



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 10:04 PM 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

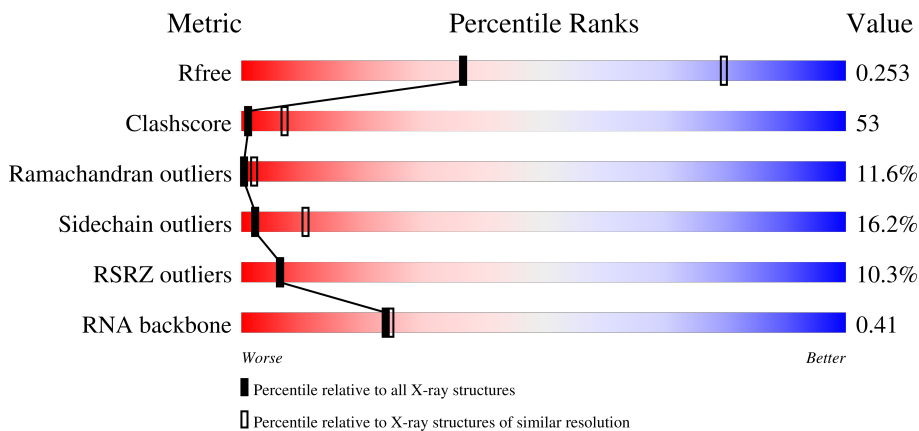
1 Overall quality at a glance

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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)
RNA backbone	3102	1091 (3.66-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1533	
2	AB	218	
2	CB	218	
3	AC	206	

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

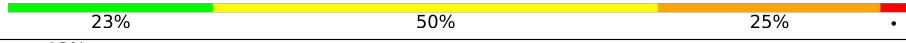
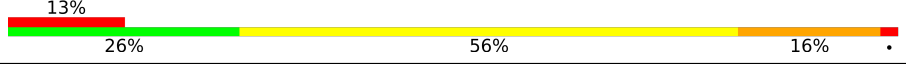
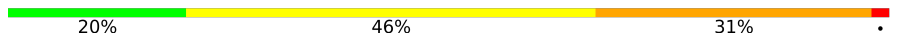
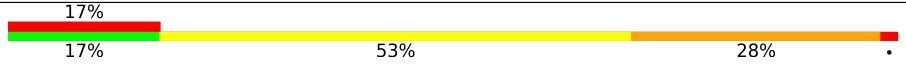
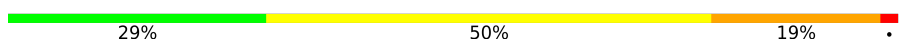
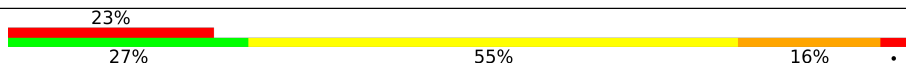
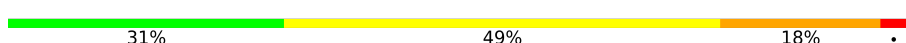
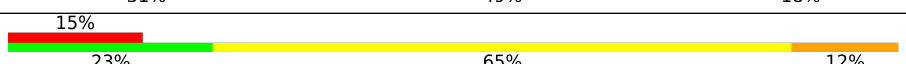
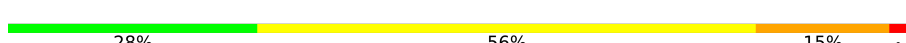
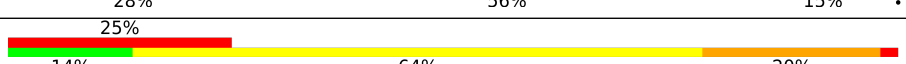
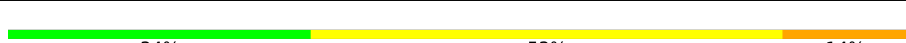
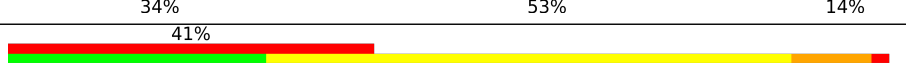
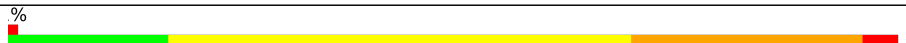
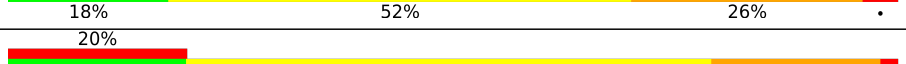
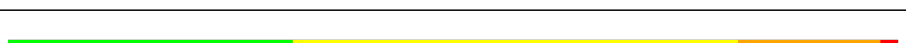

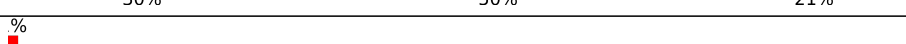
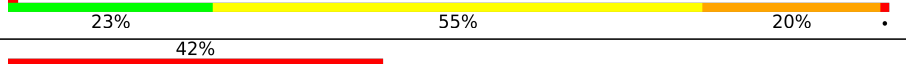


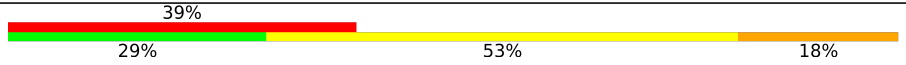
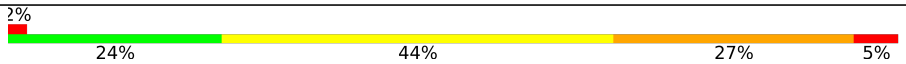
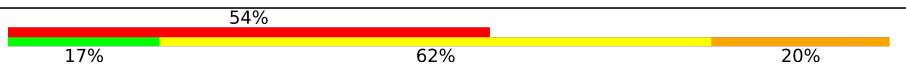
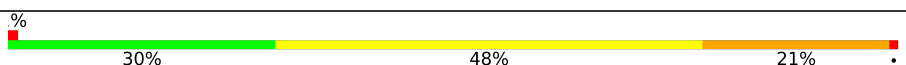
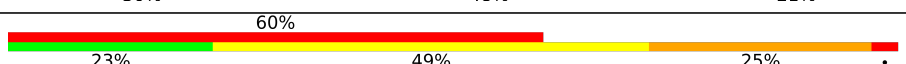
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Mol	Chain	Length	Quality of chain
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
28	BG	176	
28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

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Mol	Chain	Length	Quality of chain
31	BJ	142	 23% 50% 25% .
31	DJ	142	 13% 26% 56% 16% .
32	BK	122	 20% 46% 31% .
32	DK	122	 17% 17% 53% 28% .
33	BL	143	 29% 50% 19% .
33	DL	143	 23% 27% 55% 16% .
34	BM	136	 31% 49% 18% .
34	DM	136	 15% 23% 65% 12% .
35	BN	120	 28% 56% 15% .
35	DN	120	 25% 14% 64% 20% .
36	BO	116	 34% 53% 14% .
36	DO	116	 41% 29% 59% 9% .
37	BP	114	 18% 52% 26% .
37	DP	114	 20% 20% 59% 19% .
38	BQ	117	 32% 50% 16% .
38	DQ	117	 17% 30% 50% 21% .
39	BR	103	 23% 55% 20% .
39	DR	103	 42% 29% 54% 17% .
40	BS	110	 35% 45% 18% .
40	DS	110	 39% 29% 53% 18% .
41	BT	93	 2% 24% 44% 27% 5% .
41	DT	93	 54% 17% 62% 20% .
42	BU	102	 30% 48% 21% .
42	DU	102	 60% 23% 49% 25% .
43	BV	94	 40% 47% 13% .

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Mol	Chain	Length	Quality of chain
43	DV	94	13% 34% 53% 12%
44	BW	79	6% 13% 44% 34% 9%
44	DW	79	56% 20% 48% 24% 8%
45	BX	77	19% 60% 19%
45	DX	77	16% 22% 62% 14%
46	BY	63	5% 35% 43% 19%
46	DY	63	32% 25% 62% 13%
47	BZ	58	21% 55% 22%
47	DZ	58	3% 29% 52% 17%
48	B0	56	38% 41% 21%
48	D0	56	32% 25% 59% 16%
49	B1	50	4% 30% 50% 18%
49	D1	50	38% 26% 60% 12%
50	B2	46	2% 41% 46% 13%
50	D2	46	13% 26% 63% 11%
51	B3	64	48% 39% 9%
51	D3	64	34% 34% 47% 16%
52	B4	38	3% 29% 53% 16%
52	D4	38	58% 34% 45% 21%
53	CA	1530	3% 15% 48% 23% 14%
54	CG	150	51% 21% 64% 15%
55	CM	113	67% 26% 58% 15%
56	CP	80	14% 20% 60% 18%
57	DB	117	18% 47% 21% 15%
58	DF	178	47% 22% 53% 22%

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	CA	1624	-	-	-	X
59	MG	CA	1628	-	-	-	X
59	MG	DA	3003	-	-	-	X
59	MG	DA	3005	-	-	-	X
59	MG	DA	3007	-	-	-	X
59	MG	DA	3010	-	-	-	X
59	MG	DA	3019	-	-	-	X
59	MG	DA	3025	-	-	-	X
59	MG	DA	3027	-	-	-	X
59	MG	DA	3056	-	-	-	X
59	MG	DA	3059	-	-	-	X
59	MG	DA	3061	-	-	-	X
59	MG	DA	3062	-	-	-	X
59	MG	DA	3073	-	-	-	X
59	MG	DA	3075	-	-	-	X
59	MG	DA	3107	-	-	-	X
59	MG	DA	3108	-	-	-	X
59	MG	DA	3124	-	-	-	X
59	MG	DA	3129	-	-	-	X
59	MG	DE	301	-	-	-	X
59	MG	DJ	201	-	-	-	X

2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	CN	95	Total	C	N	O	S	0	0	0
			769	480	159	127	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	CR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
20	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

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

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

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

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

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

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

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

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

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

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

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
28	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
30	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
31	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
48	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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).

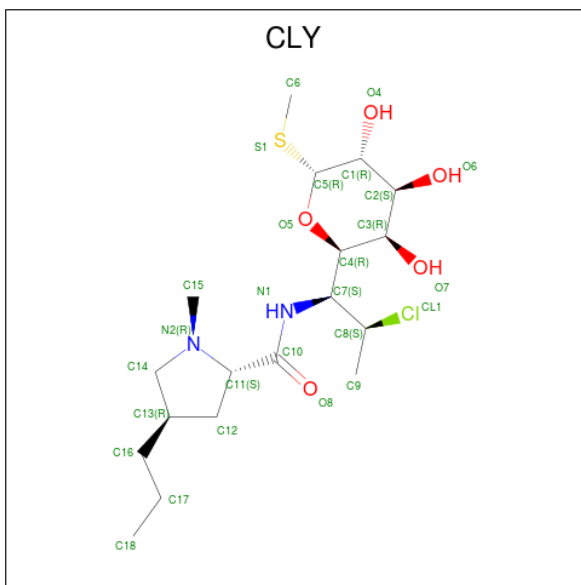
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	42	Total	Mg	0	0
			42	42		
59	AN	1	Total	Mg	0	0
			1	1		
59	BA	134	Total	Mg	0	0
			134	134		
59	BB	4	Total	Mg	0	0
			4	4		
59	BL	1	Total	Mg	0	0
			1	1		
59	CA	42	Total	Mg	0	0
			42	42		
59	DA	132	Total	Mg	0	0
			132	132		
59	DB	1	Total	Mg	0	0
			1	1		
59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

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

- Molecule 60 is CLINDAMYCIN (three-letter code: CLY) (formula: C₁₈H₃₃ClN₂O₅S).



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

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

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

- Molecule 62 is water.

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

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

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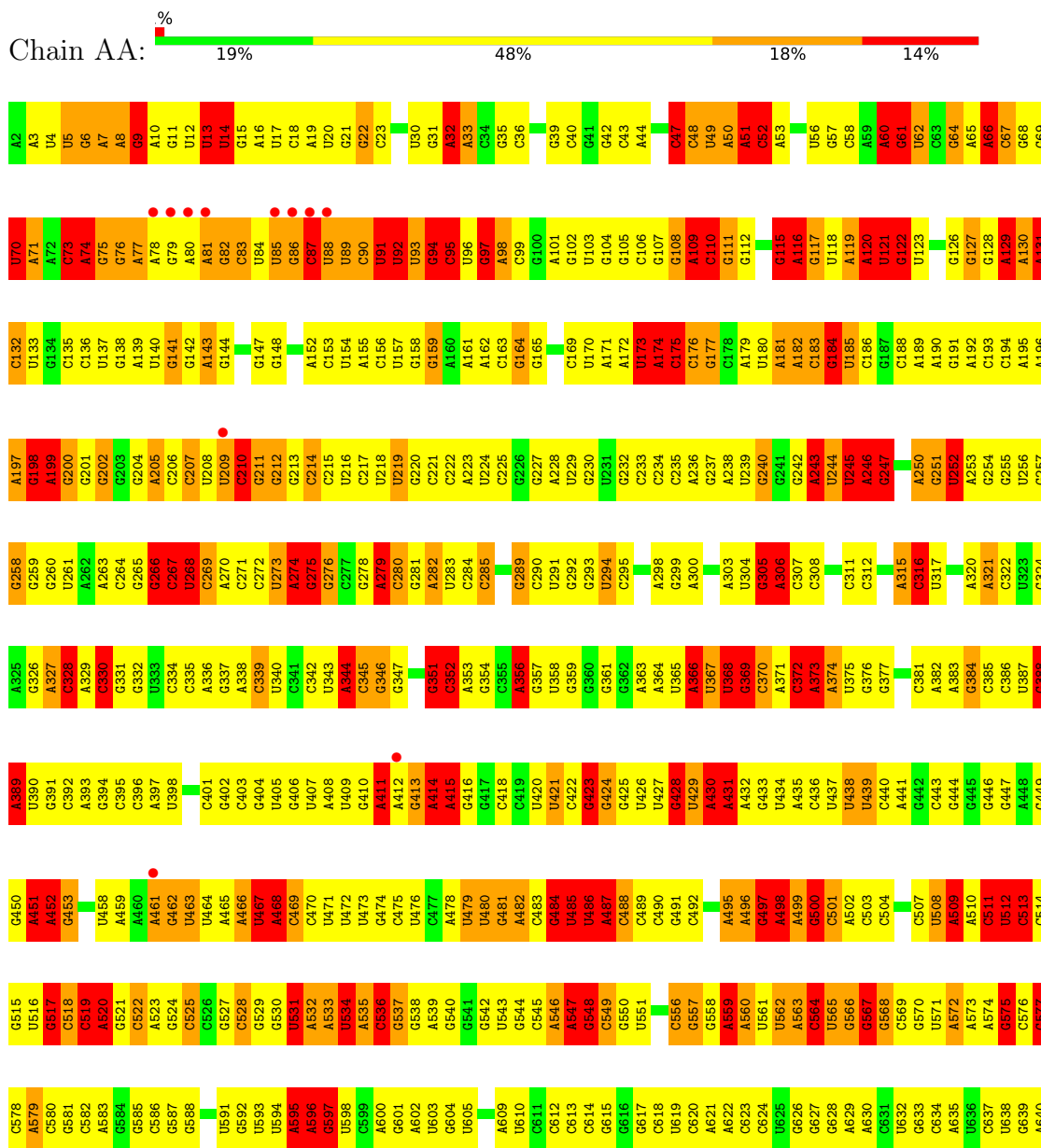
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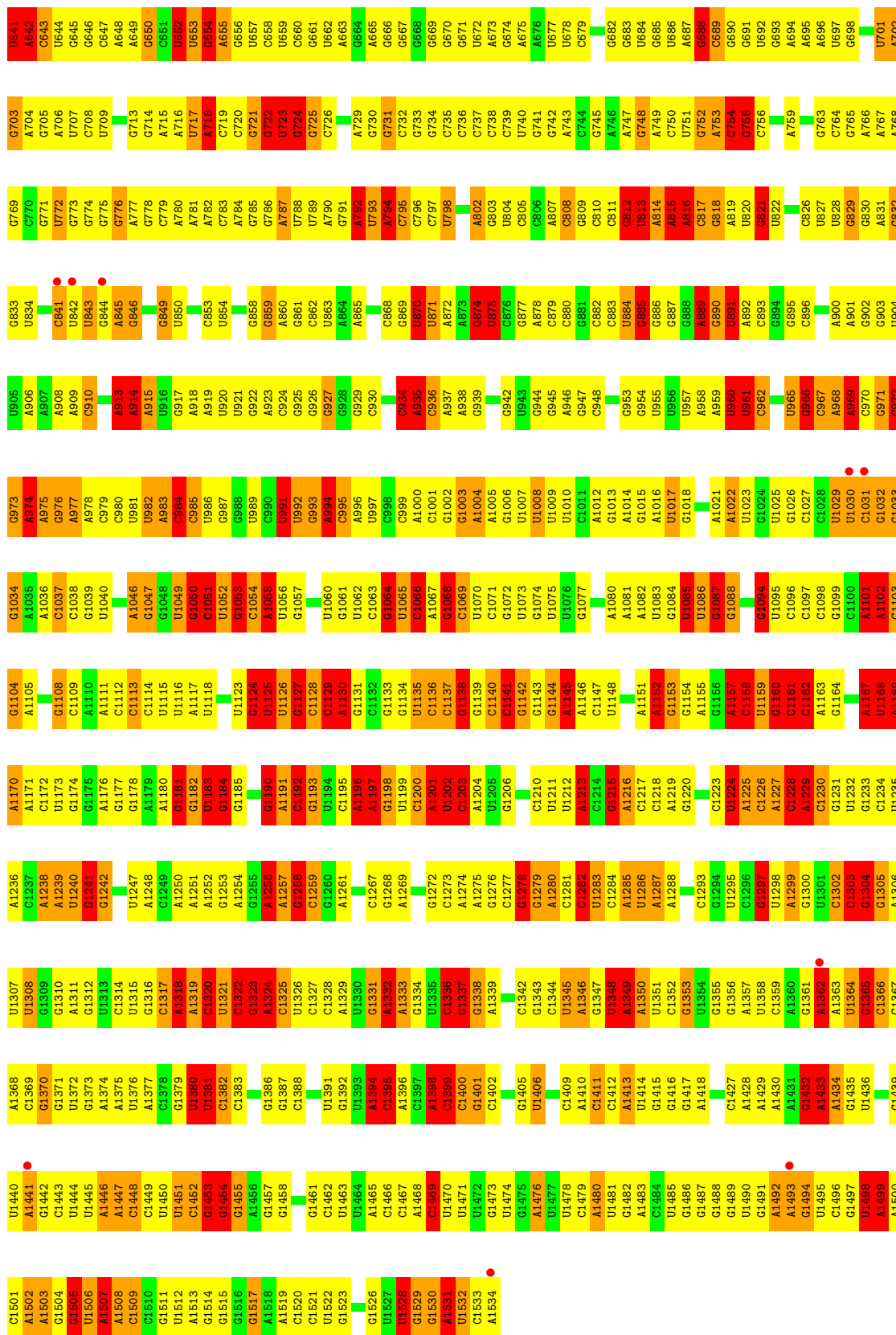
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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62	CT	3	Total O 3 3	0	0
62	CU	2	Total O 2 2	0	0
62	DA	599	Total O 599 599	0	0
62	DB	4	Total O 4 4	0	0
62	DC	9	Total O 9 9	0	0
62	DD	2	Total O 2 2	0	0
62	DE	3	Total O 3 3	0	0
62	DJ	5	Total O 5 5	0	0
62	DL	5	Total O 5 5	0	0
62	DN	3	Total O 3 3	0	0
62	DT	3	Total O 3 3	0	0
62	DU	2	Total O 2 2	0	0
62	DV	1	Total O 1 1	0	0
62	D2	2	Total O 2 2	0	0
62	D3	1	Total O 1 1	0	0
62	D4	4	Total O 4 4	0	0

3 Residue-property plots [i](#)

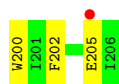
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S rRNA

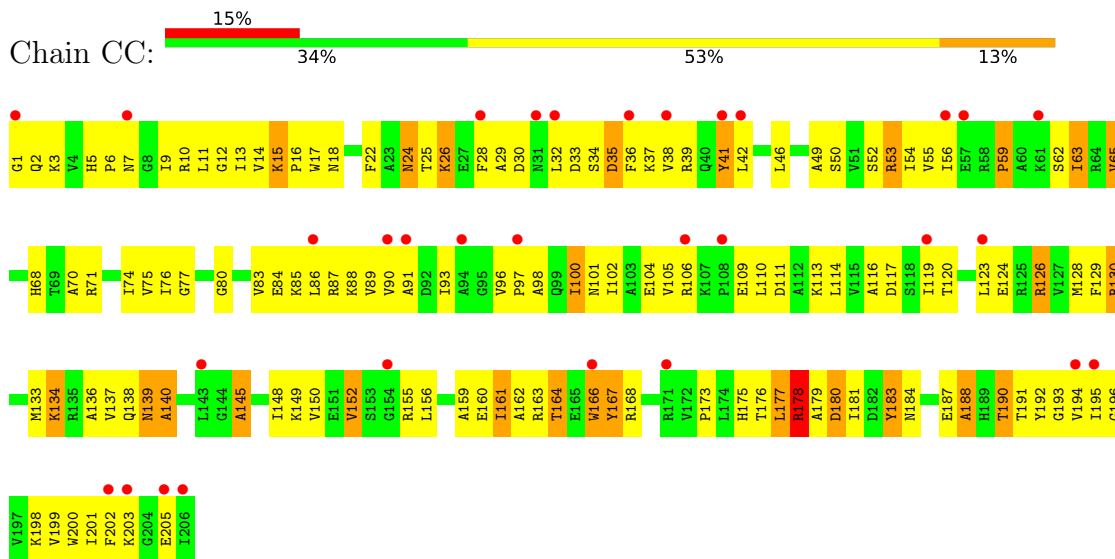




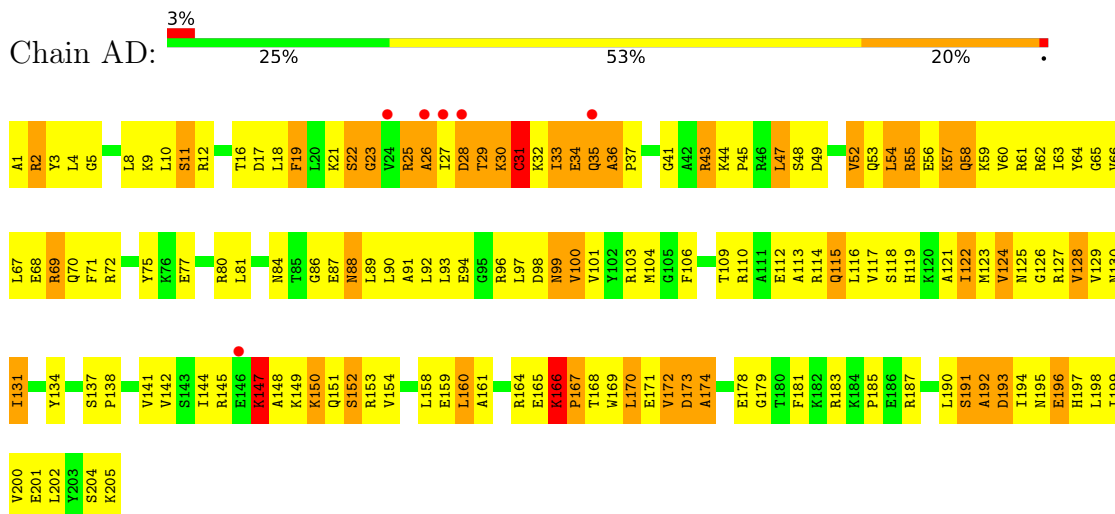
• Molecule 2: 30S ribosomal protein S2



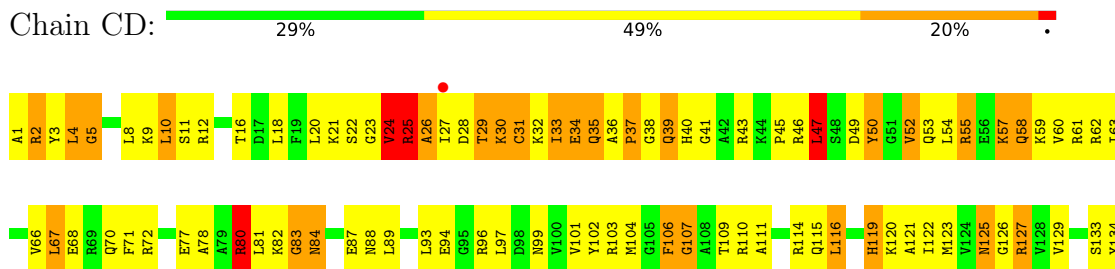
- Molecule 3: 30S ribosomal protein S3

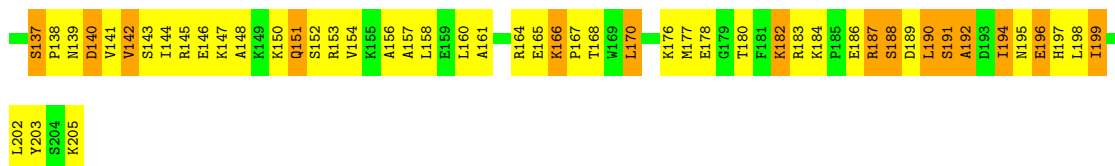


- Molecule 4: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S4

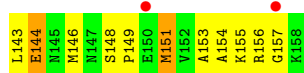
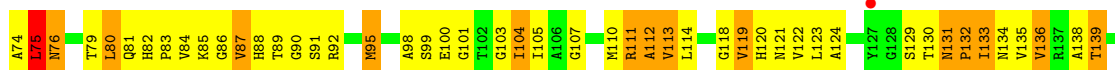
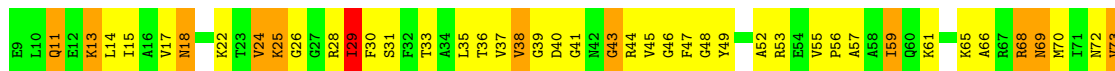




