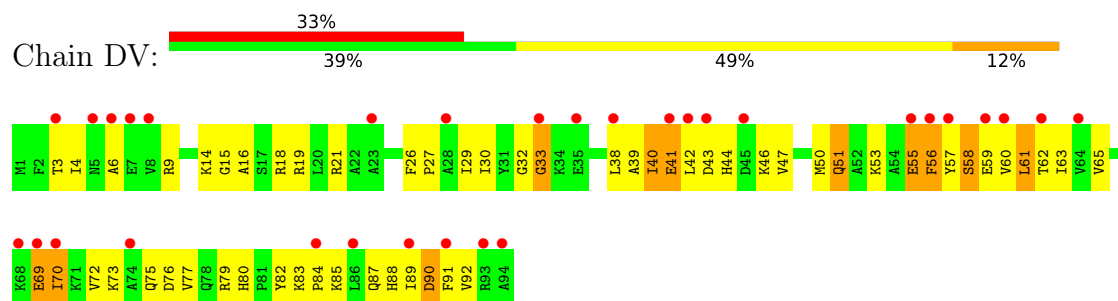
• Molecule 42: 50S ribosomal protein L24



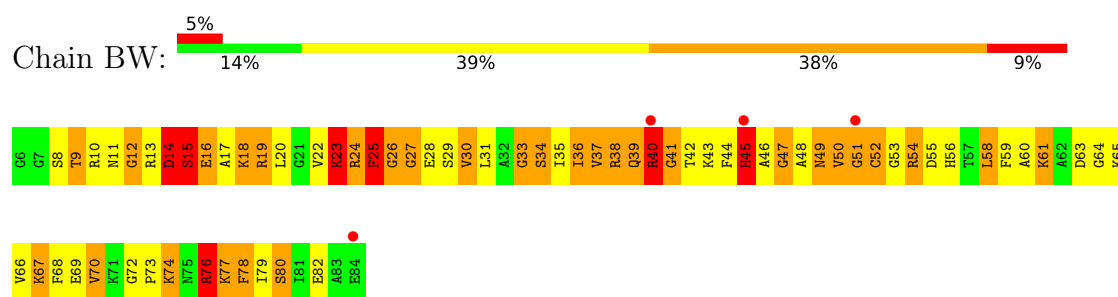
- Molecule 43: 50S ribosomal protein L25



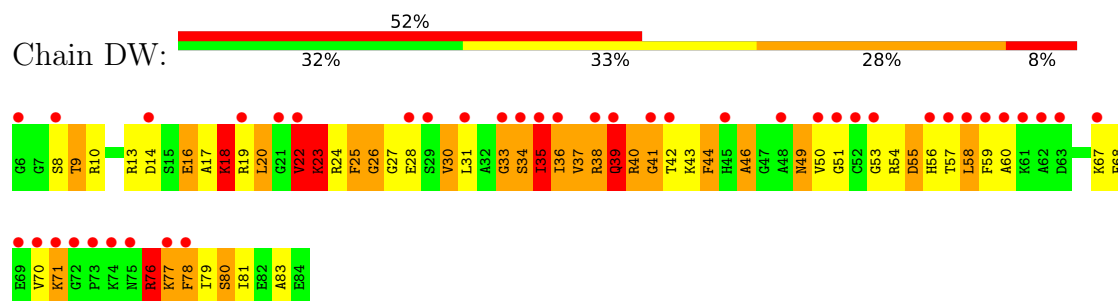
- Molecule 43: 50S ribosomal protein L25



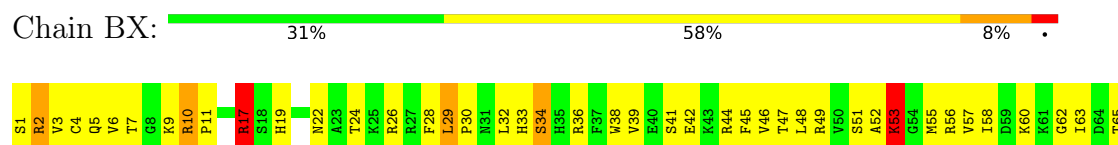
- Molecule 44: 50S ribosomal protein L27



- Molecule 44: 50S ribosomal protein L27

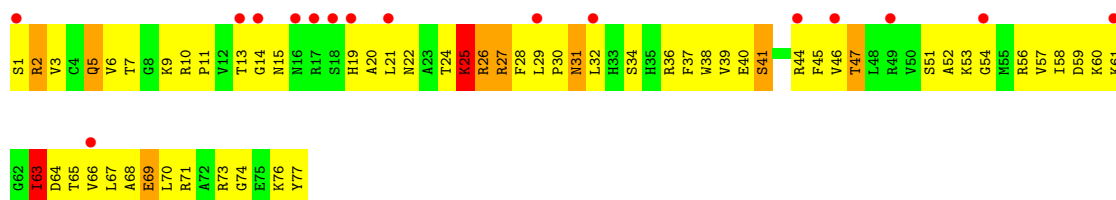


- Molecule 45: 50S ribosomal protein L28

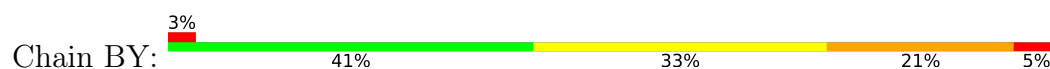




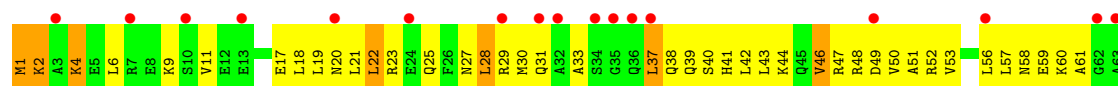
- Molecule 45: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L29



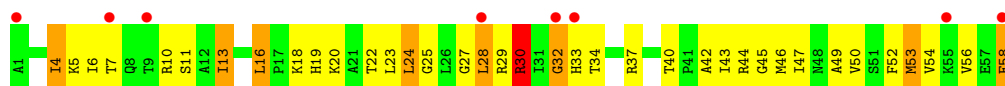
- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30



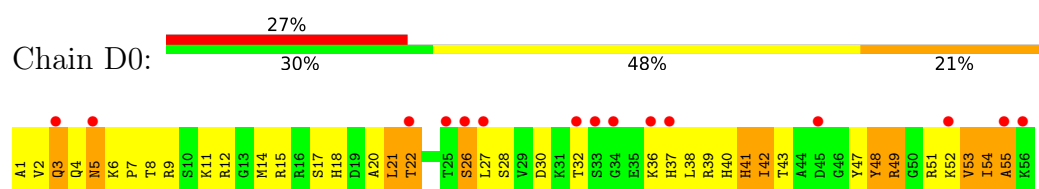
- Molecule 47: 50S ribosomal protein L30



