



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:52 AM UTC

PDB ID : 4V7V / pdb_00004v7v
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

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

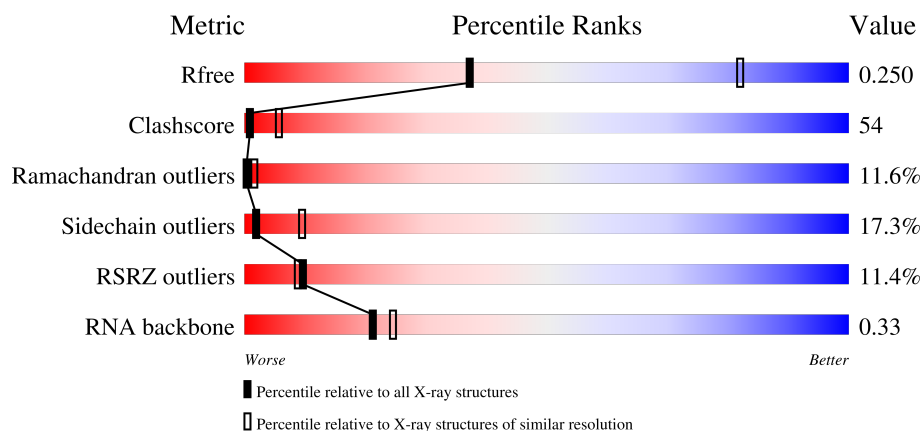
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)
RNA backbone	3983	1020 (3.58-2.98)

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% 19% 49% 22% 10%
2	AB	218	4% 21% 55% 22% .
2	CB	218	11% 23% 61% 14% .
3	AC	206	4% 32% 50% 15% .

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

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

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

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

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

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

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 284501 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

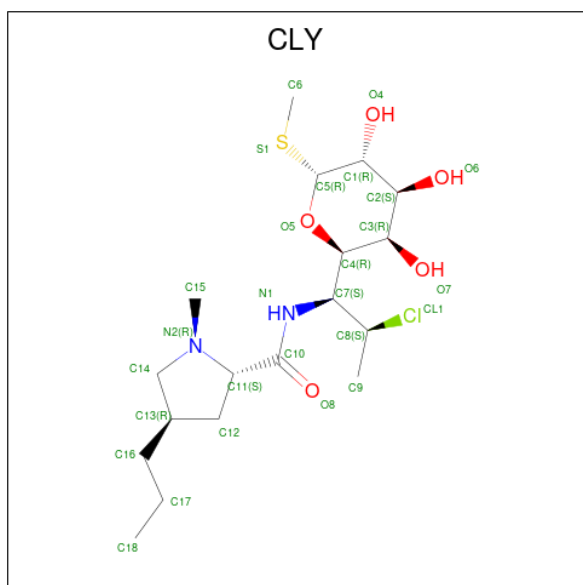
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	42	Total	Mg	0	0
			42	42		
59	AN	1	Total	Mg	0	0
			1	1		
59	BA	134	Total	Mg	0	0
			134	134		
59	BB	4	Total	Mg	0	0
			4	4		
59	BL	1	Total	Mg	0	0
			1	1		
59	CA	42	Total	Mg	0	0
			42	42		
59	DA	132	Total	Mg	0	0
			132	132		
59	DB	1	Total	Mg	0	0
			1	1		
59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

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

- Molecule 60 is CLINDAMYCIN (CCD ID: CLY) (formula: $C_{18}H_{33}ClN_2O_5S$).



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

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 62 is water.

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

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

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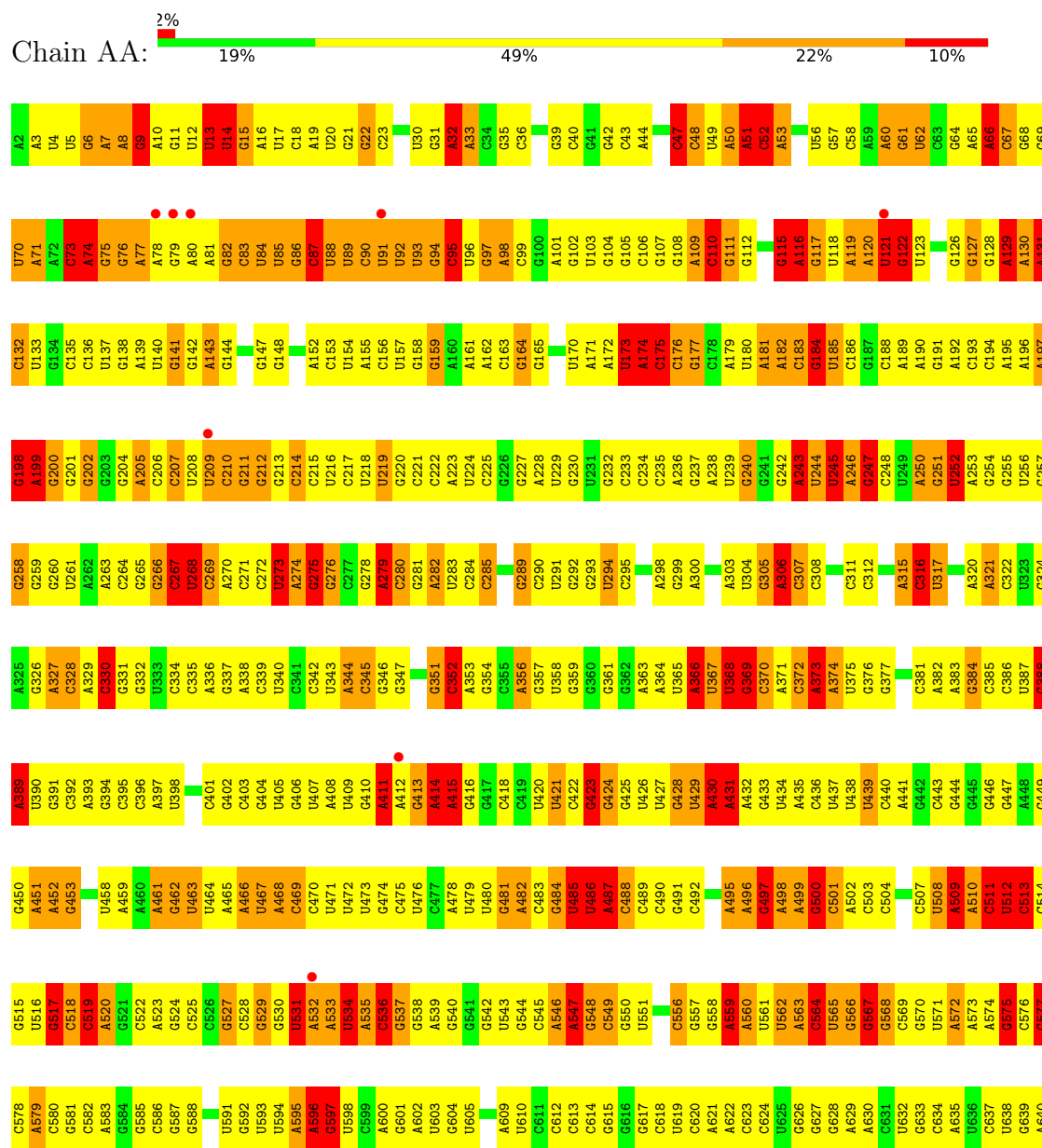
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CN	3	Total 3	O 3	0	0
62	CT	3	Total 3	O 3	0	0
62	CU	2	Total 2	O 2	0	0
62	DA	599	Total 599	O 599	0	0
62	DB	4	Total 4	O 4	0	0
62	DC	9	Total 9	O 9	0	0
62	DD	2	Total 2	O 2	0	0
62	DE	3	Total 3	O 3	0	0
62	DJ	5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

3 Residue-property plots

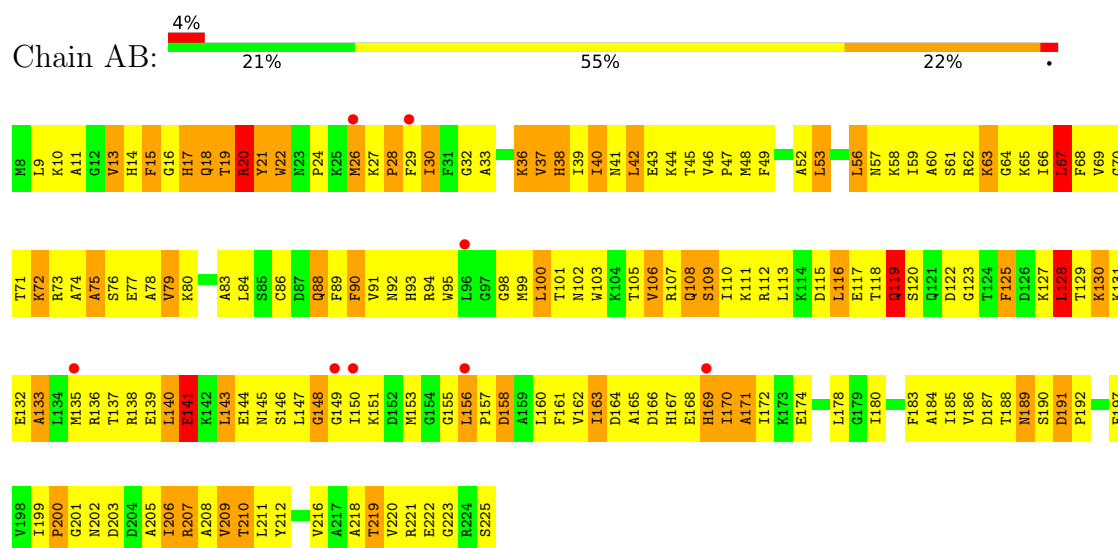
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

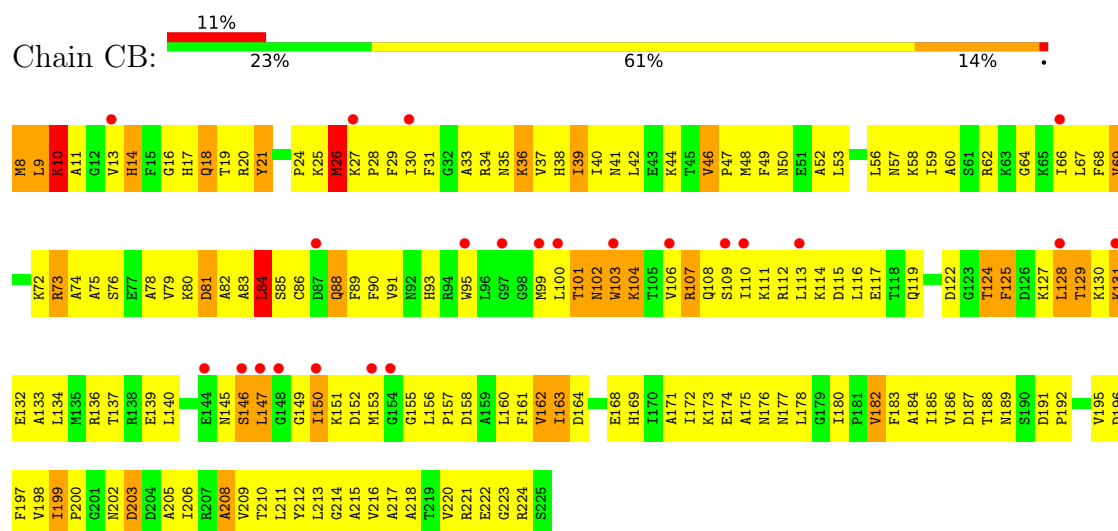




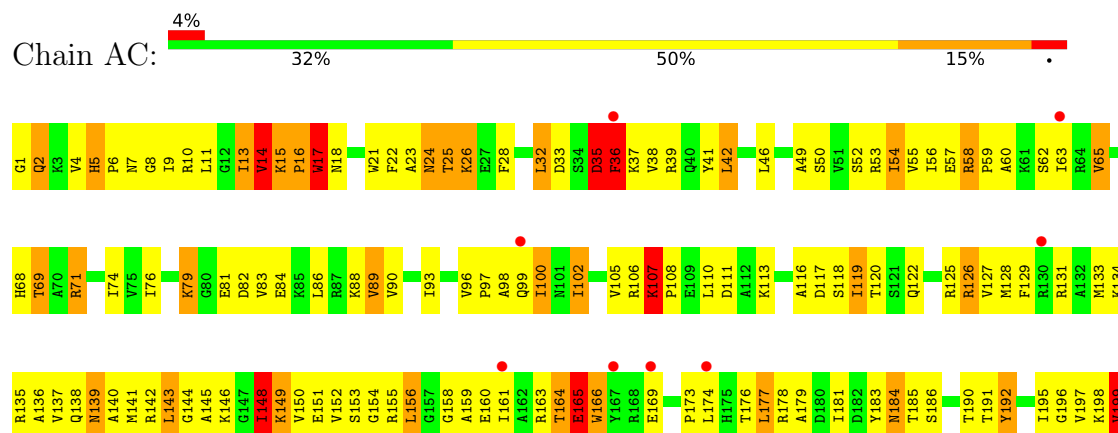
- Molecule 2: 30S ribosomal protein S2



- Molecule 2: 30S ribosomal protein S2

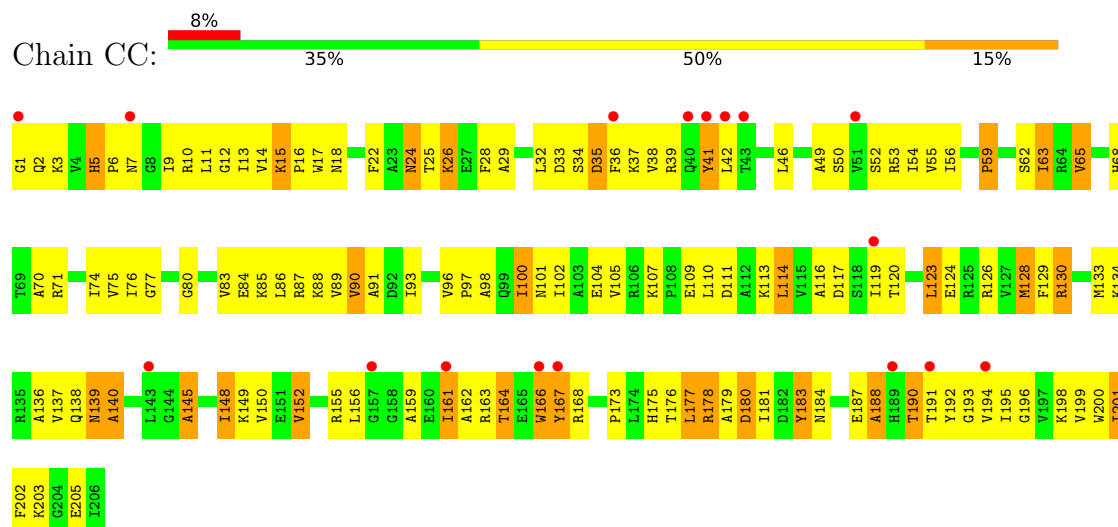


- Molecule 3: 30S ribosomal protein S3

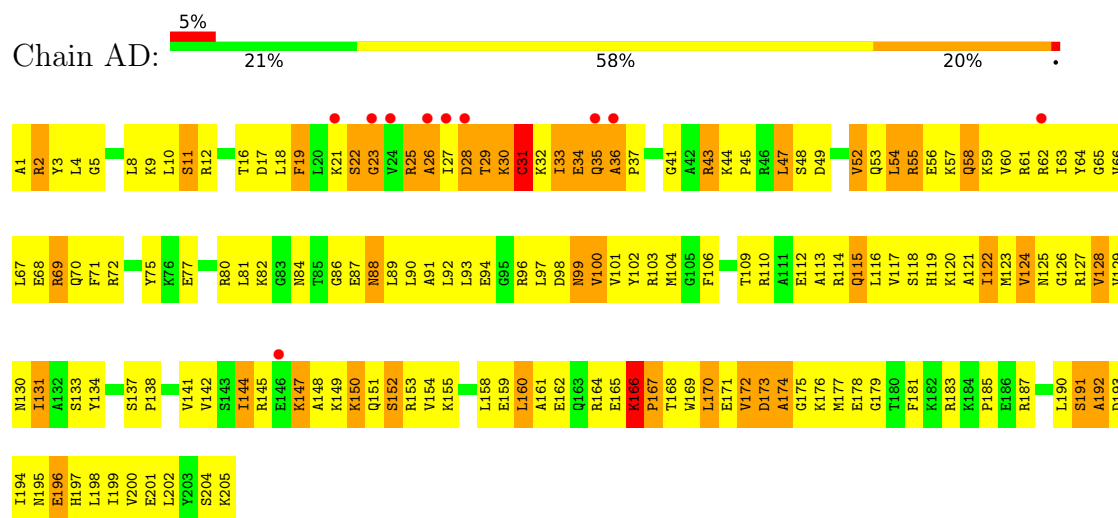




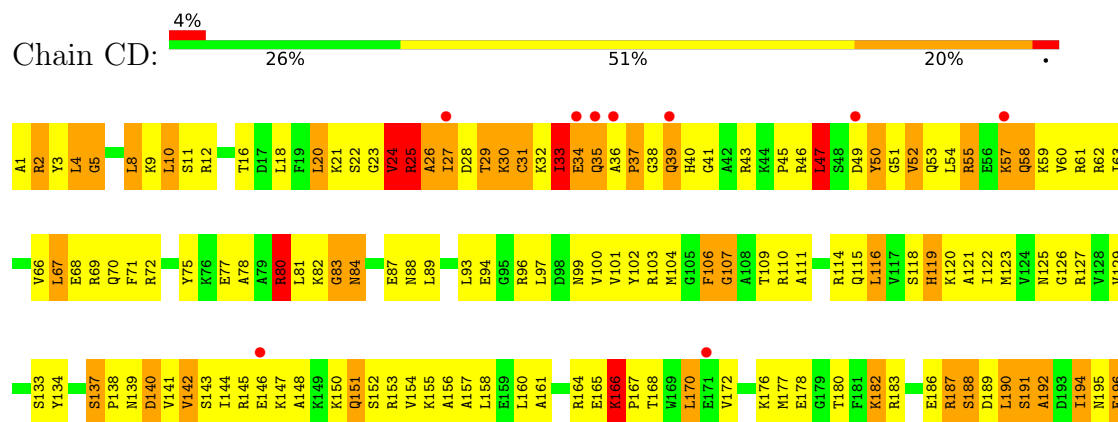
• Molecule 3: 30S ribosomal protein S3

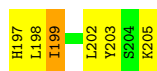


• Molecule 4: 30S ribosomal protein S4

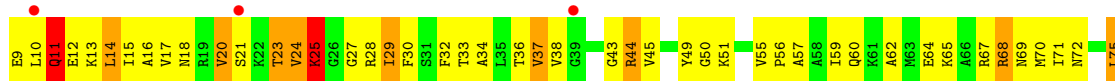


• Molecule 4: 30S ribosomal protein S4

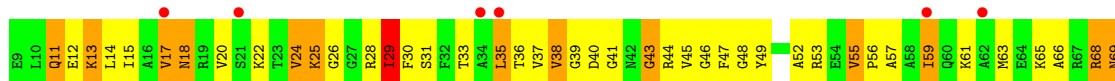




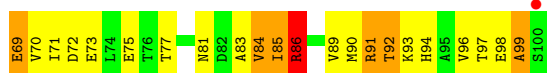
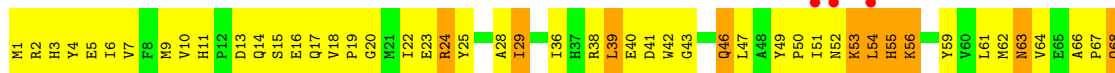
• Molecule 5: 30S ribosomal protein S5



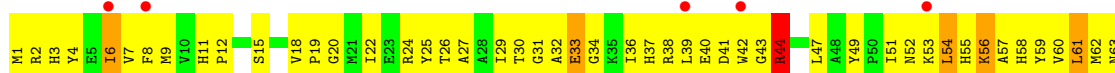
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