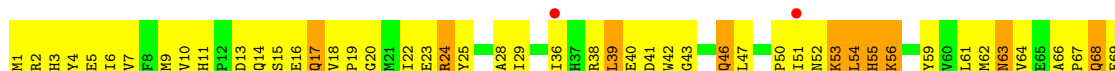
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5

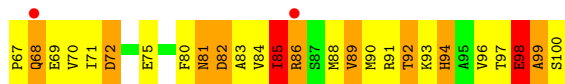
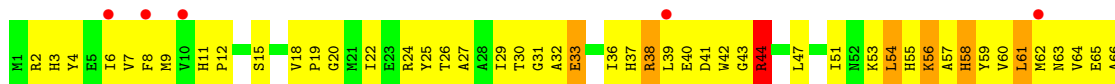


- Molecule 6: 30S ribosomal protein S6

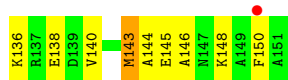


- Molecule 6: 30S ribosomal protein S6

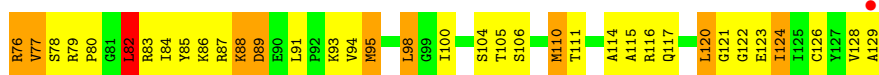
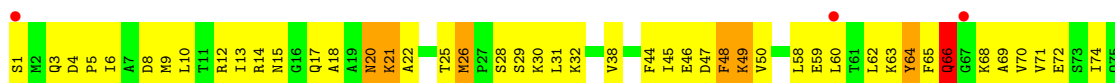




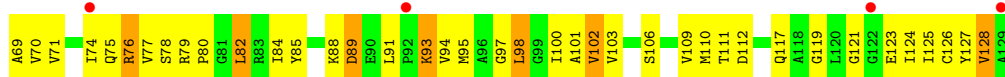
• Molecule 7: 30S ribosomal protein S7



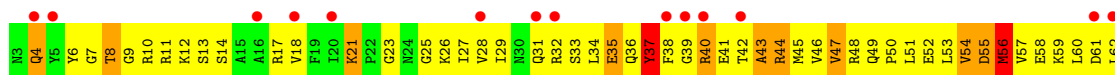
• Molecule 8: 30S ribosomal protein S8

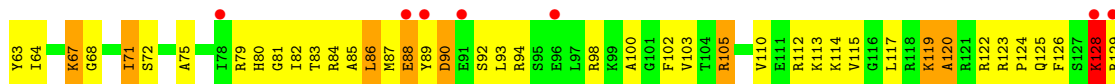


• Molecule 8: 30S ribosomal protein S8

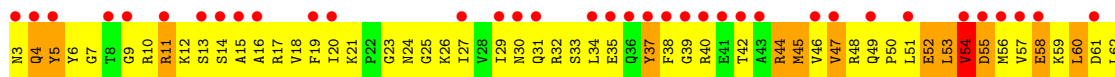


• Molecule 9: 30S ribosomal protein S9

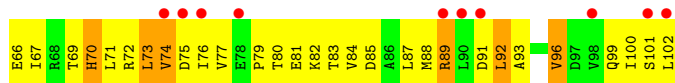
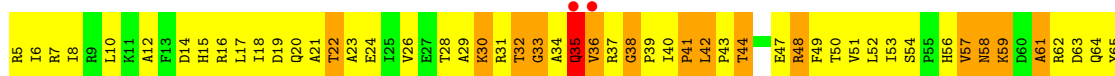
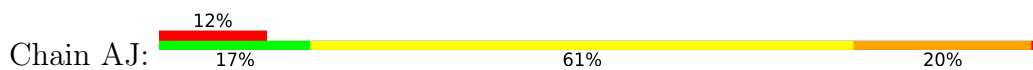




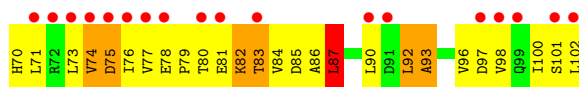
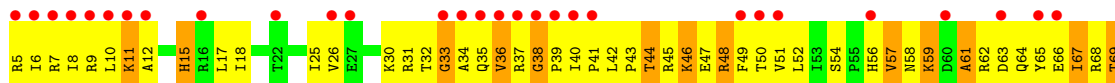
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10



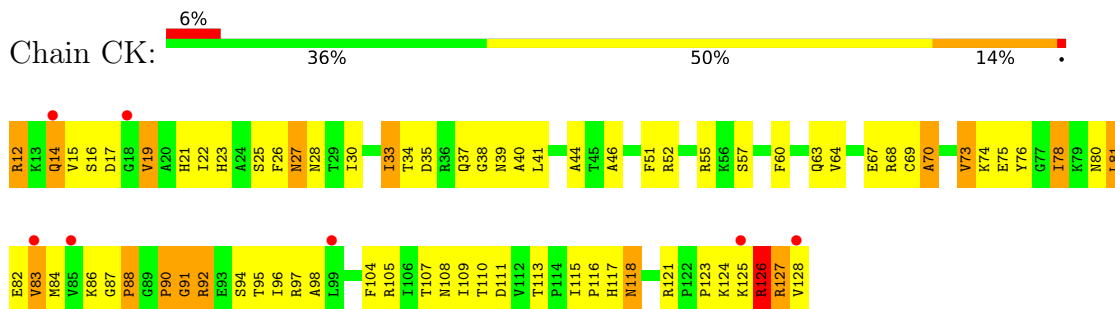
• Molecule 10: 30S ribosomal protein S10



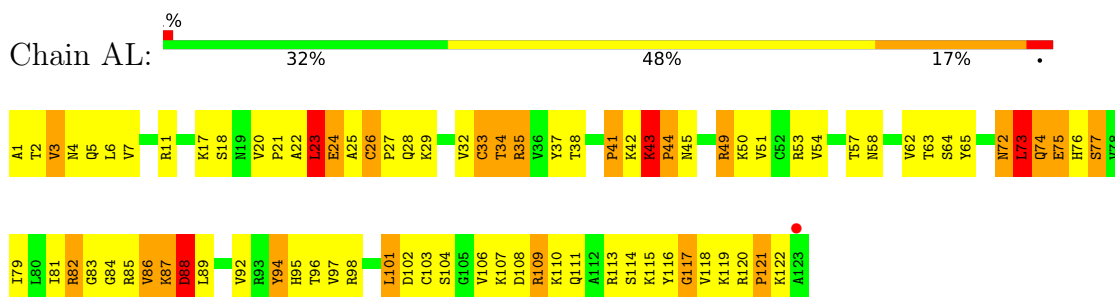
• Molecule 11: 30S ribosomal protein S11



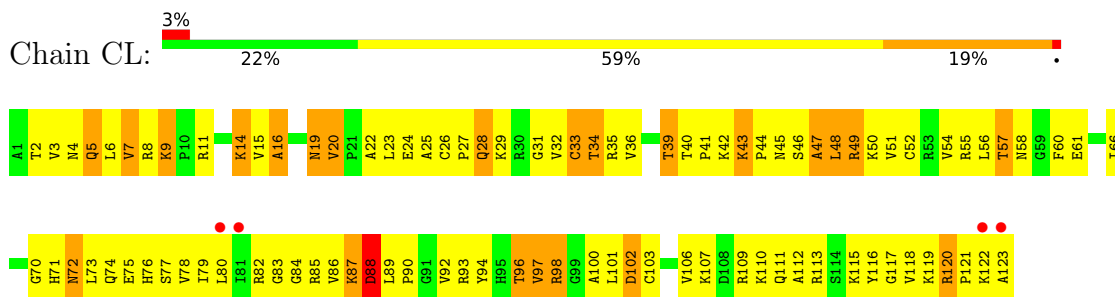
- Molecule 11: 30S ribosomal protein S11



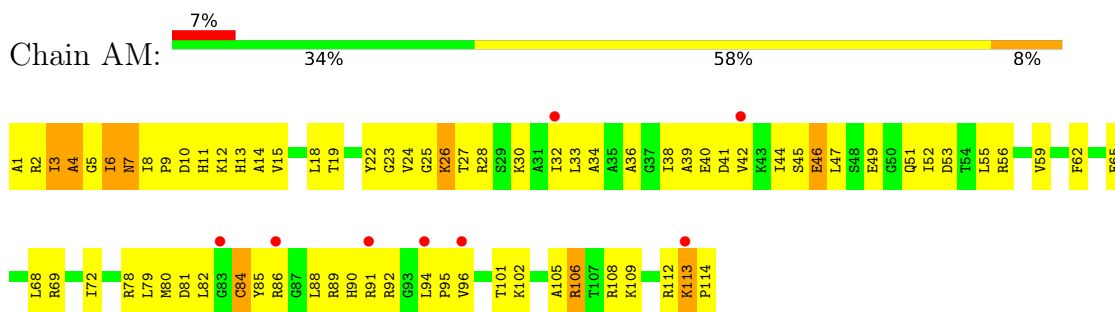
- Molecule 12: 30S ribosomal protein S12



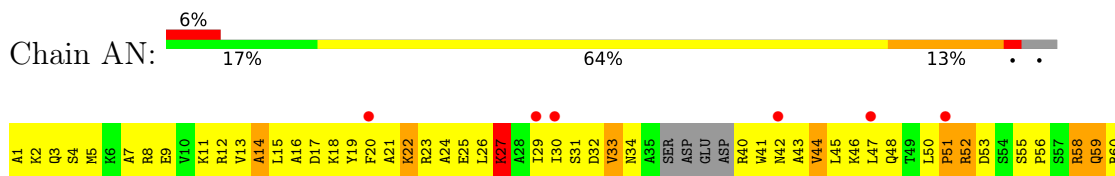
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

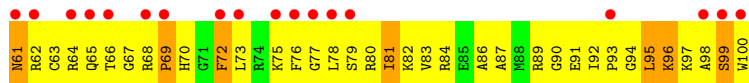
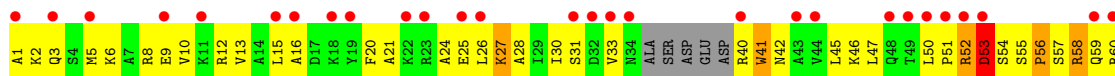


- Molecule 14: 30S ribosomal protein S14

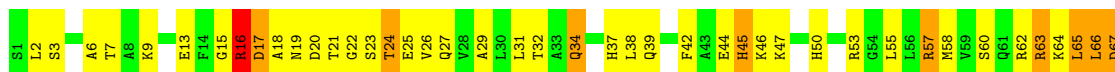




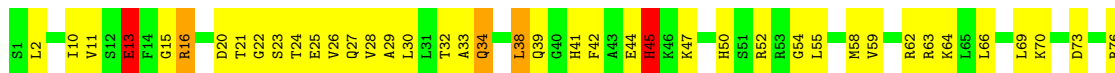
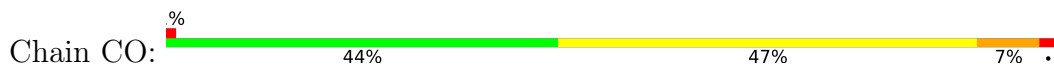
- Molecule 14: 30S ribosomal protein S14



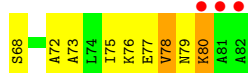
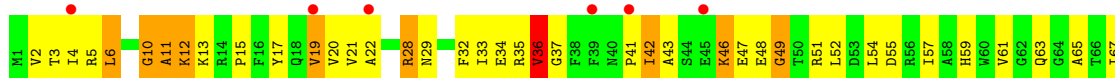
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

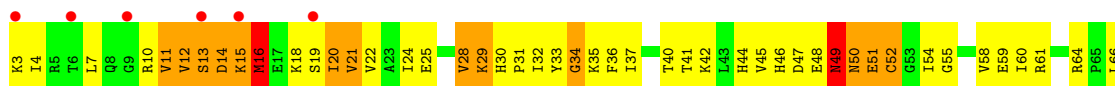


- Molecule 16: 30S ribosomal protein S16

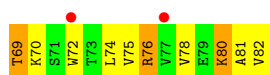


- Molecule 17: 30S ribosomal protein S17

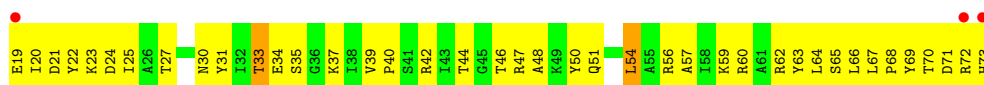




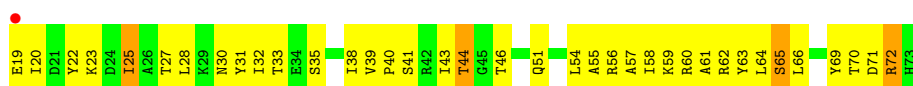
- Molecule 17: 30S ribosomal protein S17



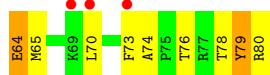
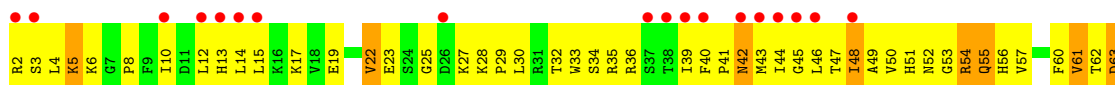
- Molecule 18: 30S ribosomal protein S18



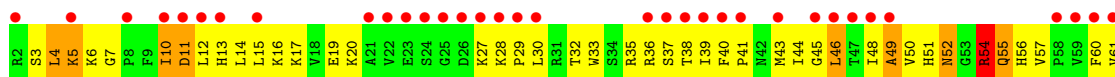
- Molecule 18: 30S ribosomal protein S18

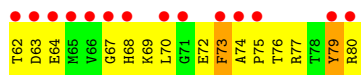


- Molecule 19: 30S ribosomal protein S19

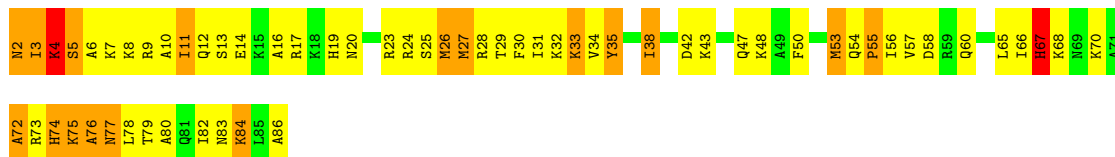
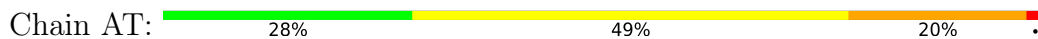


- Molecule 19: 30S ribosomal protein S19

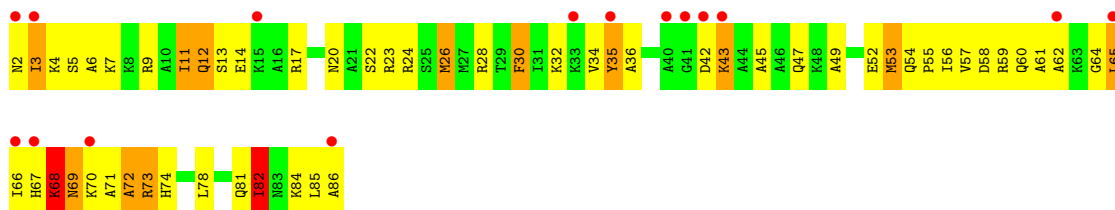




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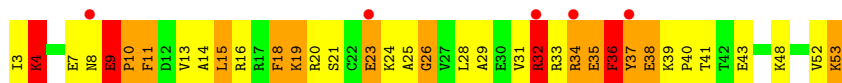
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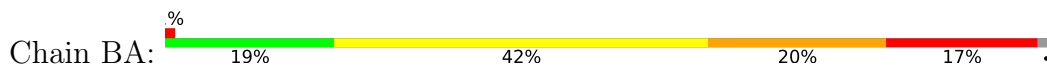
• Molecule 21: 30S ribosomal protein S21