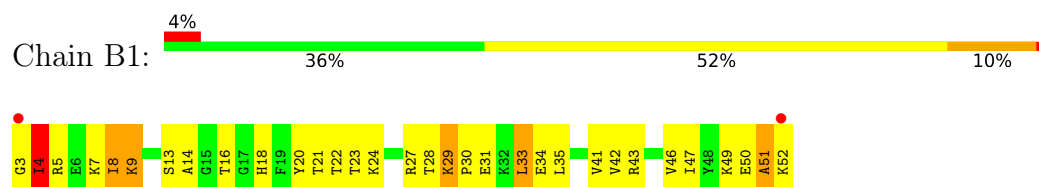
- Molecule 48: 50S ribosomal protein L32



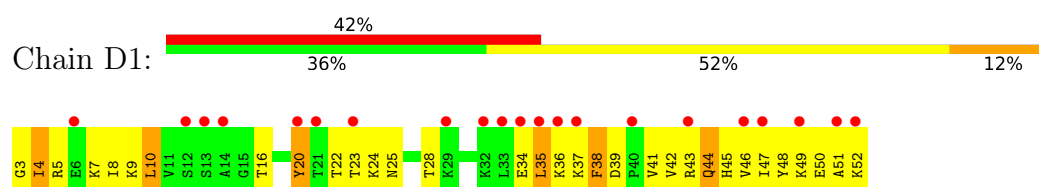
- Molecule 48: 50S ribosomal protein L32



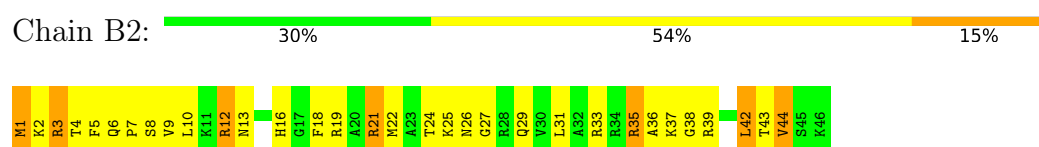
• Molecule 49: 50S ribosomal protein L33



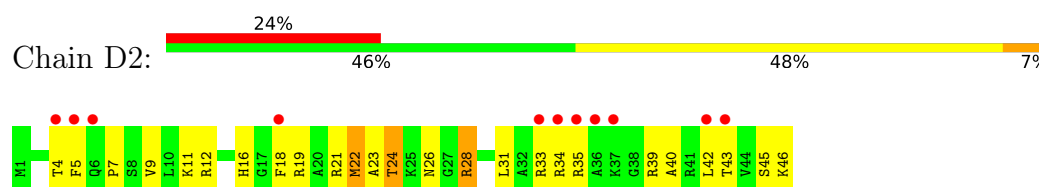
• Molecule 49: 50S ribosomal protein L33



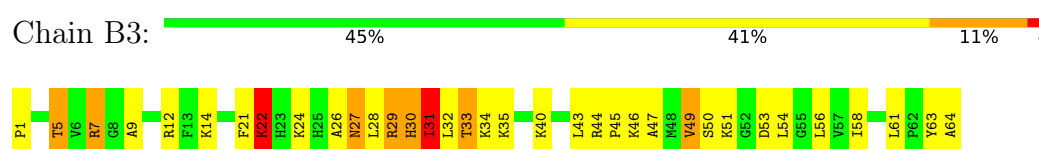
• Molecule 50: 50S ribosomal protein L34



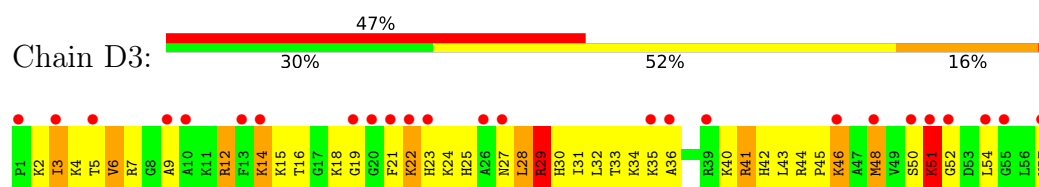
• Molecule 50: 50S ribosomal protein L34



• Molecule 51: 50S ribosomal protein L35

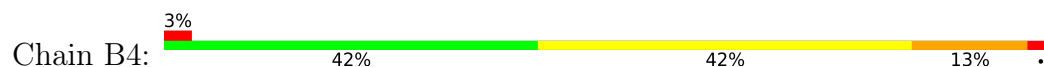


• Molecule 51: 50S ribosomal protein L35

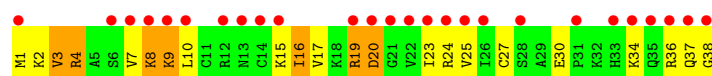




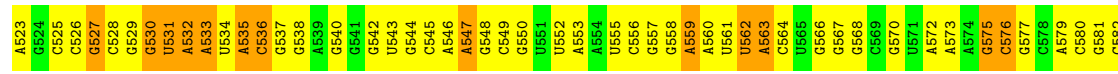
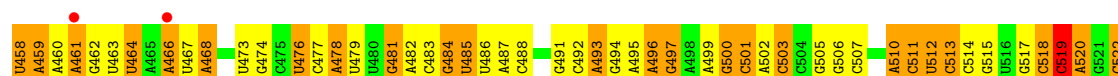
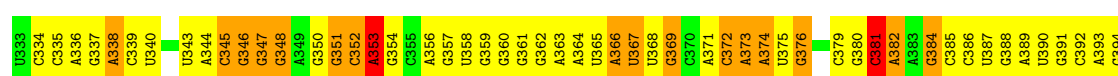
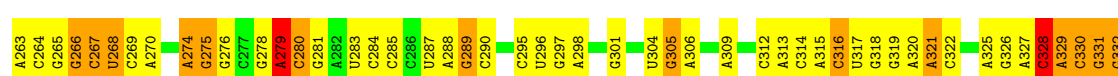
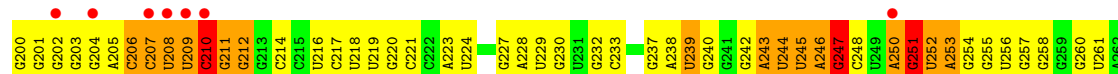
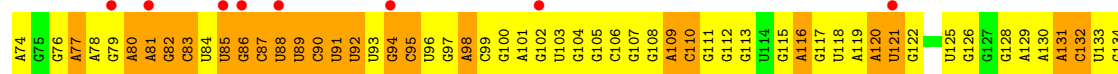
- Molecule 52: 50S ribosomal protein L36



