



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2024 – 04:25 AM EDT

PDB ID : 4V7V  
Title : Crystal structure of the E. coli ribosome bound to clindamycin.  
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.  
Deposited on : 2010-08-16  
Resolution : 3.29 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

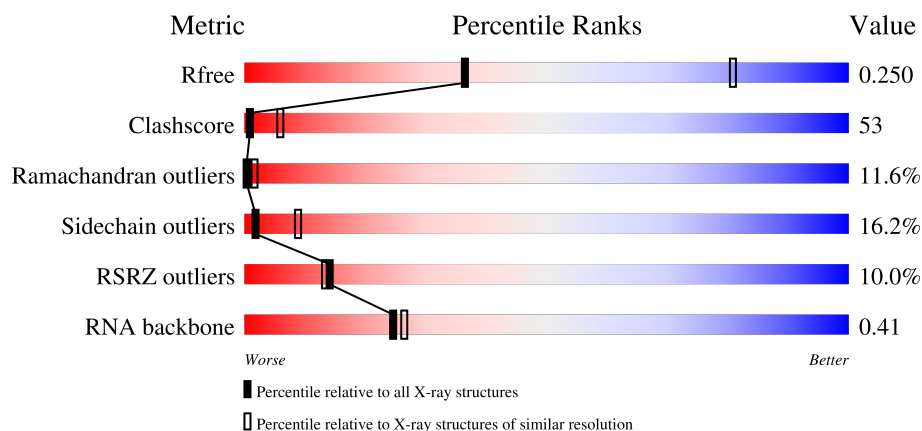
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 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))
$R_{free}$	164625	1214 (3.30-3.26)
Clashscore	180529	1265 (3.30-3.26)
Ramachandran outliers	177936	1264 (3.30-3.26)
Sidechain outliers	177891	1263 (3.30-3.26)
RSRZ outliers	164620	1215 (3.30-3.26)
RNA backbone	3690	1001 (3.60-2.96)

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  $\geq 3$ , 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	<div> <div>19%</div> <div>48%</div> <div>18%</div> <div>14%</div> </div>
2	AB	218	<div> <div>3%</div> <div>21%</div> <div>54%</div> <div>23%</div> <div>.</div> </div>
2	CB	218	<div> <div>8%</div> <div>25%</div> <div>60%</div> <div>14%</div> <div>.</div> </div>
3	AC	206	<div> <div>2%</div> <div>33%</div> <div>50%</div> <div>14%</div> <div>.</div> </div>

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

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

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Mol	Chain	Length	Quality of chain
31	BJ	142	
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	

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Mol	Chain	Length	Quality of chain
43	DV	94	
44	BW	79	
44	DW	79	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	
53	CA	1530	
54	CG	150	
55	CM	113	
56	CP	80	
57	DB	117	
58	DF	178	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3129	-	-	-	X
59	MG	DA	3025	-	-	-	X
59	MG	DA	3062	-	-	-	X
59	MG	DA	3073	-	-	-	X
59	MG	DA	3124	-	-	-	X

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 284501 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			

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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			

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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			

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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			

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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).

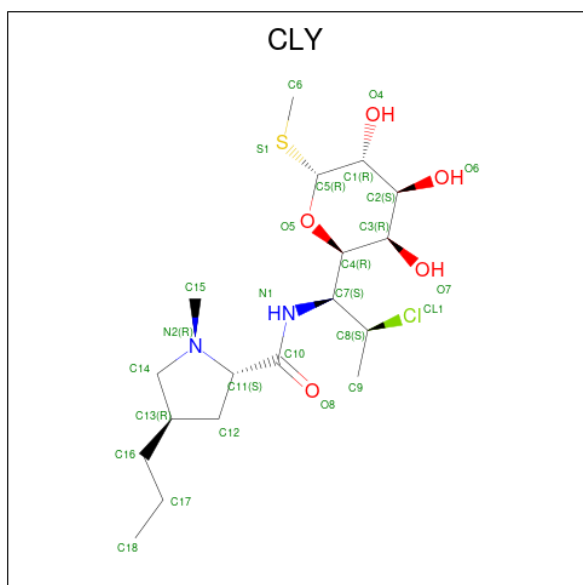
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	42	Total	Mg	0	0
			42	42		
59	AN	1	Total	Mg	0	0
			1	1		
59	BA	134	Total	Mg	0	0
			134	134		
59	BB	4	Total	Mg	0	0
			4	4		
59	BL	1	Total	Mg	0	0
			1	1		
59	CA	42	Total	Mg	0	0
			42	42		
59	DA	132	Total	Mg	0	0
			132	132		
59	DB	1	Total	Mg	0	0
			1	1		
59	DC	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DE	1	Total	Mg	0	0
			1	1		
59	DJ	1	Total	Mg	0	0
			1	1		

- Molecule 60 is CLINDAMYCIN (three-letter code: CLY) (formula:  $C_{18}H_{33}ClN_2O_5S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
60	BA	1	Total	C	Cl	N	O	S	0	0
			27	18	1	2	5	1		

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

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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AA	197	Total	O	0	0
			197	197		
62	AE	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AL	1	Total 1	O 1	0	0
62	AN	6	Total 6	O 6	0	0
62	AT	2	Total 2	O 2	0	0
62	AU	1	Total 1	O 1	0	0
62	BA	601	Total 601	O 601	0	0
62	BB	20	Total 20	O 20	0	0
62	BC	8	Total 8	O 8	0	0
62	BD	4	Total 4	O 4	0	0
62	BE	1	Total 1	O 1	0	0
62	BL	3	Total 3	O 3	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	3	Total 3	O 3	0	0
62	B2	2	Total 2	O 2	0	0
62	B3	2	Total 2	O 2	0	0
62	B4	1	Total 1	O 1	0	0
62	CA	193	Total 193	O 193	0	0
62	CE	4	Total 4	O 4	0	0
62	CI	1	Total 1	O 1	0	0
62	CL	1	Total 1	O 1	0	0

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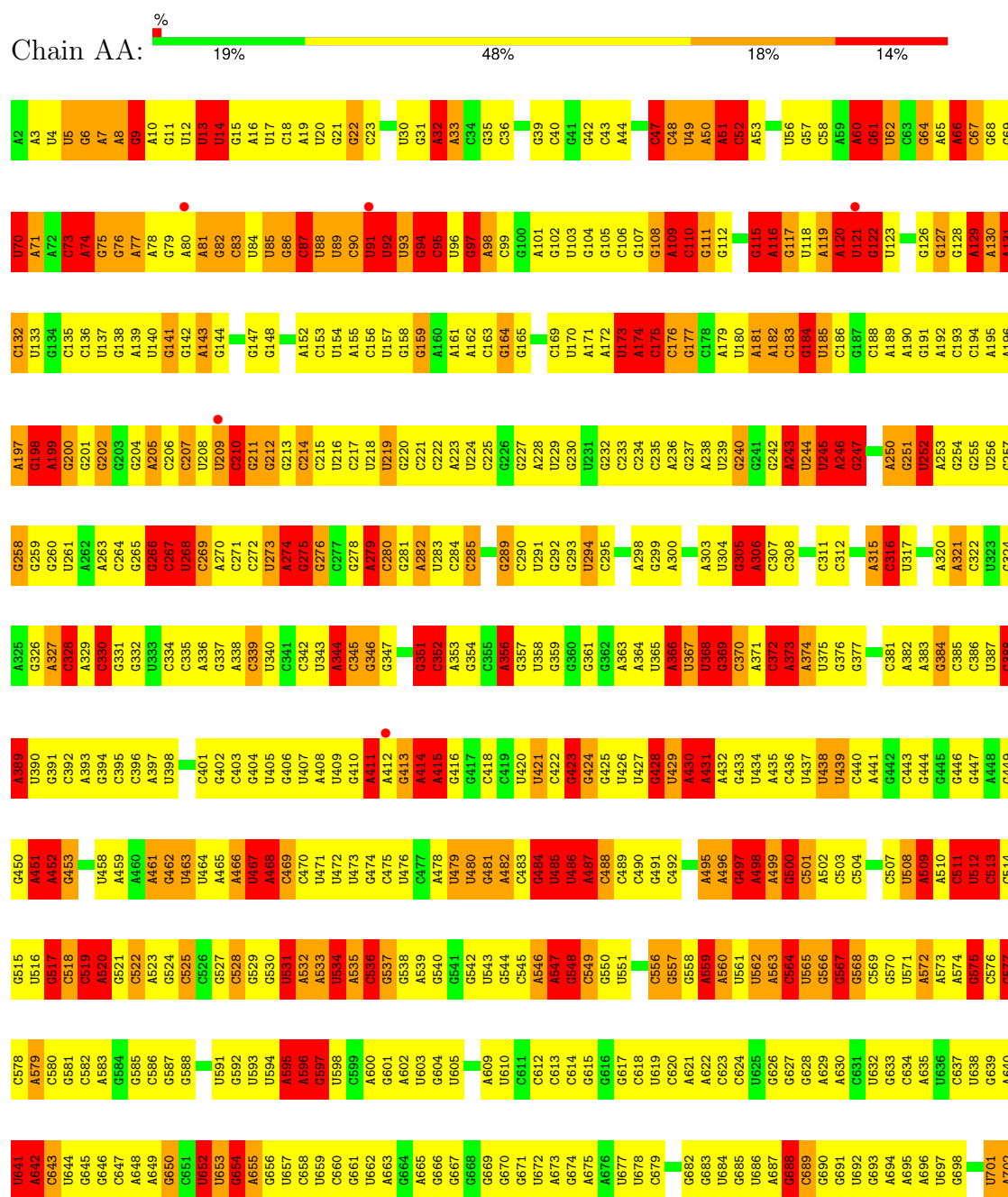
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CN	3	Total 3	O 3	0	0
62	CT	3	Total 3	O 3	0	0
62	CU	2	Total 2	O 2	0	0
62	DA	599	Total 599	O 599	0	0
62	DB	4	Total 4	O 4	0	0
62	DC	9	Total 9	O 9	0	0
62	DD	2	Total 2	O 2	0	0
62	DE	3	Total 3	O 3	0	0
62	DJ	5	Total 5	O 5	0	0
62	DL	5	Total 5	O 5	0	0
62	DN	3	Total 3	O 3	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	2	Total 2	O 2	0	0
62	D3	1	Total 1	O 1	0	0
62	D4	4	Total 4	O 4	0	0

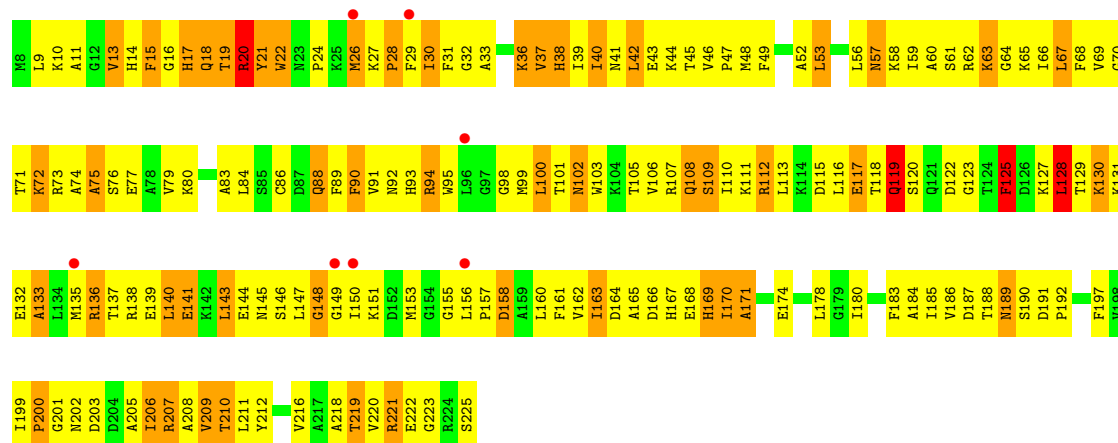
### 3 Residue-property plots

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

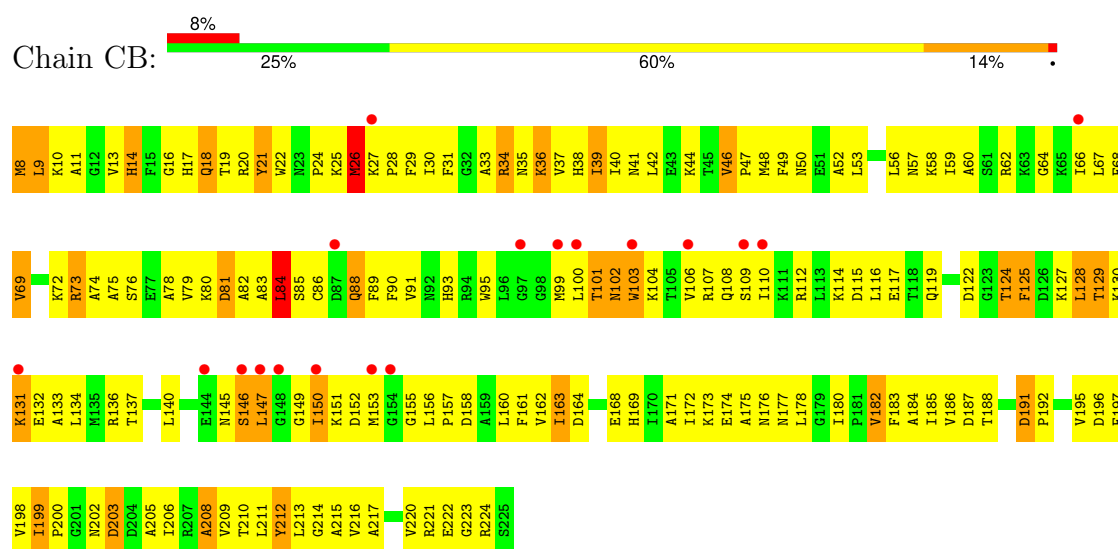
#### • Molecule 1: 16S rRNA



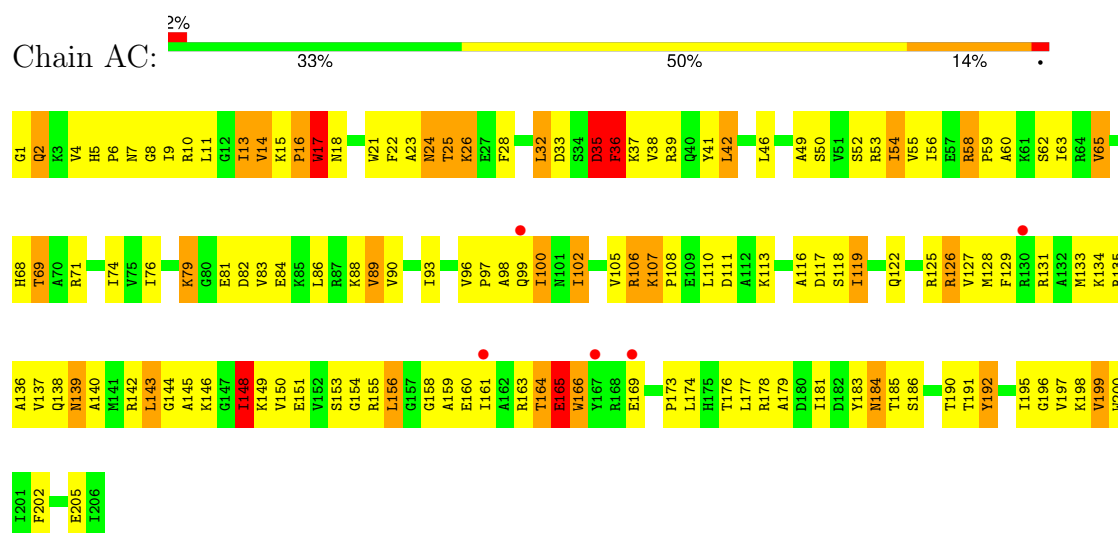




• Molecule 2: 30S ribosomal protein S2

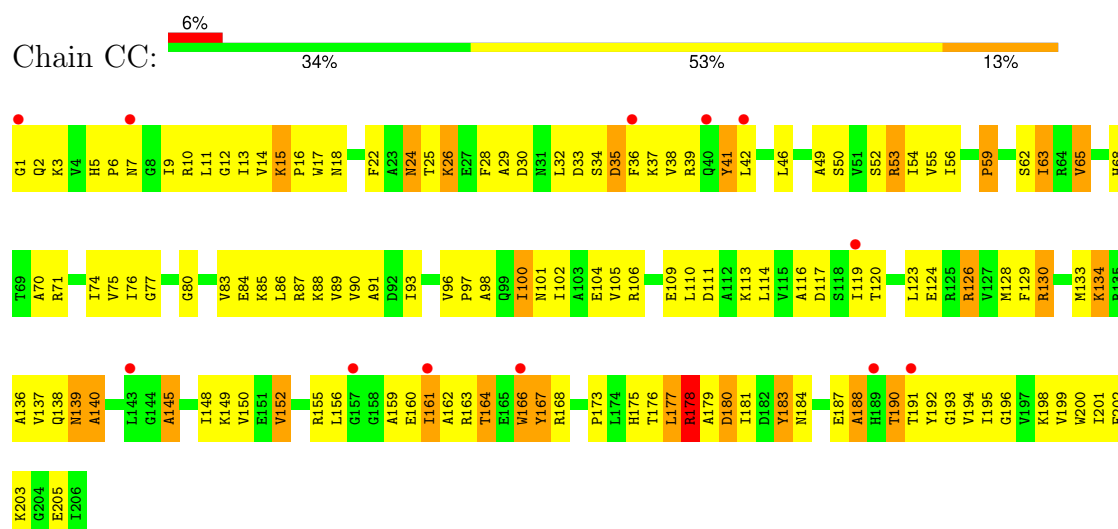


• Molecule 3: 30S ribosomal protein S3

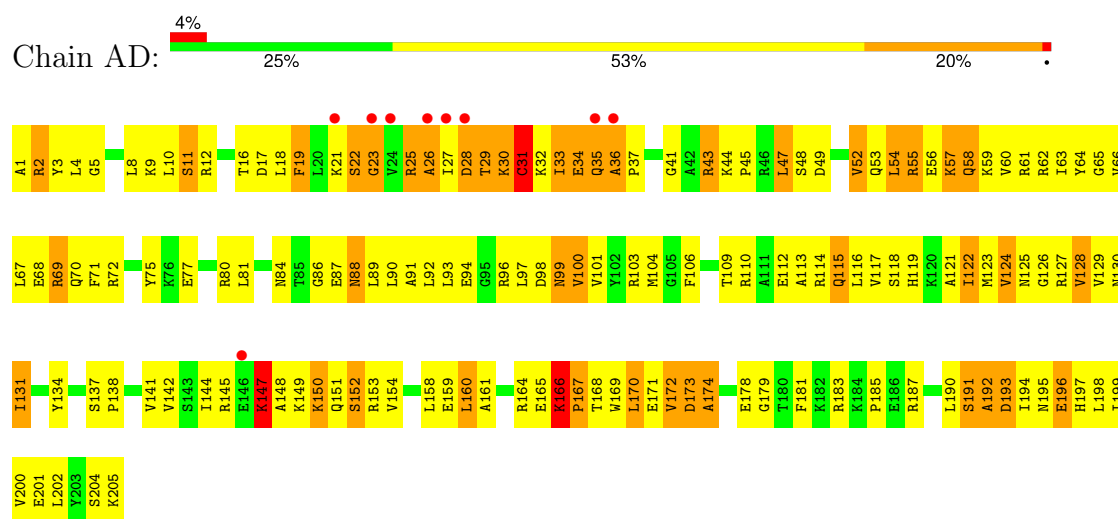


• Molecule 3: 30S ribosomal protein S3

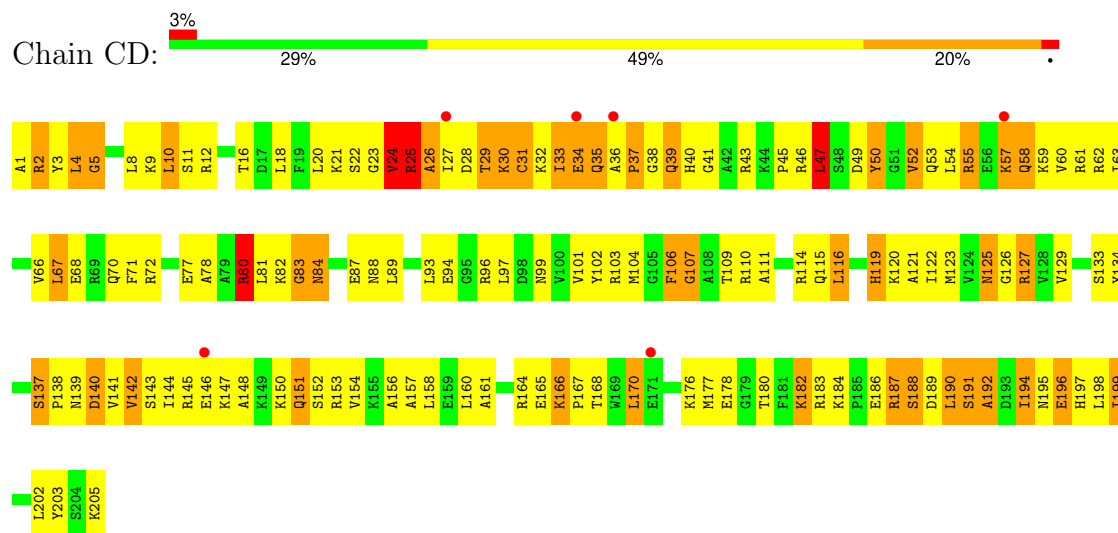




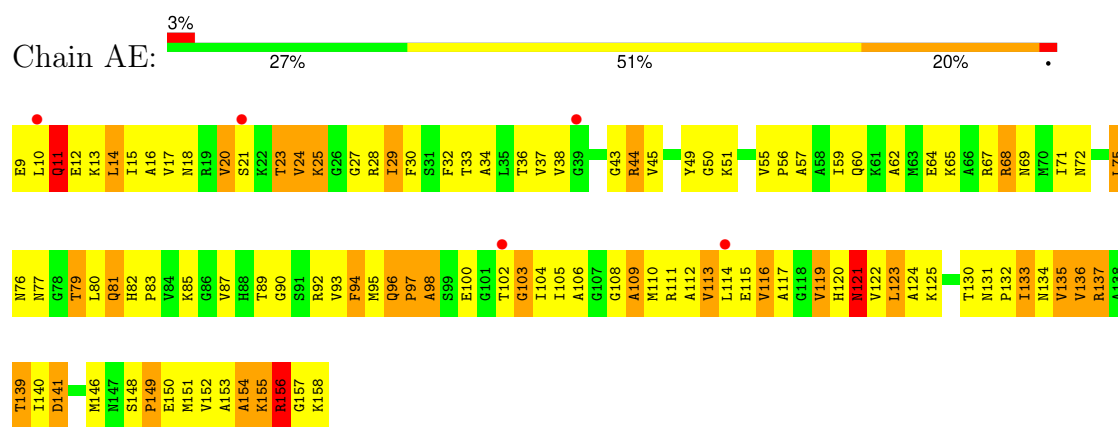
• Molecule 4: 30S ribosomal protein S4



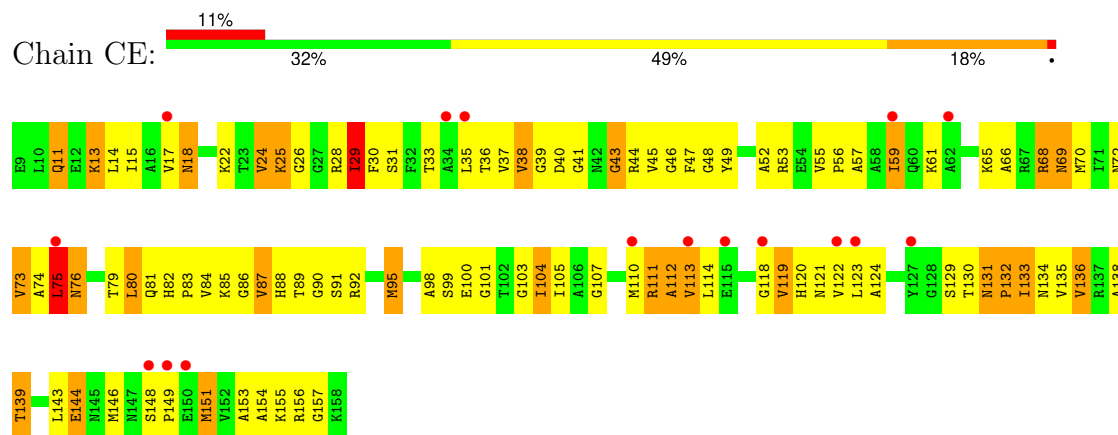
• Molecule 4: 30S ribosomal protein S4



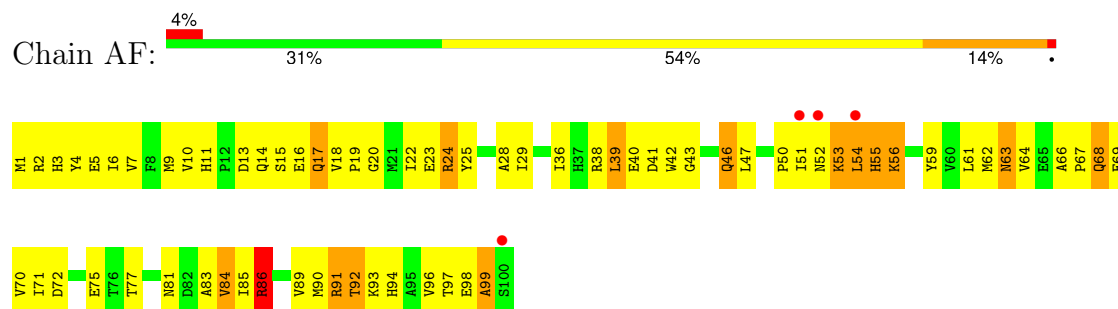
• Molecule 5: 30S ribosomal protein S5



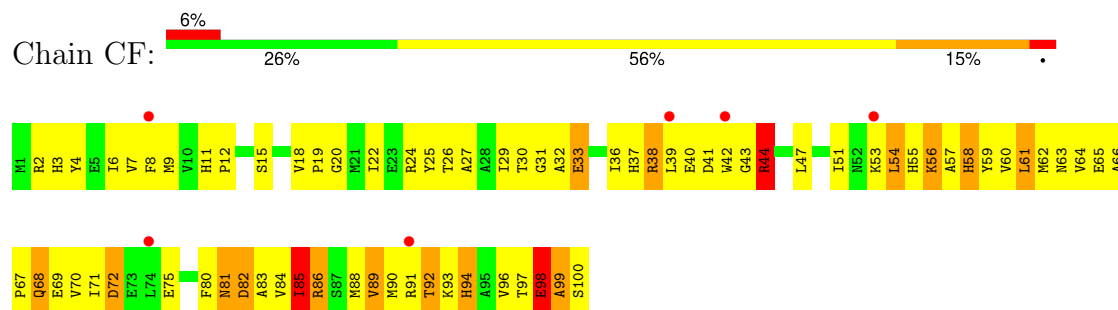
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