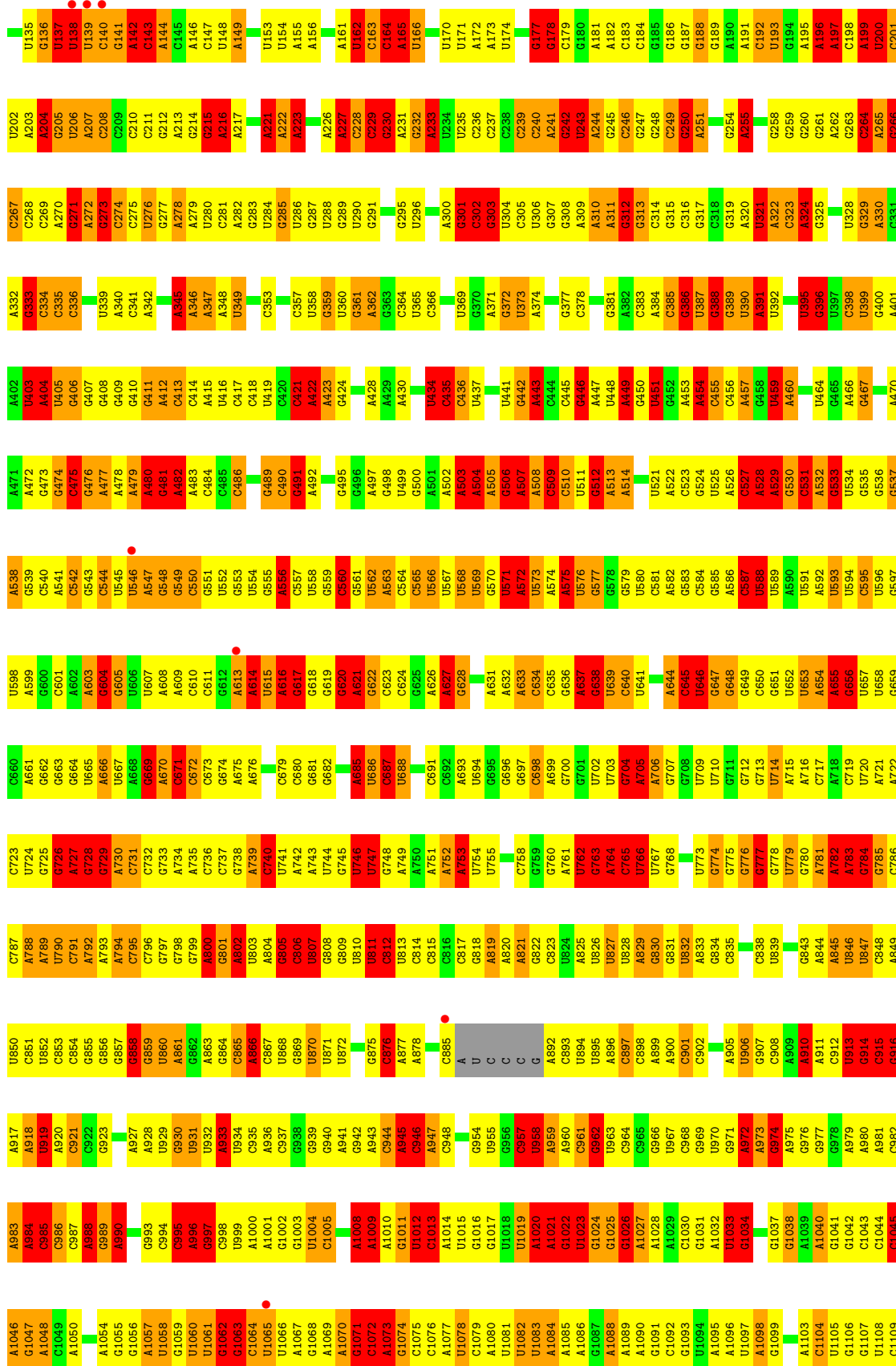


• Molecule 21: 30S ribosomal protein S21

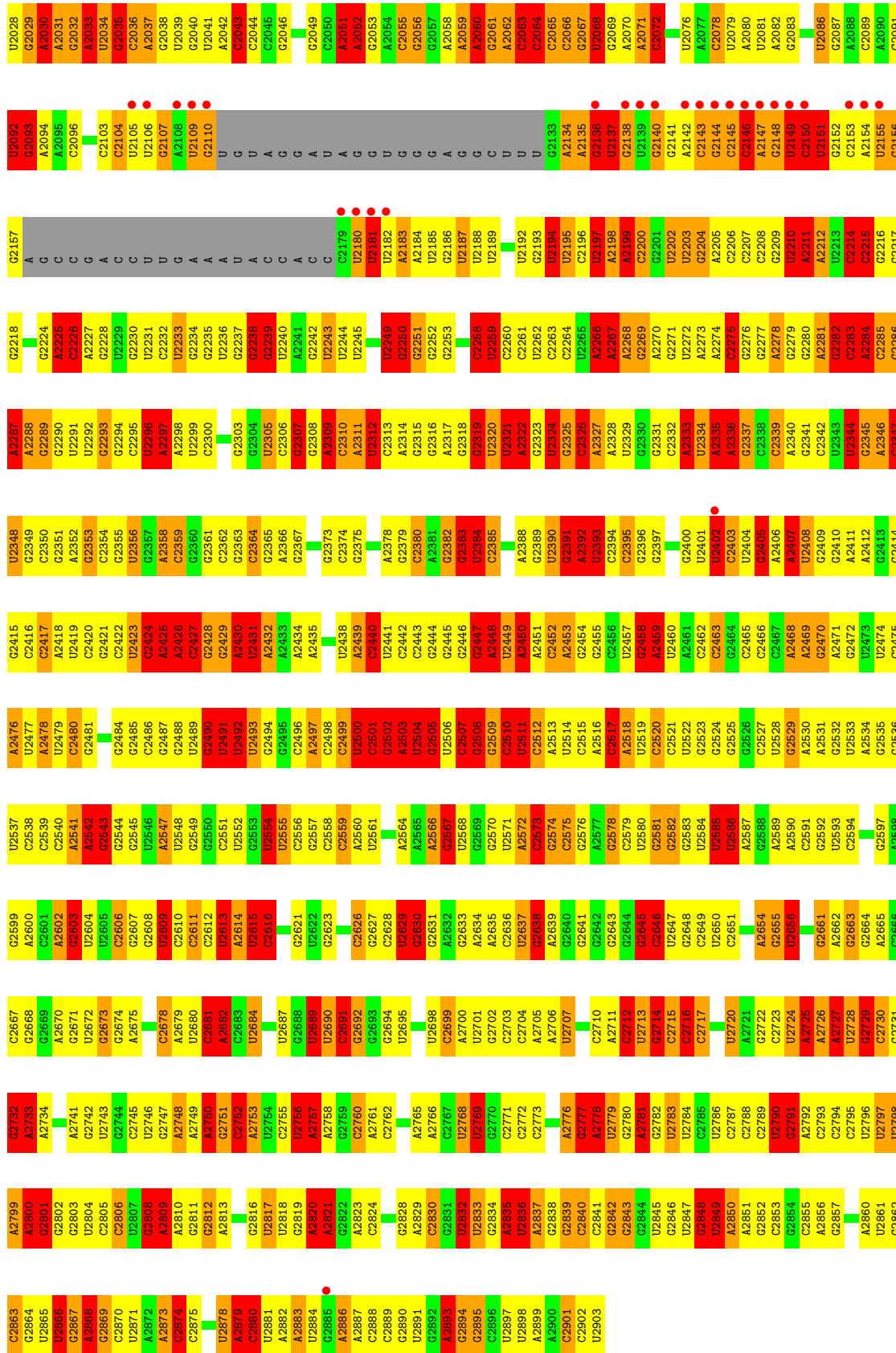


• Molecule 22: 23S rRNA

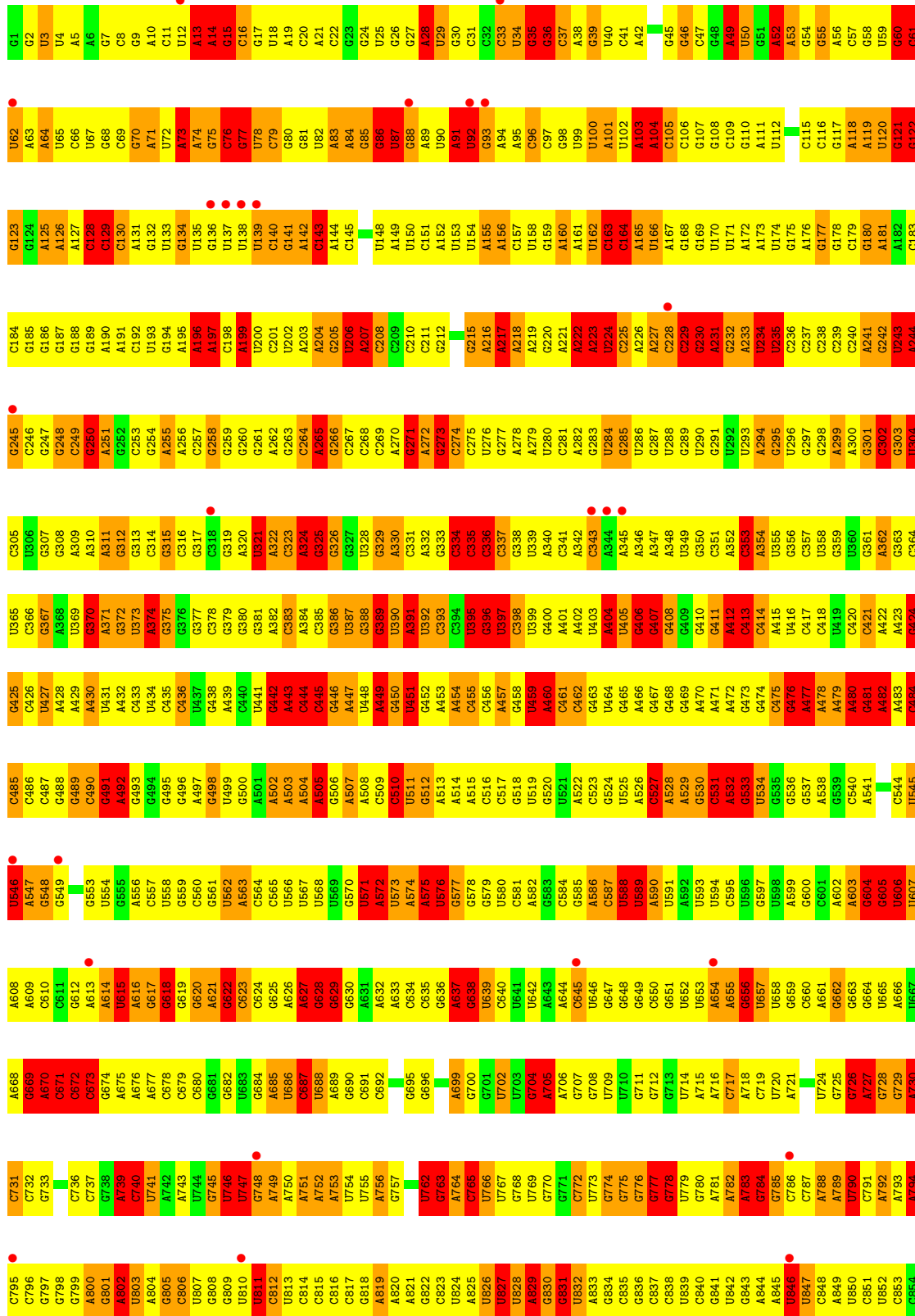
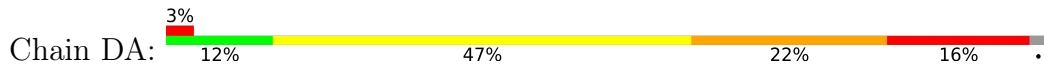




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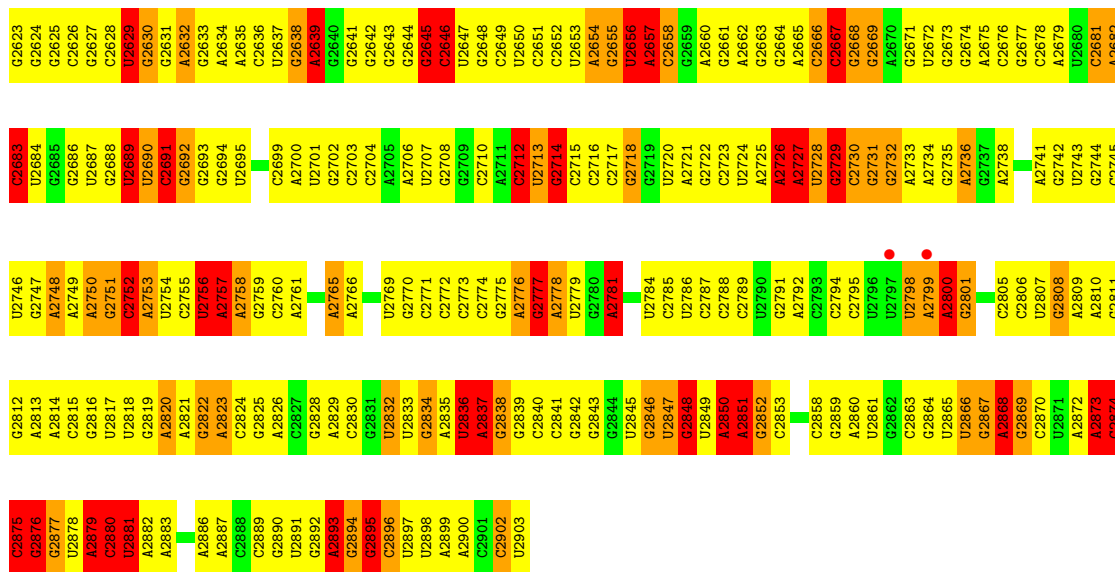


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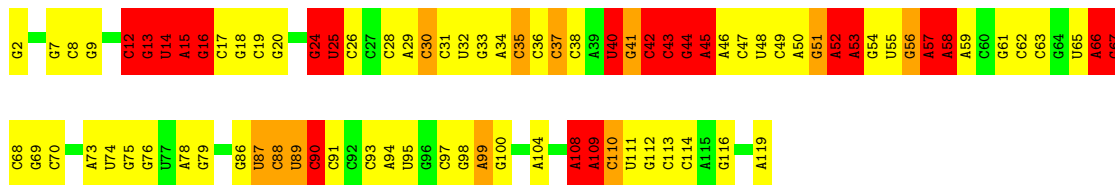


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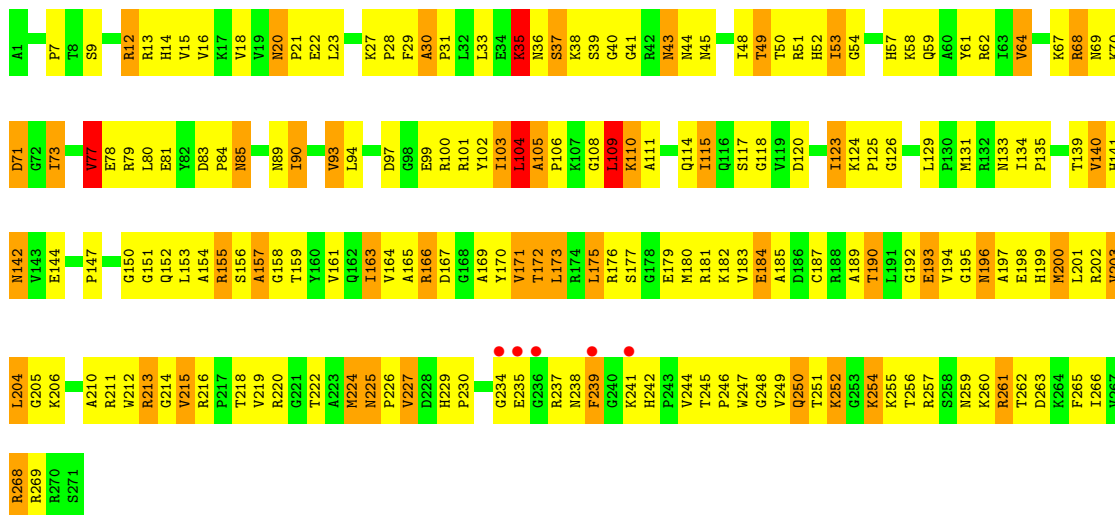
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U2585	G2524	G2457	U2393	A2333	U2272	G2209	G2148	U2022	U1952	G1884	G1817	A1757
G2586	A2525	A2458	C2394	U2334	A2273	U2210	U2149	C2023	A1952	A1885	U1818	U1758
A2587	G2526	U2460	C2395	A2335	A2274	A2211	G2150	G2024	A1953	U1886	A1819	A1759
G2588	C2527	A2461	G2396	A2336	C2275	A2212	U2151	C2025	G1954	C1887	U1820	C1760
A2589	U2528	U2462	U2397	G2337	G2276	U2213	U2092	C2026	U1955	C1888	A1821	C1761
C2590	G2529	G2463	G2398	C2338	A2277	C2214	G2093	U2096	U1956	A1889	C1822	A1762
U2591	A2530	U2464	U2401	C2339	G2278	C2215	A2094	C1957	C1957	A1890	G1823	G1763
G2592	C2531	C2465	C2402	C2340	A2279	C2216	A2095	A2031	U1957	A1891	G1824	G1764
U2593	U2532	C2466	U2403	G2341	G2279	G2217	C2096	G2032	C1961	U1895	U1825	U1765
C2594	G2533	U2467	G2404	C2342	A2280	G2218	A2097	A2033	C1962	G1896	G1826	G1766
A2595	A2534	A2468	A2405	U2343	A2281	U2219	U2098	U2034	U1963	G1897	U1827	G1767
U2596	U2535	G2470	A2406	C2344	C2282	U2220	U2099	G2035	G1964	G1898	G1828	C1768
G2597	G2536	U2471	U2407	G2345	A2283	G2221	G2100	C2036	C1965	U1898	A1829	U1769
C2598	C2537	U2472	U2408	A2346	C2284	C2222	A2101	A2037	A1966	A1899	G1830	G1770
U2599	U2538	U2473	G2409	G2347	G2285	G2223	G2102	G2038	C1967	A1900	U1833	C1771
C2600	C2539	A2474	G2410	U2348	A2286	G2224	C2103	U2039	G1968	A1901	C1833	A1772
A2601	U2540	C2475	A2411	G2349	A2287	A2225	C2104	G2040	A1969	C1902	U1834	A1773
G2602	A2541	G2476	G2412	C2350	A2288	C2226	U2105	U2041	A1970	G1903	G1835	U1774
U2603	A2542	A2477	G2413	G2351	G2289	A2227	U2106	A2042	U1971	G1904	C1836	U1775
C2604	G2543	U2478	G2414	G2352	G2290	G2228	G2107	C2043	G1972	G1905	C1837	G1776
U2605	G2544	A2478	G2415	G2353	U2291	U2229	A2108	C2044	G1973	G1906	C1838	U1777
C2606	G2545	U2479	C2416	G2354	U2292	G2230	U2109	G2045	C1974	G1907	G1839	U1778
G2607	U2546	G2481	C2417	C2355	G2293	U2231	G2110	G2046	G1975	U1910	G1840	U1779
U2608	A2547	A2482	A2418	G2356	U2294	C2232	U	C2047	G1975	G1911	A1760	C1780
G2609	U2548	C2483	U2419	U2357	U2295	C2232	U	G2048	G1980	U1911	U1761	U1781
C2610	G2549	G2484	C2420	G2357	U2296	U2233	U	G2049	A1981	A1912	C1843	C1843
U2611	G2550	G2485	G2421	A2358	A2297	G2234	A	A2042	U1982	A1913	C1844	U1782
C2612	C2551	U2486	C2422	C2359	A2298	G2235	C	C2050	U1983	C1913	G1845	A1783
U2613	U2552	G2487	G2423	G2360	U2299	U2236	C	A2051	G1984	C1914	G1846	A1784
A2614	G2553	U2488	U2424	G2361	C2300	G2237	A	A2052	G1985	U1915	A1847	A1785
U2615	U2554	U2489	C2425	C2362	C2301	G2238	C	A2053	C1986	A1916	A1786	A1786
C2616	G2555	U2490	A2426	G2363	U2302	G2239	U	A2054	U1917	A1917	A1787	A1787
U2617	C2556	G2491	G2427	C2364	G2303	U2240	C	G2055	G1989	A1918	C1788	C1788
G2618	U2557	U2492	G2428	G2365	G2304	U2241	U	G2056	C1990	A1919	A1789	A1789
C2619	C2558	A2493	G2429	A2366	U2305	U2242	G	G2057	U1991	C1920	A1853	C1790
U2620	U2559	G2494	A2430	G2367	C2306	U2243	U	A2058	G1992	G1921	A1854	C1791
C2621	A2560	U2500	G2368	A2369	G2307	U2244	U	C2059	U1993	U1922	G1857	G1792
U2622	U2561		G2369	A2370	G2308	C2248	G	A2060	C1994	C1924	A1858	C1793



• Molecule 23: 5S rRNA

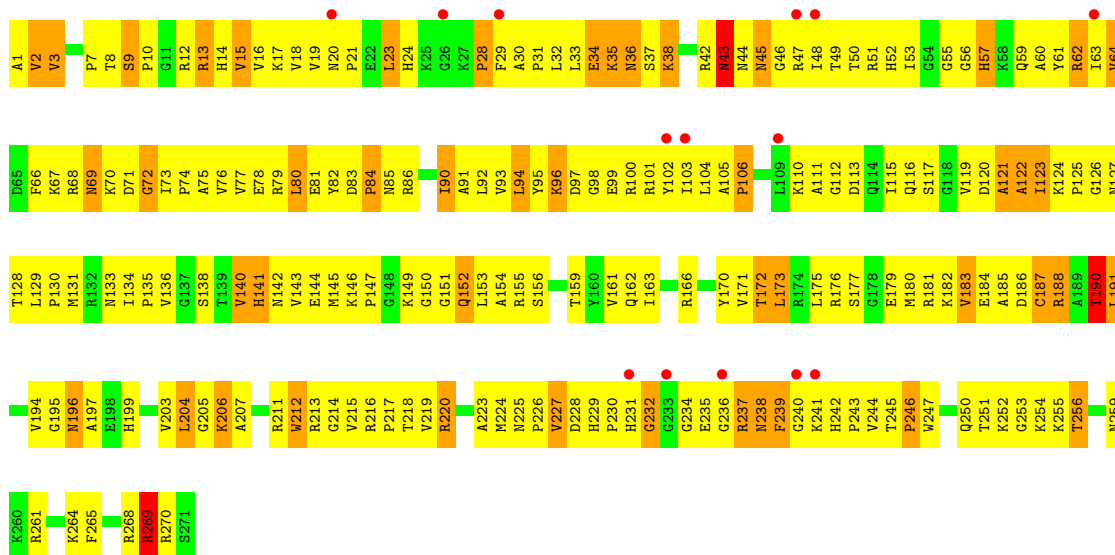


• Molecule 24: 50S ribosomal protein L2

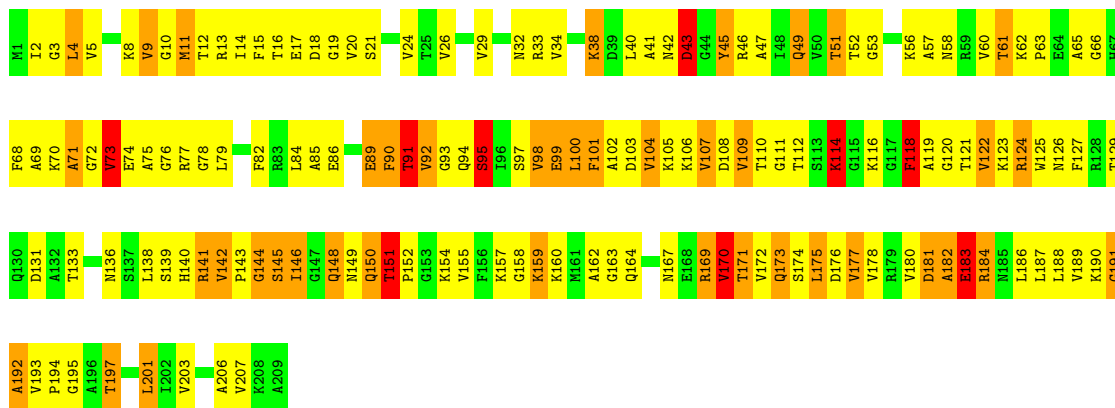


• Molecule 24: 50S ribosomal protein L2

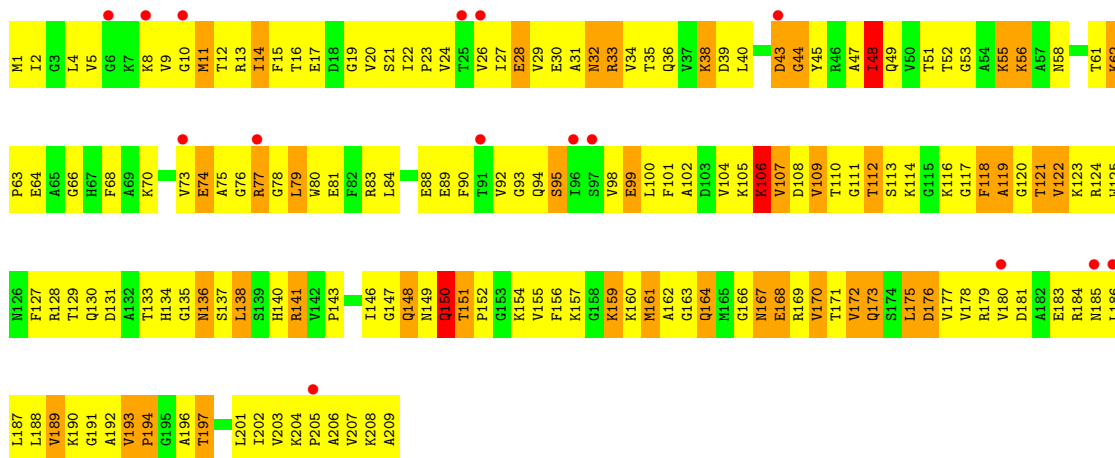
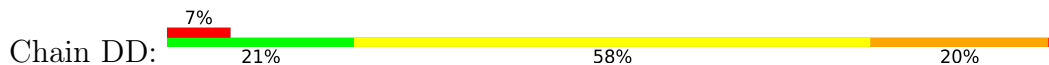