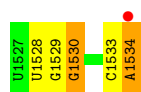
- Molecule 52: 50S ribosomal protein L36



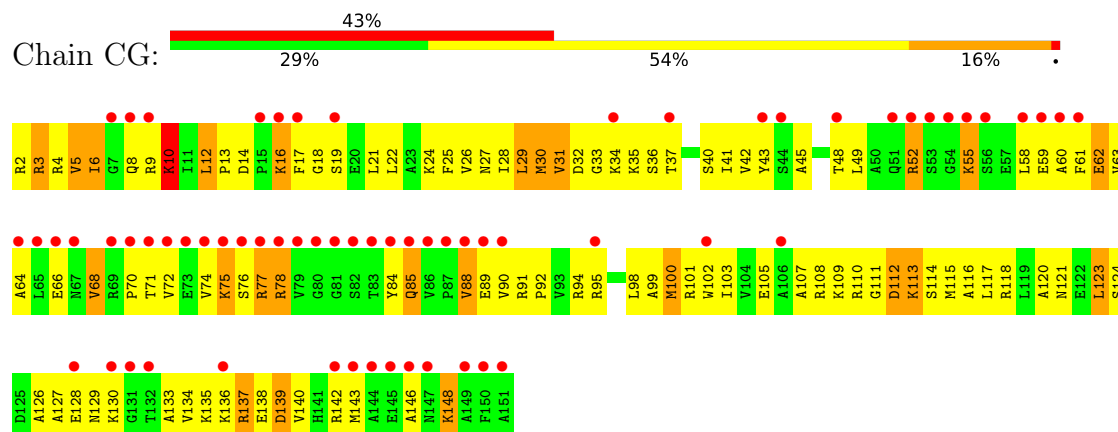
- Molecule 53: 16S rRNA



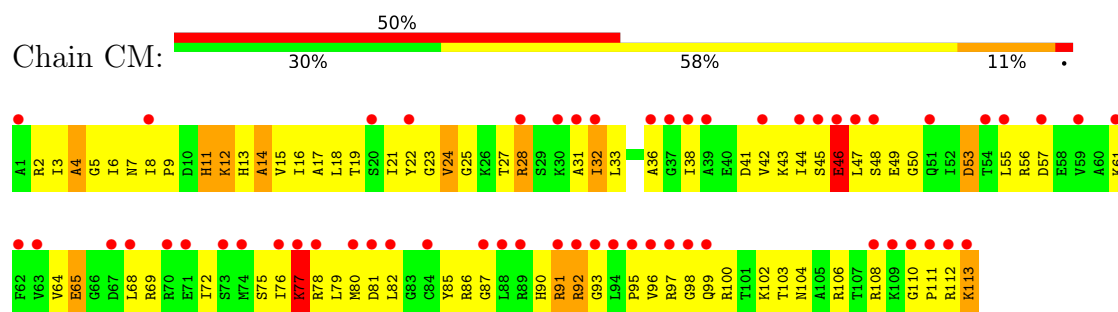
U1463	A1394	U1330	C1267	C1200	U1135	G1068	A1005	G941	U871	C726	A654	A583
U1464	C1395	G1331	G1268	A1201	C1136	C1069	G1006	G942	A872	G727	A655	G584
C1397	A1332	A1332	A1269	C1203	C1137	C1070	U1007		A873	A728		
A1468	C1398	A1333	A1270		G1138	C1071	U1008	G945	G874	A729	C658	G587
	C1399	U1335	A1271	G1206	C1139	G1072	U1009	A946	U875	G730	U659	U590
C1400	U1336	U1335	C1272	G1207	C1140	U1073	U1010	G947	A802	G731		U591
U1471	C1337	C1336	C1273	G1208	C1141	G1074	C1011	C948	G877	G732	A663	G592
U1472	G1338	C1337	A1274	C1268	G1142	U1075	A1012		A878	G733	G664	
A1476	A1339	G1338	A1275	C1209	G1143	U1076	G951		C879	G734	A665	A595
U1477	C1339	C1210	C1276	U1211	G1144	G1077	A1014		C880	C735	A666	A596
U1478	A1340	U1211	C1277	U1212	A1145	U1078	G952		C881	G736	G667	G597
C1407	C1342	U1212	G1278	A1213	A1146	G1079	G953		C882	C737	G668	U598
U1480	G1343	U1213	G1279	C1214	C1147	A1080	U1017			C738	G669	C599
U1481	C1344	U1214	A1280	G1215	U1148	A1081	G1018		G885	C739		
G1482	U1345	G1215	C1281	G1216	C1149	A1082	A1019		G886	U740	U672	G604
A1410	A1346	C1217	U1283	C1218	A1150	U1083	G959		A814	U741	A673	U605
C1411	C1347	C1218	U1284	C1219	A1151	G1084	U1021		A815	G745	A674	G606
A1483	U1348	U1285	C1284	A1219	A1152	U1085	U960		A816	U746	A675	G607
U1484	C1349	A1285	C1284	G1220	G1153	G1086	U1022		G817	A747	A676	A608
U1485	A1413	U1286	U1287	G1221	G1154	U1087	G1024		A819	G748	U677	A609
G1486	U1414	A1287	A1288	G1222	A1155	G1088	G966		U820	A749	U678	U610
G1487	U1351	A1288	C1223	C1223	A1157	U1089	G1026		U821	C750	C679	C611
G1488	C1352	A1289	C1224	U1224	C1158	U1091	U1029		U822	G751		C612
				A1225	U1159	A1092	U1030		G823	G752	U684	C613
A1491	G1356	C1293	C1294	C1226	C1159	A1093	C1031		G824	U753	G685	C614
A1492	A1357	U1295	C1295	A1227	G1160	G1094	G1032		A825	A754	U686	G615
A1493	U1358	C1296	C1296	C1228	C1161	U1095	G1033		C826	C755	A687	G616
U1495	C1359	C1297	U1297	A1229	C1162	C1096	G1034		U827	G756	G688	G617
A1496	A1360	G1298	C1298			C1097	U1035		U904	U757	C689	G618
U1497	G1361	U1298	C1298		A1167	C1098	A1036		A905	C758	G691	U619
A1430	A1362	A1299	C1300	C1237	U1168	C1099	C1037		A906	A759	U692	C623
A1431	U1363	C1301	U1301	A1238	A1169	C1100	C1038		A907	G760	G693	C624
G1432	C1364	C1302	C1302	U1240	U1170	A1101	G1039		A908	G761	A694	U625
A1434	G1365	C1303	C1303	G1241	C1171	A1102	U1040		A909	U762	A695	
A1435	C1366	G1304	C1304	G1242	U1173	C1103	C980		A910	G763	A696	
U1436	C1367	G1305	G1305	C1243	U1174	G1104	A1042		A913	G764	A629	A630
	A1368			G1244	G1175	A1105	G1043		A914	G765	C631	C632
A1437	C1369	U1308	U1308	C1245	A1176	C1106	A1046		A918	G769	U701	U633
G1438	G1370	G1309	G1310	C1246	C1177	G1107	G1047		A919	C770	A702	
U1506	U1371	C1310	C1310	U1247	G1178	G1108	C985		A920	G771	G703	G633
A1507	C1372	A1311	A1311	A1248	A1179	G1109	U920		U921	G775	A704	
A1508	G1373	C1312	C1312	C1249	A1180	C1113	U1049		G922	G776	G705	U636
C1509	A1374	U1313	U1313	A1250	G1181	C1114	G1050		A923	A777	U707	U638
C1510	A1375	C1314	C1314	A1251	G1182		C1051				C708	U639
G1511		U1315	U1315	A1252	U1183	C1118	U1052		G926	A780	U709	A640
U1512	C1378	C1316	C1316	A1253	G1184	C1119	G1053		G927	A781		U641
A1513	A1447	C1317	C1317	U1254	C1185	U1123	C1054		G928	A782	A712	A642
G1514	U1380	A1318	A1318	G1255	G1186	G1124	A1055		G929		G713	C643
U1515	U1381	C1319	C1319	A1256		U1125	U1056		C930			U644
G1516	C1382	A1319	A1319	A1257	G1190	U1126	G1057		C931	G785	U717	G645
U1451	C1383	C1320	C1320	U1258	A1191	U1127	U1060		G932	G786	A718	G646
C1452		U1321	U1321	C1259	C1192	C1128	G1061		C933	A787	C719	C647
A1519	G1386	C1322	C1322	U1260	G1193	C1129	U1062		C934		G720	A648
C1520	G1387	G1323	G1323	A1261	U1194	C1130	C1063		C935	A790	G721	A649
C1521	C1388	A1324	A1324	C1262	C1195	U1131	G1064		C936	G791	G722	G650
G1455	C1389	C1325	C1325	C1263	A1196	C1132	U1065		A937	U792	U723	C651
U1456	U1390	U1326	U1326	U1264	A1197	G1133	C1066			G793	G724	U652
G1457	U1391	C1327	C1327	C1265	G1198	C1134	A1067			A794		U653
G1458	C1392	A1329	A1329	G1266	U1199							