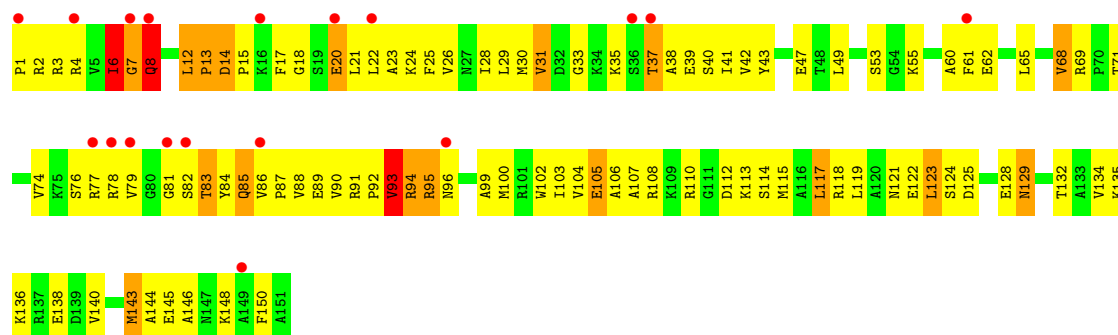


• Molecule 6: 30S ribosomal protein S6

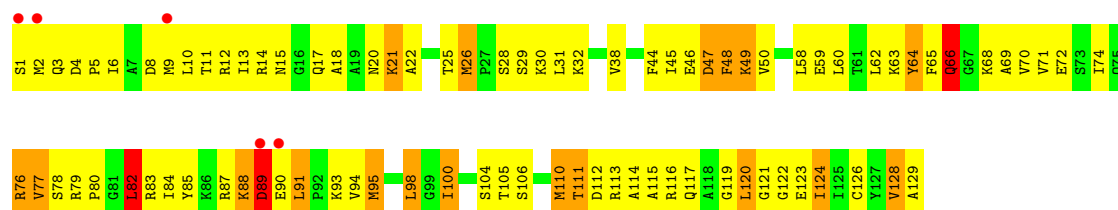




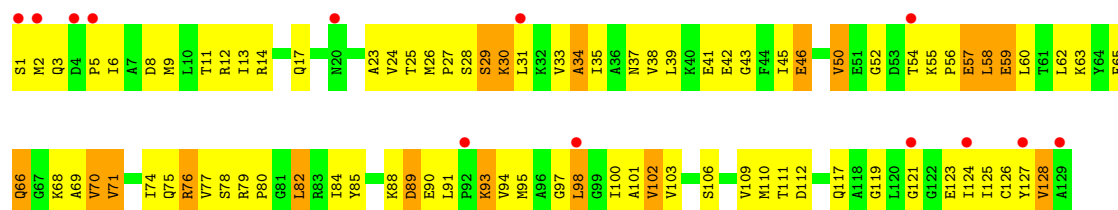
• Molecule 7: 30S ribosomal protein S7



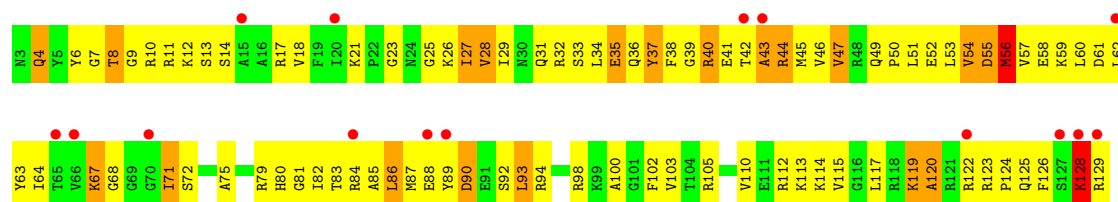
• Molecule 8: 30S ribosomal protein S8



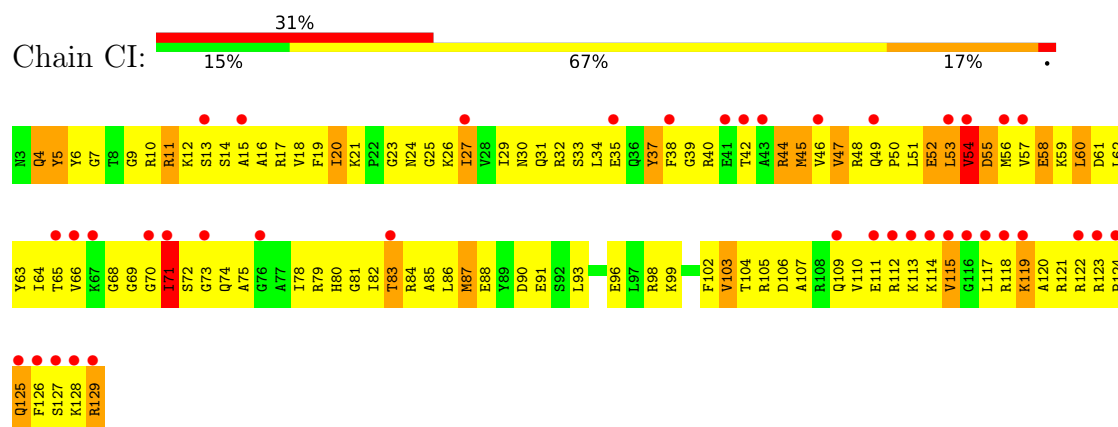
• Molecule 8: 30S ribosomal protein S8



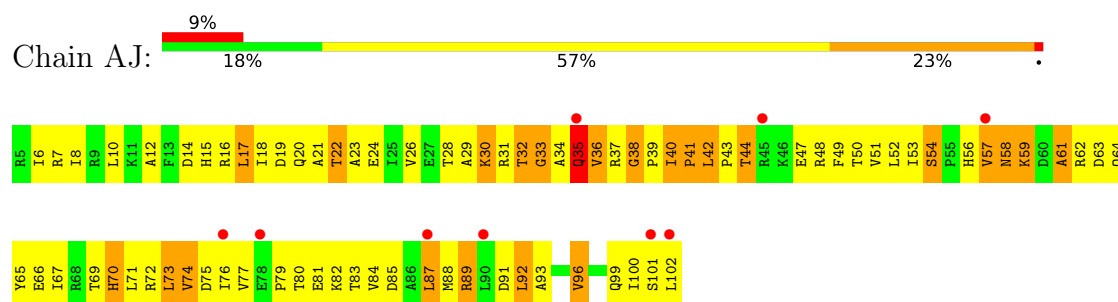
• Molecule 9: 30S ribosomal protein S9



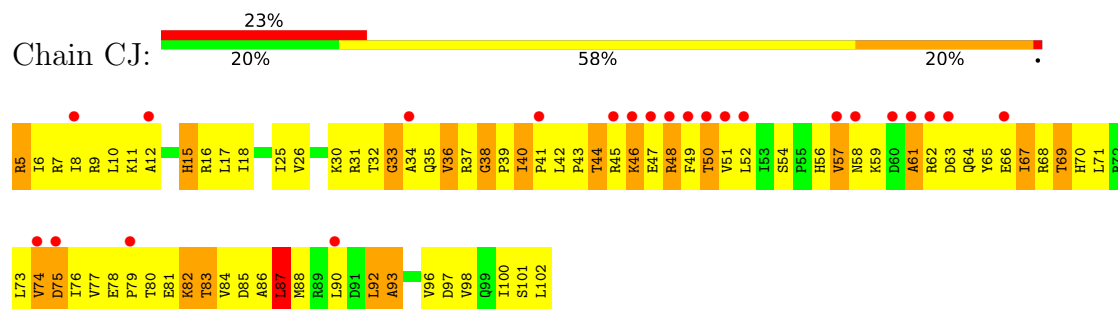
- Molecule 9: 30S ribosomal protein S9



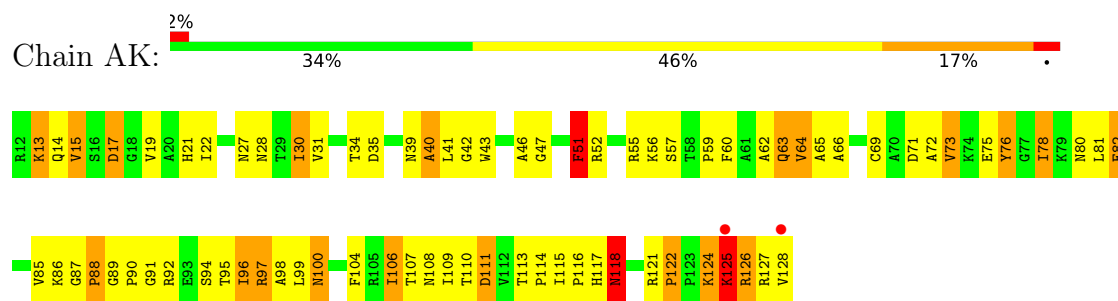
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

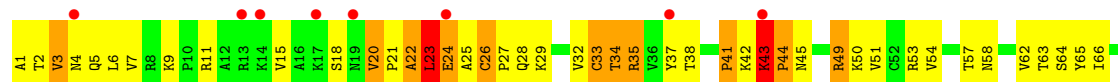


- Molecule 11: 30S ribosomal protein S11

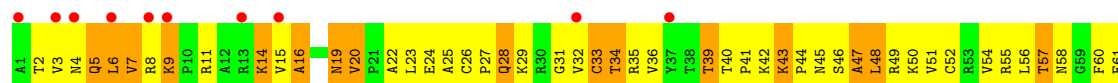




• Molecule 12: 30S ribosomal protein S12



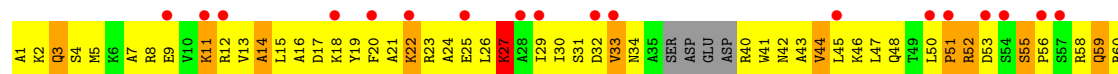
• Molecule 12: 30S ribosomal protein S12



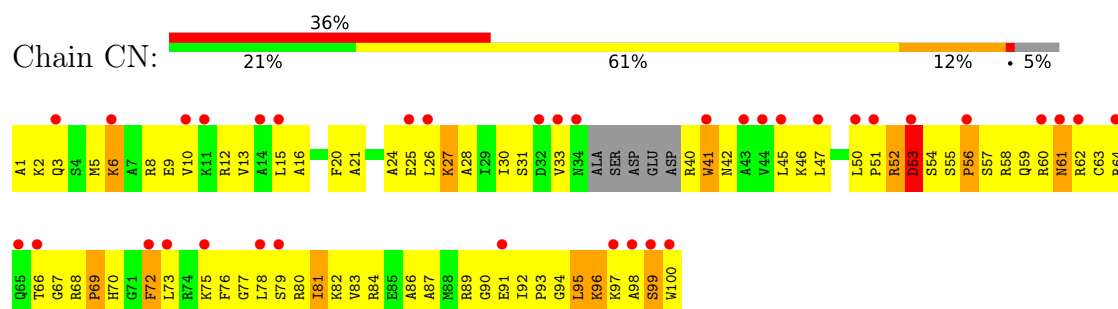
• Molecule 13: 30S ribosomal protein S13



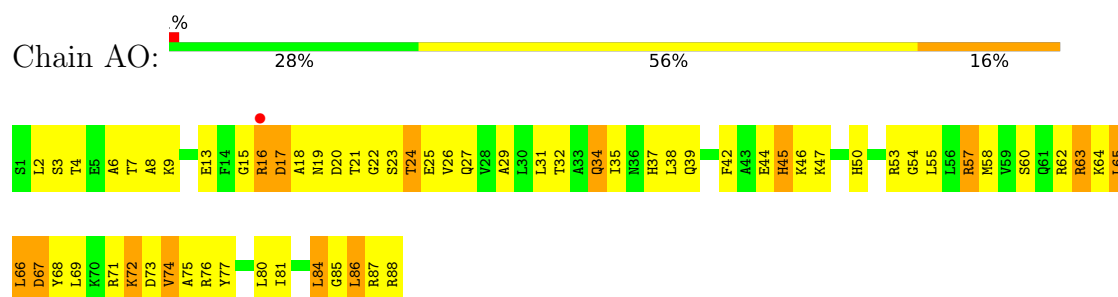
• Molecule 14: 30S ribosomal protein S14



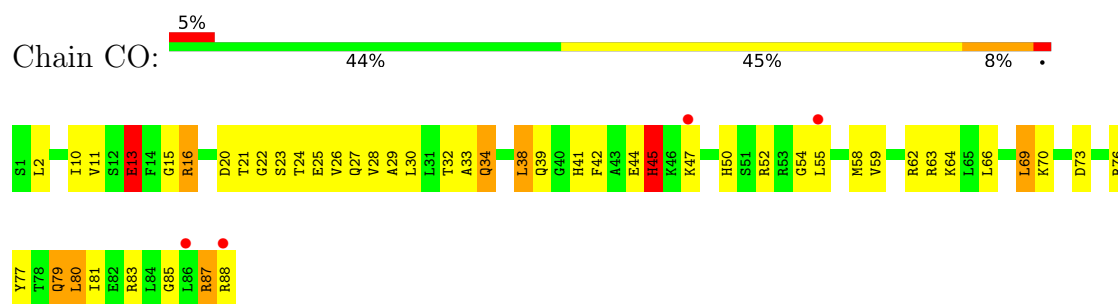
• Molecule 14: 30S ribosomal protein S14



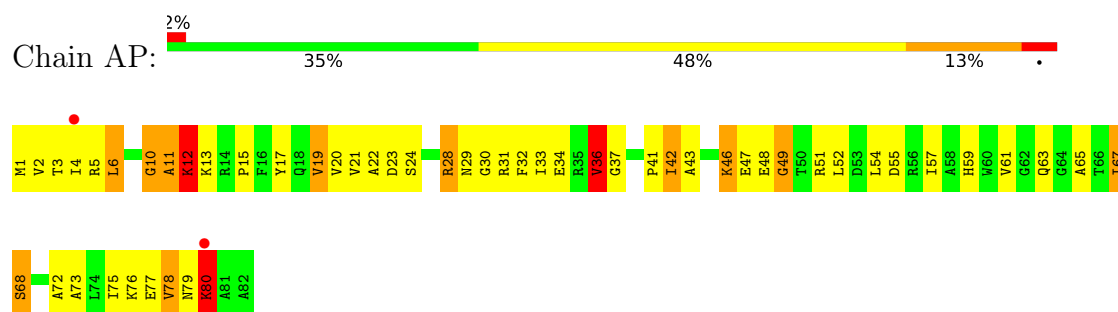
• Molecule 15: 30S ribosomal protein S15



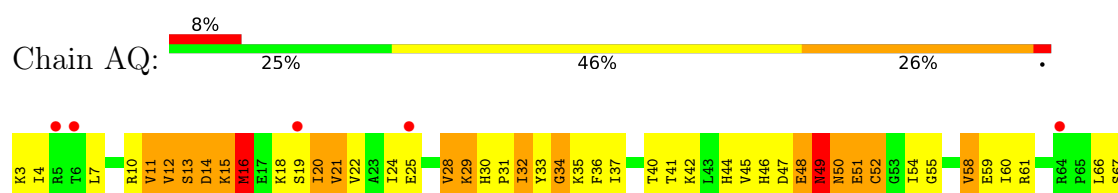
• Molecule 15: 30S ribosomal protein S15

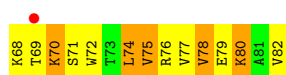


• Molecule 16: 30S ribosomal protein S16

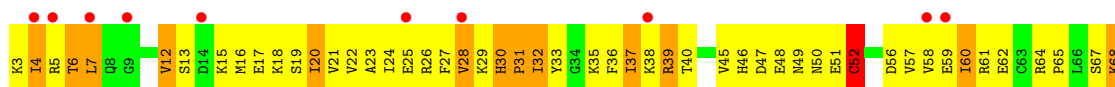


• Molecule 17: 30S ribosomal protein S17





- Molecule 17: 30S ribosomal protein S17



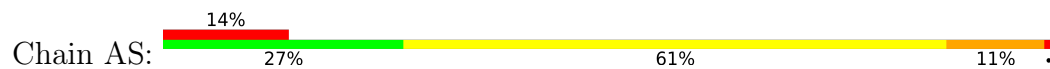
- Molecule 18: 30S ribosomal protein S18



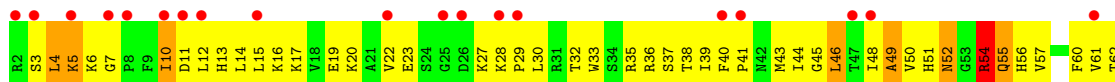
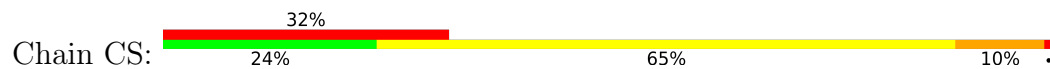
- Molecule 18: 30S ribosomal protein S18



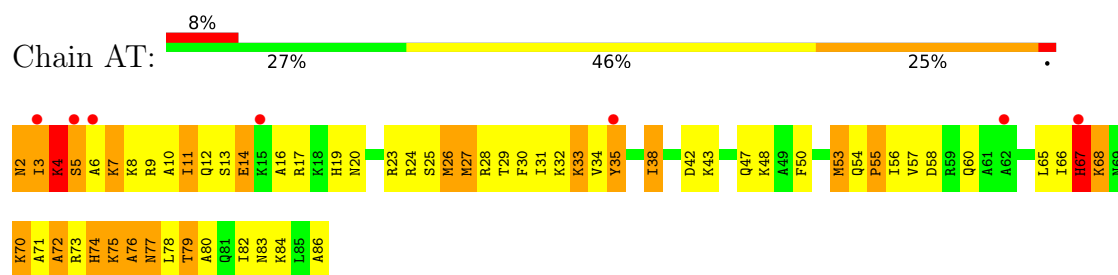
- Molecule 19: 30S ribosomal protein S19



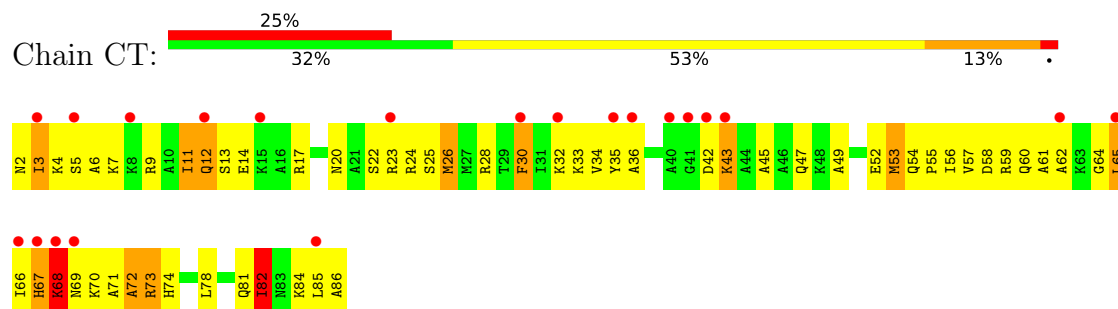
- Molecule 19: 30S ribosomal protein S19



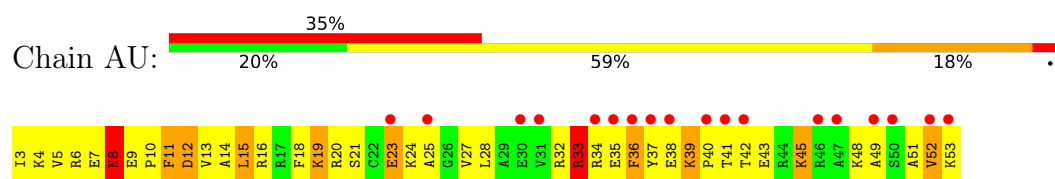
- Molecule 20: 30S ribosomal protein S20



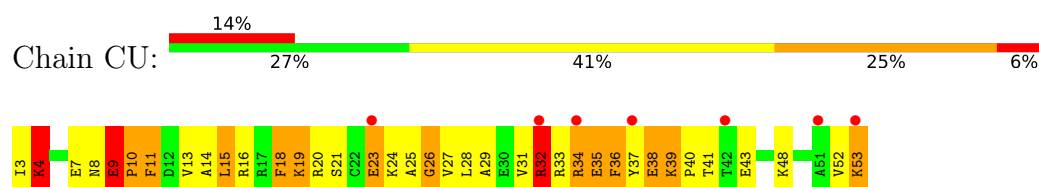
- Molecule 20: 30S ribosomal protein S20



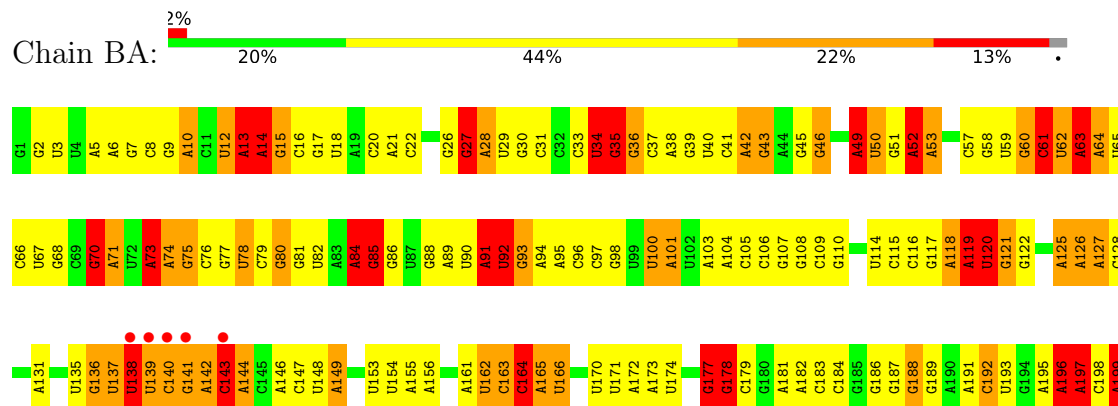
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