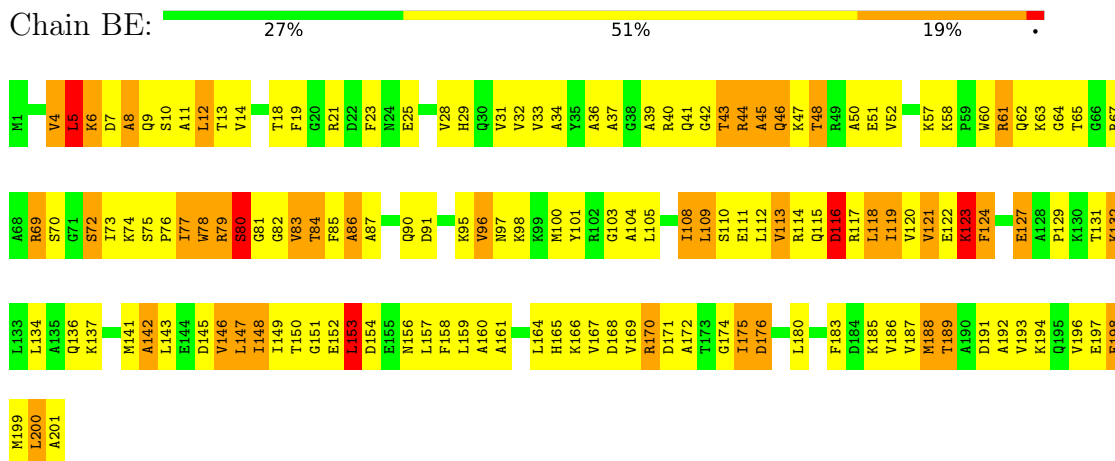
• Molecule 25: 50S ribosomal protein L3



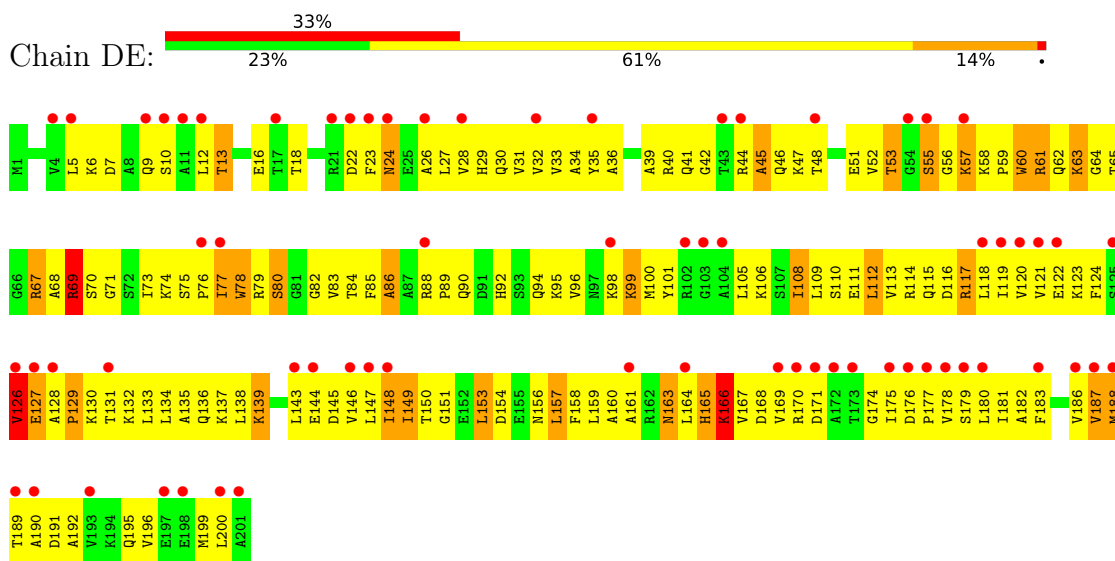
• Molecule 25: 50S ribosomal protein L3



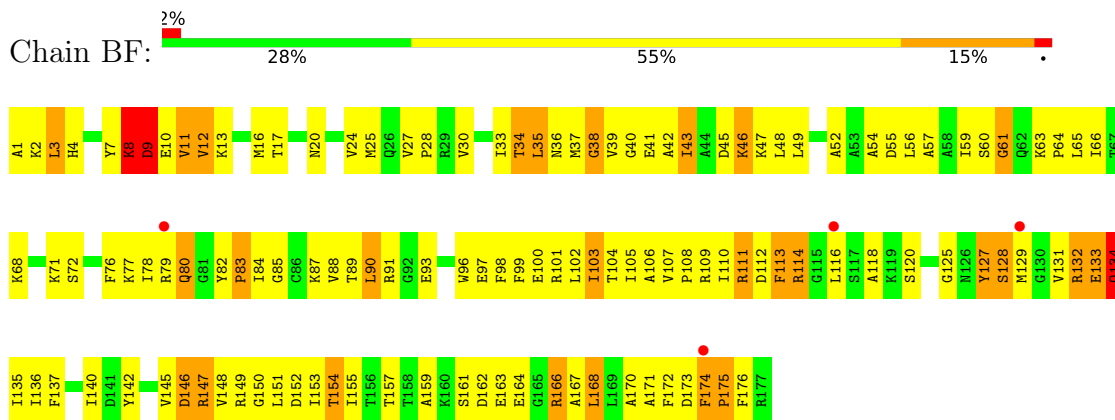
- Molecule 26: 50S ribosomal protein L4



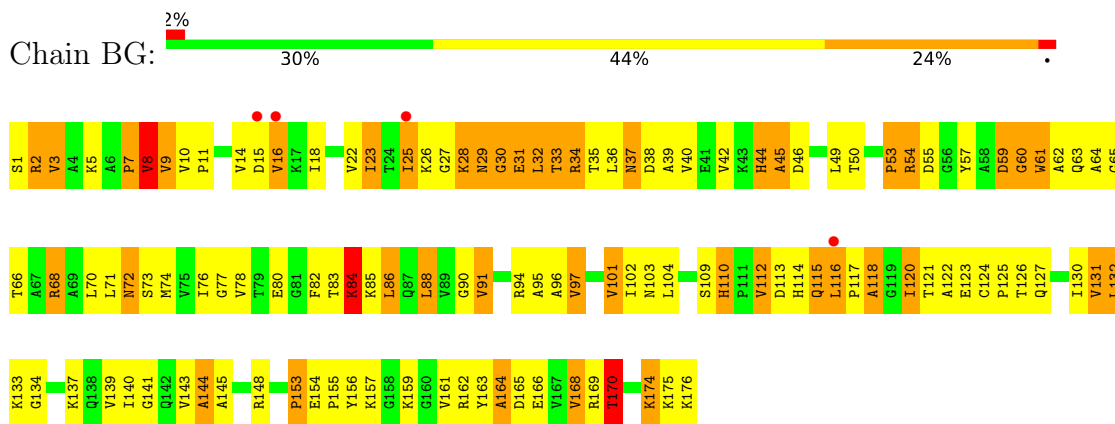
- Molecule 26: 50S ribosomal protein L4



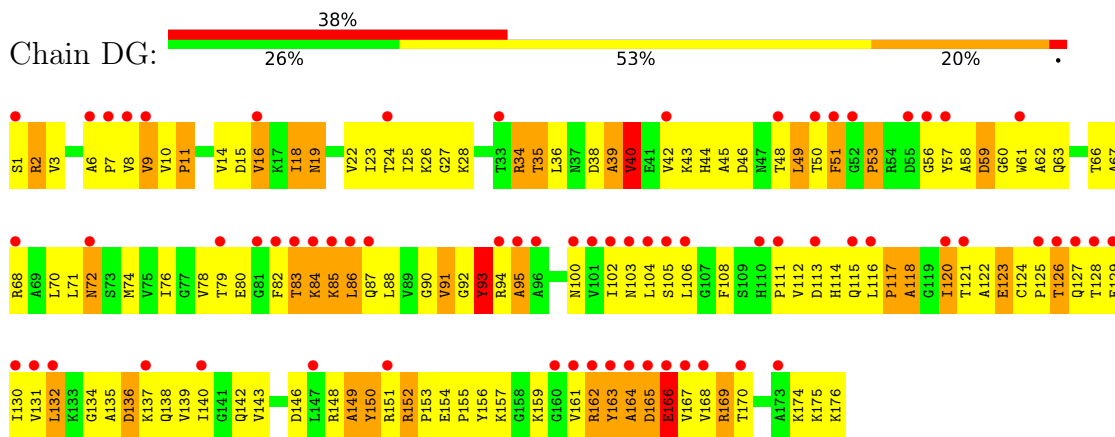
- Molecule 27: 50S ribosomal protein L5



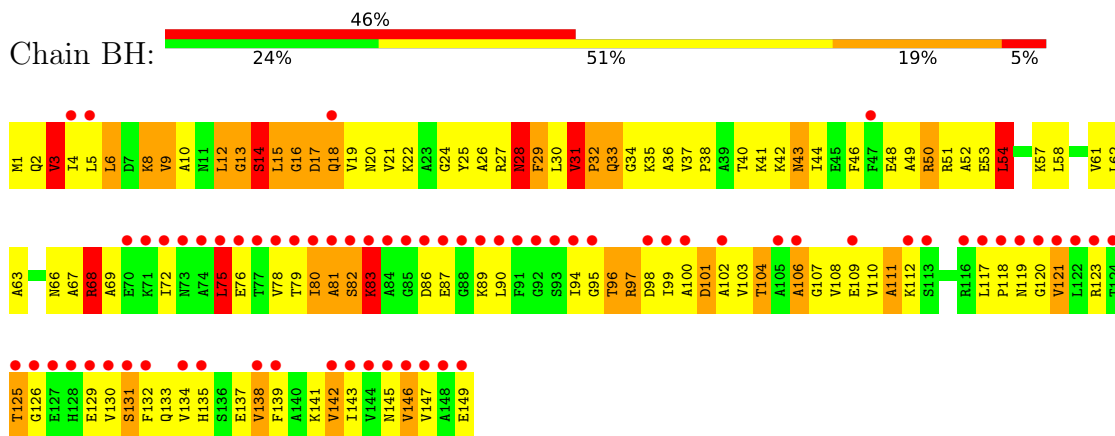
- Molecule 28: 50S ribosomal protein L6



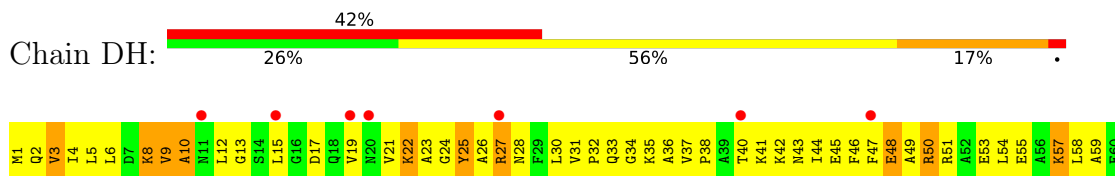
• Molecule 28: 50S ribosomal protein L6

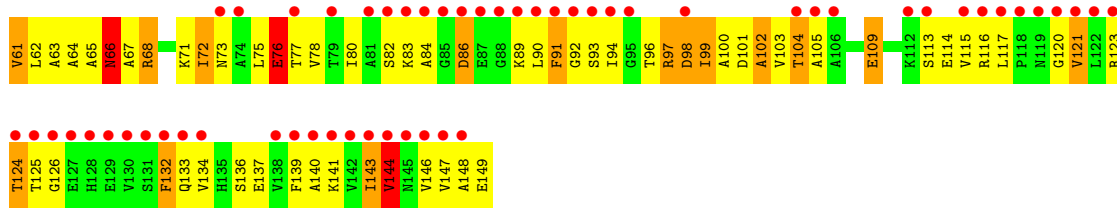


• Molecule 29: 50S ribosomal protein L9

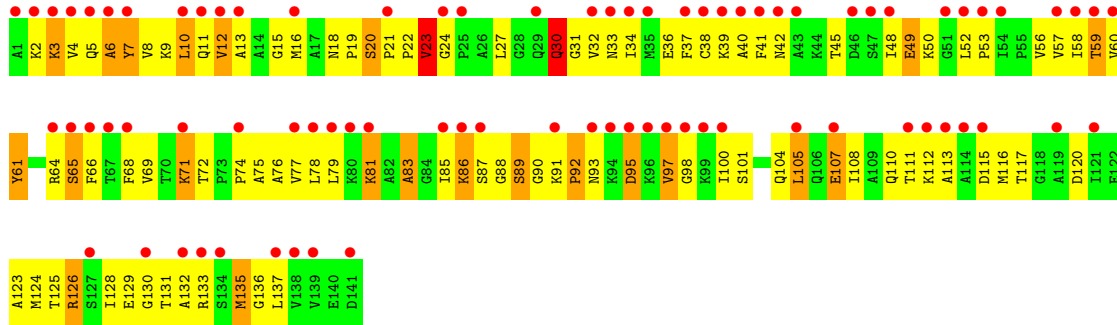


• Molecule 29: 50S ribosomal protein L9

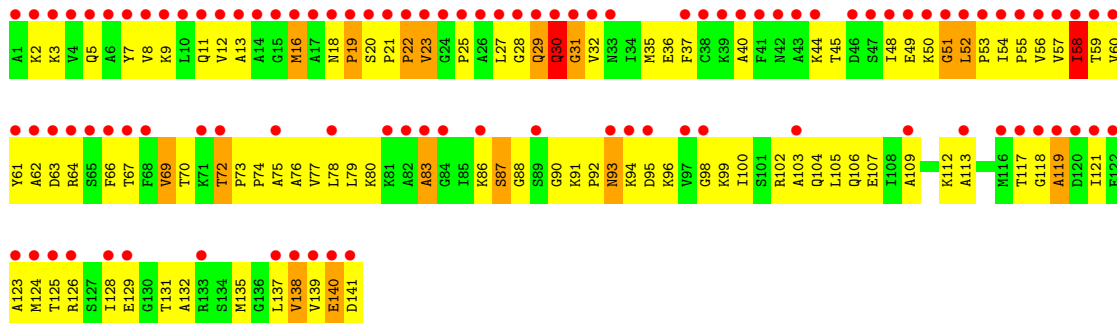
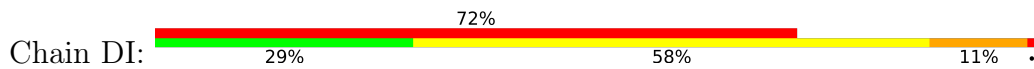




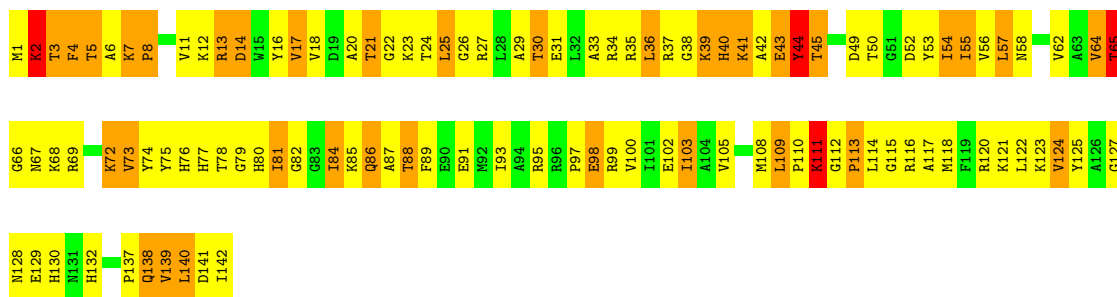
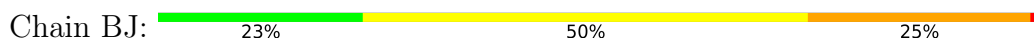
• Molecule 30: 50S ribosomal protein L11



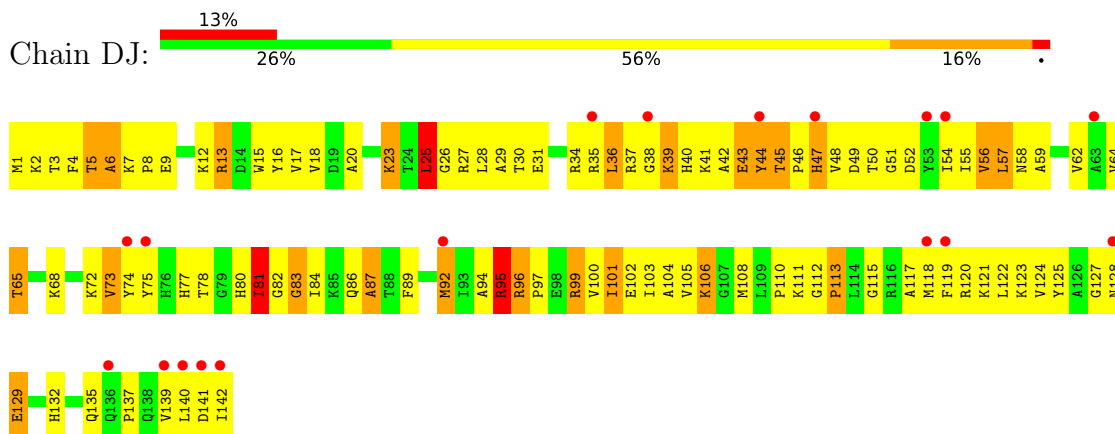
• Molecule 30: 50S ribosomal protein L11



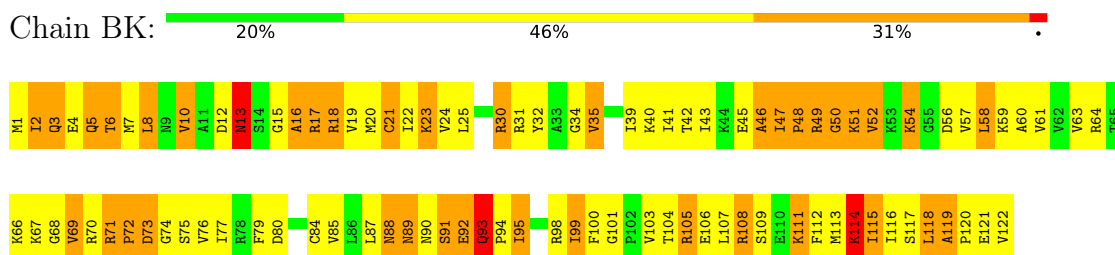
• Molecule 31: 50S ribosomal protein L13



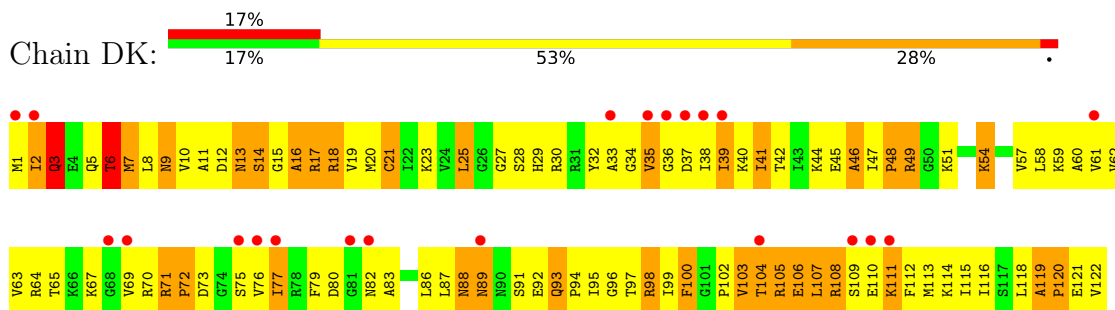
• Molecule 31: 50S ribosomal protein L13



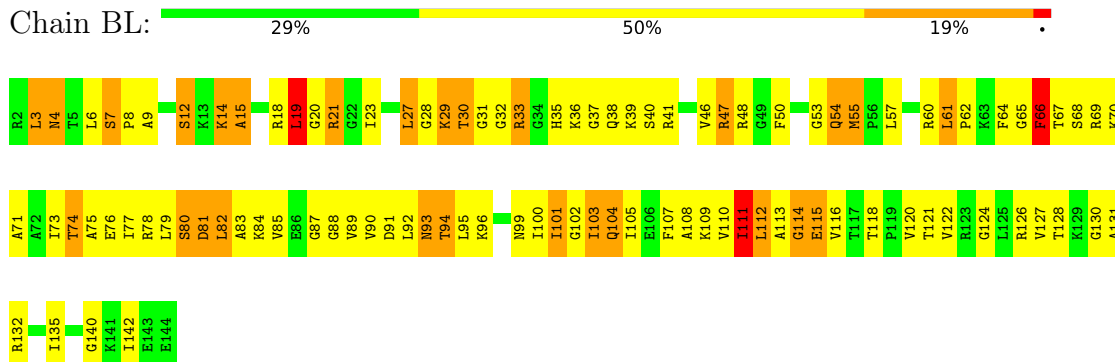
• Molecule 32: 50S ribosomal protein L14



• Molecule 32: 50S ribosomal protein L14

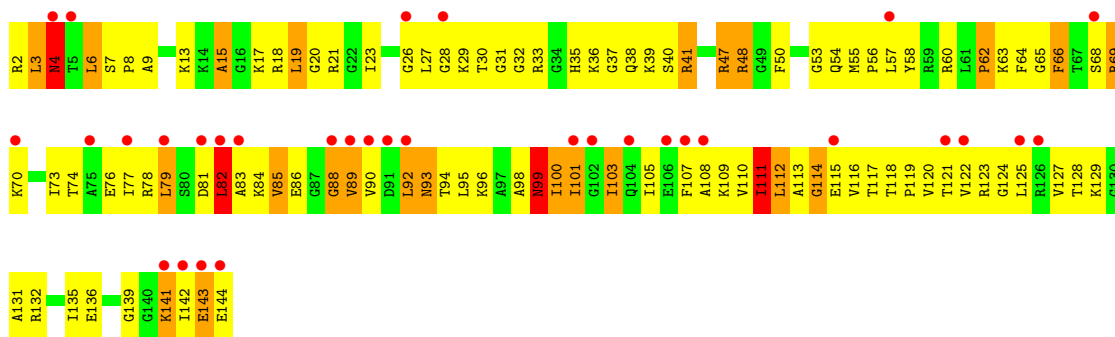


• Molecule 33: 50S ribosomal protein L15



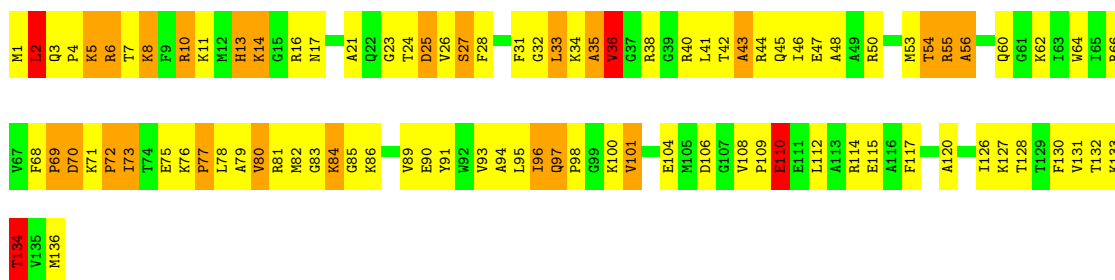
• Molecule 33: 50S ribosomal protein L15





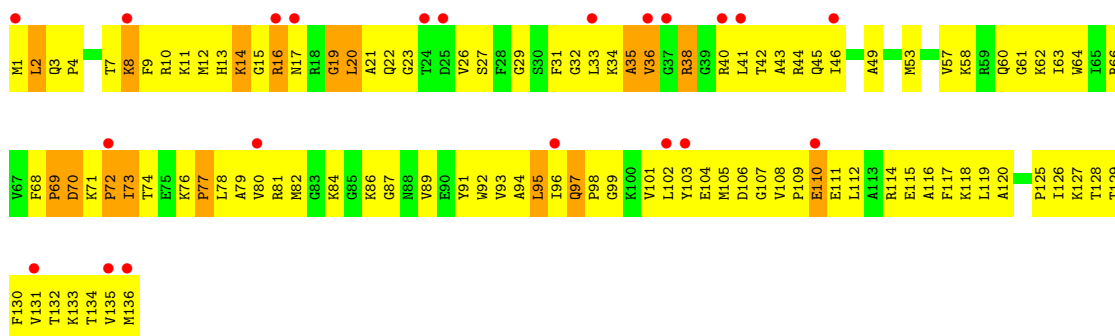
- Molecule 34: 50S ribosomal protein L16