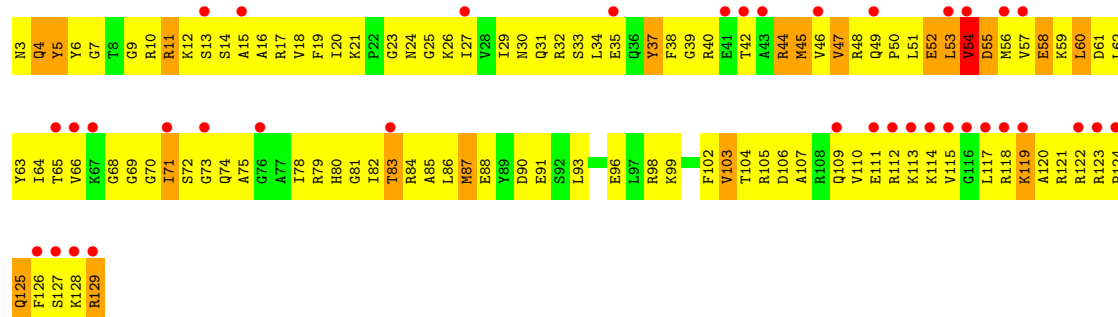


• Molecule 6: 30S ribosomal protein S6

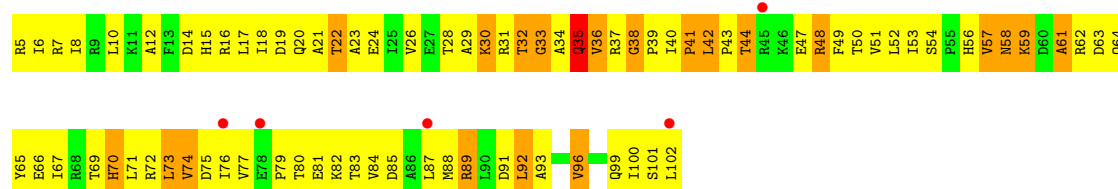


• Molecule 7: 30S ribosomal protein S7

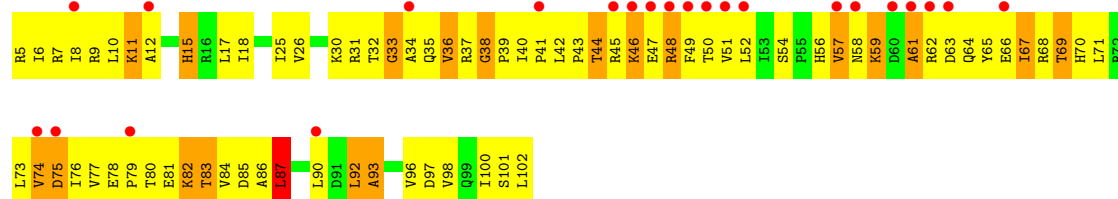




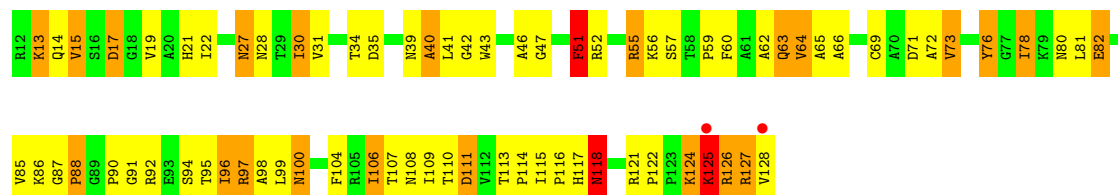
• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

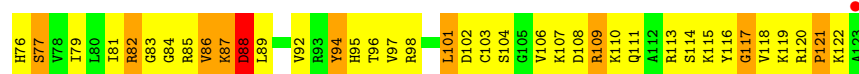


• Molecule 11: 30S ribosomal protein S11

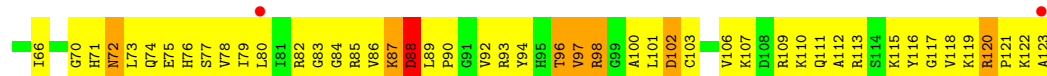
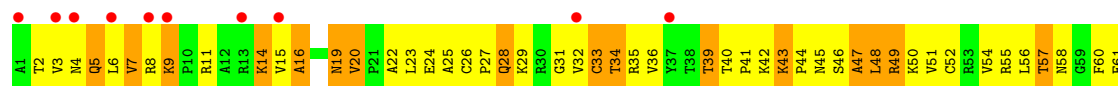




• Molecule 12: 30S ribosomal protein S12



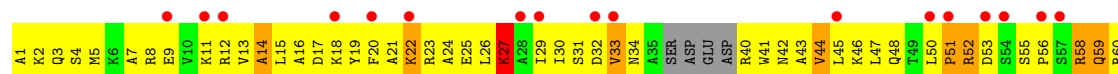
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13

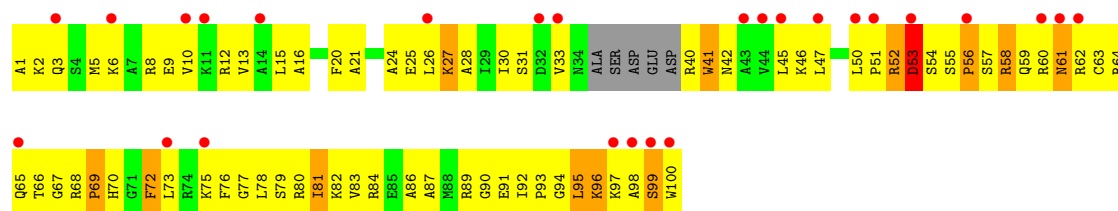


• Molecule 14: 30S ribosomal protein S14

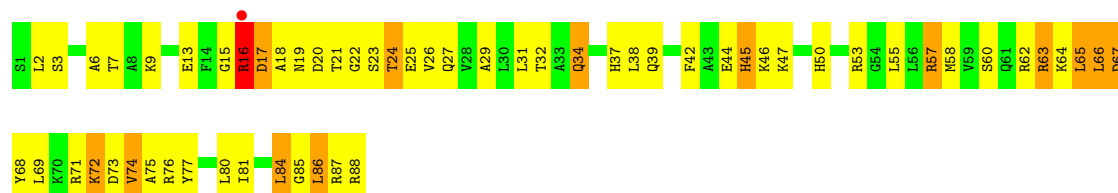


• Molecule 14: 30S ribosomal protein S14

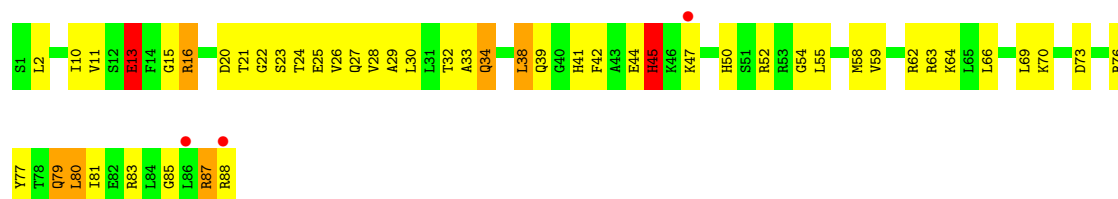




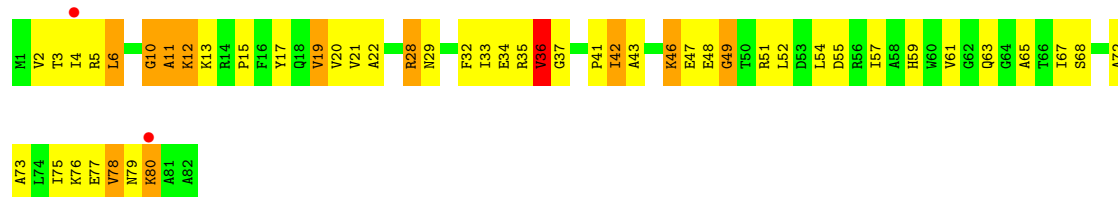
• Molecule 15: 30S ribosomal protein S15



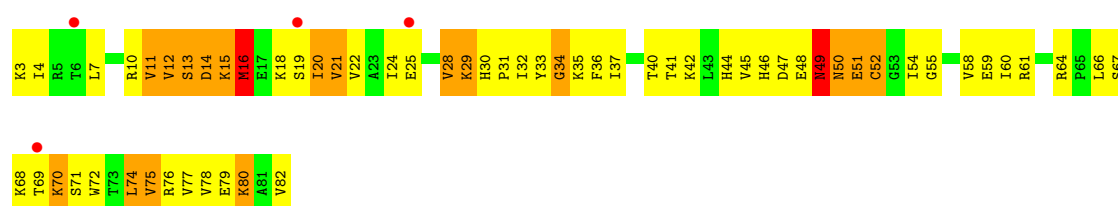
• Molecule 15: 30S ribosomal protein S15



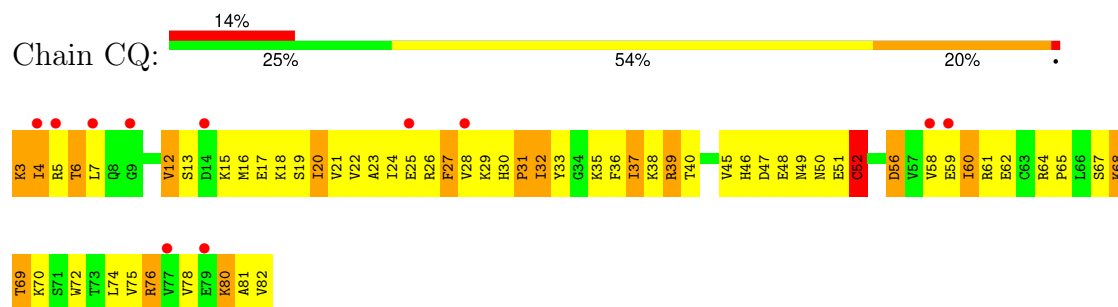
• Molecule 16: 30S ribosomal protein S16



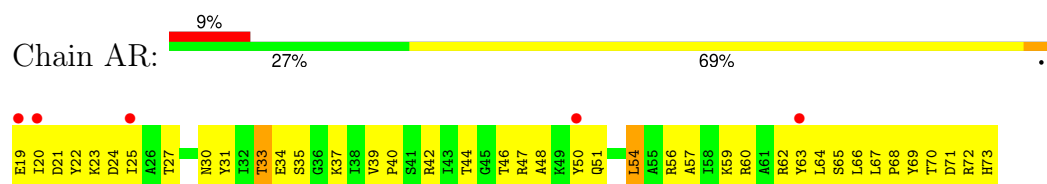
• Molecule 17: 30S ribosomal protein S17



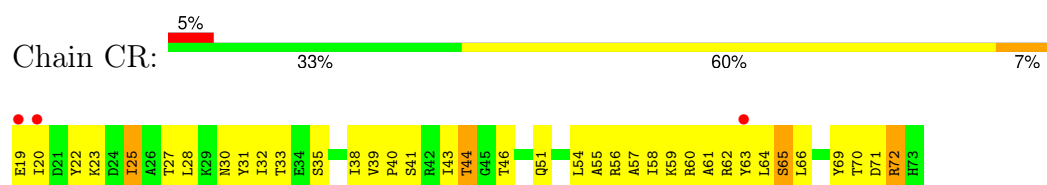
## ● Molecule 17: 30S ribosomal protein S17



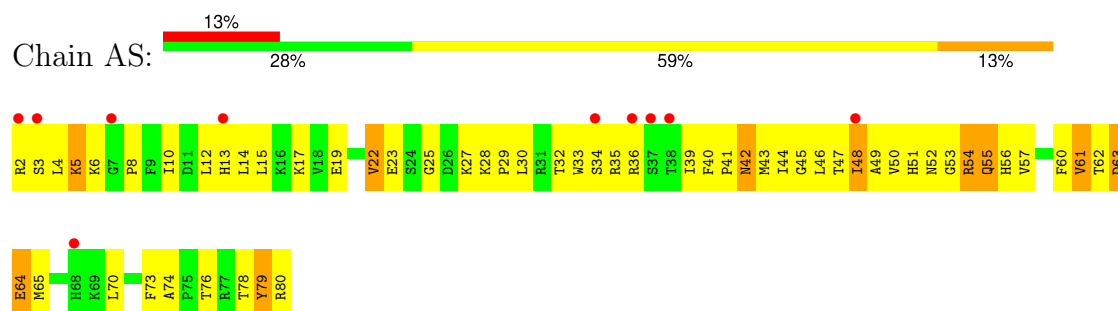
## ● Molecule 18: 30S ribosomal protein S18



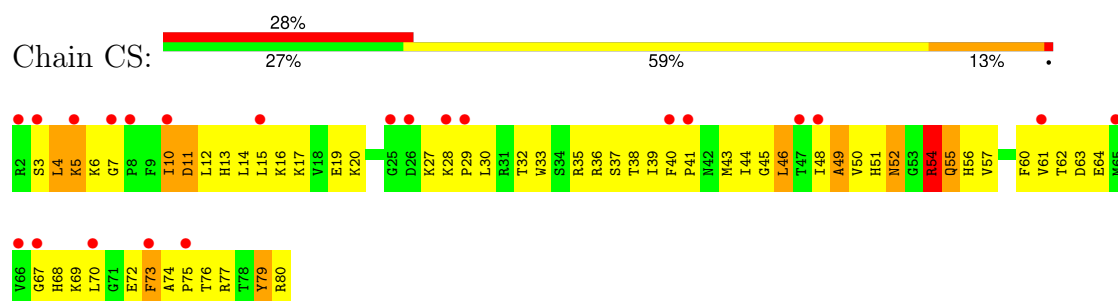
## ● Molecule 18: 30S ribosomal protein S18



## ● Molecule 19: 30S ribosomal protein S19

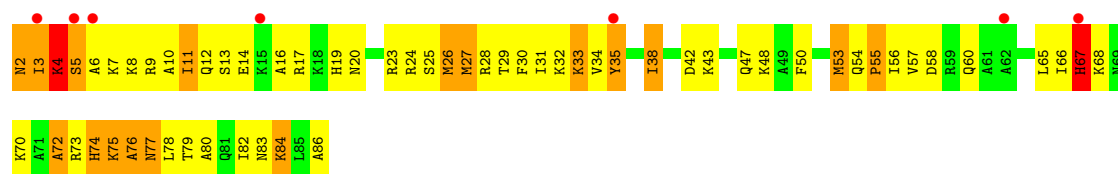


## ● Molecule 19: 30S ribosomal protein S19

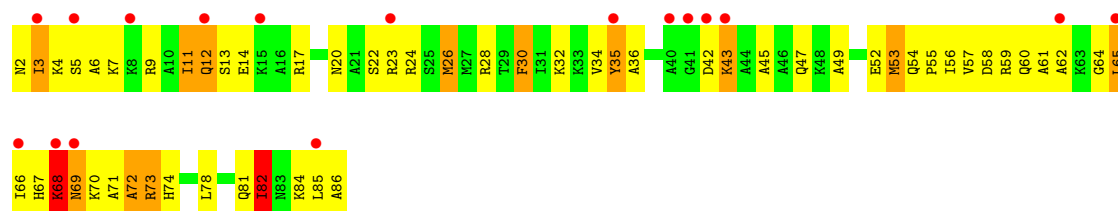


## ● Molecule 20: 30S ribosomal protein S20

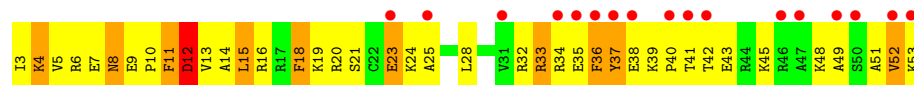




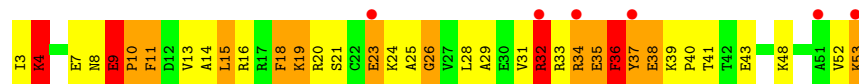
• Molecule 20: 30S ribosomal protein S20



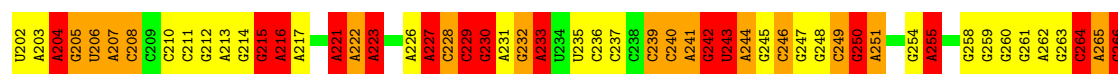
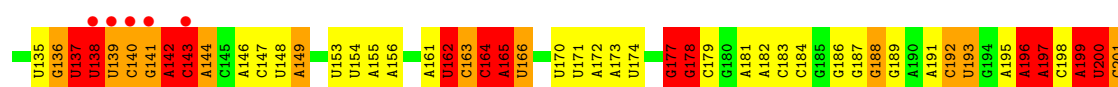
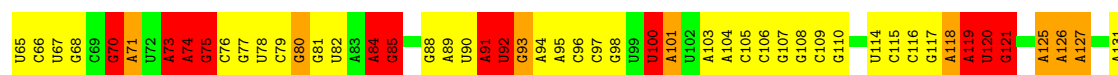
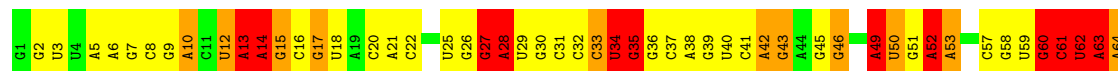
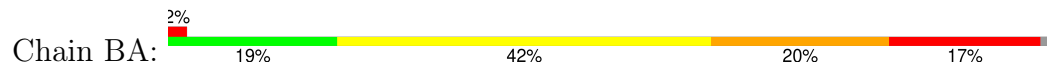
• Molecule 21: 30S ribosomal protein S21