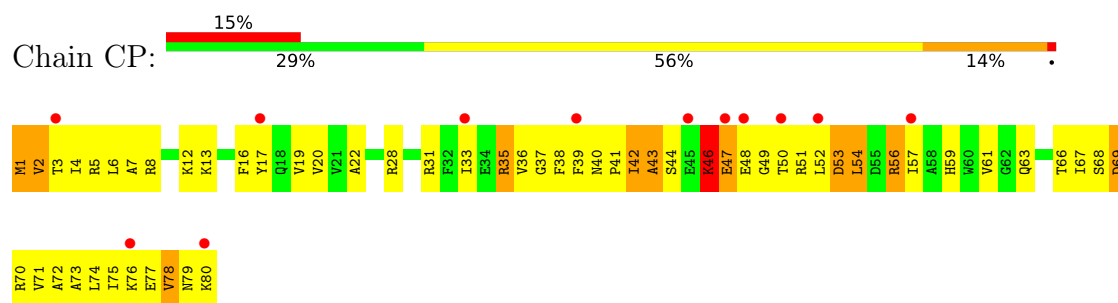
• Molecule 54: 30S ribosomal protein S7



• Molecule 55: 30S ribosomal protein S13



• Molecule 56: 30S ribosomal protein S16

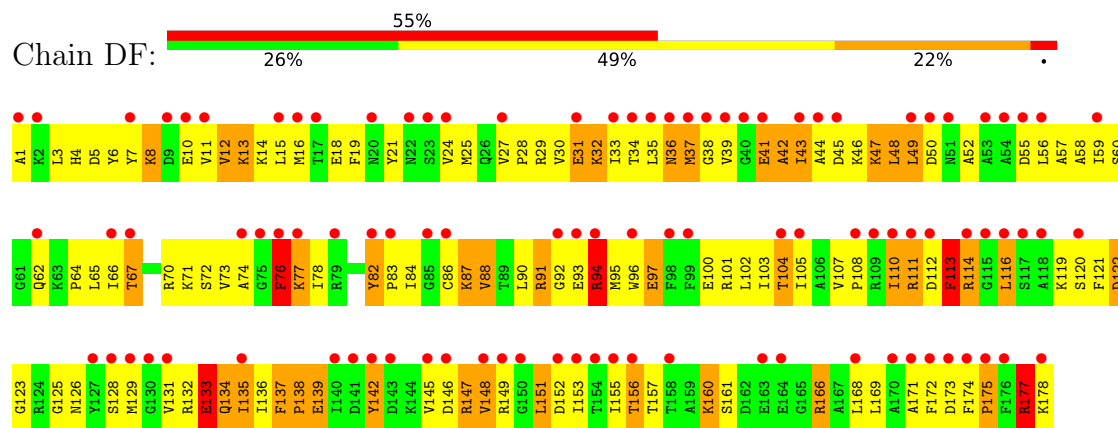


• Molecule 57: 5S rRNA



● Molecule 58: 50S ribosomal protein L5

Chain DF:



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)	Xtriage
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	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.45	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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
39	BR	20	VAL
50	B2	9	VAL
39	DR	58	VAL
40	BS	48	LYS
44	BW	14	ASP

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

Mol	Chain	Res	Type
41	BT	91	GLN
3	CC	31	ASN
42	DU	44	HIS
43	BV	44	HIS
47	BZ	33	HIS

5.3.3 RNA ⓘ

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
53	CA	512	U
22	DA	52	A
22	DA	2492	U
53	CA	701	U
53	CA	1142	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:

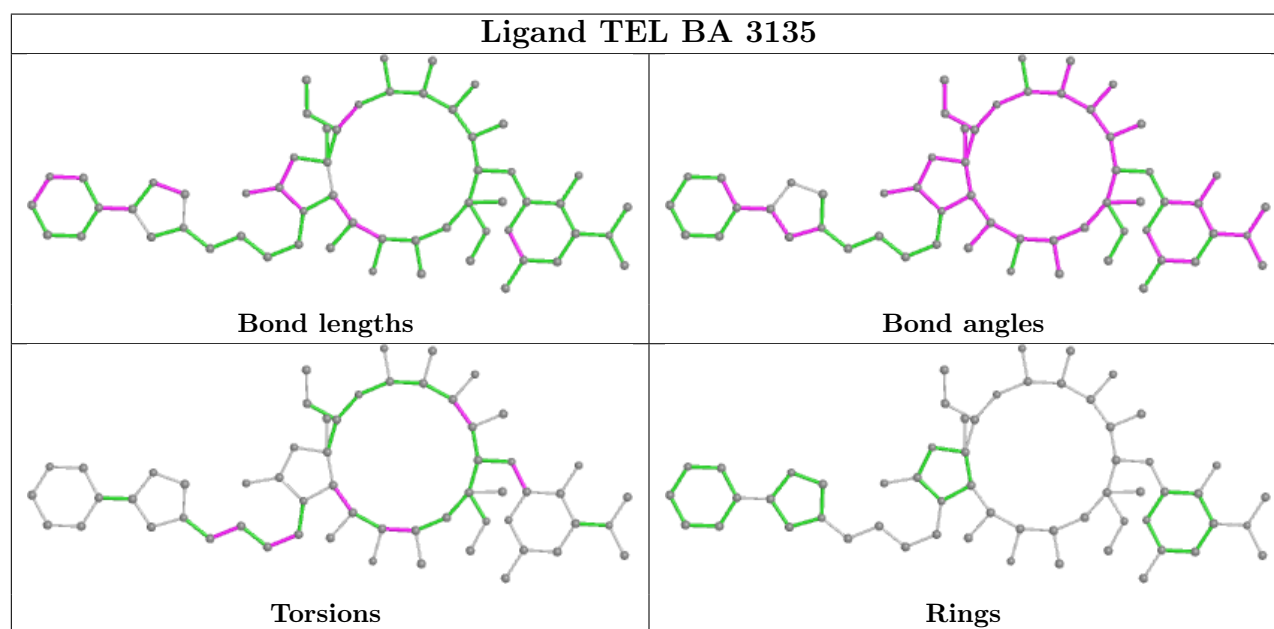
Mol	Chain	Res	Type	Atoms
60	BA	3135	TEL	C2-C3-C7-C12
60	BA	3135	TEL	C2-C3-C7-C13
60	BA	3135	TEL	O18-C13-C19-C23
60	BA	3135	TEL	N6-C11-C17-C22
60	BA	3135	TEL	C17-C22-C27-N31

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1533/1533 (100%)	-0.42	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	45, 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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, 75, 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

Continued on next page...

Continued from previous page...

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 ⓘ

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(\AA^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	DA	3106	1/1	0.45	0.74	316,316,316,316	0
59	MG	CA	1618	1/1	0.45	0.30	146,146,146,146	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	CA	1628	1/1	0.56	0.16	165,165,165,165	0
59	MG	DA	3090	1/1	0.56	0.11	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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	3024	1/1	0.58	0.20	100,100,100,100	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	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	3132	1/1	0.62	0.87	185,185,185,185	0
59	MG	DA	3026	1/1	0.62	0.91	258,258,258,258	0
59	MG	DA	3015	1/1	0.63	0.74	176,176,176,176	0
59	MG	DA	3010	1/1	0.63	0.57	195,195,195,195	0
59	MG	DA	3083	1/1	0.63	0.29	204,204,204,204	0
59	MG	DA	3003	1/1	0.65	0.82	229,229,229,229	0
59	MG	DA	3014	1/1	0.66	0.37	133,133,133,133	0
59	MG	DA	3079	1/1	0.66	0.89	200,200,200,200	0
59	MG	DA	3001	1/1	0.66	0.09	149,149,149,149	0
59	MG	DA	3064	1/1	0.66	0.66	280,280,280,280	0
59	MG	DA	3099	1/1	0.66	0.19	164,164,164,164	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	3038	1/1	0.67	0.12	203,203,203,203	0
59	MG	AA	1616	1/1	0.68	0.14	106,106,106,106	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	DA	3078	1/1	0.69	0.24	182,182,182,182	0
59	MG	CA	1613	1/1	0.70	0.15	107,107,107,107	0
59	MG	CA	1615	1/1	0.70	0.30	170,170,170,170	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	CA	1610	1/1	0.72	0.06	151,151,151,151	0
59	MG	DA	3062	1/1	0.72	0.56	213,213,213,213	0
59	MG	DA	3032	1/1	0.72	0.19	131,131,131,131	0
59	MG	DA	3050	1/1	0.72	0.28	160,160,160,160	0
59	MG	DA	3098	1/1	0.73	0.33	151,151,151,151	0

Continued on next page...

Continued from previous page...