Chain BM: 31% 49% 18%



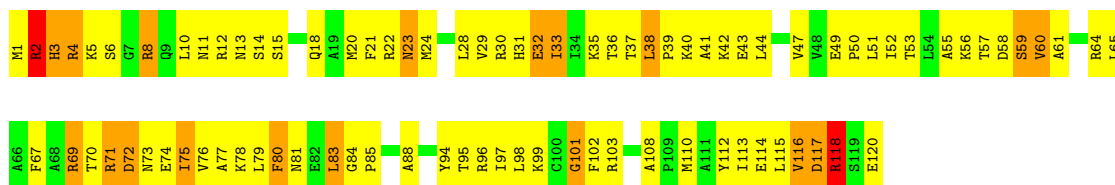
- Molecule 34: 50S ribosomal protein L16

Chain DM: 15% 23% 65% 12%

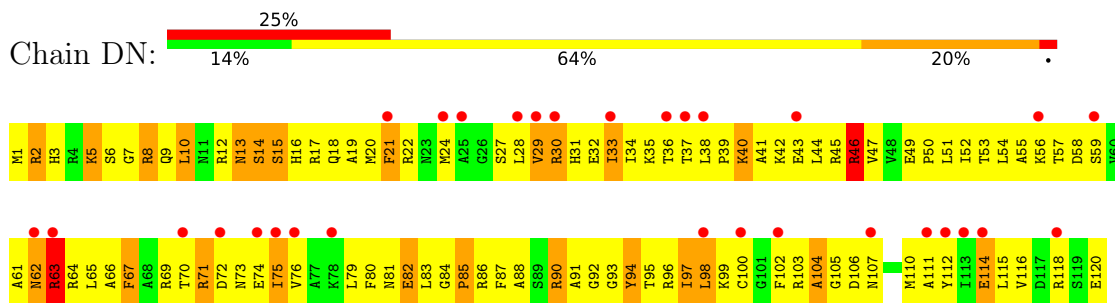


- Molecule 35: 50S ribosomal protein L17

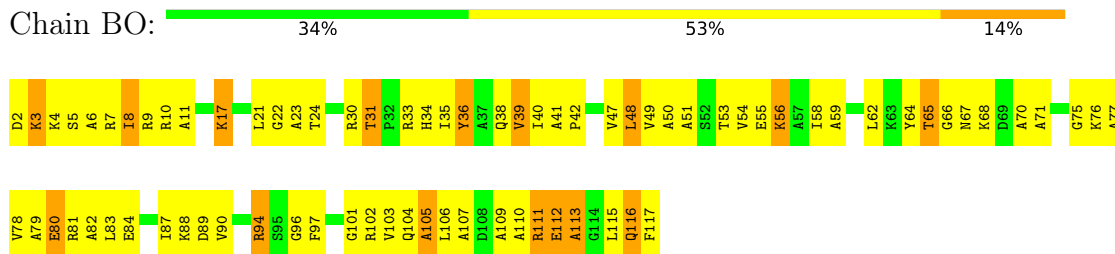
Chain BN: 28% 56% 15%



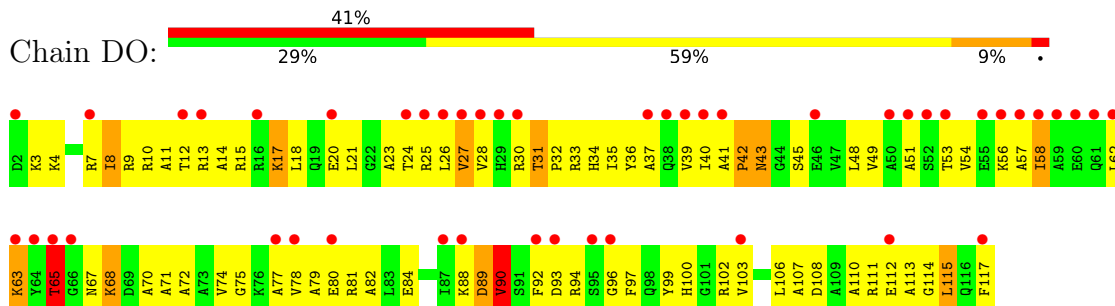
- Molecule 35: 50S ribosomal protein L17



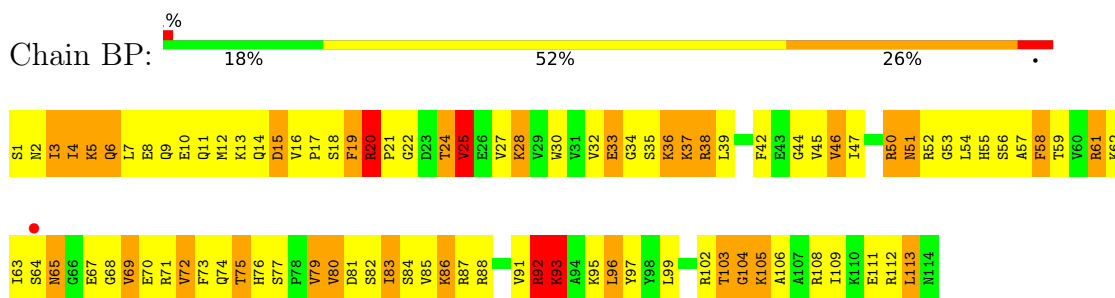
• Molecule 36: 50S ribosomal protein L18



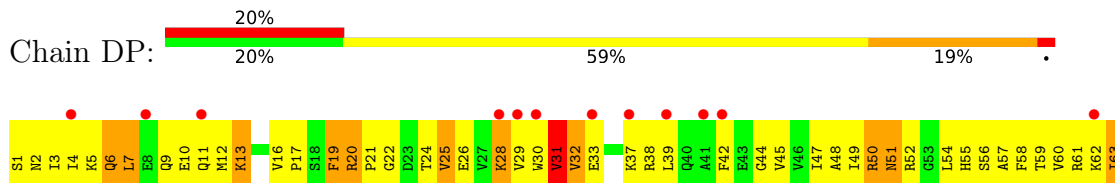
• Molecule 36: 50S ribosomal protein L18

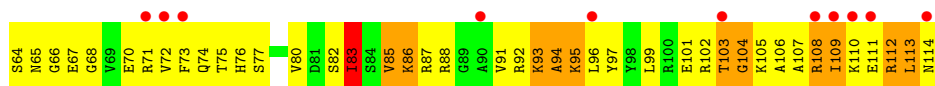


• Molecule 37: 50S ribosomal protein L19

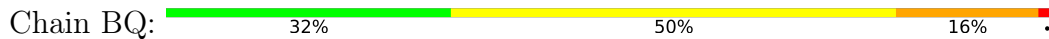


• Molecule 37: 50S ribosomal protein L19

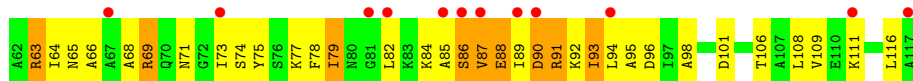
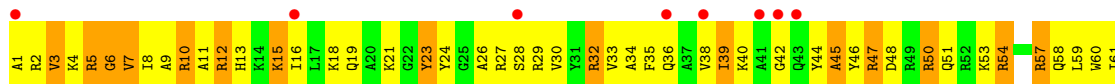




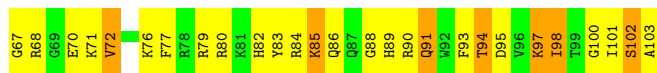
• Molecule 38: 50S ribosomal protein L20



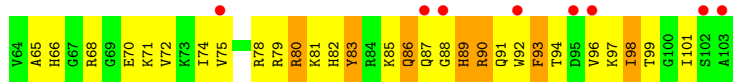
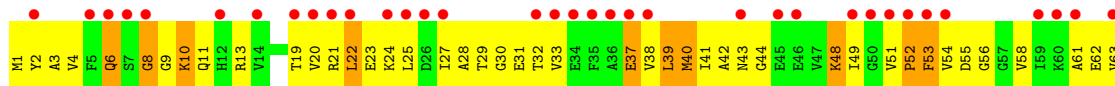
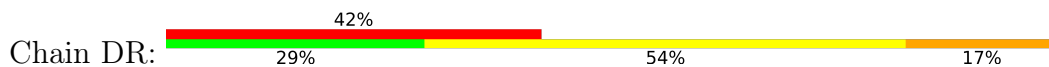
• Molecule 38: 50S ribosomal protein L20



• Molecule 39: 50S ribosomal protein L21

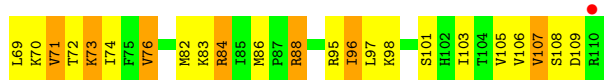
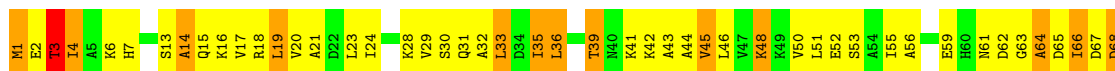


• Molecule 39: 50S ribosomal protein L21

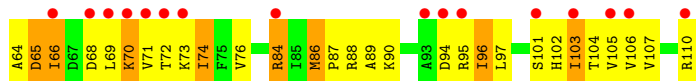
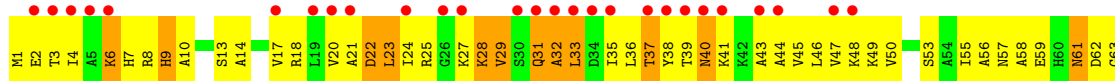


• Molecule 40: 50S ribosomal protein L22





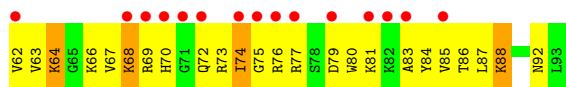
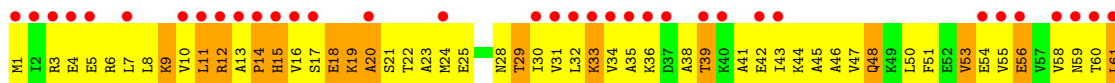
• Molecule 40: 50S ribosomal protein L22



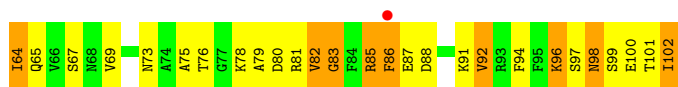
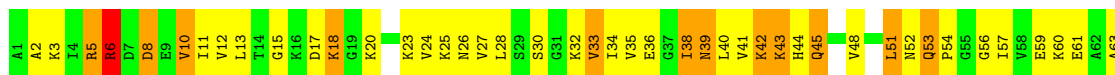
• Molecule 41: 50S ribosomal protein L23



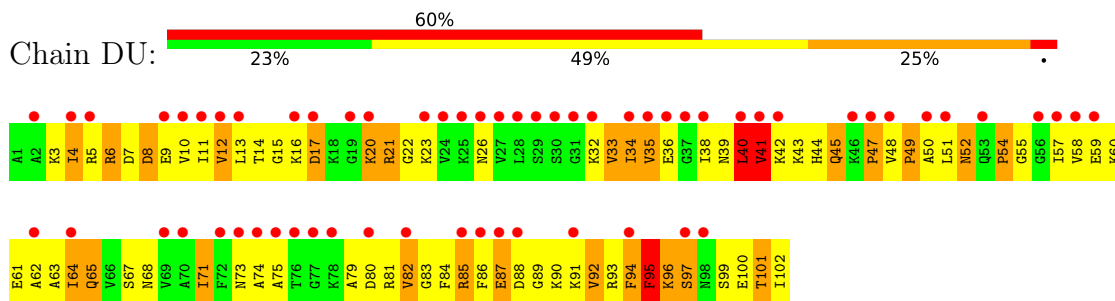
• Molecule 41: 50S ribosomal protein L23



• Molecule 42: 50S ribosomal protein L24



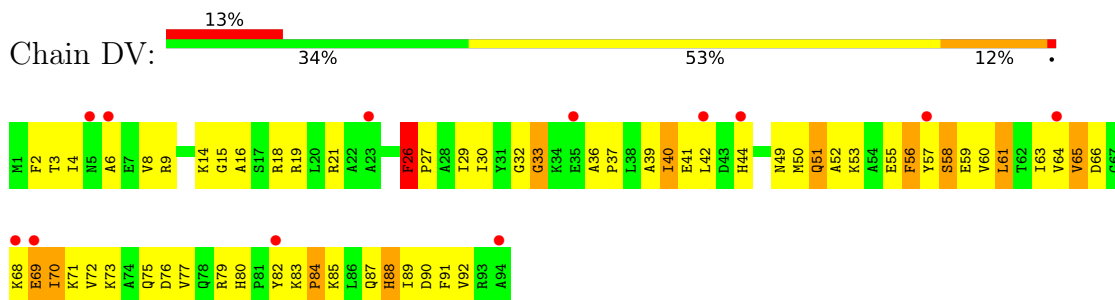
• Molecule 42: 50S ribosomal protein L24



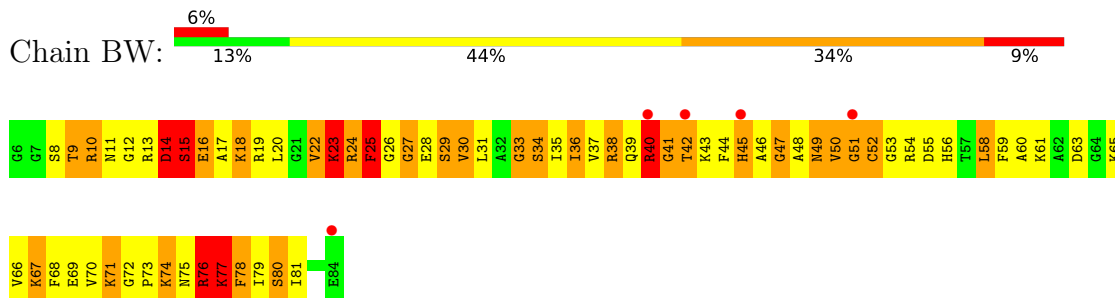
- Molecule 43: 50S ribosomal protein L25



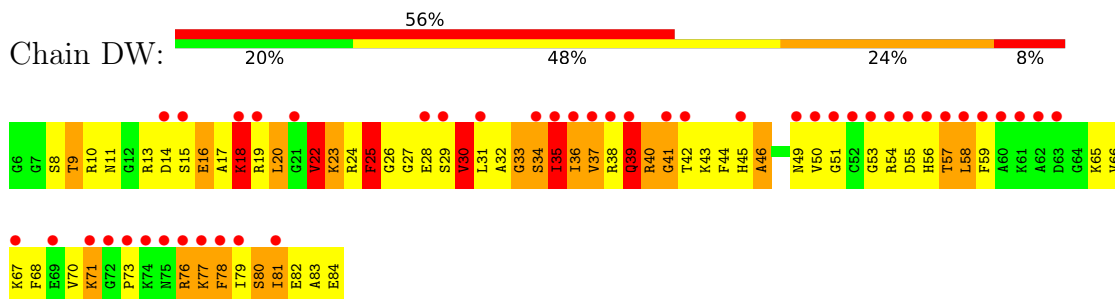
- Molecule 43: 50S ribosomal protein L25



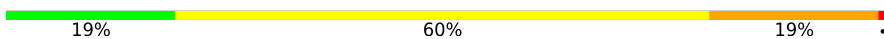
- Molecule 44: 50S ribosomal protein L27

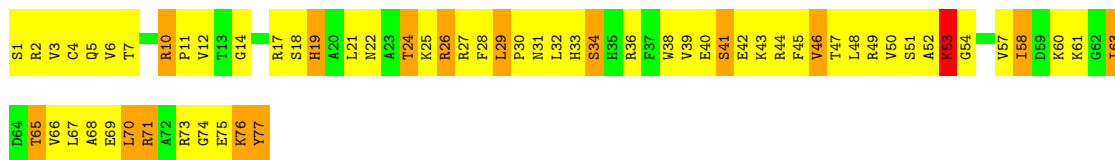


- Molecule 44: 50S ribosomal protein L27



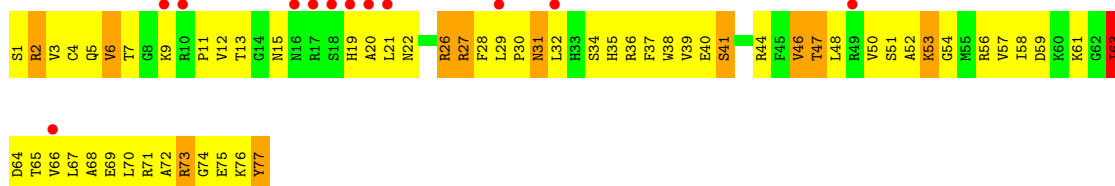
- Molecule 45: 50S ribosomal protein L28

Chain BX: 



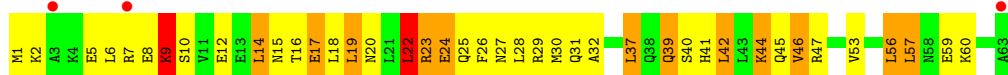
- Molecule 45: 50S ribosomal protein L28

Chain DX: 



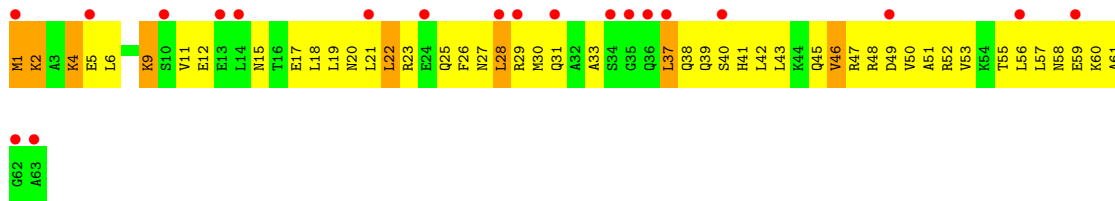
- Molecule 46: 50S ribosomal protein L29

Chain BY: 



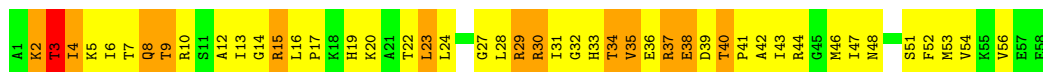
- Molecule 46: 50S ribosomal protein L29

Chain DY: 

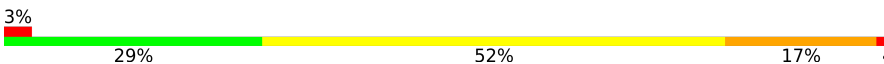


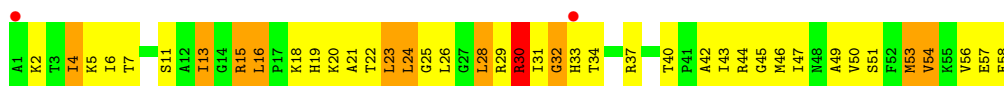
- Molecule 47: 50S ribosomal protein L30

Chain BZ: 

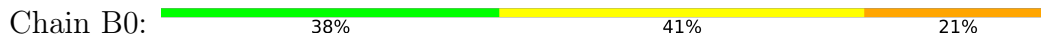


- Molecule 47: 50S ribosomal protein L30

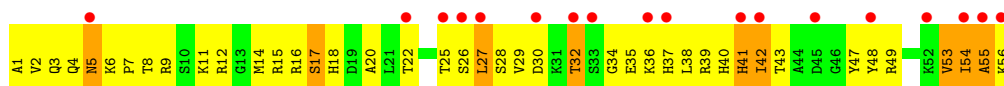
Chain DZ: 



- Molecule 48: 50S ribosomal protein L32



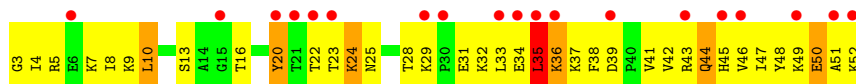
- Molecule 48: 50S ribosomal protein L32



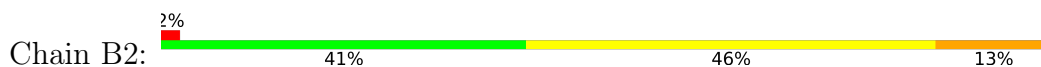
- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34



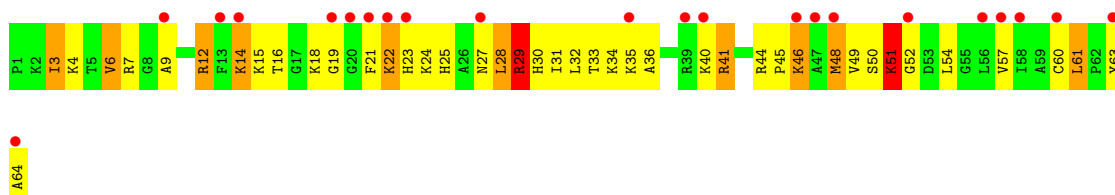
- Molecule 51: 50S ribosomal protein L35

Chain B3: 



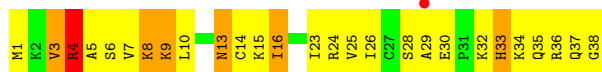
• Molecule 51: 50S ribosomal protein L35

Chain D3: 



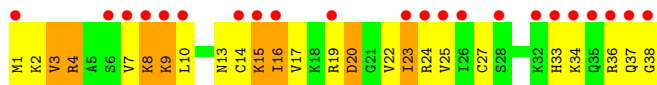
• Molecule 52: 50S ribosomal protein L36

Chain B4: 




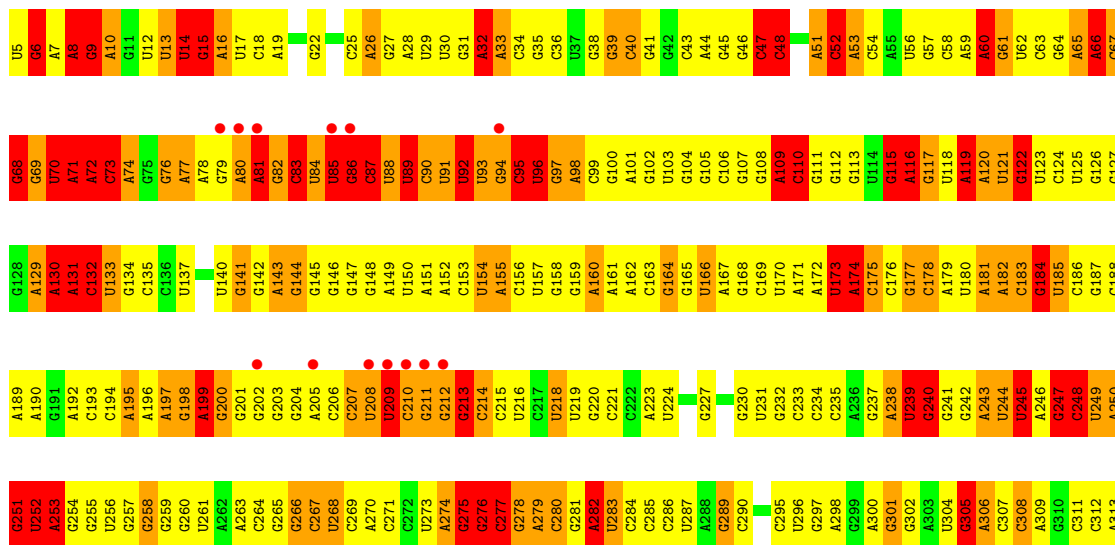
• Molecule 52: 50S ribosomal protein L36