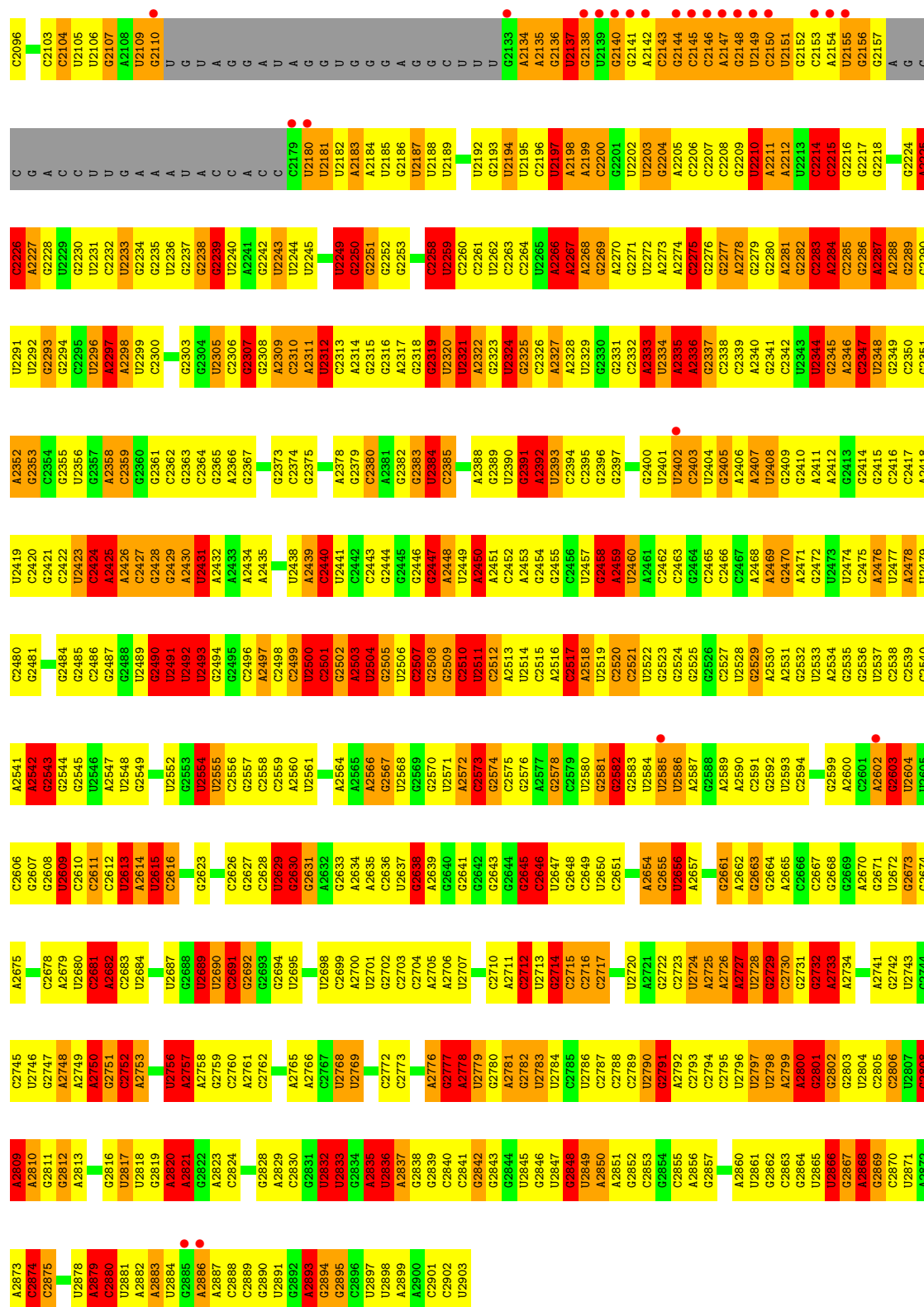


- Molecule 22: 23S rRNA

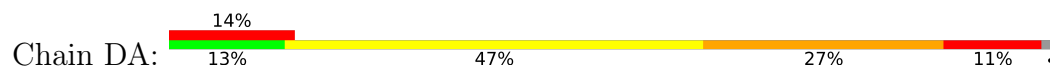




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A2031	C1962	A1889	U1827	C1764	G1699	A1635	G1568	A1496	A1431	G1369	G1303	A1241	U1174
G2032	U1963	C1765	A1828	U1765	A1700	U1636	A1569	U1497	A1432	G1370	G1304	U1242	A1176
A2033	G1964	G1766	G1829	U1766	A1701	U1637	A1570	U1498	A1433	G1371	C1305	U1243	A1175
U2034	C1965	G1767	G1830	G1767	G1702	C1638	A1571	G1500	A1434	U1372	C1306	G1245	G1177
G2035	A1900	G1768	G1831	G1768	G1703	C1639	G1572	G1501	G1435	A1373	G1309	A1246	C1178
C2036	A1901	U1769	C1832	U1769	C1706	G1641	U1576	G1502	G1436	G1374	G1310	A1247	G1179
A2037	C1902	G1770	G1833	G1770	G1707	G1642	C1437	A1503	C1438	U1375	G1311	A1248	U1180
G2038	G1903	A1773	G1834	U1773	G1708	G1643	C1438	A1504	G1439	G1376	G1312	G1249	U1181
U2039	G1904	A1774	G1835	C1774	G1709	G1644	A1579	A1505	U1440	G1377	U1312	U1250	G1182
G2040	C1905	G1775	G1836	U1775	G1710	G1645	A1580	U1506	U1441	G1378	U1313	G1251	G1183
U2041	G1906	G1776	G1837	U1776	G1711	G1646	C1581	G1507	G1442	U1379	G1314	G1252	U1184
A2042	G1907	U1777	G1840	U1777	U1712	U1647	C1582	A1508	G1444	G1380	C1315	G1253	G1185
C2043	G1910	U1778	G1841	U1778	A1713	U1648	A1583	A1509	G1445	G1381	U1316	A1253	G1186
G2044	U1911	U1779	G1842	U1779	A1714	G1649	U1584	A1510	C1446	G1382	U1317	A1254	U1187
C2045	A1912	G1780	G1843	U1780	G1715	A1650	C1585	A1511	C1447	U1383	G1318	U1255	U1188
G2046	G1913	A1781	G1844	U1781	G1716	G1651	A1586	G1511	G1450	A1384	C1319	G1256	A1189
C2047	U1914	U1782	G1845	U1782	G1717	A1652	G1587	C1512	G1451	A1385	C1320	G1257	G1190
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C2049	U1916	G1784	A1847	U1784	G1719	A1654	U1589	G1514	G1453	A1387	A1322	G1259	C1196
A2051	U1917	A1785	G1848	U1785	U1720	C1656	A1591	A1515	G1454	G1388	C1323	A1260	G1197
A2052	G1918	A1786	G1849	U1786	G1721	U1657	C1592	G1516	G1455	G1389	G1324	G1261	U1198
G2053	C1985	G1787	G1850	U1787	G1722	C1658	A1593	G1521	G1456	A1392	U1325	G1262	U1199
A2054	A1919	C1788	U1851	G1788	G1723	G1659	U1594	G1522	U1457	A1393	U1326	G1263	C1200
C2055	G1920	U1789	U1852	G1789	G1724	G1660	C1595	U1523	U1458	U1394	A1327	G1265	U1201
G2056	G1921	G1790	A1853	U1790	U1725	G1661	A1596	G1524	G1459	A1395	U1328	U1267	U1202
C2057	U1922	A1791	G1854	G1791	C1726	U1662	A1597	A1525	U1460	U1396	C1330	A1268	G1203
A2058	C1994	G1792	U1855	G1792	G1727	G1663	A1598	G1533	C1461	U1397	G1331	G1270	A1204
G2059	U1995	A1794	U1856	U1794	C1728	A1664	U1599	G1534	C1462	C1399	G1332	G1271	A1205
A2060	C1996	G1795	G1857	C1795	U1729	A1665	A1602	U1535	G1465	U1400	G1333	A1272	G1206
G2061	G1928	U1796	A1858	U1796	C1730	G1666	A1603	A1536	U1466	G1401	C1335	U1273	C1207
A2062	G1929	G1797	U1859	G1797	G1731	G1667	A1604	G1537	U1467	U1402	C1336	A1274	G1210
C2063	U1930	U1798	G1860	U1798	G1732	A1668	C1605	G1538	U1468	A1403	G1337	A1275	G1211
G2064	U1931	G1799	G1861	G1799	G1733	A1669	C1606	U1539	U1469	A1404	G1338	G1276	G1212
C2065	A1932	C1800	G1862	C1800	G1734	C1670	C1607	U1540	A1470	C1404	G1339	G1278	A1213
G2066	U1933	A1801	G1863	A1801	G1735	U1671	A1608	C1541	G1471	U1405	U1340	G1279	A1214
A2067	C1935	A1802	U1864	A1802	U1736	A1672	U1609	U1542	G1472	G1409	G1341	G1280	G1218
U2068	A1936	A1803	U1865	A1803	U1737	G1673	A1610	U1543	G1473	G1410	A1342	U1281	U1219
G2069	U1937	C1804	G1866	G1804	G1738	G1674	C1611	G1544	U1474	U1411	G1343	U1282	G1220
A2070	U1939	A1805	G1867	C1805	A1739	A1675	G1612	G1546	G1475	U1412	U1344	G1283	C1221
C2071	U1940	G1806	C1868	A1806	G1740	A1676	G1613	A1549	U1476	U1413	A1284	U1285	U1222
G2072	A1808	U1744	G1869	A1808	A1744	U1680	A1614	C1550	A1477	C1414	A1285	A1286	G1223
U2076	C1809	A1745	A1869	G1810	A1745	G1681	C1615	G1551	G1478	U1415	C1348	A1287	U1224
A2077	A1810	U1746	A1870	G1811	A1746	G1682	A1616	G1552	G1479	G1416	C1349	G1288	G1225
C2078	G1812	A1747	G1873	U1812	U1747	U1683	C1617	A1553	U1481	C1417	G1352	G1289	A1226
U2079	G1813	C1748	G1874	G1813	G1748	G1684	A1618	G1554	U1482	G1418	A1353	G1290	G1227
A2080	U1946	A1749	G1875	G1814	A1749	C1685	G1619	C1556	G1483	A1419	A1354	G1291	G1228
U2081	C1947	G1750	G1876	A1815	G1750	U1686	G1622	C1557	U1484	A1420	G1355	G1292	C1229
A2082	U1951	G1816	A1877	C1816	A1754	U1688	G1623	C1558	U1485	G1421	C1356	C1293	A1230
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U2086	C1953	U1818	A1879	A1818	G1756	A1690	G1625	G1560	U1487	G1423	G1358	G1296	G1234
C2087	G1954	A1819	C1879	C1819	U1757	C1691	G1626	G1561	G1488	G1424	A1359	G1297	U1235
G2088	U1955	A1820	U1882	U1820	A1757	U1692	A1628	U1562	G1489	G1425	G1360	C1298	G1236
C2089	C1956	G1821	U1883	U1821	U1758	U1693	G1627	U1563	G1491	G1426	C1363	G1299	A1237
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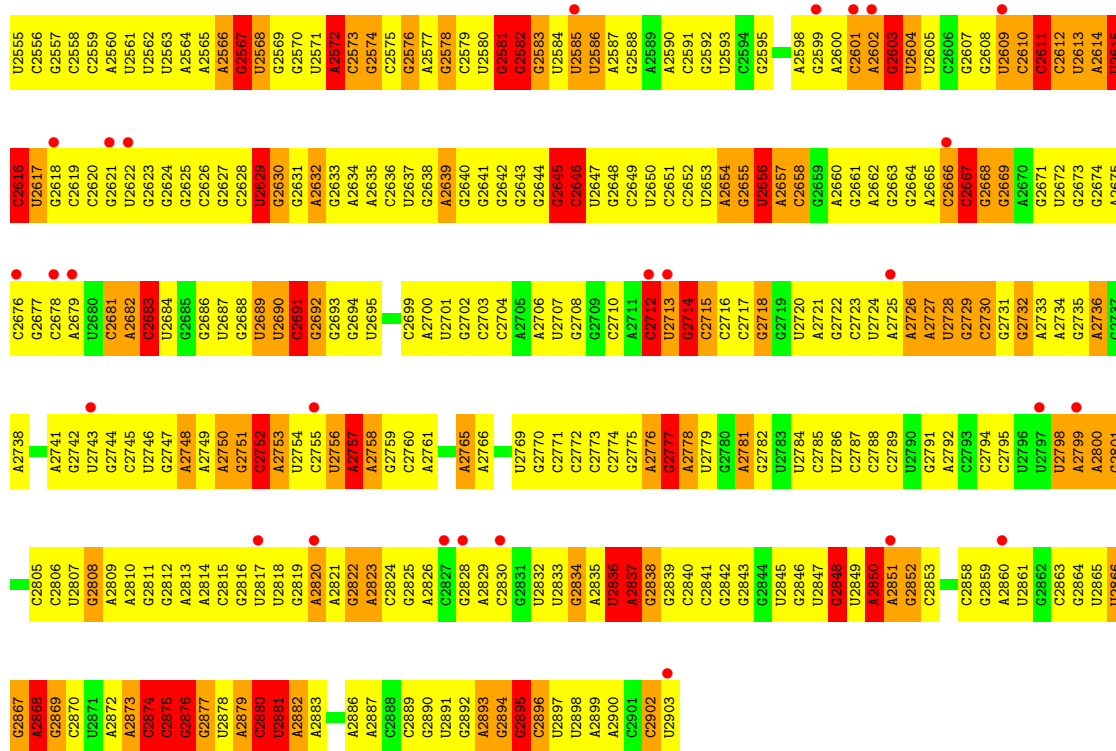
- Molecule 22: 23S rRNA





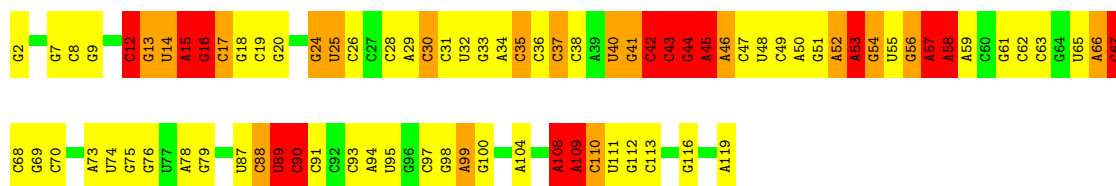


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A2497	G2428	G2365	U2244	G2057	U1993	C1924	G1857	G1791	G1730
C2498	G2429	A2366	U2245	U2057	U1993	C1924	G1857	G1791	G1731
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G2502	A2433	G2370	G2250	A2062	A1998	A1928	G1862	A1735	G1735
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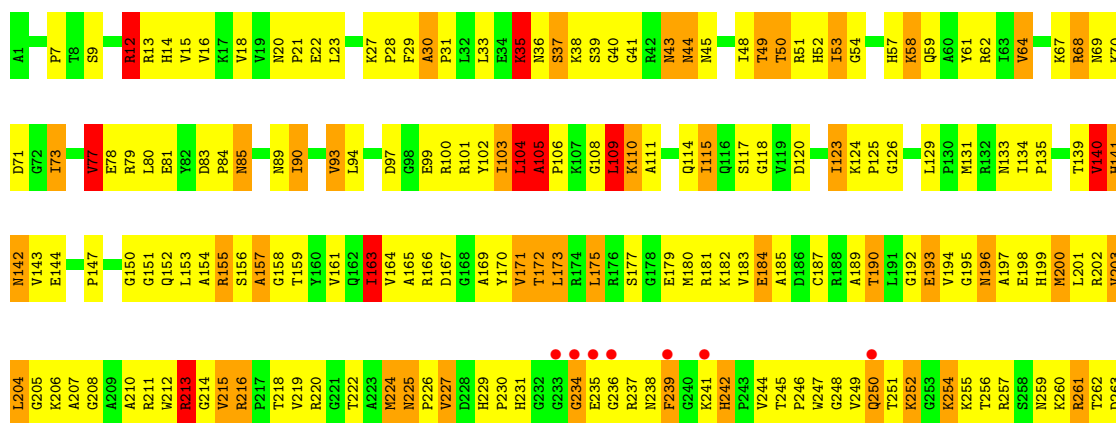
• Molecule 23: 5S rRNA