• Molecule 21: 30S ribosomal protein S21



• Molecule 22: 23S rRNA





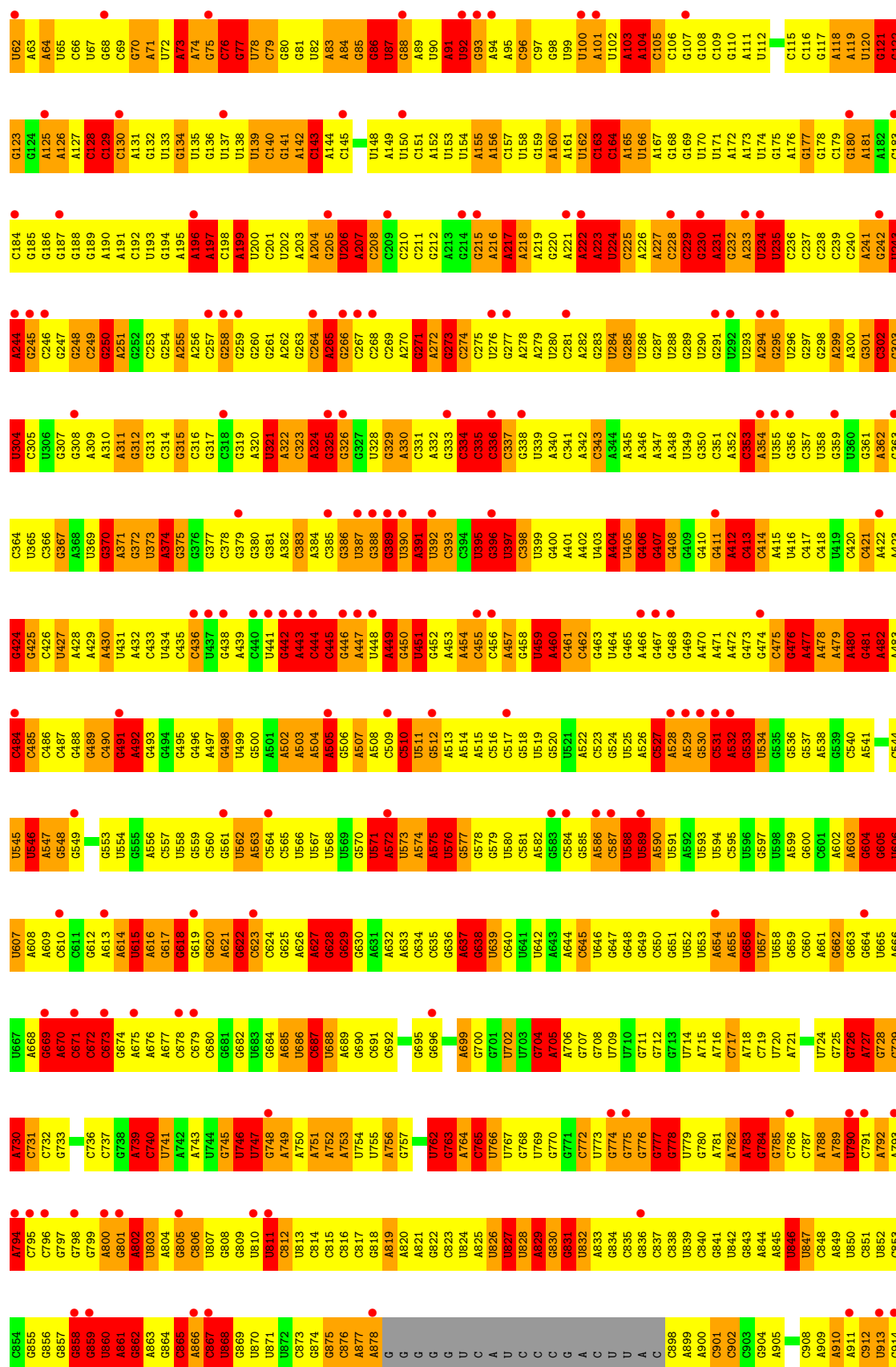
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U1174	A1111	G1047	A984	A918	C851	A788	U724	A661	A599	G539	A472	U403	G353	C268
A1175	C985	A1048	C986	U919	U852	A789	G725	G663	G600	C540	A473	U404	C334	C269
G1049	U1113	C1049	C987	A920	C853	U790	G726	G664	C601	A541	G474	U405	C335	A270
A1050	G1114	C1050	C988	C921	G854	C791	G727	U665	A602	C542	C475	U406	C336	G271
	G1115		A988	C922	G855	A792	G728	U666	A603	G543	G476	G407		A272
	G1116	A1054	G989	G923	G856	U793	G729	U667	G604	C544	A477	G408	G273	G274
	G1117	G1055	A990		G857	A794	A730	U668	G605	U545	A478	G409	U339	C275
	C1118	A1056	G991	A927	G858	C795	C731	U669	A606	U546	A479	G410	A340	C276
	U1119	A1057	G992	A928	G859	C796	C732	G670	U607	A547	A480	G411	A342	U277
	G1120	U1058	C994	U929	U860	G797	G733	A670	A608	C548	G481	A412	U278	G277
		G1059	C995	G930	G861	U798	A734	C671	A609	C549	A482	C413	A345	A279
	G1125	U1060	A986	U931	G862	G799	A735	C672	C510	C550	A483	C414	A346	A280
	A1126	U1061	G997	U932	A863	C673	C736	A676	C611	G551	C484	A415	A347	U281
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	U1189	C1064	A1000	C935	A866	U803	A739		A614	C554		U419	C353	U284
	U1190	U1065	A1001	A936	C867	A804	C740	U615	G499	C555	C490	C420		G285
	G1131	U1066	G1002	C937	U868	G805	U741	G616	A616	A556	C491	C421	C357	U286
	U1132	A1067	G1003	G938	G869	C806	A742	G617	G617	C557	A492	A422	U358	G287
	U1133	G1068	U1004	G939	U870	U807	A743	G618	G618	U558		A423	U359	U288
	A1134	A1069	C1005	G940	U871	G808	U744	G619	G619	C559		G424	U360	G289
	C1135	A1070		A941	U872	G809	G745	G620	G620	C560			G361	U290
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	G1137	A1072	A1009	A943	C876	U811	U747	U686	G622	U562	A497	A429	G363	G295
	G1138	A1073	A1010	C944	A877	C812	G748	C887	C523	A563		A430	C364	U296
	U1139	G1074	G1011	A945	A878	U813	A749	U688	C624	C564			C365	
	C1140	C1075	U1012	C946	U878	C814	A750	G625	G625	C565			C366	
	U1141	C1076	C1013	A947		C815	G751	A626	A626	U566	A501	U434		A300
	A1142	A1077	A1014	C948	C985	G816	A752	G692	A627	U567	A502	C435	U369	G301
	A1143	U1078	U1015		A	C817	A753	A693	G628	U568	A503	C436	G370	G302
	C1144	C1079	G1016	G954	U	G818	U754	U694	A631	G570	A504	U437	A371	U304
	C1145	A1080	G1017	U955	C	A819	U755	U695	A632	U571	G506	U441	G372	C305
	C1146	U1081	U1018	C956	C	A820	C758	G696	A633	A572	A507	G442	U373	U306
	U1148	U1082	U1019	C957	C	A821	G759	G697	A634	U573	A508	A443	A374	G307
	G1149	U1083	A1020	U958	G	C822	G760	C698	C634	A574	C509	C444		G308
	C1150	A1084	A1021	A959	A892	C823	A761	A699	C635	A575	C510	C445	G377	A309
	A1151	A1085	G1022	A960	C893	U824		G700	G636	U576	U511	G446	C378	A310
	G1152	A1086	U1023	C961	U894	A825	G762	G701	A637	G577	G512	A447	G381	A311
	C1153	G1087	G1024	G962	U895	U826	G763	G702	G638	U578	A513	U448	A382	G312
	G1154	A1088	G1025	U963	A896	U827	A764	U703	U639	G579	A514	A449	A383	G313
	U1155	U1089	G1026	C964	C897	U828	C765	G704	C640	U580		G450	A384	G314
	A1156	A1090	A1027	C965	C898	A829	U766	A705	U641	C581	U521	U451	C385	G315
	G1157	C1091	A1028	G966	A899	G830	U767	A706		A582	A522	G452	C386	G316
	C1158	C1092	A1029	U967	A900	G831	G768	G707	A644	G583	C523	A453	G387	G317
	U1159	G1093	C1030	C968	C901	U832		G708	C645	C584	G524	A454	G388	C318
	A1160	A1095	G1031	G969	C902	U833	G773	U709	U646	U585	C525	A455	G389	G319
	G1161	U1096	A1032	U970	A905	G834	G774	U710	G647	U586	A526	C456	U390	A320
	C1162	U1097	U1033	G971	U906	C835	G775	G711	G648	A587	C527	A457	A391	U321
	G1163	A1098	G1034	A972	G907		G776	G712	G649	U588	A528	G458	U392	A322
	C1164	G1099		G973	C908	C838	G777	G713	C650	U589	A529	A459	U393	C323
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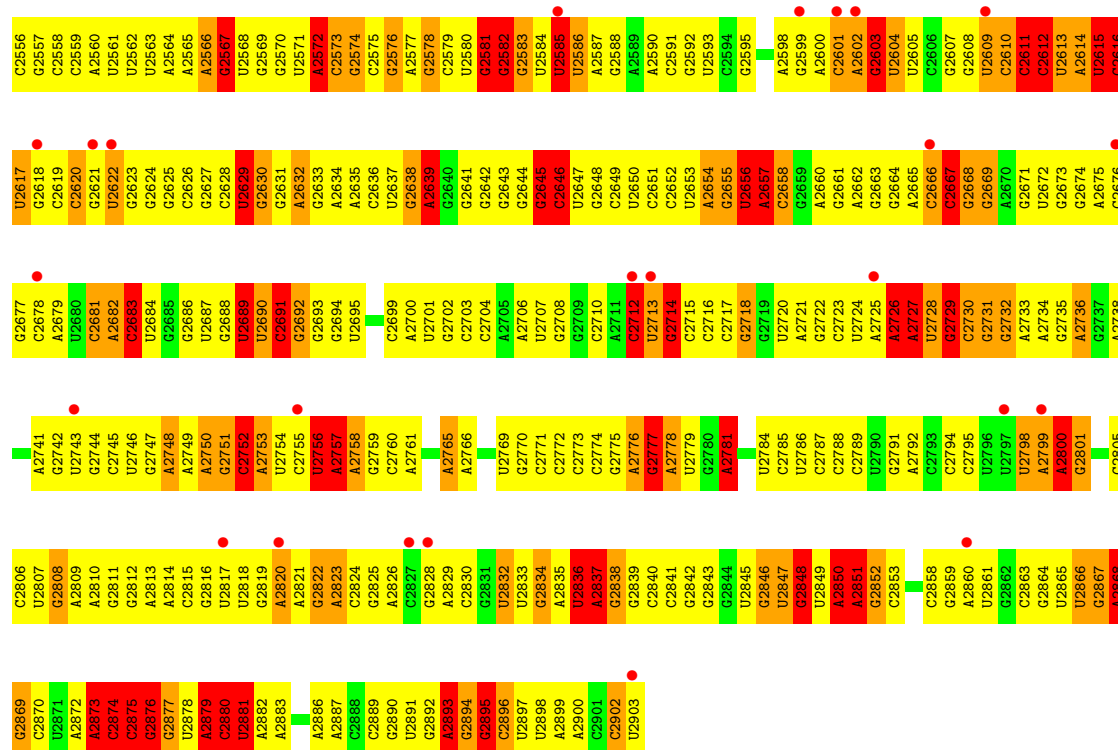
Response	Percentage
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Yes	12%
Yes, but not in the way the U.S. is currently acting	47%
Yes, but only if other countries take action first	22%
No opinion	16%





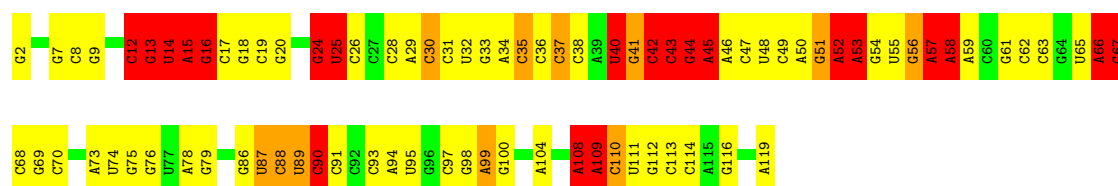
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C2439	C2374	C2313	G2254	U2189	C	C2065	G2000	U1931	G1799	A1739	G1739
A2440	G2375	A2314	C2254	G2190	U	G2066	C2001	A1932	C1800	A1740	G1740
U2441	A2377	G2315	G2255	U2191	U	G2067	U2007	G1933	A1801	G1740	C1741
C2442	A2378	G2316	G2256	U2192	U	U2068	G2008	C1934	A1802	C1741	U1742
G2443	G2379	A2317	U2257	U2195	G2133	G2069	C2009	G1935	A1803	G1743	G1743
C2444	C2380	G2318	C2258	C2196	A2134	A2070	A2009	U1936	C1804	A1744	A1744
G2445	C2381	U2320	U2259	U2197	G2135	C2071	G2010	A1937	A1805	A1745	A1745
G2446	G2382	U2321	C2260	U2198	G2136	C2072	U2011	U1938	G1806	U1746	U1746
G2447	C2383	U2322	U2261	A2199	U2137	C2073	G2012	U1939	G1807	U1747	U1747
C2448	U2384	A2323	U2262	C2200	G2138	U2074	A2013	U1940	A1808	C1748	C1748
U2449	C2385	U2324	C2263	G2201	U2139	U2075	A2014	A1876	A1809	U1751	U1751
A2450	A2386	U2325	C2264	U2202	G2140	U2076	A2015	C1941	A1810	G1752	G1752
U2451	U2387	G2325	U2265	U2203	G2141	C2077	U2016	U1943	G1811	G1753	G1753
U2452	C2388	G2326	A2266	U2204	A2142	C2078	U2017	U1944	G1812	A1754	A1754
C2453	G2389	U2327	A2267	G2205	C2143	U2079	G2018	G1945	G1813	G1755	G1755
G2454	U2390	U2328	A2268	A2205	G2144	A2080	A2019	U1946	A1814	A1756	A1756
C2455	C2391	G2330	C2269	C2206	C2145	U2085	A2020	U1947	A1815	G1757	G1757
G2456	U2392	U2331	A2270	C2207	C2146	U2086	C2021	U1951	C1816	U1758	U1758
U2457	C2393	C2332	G2271	C2208	A2147	U2087	G2022	C1957	G1817	A1759	A1759
C2458	U2394	U2333	U2272	G2209	G2148	C2088	C2023	U1952	G1818	C1760	C1760
A2459	C2395	U2334	A2273	U2210	U2149	A2088	G2024	A1953	U1819	G1761	G1761
U2460	C2396	A2335	A2274	A2211	C2150	U2091	G2025	G1954	U1820	G1762	G1762
A2461	U2397	U2336	C2275	U2212	U2151	U2092	U2026	U1955	A1821	G1763	G1763
C2462	C2401	C2337	G2276	U2213	G2152	G2093	G2029	U1956	A1822	G1764	G1764
G2463	U2402	C2338	G2277	C2214	C2153	A2094	A2030	C1957	G1823	U1765	U1765
C2464	C2403	C2339	A2278	C2215	U2154	A2095	A2031	C1961	G1824	G1766	G1766
U2465	U2404	A2340	G2279	G2216	U2155	C2096	G2032	C1962	U1825	G1767	G1767
C2466	G2405	G2341	G2280	G2217	G2156	U2097	A2033	U1963	G1826	C1768	C1768
A2467	U2406	U2342	A2281	G2218	G2157	U2098	G2034	G1964	U1827	G1769	G1769
U2468	C2407	U2343	C2282	U2219	A	U2099	G2035	C1965	A1829	G1770	G1770
C2469	U2408	G2345	C2283	G2220	G	G2100	C2036	A1966	C1830	A1771	A1771
G2470	C2409	A2346	A2284	G2221	C	A2101	A2037	C1967	C1833	A1772	A1772
U2471	G2410	C2347	C2285	C2222	G	G2102	G2038	G1968	U1834	C1773	C1773
A2411	A2411	U2348	G2286	G2223	A	C2103	U2039	A1969	G1835	U1774	U1774
C2412	U2412	G2349	A2287	G2224	C	U2104	G2040	A1970	C1836	G1775	G1775
U2413	G2413	C2350	A2288	A2225	C	U2105	U2041	G1971	C1837	G1776	G1776
G2414	G2414	G2351	C2289	C2226	U	U2106	A2042	G1972	C1838	U1777	U1777
U2415	U2415	A2352	U2290	A2227	U	G2107	C2043	G1973	G1839	U1778	U1778
C2416	C2416	C2353	U2291	G2228	G	A2108	C2044	C1974	G1840	U1779	U1779
U2417	U2417	G2354	U2292	U2229	A	U2109	G2045	G1975	A1780	A1780	A1780
A2418	A2418	C2355	G2293	G2230	A	G2110	G2046	C1976	C1843	U1781	U1781
U2419	U2419	U2356	C2294	U2231	A	U	C2047	G1980	C1844	U1782	U1782
C2420	U2420	G2357	U2295	C2232	U	G	G2048	A1981	G1845	A1783	A1783
U2421	G2421	C2358	U2296	U2233	A	U	G2049	U1982	G1846	G1784	G1784
C2422	U2422	A2359	A2297	G2234	C	A	C2050	G1983	U1915	A1785	A1785
U2423	U2423	C2360	U2298	G2235	C	G	A2051	G1984	A1916	A1786	A1786
C2424	C2424	G2361	U2299	U2236	A	G	A2052	C1985	U1917	A1787	A1787
U2425	U2425	C2362	C2300	G2237	C	U	A2053	G1989	G1849	C1788	C1788
A2426	A2426	G2363	U2302	G2238	C	U	A2054				
				G2239							



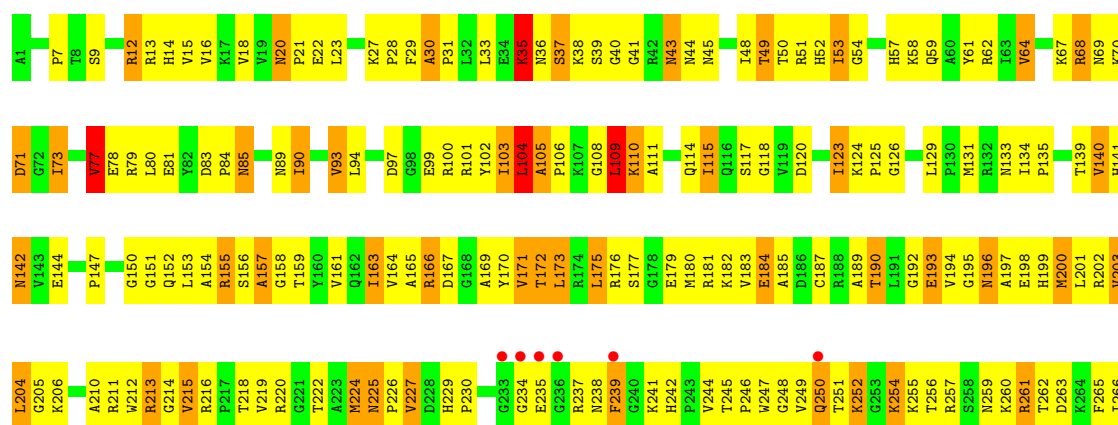
### • Molecule 23: 5S rRNA

Chain BB: 28% 45% 9% 18%



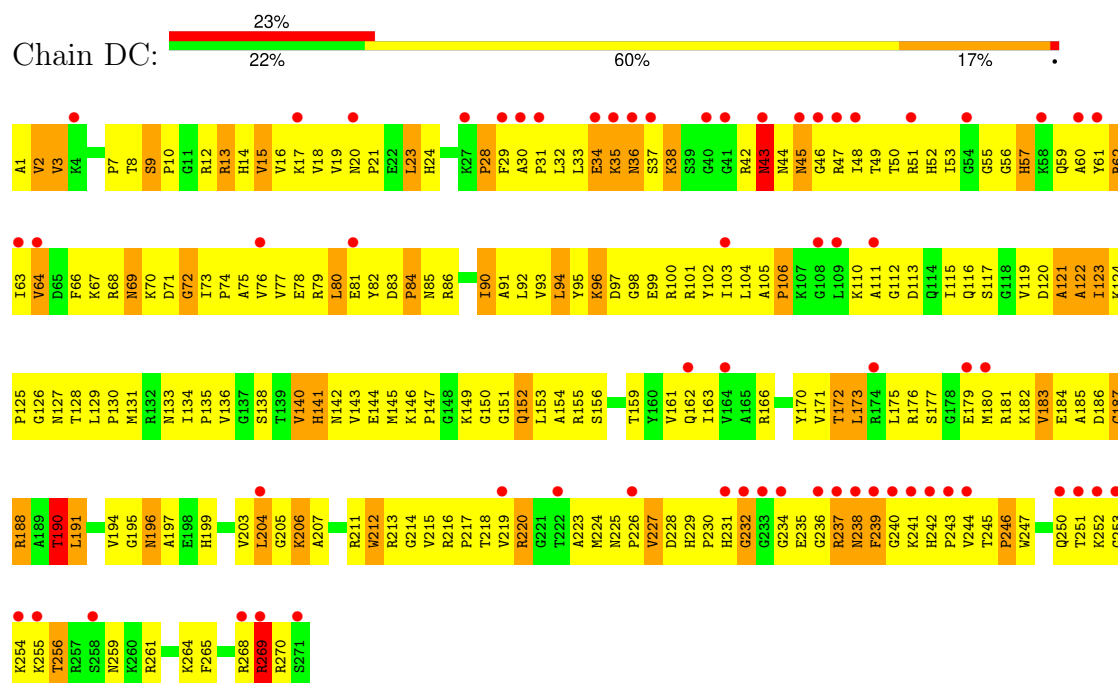
### • Molecule 24: 50S ribosomal protein L2