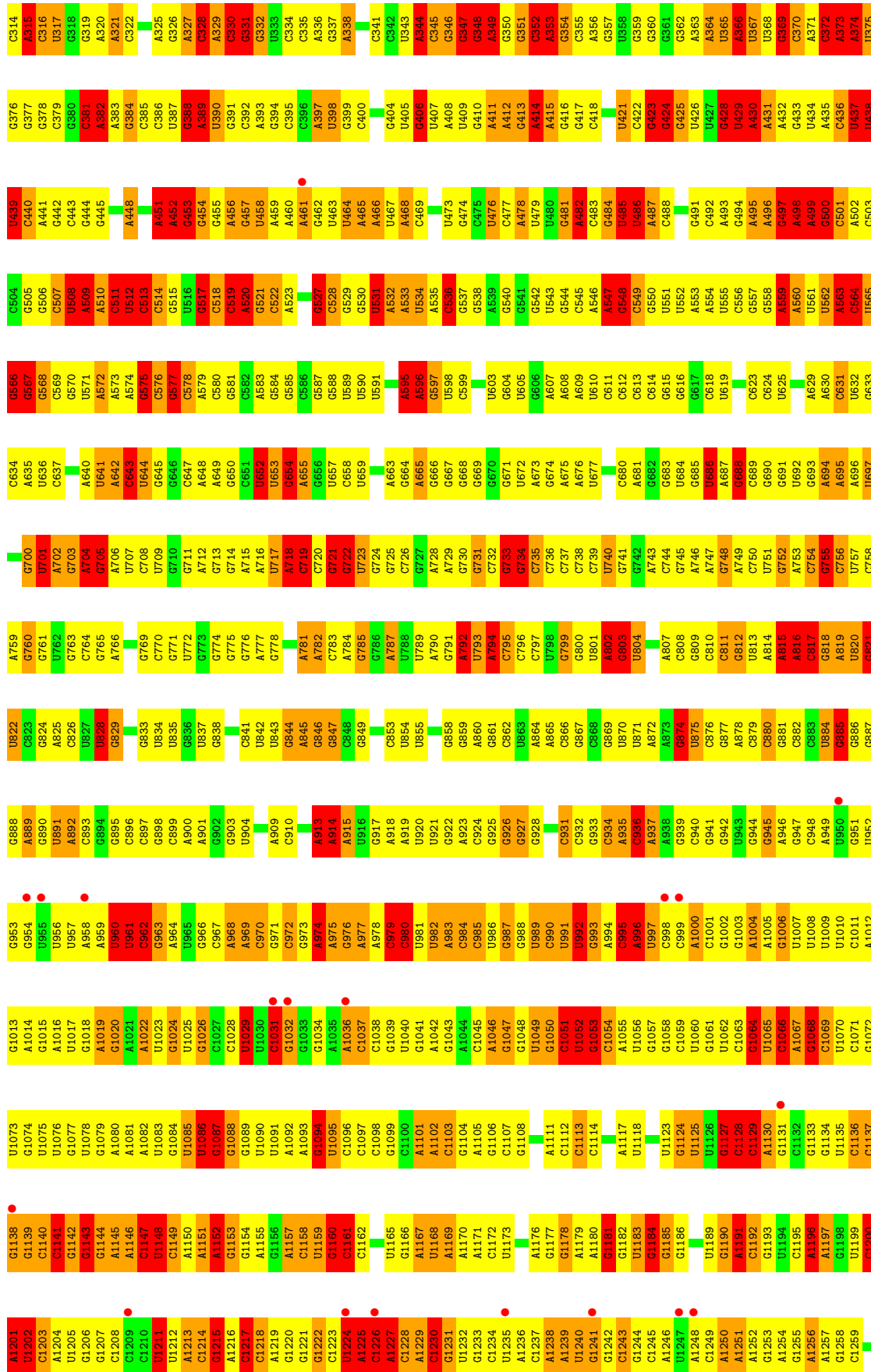
Chain D4: 

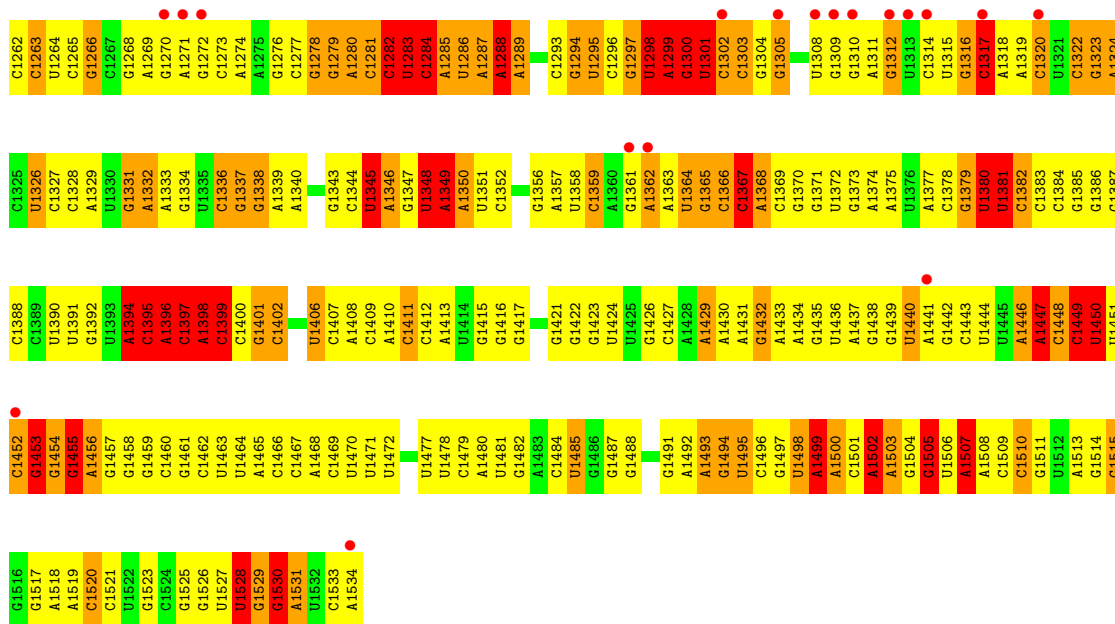


• Molecule 53: 16S rRNA

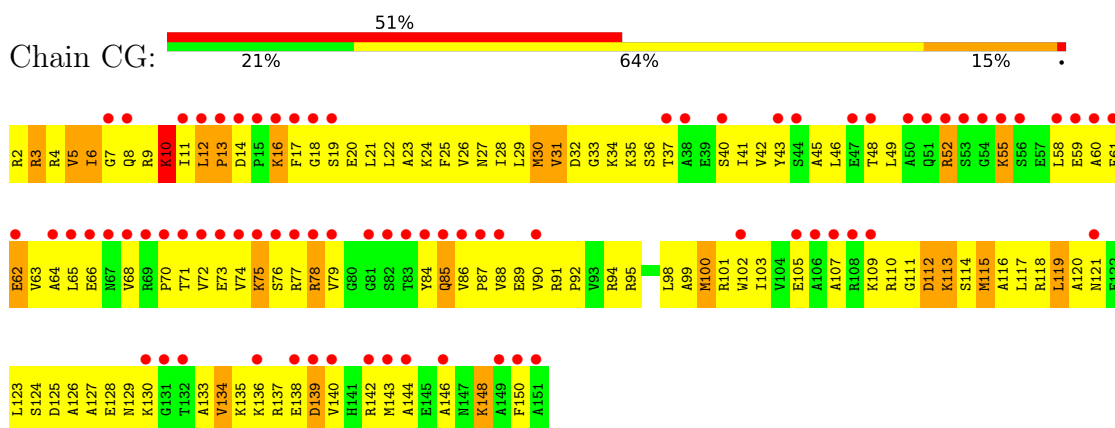
Chain CA: 



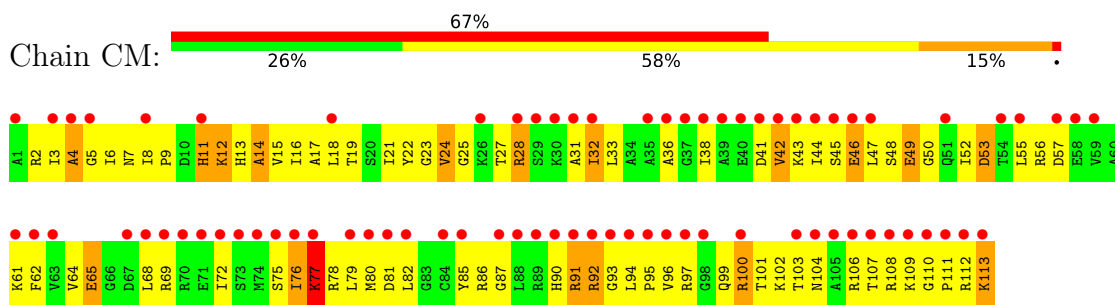




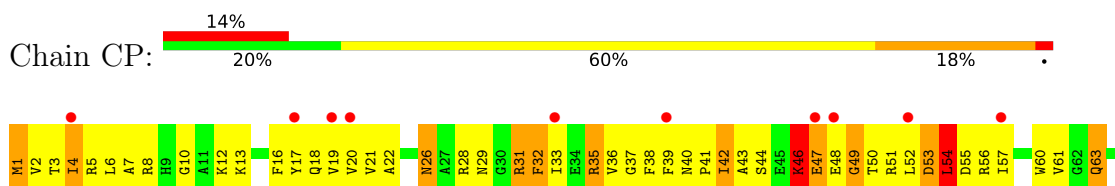
• Molecule 54: 30S ribosomal protein S7

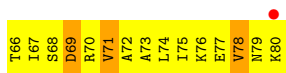


• Molecule 55: 30S ribosomal protein S13

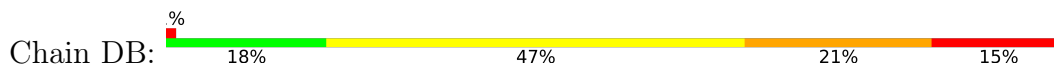


• Molecule 56: 30S ribosomal protein S16

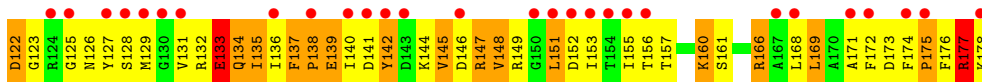
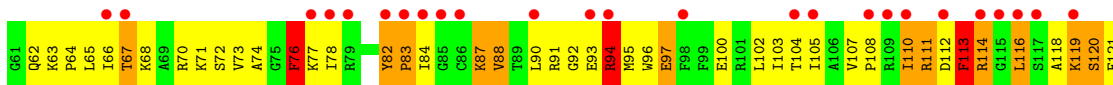
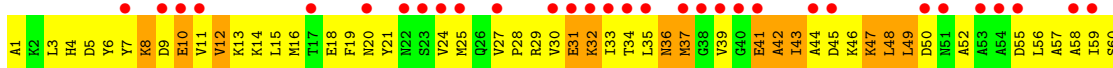




• Molecule 57: 5S rRNA



• Molecule 58: 50S ribosomal protein L5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.26Å)	Xtrriage
Refinement program	PHENIX ?, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.189 , 0.241 0.202 , 0.253	Depositor DCC
R_{free} test set	14080 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtrriage
Anisotropy	0.324	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 77.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284501	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.50	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	121 (56%)	65 (30%)	30 (14%)	0	1
2	CB	216/218 (99%)	145 (67%)	54 (25%)	17 (8%)	1	6
3	AC	204/206 (99%)	154 (76%)	33 (16%)	17 (8%)	1	6
3	CC	204/206 (99%)	147 (72%)	40 (20%)	17 (8%)	1	6
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	6
6	CF	98/100 (98%)	62 (63%)	27 (28%)	9 (9%)	1	4
7	AG	149/151 (99%)	107 (72%)	34 (23%)	8 (5%)	2	12
8	AH	127/129 (98%)	92 (72%)	27 (21%)	8 (6%)	1	10
8	CH	127/129 (98%)	87 (68%)	30 (24%)	10 (8%)	1	6
9	AI	125/127 (98%)	83 (66%)	31 (25%)	11 (9%)	1	5
9	CI	125/127 (98%)	87 (70%)	29 (23%)	9 (7%)	1	8
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	3
11	CK	115/117 (98%)	89 (77%)	17 (15%)	9 (8%)	1	6
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	8
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	9
15	AO	86/88 (98%)	58 (67%)	22 (26%)	6 (7%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CO	86/88 (98%)	68 (79%)	15 (17%)	3 (4%)	3	22
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%)	8	35
18	CR	53/55 (96%)	40 (76%)	11 (21%)	2 (4%)	3	20
19	AS	77/79 (98%)	56 (73%)	14 (18%)	7 (9%)	1	4
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	4
20	AT	83/85 (98%)	54 (65%)	20 (24%)	9 (11%)	0	3
20	CT	83/85 (98%)	55 (66%)	21 (25%)	7 (8%)	1	5
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	8
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	3
26	DE	199/201 (99%)	122 (61%)	51 (26%)	26 (13%)	0	1
27	BF	175/177 (99%)	127 (73%)	33 (19%)	15 (9%)	1	5
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	2
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	1
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	9
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%)	1	5
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	10
36	DO	114/116 (98%)	76 (67%)	26 (23%)	12 (10%)	0	3
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	10
38	DQ	115/117 (98%)	78 (68%)	24 (21%)	13 (11%)	0	2
39	BR	101/103 (98%)	76 (75%)	16 (16%)	9 (9%)	1	5
39	DR	101/103 (98%)	67 (66%)	25 (25%)	9 (9%)	1	5
40	BS	108/110 (98%)	77 (71%)	25 (23%)	6 (6%)	2	12
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	1
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%)	6	31
43	DV	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	1	7
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	6
45	DX	75/77 (97%)	46 (61%)	24 (32%)	5 (7%)	1	9
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	6
47	BZ	56/58 (97%)	44 (79%)	10 (18%)	2 (4%)	3	21
47	DZ	56/58 (97%)	35 (62%)	15 (27%)	6 (11%)	0	3
48	B0	54/56 (96%)	42 (78%)	8 (15%)	4 (7%)	1	7
48	D0	54/56 (96%)	37 (68%)	12 (22%)	5 (9%)	0	4
49	B1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	D1	48/50 (96%)	33 (69%)	10 (21%)	5 (10%)	0	3
50	B2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	6	30
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	9
51	D3	62/64 (97%)	40 (64%)	17 (27%)	5 (8%)	1	6
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	7
55	CM	111/113 (98%)	63 (57%)	36 (32%)	12 (11%)	0	3
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	147 (82%)	33 (18%)	1	7
2	CB	180/180 (100%)	152 (84%)	28 (16%)	2	12
3	AC	170/170 (100%)	140 (82%)	30 (18%)	2	8
3	CC	170/170 (100%)	153 (90%)	17 (10%)	7	28
4	AD	172/172 (100%)	142 (83%)	30 (17%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/172 (100%)	140 (81%)	32 (19%)	1	7
5	AE	113/113 (100%)	87 (77%)	26 (23%)	1	3
5	CE	113/113 (100%)	92 (81%)	21 (19%)	1	7
6	AF	87/87 (100%)	74 (85%)	13 (15%)	3	13
6	CF	87/87 (100%)	73 (84%)	14 (16%)	2	11
7	AG	124/124 (100%)	109 (88%)	15 (12%)	5	21
8	AH	104/104 (100%)	90 (86%)	14 (14%)	4	17
8	CH	104/104 (100%)	91 (88%)	13 (12%)	4	19
9	AI	105/105 (100%)	87 (83%)	18 (17%)	2	9
9	CI	105/105 (100%)	92 (88%)	13 (12%)	4	20
10	AJ	86/86 (100%)	74 (86%)	12 (14%)	3	16
10	CJ	86/86 (100%)	77 (90%)	9 (10%)	7	26
11	AK	90/90 (100%)	72 (80%)	18 (20%)	1	5
11	CK	90/90 (100%)	77 (86%)	13 (14%)	3	15
12	AL	103/103 (100%)	85 (82%)	18 (18%)	2	8
12	CL	103/103 (100%)	86 (84%)	17 (16%)	2	10
13	AM	92/92 (100%)	88 (96%)	4 (4%)	29	59
14	AN	79/83 (95%)	72 (91%)	7 (9%)	9	32
14	CN	79/83 (95%)	68 (86%)	11 (14%)	3	16
15	AO	76/76 (100%)	67 (88%)	9 (12%)	5	21
15	CO	76/76 (100%)	68 (90%)	8 (10%)	7	26
16	AP	65/65 (100%)	58 (89%)	7 (11%)	6	25
17	AQ	74/74 (100%)	60 (81%)	14 (19%)	1	6
17	CQ	74/74 (100%)	62 (84%)	12 (16%)	2	10
18	AR	48/48 (100%)	46 (96%)	2 (4%)	30	60
18	CR	48/48 (100%)	44 (92%)	4 (8%)	11	35
19	AS	70/70 (100%)	63 (90%)	7 (10%)	7	28
19	CS	70/70 (100%)	63 (90%)	7 (10%)	7	28
20	AT	65/65 (100%)	50 (77%)	15 (23%)	1	3
20	CT	65/65 (100%)	55 (85%)	10 (15%)	2	12
21	AU	44/44 (100%)	37 (84%)	7 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	44/44 (100%)	36 (82%)	8 (18%)	1	7
24	BC	216/216 (100%)	166 (77%)	50 (23%)	1	3
24	DC	216/216 (100%)	189 (88%)	27 (12%)	4	19
25	BD	164/164 (100%)	131 (80%)	33 (20%)	1	5
25	DD	164/164 (100%)	139 (85%)	25 (15%)	3	12
26	BE	165/165 (100%)	126 (76%)	39 (24%)	1	2
26	DE	165/165 (100%)	148 (90%)	17 (10%)	7	26
27	BF	148/148 (100%)	124 (84%)	24 (16%)	2	10
28	BG	137/137 (100%)	107 (78%)	30 (22%)	1	3
28	DG	137/137 (100%)	121 (88%)	16 (12%)	5	22
29	BH	114/114 (100%)	96 (84%)	18 (16%)	2	11
29	DH	114/114 (100%)	98 (86%)	16 (14%)	3	16
30	BI	109/109 (100%)	91 (84%)	18 (16%)	2	10
30	DI	109/109 (100%)	103 (94%)	6 (6%)	21	52
31	BJ	116/116 (100%)	84 (72%)	32 (28%)	0	1
31	DJ	116/116 (100%)	103 (89%)	13 (11%)	6	23
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%)	4	19
34	BM	109/109 (100%)	87 (80%)	22 (20%)	1	5
34	DM	109/109 (100%)	103 (94%)	6 (6%)	21	52
35	BN	100/100 (100%)	83 (83%)	17 (17%)	2	9
35	DN	100/100 (100%)	80 (80%)	20 (20%)	1	5
36	BO	86/86 (100%)	71 (83%)	15 (17%)	2	8
36	DO	86/86 (100%)	78 (91%)	8 (9%)	9	30
37	BP	99/99 (100%)	72 (73%)	27 (27%)	0	1
37	DP	99/99 (100%)	89 (90%)	10 (10%)	7	27
38	BQ	89/89 (100%)	72 (81%)	17 (19%)	1	6
38	DQ	89/89 (100%)	75 (84%)	14 (16%)	2	12
39	BR	84/84 (100%)	66 (79%)	18 (21%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DR	84/84 (100%)	71 (84%)	13 (16%)	2	12
40	BS	93/93 (100%)	74 (80%)	19 (20%)	1	4
40	DS	93/93 (100%)	79 (85%)	14 (15%)	3	13
41	BT	80/80 (100%)	59 (74%)	21 (26%)	0	1
41	DT	80/80 (100%)	74 (92%)	6 (8%)	13	39
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	4
42	DU	83/83 (100%)	73 (88%)	10 (12%)	5	21
43	BV	78/78 (100%)	61 (78%)	17 (22%)	1	3
43	DV	78/78 (100%)	70 (90%)	8 (10%)	7	26
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%)	3	13
46	BY	55/55 (100%)	45 (82%)	10 (18%)	1	7
46	DY	55/55 (100%)	52 (94%)	3 (6%)	21	52
47	BZ	48/48 (100%)	32 (67%)	16 (33%)	0	0
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	2	10
48	B0	47/47 (100%)	34 (72%)	13 (28%)	0	1
48	D0	47/47 (100%)	40 (85%)	7 (15%)	3	13
49	B1	45/45 (100%)	38 (84%)	7 (16%)	2	12
49	D1	45/45 (100%)	41 (91%)	4 (9%)	9	32
50	B2	38/38 (100%)	31 (82%)	7 (18%)	1	7
50	D2	38/38 (100%)	35 (92%)	3 (8%)	12	37
51	B3	51/51 (100%)	45 (88%)	6 (12%)	5	21
51	D3	51/51 (100%)	40 (78%)	11 (22%)	1	4
52	B4	34/34 (100%)	29 (85%)	5 (15%)	3	14
52	D4	34/34 (100%)	29 (85%)	5 (15%)	3	14
54	CG	123/123 (100%)	104 (85%)	19 (15%)	2	12
55	CM	91/91 (100%)	81 (89%)	10 (11%)	6	24
56	CP	65/65 (100%)	54 (83%)	11 (17%)	2	9
58	DF	149/149 (100%)	127 (85%)	22 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9331/9339 (100%)	7816 (84%)	1515 (16%)	2 10

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 [i](#)

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 monosaccharides 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	-	25,28,28	1.49	4 (16%)	29,40,40	1.52	8 (27%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3135	CLY	C14-N2	3.38	1.51	1.47
60	BA	3135	CLY	C15-N2	2.88	1.52	1.46
60	BA	3135	CLY	O5-C4	2.75	1.48	1.44
60	BA	3135	CLY	C6-S1	2.24	1.84	1.79

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	-3.28	109.28	116.58
60	BA	3135	CLY	C10-C11-N2	-2.62	107.53	112.40
60	BA	3135	CLY	O4-C1-C2	-2.38	104.84	110.35
60	BA	3135	CLY	C9-C8-CL1	-2.17	105.14	108.76
60	BA	3135	CLY	C15-N2-C14	2.16	115.39	112.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