Chain BB: 30% 42% 15% 13%



• Molecule 24: 50S ribosomal protein L2

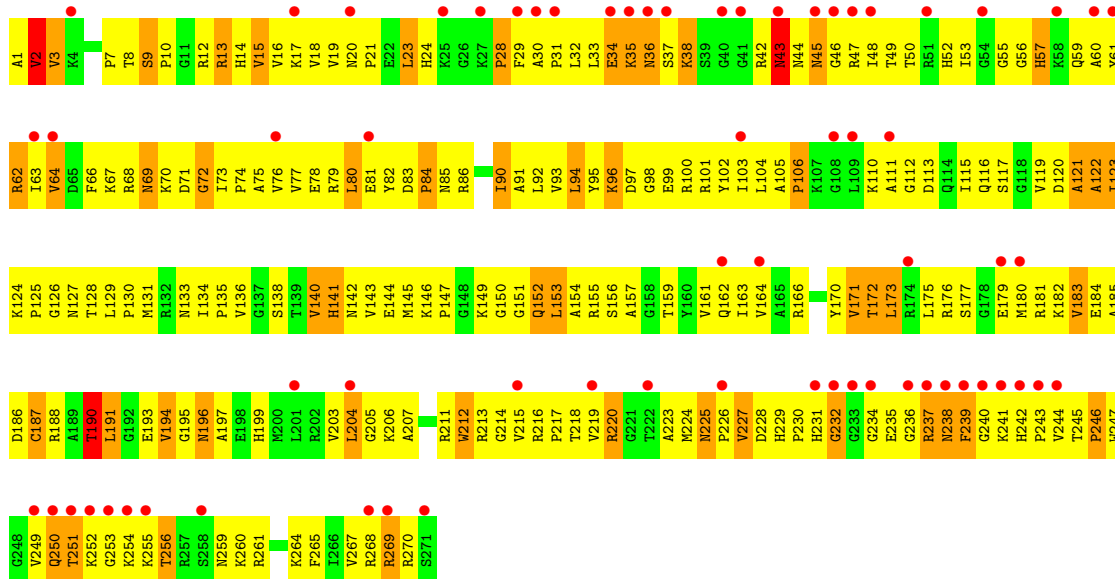
Chain BC: 3% 29% 51% 17%



K264
F266
I266
V267
R268
R269
R270
S271

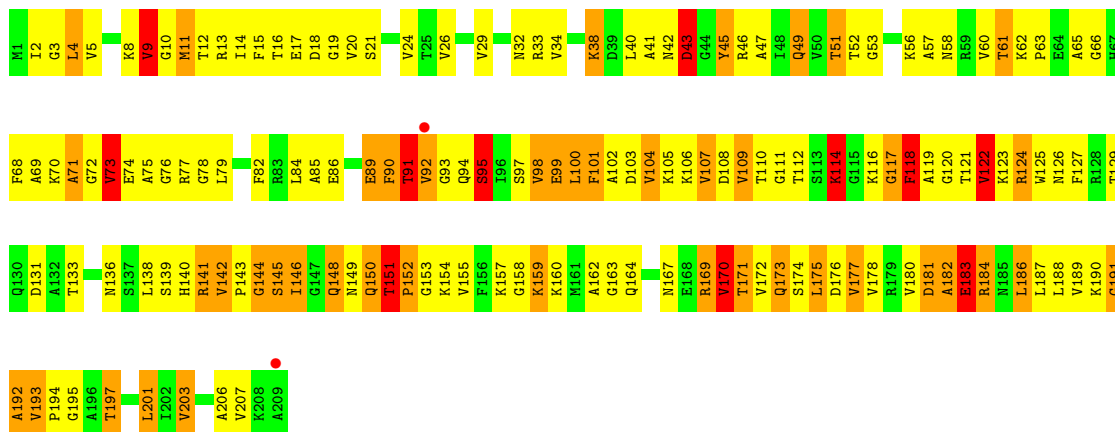
• Molecule 24: 50S ribosomal protein L2

Chain DC: 25% 20% 60% 19%



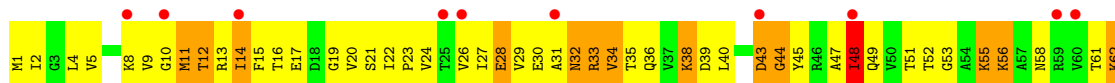
• Molecule 25: 50S ribosomal protein L3

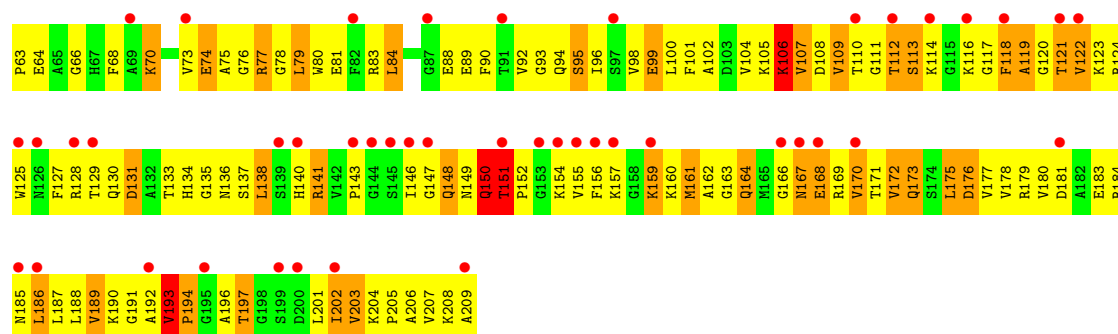
Chain BD: 25% 48% 21% 5%



• Molecule 25: 50S ribosomal protein L3

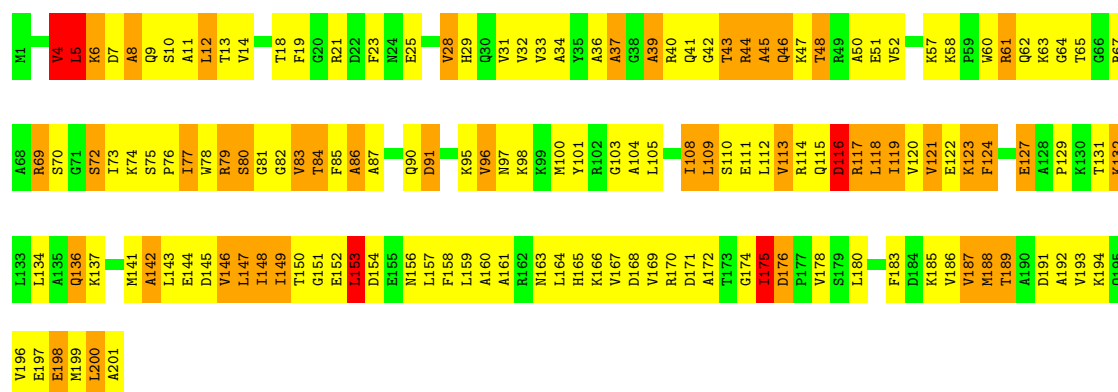
Chain DD: 26% 20% 55% 23%





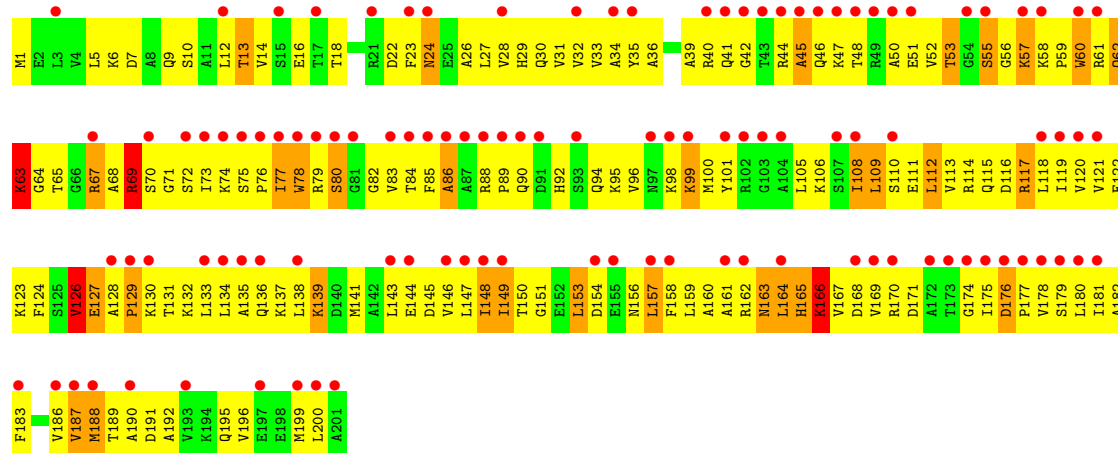
• Molecule 26: 50S ribosomal protein L4

Chain BE: 25% 50% 22%



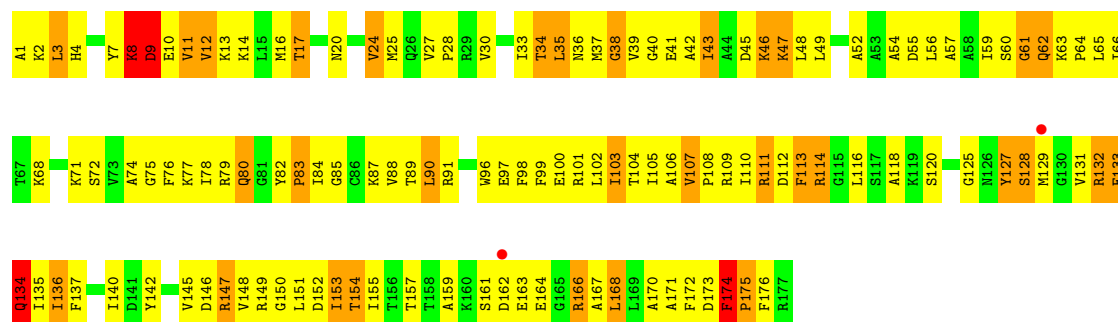
• Molecule 26: 50S ribosomal protein L4

Chain DE: 20% 54% 63% 15%

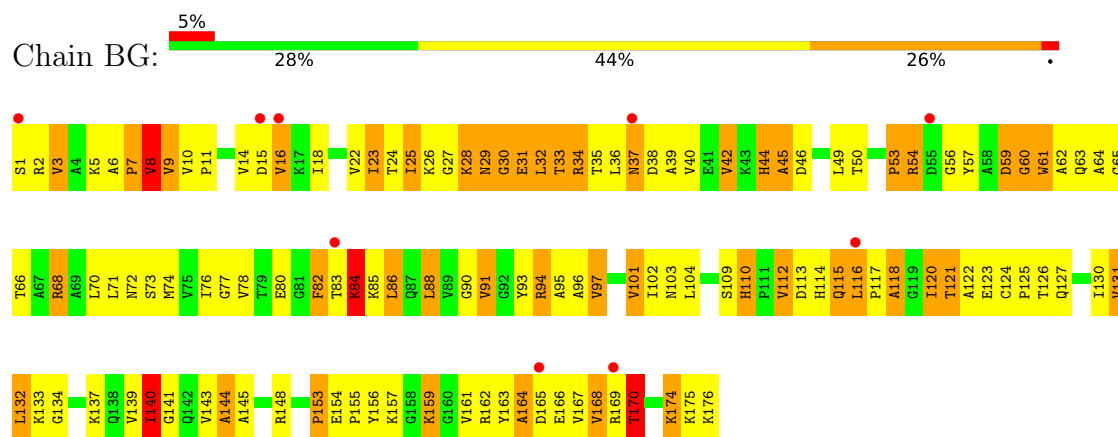


• Molecule 27: 50S ribosomal protein L5

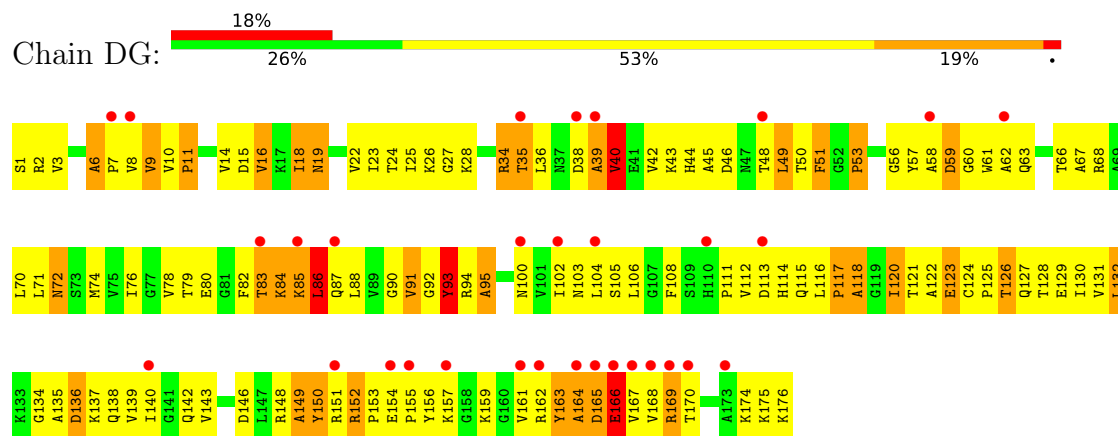
Chain BF: 27% 53% 18%



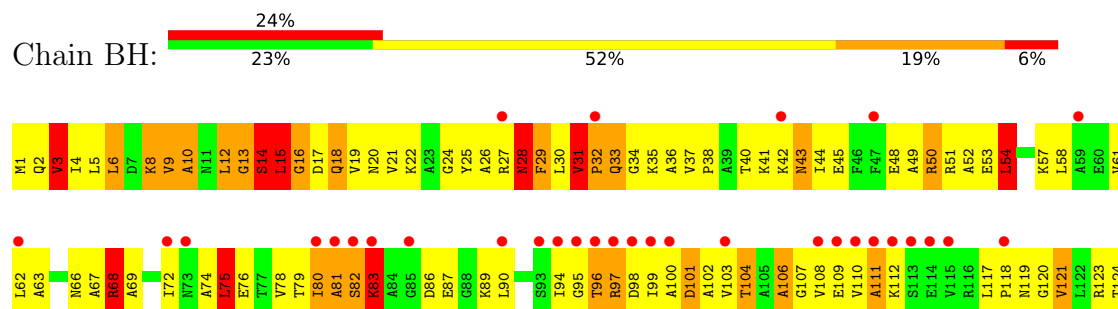
• Molecule 28: 50S ribosomal protein L6



• Molecule 28: 50S ribosomal protein L6

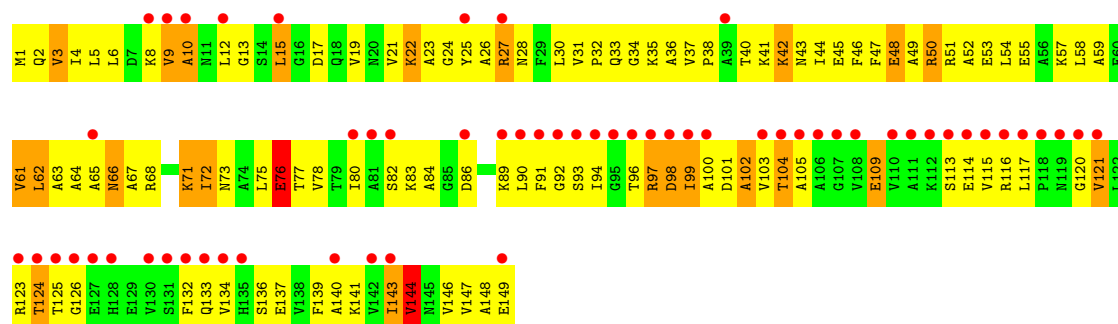


• Molecule 29: 50S ribosomal protein L9

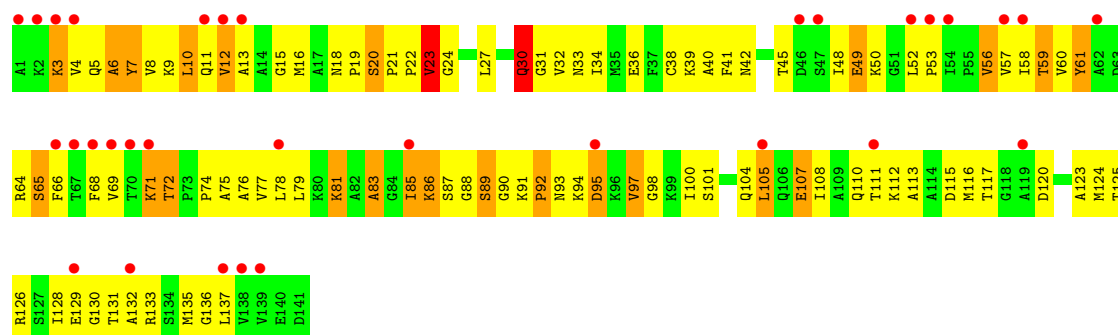




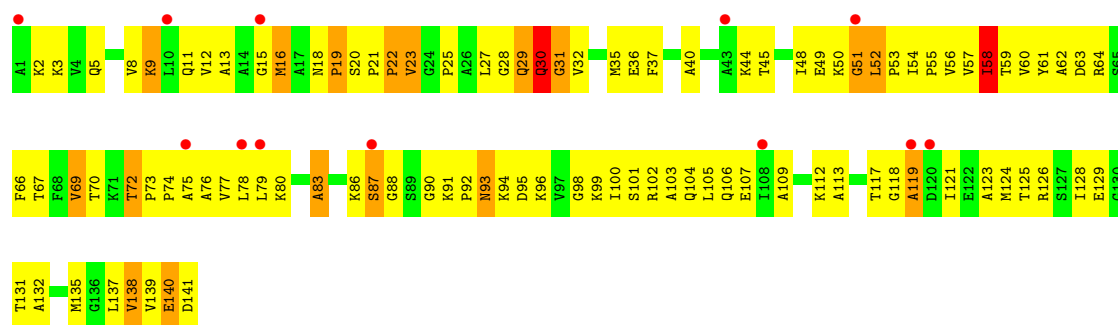
• Molecule 29: 50S ribosomal protein L9



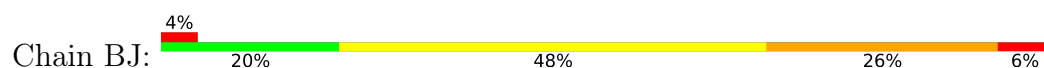
• Molecule 30: 50S ribosomal protein L11

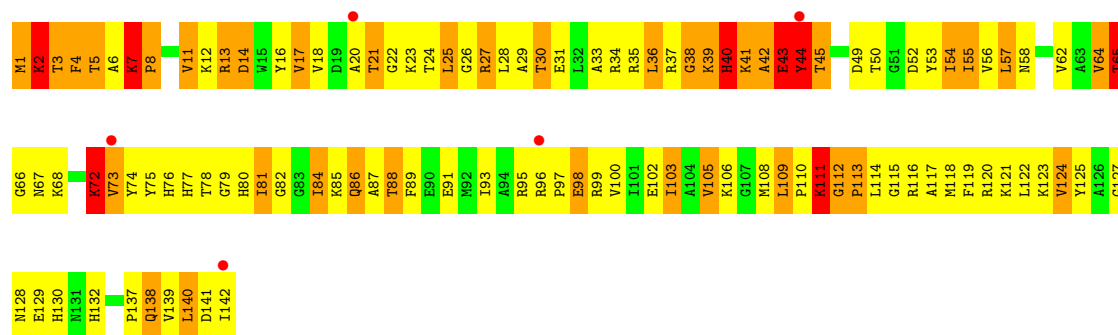


• Molecule 30: 50S ribosomal protein L11

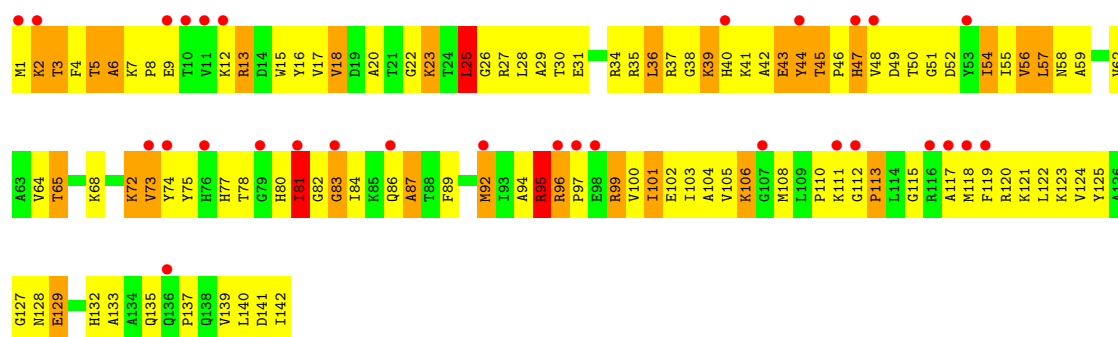


• Molecule 31: 50S ribosomal protein L13

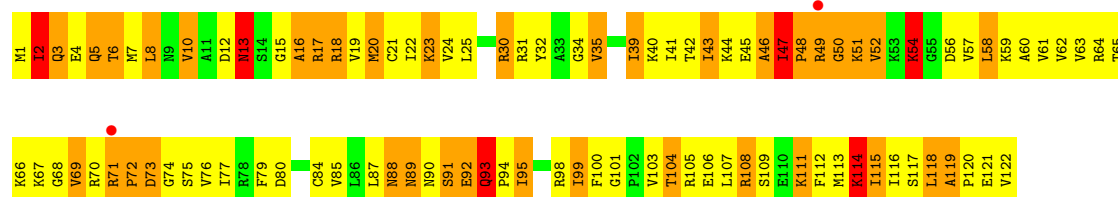
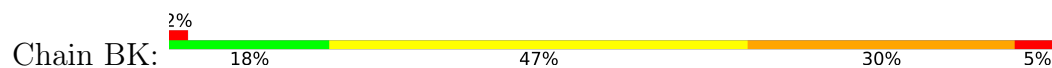




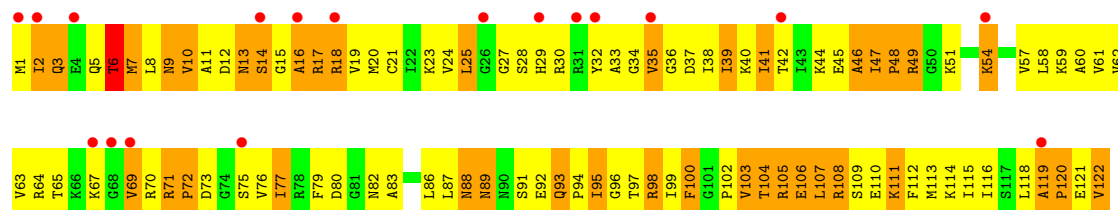
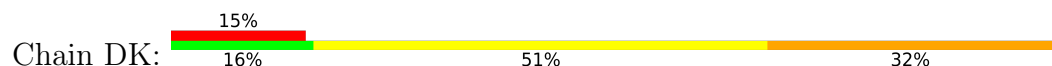
• Molecule 31: 50S ribosomal protein L13



• Molecule 32: 50S ribosomal protein L14

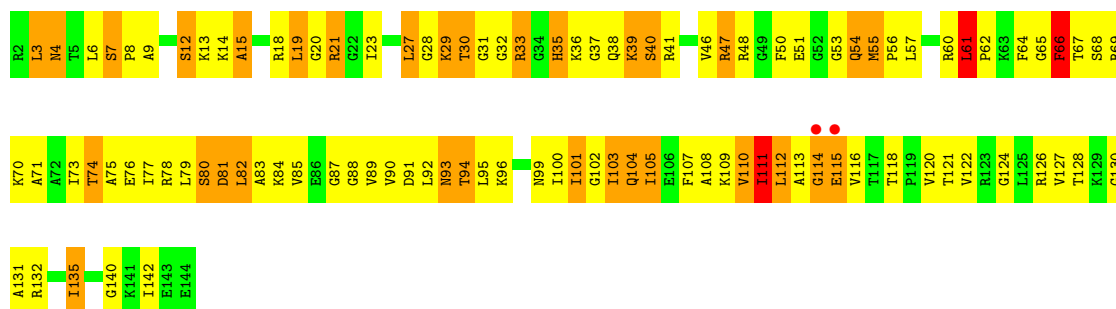


• Molecule 32: 50S ribosomal protein L14

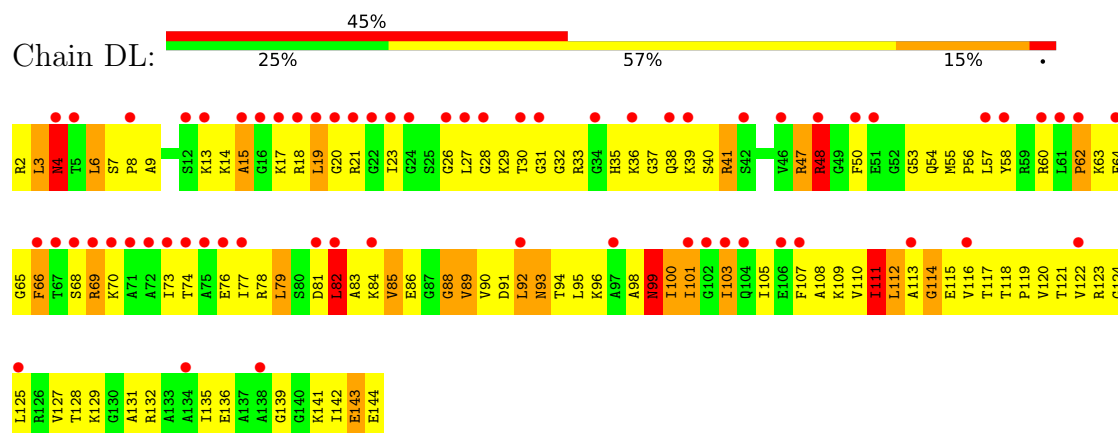


• Molecule 33: 50S ribosomal protein L15

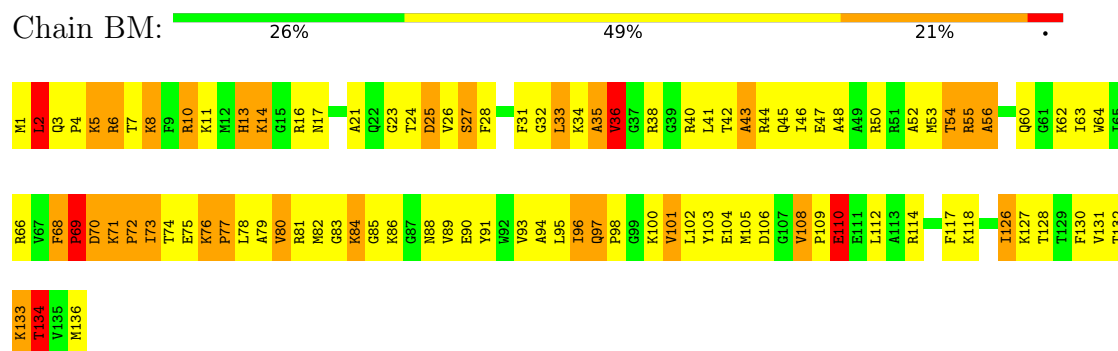




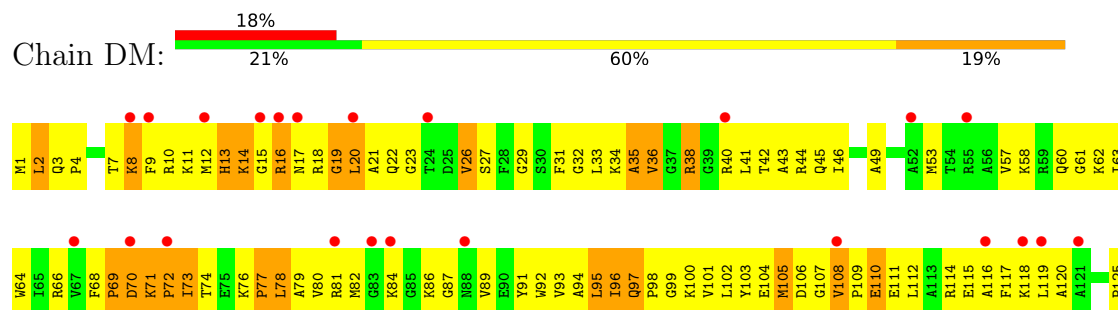
• Molecule 33: 50S ribosomal protein L15

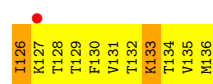


• Molecule 34: 50S ribosomal protein L16



• Molecule 34: 50S ribosomal protein L16

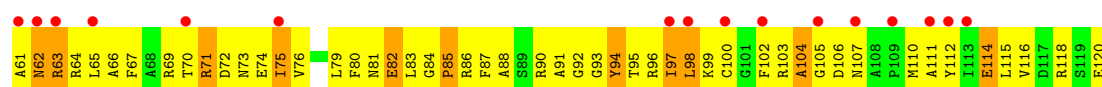
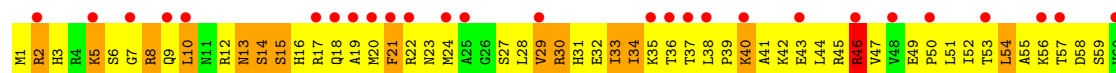




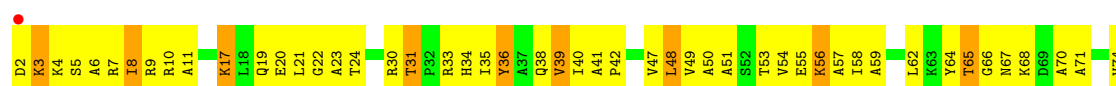
- Molecule 35: 50S ribosomal protein L17



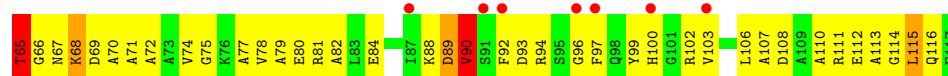
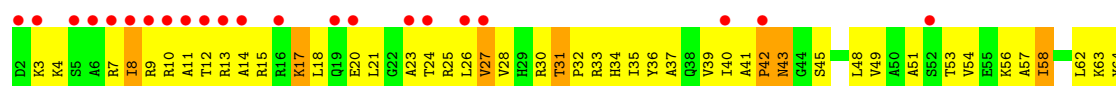
- Molecule 35: 50S ribosomal protein L17



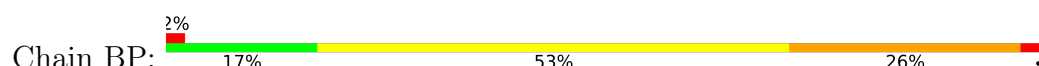
- Molecule 36: 50S ribosomal protein L18

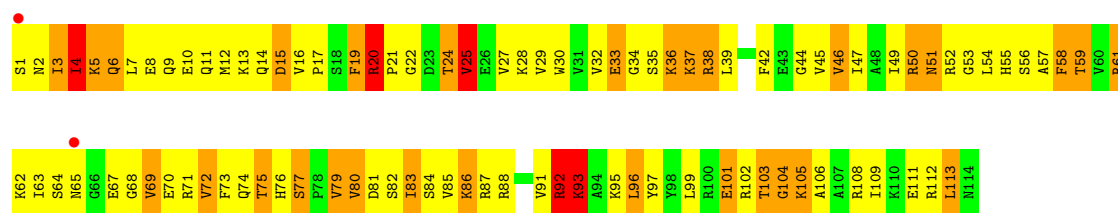


- Molecule 36: 50S ribosomal protein L18

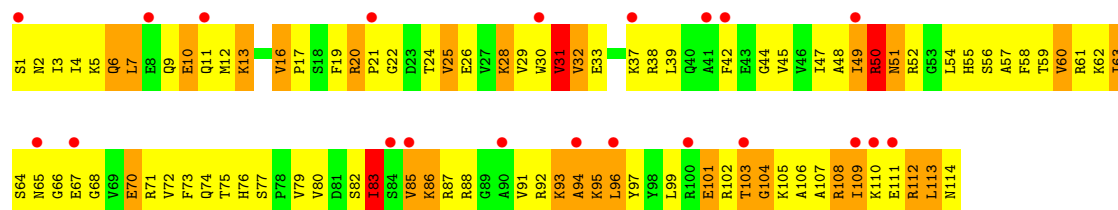


- Molecule 37: 50S ribosomal protein L19

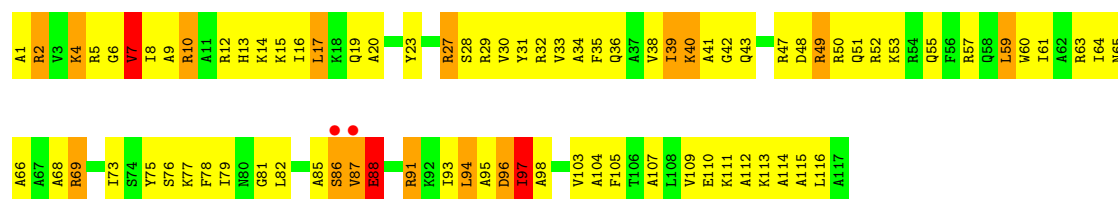




• Molecule 37: 50S ribosomal protein L19



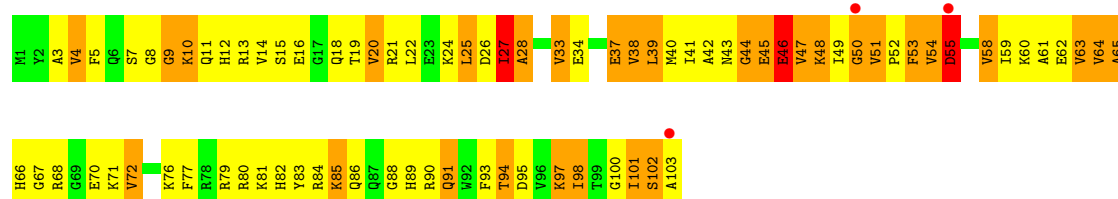
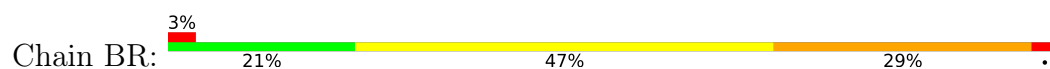
• Molecule 38: 50S ribosomal protein L20



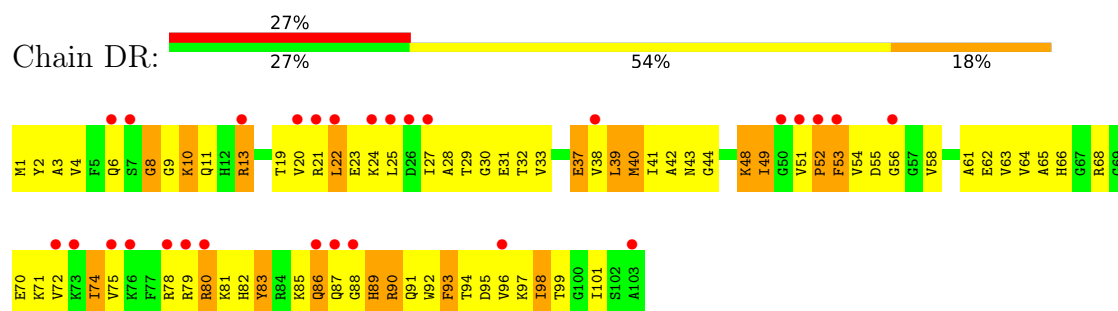
• Molecule 38: 50S ribosomal protein L20



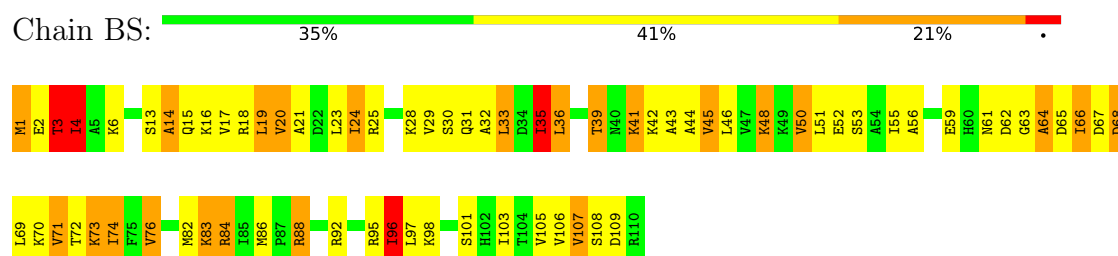
• Molecule 39: 50S ribosomal protein L21