Chain BC: 2% 31% 50% 17%

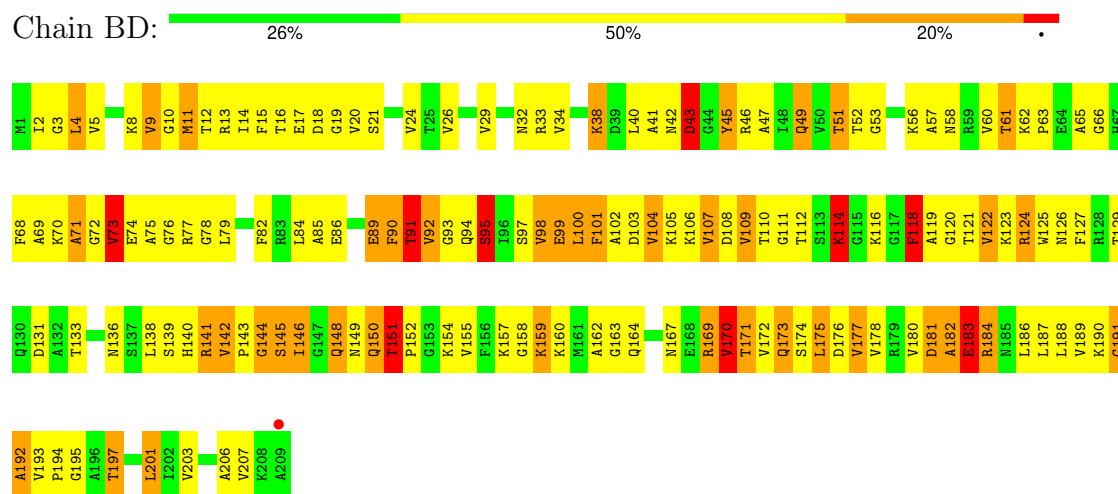




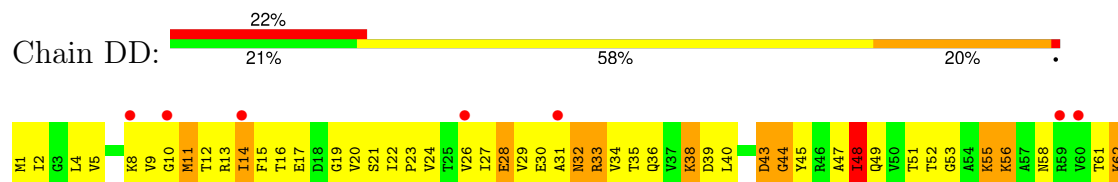
• Molecule 24: 50S ribosomal protein L2



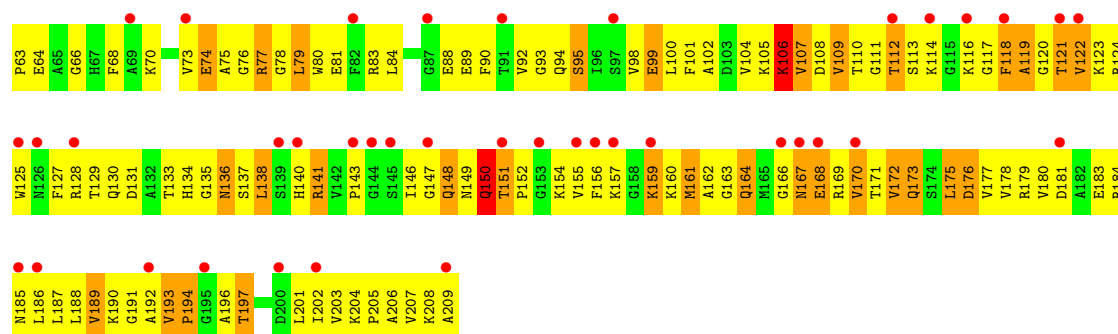
• Molecule 25: 50S ribosomal protein L3



• Molecule 25: 50S ribosomal protein L3

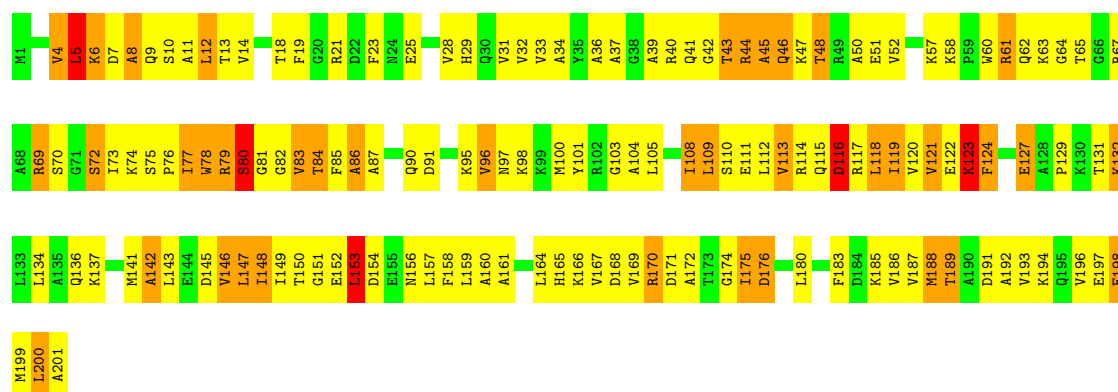






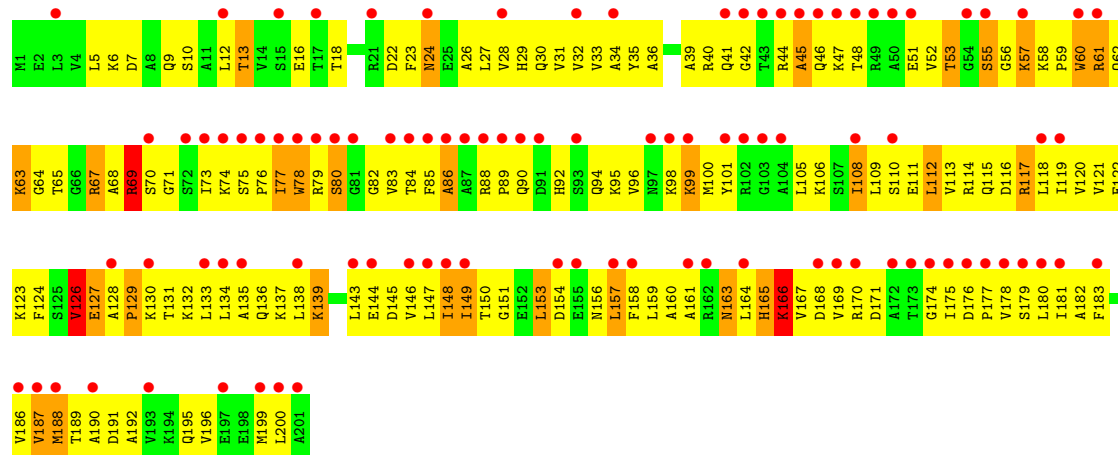
• Molecule 26: 50S ribosomal protein L4

Chain BE: 27% 51% 19%



• Molecule 26: 50S ribosomal protein L4

Chain DE: 23% 49% 61% 14%

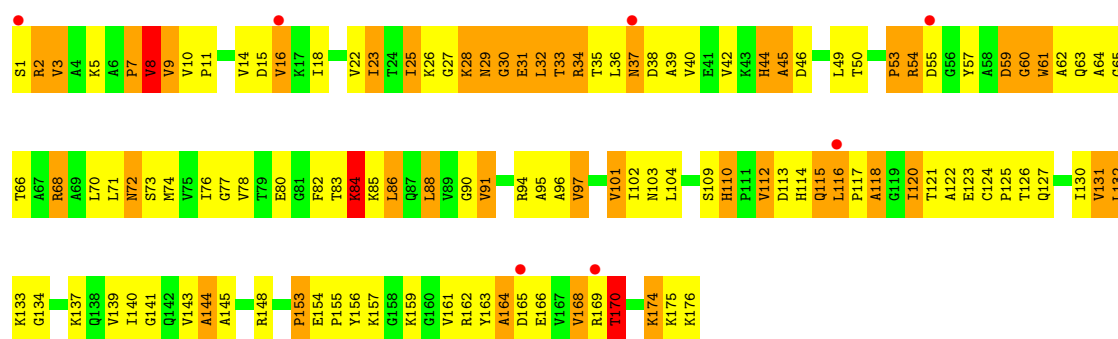


• Molecule 27: 50S ribosomal protein L5

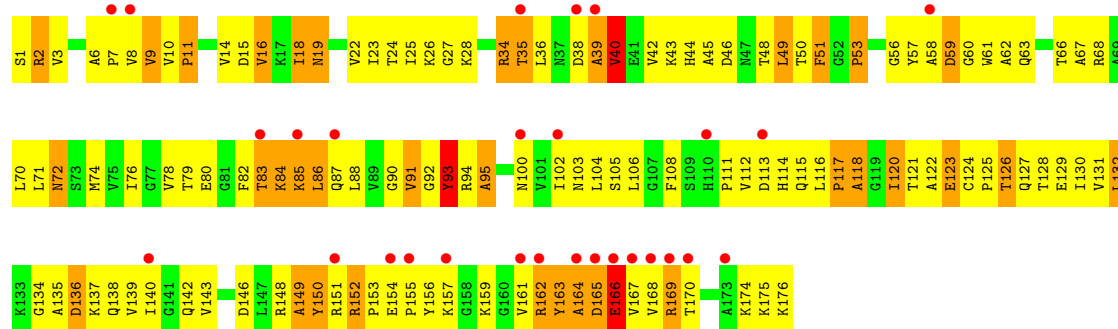
Chain BF: 28% 55% 15%



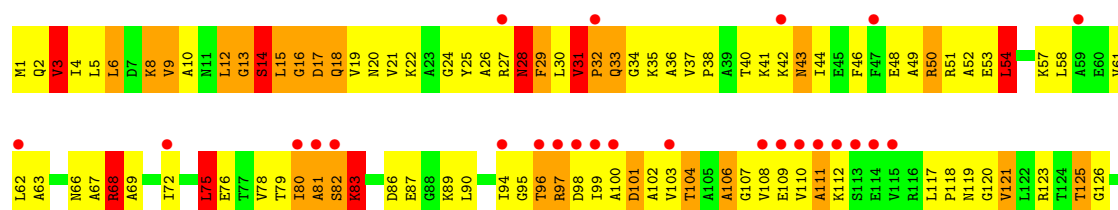
• Molecule 28: 50S ribosomal protein L6

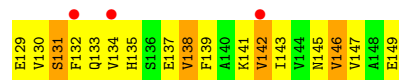


• Molecule 28: 50S ribosomal protein L6

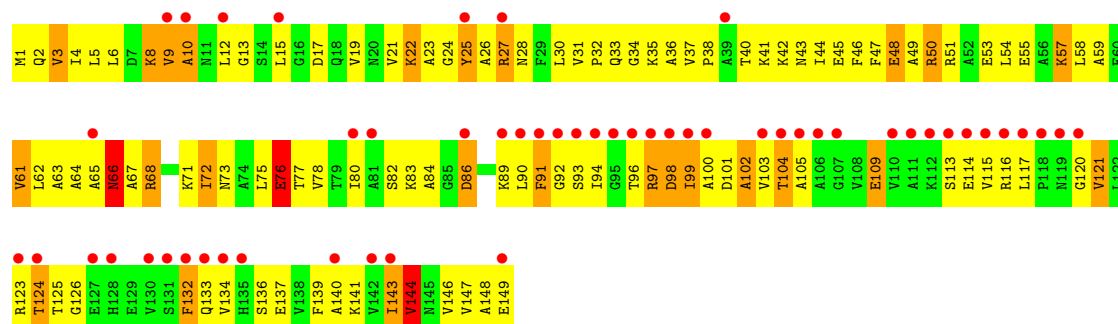


• Molecule 29: 50S ribosomal protein L9

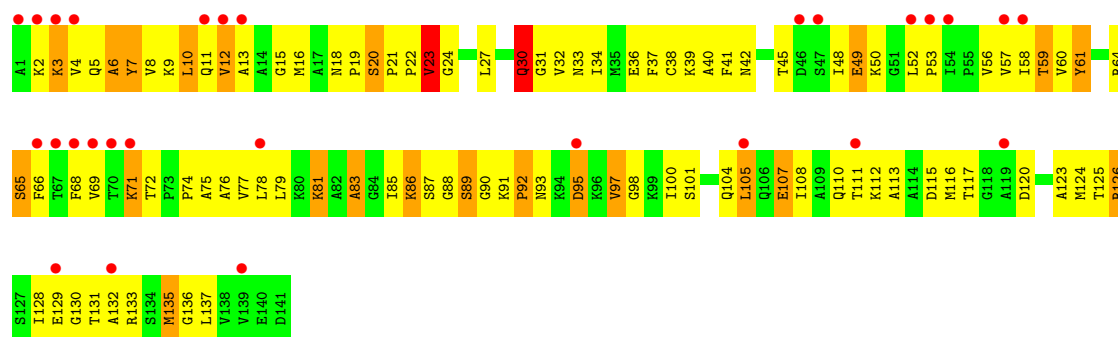




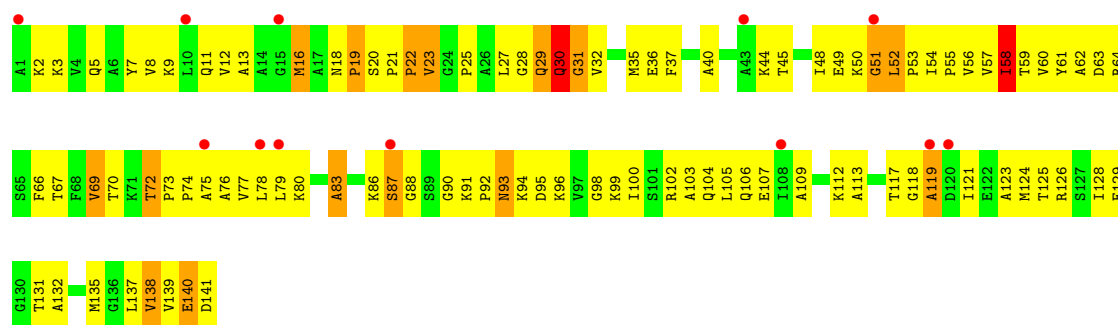
• Molecule 29: 50S ribosomal protein L9



• Molecule 30: 50S ribosomal protein L11

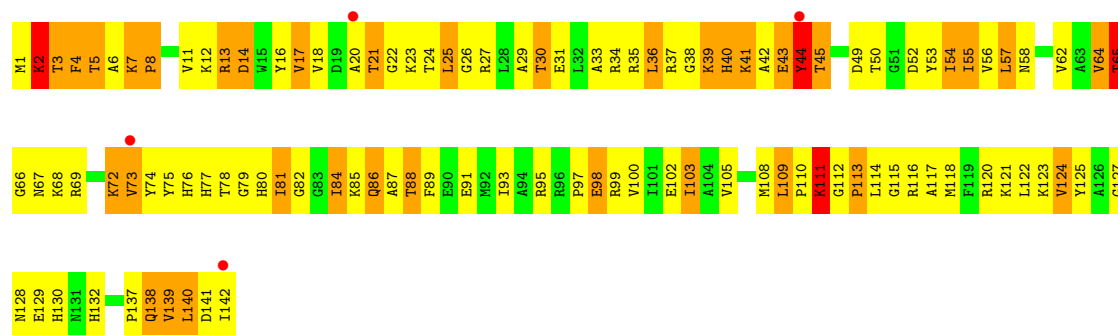


• Molecule 30: 50S ribosomal protein L11

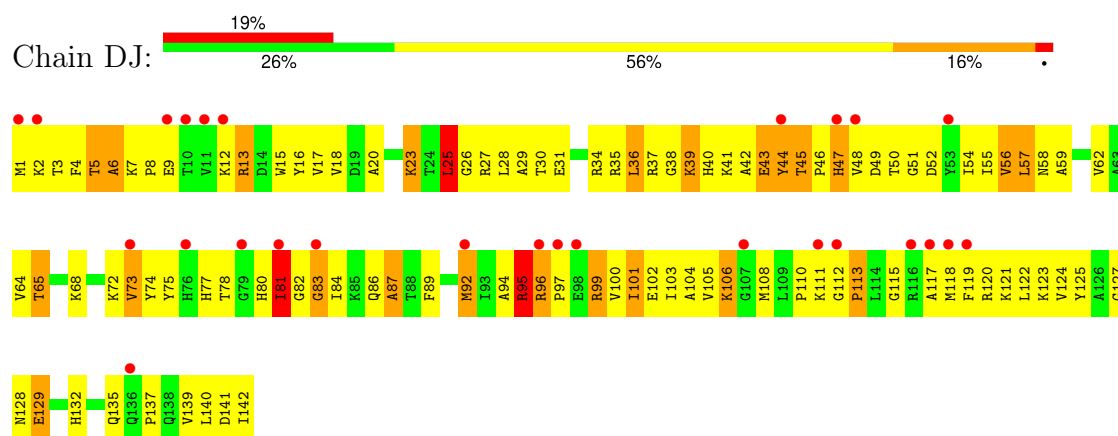


• Molecule 31: 50S ribosomal protein L13

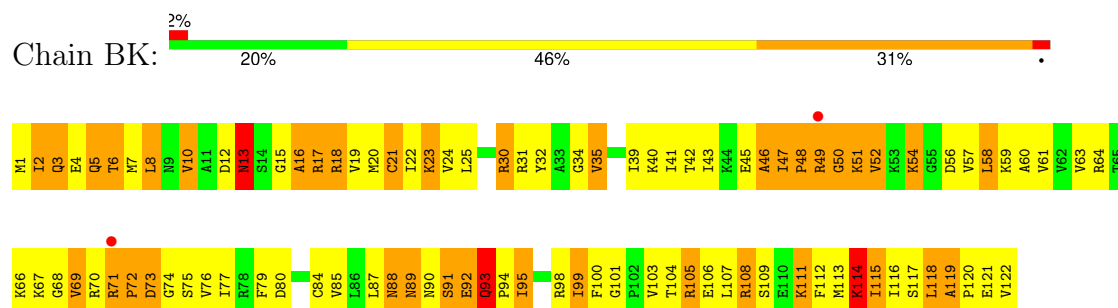




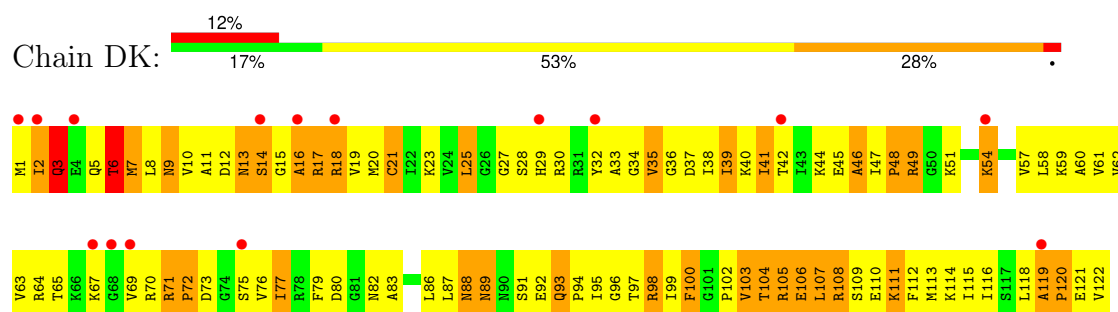
• Molecule 31: 50S ribosomal protein L13



• Molecule 32: 50S ribosomal protein L14



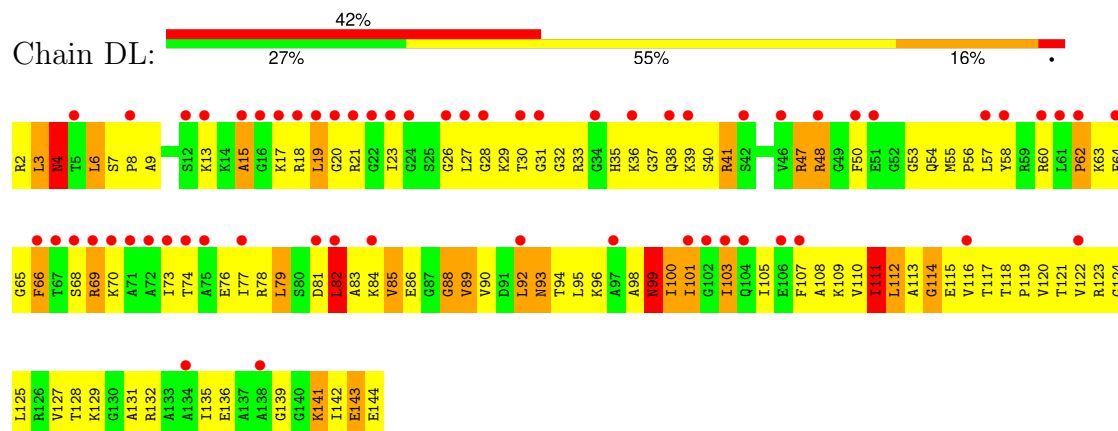
• Molecule 32: 50S ribosomal protein L14



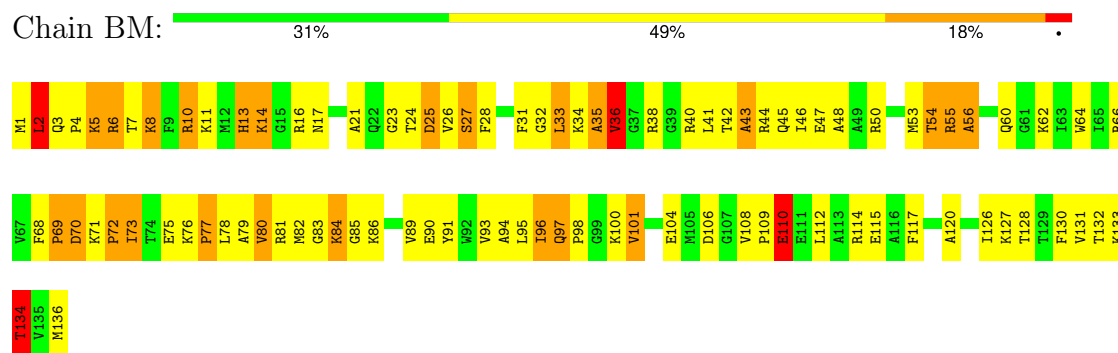
• Molecule 33: 50S ribosomal protein L15



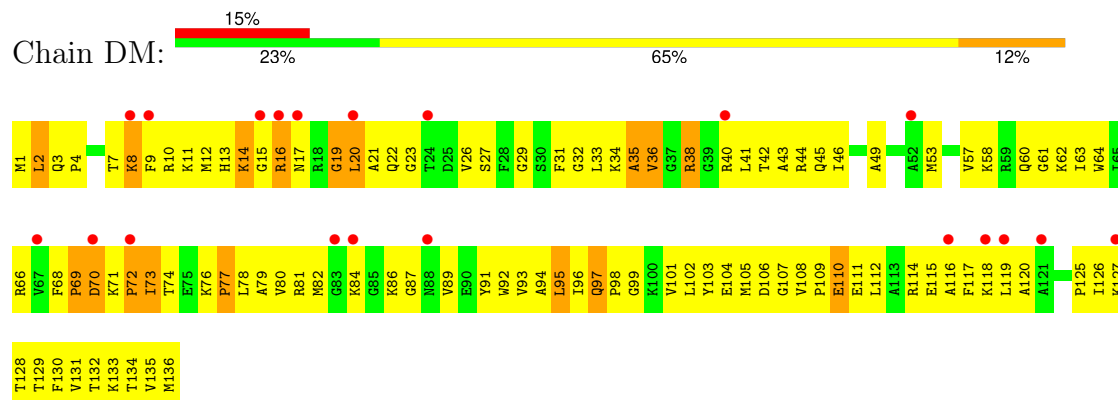
- Molecule 33: 50S ribosomal protein L15



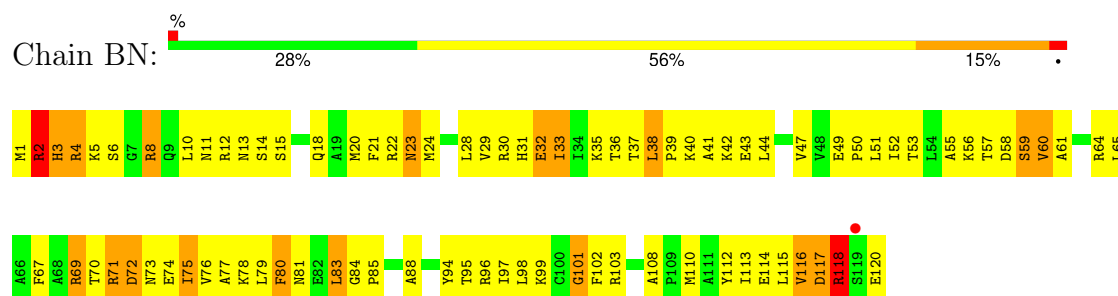
- Molecule 34: 50S ribosomal protein L16



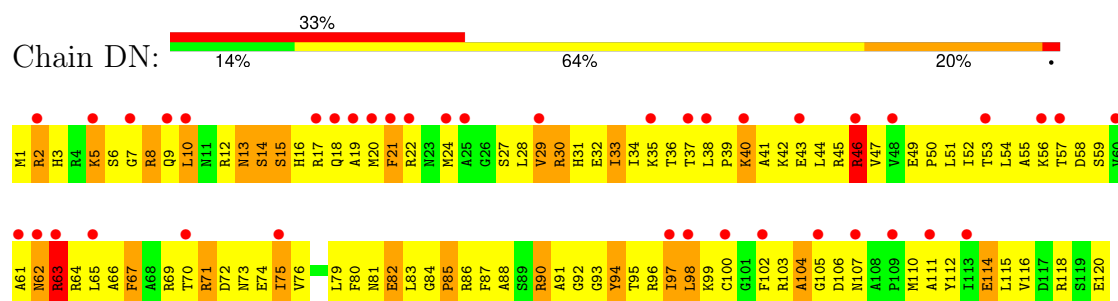
- Molecule 34: 50S ribosomal protein L16



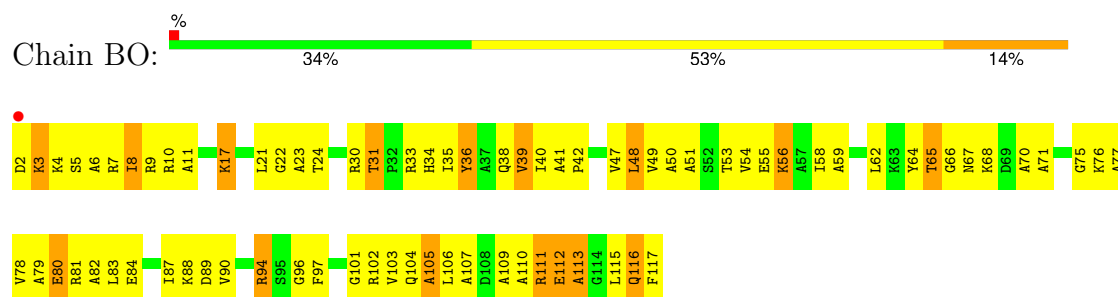
- Molecule 35: 50S ribosomal protein L17



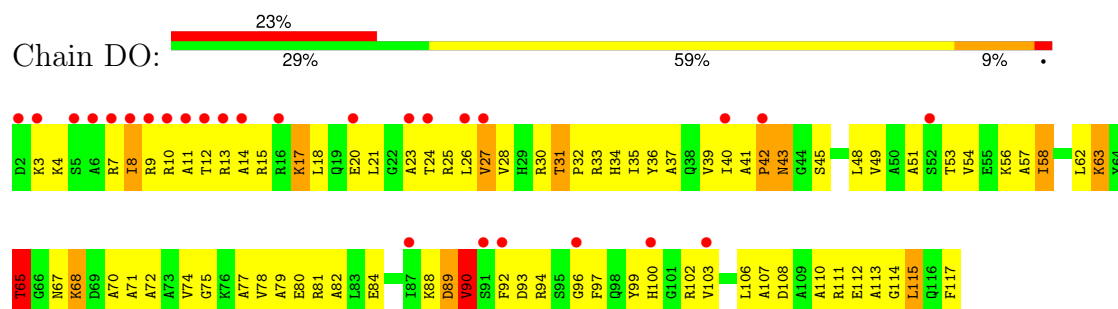
- Molecule 35: 50S ribosomal protein L17



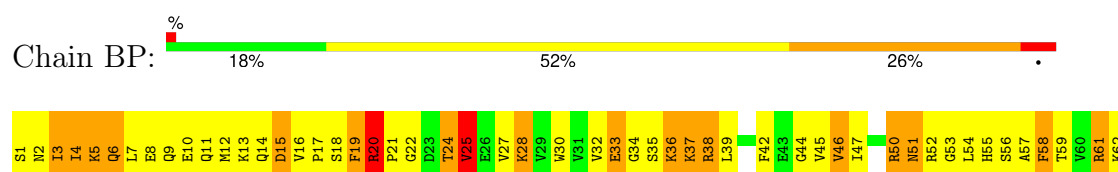
- Molecule 36: 50S ribosomal protein L18

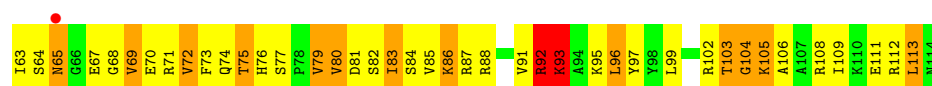


- Molecule 36: 50S ribosomal protein L18

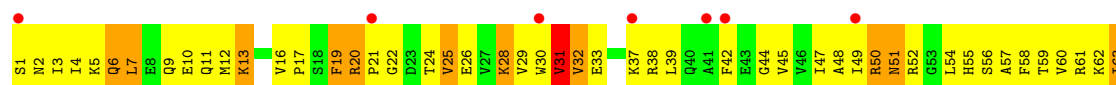


- Molecule 37: 50S ribosomal protein L19

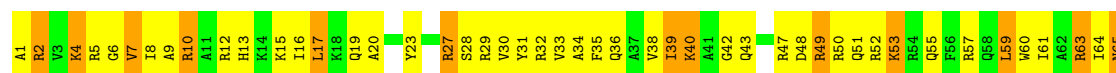




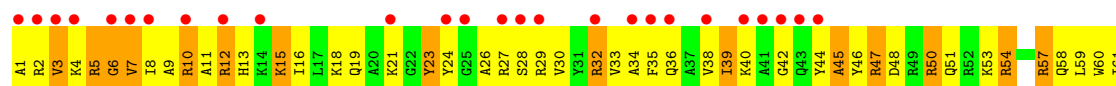
• Molecule 37: 50S ribosomal protein L19



• Molecule 38: 50S ribosomal protein L20



• Molecule 38: 50S ribosomal protein L20

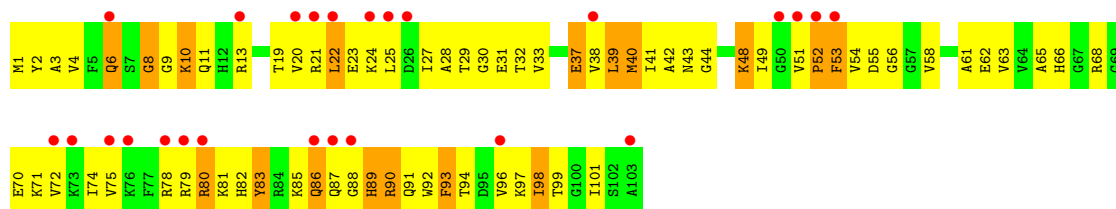


• Molecule 39: 50S ribosomal protein L21



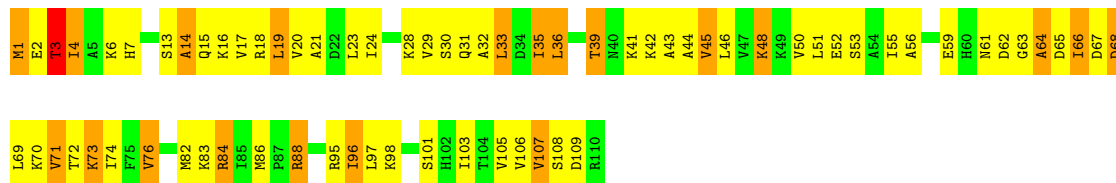
• Molecule 39: 50S ribosomal protein L21