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	CA	1620	1/1	0.73	0.15	164,164,164,164	0
59	MG	DA	3030	1/1	0.74	0.31	104,104,104,104	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	CA	1637	1/1	0.75	0.11	170,170,170,170	0
59	MG	AA	1627	1/1	0.75	0.37	137,137,137,137	0
59	MG	DA	3071	1/1	0.75	0.18	74,74,74,74	0
59	MG	DA	3035	1/1	0.75	0.14	79,79,79,79	0
59	MG	DA	3113	1/1	0.76	0.12	121,121,121,121	0
59	MG	DA	3087	1/1	0.76	0.28	152,152,152,152	0
59	MG	DA	3041	1/1	0.76	0.15	110,110,110,110	0
59	MG	DA	3116	1/1	0.76	0.12	54,54,54,54	0
59	MG	DA	3059	1/1	0.76	0.39	197,197,197,197	0
59	MG	DA	3036	1/1	0.77	0.58	222,222,222,222	0
59	MG	DA	3033	1/1	0.77	0.32	132,132,132,132	0
61	ZN	D4	101	1/1	0.77	0.10	157,157,157,157	0
59	MG	DA	3056	1/1	0.77	0.18	72,72,72,72	0
59	MG	DA	3053	1/1	0.77	0.25	98,98,98,98	0
59	MG	AA	1619	1/1	0.77	0.69	209,209,209,209	0
59	MG	BA	3068	1/1	0.77	0.09	151,151,151,151	0
59	MG	DA	3021	1/1	0.78	0.15	83,83,83,83	0
59	MG	DA	3104	1/1	0.78	0.16	33,33,33,33	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	AA	1626	1/1	0.79	0.10	52,52,52,52	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	CA	1601	1/1	0.79	0.10	120,120,120,120	0
59	MG	DA	3048	1/1	0.80	0.15	95,95,95,95	0
59	MG	AA	1603	1/1	0.80	0.14	131,131,131,131	0
59	MG	BA	3007	1/1	0.80	0.15	104,104,104,104	0
59	MG	CA	1623	1/1	0.80	0.17	121,121,121,121	0
59	MG	BA	3018	1/1	0.80	0.14	44,44,44,44	0
59	MG	CA	1608	1/1	0.80	0.17	44,44,44,44	0
59	MG	DA	3115	1/1	0.80	0.21	126,126,126,126	0
59	MG	CA	1602	1/1	0.81	0.16	145,145,145,145	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	1626	1/1	0.81	0.40	196,196,196,196	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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	CA	1612	1/1	0.82	0.41	113,113,113,113	0
59	MG	AA	1623	1/1	0.82	0.12	89,89,89,89	0
59	MG	DA	3017	1/1	0.82	0.13	51,51,51,51	0
59	MG	CA	1616	1/1	0.82	0.39	203,203,203,203	0
59	MG	DA	3031	1/1	0.82	0.18	76,76,76,76	0
59	MG	DB	201	1/1	0.82	0.10	88,88,88,88	0
59	MG	DA	3122	1/1	0.83	0.15	94,94,94,94	0
59	MG	DA	3124	1/1	0.83	0.18	70,70,70,70	0
59	MG	DA	3095	1/1	0.83	0.20	122,122,122,122	0
59	MG	DA	3013	1/1	0.83	0.38	189,189,189,189	0
59	MG	BA	3089	1/1	0.83	0.13	95,95,95,95	0
59	MG	DA	3096	1/1	0.83	0.14	93,93,93,93	0
59	MG	DA	3094	1/1	0.84	0.26	134,134,134,134	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	3076	1/1	0.84	0.25	149,149,149,149	0
59	MG	AA	1638	1/1	0.84	0.17	47,47,47,47	0
59	MG	CE	201	1/1	0.84	0.27	132,132,132,132	0
59	MG	AA	1630	1/1	0.84	0.37	189,189,189,189	0
59	MG	DA	3070	1/1	0.85	0.13	60,60,60,60	0
59	MG	DA	3055	1/1	0.85	0.11	72,72,72,72	0
59	MG	CA	1625	1/1	0.85	0.17	48,48,48,48	0
59	MG	AA	1639	1/1	0.85	0.12	109,109,109,109	0
59	MG	BB	201	1/1	0.85	0.28	228,228,228,228	0
59	MG	BA	3085	1/1	0.85	0.20	124,124,124,124	0
59	MG	DA	3118	1/1	0.85	0.10	59,59,59,59	0
59	MG	DA	3046	1/1	0.85	0.24	125,125,125,125	0
59	MG	AA	1602	1/1	0.85	0.12	152,152,152,152	0
59	MG	DA	3128	1/1	0.86	0.31	116,116,116,116	0
59	MG	BA	3057	1/1	0.86	0.14	147,147,147,147	0
59	MG	CA	1636	1/1	0.87	0.30	119,119,119,119	0
59	MG	DA	3042	1/1	0.87	0.20	99,99,99,99	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	BA	3004	1/1	0.87	0.24	156,156,156,156	0
59	MG	DA	3073	1/1	0.87	0.08	148,148,148,148	0
59	MG	BA	3045	1/1	0.87	0.14	30,30,30,30	0
59	MG	AA	1625	1/1	0.87	0.08	64,64,64,64	0
59	MG	DA	3075	1/1	0.88	0.41	172,172,172,172	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	1627	1/1	0.88	1.25	237,237,237,237	0
59	MG	BA	3059	1/1	0.88	0.33	129,129,129,129	0
59	MG	AA	1637	1/1	0.88	0.12	96,96,96,96	0
59	MG	DA	3100	1/1	0.88	0.33	105,105,105,105	0
59	MG	DA	3121	1/1	0.88	0.13	122,122,122,122	0
59	MG	CA	1631	1/1	0.89	0.10	160,160,160,160	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	BA	3055	1/1	0.89	0.35	215,215,215,215	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	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	DA	3117	1/1	0.90	0.20	73,73,73,73	0
59	MG	BA	3131	1/1	0.90	0.40	184,184,184,184	0
59	MG	CA	1638	1/1	0.90	0.09	141,141,141,141	0
59	MG	DA	3103	1/1	0.90	0.17	76,76,76,76	0
59	MG	CA	1606	1/1	0.90	0.16	54,54,54,54	0
59	MG	AA	1614	1/1	0.90	0.17	156,156,156,156	0
59	MG	BB	202	1/1	0.90	0.06	64,64,64,64	0
59	MG	BA	3005	1/1	0.90	0.11	75,75,75,75	0
59	MG	DA	3012	1/1	0.90	0.21	41,41,41,41	0
59	MG	DA	3081	1/1	0.90	0.28	78,78,78,78	0
59	MG	CA	1629	1/1	0.91	0.24	126,126,126,126	0
59	MG	DA	3009	1/1	0.91	0.14	100,100,100,100	0
59	MG	AA	1607	1/1	0.91	0.07	105,105,105,105	0
59	MG	AA	1621	1/1	0.91	0.17	143,143,143,143	0
59	MG	CA	1621	1/1	0.91	0.18	50,50,50,50	0
59	MG	AA	1641	1/1	0.91	0.23	148,148,148,148	0
59	MG	DC	302	1/1	0.91	0.31	159,159,159,159	0
59	MG	DA	3119	1/1	0.91	0.11	67,67,67,67	0
59	MG	BA	3034	1/1	0.91	0.28	197,197,197,197	0
59	MG	DA	3029	1/1	0.91	0.94	142,142,142,142	0
59	MG	BA	3070	1/1	0.91	0.21	135,135,135,135	0
59	MG	CA	1611	1/1	0.91	0.19	111,111,111,111	0
59	MG	BA	3103	1/1	0.91	0.17	21,21,21,21	0
59	MG	DA	3080	1/1	0.91	0.11	152,152,152,152	0
59	MG	BA	3010	1/1	0.92	0.07	17,17,17,17	0
59	MG	DA	3023	1/1	0.92	0.14	111,111,111,111	0
59	MG	DA	3052	1/1	0.92	0.12	56,56,56,56	0