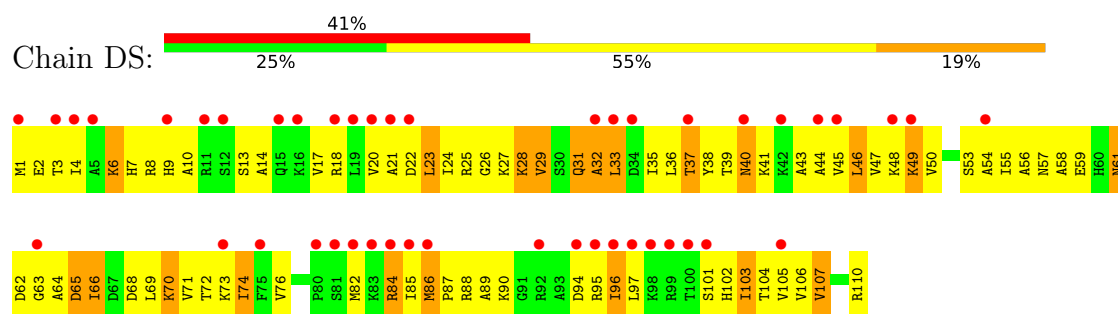
- Molecule 39: 50S ribosomal protein L21



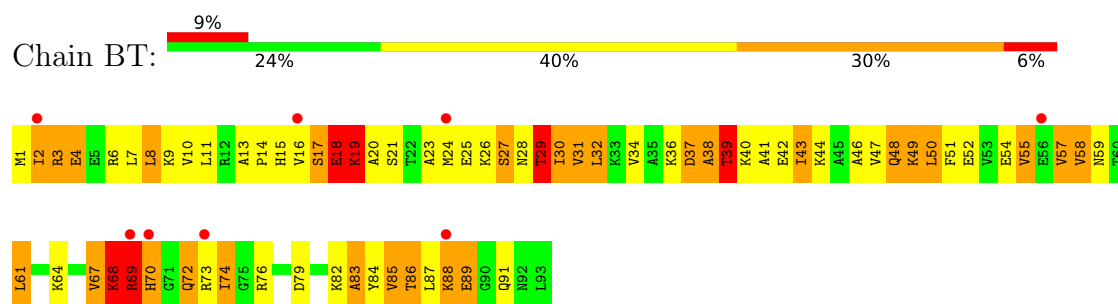
- Molecule 40: 50S ribosomal protein L22



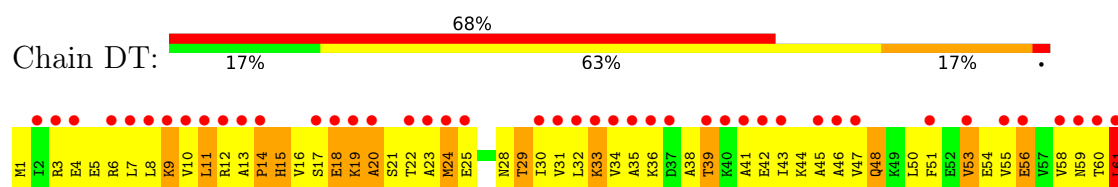
- Molecule 40: 50S ribosomal protein L22

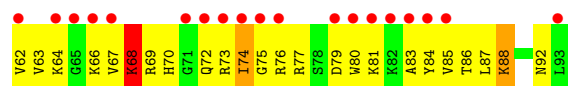


- Molecule 41: 50S ribosomal protein L23

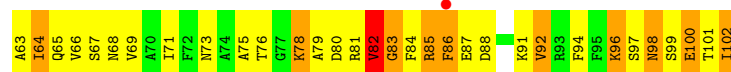
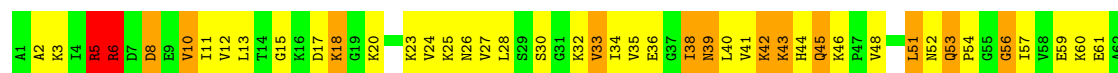


- Molecule 41: 50S ribosomal protein L23

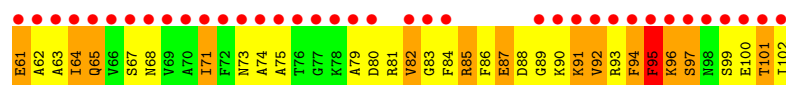
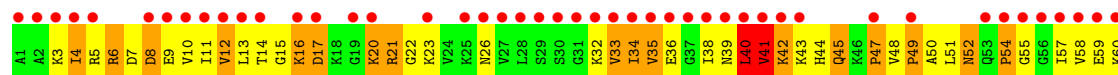
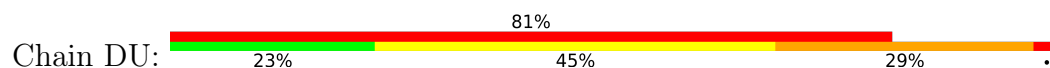




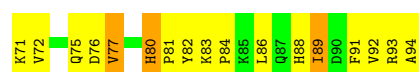
• Molecule 42: 50S ribosomal protein L24



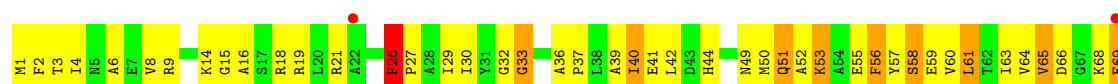
• Molecule 42: 50S ribosomal protein L24



• Molecule 43: 50S ribosomal protein L25

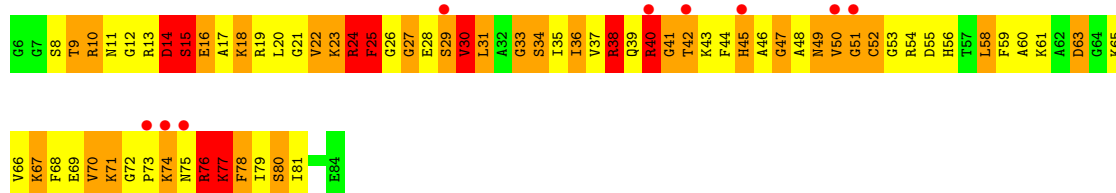


• Molecule 43: 50S ribosomal protein L25

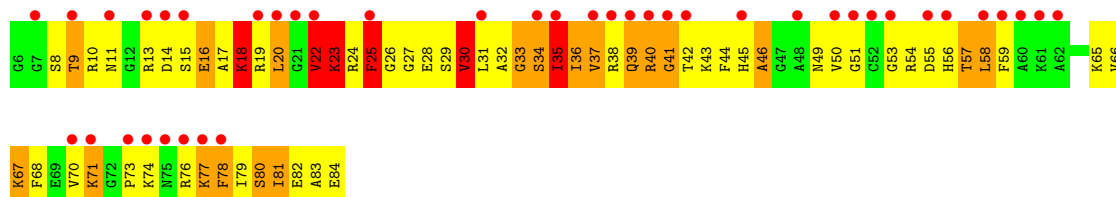
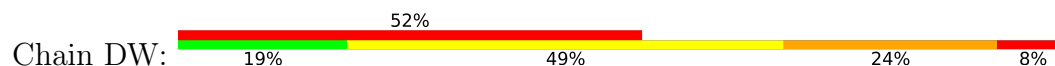


• Molecule 44: 50S ribosomal protein L27

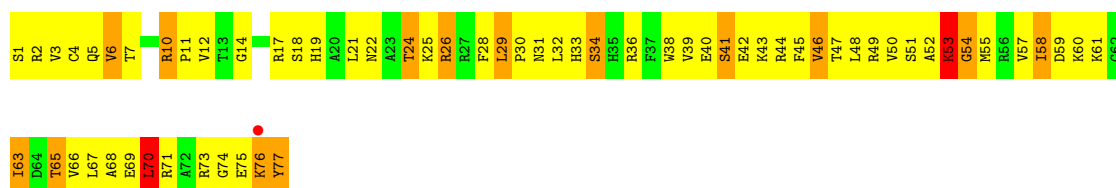




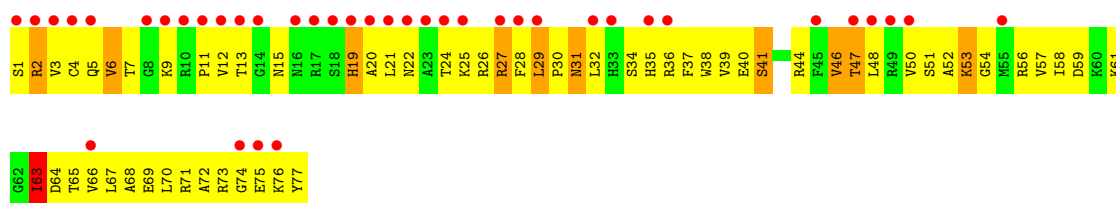
• Molecule 44: 50S ribosomal protein L27



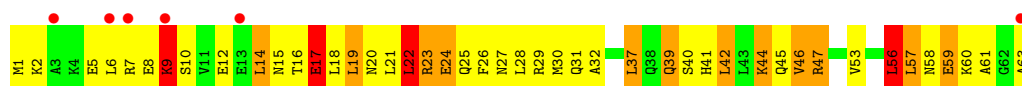
• Molecule 45: 50S ribosomal protein L28



• Molecule 45: 50S ribosomal protein L28



• Molecule 46: 50S ribosomal protein L29

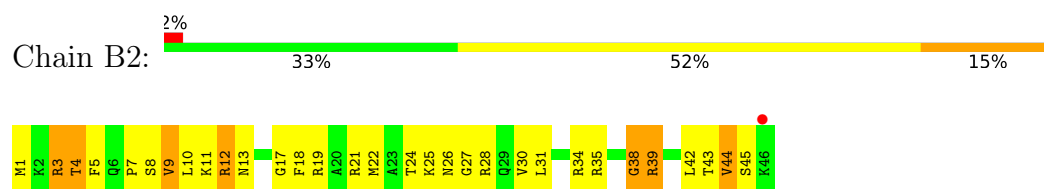


• Molecule 46: 50S ribosomal protein L29

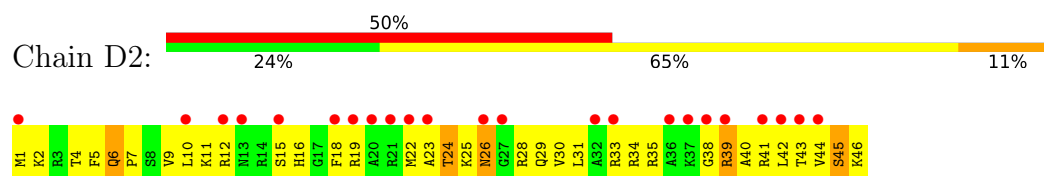




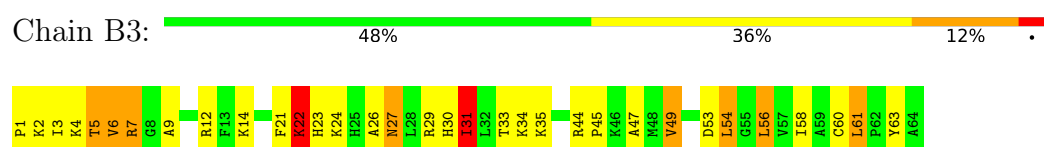
- Molecule 50: 50S ribosomal protein L34



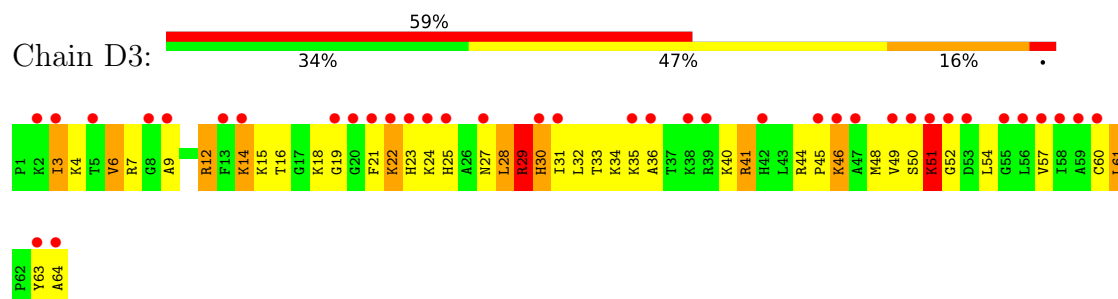
- Molecule 50: 50S ribosomal protein L34



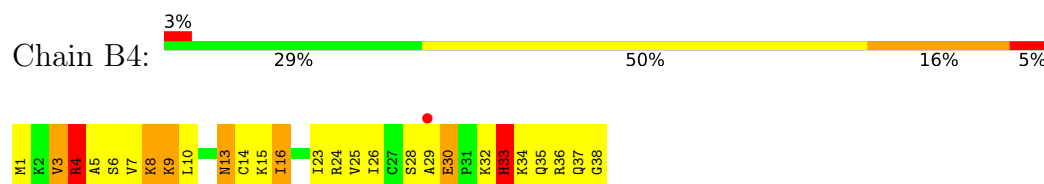
- Molecule 51: 50S ribosomal protein L35



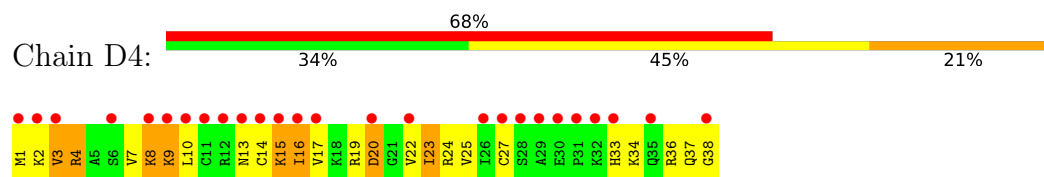
- Molecule 51: 50S ribosomal protein L35



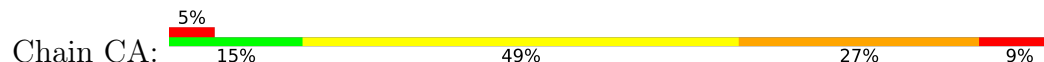
- Molecule 52: 50S ribosomal protein L36



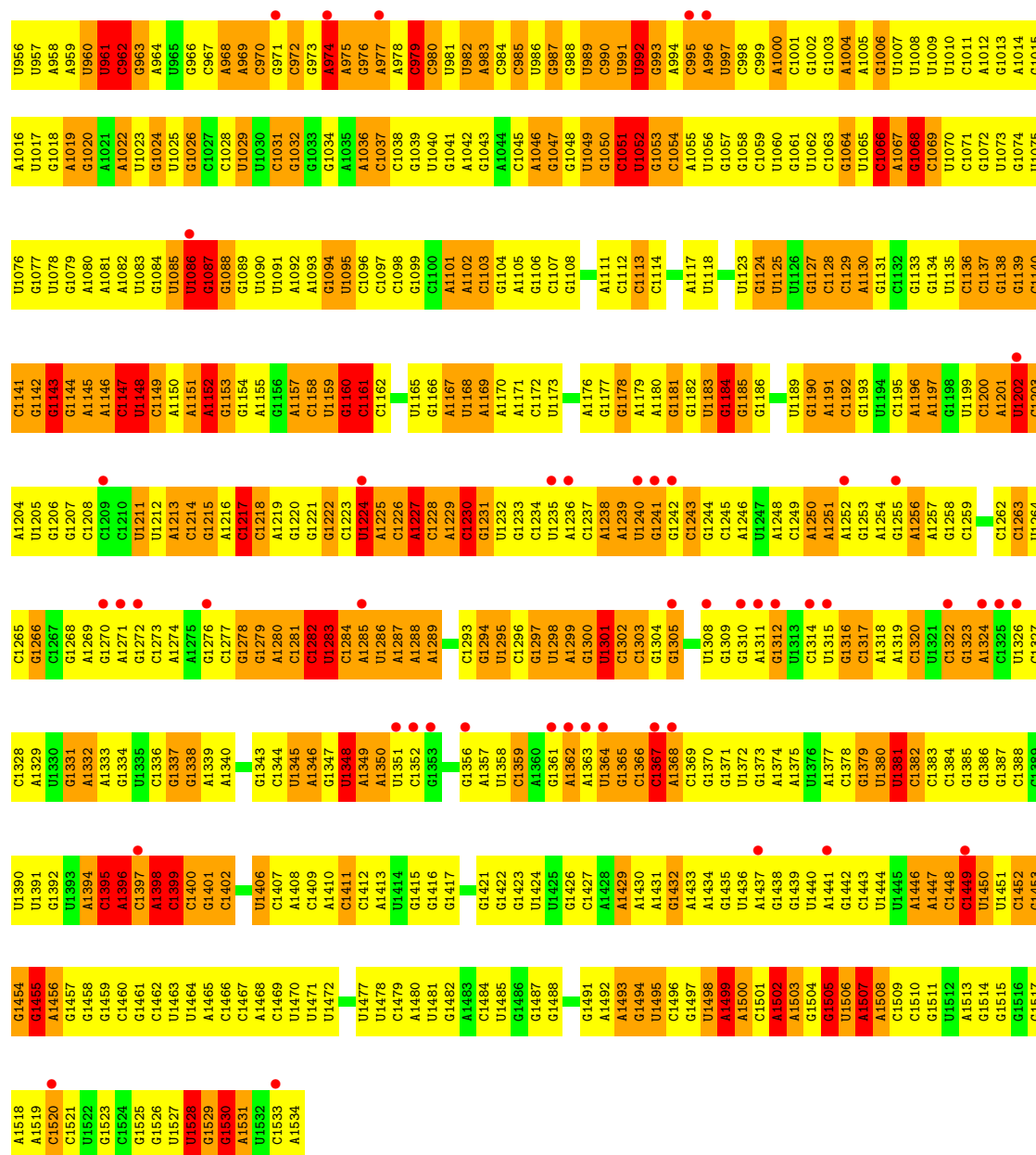
- Molecule 52: 50S ribosomal protein L36



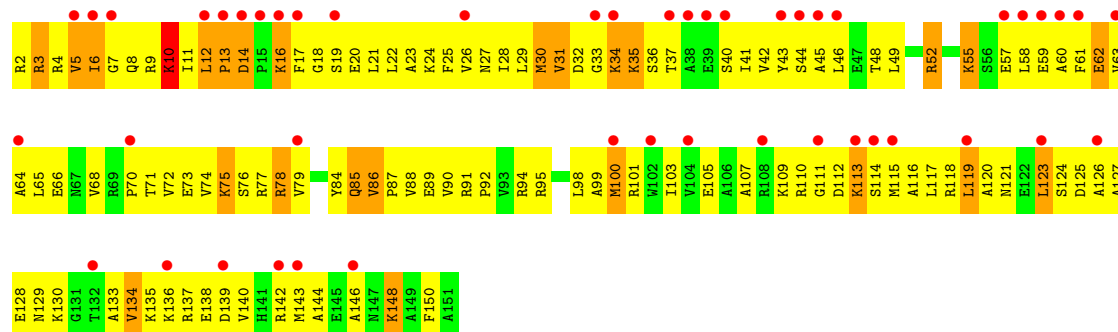
- Molecule 53: 16S rRNA



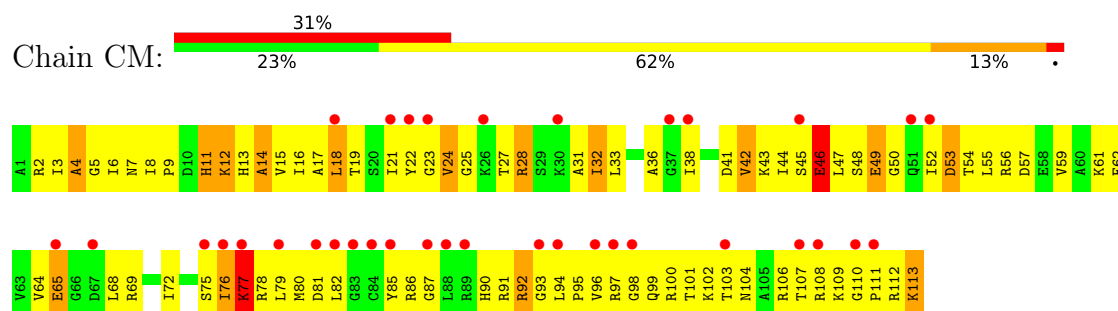
U891	A825	U762	A702	C637	C569	G442	C379	A315	U252	A190	A129	G69	U5
A892	C826	G763	G703	A640	G570	C443	G380	A316	A253	G191	A130	U70	G6
G893	U827	G764	A704	A641	U571	G444	C381	U317	G254	A192	A131	A71	A7
G894	G765	G765	G705	U641	A509	G445	A382	G318	G255	C193	A132	A72	A8
G895	G829	A766	A706	A642	A573		A383	G319	U256	C194	U133	C73	G9
G896			U707	G643	U512		G384	A320	G257	A195	G134	A74	A10
G897			C708	G644	G576		C395	A321	G258	A196	C135	G75	
G898	U834	G770	U709	G645	C576	A451	C386	C322	G259	A197	G136	G76	U13
G899	U835	G771	G710	G646	C577	A452	U387		U261	G198	U137	A77	U14
A900	U836	U772	G578	C578	U516	G453	G388	A325	A263	A262		A78	A15
A901	U837	G773	A712	G454	A579	G454	A389	G326	C264	G201	U140	G79	U16
G902	G838	G774	C518	A649	C580	A455	U390	G327	A265	G202	G141	A80	U17
G903		G775	G713	A649	C581	A456	G391	A328	G266	G203	G142	A81	C18
U904		G776	A715	G650	A582	C457	C392	A329	G267	G204	A143	G82	A19
		A777	U716	G651	G583	U458	A393	G330	U268	G205	G144	C83	
		A778	U717	U652	C584	A459	G394	G331	C271	A206	G145	U84	G22
C910			A718	G654	G585	A460	C395	G332	G275	C206	G146		
			C719	A655	C586	A461	C396	U333	G269	C207	G147	U85	
A913	A845	A781	G720	A656	G587	C462	A397	C334	U268	U208	G148	C87	C25
A914	G846	A782	G721	U657	G588	U463	U398	C335	A270	U209	A149	C88	A26
A915	G847	A783	G722	U658	U589	U464	G399	A336	C272	G210	U150	U88	C27
A916	G848	G785	U723	U659	C584	A465	C400	G337	U273	G211	U151	U89	A28
G917	G849	G786	G724	U659	U591	A466		A338	G274	G212	C90	U90	U29
A918		A787	G725			U467	U405		G275	G213	A152	U91	U30
A919		U788	C726			A468	G406	U343	G276	C214	U153	U92	G31
U920	U854	U789	G727			C469	G407	A344	C277	C215	A155	U93	A32
U921	U855	A790	A728				U408	A345	G278	U216	C156	G94	A33
G922		G791	U729			U473	A408	G346	A279	C217	C156	C95	C34
A923	G859	A792	C730			G474	U409	G347	U280	U218	U157	U96	G35
C924	A860	G793	G731			C475	G410	G348	G281	U219	G158	G97	C36
G925	G861	A794	C732			U476	A411	A349	U282	G220	A160	U98	U37
G926	C862	C795	G733			C477	A412	G350	U283	C221	A161	C99	G38
U927	U863	G796	G734			A478	G413	G351	C284	C222	A162	G100	C39
G928	A864	C797	C735			U479	A414	C352	C285	U224	C163	A101	C40
	G865	U798	C736			U480	A415	A353	C286		G164	G102	G41
C931	C866	G799	C737			G481	G416	G354	U287		U165	U103	G42
C932	G867	G800	C738			A482	G417	C355	A288		U166	G104	C43
C933	C868	U801	C739			C483	C418	A356	G289		A167	G105	A44
G934	G869	A802	U740			G484		G357	C290		A167	C106	G45
A935	U870	G803	G741			U485	U421	U358		G230	G168	G107	G46
C936	U871	U804	G742			U486	C422	G359	U296	U231	C169	G108	C47
A937	A872		A743			A487	G423	G360	G301	C233	U170	A109	C48
A938	A873		G744				G424	G361	A298	C234	A171	C110	
C939	G874		G745				G425	G362	G299	U235	U172	G111	A51
C940	U875		A746				U426	A363	G299	A236	A174	G112	C52
C876	G877		C747			G491	U427	A364	A300	G237	C175	G113	C53
G941	G878		U748			C492	G428	U365	G302	A238	C176	G114	C54
U943	A878		C749			A493	U429	A366	A303	U239	G177	G115	A55
G944	C879		C750			G494	A430	U367	G303	G240	G178	U56	U56
G945	C880		U751			A495	A431	U368	A304	G241	A179	G57	C58
A946	G881		G752			A496	A432	G369	G305	G242	U180	U58	A59
G947	C882		A753			A497	G433	C370	A306	A243	U181	A120	A60
C948	U883		C754			A498	U434	A371	C307	U244	A182	G61	U121
A949	G884		G755			A499	U435	C372	U308	U245	C183	U62	U62
	G885		C756			C501	A436	A373	A309	A246	G184	C63	C63
G950	A885		U757			A502	U437	A374	G310	G247	U185	C124	G64
G951	G886		C758			C503	U438	U375	C311	C248	C186	U125	A65
U952	C887		A759			G504	U439	G376	C312	U249	G187	U126	A66
G953	A888		C760			G505	U440	G377	A313	G127	C188	G127	C67
G954	U889		G761			G506	A441	G378	C314	G251	A189	G128	G68