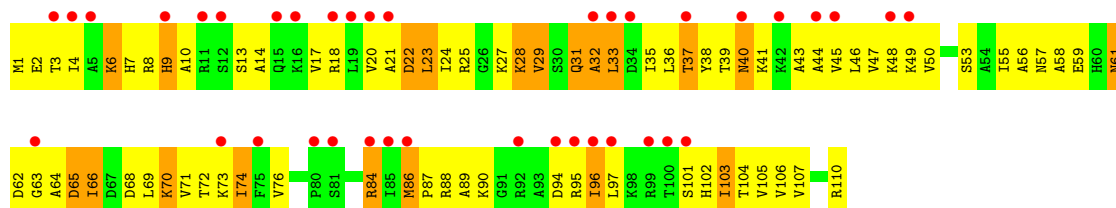
• Molecule 40: 50S ribosomal protein L22

Chain BS: 35% 45% 18%



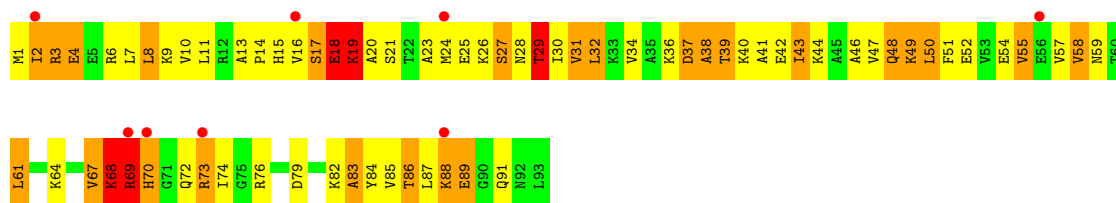
• Molecule 40: 50S ribosomal protein L22

Chain DS: 29% 53% 18%



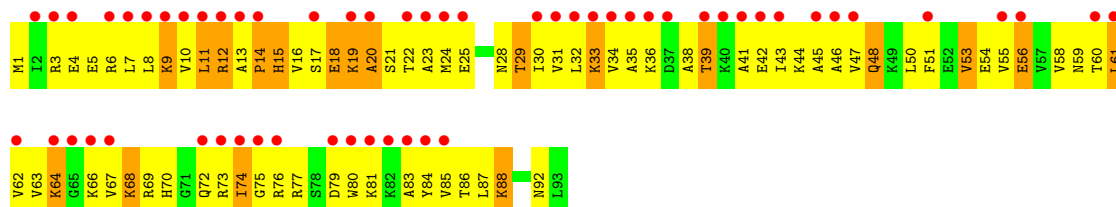
• Molecule 41: 50S ribosomal protein L23

Chain BT: 9% 24% 44% 27% 5%



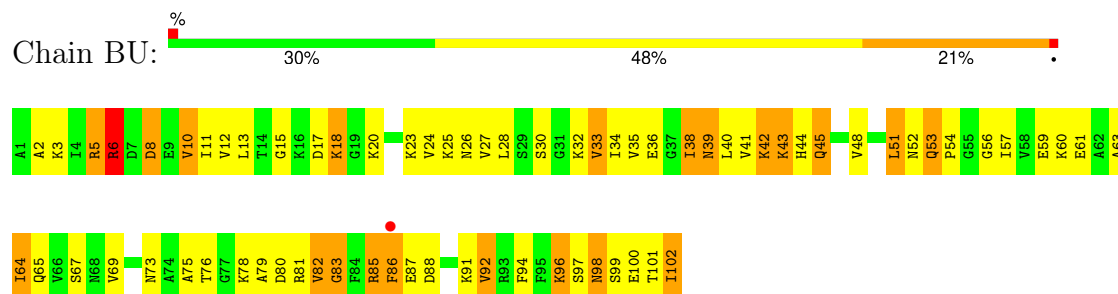
• Molecule 41: 50S ribosomal protein L23

Chain DT: 17% 61% 62% 20%

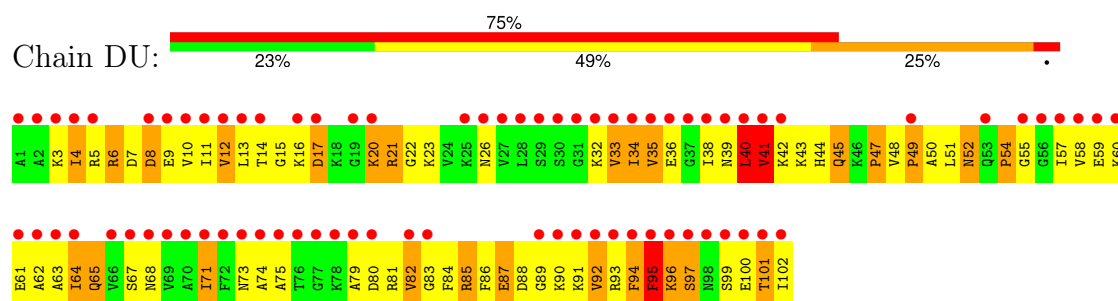




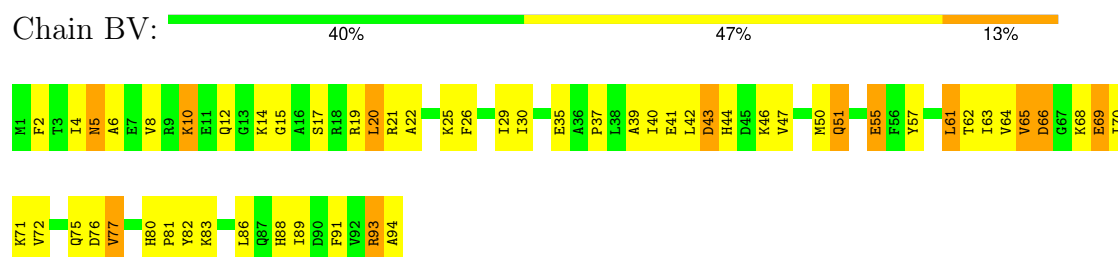
- Molecule 42: 50S ribosomal protein L24



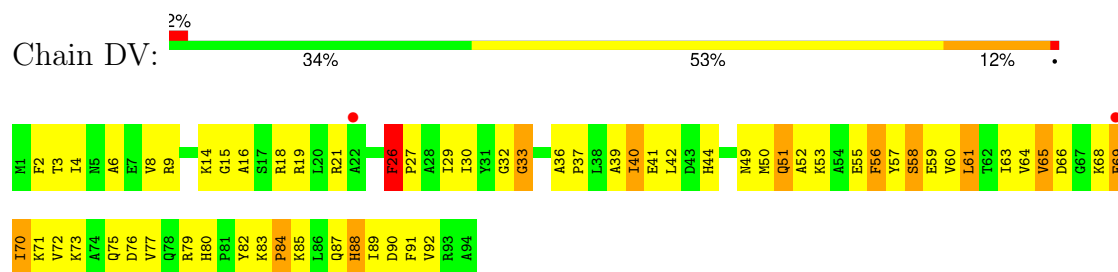
- Molecule 42: 50S ribosomal protein L24



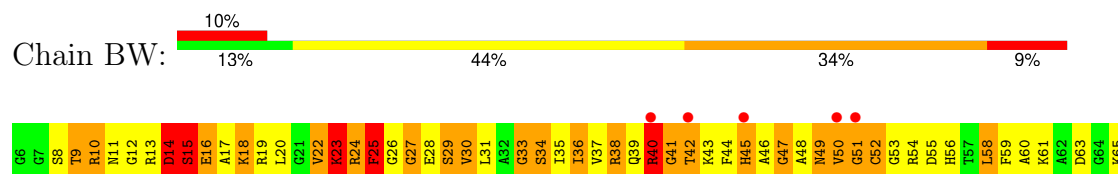
- Molecule 43: 50S ribosomal protein L25



- Molecule 43: 50S ribosomal protein L25

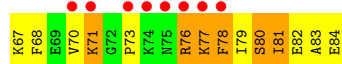
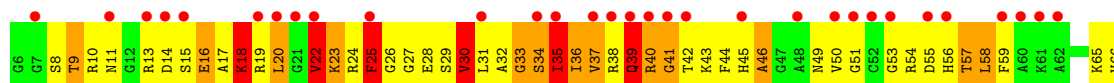
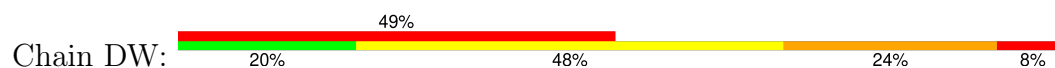


- Molecule 44: 50S ribosomal protein L27





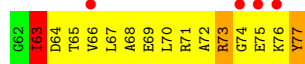
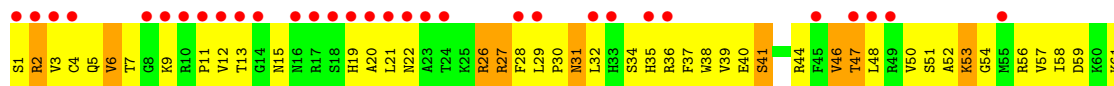
• Molecule 44: 50S ribosomal protein L27



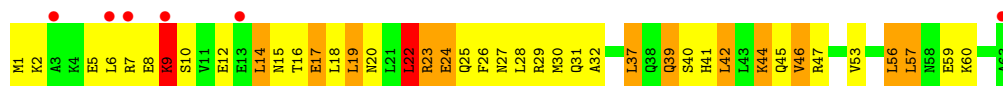
• Molecule 45: 50S ribosomal protein L28



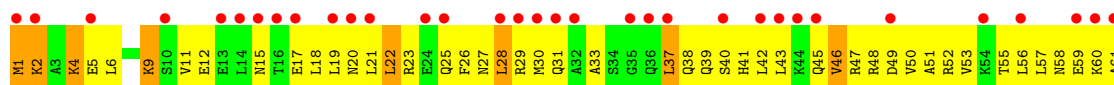
• Molecule 45: 50S ribosomal protein L28



• Molecule 46: 50S ribosomal protein L29



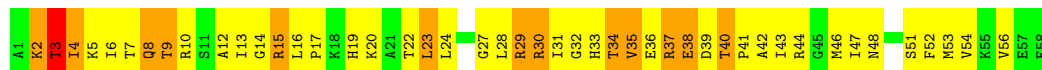
• Molecule 46: 50S ribosomal protein L29





- Molecule 47: 50S ribosomal protein L30

Chain BZ: 21% 55% 22%



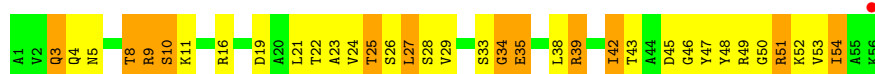
- Molecule 47: 50S ribosomal protein L30

Chain DZ: 19% 29% 52% 17%



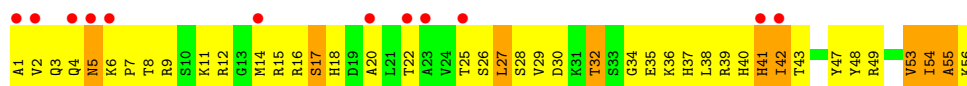
- Molecule 48: 50S ribosomal protein L32

Chain B0: 2% 38% 41% 21%



- Molecule 48: 50S ribosomal protein L32

Chain D0: 21% 25% 59% 16%



- Molecule 49: 50S ribosomal protein L33

Chain B1: 2% 30% 50% 18%

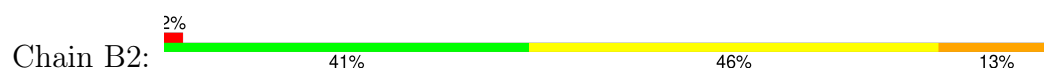


- Molecule 49: 50S ribosomal protein L33

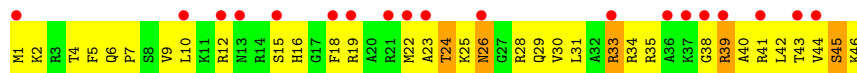
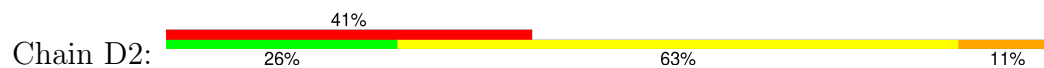
Chain D1: 28% 26% 60% 12%



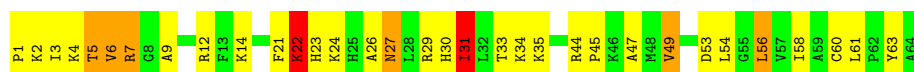
- Molecule 50: 50S ribosomal protein L34



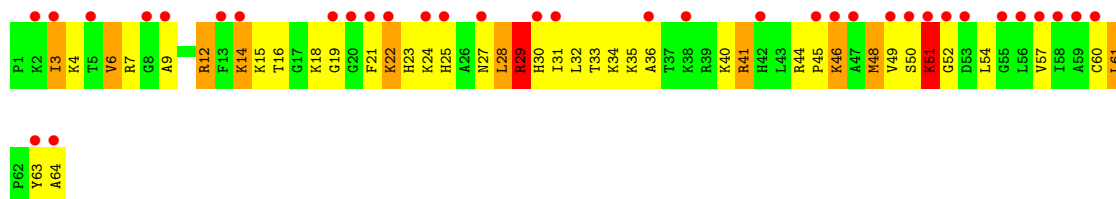
- Molecule 50: 50S ribosomal protein L34



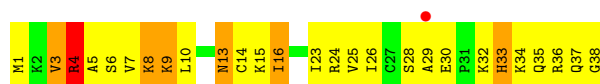
- Molecule 51: 50S ribosomal protein L35



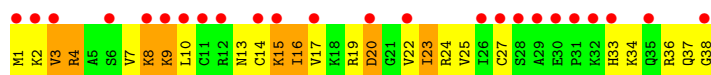
- Molecule 51: 50S ribosomal protein L35



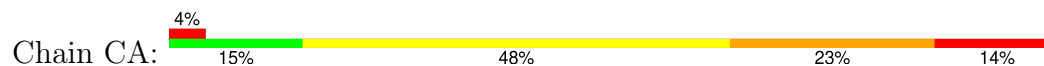
- Molecule 52: 50S ribosomal protein L36



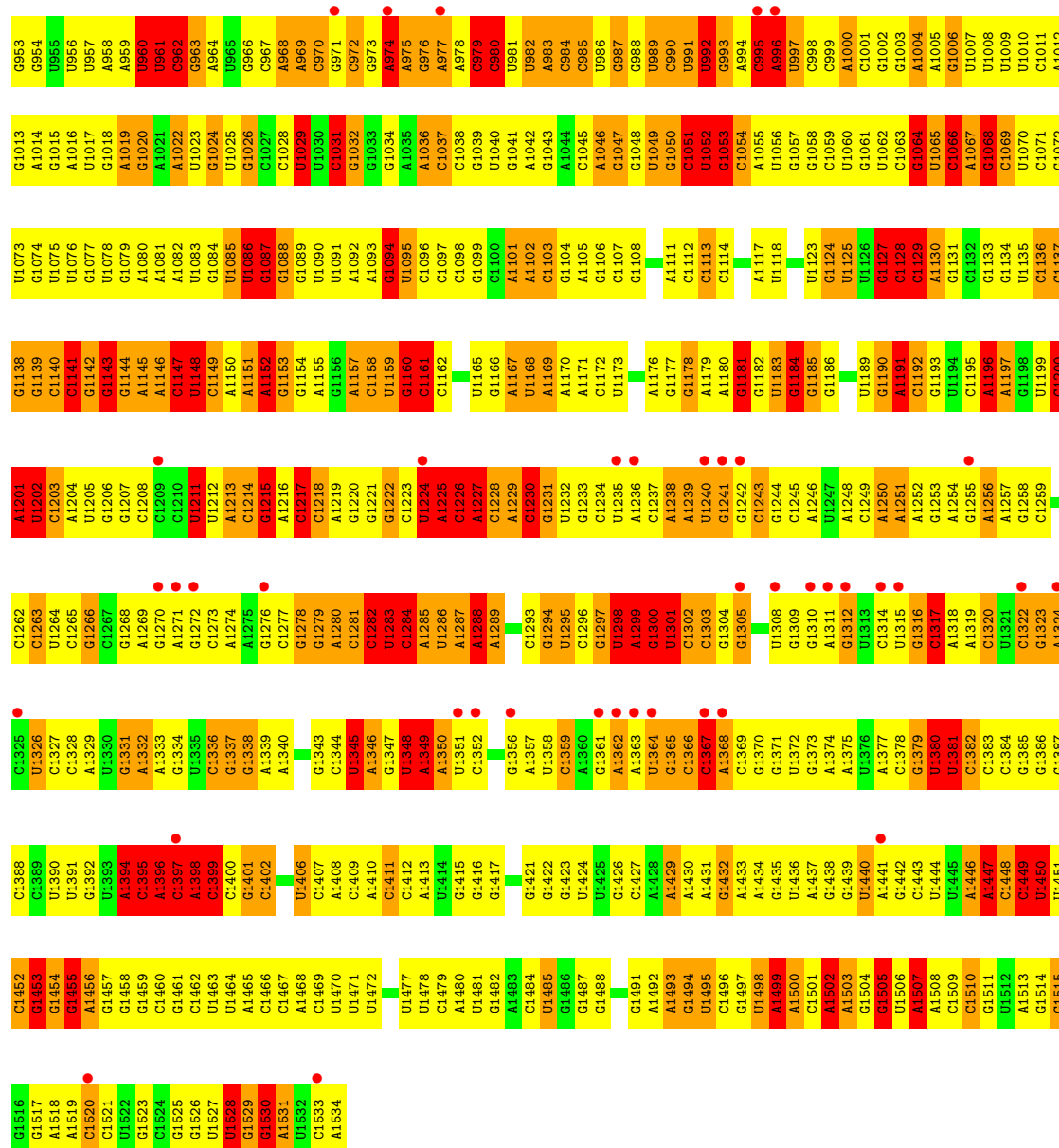
- Molecule 52: 50S ribosomal protein L36



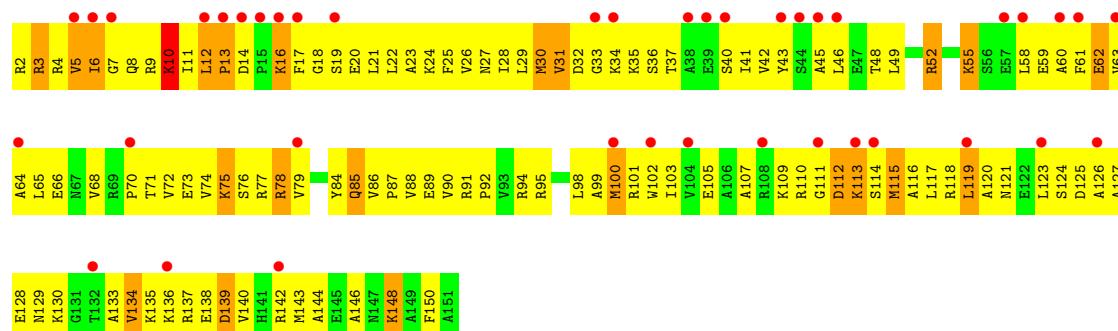
- Molecule 53: 16S rRNA





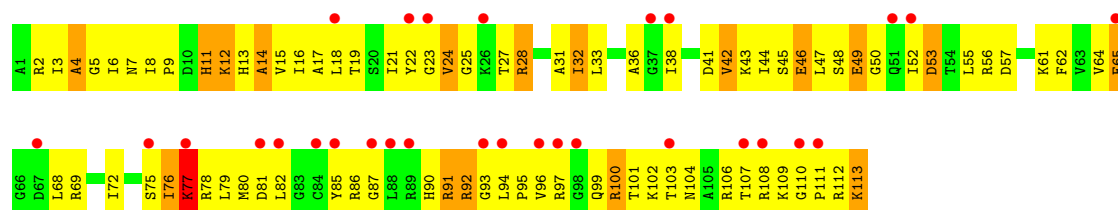


### • Molecule 54: 30S ribosomal protein S7



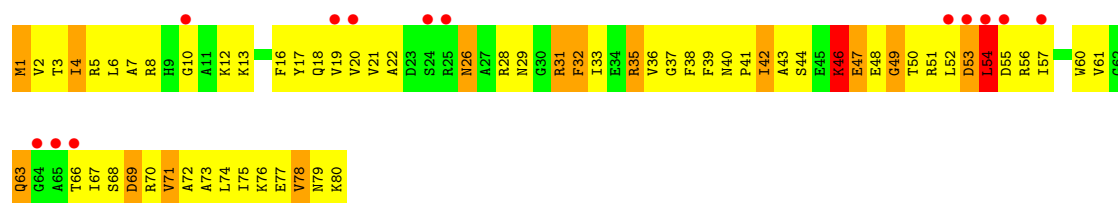
- Molecule 55: 30S ribosomal protein S13

Chain CM: 




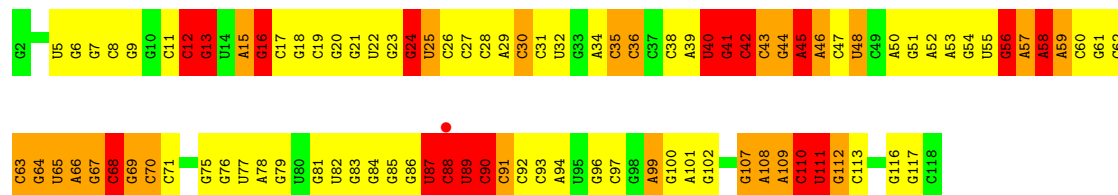
- Molecule 56: 30S ribosomal protein S16

Chain CP: 



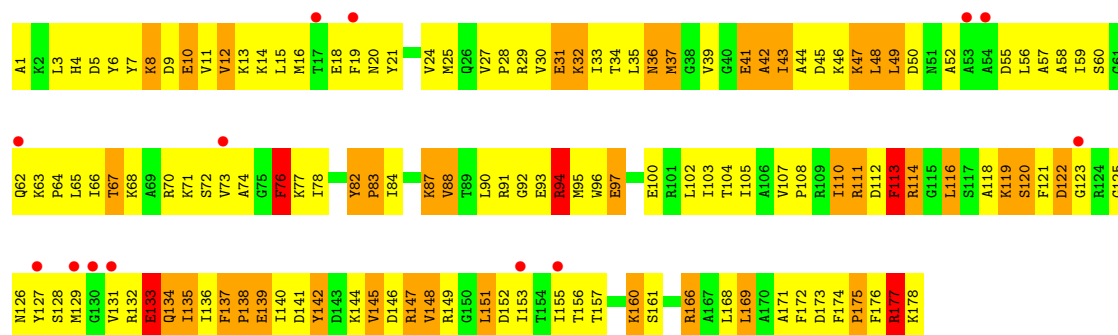
- Molecule 57: 5S rRNA

Chain DB: 



- 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, $\alpha$ , $\beta$ , $\gamma$	211.08Å 434.46Å 618.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.35 – 3.29 76.35 – 3.29	Depositor EDS
% Data completeness (in resolution range)	77.5 (76.35-3.29) 77.5 (76.35-3.29)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 3.26Å)	Xtriage
Refinement program	PHENIX, PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.189 , 0.241 0.201 , 0.250	Depositor DCC
$R_{free}$ test set	14080 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.6	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 76.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	284501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, MG, CLY