59	MG	BA	3108	1/1	0.92	0.09	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3115	1/1	0.92	0.10	7,7,7,7	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
59	MG	BA	3114	1/1	0.92	0.15	8,8,8,8	0
59	MG	DA	3093	1/1	0.92	0.17	234,234,234,234	0
59	MG	DA	3114	1/1	0.92	0.10	147,147,147,147	0
59	MG	BA	3023	1/1	0.92	0.10	16,16,16,16	0
59	MG	DA	3068	1/1	0.92	0.16	67,67,67,67	0
59	MG	CA	1639	1/1	0.92	0.22	161,161,161,161	0
59	MG	AA	1620	1/1	0.92	0.10	126,126,126,126	0
59	MG	BA	3067	1/1	0.93	0.12	17,17,17,17	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	3001	1/1	0.93	0.09	117,117,117,117	0
59	MG	BB	204	1/1	0.93	0.08	23,23,23,23	0
59	MG	BA	3118	1/1	0.93	0.14	23,23,23,23	0
59	MG	DA	3105	1/1	0.93	0.20	61,61,61,61	0
59	MG	BA	3077	1/1	0.93	0.13	38,38,38,38	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	DA	3131	1/1	0.93	0.17	91,91,91,91	0
59	MG	BA	3129	1/1	0.93	1.07	243,243,243,243	0
59	MG	CA	1633	1/1	0.93	0.14	138,138,138,138	0
59	MG	DA	3065	1/1	0.93	0.17	77,77,77,77	0
59	MG	BB	203	1/1	0.94	0.11	34,34,34,34	0
59	MG	CA	1630	1/1	0.94	0.27	126,126,126,126	0
59	MG	BA	3121	1/1	0.94	0.13	35,35,35,35	0
59	MG	BA	3074	1/1	0.94	0.17	85,85,85,85	0
59	MG	BA	3073	1/1	0.94	0.17	17,17,17,17	0
59	MG	BA	3076	1/1	0.94	0.10	119,119,119,119	0
59	MG	BA	3078	1/1	0.94	0.20	31,31,31,31	0
59	MG	AA	1636	1/1	0.94	0.32	199,199,199,199	0
59	MG	BA	3048	1/1	0.94	0.17	101,101,101,101	0
59	MG	BA	3047	1/1	0.94	0.09	151,151,151,151	0
59	MG	AA	1631	1/1	0.94	0.17	168,168,168,168	0
59	MG	AA	1624	1/1	0.94	0.15	102,102,102,102	0
59	MG	BA	3133	1/1	0.94	0.26	146,146,146,146	0
59	MG	BA	3060	1/1	0.94	0.30	188,188,188,188	0
59	MG	BA	3122	1/1	0.94	0.71	155,155,155,155	0
59	MG	BA	3088	1/1	0.94	0.10	62,62,62,62	0
59	MG	DA	3101	1/1	0.94	0.13	75,75,75,75	0
59	MG	AA	1633	1/1	0.94	0.10	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1635	1/1	0.94	0.14	73,73,73,73	0
59	MG	BA	3127	1/1	0.94	0.14	2,2,2,2	0
59	MG	BA	3024	1/1	0.94	0.12	18,18,18,18	0
59	MG	AA	1618	1/1	0.94	0.18	87,87,87,87	0
59	MG	BA	3081	1/1	0.94	0.18	92,92,92,92	0
59	MG	AA	1613	1/1	0.95	0.08	50,50,50,50	0
59	MG	BA	3086	1/1	0.95	0.12	134,134,134,134	0
59	MG	BA	3110	1/1	0.95	0.16	89,89,89,89	0
59	MG	BA	3036	1/1	0.95	0.34	187,187,187,187	0
59	MG	BA	3132	1/1	0.95	0.13	1,1,1,1	0
59	MG	DA	3034	1/1	0.95	0.17	78,78,78,78	0
59	MG	BA	3046	1/1	0.95	0.08	12,12,12,12	0
59	MG	AA	1610	1/1	0.95	0.11	201,201,201,201	0
59	MG	BA	3124	1/1	0.95	0.14	33,33,33,33	0
59	MG	BA	3017	1/1	0.95	0.11	33,33,33,33	0
59	MG	BA	3037	1/1	0.95	0.17	24,24,24,24	0
59	MG	BA	3083	1/1	0.95	0.17	37,37,37,37	0
59	MG	AA	1609	1/1	0.95	0.12	54,54,54,54	0
59	MG	BA	3091	1/1	0.95	0.07	49,49,49,49	0
59	MG	CA	1634	1/1	0.95	0.09	74,74,74,74	0
59	MG	BA	3033	1/1	0.95	0.21	14,14,14,14	0
59	MG	CA	1641	1/1	0.95	0.12	82,82,82,82	0
59	MG	AA	1605	1/1	0.95	0.12	52,52,52,52	0
59	MG	AA	1640	1/1	0.95	0.04	84,84,84,84	0
59	MG	BA	3062	1/1	0.95	0.18	5,5,5,5	0
59	MG	AA	1604	1/1	0.95	0.09	121,121,121,121	0
59	MG	AA	1643	1/1	0.95	0.12	43,43,43,43	0
59	MG	BA	3095	1/1	0.95	0.19	117,117,117,117	0
59	MG	AA	1612	1/1	0.95	0.10	85,85,85,85	0
59	MG	BA	3071	1/1	0.95	0.11	7,7,7,7	0
59	MG	BA	3097	1/1	0.95	0.10	33,33,33,33	0
59	MG	BA	3063	1/1	0.95	0.13	12,12,12,12	0
59	MG	CA	1604	1/1	0.95	0.05	57,57,57,57	0
59	MG	BA	3101	1/1	0.95	0.09	18,18,18,18	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	3032	1/1	0.96	0.12	25,25,25,25	0
59	MG	BA	3096	1/1	0.96	0.14	93,93,93,93	0
59	MG	DA	3066	1/1	0.96	0.14	61,61,61,61	0
59	MG	BA	3109	1/1	0.96	0.16	112,112,112,112	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3025	1/1	0.96	0.18	104,104,104,104	0
61	ZN	B4	101	1/1	0.96	0.07	118,118,118,118	0
59	MG	BA	3011	1/1	0.96	0.21	126,126,126,126	0
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	1606	1/1	0.96	0.08	72,72,72,72	0
59	MG	AA	1601	1/1	0.96	0.10	77,77,77,77	0
59	MG	BA	3002	1/1	0.96	0.10	85,85,85,85	0
59	MG	AA	1615	1/1	0.96	0.10	128,128,128,128	0
59	MG	BA	3049	1/1	0.96	0.13	6,6,6,6	0
59	MG	BA	3022	1/1	0.96	0.16	5,5,5,5	0
59	MG	BA	3116	1/1	0.96	0.14	71,71,71,71	0
59	MG	BA	3051	1/1	0.96	0.17	24,24,24,24	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	3015	1/1	0.96	0.17	95,95,95,95	0
59	MG	BA	3102	1/1	0.96	0.21	9,9,9,9	0
59	MG	BA	3016	1/1	0.96	0.09	4,4,4,4	0
59	MG	BA	3029	1/1	0.97	0.10	52,52,52,52	0
59	MG	BA	3026	1/1	0.97	0.08	32,32,32,32	0
59	MG	BA	3119	1/1	0.97	0.07	47,47,47,47	0
59	MG	BA	3111	1/1	0.97	0.15	38,38,38,38	0
59	MG	BA	3035	1/1	0.97	0.10	5,5,5,5	0
59	MG	CA	1632	1/1	0.97	0.09	65,65,65,65	0
59	MG	BA	3120	1/1	0.97	0.21	3,3,3,3	0
59	MG	BA	3065	1/1	0.97	0.11	20,20,20,20	0
59	MG	BA	3058	1/1	0.97	0.04	47,47,47,47	0
59	MG	BA	3066	1/1	0.97	0.10	21,21,21,21	0
59	MG	BA	3072	1/1	0.97	0.21	97,97,97,97	0
60	TEL	BA	3135	58/58	0.97	0.22	0,23,68,74	0
59	MG	BA	3075	1/1	0.97	0.06	26,26,26,26	0
59	MG	BA	3064	1/1	0.97	0.13	5,5,5,5	0
59	MG	BA	3098	1/1	0.97	0.13	26,26,26,26	0
59	MG	CA	1609	1/1	0.97	0.12	97,97,97,97	0
59	MG	BA	3130	1/1	0.97	0.14	108,108,108,108	0
59	MG	AA	1634	1/1	0.97	0.08	62,62,62,62	0
59	MG	BA	3056	1/1	0.97	0.31	219,219,219,219	0
59	MG	BA	3107	1/1	0.97	0.16	12,12,12,12	0
59	MG	BA	3027	1/1	0.97	0.17	119,119,119,119	0
59	MG	DA	3054	1/1	0.97	0.14	70,70,70,70	0
59	MG	BA	3061	1/1	0.97	0.17	11,11,11,11	0
59	MG	BA	3012	1/1	0.97	0.13	1,1,1,1	0