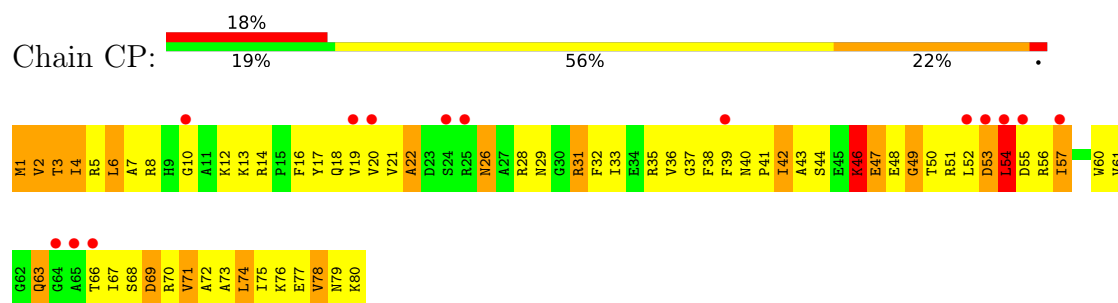
● Molecule 54: 30S ribosomal protein S7



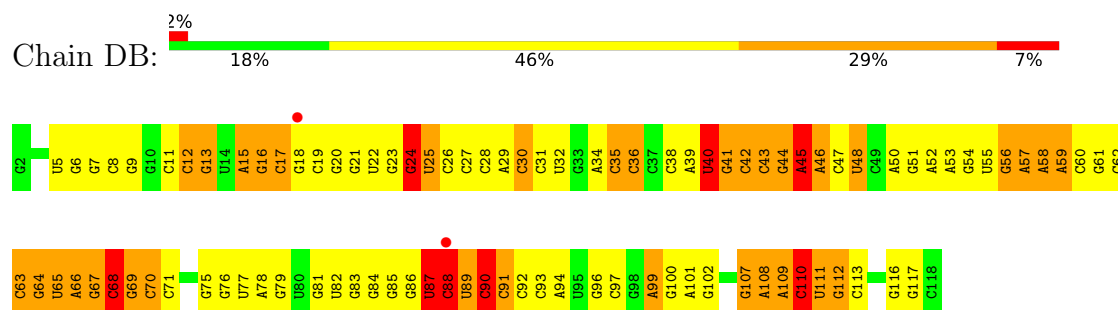
- Molecule 55: 30S ribosomal protein S13



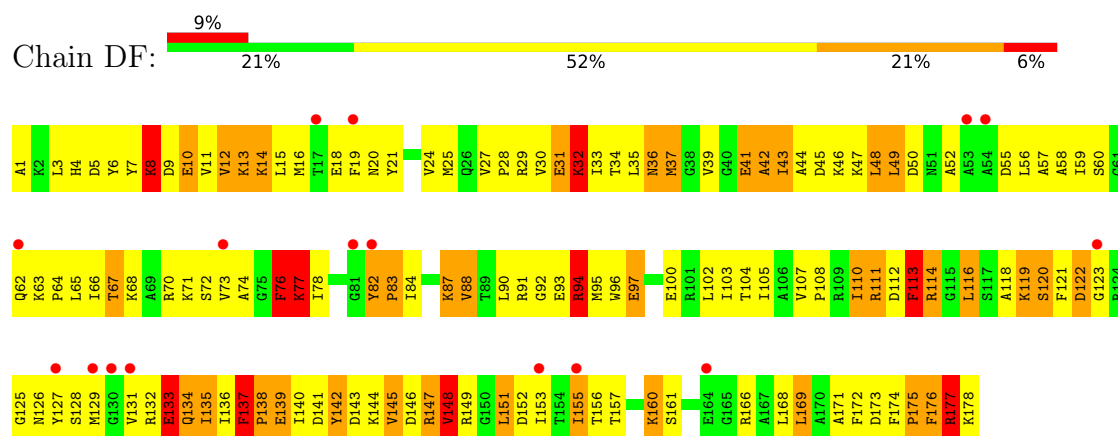
- Molecule 56: 30S ribosomal protein S16



- 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)	Xtriage
Refinement program	PHENIX, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.189 , 0.241 0.201 , 0.250	Depositor DCC
R_{free} test set	14080 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284501	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.32	1/36834 (0.0%)	0.94	229/57462 (0.4%)
2	AB	0.29	0/1736	0.76	5/2338 (0.2%)
2	CB	0.29	0/1736	0.81	2/2338 (0.1%)
3	AC	0.33	0/1652	0.85	10/2225 (0.4%)
3	CC	0.30	0/1652	0.76	4/2225 (0.2%)
4	AD	0.36	0/1665	0.81	0/2227
4	CD	0.42	0/1665	0.85	3/2227 (0.1%)
5	AE	0.40	0/1119	0.87	4/1504 (0.3%)
5	CE	0.47	1/1119 (0.1%)	0.90	2/1504 (0.1%)
6	AF	0.37	0/836	0.76	0/1128
6	CF	0.33	0/836	0.80	1/1128 (0.1%)
7	AG	0.30	0/1196	0.81	3/1602 (0.2%)
8	AH	0.39	0/989	0.94	5/1326 (0.4%)
8	CH	0.36	0/989	0.84	0/1326
9	AI	0.29	0/1034	0.77	0/1375
9	CI	0.27	0/1034	0.73	0/1375
10	AJ	0.32	0/797	0.87	4/1077 (0.4%)
10	CJ	0.29	0/797	0.79	3/1077 (0.3%)
11	AK	0.35	0/893	0.93	4/1205 (0.3%)
11	CK	0.33	0/893	0.83	0/1205
12	AL	0.48	0/969	1.04	3/1300 (0.2%)
12	CL	0.37	0/969	0.87	2/1300 (0.2%)
13	AM	0.31	0/893	0.79	0/1193
14	AN	0.33	0/785	0.78	3/1043 (0.3%)
14	CN	0.26	0/780	0.75	0/1036
15	AO	0.36	0/722	0.69	0/964
15	CO	0.32	0/722	0.70	0/964
16	AP	0.41	0/659	0.85	0/884
17	AQ	0.41	0/658	0.86	0/881
17	CQ	0.35	0/658	0.82	2/881 (0.2%)
18	AR	0.36	0/463	0.78	0/621
18	CR	0.33	0/463	0.75	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AS	0.28	0/653	0.78	0/877
19	CS	0.24	0/653	0.78	0/877
20	AT	0.39	0/671	0.81	2/888 (0.2%)
20	CT	0.33	0/671	0.90	2/888 (0.2%)
21	AU	0.30	0/431	0.84	1/570 (0.2%)
21	CU	0.36	0/431	0.88	0/570
22	BA	0.44	5/68626 (0.0%)	1.13	696/107056 (0.7%)
22	DA	0.30	1/68314 (0.0%)	0.94	404/106569 (0.4%)
23	BB	0.41	0/2828	1.09	24/4410 (0.5%)
24	BC	0.53	1/2122 (0.0%)	1.06	15/2852 (0.5%)
24	DC	0.37	0/2122	0.87	2/2852 (0.1%)
25	BD	0.65	0/1586	1.06	5/2134 (0.2%)
25	DD	0.34	0/1586	0.87	5/2134 (0.2%)
26	BE	0.55	0/1571	0.97	3/2113 (0.1%)
26	DE	0.31	0/1571	0.81	2/2113 (0.1%)
27	BF	0.39	0/1435	0.87	3/1926 (0.2%)
28	BG	0.46	0/1343	0.94	5/1816 (0.3%)
28	DG	0.28	0/1343	0.76	2/1816 (0.1%)
29	BH	0.35	0/1122	0.77	1/1515 (0.1%)
29	DH	0.34	0/1122	0.83	3/1515 (0.2%)
30	BI	0.35	0/1046	0.88	4/1410 (0.3%)
30	DI	0.29	0/1046	0.81	0/1410
31	BJ	0.72	1/1152 (0.1%)	1.27	12/1551 (0.8%)
31	DJ	0.34	0/1152	0.85	0/1551
32	BK	0.63	0/948	0.98	3/1268 (0.2%)
32	DK	0.36	0/948	0.84	2/1268 (0.2%)
33	BL	0.57	0/1054	1.04	5/1403 (0.4%)
33	DL	0.31	0/1054	0.78	0/1403
34	BM	0.60	0/1093	1.11	8/1460 (0.5%)
34	DM	0.34	0/1093	0.87	4/1460 (0.3%)
35	BN	0.57	0/974	1.00	3/1301 (0.2%)
35	DN	0.34	0/974	0.87	2/1301 (0.2%)
36	BO	0.53	0/902	0.92	1/1209 (0.1%)
36	DO	0.28	0/902	0.73	0/1209
37	BP	0.58	0/929	0.99	3/1242 (0.2%)
37	DP	0.33	0/929	0.81	5/1242 (0.4%)
38	BQ	0.71	0/960	1.00	3/1278 (0.2%)
38	DQ	0.31	0/960	0.74	1/1278 (0.1%)
39	BR	0.63	0/829	1.03	4/1107 (0.4%)
39	DR	0.31	0/829	0.73	1/1107 (0.1%)
40	BS	0.69	0/864	1.02	2/1156 (0.2%)
40	DS	0.35	0/864	0.77	0/1156
41	BT	0.57	0/745	0.97	3/994 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	DT	0.28	0/745	0.72	0/994
42	BU	0.52	0/788	1.05	8/1051 (0.8%)
42	DU	0.28	0/788	0.80	1/1051 (0.1%)
43	BV	0.51	0/766	0.95	5/1025 (0.5%)
43	DV	0.30	0/766	0.79	2/1025 (0.2%)
44	BW	0.66	0/603	1.02	4/797 (0.5%)
44	DW	0.29	0/603	0.71	0/797
45	BX	0.51	0/635	0.96	1/848 (0.1%)
45	DX	0.34	0/635	0.90	2/848 (0.2%)
46	BY	0.45	0/510	0.88	3/677 (0.4%)
46	DY	0.25	0/510	0.72	0/677
47	BZ	0.67	0/453	1.09	2/605 (0.3%)
47	DZ	0.33	0/453	0.81	1/605 (0.2%)
48	B0	0.59	0/450	0.94	1/599 (0.2%)
48	D0	0.30	0/450	0.74	0/599
49	B1	0.42	0/417	0.93	4/554 (0.7%)
49	D1	0.31	0/417	0.77	0/554
50	B2	0.60	0/380	1.00	3/498 (0.6%)
50	D2	0.33	0/380	0.96	2/498 (0.4%)
51	B3	0.57	0/513	0.99	2/676 (0.3%)
51	D3	0.32	0/513	0.81	0/676
52	B4	0.69	0/303	1.22	4/397 (1.0%)
52	D4	0.49	0/303	0.69	0/397
53	CA	0.31	1/36762 (0.0%)	0.90	173/57350 (0.3%)
54	CG	0.27	0/1188	0.84	4/1591 (0.3%)
55	CM	0.25	0/885	0.66	0/1181
56	CP	0.36	0/649	0.86	3/870 (0.3%)
57	DB	0.31	1/2803 (0.0%)	0.81	10/4371 (0.2%)
58	DF	0.27	0/1444	0.79	6/1937 (0.3%)
All	All	0.38	12/306773 (0.0%)	0.97	1771/458565 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	BD	0	1
31	BJ	0	1
35	BN	0	1
58	DF	0	1
All	All	0	4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	CA	1396	A	O3'-P	-13.06	1.41	1.61
1	AA	1047	G	O3'-P	-10.83	1.45	1.61
22	BA	1905	C	O3'-P	-9.77	1.46	1.61
5	CE	73	VAL	C-N	8.83	1.46	1.33
22	BA	2197	U	O3'-P	-7.99	1.49	1.61

The worst 5 of 1771 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	DA	2586	U	N1-C1'-C2'	-12.98	92.53	112.00
1	AA	1047	G	P-O3'-C3'	-12.81	100.98	120.20
22	BA	627	A	P-O3'-C3'	12.41	138.81	120.20
22	BA	531	C	P-O3'-C3'	12.38	138.77	120.20
22	BA	2424	C	P-O3'-C3'	-12.23	101.86	120.20

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

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	1984	0
2	AB	1705	0	1731	291	0
2	CB	1705	0	1732	245	0
3	AC	1625	0	1699	184	0
3	CC	1625	0	1699	197	0
4	AD	1643	0	1710	258	0
4	CD	1643	0	1710	236	0
5	AE	1106	0	1148	213	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	CE	1106	0	1148	154	0
6	AF	818	0	808	122	0
6	CF	818	0	808	126	0
7	AG	1182	0	1240	130	0
8	AH	979	0	1034	150	0
8	CH	979	0	1034	133	0
9	AI	1022	0	1070	135	0
9	CI	1022	0	1070	167	0
10	AJ	787	0	828	142	0
10	CJ	787	0	828	151	0
11	AK	877	0	887	145	0
11	CK	877	0	887	133	0
12	AL	955	0	1019	131	0
12	CL	955	0	1019	160	0
13	AM	884	0	944	98	0
14	AN	774	0	827	148	0
14	CN	769	0	822	134	0
15	AO	714	0	737	92	0
15	CO	714	0	737	62	0
16	AP	649	0	666	83	0
17	AQ	649	0	691	102	0
17	CQ	649	0	691	113	0
18	AR	456	0	478	59	0
18	CR	456	0	478	60	0
19	AS	638	0	665	75	0
19	CS	638	0	665	109	0
20	AT	665	0	714	99	0
20	CT	665	0	714	92	0
21	AU	426	0	449	119	0
21	CU	426	0	449	97	0
22	BA	61274	0	30819	3243	0
22	DA	60995	0	30679	5238	0
23	BB	2529	0	1281	118	0
24	BC	2083	0	2157	300	0
24	DC	2083	0	2157	357	0
25	BD	1565	0	1616	274	0
25	DD	1565	0	1616	298	0
26	BE	1552	0	1619	212	0
26	DE	1552	0	1619	281	0
27	BF	1411	0	1447	213	0
28	BG	1323	0	1374	221	0
28	DG	1323	0	1374	206	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BH	1111	0	1148	175	0
29	DH	1111	0	1148	181	0
30	BI	1032	0	1088	121	0
30	DI	1032	0	1088	125	0
31	BJ	1129	0	1162	229	0
31	DJ	1129	0	1162	209	0
32	BK	939	0	1012	167	0
32	DK	939	0	1012	190	0
33	BL	1045	0	1117	177	0
33	DL	1045	0	1117	197	0
34	BM	1074	0	1157	153	0
34	DM	1074	0	1157	158	0
35	BN	961	0	1000	132	0
35	DN	961	0	1000	213	0
36	BO	892	0	923	95	0
36	DO	892	0	923	113	0
37	BP	917	0	965	205	0
37	DP	917	0	965	179	0
38	BQ	947	0	1022	196	0
38	DQ	947	0	1022	184	0
39	BR	816	0	839	144	0
39	DR	816	0	839	142	0
40	BS	857	0	922	118	0
40	DS	857	0	922	140	0
41	BT	739	0	807	163	0
41	DT	739	0	807	164	0
42	BU	780	0	834	87	0
42	DU	780	0	834	134	0
43	BV	753	0	780	83	0
43	DV	753	0	780	110	0
44	BW	596	0	610	234	0
44	DW	596	0	610	180	0
45	BX	625	0	655	109	0
45	DX	625	0	655	116	0
46	BY	509	0	543	71	0
46	DY	509	0	543	108	0
47	BZ	449	0	491	60	0
47	DZ	449	0	491	60	0
48	B0	444	0	461	33	0
48	D0	444	0	461	76	0
49	B1	410	0	440	61	0
49	D1	410	0	440	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	B2	377	0	418	42	0
50	D2	377	0	418	68	0
51	B3	504	0	574	54	0
51	D3	504	0	574	68	0
52	B4	302	0	340	48	0
52	D4	302	0	342	42	0
53	CA	32831	0	16521	2402	0
54	CG	1175	0	1230	199	0
55	CM	877	0	937	171	0
56	CP	639	0	656	109	0
57	DB	2507	0	1270	232	0
58	DF	1420	0	1460	295	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	25584	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 54.

The worst 5 of 25584 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:900:A:C2'	22:BA:901:C:H5'	1.40	1.46
2:AB:108:GLN:O	2:AB:110:ILE:N	1.58	1.37
22:BA:1073:A:C2'	22:BA:1074:G:H5''	1.54	1.35
2:CB:93:HIS:CG	2:CB:145:ASN:O	1.88	1.27
28:BG:84:LYS:HG3	28:BG:132:LEU:N	1.49	1.26

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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

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

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

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

5 of 1303 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	152 (84%)	28 (16%)	2	12
2	CB	180/180 (100%)	154 (86%)	26 (14%)	3	15
3	AC	170/170 (100%)	135 (79%)	35 (21%)	1	5
3	CC	170/170 (100%)	155 (91%)	15 (9%)	9	32
4	AD	172/172 (100%)	143 (83%)	29 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/172 (100%)	139 (81%)	33 (19%)	1	6
5	AE	113/113 (100%)	84 (74%)	29 (26%)	0	2
5	CE	113/113 (100%)	88 (78%)	25 (22%)	1	4
6	AF	87/87 (100%)	73 (84%)	14 (16%)	2	12
6	CF	87/87 (100%)	77 (88%)	10 (12%)	5	22
7	AG	124/124 (100%)	107 (86%)	17 (14%)	3	16
8	AH	104/104 (100%)	89 (86%)	15 (14%)	3	15
8	CH	104/104 (100%)	91 (88%)	13 (12%)	4	19
9	AI	105/105 (100%)	89 (85%)	16 (15%)	3	13
9	CI	105/105 (100%)	89 (85%)	16 (15%)	3	13
10	AJ	86/86 (100%)	74 (86%)	12 (14%)	3	16
10	CJ	86/86 (100%)	77 (90%)	9 (10%)	6	25
11	AK	90/90 (100%)	75 (83%)	15 (17%)	2	11
11	CK	90/90 (100%)	76 (84%)	14 (16%)	2	12
12	AL	103/103 (100%)	82 (80%)	21 (20%)	1	5
12	CL	103/103 (100%)	86 (84%)	17 (16%)	2	11
13	AM	92/92 (100%)	87 (95%)	5 (5%)	20	48
14	AN	79/83 (95%)	73 (92%)	6 (8%)	12	38
14	CN	79/83 (95%)	69 (87%)	10 (13%)	4	19
15	AO	76/76 (100%)	68 (90%)	8 (10%)	6	25
15	CO	76/76 (100%)	67 (88%)	9 (12%)	5	21
16	AP	65/65 (100%)	54 (83%)	11 (17%)	2	10
17	AQ	74/74 (100%)	57 (77%)	17 (23%)	1	3
17	CQ	74/74 (100%)	61 (82%)	13 (18%)	2	9
18	AR	48/48 (100%)	45 (94%)	3 (6%)	16	44
18	CR	48/48 (100%)	43 (90%)	5 (10%)	7	25
19	AS	70/70 (100%)	61 (87%)	9 (13%)	4	18
19	CS	70/70 (100%)	65 (93%)	5 (7%)	13	40
20	AT	65/65 (100%)	48 (74%)	17 (26%)	0	2
20	CT	65/65 (100%)	57 (88%)	8 (12%)	4	20
21	AU	44/44 (100%)	36 (82%)	8 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	44/44 (100%)	36 (82%)	8 (18%)	2	8
24	BC	216/216 (100%)	167 (77%)	49 (23%)	1	4
24	DC	216/216 (100%)	182 (84%)	34 (16%)	2	12
25	BD	164/164 (100%)	126 (77%)	38 (23%)	1	3
25	DD	164/164 (100%)	131 (80%)	33 (20%)	1	6
26	BE	165/165 (100%)	122 (74%)	43 (26%)	0	2
26	DE	165/165 (100%)	147 (89%)	18 (11%)	6	23
27	BF	148/148 (100%)	118 (80%)	30 (20%)	1	5
28	BG	137/137 (100%)	106 (77%)	31 (23%)	1	4
28	DG	137/137 (100%)	122 (89%)	15 (11%)	6	23
29	BH	114/114 (100%)	97 (85%)	17 (15%)	3	14
29	DH	114/114 (100%)	102 (90%)	12 (10%)	6	25
30	BI	109/109 (100%)	95 (87%)	14 (13%)	4	19
30	DI	109/109 (100%)	104 (95%)	5 (5%)	24	53
31	BJ	116/116 (100%)	83 (72%)	33 (28%)	0	1
31	DJ	116/116 (100%)	98 (84%)	18 (16%)	2	13
32	BK	103/103 (100%)	74 (72%)	29 (28%)	0	1
32	DK	103/103 (100%)	79 (77%)	24 (23%)	1	3
33	BL	102/102 (100%)	67 (66%)	35 (34%)	0	1
33	DL	102/102 (100%)	88 (86%)	14 (14%)	3	16
34	BM	109/109 (100%)	84 (77%)	25 (23%)	1	4
34	DM	109/109 (100%)	98 (90%)	11 (10%)	7	26
35	BN	100/100 (100%)	84 (84%)	16 (16%)	2	12
35	DN	100/100 (100%)	82 (82%)	18 (18%)	2	8
36	BO	86/86 (100%)	68 (79%)	18 (21%)	1	5
36	DO	86/86 (100%)	79 (92%)	7 (8%)	11	36
37	BP	99/99 (100%)	70 (71%)	29 (29%)	0	1
37	DP	99/99 (100%)	86 (87%)	13 (13%)	4	18
38	BQ	89/89 (100%)	74 (83%)	15 (17%)	2	10
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	3	15
39	BR	84/84 (100%)	58 (69%)	26 (31%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DR	84/84 (100%)	70 (83%)	14 (17%)	2	11
40	BS	93/93 (100%)	67 (72%)	26 (28%)	0	1
40	DS	93/93 (100%)	78 (84%)	15 (16%)	2	12
41	BT	80/80 (100%)	56 (70%)	24 (30%)	0	1
41	DT	80/80 (100%)	73 (91%)	7 (9%)	9	32
42	BU	83/83 (100%)	65 (78%)	18 (22%)	1	5
42	DU	83/83 (100%)	70 (84%)	13 (16%)	2	12
43	BV	78/78 (100%)	60 (77%)	18 (23%)	1	4
43	DV	78/78 (100%)	69 (88%)	9 (12%)	5	22
44	BW	59/59 (100%)	39 (66%)	20 (34%)	0	1
44	DW	59/59 (100%)	44 (75%)	15 (25%)	0	2
45	BX	67/67 (100%)	52 (78%)	15 (22%)	1	4
45	DX	67/67 (100%)	60 (90%)	7 (10%)	7	25
46	BY	55/55 (100%)	43 (78%)	12 (22%)	1	5
46	DY	55/55 (100%)	51 (93%)	4 (7%)	13	39
47	BZ	48/48 (100%)	31 (65%)	17 (35%)	0	0
47	DZ	48/48 (100%)	37 (77%)	11 (23%)	1	4
48	B0	47/47 (100%)	37 (79%)	10 (21%)	1	5
48	D0	47/47 (100%)	41 (87%)	6 (13%)	4	19
49	B1	45/45 (100%)	36 (80%)	9 (20%)	1	6
49	D1	45/45 (100%)	40 (89%)	5 (11%)	6	23
50	B2	38/38 (100%)	32 (84%)	6 (16%)	2	12
50	D2	38/38 (100%)	36 (95%)	2 (5%)	20	49
51	B3	51/51 (100%)	44 (86%)	7 (14%)	3	16
51	D3	51/51 (100%)	40 (78%)	11 (22%)	1	5
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%)	105 (85%)	18 (15%)	3	15
55	CM	91/91 (100%)	81 (89%)	10 (11%)	6	23
56	CP	65/65 (100%)	52 (80%)	13 (20%)	1	6
58	DF	149/149 (100%)	122 (82%)	27 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9331/9339 (100%)	7718 (83%)	1613 (17%)	2 9

5 of 1613 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	B1	16	THR
55	CM	12	LYS
51	D3	27	ASN
2	CB	14	HIS
49	B1	11	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 365 such sidechains are listed below:

Mol	Chain	Res	Type
9	CI	3	ASN
28	DG	37	ASN
10	CJ	70	HIS
19	CS	52	ASN
32	DK	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	507 (33%)	233 (15%)
22	BA	2850/2903 (98%)	980 (34%)	473 (16%)
22	DA	2839/2903 (97%)	1097 (38%)	506 (17%)
23	BB	117/118 (99%)	36 (30%)	18 (15%)
53	CA	1529/1530 (99%)	561 (36%)	236 (15%)
57	DB	116/117 (99%)	39 (33%)	15 (12%)
All	All	8983/9104 (98%)	3220 (35%)	1481 (16%)

5 of 3220 RNA backbone outliers are listed below:

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

5 of 1481 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	CA	1227	A
22	DA	1025	G
53	CA	1498	U
53	CA	1224	U
22	DA	424	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

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

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	CLY	BA	3135	-	-	2/21/53/53	0/2/2/2

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

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

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

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

There are no chirality outliers.