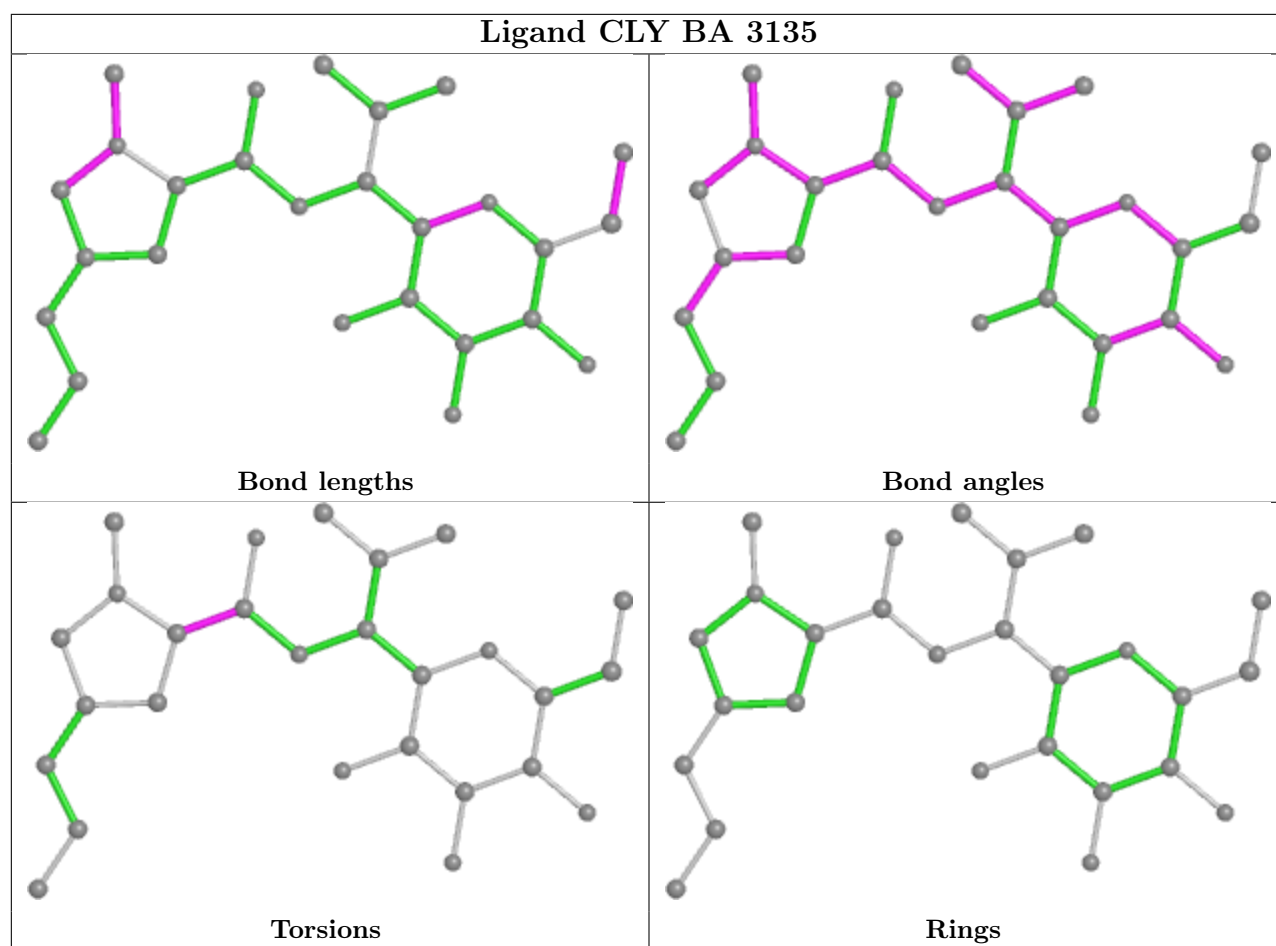
Mol	Chain	Res	Type	Atoms
60	BA	3135	CLY	N1-C10-C11-C12
60	BA	3135	CLY	N1-C10-C11-N2

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	AA	1533/1533 (100%)	-0.56	20 (1%) 77 76	26, 75, 180, 427	0
2	AB	218/218 (100%)	1.35	47 (21%) 0 1	111, 151, 210, 294	0
2	CB	218/218 (100%)	1.86	91 (41%) 0 0	125, 161, 248, 300	0
3	AC	206/206 (100%)	0.38	10 (4%) 29 28	51, 97, 147, 208	0
3	CC	206/206 (100%)	0.93	31 (15%) 2 2	74, 144, 225, 261	0
4	AD	205/205 (100%)	-0.02	6 (2%) 51 50	43, 83, 164, 311	0
4	CD	205/205 (100%)	-0.27	1 (0%) 91 91	31, 59, 113, 227	0
5	AE	150/150 (100%)	0.15	4 (2%) 54 52	55, 78, 148, 255	0
5	CE	150/150 (100%)	0.26	3 (2%) 65 63	55, 85, 149, 258	0
6	AF	100/100 (100%)	-0.06	2 (2%) 65 63	53, 90, 143, 171	0
6	CF	100/100 (100%)	0.46	7 (7%) 16 16	72, 107, 167, 226	0
7	AG	151/151 (100%)	0.39	13 (8%) 10 10	67, 129, 199, 248	0
8	AH	129/129 (100%)	0.17	4 (3%) 49 48	38, 71, 123, 214	0
8	CH	129/129 (100%)	0.46	7 (5%) 25 24	53, 100, 161, 214	0
9	AI	127/127 (100%)	0.90	21 (16%) 1 2	66, 125, 243, 279	0
9	CI	127/127 (100%)	2.01	51 (40%) 0 0	111, 184, 282, 308	0
10	AJ	98/98 (100%)	0.62	12 (12%) 4 4	60, 114, 210, 262	0
10	CJ	98/98 (100%)	2.43	47 (47%) 0 0	103, 188, 266, 292	0
11	AK	117/117 (100%)	0.46	5 (4%) 35 33	36, 98, 174, 203	0
11	CK	117/117 (100%)	0.38	7 (5%) 21 21	55, 104, 165, 196	0
12	AL	123/123 (100%)	-0.27	1 (0%) 86 86	15, 54, 116, 167	0
12	CL	123/123 (100%)	0.28	4 (3%) 46 44	36, 73, 121, 188	0
13	AM	114/114 (100%)	0.45	8 (7%) 16 16	76, 125, 196, 274	0
14	AN	96/100 (96%)	0.27	6 (6%) 20 20	59, 102, 195, 267	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	CN	95/100 (95%)	2.30	46 (48%) 0 0	109, 221, 327, 373	0
15	AO	88/88 (100%)	-0.41	0 100 100	36, 70, 123, 182	0
15	CO	88/88 (100%)	0.07	1 (1%) 80 80	59, 103, 158, 277	0
16	AP	82/82 (100%)	0.51	9 (10%) 5 5	44, 74, 148, 243	0
17	AQ	80/80 (100%)	0.48	7 (8%) 10 10	29, 78, 141, 267	0
17	CQ	80/80 (100%)	0.86	13 (16%) 1 2	48, 106, 161, 199	0
18	AR	55/55 (100%)	0.06	3 (5%) 25 24	60, 86, 161, 196	0
18	CR	55/55 (100%)	0.16	1 (1%) 68 66	47, 92, 186, 230	0
19	AS	79/79 (100%)	1.52	21 (26%) 0 0	79, 127, 199, 277	0
19	CS	79/79 (100%)	3.17	48 (60%) 0 0	181, 371, 451, 469	0
20	AT	85/85 (100%)	-0.08	0 100 100	43, 76, 116, 143	0
20	CT	85/85 (100%)	1.02	15 (17%) 1 1	58, 117, 197, 268	0
21	AU	51/51 (100%)	1.78	21 (41%) 0 0	88, 157, 204, 230	0
21	CU	51/51 (100%)	0.54	5 (9%) 7 7	58, 111, 182, 320	0
22	BA	2854/2903 (98%)	-0.51	36 (1%) 77 76	4, 28, 155, 403	0
22	DA	2841/2903 (97%)	0.22	83 (2%) 51 50	49, 122, 252, 460	0
23	BB	118/118 (100%)	-0.61	0 100 100	13, 43, 77, 106	0
24	BC	271/271 (100%)	-0.34	5 (1%) 68 66	5, 39, 81, 171	0
24	DC	271/271 (100%)	0.43	14 (5%) 27 25	51, 96, 147, 192	0
25	BD	209/209 (100%)	-0.43	0 100 100	3, 23, 72, 171	0
25	DD	209/209 (100%)	0.54	15 (7%) 15 15	50, 111, 176, 290	0
26	BE	201/201 (100%)	-0.28	0 100 100	2, 37, 98, 185	0
26	DE	201/201 (100%)	1.66	67 (33%) 0 0	62, 197, 394, 486	0
27	BF	177/177 (100%)	0.09	4 (2%) 60 58	27, 70, 127, 197	0
28	BG	176/176 (100%)	-0.03	4 (2%) 60 58	23, 60, 119, 204	0
28	DG	176/176 (100%)	1.63	67 (38%) 0 0	95, 195, 279, 335	0
29	BH	149/149 (100%)	3.03	68 (45%) 0 0	40, 177, 291, 362	0
29	DH	149/149 (100%)	3.28	63 (42%) 0 0	82, 181, 277, 319	0
30	BI	141/141 (100%)	3.00	80 (56%) 0 0	162, 269, 338, 374	0
30	DI	141/141 (100%)	3.53	101 (71%) 0 0	210, 324, 369, 408	0
31	BJ	142/142 (100%)	-0.50	0 100 100	6, 21, 60, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
31	DJ	142/142 (100%)	0.83	18 (12%) 3 3	63, 102, 163, 184	0
32	BK	122/122 (100%)	-0.45	0 100 100	7, 26, 74, 263	0
32	DK	122/122 (100%)	0.97	21 (17%) 1 1	52, 95, 164, 236	0
33	BL	143/143 (100%)	-0.42	0 100 100	3, 35, 77, 103	0
33	DL	143/143 (100%)	1.35	33 (23%) 0 1	58, 159, 278, 348	0
34	BM	136/136 (100%)	-0.47	0 100 100	4, 26, 66, 135	0
34	DM	136/136 (100%)	0.87	21 (15%) 2 2	44, 105, 164, 196	0
35	BN	120/120 (100%)	-0.54	0 100 100	6, 20, 43, 151	0
35	DN	120/120 (100%)	1.33	30 (25%) 0 0	79, 127, 200, 268	0
36	BO	116/116 (100%)	-0.24	0 100 100	26, 43, 77, 126	0
36	DO	116/116 (100%)	2.03	47 (40%) 0 0	124, 168, 240, 292	0
37	BP	114/114 (100%)	-0.29	1 (0%) 84 84	9, 35, 83, 148	0
37	DP	114/114 (100%)	1.04	23 (20%) 1 1	62, 114, 174, 238	0
38	BQ	117/117 (100%)	-0.57	0 100 100	3, 16, 43, 199	0
38	DQ	117/117 (100%)	1.03	20 (17%) 1 1	66, 103, 194, 288	0
39	BR	103/103 (100%)	-0.45	1 (0%) 82 82	4, 31, 80, 180	0
39	DR	103/103 (100%)	2.02	43 (41%) 0 0	67, 130, 227, 316	0
40	BS	110/110 (100%)	-0.50	1 (0%) 84 84	4, 17, 52, 175	0
40	DS	110/110 (100%)	1.79	43 (39%) 0 0	59, 130, 231, 279	0
41	BT	93/93 (100%)	-0.03	2 (2%) 62 59	19, 43, 128, 185	0
41	DT	93/93 (100%)	2.64	50 (53%) 0 0	123, 205, 306, 347	0
42	BU	102/102 (100%)	-0.11	1 (0%) 82 82	18, 49, 120, 241	0
42	DU	102/102 (100%)	3.05	61 (59%) 0 0	123, 285, 434, 557	0
43	BV	94/94 (100%)	-0.07	0 100 100	15, 43, 86, 142	0
43	DV	94/94 (100%)	0.85	12 (12%) 3 3	97, 143, 194, 233	0
44	BW	79/79 (100%)	0.02	5 (6%) 20 20	10, 30, 105, 223	0
44	DW	79/79 (100%)	2.38	44 (55%) 0 0	82, 140, 238, 284	0
45	BX	77/77 (100%)	-0.41	0 100 100	11, 42, 84, 117	0
45	DX	77/77 (100%)	0.95	12 (15%) 2 2	78, 117, 171, 236	0
46	BY	63/63 (100%)	0.17	3 (4%) 30 29	30, 66, 136, 222	0
46	DY	63/63 (100%)	1.97	20 (31%) 0 0	143, 309, 433, 440	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	BZ	58/58 (100%)	-0.45	0 100 100	8, 22, 56, 111	0
47	DZ	58/58 (100%)	0.30	2 (3%) 45 43	78, 119, 208, 217	0
48	B0	56/56 (100%)	-0.61	0 100 100	3, 24, 70, 159	0
48	D0	56/56 (100%)	1.28	18 (32%) 0 0	63, 139, 242, 298	0
49	B1	50/50 (100%)	0.29	2 (4%) 38 36	22, 48, 99, 165	0
49	D1	50/50 (100%)	1.99	19 (38%) 0 0	99, 170, 210, 236	0
50	B2	46/46 (100%)	-0.54	1 (2%) 62 59	7, 26, 52, 155	0
50	D2	46/46 (100%)	0.94	6 (13%) 3 3	81, 118, 175, 233	0
51	B3	64/64 (100%)	-0.58	0 100 100	5, 23, 44, 70	0
51	D3	64/64 (100%)	1.61	22 (34%) 0 0	65, 128, 183, 257	0
52	B4	38/38 (100%)	0.03	1 (2%) 56 52	21, 45, 86, 124	0
52	D4	38/38 (100%)	2.45	22 (57%) 0 0	79, 137, 187, 227	0
53	CA	1530/1530 (100%)	-0.05	50 (3%) 46 44	34, 102, 281, 444	0
54	CG	150/150 (100%)	2.27	76 (50%) 0 0	107, 224, 298, 322	0
55	CM	113/113 (100%)	3.02	76 (67%) 0 0	182, 402, 494, 538	0
56	CP	80/80 (100%)	0.90	11 (13%) 2 2	51, 94, 155, 236	0
57	DB	117/117 (100%)	-0.05	1 (0%) 84 84	95, 169, 224, 274	0
58	DF	178/178 (100%)	2.03	84 (47%) 0 0	183, 225, 286, 338	0
All	All	20431/20551 (99%)	0.34	2108 (10%) 6 6	2, 94, 269, 557	0

The worst 5 of 2108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DH	92	GLY	29.7
29	DH	124	THR	23.0
29	DH	91	PHE	21.8
29	DH	105	ALA	21.1
30	BI	67	THR	15.3

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

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

6.3 Carbohydrates i

There are no monosaccharides in this entry.