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	0.50	2/36834 (0.0%)	1.24	439/57462 (0.8%)
2	AB	0.24	0/1736	0.44	0/2338
2	CB	0.23	0/1736	0.44	0/2338
3	AC	0.26	0/1652	0.48	0/2225
3	CC	0.22	0/1652	0.42	0/2225
4	AD	0.29	0/1665	0.50	0/2227
4	CD	0.32	0/1665	0.55	0/2227
5	AE	0.31	0/1119	0.56	0/1504
5	CE	0.35	1/1119 (0.1%)	0.53	0/1504
6	AF	0.28	0/836	0.47	0/1128
6	CF	0.26	0/836	0.48	0/1128
7	AG	0.23	0/1196	0.45	0/1602
8	AH	0.30	0/989	0.52	0/1326
8	CH	0.26	0/989	0.49	0/1326
9	AI	0.24	0/1034	0.45	0/1375
9	CI	0.21	0/1034	0.41	0/1375
10	AJ	0.24	0/797	0.47	0/1077
10	CJ	0.21	0/797	0.45	0/1077
11	AK	0.26	0/893	0.51	0/1205
11	CK	0.26	0/893	0.50	0/1205
12	AL	0.35	0/969	0.66	1/1300 (0.1%)
12	CL	0.29	0/969	0.54	0/1300
13	AM	0.23	0/893	0.47	0/1193
14	AN	0.26	0/785	0.46	0/1043
14	CN	0.21	0/780	0.37	0/1036
15	AO	0.29	0/722	0.45	0/964
15	CO	0.25	0/722	0.42	0/964
16	AP	0.30	0/659	0.48	0/884
17	AQ	0.35	0/658	0.56	0/881
17	CQ	0.27	0/658	0.49	0/881
18	AR	0.28	0/463	0.47	0/621
18	CR	0.26	0/463	0.45	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	AS	0.24	0/653	0.43	0/877
19	CS	0.20	0/653	0.41	0/877
20	AT	0.31	0/671	0.52	0/888
20	CT	0.25	0/671	0.49	0/888
21	AU	0.27	0/431	0.45	0/570
21	CU	0.32	0/431	0.57	0/570
22	BA	0.73	7/68626 (0.0%)	1.54	1278/107056 (1.2%)
22	DA	0.45	2/68314 (0.0%)	1.23	934/106569 (0.9%)
23	BB	0.68	0/2828	1.42	40/4410 (0.9%)
24	BC	0.40	0/2122	0.67	0/2852
24	DC	0.29	0/2122	0.51	0/2852
25	BD	0.51	0/1586	0.72	1/2134 (0.0%)
25	DD	0.28	0/1586	0.54	0/2134
26	BE	0.42	0/1571	0.63	0/2113
26	DE	0.24	0/1571	0.46	0/2113
27	BF	0.32	0/1435	0.52	0/1926
28	BG	0.36	0/1343	0.59	0/1816
28	DG	0.22	0/1343	0.44	0/1816
29	BH	0.27	0/1122	0.47	0/1515
29	DH	0.25	0/1122	0.51	2/1515 (0.1%)
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.20	0/1046	0.42	0/1410
31	BJ	0.52	0/1152	0.77	0/1551
31	DJ	0.26	0/1152	0.55	1/1551 (0.1%)
32	BK	0.49	0/948	0.71	0/1268
32	DK	0.29	0/948	0.52	0/1268
33	BL	0.41	0/1054	0.71	1/1403 (0.1%)
33	DL	0.25	0/1054	0.50	0/1403
34	BM	0.46	0/1093	0.68	0/1460
34	DM	0.27	0/1093	0.46	0/1460
35	BN	0.42	0/974	0.68	0/1301
35	DN	0.26	0/974	0.48	0/1301
36	BO	0.39	0/902	0.59	0/1209
36	DO	0.21	0/902	0.40	0/1209
37	BP	0.45	0/929	0.71	0/1242
37	DP	0.27	0/929	0.47	0/1242
38	BQ	0.55	0/960	0.69	0/1278
38	DQ	0.27	0/960	0.44	0/1278
39	BR	0.54	0/829	0.72	0/1107
39	DR	0.26	0/829	0.49	0/1107
40	BS	0.51	0/864	0.73	0/1156
40	DS	0.26	0/864	0.50	0/1156
41	BT	0.43	0/745	0.68	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
41	DT	0.22	0/745	0.45	0/994
42	BU	0.39	0/788	0.67	0/1051
42	DU	0.22	0/788	0.45	0/1051
43	BV	0.41	0/766	0.60	0/1025
43	DV	0.23	0/766	0.42	0/1025
44	BW	0.49	0/603	0.77	0/797
44	DW	0.25	0/603	0.46	0/797
45	BX	0.39	0/635	0.66	0/848
45	DX	0.26	0/635	0.52	0/848
46	BY	0.36	0/510	0.60	0/677
46	DY	0.21	0/510	0.42	0/677
47	BZ	0.51	0/453	0.73	0/605
47	DZ	0.25	0/453	0.50	0/605
48	B0	0.44	0/450	0.69	0/599
48	D0	0.26	0/450	0.48	0/599
49	B1	0.36	0/417	0.54	0/554
49	D1	0.24	0/417	0.44	0/554
50	B2	0.45	0/380	0.62	0/498
50	D2	0.25	0/380	0.47	0/498
51	B3	0.44	0/513	0.62	0/676
51	D3	0.25	0/513	0.49	0/676
52	B4	0.47	0/303	0.74	0/397
52	D4	0.32	0/303	0.45	0/397
53	CA	0.46	3/36762 (0.0%)	1.18	421/57350 (0.7%)
54	CG	0.21	0/1188	0.42	0/1591
55	CM	0.19	0/885	0.39	0/1181
56	CP	0.27	0/649	0.49	0/870
57	DB	0.43	1/2803 (0.0%)	1.07	30/4371 (0.7%)
58	DF	0.22	0/1444	0.45	0/1937
All	All	0.51	16/306773 (0.0%)	1.17	3148/458565 (0.7%)

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
31	BJ	0	1
35	BN	0	1
58	DF	0	1
All	All	0	4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	CA	1396	A	O3'-P	-16.33	1.41	1.61
1	AA	1047	G	O3'-P	-13.54	1.45	1.61
22	BA	1905	C	O3'-P	-12.21	1.46	1.61
22	BA	2197	U	O3'-P	-9.98	1.49	1.61
22	BA	876	C	O3'-P	-9.54	1.49	1.61

The worst 5 of 3148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	DA	2586	U	N1-C1'-C2'	-16.52	92.53	114.00
22	BA	627	A	P-O3'-C3'	15.92	138.81	119.70
22	BA	531	C	P-O3'-C3'	15.89	138.77	119.70
1	AA	1047	G	P-O3'-C3'	-15.60	100.98	119.70
22	BA	2068	U	N1-C1'-C2'	-15.16	94.30	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	BD	9	VAL	Peptide
31	BJ	43	GLU	Peptide
35	BN	101	GLY	Peptide
58	DF	177	ARG	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32895	0	16553	1994	0
2	AB	1705	0	1731	279	0
2	CB	1705	0	1732	233	0
3	AC	1625	0	1699	178	0
3	CC	1625	0	1699	193	0
4	AD	1643	0	1710	243	0
4	CD	1643	0	1710	224	0
5	AE	1106	0	1148	206	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	CE	1106	0	1148	145	0
6	AF	818	0	808	111	0
6	CF	818	0	808	117	0
7	AG	1182	0	1240	130	0
8	AH	979	0	1034	136	0
8	CH	979	0	1034	126	0
9	AI	1022	0	1070	133	0
9	CI	1022	0	1070	164	0
10	AJ	787	0	828	141	0
10	CJ	787	0	828	148	0
11	AK	877	0	887	140	0
11	CK	877	0	887	128	0
12	AL	955	0	1019	127	0
12	CL	955	0	1019	156	0
13	AM	884	0	944	94	0
14	AN	774	0	827	136	0
14	CN	769	0	822	130	0
15	AO	714	0	737	84	0
15	CO	714	0	737	61	0
16	AP	649	0	666	79	0
17	AQ	649	0	691	100	0
17	CQ	649	0	691	112	0
18	AR	456	0	478	53	0
18	CR	456	0	478	57	0
19	AS	638	0	665	74	0
19	CS	638	0	665	109	0
20	AT	665	0	714	97	0
20	CT	665	0	714	86	0
21	AU	426	0	449	116	0
21	CU	426	0	449	92	0
22	BA	61274	0	30819	3248	0
22	DA	60995	0	30679	5259	0
23	BB	2529	0	1281	118	0
24	BC	2083	0	2157	287	0
24	DC	2083	0	2157	345	0
25	BD	1565	0	1616	269	0
25	DD	1565	0	1616	291	0
26	BE	1552	0	1619	203	0
26	DE	1552	0	1619	266	0
27	BF	1411	0	1447	208	0
28	BG	1323	0	1374	211	0
28	DG	1323	0	1374	199	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BH	1111	0	1148	166	0
29	DH	1111	0	1148	175	0
30	BI	1032	0	1088	114	0
30	DI	1032	0	1088	120	0
31	BJ	1129	0	1162	216	0
31	DJ	1129	0	1162	202	0
32	BK	939	0	1012	164	0
32	DK	939	0	1012	183	0
33	BL	1045	0	1117	169	0
33	DL	1045	0	1117	192	0
34	BM	1074	0	1157	146	0
34	DM	1074	0	1157	150	0
35	BN	961	0	1000	123	0
35	DN	961	0	1000	207	0
36	BO	892	0	923	92	0
36	DO	892	0	923	107	0
37	BP	917	0	965	195	0
37	DP	917	0	965	172	0
38	BQ	947	0	1022	191	0
38	DQ	947	0	1022	180	0
39	BR	816	0	839	138	0
39	DR	816	0	839	137	0
40	BS	857	0	922	110	0
40	DS	857	0	922	131	0
41	BT	739	0	807	156	0
41	DT	739	0	807	159	0
42	BU	780	0	834	84	0
42	DU	780	0	834	133	0
43	BV	753	0	780	76	0
43	DV	753	0	780	108	0
44	BW	596	0	610	229	0
44	DW	596	0	610	174	0
45	BX	625	0	655	104	0
45	DX	625	0	655	114	0
46	BY	509	0	543	69	0
46	DY	509	0	543	102	0
47	BZ	449	0	491	58	0
47	DZ	449	0	491	58	0
48	B0	444	0	461	32	0
48	D0	444	0	461	75	0
49	B1	410	0	440	57	0
49	D1	410	0	440	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	B2	377	0	418	36	0
50	D2	377	0	418	66	0
51	B3	504	0	574	53	0
51	D3	504	0	574	67	0
52	B4	302	0	340	47	0
52	D4	302	0	342	41	0
53	CA	32831	0	16521	2416	0
54	CG	1175	0	1230	194	0
55	CM	877	0	937	167	0
56	CP	639	0	656	101	0
57	DB	2507	0	1270	234	0
58	DF	1420	0	1460	282	0
59	AA	42	0	0	0	0
59	AN	1	0	0	0	0
59	BA	134	0	0	0	0
59	BB	4	0	0	0	0
59	BL	1	0	0	0	0
59	CA	42	0	0	0	0
59	DA	132	0	0	0	0
59	DB	1	0	0	0	0
59	DC	2	0	0	0	0
59	DE	1	0	0	0	0
59	DJ	1	0	0	0	0
60	BA	27	0	32	2	0
61	B4	1	0	0	0	0
61	D4	1	0	0	0	0
62	AA	197	0	0	5	0
62	AE	1	0	0	0	0
62	AL	1	0	0	0	0
62	AN	6	0	0	2	0
62	AT	2	0	0	0	0
62	AU	1	0	0	0	0
62	B2	2	0	0	0	0
62	B3	2	0	0	1	0
62	B4	1	0	0	0	0
62	BA	601	0	0	48	0
62	BB	20	0	0	1	0
62	BC	8	0	0	0	0
62	BD	4	0	0	1	0
62	BE	1	0	0	1	0
62	BL	3	0	0	1	0
62	BN	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	BQ	1	0	0	0	0
62	BR	1	0	0	1	0
62	BT	3	0	0	0	0
62	CA	193	0	0	7	0
62	CE	4	0	0	0	0
62	CI	1	0	0	0	0
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	2	0	0	0	0
62	D3	1	0	0	0	0
62	D4	4	0	0	0	0
62	DA	599	0	0	28	0
62	DB	4	0	0	0	0
62	DC	9	0	0	2	0
62	DD	2	0	0	0	0
62	DE	3	0	0	0	0
62	DJ	5	0	0	0	0
62	DL	5	0	0	1	0
62	DN	3	0	0	0	0
62	DT	3	0	0	1	0
62	DU	2	0	0	0	0
62	DV	1	0	0	0	0
All	All	284501	0	190871	25099	0

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 53.

The worst 5 of 25099 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)
22:BA:900:A:C2'	22:BA:901:C:H5'	1.40	1.46
2:AB:108:GLN:O	2:AB:110:ILE:N	1.58	1.37
22:BA:1073:A:C2'	22:BA:1074:G:H5''	1.54	1.35
2:CB:93:HIS:CG	2:CB:145:ASN:O	1.88	1.27
28:BG:84:LYS:HG3	28:BG:132:LEU:N	1.49	1.26

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	121 (56%)	65 (30%)	30 (14%)	0	1
2	CB	216/218 (99%)	145 (67%)	54 (25%)	17 (8%)	1	5
3	AC	204/206 (99%)	154 (76%)	33 (16%)	17 (8%)	0	4
3	CC	204/206 (99%)	147 (72%)	40 (20%)	17 (8%)	0	4
4	AD	203/205 (99%)	134 (66%)	42 (21%)	27 (13%)	0	1
4	CD	203/205 (99%)	139 (68%)	38 (19%)	26 (13%)	0	1
5	AE	148/150 (99%)	105 (71%)	26 (18%)	17 (12%)	0	2
5	CE	148/150 (99%)	110 (74%)	23 (16%)	15 (10%)	0	3
6	AF	98/100 (98%)	71 (72%)	19 (19%)	8 (8%)	1	5
6	CF	98/100 (98%)	62 (63%)	27 (28%)	9 (9%)	0	3
7	AG	149/151 (99%)	107 (72%)	34 (23%)	8 (5%)	1	10
8	AH	127/129 (98%)	92 (72%)	27 (21%)	8 (6%)	1	8
8	CH	127/129 (98%)	87 (68%)	30 (24%)	10 (8%)	1	5
9	AI	125/127 (98%)	83 (66%)	31 (25%)	11 (9%)	0	4
9	CI	125/127 (98%)	87 (70%)	29 (23%)	9 (7%)	1	6
10	AJ	96/98 (98%)	64 (67%)	19 (20%)	13 (14%)	0	1
10	CJ	96/98 (98%)	58 (60%)	24 (25%)	14 (15%)	0	1
11	AK	115/117 (98%)	85 (74%)	18 (16%)	12 (10%)	0	2
11	CK	115/117 (98%)	89 (77%)	17 (15%)	9 (8%)	1	5
12	AL	121/123 (98%)	84 (69%)	21 (17%)	16 (13%)	0	1
12	CL	121/123 (98%)	84 (69%)	25 (21%)	12 (10%)	0	3
13	AM	112/114 (98%)	87 (78%)	17 (15%)	8 (7%)	1	6
14	AN	92/100 (92%)	54 (59%)	23 (25%)	15 (16%)	0	1
14	CN	91/100 (91%)	58 (64%)	27 (30%)	6 (7%)	1	7
15	AO	86/88 (98%)	58 (67%)	22 (26%)	6 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CO	86/88 (98%)	68 (79%)	15 (17%)	3 (4%)	3	18
16	AP	80/82 (98%)	58 (72%)	13 (16%)	9 (11%)	0	2
17	AQ	78/80 (98%)	46 (59%)	20 (26%)	12 (15%)	0	1
17	CQ	78/80 (98%)	60 (77%)	8 (10%)	10 (13%)	0	1
18	AR	53/55 (96%)	39 (74%)	13 (24%)	1 (2%)	6	30
18	CR	53/55 (96%)	40 (76%)	11 (21%)	2 (4%)	2	16
19	AS	77/79 (98%)	56 (73%)	14 (18%)	7 (9%)	0	3
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	0	3
20	AT	83/85 (98%)	54 (65%)	20 (24%)	9 (11%)	0	2
20	CT	83/85 (98%)	55 (66%)	21 (25%)	7 (8%)	0	4
21	AU	49/51 (96%)	25 (51%)	17 (35%)	7 (14%)	0	1
21	CU	49/51 (96%)	24 (49%)	11 (22%)	14 (29%)	0	0
24	BC	269/271 (99%)	197 (73%)	53 (20%)	19 (7%)	1	6
24	DC	269/271 (99%)	177 (66%)	55 (20%)	37 (14%)	0	1
25	BD	207/209 (99%)	140 (68%)	38 (18%)	29 (14%)	0	1
25	DD	207/209 (99%)	134 (65%)	39 (19%)	34 (16%)	0	1
26	BE	199/201 (99%)	143 (72%)	35 (18%)	21 (11%)	0	2
26	DE	199/201 (99%)	122 (61%)	51 (26%)	26 (13%)	0	1
27	BF	175/177 (99%)	127 (73%)	33 (19%)	15 (9%)	0	4
28	BG	174/176 (99%)	115 (66%)	32 (18%)	27 (16%)	0	1
28	DG	174/176 (99%)	100 (58%)	43 (25%)	31 (18%)	0	1
29	BH	147/149 (99%)	67 (46%)	46 (31%)	34 (23%)	0	0
29	DH	147/149 (99%)	71 (48%)	58 (40%)	18 (12%)	0	1
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	0	3
30	DI	139/141 (99%)	78 (56%)	43 (31%)	18 (13%)	0	1
31	BJ	140/142 (99%)	101 (72%)	23 (16%)	16 (11%)	0	2
31	DJ	140/142 (99%)	90 (64%)	30 (21%)	20 (14%)	0	1
32	BK	120/122 (98%)	83 (69%)	15 (12%)	22 (18%)	0	0
32	DK	120/122 (98%)	83 (69%)	13 (11%)	24 (20%)	0	0
33	BL	141/143 (99%)	104 (74%)	28 (20%)	9 (6%)	1	7
33	DL	141/143 (99%)	81 (57%)	42 (30%)	18 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BM	134/136 (98%)	91 (68%)	25 (19%)	18 (13%)	0	1
34	DM	134/136 (98%)	93 (69%)	24 (18%)	17 (13%)	0	1
35	BN	118/120 (98%)	87 (74%)	21 (18%)	10 (8%)	0	4
35	DN	118/120 (98%)	72 (61%)	30 (25%)	16 (14%)	0	1
36	BO	114/116 (98%)	87 (76%)	20 (18%)	7 (6%)	1	8
36	DO	114/116 (98%)	76 (67%)	26 (23%)	12 (10%)	0	2
37	BP	112/114 (98%)	75 (67%)	21 (19%)	16 (14%)	0	1
37	DP	112/114 (98%)	65 (58%)	27 (24%)	20 (18%)	0	1
38	BQ	115/117 (98%)	91 (79%)	17 (15%)	7 (6%)	1	8
38	DQ	115/117 (98%)	78 (68%)	24 (21%)	13 (11%)	0	2
39	BR	101/103 (98%)	76 (75%)	16 (16%)	9 (9%)	0	4
39	DR	101/103 (98%)	67 (66%)	25 (25%)	9 (9%)	0	4
40	BS	108/110 (98%)	77 (71%)	25 (23%)	6 (6%)	1	9
40	DS	108/110 (98%)	75 (69%)	21 (19%)	12 (11%)	0	2
41	BT	91/93 (98%)	55 (60%)	19 (21%)	17 (19%)	0	0
41	DT	91/93 (98%)	47 (52%)	28 (31%)	16 (18%)	0	1
42	BU	100/102 (98%)	63 (63%)	22 (22%)	15 (15%)	0	1
42	DU	100/102 (98%)	50 (50%)	23 (23%)	27 (27%)	0	0
43	BV	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	5	26
43	DV	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	1	5
44	BW	77/79 (98%)	27 (35%)	25 (32%)	25 (32%)	0	0
44	DW	77/79 (98%)	34 (44%)	22 (29%)	21 (27%)	0	0
45	BX	75/77 (97%)	54 (72%)	15 (20%)	6 (8%)	1	5
45	DX	75/77 (97%)	46 (61%)	24 (32%)	5 (7%)	1	7
46	BY	61/63 (97%)	37 (61%)	16 (26%)	8 (13%)	0	1
46	DY	61/63 (97%)	40 (66%)	16 (26%)	5 (8%)	1	5
47	BZ	56/58 (97%)	44 (79%)	10 (18%)	2 (4%)	3	17
47	DZ	56/58 (97%)	35 (62%)	15 (27%)	6 (11%)	0	2
48	B0	54/56 (96%)	42 (78%)	8 (15%)	4 (7%)	1	6
48	D0	54/56 (96%)	37 (68%)	12 (22%)	5 (9%)	0	3
49	B1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	D1	48/50 (96%)	33 (69%)	10 (21%)	5 (10%)	0	2
50	B2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	5	25
50	D2	44/46 (96%)	32 (73%)	6 (14%)	6 (14%)	0	1
51	B3	62/64 (97%)	50 (81%)	8 (13%)	4 (6%)	1	7
51	D3	62/64 (97%)	40 (64%)	17 (27%)	5 (8%)	1	5
52	B4	36/38 (95%)	28 (78%)	4 (11%)	4 (11%)	0	2
52	D4	36/38 (95%)	24 (67%)	6 (17%)	6 (17%)	0	1
54	CG	148/150 (99%)	103 (70%)	34 (23%)	11 (7%)	1	6
55	CM	111/113 (98%)	63 (57%)	36 (32%)	12 (11%)	0	2
56	CP	78/80 (98%)	50 (64%)	19 (24%)	9 (12%)	0	2
58	DF	176/178 (99%)	98 (56%)	46 (26%)	32 (18%)	0	1
All	All	11238/11447 (98%)	7490 (67%)	2445 (22%)	1303 (12%)	0	2

5 of 1303 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	20	ARG
2	AB	21	TYR
2	AB	37	VAL
2	AB	40	ILE
2	AB	75	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	147 (82%)	33 (18%)	1	6
2	CB	180/180 (100%)	152 (84%)	28 (16%)	2	10
3	AC	170/170 (100%)	140 (82%)	30 (18%)	1	7
3	CC	170/170 (100%)	153 (90%)	17 (10%)	6	23
4	AD	172/172 (100%)	142 (83%)	30 (17%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/172 (100%)	140 (81%)	32 (19%)	1	5
5	AE	113/113 (100%)	87 (77%)	26 (23%)	0	2
5	CE	113/113 (100%)	92 (81%)	21 (19%)	1	5
6	AF	87/87 (100%)	74 (85%)	13 (15%)	2	11
6	CF	87/87 (100%)	73 (84%)	14 (16%)	2	9
7	AG	124/124 (100%)	109 (88%)	15 (12%)	4	17
8	AH	104/104 (100%)	90 (86%)	14 (14%)	3	14
8	CH	104/104 (100%)	91 (88%)	13 (12%)	3	16
9	AI	105/105 (100%)	87 (83%)	18 (17%)	1	8
9	CI	105/105 (100%)	92 (88%)	13 (12%)	4	17
10	AJ	86/86 (100%)	74 (86%)	12 (14%)	3	14
10	CJ	86/86 (100%)	77 (90%)	9 (10%)	5	22
11	AK	90/90 (100%)	72 (80%)	18 (20%)	1	4
11	CK	90/90 (100%)	77 (86%)	13 (14%)	2	13
12	AL	103/103 (100%)	85 (82%)	18 (18%)	1	7
12	CL	103/103 (100%)	86 (84%)	17 (16%)	2	9
13	AM	92/92 (100%)	88 (96%)	4 (4%)	25	52
14	AN	79/83 (95%)	72 (91%)	7 (9%)	8	28
14	CN	79/83 (95%)	68 (86%)	11 (14%)	3	14
15	AO	76/76 (100%)	67 (88%)	9 (12%)	4	18
15	CO	76/76 (100%)	68 (90%)	8 (10%)	5	22
16	AP	65/65 (100%)	58 (89%)	7 (11%)	5	21
17	AQ	74/74 (100%)	60 (81%)	14 (19%)	1	5
17	CQ	74/74 (100%)	62 (84%)	12 (16%)	2	9
18	AR	48/48 (100%)	46 (96%)	2 (4%)	25	53
18	CR	48/48 (100%)	44 (92%)	4 (8%)	9	30
19	AS	70/70 (100%)	63 (90%)	7 (10%)	6	23
19	CS	70/70 (100%)	63 (90%)	7 (10%)	6	23
20	AT	65/65 (100%)	50 (77%)	15 (23%)	0	2
20	CT	65/65 (100%)	55 (85%)	10 (15%)	2	10
21	AU	44/44 (100%)	37 (84%)	7 (16%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	44/44 (100%)	36 (82%)	8 (18%)	1	6
24	BC	216/216 (100%)	166 (77%)	50 (23%)	0	2
24	DC	216/216 (100%)	189 (88%)	27 (12%)	3	16
25	BD	164/164 (100%)	131 (80%)	33 (20%)	1	4
25	DD	164/164 (100%)	139 (85%)	25 (15%)	2	11
26	BE	165/165 (100%)	126 (76%)	39 (24%)	0	2
26	DE	165/165 (100%)	148 (90%)	17 (10%)	6	22
27	BF	148/148 (100%)	124 (84%)	24 (16%)	2	9
28	BG	137/137 (100%)	107 (78%)	30 (22%)	1	3
28	DG	137/137 (100%)	121 (88%)	16 (12%)	4	18
29	BH	114/114 (100%)	96 (84%)	18 (16%)	2	9
29	DH	114/114 (100%)	98 (86%)	16 (14%)	3	14
30	BI	109/109 (100%)	91 (84%)	18 (16%)	2	9
30	DI	109/109 (100%)	103 (94%)	6 (6%)	18	45
31	BJ	116/116 (100%)	84 (72%)	32 (28%)	0	1
31	DJ	116/116 (100%)	103 (89%)	13 (11%)	5	19
32	BK	103/103 (100%)	78 (76%)	25 (24%)	0	2
32	DK	103/103 (100%)	82 (80%)	21 (20%)	1	4
33	BL	102/102 (100%)	71 (70%)	31 (30%)	0	1
33	DL	102/102 (100%)	89 (87%)	13 (13%)	3	16
34	BM	109/109 (100%)	87 (80%)	22 (20%)	1	4
34	DM	109/109 (100%)	103 (94%)	6 (6%)	18	45
35	BN	100/100 (100%)	83 (83%)	17 (17%)	1	8
35	DN	100/100 (100%)	80 (80%)	20 (20%)	1	4
36	BO	86/86 (100%)	71 (83%)	15 (17%)	1	7
36	DO	86/86 (100%)	78 (91%)	8 (9%)	7	26
37	BP	99/99 (100%)	72 (73%)	27 (27%)	0	1
37	DP	99/99 (100%)	89 (90%)	10 (10%)	6	23
38	BQ	89/89 (100%)	72 (81%)	17 (19%)	1	5
38	DQ	89/89 (100%)	75 (84%)	14 (16%)	2	10
39	BR	84/84 (100%)	66 (79%)	18 (21%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DR	84/84 (100%)	71 (84%)	13 (16%)	2	10
40	BS	93/93 (100%)	74 (80%)	19 (20%)	1	4
40	DS	93/93 (100%)	79 (85%)	14 (15%)	2	11
41	BT	80/80 (100%)	59 (74%)	21 (26%)	0	1
41	DT	80/80 (100%)	74 (92%)	6 (8%)	11	34
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	4
42	DU	83/83 (100%)	73 (88%)	10 (12%)	4	17
43	BV	78/78 (100%)	61 (78%)	17 (22%)	1	3
43	DV	78/78 (100%)	70 (90%)	8 (10%)	6	22
44	BW	59/59 (100%)	41 (70%)	18 (30%)	0	1
44	DW	59/59 (100%)	44 (75%)	15 (25%)	0	2
45	BX	67/67 (100%)	51 (76%)	16 (24%)	0	2
45	DX	67/67 (100%)	57 (85%)	10 (15%)	2	11
46	BY	55/55 (100%)	45 (82%)	10 (18%)	1	6
46	DY	55/55 (100%)	52 (94%)	3 (6%)	18	45
47	BZ	48/48 (100%)	32 (67%)	16 (33%)	0	0
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	2	8
48	B0	47/47 (100%)	34 (72%)	13 (28%)	0	1
48	D0	47/47 (100%)	40 (85%)	7 (15%)	2	11
49	B1	45/45 (100%)	38 (84%)	7 (16%)	2	10
49	D1	45/45 (100%)	41 (91%)	4 (9%)	8	28
50	B2	38/38 (100%)	31 (82%)	7 (18%)	1	6
50	D2	38/38 (100%)	35 (92%)	3 (8%)	10	32
51	B3	51/51 (100%)	45 (88%)	6 (12%)	4	18
51	D3	51/51 (100%)	40 (78%)	11 (22%)	1	3
52	B4	34/34 (100%)	29 (85%)	5 (15%)	2	12
52	D4	34/34 (100%)	29 (85%)	5 (15%)	2	12
54	CG	123/123 (100%)	104 (85%)	19 (15%)	2	10
55	CM	91/91 (100%)	81 (89%)	10 (11%)	5	20
56	CP	65/65 (100%)	54 (83%)	11 (17%)	1	8
58	DF	149/149 (100%)	127 (85%)	22 (15%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9331/9339 (100%)	7816 (84%)	1515 (16%)	<b>2</b> <b>9</b>