All (2) torsion outliers are listed below:

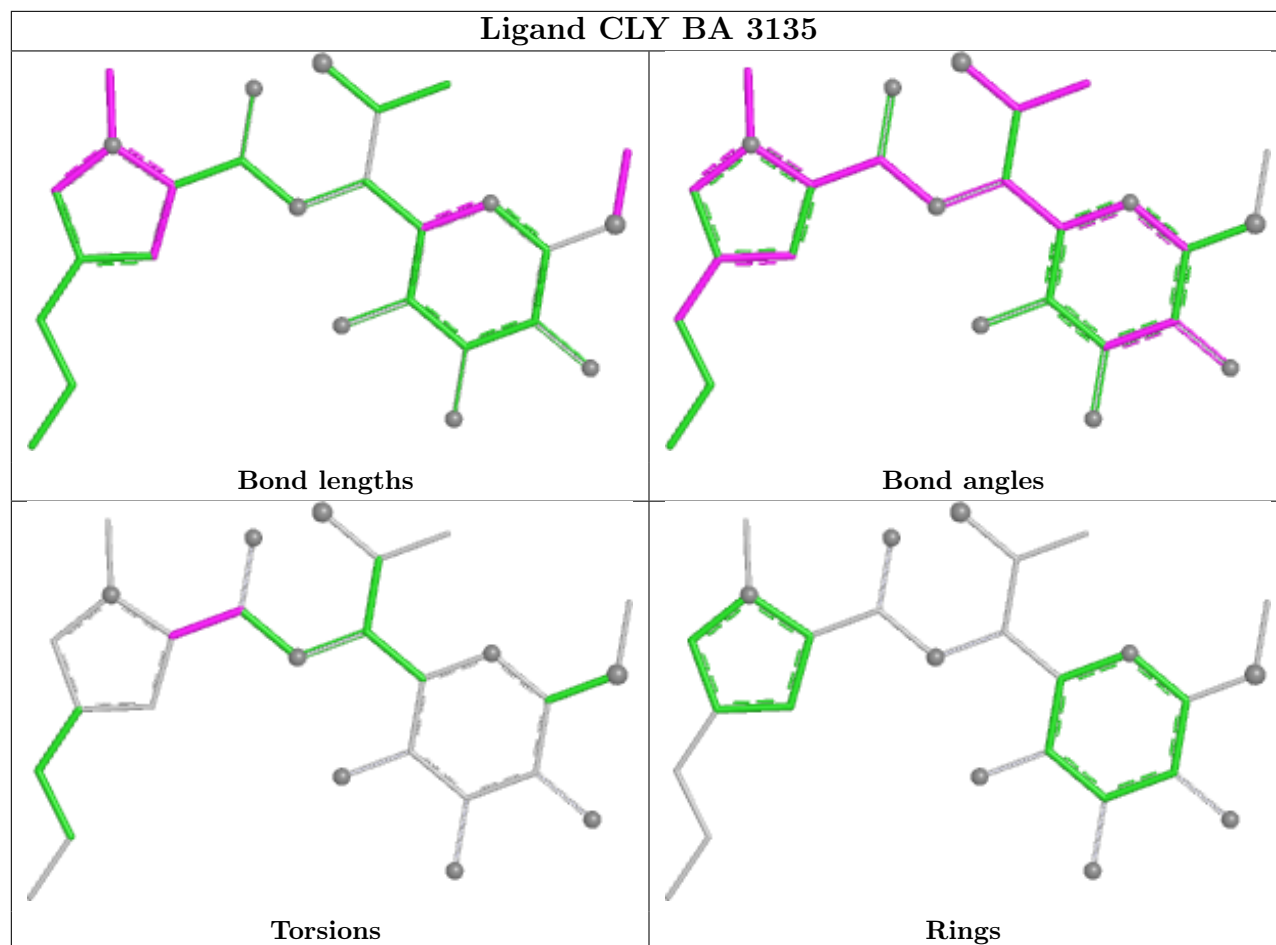
Mol	Chain	Res	Type	Atoms
60	BA	3135	CLY	N1-C10-C11-C12
60	BA	3135	CLY	N1-C10-C11-N2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	3135	CLY	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.39	25 (1%) 70 52	26, 75, 180, 427	0
2	AB	218/218 (100%)	0.55	8 (3%) 45 30	111, 151, 210, 294	0
2	CB	218/218 (100%)	0.87	23 (10%) 11 10	125, 161, 248, 300	0
3	AC	206/206 (100%)	0.14	8 (3%) 43 29	51, 97, 147, 208	0
3	CC	206/206 (100%)	0.65	17 (8%) 17 14	74, 144, 225, 261	0
4	AD	205/205 (100%)	0.26	10 (4%) 35 24	43, 83, 164, 311	0
4	CD	205/205 (100%)	0.28	9 (4%) 39 25	31, 59, 113, 227	0
5	AE	150/150 (100%)	0.50	6 (4%) 42 28	55, 78, 148, 255	0
5	CE	150/150 (100%)	0.89	19 (12%) 8 7	55, 85, 149, 258	0
6	AF	100/100 (100%)	0.34	4 (4%) 42 28	53, 90, 143, 171	0
6	CF	100/100 (100%)	0.54	7 (7%) 22 16	72, 107, 167, 226	0
7	AG	151/151 (100%)	0.73	18 (11%) 9 8	67, 129, 199, 248	0
8	AH	129/129 (100%)	0.09	5 (3%) 43 29	38, 71, 123, 214	0
8	CH	129/129 (100%)	0.69	13 (10%) 12 10	53, 100, 161, 214	0
9	AI	127/127 (100%)	0.91	15 (11%) 9 8	66, 125, 243, 279	0
9	CI	127/127 (100%)	1.62	40 (31%) 1 1	111, 184, 282, 308	0
10	AJ	98/98 (100%)	0.59	9 (9%) 14 11	60, 114, 210, 262	0
10	CJ	98/98 (100%)	1.47	23 (23%) 2 2	103, 188, 266, 292	0
11	AK	117/117 (100%)	0.18	2 (1%) 69 50	36, 98, 174, 203	0
11	CK	117/117 (100%)	0.33	5 (4%) 40 26	55, 104, 165, 196	0
12	AL	123/123 (100%)	0.11	9 (7%) 21 16	15, 54, 116, 167	0
12	CL	123/123 (100%)	0.51	12 (9%) 13 11	36, 73, 121, 188	0
13	AM	114/114 (100%)	0.65	9 (7%) 18 14	76, 125, 196, 274	0
14	AN	96/100 (96%)	1.02	19 (19%) 3 2	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%)	1.77	36 (37%) 1 1	109, 221, 327, 373	0
15	AO	88/88 (100%)	-0.01	1 (1%) 78 61	36, 70, 123, 182	0
15	CO	88/88 (100%)	0.64	4 (4%) 38 25	59, 103, 158, 277	0
16	AP	82/82 (100%)	0.34	2 (2%) 59 40	44, 74, 148, 243	0
17	AQ	80/80 (100%)	0.36	6 (7%) 20 15	29, 78, 141, 267	0
17	CQ	80/80 (100%)	0.95	12 (15%) 5 5	48, 106, 161, 199	0
18	AR	55/55 (100%)	0.27	5 (9%) 15 12	60, 86, 161, 196	0
18	CR	55/55 (100%)	0.41	3 (5%) 30 21	47, 92, 186, 230	0
19	AS	79/79 (100%)	0.99	11 (13%) 6 5	79, 127, 199, 277	0
19	CS	79/79 (100%)	1.43	25 (31%) 1 1	181, 371, 451, 469	0
20	AT	85/85 (100%)	0.39	7 (8%) 17 14	43, 76, 116, 143	0
20	CT	85/85 (100%)	1.27	21 (24%) 2 1	58, 117, 197, 268	0
21	AU	51/51 (100%)	1.65	18 (35%) 1 1	88, 157, 204, 230	0
21	CU	51/51 (100%)	1.04	7 (13%) 6 6	58, 111, 182, 320	0
22	BA	2854/2903 (98%)	-0.71	48 (1%) 69 50	4, 28, 155, 403	0
22	DA	2841/2903 (97%)	1.06	413 (14%) 6 5	49, 122, 252, 460	0
23	BB	118/118 (100%)	-0.62	0 100 100	13, 43, 77, 106	0
24	BC	271/271 (100%)	-0.00	7 (2%) 57 38	5, 39, 81, 171	0
24	DC	271/271 (100%)	1.36	67 (24%) 2 1	51, 96, 147, 192	0
25	BD	209/209 (100%)	-0.30	2 (0%) 79 63	3, 23, 72, 171	0
25	DD	209/209 (100%)	1.41	54 (25%) 1 1	50, 111, 176, 290	0
26	BE	201/201 (100%)	-0.31	0 100 100	2, 37, 98, 185	0
26	DE	201/201 (100%)	2.38	109 (54%) 0 0	62, 197, 394, 486	0
27	BF	177/177 (100%)	0.01	2 (1%) 78 61	27, 70, 127, 197	0
28	BG	176/176 (100%)	0.09	9 (5%) 33 23	23, 60, 119, 204	0
28	DG	176/176 (100%)	1.14	31 (17%) 4 3	95, 195, 279, 335	0
29	BH	149/149 (100%)	1.23	36 (24%) 2 1	40, 177, 291, 362	0
29	DH	149/149 (100%)	1.93	59 (39%) 1 1	82, 181, 277, 319	0
30	BI	141/141 (100%)	1.50	32 (22%) 2 2	162, 269, 338, 374	0
30	DI	141/141 (100%)	0.90	12 (8%) 16 13	210, 324, 369, 408	0
31	BJ	142/142 (100%)	-0.22	5 (3%) 47 31	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%)	1.21	30 (21%) 2 2	63, 102, 163, 184	0
32	BK	122/122 (100%)	-0.25	2 (1%) 70 52	7, 26, 74, 263	0
32	DK	122/122 (100%)	0.99	18 (14%) 5 5	52, 95, 164, 236	0
33	BL	143/143 (100%)	-0.12	2 (1%) 73 55	3, 35, 77, 103	0
33	DL	143/143 (100%)	2.16	64 (44%) 0 0	58, 159, 278, 348	0
34	BM	136/136 (100%)	-0.38	0 100 100	4, 26, 66, 135	0
34	DM	136/136 (100%)	1.01	24 (17%) 4 3	44, 105, 164, 196	0
35	BN	120/120 (100%)	-0.40	1 (0%) 82 68	6, 20, 43, 151	0
35	DN	120/120 (100%)	1.84	43 (35%) 1 1	79, 127, 200, 268	0
36	BO	116/116 (100%)	-0.01	1 (0%) 81 65	26, 43, 77, 126	0
36	DO	116/116 (100%)	1.25	29 (25%) 2 1	124, 168, 240, 292	0
37	BP	114/114 (100%)	-0.24	2 (1%) 67 49	9, 35, 83, 148	0
37	DP	114/114 (100%)	1.31	21 (18%) 3 3	62, 114, 174, 238	0
38	BQ	117/117 (100%)	-0.34	2 (1%) 69 50	3, 16, 43, 199	0
38	DQ	117/117 (100%)	1.66	42 (35%) 1 1	66, 103, 194, 288	0
39	BR	103/103 (100%)	-0.21	3 (2%) 53 35	4, 31, 80, 180	0
39	DR	103/103 (100%)	1.60	28 (27%) 1 1	67, 130, 227, 316	0
40	BS	110/110 (100%)	-0.42	0 100 100	4, 17, 52, 175	0
40	DS	110/110 (100%)	1.98	45 (40%) 0 1	59, 130, 231, 279	0
41	BT	93/93 (100%)	0.49	8 (8%) 16 13	19, 43, 128, 185	0
41	DT	93/93 (100%)	2.70	63 (67%) 0 0	123, 205, 306, 347	0
42	BU	102/102 (100%)	0.19	1 (0%) 79 63	18, 49, 120, 241	0
42	DU	102/102 (100%)	3.69	83 (81%) 0 0	123, 285, 434, 557	0
43	BV	94/94 (100%)	-0.12	0 100 100	15, 43, 86, 142	0
43	DV	94/94 (100%)	0.33	3 (3%) 50 34	97, 143, 194, 233	0
44	BW	79/79 (100%)	0.41	9 (11%) 10 9	10, 30, 105, 223	0
44	DW	79/79 (100%)	2.32	41 (51%) 0 0	82, 140, 238, 284	0
45	BX	77/77 (100%)	-0.07	1 (1%) 75 56	11, 42, 84, 117	0
45	DX	77/77 (100%)	2.24	39 (50%) 0 0	78, 117, 171, 236	0
46	BY	63/63 (100%)	0.55	6 (9%) 14 11	30, 66, 136, 222	0
46	DY	63/63 (100%)	2.61	35 (55%) 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%)	-0.29	0 100 100	8, 22, 56, 111	0
47	DZ	58/58 (100%)	1.22	12 (20%) 2 2	78, 119, 208, 217	0
48	B0	56/56 (100%)	-0.33	1 (1%) 67 49	3, 24, 70, 159	0
48	D0	56/56 (100%)	1.59	12 (21%) 2 2	63, 139, 242, 298	0
49	B1	50/50 (100%)	-0.14	1 (2%) 65 46	22, 48, 99, 165	0
49	D1	50/50 (100%)	1.49	15 (30%) 1 1	99, 170, 210, 236	0
50	B2	46/46 (100%)	-0.04	1 (2%) 62 43	7, 26, 52, 155	0
50	D2	46/46 (100%)	2.20	23 (50%) 0 0	81, 118, 175, 233	0
51	B3	64/64 (100%)	-0.41	0 100 100	5, 23, 44, 70	0
51	D3	64/64 (100%)	2.64	38 (59%) 0 0	65, 128, 183, 257	0
52	B4	38/38 (100%)	0.06	1 (2%) 57 38	21, 45, 86, 124	0
52	D4	38/38 (100%)	2.63	26 (68%) 0 0	79, 137, 187, 227	0
53	CA	1530/1530 (100%)	0.41	81 (5%) 32 22	34, 102, 281, 444	0
54	CG	150/150 (100%)	1.59	47 (31%) 1 1	107, 224, 298, 322	0
55	CM	113/113 (100%)	1.74	35 (30%) 1 1	182, 402, 494, 538	0
56	CP	80/80 (100%)	1.06	14 (17%) 4 4	51, 94, 155, 236	0
57	DB	117/117 (100%)	0.46	2 (1%) 69 50	95, 169, 224, 274	0
58	DF	178/178 (100%)	0.83	16 (8%) 15 12	183, 225, 286, 338	0
All	All	20431/20551 (99%)	0.48	2330 (11%) 10 9	2, 94, 269, 557	0

The worst 5 of 2330 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	DU	30	SER	15.7
26	DE	103	GLY	11.9
26	DE	104	ALA	10.6
37	DP	109	ILE	10.5
38	DQ	7	VAL	10.4