Continued on next page...

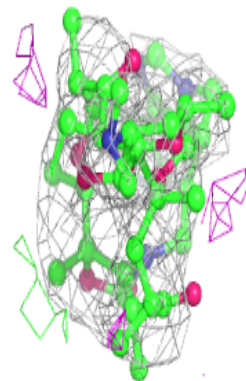
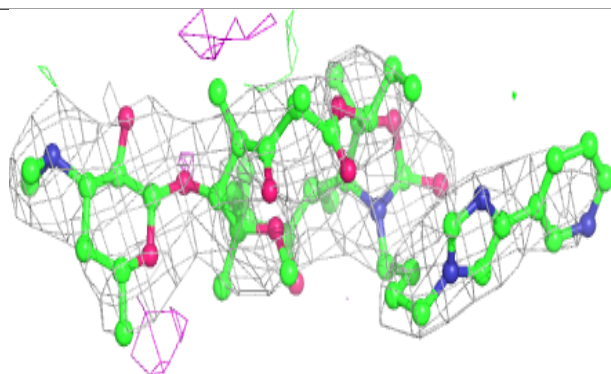
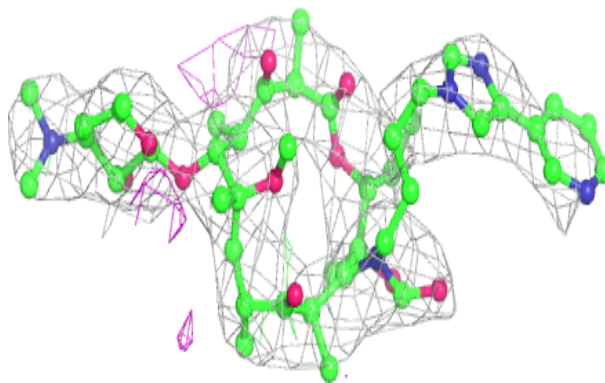
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	1624	1/1	0.97	0.26	128,128,128,128	0
59	MG	BA	3052	1/1	0.98	0.16	46,46,46,46	0
59	MG	BA	3123	1/1	0.98	0.14	11,11,11,11	0
59	MG	BA	3094	1/1	0.98	0.06	22,22,22,22	0
59	MG	BA	3014	1/1	0.98	0.21	44,44,44,44	0
59	MG	AA	1608	1/1	0.98	0.22	47,47,47,47	0
59	MG	BA	3084	1/1	0.98	0.16	3,3,3,3	0
59	MG	BA	3087	1/1	0.98	0.12	36,36,36,36	0
59	MG	BA	3050	1/1	0.98	0.09	33,33,33,33	0
59	MG	BA	3006	1/1	0.98	0.07	31,31,31,31	0
59	MG	BA	3013	1/1	0.98	0.19	1,1,1,1	0
59	MG	BA	3100	1/1	0.98	0.13	85,85,85,85	0
59	MG	BA	3053	1/1	0.98	0.15	6,6,6,6	0
59	MG	BA	3079	1/1	0.98	0.17	11,11,11,11	0
59	MG	BA	3093	1/1	0.98	0.07	35,35,35,35	0
59	MG	BA	3030	1/1	0.98	0.17	9,9,9,9	0
59	MG	CA	1605	1/1	0.98	0.14	32,32,32,32	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	AA	1611	1/1	0.98	0.07	60,60,60,60	0
59	MG	BA	3112	1/1	0.98	0.09	41,41,41,41	0
59	MG	BA	3082	1/1	0.98	0.11	109,109,109,109	0
59	MG	BA	3080	1/1	0.98	0.04	26,26,26,26	0
59	MG	BA	3128	1/1	0.98	0.12	15,15,15,15	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	3054	1/1	0.98	0.09	58,58,58,58	0
59	MG	AA	1642	1/1	0.98	0.14	36,36,36,36	0
59	MG	BA	3126	1/1	0.98	0.15	18,18,18,18	0
59	MG	BA	3039	1/1	0.99	0.16	8,8,8,8	0
59	MG	BA	3099	1/1	0.99	0.20	8,8,8,8	0
59	MG	BA	3019	1/1	0.99	0.18	13,13,13,13	0
59	MG	BA	3044	1/1	0.99	0.06	43,43,43,43	0
59	MG	AA	1622	1/1	0.99	0.19	40,40,40,40	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	3042	1/1	0.99	0.11	16,16,16,16	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.

Electron density around TEL BA 3135:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.