5 of 1515 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CC	160	GLU
20	CT	11	ILE
4	CD	142	VAL
3	CC	152	VAL
9	CI	83	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 355 such sidechains are listed below:

Mol	Chain	Res	Type
10	CJ	70	HIS
30	DI	106	GLN
12	CL	72	ASN
24	DC	59	GLN
35	DN	31	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	482 (31%)	233 (15%)
22	BA	2850/2903 (98%)	900 (31%)	473 (16%)
22	DA	2839/2903 (97%)	1062 (37%)	506 (17%)
23	BB	117/118 (99%)	32 (27%)	18 (15%)
53	CA	1529/1530 (99%)	548 (35%)	236 (15%)
57	DB	116/117 (99%)	38 (32%)	15 (12%)
All	All	8983/9104 (98%)	3062 (34%)	1481 (16%)

5 of 3062 RNA backbone outliers are listed below:

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



5 of 1481 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	CA	1227	A
22	DA	1025	G
53	CA	1498	U
53	CA	1224	U
22	DA	424	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 364 ligands modelled in this entry, 363 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
60	CLY	BA	3135	-	26,28,28	1.52	6 (23%)	31,40,40	1.49	8 (25%)

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	CLY	BA	3135	-	-	2/21/53/53	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3135	CLY	C14-N2	3.44	1.51	1.47
60	BA	3135	CLY	C15-N2	2.80	1.52	1.46
60	BA	3135	CLY	O5-C4	2.77	1.48	1.44
60	BA	3135	CLY	C6-S1	2.26	1.84	1.79
60	BA	3135	CLY	C12-C11	-2.17	1.50	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	3135	CLY	C11-C10-N1	-3.30	109.28	116.52
60	BA	3135	CLY	C10-C11-N2	-2.39	107.53	112.39
60	BA	3135	CLY	O4-C1-C2	-2.35	104.84	110.38
60	BA	3135	CLY	C12-C13-C16	-2.33	112.01	114.68
60	BA	3135	CLY	C9-C8-CL1	-2.25	105.14	108.70

There are no chirality outliers.

All (2) torsion outliers are listed below:

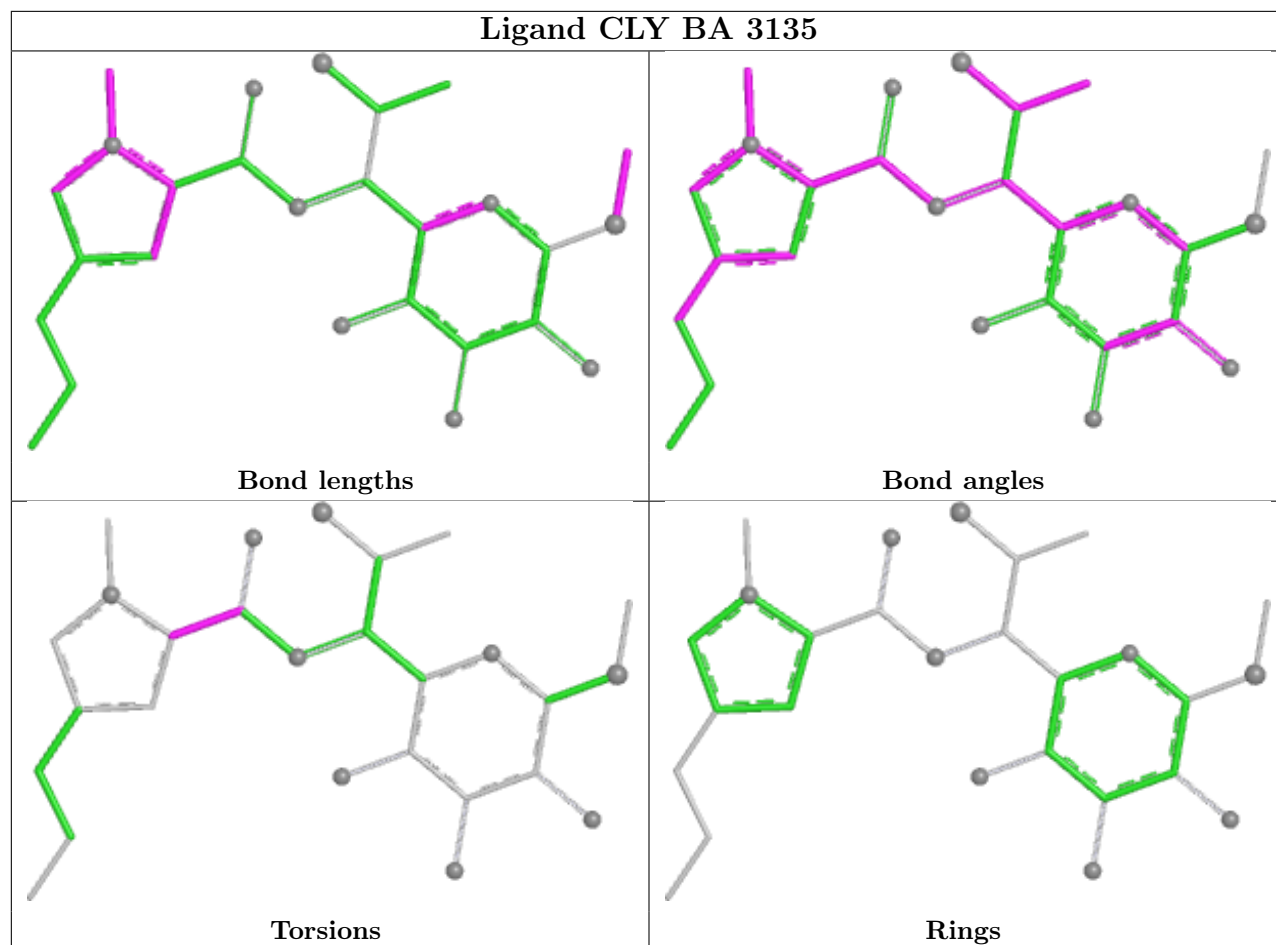
Mol	Chain	Res	Type	Atoms
60	BA	3135	CLY	N1-C10-C11-C12
60	BA	3135	CLY	N1-C10-C11-N2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	3135	CLY	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	AA	1533/1533 (100%)	-0.44	19 (1%) 76 63	26, 75, 180, 427	0
2	AB	218/218 (100%)	0.40	7 (3%) 50 37	111, 151, 210, 294	0
2	CB	218/218 (100%)	0.73	18 (8%) 19 17	125, 161, 248, 300	0
3	AC	206/206 (100%)	-0.00	5 (2%) 59 44	51, 97, 147, 208	0
3	CC	206/206 (100%)	0.51	12 (5%) 30 24	74, 144, 225, 261	0
4	AD	205/205 (100%)	0.12	9 (4%) 39 30	43, 83, 164, 311	0
4	CD	205/205 (100%)	0.13	6 (2%) 54 39	31, 59, 113, 227	0
5	AE	150/150 (100%)	0.36	5 (3%) 49 36	55, 78, 148, 255	0
5	CE	150/150 (100%)	0.75	16 (10%) 12 12	55, 85, 149, 258	0
6	AF	100/100 (100%)	0.20	4 (4%) 43 32	53, 90, 143, 171	0
6	CF	100/100 (100%)	0.40	6 (6%) 29 23	72, 107, 167, 226	0
7	AG	151/151 (100%)	0.59	17 (11%) 11 11	67, 129, 199, 248	0
8	AH	129/129 (100%)	-0.06	4 (3%) 51 38	38, 71, 123, 214	0
8	CH	129/129 (100%)	0.55	11 (8%) 18 16	53, 100, 161, 214	0
9	AI	127/127 (100%)	0.77	11 (8%) 17 16	66, 125, 243, 279	0
9	CI	127/127 (100%)	1.47	37 (29%) 1 1	111, 184, 282, 308	0
10	AJ	98/98 (100%)	0.45	5 (5%) 34 27	60, 114, 210, 262	0
10	CJ	98/98 (100%)	1.32	23 (23%) 2 2	103, 188, 266, 292	0
11	AK	117/117 (100%)	0.04	2 (1%) 69 54	36, 98, 174, 203	0
11	CK	117/117 (100%)	0.18	4 (3%) 48 35	55, 104, 165, 196	0
12	AL	123/123 (100%)	-0.03	9 (7%) 22 19	15, 54, 116, 167	0
12	CL	123/123 (100%)	0.37	12 (9%) 14 14	36, 73, 121, 188	0
13	AM	114/114 (100%)	0.51	4 (3%) 47 35	76, 125, 196, 274	0
14	AN	96/100 (96%)	0.88	18 (18%) 4 3	59, 102, 195, 267	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
14	CN	95/100 (95%)	1.63	26 (27%)	2 1	109, 221, 327, 373	0
15	AO	88/88 (100%)	-0.16	1 (1%)	77 66	36, 70, 123, 182	0
15	CO	88/88 (100%)	0.50	3 (3%)	48 35	59, 103, 158, 277	0
16	AP	82/82 (100%)	0.20	2 (2%)	59 44	44, 74, 148, 243	0
17	AQ	80/80 (100%)	0.22	4 (5%)	35 27	29, 78, 141, 267	0
17	CQ	80/80 (100%)	0.81	11 (13%)	8 8	48, 106, 161, 199	0
18	AR	55/55 (100%)	0.12	5 (9%)	16 15	60, 86, 161, 196	0
18	CR	55/55 (100%)	0.27	3 (5%)	32 25	47, 92, 186, 230	0
19	AS	79/79 (100%)	0.85	10 (12%)	9 9	79, 127, 199, 277	0
19	CS	79/79 (100%)	1.28	22 (27%)	2 1	181, 371, 451, 469	0
20	AT	85/85 (100%)	0.25	7 (8%)	19 17	43, 76, 116, 143	0
20	CT	85/85 (100%)	1.13	17 (20%)	3 3	58, 117, 197, 268	0
21	AU	51/51 (100%)	1.51	17 (33%)	1 1	88, 157, 204, 230	0
21	CU	51/51 (100%)	0.91	6 (11%)	10 10	58, 111, 182, 320	0
22	BA	2854/2903 (98%)	-0.75	45 (1%)	70 56	4, 28, 155, 403	0
22	DA	2841/2903 (97%)	0.97	363 (12%)	9 9	49, 122, 252, 460	0
23	BB	118/118 (100%)	-0.65	0	100 100	13, 43, 77, 106	0
24	BC	271/271 (100%)	-0.15	6 (2%)	62 47	5, 39, 81, 171	0
24	DC	271/271 (100%)	1.22	63 (23%)	2 2	51, 96, 147, 192	0
25	BD	209/209 (100%)	-0.45	1 (0%)	87 79	3, 23, 72, 171	0
25	DD	209/209 (100%)	1.27	46 (22%)	3 2	50, 111, 176, 290	0
26	BE	201/201 (100%)	-0.46	0	100 100	2, 37, 98, 185	0
26	DE	201/201 (100%)	2.24	99 (49%)	0 0	62, 197, 394, 486	0
27	BF	177/177 (100%)	-0.13	2 (1%)	77 66	27, 70, 127, 197	0
28	BG	176/176 (100%)	-0.05	7 (3%)	43 32	23, 60, 119, 204	0
28	DG	176/176 (100%)	1.00	28 (15%)	6 5	95, 195, 279, 335	0
29	BH	149/149 (100%)	1.08	28 (18%)	4 3	40, 177, 291, 362	0
29	DH	149/149 (100%)	1.79	53 (35%)	1 1	82, 181, 277, 319	0
30	BI	141/141 (100%)	1.35	28 (19%)	3 3	162, 269, 338, 374	0
30	DI	141/141 (100%)	0.76	12 (8%)	18 16	210, 324, 369, 408	0
31	BJ	142/142 (100%)	-0.36	4 (2%)	55 40	6, 21, 60, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
31	DJ	142/142 (100%)	1.07	27 (19%) 4 3	63, 102, 163, 184	0
32	BK	122/122 (100%)	-0.39	2 (1%) 70 56	7, 26, 74, 263	0
32	DK	122/122 (100%)	0.85	15 (12%) 9 9	52, 95, 164, 236	0
33	BL	143/143 (100%)	-0.26	1 (0%) 84 74	3, 35, 77, 103	0
33	DL	143/143 (100%)	2.02	60 (41%) 1 0	58, 159, 278, 348	0
34	BM	136/136 (100%)	-0.52	0 100 100	4, 26, 66, 135	0
34	DM	136/136 (100%)	0.87	20 (14%) 7 6	44, 105, 164, 196	0
35	BN	120/120 (100%)	-0.55	1 (0%) 82 72	6, 20, 43, 151	0
35	DN	120/120 (100%)	1.69	40 (33%) 1 1	79, 127, 200, 268	0
36	BO	116/116 (100%)	-0.15	1 (0%) 81 70	26, 43, 77, 126	0
36	DO	116/116 (100%)	1.10	27 (23%) 2 2	124, 168, 240, 292	0
37	BP	114/114 (100%)	-0.38	1 (0%) 81 70	9, 35, 83, 148	0
37	DP	114/114 (100%)	1.16	18 (15%) 6 5	62, 114, 174, 238	0
38	BQ	117/117 (100%)	-0.48	2 (1%) 69 54	3, 16, 43, 199	0
38	DQ	117/117 (100%)	1.52	36 (30%) 1 1	66, 103, 194, 288	0
39	BR	103/103 (100%)	-0.35	2 (1%) 66 51	4, 31, 80, 180	0
39	DR	103/103 (100%)	1.45	25 (24%) 2 1	67, 130, 227, 316	0
40	BS	110/110 (100%)	-0.56	0 100 100	4, 17, 52, 175	0
40	DS	110/110 (100%)	1.84	38 (34%) 1 1	59, 130, 231, 279	0
41	BT	93/93 (100%)	0.35	8 (8%) 18 16	19, 43, 128, 185	0
41	DT	93/93 (100%)	2.56	57 (61%) 0 0	123, 205, 306, 347	0
42	BU	102/102 (100%)	0.05	1 (0%) 79 67	18, 49, 120, 241	0
42	DU	102/102 (100%)	3.55	77 (75%) 0 0	123, 285, 434, 557	0
43	BV	94/94 (100%)	-0.26	0 100 100	15, 43, 86, 142	0
43	DV	94/94 (100%)	0.19	2 (2%) 63 49	97, 143, 194, 233	0
44	BW	79/79 (100%)	0.27	8 (10%) 14 13	10, 30, 105, 223	0
44	DW	79/79 (100%)	2.17	39 (49%) 0 0	82, 140, 238, 284	0
45	BX	77/77 (100%)	-0.21	1 (1%) 74 61	11, 42, 84, 117	0
45	DX	77/77 (100%)	2.10	35 (45%) 1 0	78, 117, 171, 236	0
46	BY	63/63 (100%)	0.41	6 (9%) 15 14	30, 66, 136, 222	0
46	DY	63/63 (100%)	2.47	35 (55%) 0 0	143, 309, 433, 440	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
47	BZ	58/58 (100%)	-0.43	0 100 100	8, 22, 56, 111	0
47	DZ	58/58 (100%)	1.08	11 (18%) 4 3	78, 119, 208, 217	0
48	B0	56/56 (100%)	-0.47	1 (1%) 67 53	3, 24, 70, 159	0
48	D0	56/56 (100%)	1.44	12 (21%) 3 2	63, 139, 242, 298	0
49	B1	50/50 (100%)	-0.28	1 (2%) 64 50	22, 48, 99, 165	0
49	D1	50/50 (100%)	1.34	14 (28%) 2 1	99, 170, 210, 236	0
50	B2	46/46 (100%)	-0.18	1 (2%) 62 47	7, 26, 52, 155	0
50	D2	46/46 (100%)	2.07	19 (41%) 1 0	81, 118, 175, 233	0
51	B3	64/64 (100%)	-0.55	0 100 100	5, 23, 44, 70	0
51	D3	64/64 (100%)	2.50	35 (54%) 0 0	65, 128, 183, 257	0
52	B4	38/38 (100%)	-0.08	1 (2%) 57 42	21, 45, 86, 124	0
52	D4	38/38 (100%)	2.49	24 (63%) 0 0	79, 137, 187, 227	0
53	CA	1530/1530 (100%)	0.34	68 (4%) 39 30	34, 102, 281, 444	0
54	CG	150/150 (100%)	1.44	40 (26%) 2 1	107, 224, 298, 322	0
55	CM	113/113 (100%)	1.59	29 (25%) 2 1	182, 402, 494, 538	0
56	CP	80/80 (100%)	0.92	13 (16%) 5 5	51, 94, 155, 236	0
57	DB	117/117 (100%)	0.39	1 (0%) 81 70	95, 169, 224, 274	0
58	DF	178/178 (100%)	0.68	13 (7%) 22 19	183, 225, 286, 338	0
All	All	20431/20551 (99%)	0.37	2051 (10%) 14 13	2, 94, 269, 557	0

The worst 5 of 2051 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	DU	30	SER	15.4
26	DE	103	GLY	11.7
26	DE	104	ALA	10.4
37	DP	109	ILE	10.4
38	DQ	7	VAL	10.2