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	DA	3129	1/1	0.24	0.23	233,233,233,233	0
59	MG	DA	3062	1/1	0.26	0.60	211,211,211,211	0
59	MG	DA	3003	1/1	0.27	0.21	236,236,236,236	0
59	MG	DA	3108	1/1	0.34	0.23	185,185,185,185	0
59	MG	DA	3124	1/1	0.36	0.46	176,176,176,176	0
59	MG	DA	3018	1/1	0.39	0.23	226,226,226,226	0
59	MG	DA	3019	1/1	0.40	0.38	247,247,247,247	0
59	MG	CA	1627	1/1	0.47	0.25	181,181,181,181	0
59	MG	CA	1602	1/1	0.50	0.27	175,175,175,175	0
59	MG	CA	1622	1/1	0.50	0.13	226,226,226,226	0
59	MG	DJ	201	1/1	0.53	0.26	230,230,230,230	0
59	MG	DA	3057	1/1	0.55	0.20	227,227,227,227	0
59	MG	DC	301	1/1	0.59	0.20	145,145,145,145	0
59	MG	DA	3122	1/1	0.62	0.18	153,153,153,153	0
59	MG	CA	1619	1/1	0.63	0.17	214,214,214,214	0
59	MG	DA	3010	1/1	0.63	0.31	218,218,218,218	0
59	MG	CA	1616	1/1	0.65	0.14	254,254,254,254	0
59	MG	DA	3027	1/1	0.65	0.36	253,253,253,253	0
59	MG	DA	3105	1/1	0.65	0.24	262,262,262,262	0
59	MG	DA	3119	1/1	0.67	0.15	93,93,93,93	0
59	MG	BB	201	1/1	0.68	0.12	222,222,222,222	0
59	MG	DA	3007	1/1	0.68	0.12	254,254,254,254	0
59	MG	DA	3110	1/1	0.68	0.13	153,153,153,153	0
59	MG	DA	3021	1/1	0.69	0.24	199,199,199,199	0
59	MG	DA	3109	1/1	0.69	0.11	174,174,174,174	0
59	MG	DA	3107	1/1	0.69	0.18	161,161,161,161	0
59	MG	DA	3073	1/1	0.70	0.56	274,274,274,274	0
59	MG	CA	1628	1/1	0.70	0.19	260,260,260,260	0
59	MG	DA	3015	1/1	0.70	0.16	183,183,183,183	0
59	MG	DA	3132	1/1	0.71	0.21	174,174,174,174	0
59	MG	DA	3048	1/1	0.72	0.09	218,218,218,218	0
59	MG	DA	3013	1/1	0.72	0.17	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3114	1/1	0.73	0.28	167,167,167,167	0
59	MG	DC	302	1/1	0.73	0.13	129,129,129,129	0
59	MG	DA	3061	1/1	0.73	0.35	229,229,229,229	0
59	MG	DA	3005	1/1	0.75	0.23	309,309,309,309	0
59	MG	DA	3025	1/1	0.76	0.41	278,278,278,278	0
59	MG	CA	1607	1/1	0.77	0.11	121,121,121,121	0
59	MG	CA	1601	1/1	0.77	0.15	156,156,156,156	0
59	MG	DA	3049	1/1	0.78	0.15	172,172,172,172	0
59	MG	DE	301	1/1	0.78	0.26	131,131,131,131	0
59	MG	DA	3117	1/1	0.78	0.12	71,71,71,71	0
59	MG	CA	1629	1/1	0.79	0.13	197,197,197,197	0
59	MG	DA	3052	1/1	0.79	0.14	89,89,89,89	0
59	MG	DA	3006	1/1	0.79	0.15	211,211,211,211	0
59	MG	DA	3001	1/1	0.79	0.16	151,151,151,151	0
59	MG	DA	3042	1/1	0.79	0.12	161,161,161,161	0
59	MG	DA	3063	1/1	0.79	0.16	278,278,278,278	0
59	MG	AA	1618	1/1	0.79	0.24	197,197,197,197	0
59	MG	DA	3087	1/1	0.79	0.16	179,179,179,179	0
59	MG	CA	1639	1/1	0.80	0.10	165,165,165,165	0
59	MG	DA	3091	1/1	0.80	0.18	116,116,116,116	0
59	MG	CA	1623	1/1	0.81	0.15	124,124,124,124	0
59	MG	CA	1632	1/1	0.81	0.12	156,156,156,156	0
59	MG	DA	3017	1/1	0.81	0.16	204,204,204,204	0
59	MG	DA	3131	1/1	0.81	0.20	212,212,212,212	0
59	MG	DA	3044	1/1	0.81	0.10	156,156,156,156	0
59	MG	AA	1629	1/1	0.81	0.13	180,180,180,180	0
59	MG	AA	1610	1/1	0.81	0.12	190,190,190,190	0
59	MG	DA	3090	1/1	0.81	0.20	165,165,165,165	0
59	MG	DA	3002	1/1	0.81	0.17	180,180,180,180	0
59	MG	CA	1631	1/1	0.82	0.18	93,93,93,93	0
59	MG	BA	3129	1/1	0.82	0.46	214,214,214,214	0
59	MG	BA	3024	1/1	0.82	0.29	166,166,166,166	0
59	MG	BA	3047	1/1	0.82	0.15	111,111,111,111	0
59	MG	BA	3068	1/1	0.83	0.10	117,117,117,117	0
59	MG	DA	3092	1/1	0.83	0.15	229,229,229,229	0
59	MG	AA	1617	1/1	0.83	0.11	115,115,115,115	0
59	MG	DA	3075	1/1	0.83	0.22	174,174,174,174	0
59	MG	AA	1630	1/1	0.83	0.14	189,189,189,189	0
59	MG	CA	1634	1/1	0.83	0.11	131,131,131,131	0
59	MG	DA	3126	1/1	0.83	0.23	200,200,200,200	0
59	MG	DA	3082	1/1	0.84	0.10	197,197,197,197	0
59	MG	CA	1614	1/1	0.84	0.16	210,210,210,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3056	1/1	0.84	0.30	197,197,197,197	0
59	MG	CA	1625	1/1	0.84	0.12	100,100,100,100	0
59	MG	DA	3024	1/1	0.84	0.14	89,89,89,89	0
59	MG	DA	3097	1/1	0.84	0.13	144,144,144,144	0
59	MG	DA	3128	1/1	0.85	0.44	214,214,214,214	0
59	MG	DA	3081	1/1	0.85	0.12	142,142,142,142	0
59	MG	CA	1618	1/1	0.85	0.08	113,113,113,113	0
59	MG	DA	3068	1/1	0.85	0.20	209,209,209,209	0
59	MG	CA	1636	1/1	0.86	0.17	181,181,181,181	0
59	MG	CA	1620	1/1	0.86	0.11	168,168,168,168	0
59	MG	DA	3071	1/1	0.86	0.12	133,133,133,133	0
59	MG	DA	3112	1/1	0.86	0.13	131,131,131,131	0
59	MG	DA	3046	1/1	0.86	0.14	151,151,151,151	0
59	MG	CA	1617	1/1	0.86	0.09	199,199,199,199	0
59	MG	DA	3077	1/1	0.86	0.17	222,222,222,222	0
59	MG	DA	3078	1/1	0.86	0.20	180,180,180,180	0
59	MG	DA	3037	1/1	0.86	0.11	197,197,197,197	0
59	MG	CA	1624	1/1	0.87	0.22	165,165,165,165	0
59	MG	CA	1610	1/1	0.87	0.10	152,152,152,152	0
59	MG	DA	3083	1/1	0.87	0.15	204,204,204,204	0
59	MG	DA	3099	1/1	0.87	0.21	68,68,68,68	0
59	MG	AA	1619	1/1	0.87	0.11	156,156,156,156	0
59	MG	AA	1636	1/1	0.87	0.14	124,124,124,124	0
59	MG	CA	1615	1/1	0.88	0.08	172,172,172,172	0
59	MG	BA	3110	1/1	0.88	0.17	92,92,92,92	0
59	MG	DA	3032	1/1	0.88	0.12	121,121,121,121	0
59	MG	DA	3074	1/1	0.88	0.24	190,190,190,190	0
59	MG	AA	1614	1/1	0.88	0.32	194,194,194,194	0
59	MG	BA	3131	1/1	0.88	0.16	154,154,154,154	0
59	MG	DA	3094	1/1	0.89	0.11	107,107,107,107	0
59	MG	DA	3096	1/1	0.89	0.14	102,102,102,102	0
59	MG	BA	3117	1/1	0.89	0.15	157,157,157,157	0
59	MG	DA	3038	1/1	0.89	0.09	102,102,102,102	0
59	MG	BA	3055	1/1	0.89	0.23	205,205,205,205	0
59	MG	AA	1627	1/1	0.89	0.11	132,132,132,132	0
59	MG	DA	3070	1/1	0.89	0.09	56,56,56,56	0
59	MG	AA	1612	1/1	0.89	0.10	105,105,105,105	0
59	MG	BA	3011	1/1	0.90	0.22	102,102,102,102	0
59	MG	AA	1631	1/1	0.90	0.08	91,91,91,91	0
59	MG	CA	1637	1/1	0.90	0.15	74,74,74,74	0
59	MG	DA	3034	1/1	0.90	0.18	125,125,125,125	0
59	MG	DA	3086	1/1	0.90	0.07	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	DA	3035	1/1	0.90	0.13	194,194,194,194	0
59	MG	DA	3098	1/1	0.90	0.11	172,172,172,172	0
59	MG	DA	3033	1/1	0.91	0.12	95,95,95,95	0
59	MG	DA	3085	1/1	0.91	0.08	87,87,87,87	0
59	MG	BA	3111	1/1	0.91	0.17	77,77,77,77	0
59	MG	DA	3011	1/1	0.91	0.12	127,127,127,127	0
59	MG	DB	201	1/1	0.91	0.09	104,104,104,104	0
59	MG	CA	1603	1/1	0.91	0.24	162,162,162,162	0
59	MG	DA	3080	1/1	0.91	0.18	108,108,108,108	0
59	MG	DA	3072	1/1	0.91	0.08	187,187,187,187	0
59	MG	BA	3069	1/1	0.91	0.17	151,151,151,151	0
59	MG	DA	3084	1/1	0.92	0.16	144,144,144,144	0
59	MG	AA	1628	1/1	0.92	0.08	69,69,69,69	0
59	MG	DA	3008	1/1	0.92	0.12	148,148,148,148	0
59	MG	AA	1639	1/1	0.92	0.09	108,108,108,108	0
59	MG	DA	3059	1/1	0.92	0.44	200,200,200,200	0
59	MG	AN	201	1/1	0.92	0.09	159,159,159,159	0
59	MG	BA	3003	1/1	0.92	0.10	69,69,69,69	0
59	MG	AA	1608	1/1	0.92	0.18	68,68,68,68	0
59	MG	DA	3030	1/1	0.92	0.08	68,68,68,68	0
59	MG	DA	3016	1/1	0.92	0.11	87,87,87,87	0
59	MG	BA	3090	1/1	0.92	0.16	128,128,128,128	0
59	MG	BA	3014	1/1	0.93	0.09	68,68,68,68	0
59	MG	DA	3040	1/1	0.93	0.05	70,70,70,70	0
59	MG	DA	3125	1/1	0.93	0.12	82,82,82,82	0
59	MG	BA	3056	1/1	0.93	0.24	169,169,169,169	0
59	MG	DA	3127	1/1	0.93	0.13	142,142,142,142	0
59	MG	BA	3060	1/1	0.93	0.22	210,210,210,210	0
59	MG	DA	3029	1/1	0.93	0.12	112,112,112,112	0
59	MG	AA	1626	1/1	0.93	0.15	117,117,117,117	0
59	MG	DA	3004	1/1	0.93	0.12	114,114,114,114	0
59	MG	CA	1612	1/1	0.93	0.17	136,136,136,136	0
59	MG	BA	3046	1/1	0.93	0.11	149,149,149,149	0
59	MG	BA	3086	1/1	0.93	0.10	131,131,131,131	0
59	MG	DA	3036	1/1	0.93	0.12	82,82,82,82	0
59	MG	AA	1638	1/1	0.93	0.10	116,116,116,116	0
59	MG	DA	3111	1/1	0.94	0.10	109,109,109,109	0
59	MG	BA	3133	1/1	0.94	0.11	139,139,139,139	0
59	MG	DA	3047	1/1	0.94	0.09	95,95,95,95	0
59	MG	DA	3089	1/1	0.94	0.05	99,99,99,99	0
59	MG	DA	3118	1/1	0.94	0.08	76,76,76,76	0
59	MG	BA	3001	1/1	0.94	0.10	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1635	1/1	0.94	0.08	194,194,194,194	0
59	MG	DA	3050	1/1	0.94	0.09	106,106,106,106	0
59	MG	DA	3026	1/1	0.94	0.09	109,109,109,109	0
59	MG	BA	3124	1/1	0.94	0.07	25,25,25,25	0
59	MG	DA	3028	1/1	0.94	0.22	143,143,143,143	0
59	MG	DA	3079	1/1	0.94	0.10	142,142,142,142	0
59	MG	DA	3058	1/1	0.94	0.13	204,204,204,204	0
59	MG	DA	3130	1/1	0.94	0.12	85,85,85,85	0
59	MG	DA	3100	1/1	0.94	0.08	78,78,78,78	0
59	MG	DA	3103	1/1	0.94	0.14	44,44,44,44	0
59	MG	CA	1641	1/1	0.94	0.15	79,79,79,79	0
59	MG	DA	3041	1/1	0.94	0.10	82,82,82,82	0
59	MG	BA	3097	1/1	0.94	0.11	45,45,45,45	0
59	MG	BA	3085	1/1	0.94	0.07	100,100,100,100	0
59	MG	DA	3045	1/1	0.94	0.10	78,78,78,78	0
59	MG	CA	1633	1/1	0.95	0.10	63,63,63,63	0
59	MG	BA	3072	1/1	0.95	0.12	139,139,139,139	0
59	MG	BA	3109	1/1	0.95	0.18	124,124,124,124	0
59	MG	BA	3074	1/1	0.95	0.10	93,93,93,93	0
59	MG	CA	1638	1/1	0.95	0.07	130,130,130,130	0
59	MG	BA	3076	1/1	0.95	0.11	114,114,114,114	0
59	MG	CA	1640	1/1	0.95	0.12	157,157,157,157	0
59	MG	DA	3093	1/1	0.95	0.14	114,114,114,114	0
59	MG	AA	1607	1/1	0.95	0.09	103,103,103,103	0
59	MG	DA	3113	1/1	0.95	0.11	148,148,148,148	0
59	MG	AA	1602	1/1	0.95	0.08	152,152,152,152	0
59	MG	CA	1630	1/1	0.95	0.08	131,131,131,131	0
59	MG	BA	3058	1/1	0.95	0.15	107,107,107,107	0
59	MG	BA	3096	1/1	0.95	0.17	102,102,102,102	0
59	MG	DA	3121	1/1	0.95	0.07	84,84,84,84	0
59	MG	DA	3014	1/1	0.96	0.24	172,172,172,172	0
59	MG	CA	1613	1/1	0.96	0.07	105,105,105,105	0
59	MG	DA	3076	1/1	0.96	0.06	93,93,93,93	0
59	MG	AA	1615	1/1	0.96	0.06	120,120,120,120	0
59	MG	BA	3026	1/1	0.96	0.10	133,133,133,133	0
59	MG	BA	3033	1/1	0.96	0.18	162,162,162,162	0
59	MG	BA	3002	1/1	0.96	0.09	85,85,85,85	0
59	MG	BA	3070	1/1	0.96	0.07	53,53,53,53	0
59	MG	DA	3101	1/1	0.96	0.06	67,67,67,67	0
59	MG	BA	3100	1/1	0.96	0.23	89,89,89,89	0
59	MG	DA	3104	1/1	0.96	0.07	47,47,47,47	0
59	MG	BA	3105	1/1	0.96	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3106	1/1	0.96	0.14	92,92,92,92	0
59	MG	CA	1635	1/1	0.96	0.09	95,95,95,95	0
59	MG	DA	3067	1/1	0.96	0.08	83,83,83,83	0
59	MG	AA	1609	1/1	0.96	0.06	46,46,46,46	0
59	MG	AA	1640	1/1	0.96	0.09	154,154,154,154	0
59	MG	AA	1603	1/1	0.96	0.07	111,111,111,111	0
59	MG	BA	3081	1/1	0.96	0.14	86,86,86,86	0
59	MG	DA	3031	1/1	0.96	0.08	105,105,105,105	0
59	MG	BA	3035	1/1	0.97	0.28	171,171,171,171	0
59	MG	DA	3060	1/1	0.97	0.12	105,105,105,105	0
59	MG	DA	3012	1/1	0.97	0.06	64,64,64,64	0
59	MG	BA	3134	1/1	0.97	0.17	219,219,219,219	0
59	MG	DA	3115	1/1	0.97	0.12	65,65,65,65	0
59	MG	BA	3059	1/1	0.97	0.17	190,190,190,190	0
59	MG	DA	3065	1/1	0.97	0.09	49,49,49,49	0
59	MG	BB	202	1/1	0.97	0.06	50,50,50,50	0
59	MG	BL	201	1/1	0.97	0.07	53,53,53,53	0
59	MG	AA	1622	1/1	0.97	0.05	76,76,76,76	0
59	MG	BA	3082	1/1	0.97	0.11	114,114,114,114	0
59	MG	AA	1604	1/1	0.97	0.08	124,124,124,124	0
59	MG	DA	3043	1/1	0.97	0.12	100,100,100,100	0
59	MG	CA	1604	1/1	0.97	0.05	74,74,74,74	0
59	MG	DA	3022	1/1	0.97	0.04	69,69,69,69	0
59	MG	BA	3054	1/1	0.97	0.13	189,189,189,189	0
59	MG	CA	1608	1/1	0.97	0.12	41,41,41,41	0
59	MG	CA	1609	1/1	0.97	0.05	83,83,83,83	0
59	MG	BA	3088	1/1	0.97	0.07	50,50,50,50	0
59	MG	CA	1611	1/1	0.97	0.09	112,112,112,112	0
59	MG	AA	1606	1/1	0.97	0.07	62,62,62,62	0
59	MG	BA	3091	1/1	0.97	0.06	32,32,32,32	0
59	MG	DA	3009	1/1	0.97	0.06	69,69,69,69	0
59	MG	AA	1637	1/1	0.97	0.08	27,27,27,27	0
60	CLY	BA	3135	27/27	0.97	0.10	11,17,22,22	0
61	ZN	D4	101	1/1	0.97	0.07	161,161,161,161	0
59	MG	BA	3044	1/1	0.98	0.07	12,12,12,12	0
59	MG	BA	3007	1/1	0.98	0.07	80,80,80,80	0
59	MG	AA	1616	1/1	0.98	0.06	98,98,98,98	0
59	MG	AA	1620	1/1	0.98	0.05	117,117,117,117	0
59	MG	BA	3077	1/1	0.98	0.04	30,30,30,30	0
59	MG	CA	1621	1/1	0.98	0.19	46,46,46,46	0
59	MG	AA	1605	1/1	0.98	0.08	39,39,39,39	0
59	MG	DA	3088	1/1	0.98	0.09	87,87,87,87	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	0.98	0.04	102,102,102,102	0
59	MG	DA	3064	1/1	0.98	0.07	70,70,70,70	0
59	MG	DA	3120	1/1	0.98	0.14	109,109,109,109	0
59	MG	DA	3020	1/1	0.98	0.12	49,49,49,49	0
59	MG	DA	3066	1/1	0.98	0.05	61,61,61,61	0
59	MG	CA	1606	1/1	0.98	0.05	64,64,64,64	0
59	MG	BA	3112	1/1	0.98	0.07	47,47,47,47	0
59	MG	DA	3095	1/1	0.98	0.07	95,95,95,95	0
59	MG	DA	3069	1/1	0.98	0.09	69,69,69,69	0
59	MG	BA	3027	1/1	0.98	0.10	46,46,46,46	0
59	MG	BA	3119	1/1	0.98	0.09	51,51,51,51	0
59	MG	BA	3028	1/1	0.98	0.10	77,77,77,77	0
59	MG	BA	3030	1/1	0.98	0.05	21,21,21,21	0
59	MG	BA	3130	1/1	0.98	0.17	97,97,97,97	0
59	MG	DA	3102	1/1	0.98	0.11	86,86,86,86	0
59	MG	BA	3089	1/1	0.98	0.06	80,80,80,80	0
59	MG	AA	1613	1/1	0.98	0.05	56,56,56,56	0
59	MG	BA	3004	1/1	0.98	0.09	138,138,138,138	0
59	MG	DA	3053	1/1	0.98	0.04	67,67,67,67	0
59	MG	DA	3054	1/1	0.98	0.06	96,96,96,96	0
61	ZN	B4	101	1/1	0.98	0.08	80,80,80,80	0
59	MG	DA	3055	1/1	0.98	0.09	120,120,120,120	0
59	MG	BA	3061	1/1	0.99	0.05	20,20,20,20	0
59	MG	BA	3062	1/1	0.99	0.05	11,11,11,11	0
59	MG	BA	3065	1/1	0.99	0.03	17,17,17,17	0
59	MG	BB	203	1/1	0.99	0.03	17,17,17,17	0
59	MG	BB	204	1/1	0.99	0.06	41,41,41,41	0
59	MG	BA	3066	1/1	0.99	0.04	10,10,10,10	0
59	MG	BA	3022	1/1	0.99	0.04	8,8,8,8	0
59	MG	AA	1611	1/1	0.99	0.04	62,62,62,62	0
59	MG	BA	3025	1/1	0.99	0.09	26,26,26,26	0
59	MG	AA	1601	1/1	0.99	0.08	70,70,70,70	0
59	MG	DA	3023	1/1	0.99	0.03	87,87,87,87	0
59	MG	CA	1605	1/1	0.99	0.09	37,37,37,37	0
59	MG	BA	3073	1/1	0.99	0.07	8,8,8,8	0
59	MG	AA	1624	1/1	0.99	0.06	82,82,82,82	0
59	MG	BA	3075	1/1	0.99	0.04	29,29,29,29	0
59	MG	AA	1632	1/1	0.99	0.09	76,76,76,76	0
59	MG	BA	3029	1/1	0.99	0.10	3,3,3,3	0
59	MG	BA	3078	1/1	0.99	0.05	20,20,20,20	0
59	MG	BA	3080	1/1	0.99	0.04	34,34,34,34	0
59	MG	AA	1633	1/1	0.99	0.05	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3032	1/1	0.99	0.10	3,3,3,3	0
59	MG	BA	3083	1/1	0.99	0.03	28,28,28,28	0
59	MG	BA	3084	1/1	0.99	0.02	13,13,13,13	0
59	MG	BA	3005	1/1	0.99	0.05	87,87,87,87	0
59	MG	AA	1634	1/1	0.99	0.04	72,72,72,72	0
59	MG	BA	3087	1/1	0.99	0.03	35,35,35,35	0
59	MG	DA	3039	1/1	0.99	0.06	65,65,65,65	0
59	MG	BA	3037	1/1	0.99	0.03	5,5,5,5	0
59	MG	BA	3038	1/1	0.99	0.05	31,31,31,31	0
59	MG	BA	3041	1/1	0.99	0.03	13,13,13,13	0
59	MG	BA	3042	1/1	0.99	0.04	41,41,41,41	0
59	MG	BA	3092	1/1	0.99	0.04	56,56,56,56	0
59	MG	BA	3094	1/1	0.99	0.04	9,9,9,9	0
59	MG	CA	1626	1/1	0.99	0.11	23,23,23,23	0
59	MG	BA	3095	1/1	0.99	0.05	77,77,77,77	0
59	MG	BA	3008	1/1	0.99	0.05	7,7,7,7	0
59	MG	BA	3045	1/1	0.99	0.06	17,17,17,17	0
59	MG	BA	3010	1/1	0.99	0.04	29,29,29,29	0
59	MG	DA	3051	1/1	0.99	0.07	57,57,57,57	0
59	MG	BA	3102	1/1	0.99	0.12	3,3,3,3	0
59	MG	DA	3116	1/1	0.99	0.11	77,77,77,77	0
59	MG	BA	3103	1/1	0.99	0.06	4,4,4,4	0
59	MG	AA	1641	1/1	0.99	0.09	22,22,22,22	0
59	MG	BA	3107	1/1	0.99	0.08	5,5,5,5	0
59	MG	BA	3108	1/1	0.99	0.04	48,48,48,48	0
59	MG	BA	3049	1/1	0.99	0.06	66,66,66,66	0
59	MG	BA	3050	1/1	0.99	0.03	10,10,10,10	0
59	MG	DA	3123	1/1	0.99	0.07	61,61,61,61	0
59	MG	BA	3051	1/1	0.99	0.04	58,58,58,58	0
59	MG	BA	3053	1/1	0.99	0.04	31,31,31,31	0
59	MG	BA	3113	1/1	0.99	0.05	114,114,114,114	0
59	MG	BA	3116	1/1	0.99	0.06	76,76,76,76	0
59	MG	CA	1642	1/1	0.99	0.05	82,82,82,82	0
59	MG	AA	1642	1/1	0.99	0.04	37,37,37,37	0
59	MG	BA	3118	1/1	0.99	0.07	11,11,11,11	0
59	MG	BA	3015	1/1	0.99	0.07	55,55,55,55	0
59	MG	BA	3121	1/1	0.99	0.06	15,15,15,15	0
59	MG	BA	3122	1/1	0.99	0.14	137,137,137,137	0
59	MG	BA	3123	1/1	0.99	0.07	11,11,11,11	0
59	MG	BA	3016	1/1	0.99	0.03	2,2,2,2	0
59	MG	BA	3126	1/1	0.99	0.05	9,9,9,9	0
59	MG	BA	3057	1/1	0.99	0.04	48,48,48,48	0

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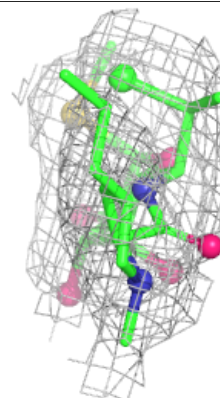
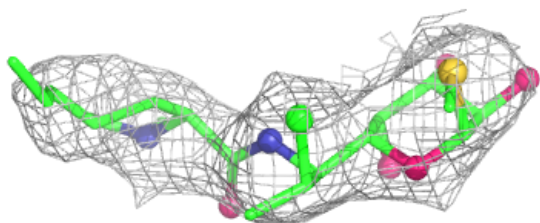
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3019	1/1	0.99	0.10	15,15,15,15	0
59	MG	BA	3020	1/1	0.99	0.05	22,22,22,22	0
59	MG	BA	3021	1/1	0.99	0.06	7,7,7,7	0
59	MG	BA	3013	1/1	1.00	0.03	1,1,1,1	0
59	MG	BA	3063	1/1	1.00	0.02	1,1,1,1	0
59	MG	BA	3114	1/1	1.00	0.05	4,4,4,4	0
59	MG	BA	3115	1/1	1.00	0.02	11,11,11,11	0
59	MG	BA	3064	1/1	1.00	0.02	18,18,18,18	0
59	MG	BA	3031	1/1	1.00	0.02	12,12,12,12	0
59	MG	AA	1621	1/1	1.00	0.10	25,25,25,25	0
59	MG	BA	3067	1/1	1.00	0.04	18,18,18,18	0
59	MG	BA	3120	1/1	1.00	0.06	4,4,4,4	0
59	MG	BA	3048	1/1	1.00	0.02	6,6,6,6	0
59	MG	BA	3023	1/1	1.00	0.03	5,5,5,5	0
59	MG	BA	3034	1/1	1.00	0.02	5,5,5,5	0
59	MG	BA	3093	1/1	1.00	0.03	36,36,36,36	0
59	MG	BA	3125	1/1	1.00	0.06	27,27,27,27	0
59	MG	BA	3071	1/1	1.00	0.02	7,7,7,7	0
59	MG	BA	3127	1/1	1.00	0.02	3,3,3,3	0
59	MG	BA	3128	1/1	1.00	0.04	19,19,19,19	0
59	MG	BA	3009	1/1	1.00	0.04	6,6,6,6	0
59	MG	BA	3052	1/1	1.00	0.02	5,5,5,5	0
59	MG	BA	3036	1/1	1.00	0.02	4,4,4,4	0
59	MG	BA	3132	1/1	1.00	0.04	1,1,1,1	0
59	MG	BA	3098	1/1	1.00	0.02	15,15,15,15	0
59	MG	BA	3099	1/1	1.00	0.05	1,1,1,1	0
59	MG	BA	3006	1/1	1.00	0.02	39,39,39,39	0
59	MG	BA	3101	1/1	1.00	0.03	11,11,11,11	0
59	MG	BA	3017	1/1	1.00	0.02	24,24,24,24	0
59	MG	BA	3039	1/1	1.00	0.13	6,6,6,6	0
59	MG	BA	3104	1/1	1.00	0.05	3,3,3,3	0
59	MG	BA	3040	1/1	1.00	0.07	11,11,11,11	0
59	MG	BA	3106	1/1	1.00	0.06	13,13,13,13	0
59	MG	BA	3079	1/1	1.00	0.02	13,13,13,13	0
59	MG	BA	3018	1/1	1.00	0.17	6,6,6,6	0
59	MG	AA	1625	1/1	1.00	0.12	30,30,30,30	0
59	MG	BA	3043	1/1	1.00	0.08	11,11,11,11	0
59	MG	BA	3012	1/1	1.00	0.02	1,1,1,1	0

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

Electron density around CLY BA 3135:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.