6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3129	1/1	-0.39	1.35	233,233,233,233	0
59	MG	DA	3124	1/1	-0.02	0.59	176,176,176,176	0
59	MG	DJ	201	1/1	0.01	2.07	230,230,230,230	0
59	MG	DA	3003	1/1	0.03	0.97	236,236,236,236	0
59	MG	DA	3013	1/1	0.26	0.24	126,126,126,126	0
59	MG	DA	3044	1/1	0.28	0.28	156,156,156,156	0
59	MG	DA	3017	1/1	0.28	0.18	204,204,204,204	0
59	MG	DA	3010	1/1	0.29	0.61	218,218,218,218	0
59	MG	DA	3025	1/1	0.34	1.37	278,278,278,278	0
59	MG	DA	3081	1/1	0.40	0.18	142,142,142,142	0
59	MG	DA	3019	1/1	0.40	2.04	247,247,247,247	0
59	MG	DA	3131	1/1	0.46	0.35	212,212,212,212	0
59	MG	DA	3001	1/1	0.49	0.19	151,151,151,151	0
59	MG	DA	3002	1/1	0.50	0.32	180,180,180,180	0
59	MG	DA	3005	1/1	0.51	1.11	309,309,309,309	0
59	MG	DA	3110	1/1	0.51	0.27	153,153,153,153	0
59	MG	DA	3061	1/1	0.52	1.00	229,229,229,229	0
59	MG	DA	3082	1/1	0.53	0.08	197,197,197,197	0
59	MG	DA	3098	1/1	0.54	0.16	172,172,172,172	0
59	MG	DA	3073	1/1	0.58	2.10	274,274,274,274	0
59	MG	DA	3007	1/1	0.59	0.65	254,254,254,254	0
59	MG	DA	3090	1/1	0.60	0.36	165,165,165,165	0
59	MG	CA	1602	1/1	0.64	0.15	175,175,175,175	0
59	MG	AA	1629	1/1	0.64	0.20	180,180,180,180	0
59	MG	DA	3016	1/1	0.64	0.15	87,87,87,87	0
59	MG	DA	3085	1/1	0.65	0.12	87,87,87,87	0
59	MG	DA	3108	1/1	0.66	0.54	185,185,185,185	0
59	MG	CA	1619	1/1	0.66	0.38	214,214,214,214	0
59	MG	DA	3030	1/1	0.66	0.13	68,68,68,68	0
59	MG	DA	3122	1/1	0.67	0.37	153,153,153,153	0
59	MG	DA	3046	1/1	0.68	0.17	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3119	1/1	0.69	0.19	93,93,93,93	0
59	MG	CA	1615	1/1	0.69	0.15	172,172,172,172	0
59	MG	CA	1616	1/1	0.69	0.39	254,254,254,254	0
59	MG	CA	1634	1/1	0.70	0.14	131,131,131,131	0
59	MG	CA	1627	1/1	0.70	0.38	181,181,181,181	0
59	MG	DA	3042	1/1	0.70	0.24	161,161,161,161	0
59	MG	DA	3132	1/1	0.70	0.35	174,174,174,174	0
59	MG	DA	3015	1/1	0.70	0.24	183,183,183,183	0
59	MG	DA	3056	1/1	0.71	0.43	197,197,197,197	0
59	MG	CA	1629	1/1	0.71	0.12	197,197,197,197	0
59	MG	DA	3117	1/1	0.71	0.22	71,71,71,71	0
59	MG	CA	1636	1/1	0.71	0.29	181,181,181,181	0
59	MG	CA	1632	1/1	0.71	0.24	156,156,156,156	0
59	MG	DA	3075	1/1	0.72	0.69	174,174,174,174	0
59	MG	CA	1624	1/1	0.72	0.69	165,165,165,165	0
59	MG	DA	3027	1/1	0.72	0.61	253,253,253,253	0
59	MG	DA	3048	1/1	0.72	0.32	218,218,218,218	0
59	MG	DA	3087	1/1	0.73	0.27	179,179,179,179	0
59	MG	BA	3011	1/1	0.73	0.21	102,102,102,102	0
59	MG	DA	3109	1/1	0.73	0.31	174,174,174,174	0
59	MG	CA	1618	1/1	0.74	0.29	113,113,113,113	0
59	MG	DA	3004	1/1	0.74	0.12	114,114,114,114	0
59	MG	CA	1614	1/1	0.74	0.26	210,210,210,210	0
59	MG	DA	3105	1/1	0.74	0.23	262,262,262,262	0
59	MG	DA	3028	1/1	0.74	0.35	143,143,143,143	0
59	MG	DA	3107	1/1	0.76	0.48	161,161,161,161	0
59	MG	DA	3049	1/1	0.76	0.23	172,172,172,172	0
59	MG	DE	301	1/1	0.76	0.47	131,131,131,131	0
59	MG	BA	3117	1/1	0.76	0.27	157,157,157,157	0
59	MG	DA	3029	1/1	0.77	0.19	112,112,112,112	0
59	MG	CA	1637	1/1	0.77	0.22	74,74,74,74	0
59	MG	DA	3038	1/1	0.77	0.14	102,102,102,102	0
59	MG	CA	1623	1/1	0.77	0.16	124,124,124,124	0
59	MG	DA	3114	1/1	0.78	0.30	167,167,167,167	0
59	MG	DA	3059	1/1	0.78	0.82	200,200,200,200	0
59	MG	DA	3006	1/1	0.78	0.11	211,211,211,211	0
59	MG	DA	3072	1/1	0.78	0.07	187,187,187,187	0
59	MG	CA	1628	1/1	0.78	1.37	260,260,260,260	0
59	MG	DA	3018	1/1	0.79	0.17	226,226,226,226	0
59	MG	AA	1627	1/1	0.79	0.18	132,132,132,132	0
59	MG	DA	3062	1/1	0.79	1.49	211,211,211,211	0
59	MG	DA	3077	1/1	0.80	0.54	222,222,222,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	DC	301	1/1	0.80	0.25	145,145,145,145	0
59	MG	DA	3008	1/1	0.81	0.13	148,148,148,148	0
59	MG	DA	3086	1/1	0.81	0.17	139,139,139,139	0
59	MG	BA	3131	1/1	0.81	0.27	154,154,154,154	0
59	MG	DA	3121	1/1	0.81	0.12	84,84,84,84	0
59	MG	CA	1620	1/1	0.81	0.13	168,168,168,168	0
59	MG	DA	3026	1/1	0.81	0.12	109,109,109,109	0
59	MG	DA	3063	1/1	0.82	0.44	278,278,278,278	0
59	MG	DA	3094	1/1	0.82	0.20	107,107,107,107	0
59	MG	DA	3092	1/1	0.83	0.27	229,229,229,229	0
59	MG	DA	3093	1/1	0.83	0.13	114,114,114,114	0
59	MG	BB	201	1/1	0.83	0.32	222,222,222,222	0
59	MG	DA	3097	1/1	0.83	0.22	144,144,144,144	0
59	MG	AA	1610	1/1	0.83	0.09	190,190,190,190	0
59	MG	DA	3128	1/1	0.83	0.72	214,214,214,214	0
59	MG	AN	201	1/1	0.83	0.25	159,159,159,159	0
59	MG	BA	3003	1/1	0.83	0.11	69,69,69,69	0
59	MG	DA	3021	1/1	0.83	0.38	199,199,199,199	0
59	MG	AA	1618	1/1	0.83	0.60	197,197,197,197	0
59	MG	AA	1619	1/1	0.83	0.11	156,156,156,156	0
59	MG	AA	1607	1/1	0.83	0.15	103,103,103,103	0
59	MG	BA	3001	1/1	0.84	0.13	116,116,116,116	0
59	MG	DA	3126	1/1	0.84	0.67	200,200,200,200	0
59	MG	DA	3127	1/1	0.84	0.25	142,142,142,142	0
59	MG	BA	3091	1/1	0.84	0.07	32,32,32,32	0
59	MG	CA	1622	1/1	0.84	0.14	226,226,226,226	0
59	MG	AA	1603	1/1	0.84	0.10	111,111,111,111	0
59	MG	DA	3083	1/1	0.84	0.17	204,204,204,204	0
59	MG	CA	1604	1/1	0.84	0.06	74,74,74,74	0
59	MG	DA	3041	1/1	0.84	0.17	82,82,82,82	0
59	MG	DA	3074	1/1	0.84	0.35	190,190,190,190	0
59	MG	DA	3058	1/1	0.85	0.18	204,204,204,204	0
59	MG	BA	3096	1/1	0.85	0.16	102,102,102,102	0
59	MG	DA	3070	1/1	0.85	0.13	56,56,56,56	0
59	MG	DA	3037	1/1	0.85	0.13	197,197,197,197	0
59	MG	DA	3100	1/1	0.85	0.12	78,78,78,78	0
59	MG	DA	3125	1/1	0.86	0.16	82,82,82,82	0
59	MG	DA	3057	1/1	0.86	0.52	227,227,227,227	0
59	MG	CA	1603	1/1	0.86	0.29	162,162,162,162	0
59	MG	CA	1617	1/1	0.86	0.23	199,199,199,199	0
59	MG	AA	1636	1/1	0.86	0.18	124,124,124,124	0
59	MG	DA	3045	1/1	0.86	0.20	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	1639	1/1	0.86	0.14	165,165,165,165	0
59	MG	CA	1607	1/1	0.86	0.25	121,121,121,121	0
59	MG	DC	302	1/1	0.86	0.27	129,129,129,129	0
59	MG	CA	1601	1/1	0.86	0.17	156,156,156,156	0
59	MG	BA	3085	1/1	0.86	0.22	100,100,100,100	0
59	MG	BA	3090	1/1	0.87	0.18	128,128,128,128	0
59	MG	BA	3074	1/1	0.87	0.24	93,93,93,93	0
59	MG	BA	3068	1/1	0.87	0.13	117,117,117,117	0
59	MG	DA	3071	1/1	0.88	0.11	133,133,133,133	0
59	MG	DA	3091	1/1	0.88	0.20	116,116,116,116	0
59	MG	DA	3106	1/1	0.88	0.20	92,92,92,92	0
59	MG	DA	3040	1/1	0.88	0.14	70,70,70,70	0
59	MG	DA	3034	1/1	0.88	0.26	125,125,125,125	0
59	MG	BA	3069	1/1	0.88	0.33	151,151,151,151	0
59	MG	DA	3064	1/1	0.88	0.14	70,70,70,70	0
59	MG	DA	3014	1/1	0.88	0.31	172,172,172,172	0
59	MG	BA	3026	1/1	0.89	0.27	133,133,133,133	0
59	MG	AA	1614	1/1	0.89	0.25	194,194,194,194	0
59	MG	CA	1633	1/1	0.89	0.13	63,63,63,63	0
59	MG	DA	3047	1/1	0.89	0.18	95,95,95,95	0
59	MG	DA	3022	1/1	0.89	0.12	69,69,69,69	0
59	MG	DA	3111	1/1	0.89	0.15	109,109,109,109	0
59	MG	DA	3096	1/1	0.89	0.16	102,102,102,102	0
59	MG	DA	3115	1/1	0.89	0.16	65,65,65,65	0
59	MG	AA	1612	1/1	0.89	0.20	105,105,105,105	0
59	MG	BA	3110	1/1	0.89	0.25	92,92,92,92	0
59	MG	AA	1628	1/1	0.89	0.11	69,69,69,69	0
59	MG	BA	3024	1/1	0.89	0.58	166,166,166,166	0
59	MG	CA	1625	1/1	0.90	0.22	100,100,100,100	0
59	MG	AA	1631	1/1	0.90	0.12	91,91,91,91	0
59	MG	AA	1635	1/1	0.90	0.18	194,194,194,194	0
59	MG	AA	1617	1/1	0.90	0.17	115,115,115,115	0
59	MG	AA	1639	1/1	0.90	0.08	108,108,108,108	0
59	MG	DA	3032	1/1	0.90	0.18	121,121,121,121	0
59	MG	DA	3011	1/1	0.90	0.17	127,127,127,127	0
59	MG	DA	3035	1/1	0.90	0.41	194,194,194,194	0
59	MG	DA	3099	1/1	0.90	0.14	68,68,68,68	0
59	MG	AA	1622	1/1	0.90	0.06	76,76,76,76	0
59	MG	DA	3101	1/1	0.90	0.10	67,67,67,67	0
59	MG	AA	1626	1/1	0.90	0.30	117,117,117,117	0
59	MG	DA	3068	1/1	0.91	0.39	209,209,209,209	0
59	MG	DA	3050	1/1	0.91	0.14	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3053	1/1	0.91	0.07	67,67,67,67	0
59	MG	BA	3089	1/1	0.91	0.12	80,80,80,80	0
59	MG	AA	1608	1/1	0.91	0.26	68,68,68,68	0
59	MG	BB	202	1/1	0.91	0.09	50,50,50,50	0
59	MG	CA	1610	1/1	0.91	0.14	152,152,152,152	0
59	MG	DA	3130	1/1	0.91	0.15	85,85,85,85	0
59	MG	DA	3095	1/1	0.91	0.09	95,95,95,95	0
59	MG	CA	1612	1/1	0.91	0.35	136,136,136,136	0
59	MG	DB	201	1/1	0.91	0.09	104,104,104,104	0
59	MG	BA	3072	1/1	0.91	0.16	139,139,139,139	0
59	MG	DA	3039	1/1	0.91	0.20	65,65,65,65	0
59	MG	BA	3129	1/1	0.91	1.04	214,214,214,214	0
59	MG	DA	3066	1/1	0.91	0.12	61,61,61,61	0
59	MG	AA	1604	1/1	0.92	0.12	124,124,124,124	0
59	MG	CA	1640	1/1	0.92	0.15	157,157,157,157	0
59	MG	AA	1640	1/1	0.92	0.09	154,154,154,154	0
59	MG	DA	3023	1/1	0.92	0.10	87,87,87,87	0
59	MG	CA	1631	1/1	0.92	0.23	93,93,93,93	0
59	MG	DA	3123	1/1	0.92	0.13	61,61,61,61	0
59	MG	BA	3082	1/1	0.92	0.16	114,114,114,114	0
59	MG	DA	3036	1/1	0.92	0.17	82,82,82,82	0
59	MG	DA	3112	1/1	0.92	0.14	131,131,131,131	0
59	MG	CA	1638	1/1	0.92	0.10	130,130,130,130	0
59	MG	BA	3086	1/1	0.93	0.16	131,131,131,131	0
59	MG	DA	3020	1/1	0.93	0.22	49,49,49,49	0
59	MG	BA	3088	1/1	0.93	0.10	50,50,50,50	0
59	MG	DA	3009	1/1	0.93	0.10	69,69,69,69	0
59	MG	DA	3089	1/1	0.93	0.09	99,99,99,99	0
59	MG	BA	3124	1/1	0.93	0.11	25,25,25,25	0
59	MG	BA	3014	1/1	0.93	0.13	68,68,68,68	0
59	MG	BA	3103	1/1	0.93	0.15	4,4,4,4	0
59	MG	CA	1606	1/1	0.93	0.09	64,64,64,64	0
59	MG	BA	3133	1/1	0.93	0.12	139,139,139,139	0
59	MG	DA	3076	1/1	0.93	0.17	93,93,93,93	0
59	MG	CA	1609	1/1	0.93	0.11	83,83,83,83	0
59	MG	DA	3079	1/1	0.93	0.12	142,142,142,142	0
59	MG	DA	3118	1/1	0.93	0.12	76,76,76,76	0
59	MG	BA	3105	1/1	0.93	0.15	42,42,42,42	0
59	MG	CA	1611	1/1	0.93	0.22	112,112,112,112	0
61	ZN	D4	101	1/1	0.93	0.07	161,161,161,161	0
59	MG	CA	1621	1/1	0.94	0.22	46,46,46,46	0
59	MG	BA	3046	1/1	0.94	0.07	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	BA	3056	1/1	0.94	0.16	169,169,169,169	0
59	MG	DA	3060	1/1	0.94	0.11	105,105,105,105	0
59	MG	DA	3080	1/1	0.94	0.20	108,108,108,108	0
59	MG	BA	3111	1/1	0.94	0.21	77,77,77,77	0
59	MG	DA	3043	1/1	0.94	0.19	100,100,100,100	0
59	MG	AA	1642	1/1	0.94	0.10	37,37,37,37	0
59	MG	DA	3084	1/1	0.94	0.40	144,144,144,144	0
59	MG	DA	3031	1/1	0.94	0.17	105,105,105,105	0
59	MG	AA	1630	1/1	0.94	0.16	189,189,189,189	0
59	MG	DA	3067	1/1	0.94	0.10	83,83,83,83	0
59	MG	DA	3088	1/1	0.94	0.20	87,87,87,87	0
59	MG	DA	3033	1/1	0.94	0.10	95,95,95,95	0
59	MG	BA	3070	1/1	0.94	0.13	53,53,53,53	0
59	MG	AA	1615	1/1	0.94	0.06	120,120,120,120	0
59	MG	AA	1625	1/1	0.94	0.23	30,30,30,30	0
59	MG	DA	3024	1/1	0.94	0.14	89,89,89,89	0
59	MG	BA	3033	1/1	0.94	0.32	162,162,162,162	0
59	MG	DA	3120	1/1	0.95	0.19	109,109,109,109	0
59	MG	AA	1609	1/1	0.95	0.13	46,46,46,46	0
59	MG	BA	3058	1/1	0.95	0.18	107,107,107,107	0
59	MG	BA	3060	1/1	0.95	0.31	210,210,210,210	0
59	MG	DA	3065	1/1	0.95	0.09	49,49,49,49	0
59	MG	DA	3103	1/1	0.95	0.20	44,44,44,44	0
59	MG	AA	1602	1/1	0.95	0.10	152,152,152,152	0
59	MG	AA	1620	1/1	0.95	0.08	117,117,117,117	0
59	MG	BA	3007	1/1	0.95	0.10	80,80,80,80	0
59	MG	DA	3052	1/1	0.95	0.18	89,89,89,89	0
59	MG	BA	3093	1/1	0.95	0.09	36,36,36,36	0
59	MG	DA	3054	1/1	0.95	0.10	96,96,96,96	0
59	MG	DA	3055	1/1	0.95	0.12	120,120,120,120	0
59	MG	BA	3134	1/1	0.95	0.20	219,219,219,219	0
59	MG	CA	1642	1/1	0.95	0.07	82,82,82,82	0
59	MG	AA	1606	1/1	0.95	0.11	62,62,62,62	0
59	MG	BA	3102	1/1	0.95	0.17	3,3,3,3	0
59	MG	BA	3049	1/1	0.95	0.13	66,66,66,66	0
59	MG	BA	3054	1/1	0.95	0.33	189,189,189,189	0
59	MG	AA	1613	1/1	0.96	0.07	56,56,56,56	0
59	MG	DA	3078	1/1	0.96	0.34	180,180,180,180	0
59	MG	BA	3106	1/1	0.96	0.12	13,13,13,13	0
59	MG	BA	3108	1/1	0.96	0.09	48,48,48,48	0
59	MG	DA	3051	1/1	0.96	0.11	57,57,57,57	0
59	MG	DA	3113	1/1	0.96	0.07	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3027	1/1	0.96	0.18	46,46,46,46	0
59	MG	BA	3030	1/1	0.96	0.09	21,21,21,21	0
59	MG	CA	1641	1/1	0.96	0.22	79,79,79,79	0
59	MG	BA	3116	1/1	0.96	0.10	76,76,76,76	0
59	MG	BA	3010	1/1	0.96	0.08	29,29,29,29	0
59	MG	BA	3123	1/1	0.96	0.15	11,11,11,11	0
59	MG	BA	3077	1/1	0.96	0.10	30,30,30,30	0
59	MG	BA	3078	1/1	0.96	0.13	20,20,20,20	0
59	MG	BA	3035	1/1	0.96	0.53	171,171,171,171	0
59	MG	BA	3132	1/1	0.96	0.15	1,1,1,1	0
59	MG	BA	3039	1/1	0.96	0.22	6,6,6,6	0
59	MG	AA	1616	1/1	0.96	0.14	98,98,98,98	0
59	MG	BA	3012	1/1	0.96	0.10	1,1,1,1	0
59	MG	BA	3050	1/1	0.96	0.11	10,10,10,10	0
59	MG	BL	201	1/1	0.96	0.13	53,53,53,53	0
59	MG	DA	3012	1/1	0.96	0.15	64,64,64,64	0
59	MG	BA	3002	1/1	0.96	0.15	85,85,85,85	0
59	MG	BA	3055	1/1	0.96	0.23	205,205,205,205	0
59	MG	CA	1630	1/1	0.96	0.06	131,131,131,131	0
59	MG	BA	3015	1/1	0.96	0.06	55,55,55,55	0
59	MG	BA	3016	1/1	0.96	0.07	2,2,2,2	0
59	MG	BA	3022	1/1	0.96	0.07	8,8,8,8	0
59	MG	AA	1638	1/1	0.96	0.10	116,116,116,116	0
59	MG	CA	1635	1/1	0.96	0.13	95,95,95,95	0
59	MG	AA	1634	1/1	0.97	0.06	72,72,72,72	0
59	MG	BA	3008	1/1	0.97	0.13	7,7,7,7	0
59	MG	CA	1626	1/1	0.97	0.22	23,23,23,23	0
59	MG	BA	3009	1/1	0.97	0.13	6,6,6,6	0
59	MG	AA	1624	1/1	0.97	0.11	82,82,82,82	0
59	MG	AA	1605	1/1	0.97	0.14	39,39,39,39	0
59	MG	BA	3066	1/1	0.97	0.12	10,10,10,10	0
59	MG	BA	3097	1/1	0.97	0.15	45,45,45,45	0
59	MG	BA	3099	1/1	0.97	0.16	1,1,1,1	0
59	MG	AA	1637	1/1	0.97	0.14	27,27,27,27	0
59	MG	BA	3034	1/1	0.97	0.10	5,5,5,5	0
59	MG	BA	3104	1/1	0.97	0.13	3,3,3,3	0
59	MG	AA	1611	1/1	0.97	0.07	62,62,62,62	0
59	MG	BA	3036	1/1	0.97	0.14	4,4,4,4	0
59	MG	CA	1608	1/1	0.97	0.22	41,41,41,41	0
59	MG	BA	3107	1/1	0.97	0.18	5,5,5,5	0
59	MG	BA	3037	1/1	0.97	0.11	5,5,5,5	0
59	MG	BA	3076	1/1	0.97	0.11	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	AA	1623	1/1	0.97	0.06	102,102,102,102	0
59	MG	CA	1613	1/1	0.97	0.10	105,105,105,105	0
59	MG	BA	3004	1/1	0.97	0.12	138,138,138,138	0
59	MG	BA	3047	1/1	0.97	0.18	111,111,111,111	0
59	MG	BA	3118	1/1	0.97	0.16	11,11,11,11	0
59	MG	BA	3119	1/1	0.97	0.07	51,51,51,51	0
59	MG	BA	3121	1/1	0.97	0.13	15,15,15,15	0
59	MG	BA	3084	1/1	0.97	0.12	13,13,13,13	0
59	MG	BA	3020	1/1	0.97	0.11	22,22,22,22	0
59	MG	DA	3069	1/1	0.97	0.14	69,69,69,69	0
59	MG	BA	3126	1/1	0.97	0.10	9,9,9,9	0
59	MG	DA	3102	1/1	0.97	0.18	86,86,86,86	0
59	MG	BA	3021	1/1	0.97	0.14	7,7,7,7	0
59	MG	BA	3130	1/1	0.97	0.26	97,97,97,97	0
59	MG	BA	3062	1/1	0.98	0.12	11,11,11,11	0
59	MG	BA	3065	1/1	0.98	0.11	17,17,17,17	0
59	MG	BA	3013	1/1	0.98	0.13	1,1,1,1	0
59	MG	BA	3023	1/1	0.98	0.10	5,5,5,5	0
59	MG	AA	1632	1/1	0.98	0.11	76,76,76,76	0
59	MG	BA	3042	1/1	0.98	0.06	41,41,41,41	0
59	MG	BA	3071	1/1	0.98	0.10	7,7,7,7	0
59	MG	BA	3044	1/1	0.98	0.13	12,12,12,12	0
59	MG	BA	3112	1/1	0.98	0.10	47,47,47,47	0
59	MG	DA	3104	1/1	0.98	0.15	47,47,47,47	0
59	MG	BA	3113	1/1	0.98	0.08	114,114,114,114	0
59	MG	BA	3114	1/1	0.98	0.15	4,4,4,4	0
59	MG	BA	3073	1/1	0.98	0.18	8,8,8,8	0
59	MG	BA	3045	1/1	0.98	0.12	17,17,17,17	0
59	MG	BA	3075	1/1	0.98	0.07	29,29,29,29	0
59	MG	BA	3025	1/1	0.98	0.12	26,26,26,26	0
59	MG	AA	1633	1/1	0.98	0.10	51,51,51,51	0
59	MG	BA	3122	1/1	0.98	0.16	137,137,137,137	0
59	MG	BA	3048	1/1	0.98	0.10	6,6,6,6	0
59	MG	BA	3080	1/1	0.98	0.06	34,34,34,34	0
59	MG	BA	3081	1/1	0.98	0.19	86,86,86,86	0
59	MG	DA	3116	1/1	0.98	0.23	77,77,77,77	0
59	MG	BA	3127	1/1	0.98	0.09	3,3,3,3	0
59	MG	AA	1601	1/1	0.98	0.11	70,70,70,70	0
59	MG	BA	3028	1/1	0.98	0.10	77,77,77,77	0
59	MG	BA	3051	1/1	0.98	0.12	58,58,58,58	0
59	MG	BA	3052	1/1	0.98	0.07	5,5,5,5	0
59	MG	BA	3087	1/1	0.98	0.11	35,35,35,35	0

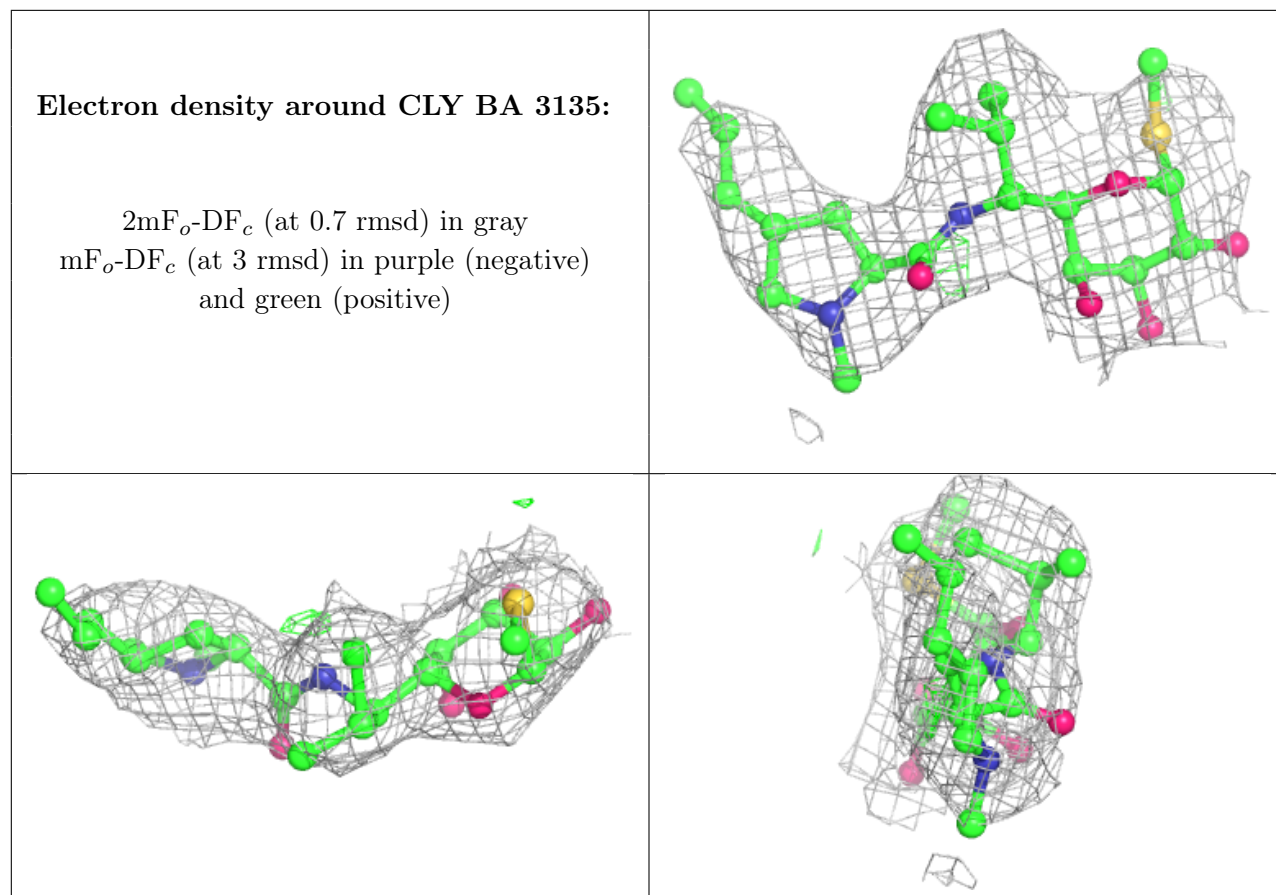
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3053	1/1	0.98	0.09	31,31,31,31	0
59	MG	BA	3029	1/1	0.98	0.18	3,3,3,3	0
59	MG	BA	3018	1/1	0.98	0.29	6,6,6,6	0
59	MG	BB	203	1/1	0.98	0.06	17,17,17,17	0
59	MG	BB	204	1/1	0.98	0.12	41,41,41,41	0
59	MG	BA	3019	1/1	0.98	0.07	15,15,15,15	0
59	MG	BA	3057	1/1	0.98	0.06	48,48,48,48	0
59	MG	BA	3094	1/1	0.98	0.08	9,9,9,9	0
59	MG	BA	3006	1/1	0.98	0.06	39,39,39,39	0
59	MG	BA	3059	1/1	0.98	0.12	190,190,190,190	0
59	MG	CA	1605	1/1	0.98	0.16	37,37,37,37	0
59	MG	BA	3098	1/1	0.98	0.07	15,15,15,15	0
59	MG	AA	1621	1/1	0.98	0.13	25,25,25,25	0
59	MG	BA	3100	1/1	0.98	0.27	89,89,89,89	0
59	MG	BA	3101	1/1	0.98	0.06	11,11,11,11	0
60	CLY	BA	3135	27/27	0.98	0.20	11,17,22,22	0
59	MG	BA	3061	1/1	0.98	0.16	20,20,20,20	0
59	MG	BA	3063	1/1	0.99	0.12	1,1,1,1	0
59	MG	BA	3031	1/1	0.99	0.13	12,12,12,12	0
59	MG	BA	3032	1/1	0.99	0.21	3,3,3,3	0
59	MG	BA	3067	1/1	0.99	0.06	18,18,18,18	0
59	MG	BA	3125	1/1	0.99	0.13	27,27,27,27	0
59	MG	BA	3092	1/1	0.99	0.10	56,56,56,56	0
59	MG	BA	3079	1/1	0.99	0.13	13,13,13,13	0
59	MG	BA	3128	1/1	0.99	0.12	19,19,19,19	0
59	MG	BA	3109	1/1	0.99	0.17	124,124,124,124	0
59	MG	BA	3038	1/1	0.99	0.16	31,31,31,31	0
59	MG	BA	3095	1/1	0.99	0.09	77,77,77,77	0
59	MG	AA	1641	1/1	0.99	0.18	22,22,22,22	0
59	MG	BA	3040	1/1	0.99	0.15	11,11,11,11	0
59	MG	BA	3083	1/1	0.99	0.09	28,28,28,28	0
59	MG	BA	3115	1/1	0.99	0.10	11,11,11,11	0
59	MG	BA	3041	1/1	0.99	0.13	13,13,13,13	0
59	MG	BA	3017	1/1	0.99	0.10	24,24,24,24	0
59	MG	BA	3043	1/1	0.99	0.18	11,11,11,11	0
59	MG	BA	3005	1/1	0.99	0.09	87,87,87,87	0
61	ZN	B4	101	1/1	0.99	0.06	80,80,80,80	0
59	MG	BA	3120	1/1	0.99	0.17	4,4,4,4	0
59	MG	BA	3064	1/1	1.00	0.08	18,18,18,18	0

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

orientation to approximate a three-dimensional view.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.