## 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	MG	DA	3129	1/1	0.27	0.23	233,233,233,233	0
59	MG	DA	3003	1/1	0.29	0.22	236,236,236,236	0
59	MG	DA	3062	1/1	0.35	0.65	211,211,211,211	0
59	MG	DA	3124	1/1	0.37	0.45	176,176,176,176	0
59	MG	DA	3018	1/1	0.40	0.23	226,226,226,226	0
59	MG	DA	3108	1/1	0.40	0.23	185,185,185,185	0
59	MG	DA	3019	1/1	0.42	0.38	247,247,247,247	0
59	MG	CA	1622	1/1	0.47	0.13	226,226,226,226	0
59	MG	CA	1602	1/1	0.47	0.27	175,175,175,175	0
59	MG	BB	201	1/1	0.50	0.14	222,222,222,222	0
59	MG	DA	3057	1/1	0.53	0.21	227,227,227,227	0
59	MG	CA	1627	1/1	0.55	0.26	181,181,181,181	0
59	MG	DA	3107	1/1	0.59	0.21	161,161,161,161	0
59	MG	DA	3010	1/1	0.60	0.32	218,218,218,218	0
59	MG	DA	3122	1/1	0.61	0.18	153,153,153,153	0
59	MG	DC	301	1/1	0.61	0.20	145,145,145,145	0
59	MG	CA	1616	1/1	0.62	0.15	254,254,254,254	0
59	MG	DA	3126	1/1	0.63	0.26	200,200,200,200	0
59	MG	DA	3027	1/1	0.64	0.36	253,253,253,253	0
59	MG	CA	1619	1/1	0.64	0.17	214,214,214,214	0
59	MG	DA	3119	1/1	0.66	0.15	93,93,93,93	0
59	MG	DA	3105	1/1	0.66	0.24	262,262,262,262	0
59	MG	DJ	201	1/1	0.66	0.27	230,230,230,230	0
59	MG	DA	3110	1/1	0.67	0.13	153,153,153,153	0
59	MG	DA	3007	1/1	0.67	0.12	254,254,254,254	0
59	MG	DA	3013	1/1	0.67	0.18	126,126,126,126	0
59	MG	DA	3109	1/1	0.67	0.11	174,174,174,174	0
59	MG	DA	3021	1/1	0.69	0.25	199,199,199,199	0
59	MG	DA	3015	1/1	0.69	0.16	183,183,183,183	0
59	MG	CA	1628	1/1	0.71	0.19	260,260,260,260	0
59	MG	DA	3048	1/1	0.71	0.09	218,218,218,218	0
59	MG	DA	3073	1/1	0.71	0.57	274,274,274,274	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3114	1/1	0.73	0.27	167,167,167,167	0
59	MG	DC	302	1/1	0.74	0.13	129,129,129,129	0
59	MG	DA	3132	1/1	0.74	0.22	174,174,174,174	0
59	MG	DA	3061	1/1	0.75	0.38	229,229,229,229	0
59	MG	CA	1601	1/1	0.75	0.15	156,156,156,156	0
59	MG	DA	3005	1/1	0.75	0.23	309,309,309,309	0
59	MG	CA	1629	1/1	0.77	0.13	197,197,197,197	0
59	MG	DA	3025	1/1	0.77	0.41	278,278,278,278	0
59	MG	CA	1607	1/1	0.77	0.12	121,121,121,121	0
59	MG	DA	3063	1/1	0.77	0.16	278,278,278,278	0
59	MG	BA	3129	1/1	0.77	0.43	214,214,214,214	0
59	MG	DA	3044	1/1	0.78	0.10	156,156,156,156	0
59	MG	DA	3087	1/1	0.78	0.17	179,179,179,179	0
59	MG	DA	3117	1/1	0.78	0.12	71,71,71,71	0
59	MG	DE	301	1/1	0.78	0.26	131,131,131,131	0
59	MG	DA	3001	1/1	0.78	0.16	151,151,151,151	0
59	MG	DA	3049	1/1	0.79	0.15	172,172,172,172	0
59	MG	DA	3006	1/1	0.79	0.15	211,211,211,211	0
59	MG	CA	1639	1/1	0.79	0.10	165,165,165,165	0
59	MG	DA	3002	1/1	0.79	0.19	180,180,180,180	0
59	MG	AA	1618	1/1	0.80	0.25	197,197,197,197	0
59	MG	DA	3052	1/1	0.80	0.14	89,89,89,89	0
59	MG	DA	3091	1/1	0.80	0.18	116,116,116,116	0
59	MG	DA	3042	1/1	0.80	0.12	161,161,161,161	0
59	MG	BA	3024	1/1	0.81	0.30	166,166,166,166	0
59	MG	DA	3090	1/1	0.81	0.20	165,165,165,165	0
59	MG	DA	3037	1/1	0.81	0.13	197,197,197,197	0
59	MG	DA	3017	1/1	0.81	0.16	204,204,204,204	0
59	MG	CA	1623	1/1	0.81	0.16	124,124,124,124	0
59	MG	CA	1631	1/1	0.82	0.19	93,93,93,93	0
59	MG	BA	3047	1/1	0.82	0.14	111,111,111,111	0
59	MG	DA	3128	1/1	0.82	0.44	214,214,214,214	0
59	MG	DA	3068	1/1	0.83	0.21	209,209,209,209	0
59	MG	CA	1620	1/1	0.83	0.12	168,168,168,168	0
59	MG	DA	3075	1/1	0.83	0.23	174,174,174,174	0
59	MG	DA	3082	1/1	0.83	0.10	197,197,197,197	0
59	MG	DA	3131	1/1	0.83	0.21	212,212,212,212	0
59	MG	CA	1634	1/1	0.83	0.12	131,131,131,131	0
59	MG	AA	1630	1/1	0.83	0.14	189,189,189,189	0
59	MG	AA	1629	1/1	0.83	0.13	180,180,180,180	0
59	MG	DA	3092	1/1	0.83	0.15	229,229,229,229	0
59	MG	DA	3097	1/1	0.83	0.14	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	CA	1614	1/1	0.84	0.16	210,210,210,210	0
59	MG	BA	3068	1/1	0.84	0.10	117,117,117,117	0
59	MG	AA	1617	1/1	0.84	0.11	115,115,115,115	0
59	MG	DA	3024	1/1	0.84	0.14	89,89,89,89	0
59	MG	DA	3081	1/1	0.84	0.12	142,142,142,142	0
59	MG	CA	1625	1/1	0.84	0.13	100,100,100,100	0
59	MG	AA	1610	1/1	0.85	0.12	190,190,190,190	0
59	MG	DA	3078	1/1	0.85	0.22	180,180,180,180	0
59	MG	CA	1632	1/1	0.85	0.12	156,156,156,156	0
59	MG	DA	3056	1/1	0.85	0.30	197,197,197,197	0
59	MG	DA	3046	1/1	0.86	0.14	151,151,151,151	0
59	MG	CA	1617	1/1	0.86	0.09	199,199,199,199	0
59	MG	DA	3071	1/1	0.86	0.12	133,133,133,133	0
59	MG	DA	3112	1/1	0.86	0.14	131,131,131,131	0
59	MG	CA	1618	1/1	0.86	0.08	113,113,113,113	0
59	MG	AA	1614	1/1	0.86	0.33	194,194,194,194	0
59	MG	AA	1636	1/1	0.87	0.15	124,124,124,124	0
59	MG	CA	1636	1/1	0.87	0.18	181,181,181,181	0
59	MG	DA	3083	1/1	0.87	0.15	204,204,204,204	0
59	MG	CA	1610	1/1	0.87	0.12	152,152,152,152	0
59	MG	BA	3117	1/1	0.87	0.16	157,157,157,157	0
59	MG	CA	1624	1/1	0.87	0.21	165,165,165,165	0
59	MG	CA	1615	1/1	0.87	0.09	172,172,172,172	0
59	MG	BA	3131	1/1	0.88	0.16	154,154,154,154	0
59	MG	DA	3032	1/1	0.88	0.12	121,121,121,121	0
59	MG	DA	3096	1/1	0.88	0.14	102,102,102,102	0
59	MG	AA	1619	1/1	0.88	0.12	156,156,156,156	0
59	MG	DA	3099	1/1	0.89	0.20	68,68,68,68	0
59	MG	DA	3074	1/1	0.89	0.24	190,190,190,190	0
59	MG	AA	1631	1/1	0.89	0.09	91,91,91,91	0
59	MG	DA	3038	1/1	0.89	0.10	102,102,102,102	0
59	MG	DA	3070	1/1	0.89	0.09	56,56,56,56	0
59	MG	BA	3110	1/1	0.89	0.17	92,92,92,92	0
59	MG	DA	3034	1/1	0.89	0.18	125,125,125,125	0
59	MG	DA	3098	1/1	0.90	0.12	172,172,172,172	0
59	MG	DA	3011	1/1	0.90	0.13	127,127,127,127	0
59	MG	CA	1603	1/1	0.90	0.25	162,162,162,162	0
59	MG	DA	3086	1/1	0.90	0.08	139,139,139,139	0
59	MG	CA	1637	1/1	0.90	0.15	74,74,74,74	0
59	MG	AA	1627	1/1	0.90	0.12	132,132,132,132	0
59	MG	BA	3011	1/1	0.90	0.21	102,102,102,102	0
59	MG	DA	3077	1/1	0.90	0.18	222,222,222,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3094	1/1	0.90	0.12	107,107,107,107	0
59	MG	AA	1612	1/1	0.90	0.10	105,105,105,105	0
59	MG	DA	3035	1/1	0.90	0.13	194,194,194,194	0
59	MG	DA	3072	1/1	0.91	0.08	187,187,187,187	0
59	MG	DA	3084	1/1	0.91	0.17	144,144,144,144	0
59	MG	DA	3085	1/1	0.91	0.08	87,87,87,87	0
59	MG	DA	3059	1/1	0.91	0.44	200,200,200,200	0
59	MG	BA	3111	1/1	0.91	0.17	77,77,77,77	0
59	MG	BA	3090	1/1	0.91	0.17	128,128,128,128	0
59	MG	BA	3046	1/1	0.91	0.11	149,149,149,149	0
59	MG	DB	201	1/1	0.91	0.10	104,104,104,104	0
59	MG	DA	3030	1/1	0.91	0.08	68,68,68,68	0
59	MG	DA	3080	1/1	0.91	0.18	108,108,108,108	0
59	MG	DA	3008	1/1	0.91	0.12	148,148,148,148	0
59	MG	DA	3033	1/1	0.91	0.12	95,95,95,95	0
59	MG	DA	3127	1/1	0.92	0.14	142,142,142,142	0
59	MG	BA	3055	1/1	0.92	0.24	205,205,205,205	0
59	MG	AN	201	1/1	0.92	0.09	159,159,159,159	0
59	MG	BA	3069	1/1	0.92	0.18	151,151,151,151	0
59	MG	DA	3004	1/1	0.92	0.12	114,114,114,114	0
59	MG	BA	3003	1/1	0.92	0.10	69,69,69,69	0
59	MG	AA	1639	1/1	0.92	0.09	108,108,108,108	0
59	MG	DA	3016	1/1	0.92	0.11	87,87,87,87	0
59	MG	DA	3125	1/1	0.92	0.12	82,82,82,82	0
59	MG	DA	3029	1/1	0.92	0.12	112,112,112,112	0
59	MG	DA	3079	1/1	0.93	0.10	142,142,142,142	0
59	MG	AA	1608	1/1	0.93	0.19	68,68,68,68	0
59	MG	DA	3026	1/1	0.93	0.09	109,109,109,109	0
59	MG	DA	3040	1/1	0.93	0.05	70,70,70,70	0
59	MG	CA	1612	1/1	0.93	0.17	136,136,136,136	0
59	MG	DA	3028	1/1	0.93	0.22	143,143,143,143	0
59	MG	BA	3085	1/1	0.93	0.07	100,100,100,100	0
59	MG	DA	3130	1/1	0.93	0.12	85,85,85,85	0
59	MG	BA	3086	1/1	0.93	0.10	131,131,131,131	0
59	MG	AA	1628	1/1	0.93	0.08	69,69,69,69	0
59	MG	AA	1626	1/1	0.93	0.17	117,117,117,117	0
59	MG	AA	1638	1/1	0.93	0.10	116,116,116,116	0
59	MG	BA	3014	1/1	0.93	0.09	68,68,68,68	0
59	MG	DA	3118	1/1	0.93	0.12	76,76,76,76	0
59	MG	DA	3036	1/1	0.93	0.12	82,82,82,82	0
59	MG	BA	3097	1/1	0.94	0.11	45,45,45,45	0
59	MG	AA	1635	1/1	0.94	0.08	194,194,194,194	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	CA	1633	1/1	0.94	0.10	63,63,63,63	0
59	MG	DA	3093	1/1	0.94	0.14	114,114,114,114	0
59	MG	DA	3058	1/1	0.94	0.14	204,204,204,204	0
59	MG	BA	3001	1/1	0.94	0.10	116,116,116,116	0
59	MG	DA	3041	1/1	0.94	0.10	82,82,82,82	0
59	MG	AA	1602	1/1	0.94	0.09	152,152,152,152	0
59	MG	BA	3124	1/1	0.94	0.07	25,25,25,25	0
59	MG	DA	3100	1/1	0.94	0.08	78,78,78,78	0
59	MG	DA	3103	1/1	0.94	0.13	44,44,44,44	0
59	MG	BA	3056	1/1	0.94	0.25	169,169,169,169	0
59	MG	DA	3047	1/1	0.94	0.09	95,95,95,95	0
59	MG	CA	1641	1/1	0.94	0.14	79,79,79,79	0
59	MG	BA	3060	1/1	0.94	0.21	210,210,210,210	0
59	MG	DA	3050	1/1	0.94	0.09	106,106,106,106	0
59	MG	DA	3111	1/1	0.94	0.10	109,109,109,109	0
59	MG	DA	3089	1/1	0.94	0.06	99,99,99,99	0
59	MG	DA	3113	1/1	0.94	0.11	148,148,148,148	0
59	MG	BA	3076	1/1	0.95	0.11	114,114,114,114	0
59	MG	AA	1603	1/1	0.95	0.07	111,111,111,111	0
59	MG	BA	3133	1/1	0.95	0.11	139,139,139,139	0
59	MG	DA	3121	1/1	0.95	0.07	84,84,84,84	0
59	MG	AA	1609	1/1	0.95	0.06	46,46,46,46	0
59	MG	BA	3058	1/1	0.95	0.15	107,107,107,107	0
59	MG	BA	3096	1/1	0.95	0.18	102,102,102,102	0
59	MG	DA	3014	1/1	0.95	0.26	172,172,172,172	0
59	MG	CA	1638	1/1	0.95	0.07	130,130,130,130	0
59	MG	BA	3033	1/1	0.95	0.18	162,162,162,162	0
59	MG	DA	3106	1/1	0.95	0.14	92,92,92,92	0
59	MG	CA	1640	1/1	0.95	0.12	157,157,157,157	0
59	MG	BA	3109	1/1	0.95	0.18	124,124,124,124	0
59	MG	AA	1607	1/1	0.95	0.09	103,103,103,103	0
59	MG	AA	1640	1/1	0.95	0.10	154,154,154,154	0
59	MG	BA	3072	1/1	0.95	0.12	139,139,139,139	0
59	MG	BA	3074	1/1	0.95	0.11	93,93,93,93	0
59	MG	DA	3045	1/1	0.95	0.10	78,78,78,78	0
59	MG	CA	1630	1/1	0.95	0.09	131,131,131,131	0
59	MG	BA	3026	1/1	0.96	0.11	133,133,133,133	0
59	MG	AA	1637	1/1	0.96	0.07	27,27,27,27	0
59	MG	CA	1635	1/1	0.96	0.08	95,95,95,95	0
59	MG	BA	3081	1/1	0.96	0.14	86,86,86,86	0
59	MG	AA	1615	1/1	0.96	0.06	120,120,120,120	0
59	MG	DA	3101	1/1	0.96	0.06	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	CA	1611	1/1	0.96	0.10	112,112,112,112	0
59	MG	DA	3104	1/1	0.96	0.07	47,47,47,47	0
59	MG	DA	3067	1/1	0.96	0.08	83,83,83,83	0
59	MG	AA	1604	1/1	0.96	0.09	124,124,124,124	0
59	MG	CA	1613	1/1	0.96	0.07	105,105,105,105	0
59	MG	DA	3031	1/1	0.96	0.08	105,105,105,105	0
59	MG	BA	3054	1/1	0.96	0.14	189,189,189,189	0
59	MG	BA	3070	1/1	0.96	0.07	53,53,53,53	0
59	MG	BA	3002	1/1	0.96	0.09	85,85,85,85	0
59	MG	BA	3100	1/1	0.96	0.23	89,89,89,89	0
59	MG	DA	3076	1/1	0.96	0.06	93,93,93,93	0
59	MG	BA	3105	1/1	0.96	0.11	42,42,42,42	0
59	MG	DA	3115	1/1	0.96	0.13	65,65,65,65	0
59	MG	BA	3059	1/1	0.97	0.17	190,190,190,190	0
59	MG	DA	3012	1/1	0.97	0.06	64,64,64,64	0
59	MG	BA	3088	1/1	0.97	0.08	50,50,50,50	0
59	MG	DA	3060	1/1	0.97	0.12	105,105,105,105	0
59	MG	AA	1622	1/1	0.97	0.05	76,76,76,76	0
59	MG	CA	1621	1/1	0.97	0.19	46,46,46,46	0
59	MG	CA	1604	1/1	0.97	0.06	74,74,74,74	0
59	MG	DA	3065	1/1	0.97	0.09	49,49,49,49	0
59	MG	DA	3066	1/1	0.97	0.06	61,61,61,61	0
59	MG	BA	3091	1/1	0.97	0.06	32,32,32,32	0
59	MG	CA	1608	1/1	0.97	0.12	41,41,41,41	0
59	MG	DA	3095	1/1	0.97	0.08	95,95,95,95	0
59	MG	CA	1609	1/1	0.97	0.06	83,83,83,83	0
59	MG	BA	3044	1/1	0.97	0.07	12,12,12,12	0
59	MG	DA	3043	1/1	0.97	0.12	100,100,100,100	0
59	MG	DA	3022	1/1	0.97	0.04	69,69,69,69	0
59	MG	BA	3004	1/1	0.97	0.10	138,138,138,138	0
59	MG	BA	3082	1/1	0.97	0.12	114,114,114,114	0
59	MG	BA	3103	1/1	0.97	0.07	4,4,4,4	0
59	MG	BA	3134	1/1	0.97	0.17	219,219,219,219	0
59	MG	AA	1606	1/1	0.97	0.07	62,62,62,62	0
59	MG	BB	202	1/1	0.97	0.06	50,50,50,50	0
59	MG	DA	3009	1/1	0.97	0.06	69,69,69,69	0
59	MG	DA	3055	1/1	0.97	0.10	120,120,120,120	0
59	MG	BL	201	1/1	0.97	0.07	53,53,53,53	0
60	CLY	BA	3135	27/27	0.97	0.10	11,17,22,22	0
61	ZN	D4	101	1/1	0.97	0.07	161,161,161,161	0
59	MG	DA	3102	1/1	0.98	0.11	86,86,86,86	0
59	MG	BA	3122	1/1	0.98	0.17	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3069	1/1	0.98	0.09	69,69,69,69	0
59	MG	BA	3010	1/1	0.98	0.05	29,29,29,29	0
59	MG	BA	3126	1/1	0.98	0.05	9,9,9,9	0
59	MG	AA	1620	1/1	0.98	0.06	117,117,117,117	0
59	MG	BA	3130	1/1	0.98	0.18	97,97,97,97	0
59	MG	AA	1605	1/1	0.98	0.08	39,39,39,39	0
59	MG	BA	3022	1/1	0.98	0.04	8,8,8,8	0
59	MG	AA	1623	1/1	0.98	0.05	102,102,102,102	0
59	MG	BA	3089	1/1	0.98	0.07	80,80,80,80	0
59	MG	AA	1613	1/1	0.98	0.05	56,56,56,56	0
59	MG	BA	3027	1/1	0.98	0.11	46,46,46,46	0
59	MG	BA	3028	1/1	0.98	0.10	77,77,77,77	0
59	MG	BA	3062	1/1	0.98	0.05	11,11,11,11	0
59	MG	BA	3030	1/1	0.98	0.05	21,21,21,21	0
59	MG	BA	3102	1/1	0.98	0.12	3,3,3,3	0
59	MG	DA	3120	1/1	0.98	0.14	109,109,109,109	0
59	MG	DA	3020	1/1	0.98	0.11	49,49,49,49	0
59	MG	CA	1606	1/1	0.98	0.05	64,64,64,64	0
59	MG	DA	3123	1/1	0.98	0.07	61,61,61,61	0
59	MG	DA	3053	1/1	0.98	0.05	67,67,67,67	0
59	MG	DA	3054	1/1	0.98	0.06	96,96,96,96	0
59	MG	DA	3088	1/1	0.98	0.09	87,87,87,87	0
59	MG	BA	3032	1/1	0.98	0.11	3,3,3,3	0
59	MG	DA	3023	1/1	0.98	0.04	87,87,87,87	0
59	MG	AA	1616	1/1	0.98	0.06	98,98,98,98	0
59	MG	BA	3107	1/1	0.98	0.09	5,5,5,5	0
59	MG	BA	3108	1/1	0.98	0.04	48,48,48,48	0
59	MG	BA	3035	1/1	0.98	0.25	171,171,171,171	0
59	MG	BA	3038	1/1	0.98	0.05	31,31,31,31	0
59	MG	BA	3007	1/1	0.98	0.07	80,80,80,80	0
59	MG	BA	3112	1/1	0.98	0.07	47,47,47,47	0
59	MG	DA	3064	1/1	0.98	0.07	70,70,70,70	0
59	MG	BA	3077	1/1	0.98	0.04	30,30,30,30	0
59	MG	BA	3118	1/1	0.98	0.07	11,11,11,11	0
61	ZN	B4	101	1/1	0.98	0.08	80,80,80,80	0
59	MG	BA	3119	1/1	0.98	0.09	51,51,51,51	0
59	MG	BA	3094	1/1	0.99	0.04	9,9,9,9	0
59	MG	BA	3095	1/1	0.99	0.05	77,77,77,77	0
59	MG	BA	3016	1/1	0.99	0.03	2,2,2,2	0
59	MG	BA	3049	1/1	0.99	0.06	66,66,66,66	0
59	MG	BA	3099	1/1	0.99	0.06	1,1,1,1	0
59	MG	BA	3050	1/1	0.99	0.04	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3051	1/1	0.99	0.05	58,58,58,58	0
59	MG	BA	3052	1/1	0.99	0.03	5,5,5,5	0
59	MG	BA	3053	1/1	0.99	0.04	31,31,31,31	0
59	MG	BA	3019	1/1	0.99	0.10	15,15,15,15	0
59	MG	CA	1626	1/1	0.99	0.11	23,23,23,23	0
59	MG	DA	3039	1/1	0.99	0.07	65,65,65,65	0
59	MG	BA	3020	1/1	0.99	0.05	22,22,22,22	0
59	MG	BA	3021	1/1	0.99	0.06	7,7,7,7	0
59	MG	BA	3057	1/1	0.99	0.04	48,48,48,48	0
59	MG	AA	1634	1/1	0.99	0.04	72,72,72,72	0
59	MG	AA	1624	1/1	0.99	0.06	82,82,82,82	0
59	MG	BA	3113	1/1	0.99	0.05	114,114,114,114	0
59	MG	BA	3114	1/1	0.99	0.05	4,4,4,4	0
59	MG	BA	3116	1/1	0.99	0.07	76,76,76,76	0
59	MG	BA	3025	1/1	0.99	0.09	26,26,26,26	0
59	MG	BA	3061	1/1	0.99	0.05	20,20,20,20	0
59	MG	AA	1625	1/1	0.99	0.12	30,30,30,30	0
59	MG	DA	3051	1/1	0.99	0.07	57,57,57,57	0
59	MG	BA	3121	1/1	0.99	0.06	15,15,15,15	0
59	MG	BA	3065	1/1	0.99	0.03	17,17,17,17	0
59	MG	BA	3123	1/1	0.99	0.07	11,11,11,11	0
59	MG	BA	3066	1/1	0.99	0.04	10,10,10,10	0
59	MG	CA	1642	1/1	0.99	0.05	82,82,82,82	0
59	MG	AA	1611	1/1	0.99	0.04	62,62,62,62	0
59	MG	BA	3127	1/1	0.99	0.03	3,3,3,3	0
59	MG	AA	1601	1/1	0.99	0.08	70,70,70,70	0
59	MG	DA	3116	1/1	0.99	0.11	77,77,77,77	0
59	MG	BA	3029	1/1	0.99	0.10	3,3,3,3	0
59	MG	BA	3005	1/1	0.99	0.05	87,87,87,87	0
59	MG	BA	3073	1/1	0.99	0.07	8,8,8,8	0
59	MG	AA	1632	1/1	0.99	0.09	76,76,76,76	0
59	MG	BA	3075	1/1	0.99	0.05	29,29,29,29	0
59	MG	BA	3008	1/1	0.99	0.05	7,7,7,7	0
59	MG	BB	203	1/1	0.99	0.03	17,17,17,17	0
59	MG	BB	204	1/1	0.99	0.06	41,41,41,41	0
59	MG	AA	1633	1/1	0.99	0.05	51,51,51,51	0
59	MG	BA	3078	1/1	0.99	0.05	20,20,20,20	0
59	MG	BA	3080	1/1	0.99	0.05	34,34,34,34	0
59	MG	BA	3037	1/1	0.99	0.04	5,5,5,5	0
59	MG	AA	1641	1/1	0.99	0.09	22,22,22,22	0
59	MG	CA	1605	1/1	0.99	0.09	37,37,37,37	0
59	MG	BA	3083	1/1	0.99	0.03	28,28,28,28	0

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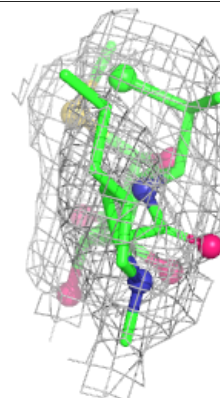
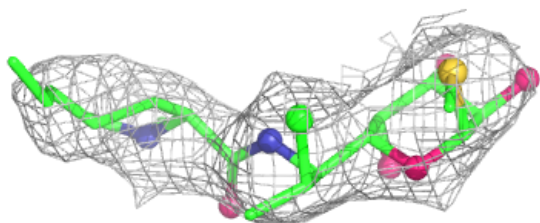
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3039	1/1	0.99	0.13	6,6,6,6	0
59	MG	BA	3041	1/1	0.99	0.04	13,13,13,13	0
59	MG	BA	3087	1/1	0.99	0.04	35,35,35,35	0
59	MG	BA	3042	1/1	0.99	0.04	41,41,41,41	0
59	MG	AA	1642	1/1	0.99	0.04	37,37,37,37	0
59	MG	BA	3045	1/1	0.99	0.06	17,17,17,17	0
59	MG	BA	3015	1/1	0.99	0.07	55,55,55,55	0
59	MG	BA	3092	1/1	0.99	0.04	56,56,56,56	0
59	MG	BA	3093	1/1	0.99	0.04	36,36,36,36	0
59	MG	AA	1621	1/1	1.00	0.09	25,25,25,25	0
59	MG	BA	3120	1/1	1.00	0.06	4,4,4,4	0
59	MG	BA	3043	1/1	1.00	0.09	11,11,11,11	0
59	MG	BA	3031	1/1	1.00	0.03	12,12,12,12	0
59	MG	BA	3023	1/1	1.00	0.04	5,5,5,5	0
59	MG	BA	3098	1/1	1.00	0.02	15,15,15,15	0
59	MG	BA	3125	1/1	1.00	0.06	27,27,27,27	0
59	MG	BA	3006	1/1	1.00	0.02	39,39,39,39	0
59	MG	BA	3079	1/1	1.00	0.02	13,13,13,13	0
59	MG	BA	3128	1/1	1.00	0.04	19,19,19,19	0
59	MG	BA	3101	1/1	1.00	0.03	11,11,11,11	0
59	MG	BA	3034	1/1	1.00	0.02	5,5,5,5	0
59	MG	BA	3048	1/1	1.00	0.02	6,6,6,6	0
59	MG	BA	3132	1/1	1.00	0.05	1,1,1,1	0
59	MG	BA	3104	1/1	1.00	0.06	3,3,3,3	0
59	MG	BA	3063	1/1	1.00	0.02	1,1,1,1	0
59	MG	BA	3106	1/1	1.00	0.06	13,13,13,13	0
59	MG	BA	3064	1/1	1.00	0.02	18,18,18,18	0
59	MG	BA	3084	1/1	1.00	0.02	13,13,13,13	0
59	MG	BA	3017	1/1	1.00	0.02	24,24,24,24	0
59	MG	BA	3036	1/1	1.00	0.02	4,4,4,4	0
59	MG	BA	3067	1/1	1.00	0.04	18,18,18,18	0
59	MG	BA	3018	1/1	1.00	0.18	6,6,6,6	0
59	MG	BA	3012	1/1	1.00	0.03	1,1,1,1	0
59	MG	BA	3013	1/1	1.00	0.03	1,1,1,1	0
59	MG	BA	3115	1/1	1.00	0.02	11,11,11,11	0
59	MG	BA	3071	1/1	1.00	0.02	7,7,7,7	0
59	MG	BA	3040	1/1	1.00	0.07	11,11,11,11	0
59	MG	BA	3009	1/1	1.00	0.04	6,6,6,6	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 CLY 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.