



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:11 PM GMT

PDB ID : 4U27
Title : Crystal structure of the E. coli ribosome bound to flopristin and linopristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-06-07
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

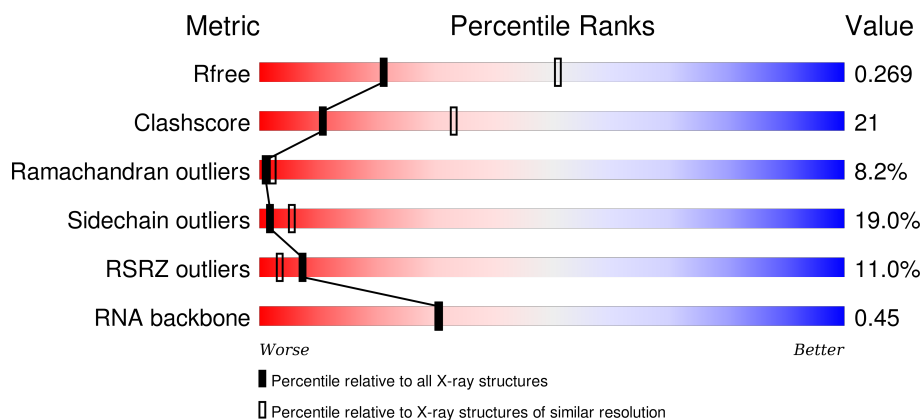
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1539	<div> <div>34%</div> <div>49%</div> <div>16%</div> </div>
1	CA	1539	<div> <div>3%</div> <div>33%</div> <div>52%</div> <div>15%</div> </div>
2	AB	218	<div> <div>9%</div> <div>25%</div> <div>45%</div> <div>23%</div> <div>6%</div> </div>
2	CB	218	<div> <div>26%</div> <div>25%</div> <div>55%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	
7	CG	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	
13	CM	114	
14	AN	100	
14	CN	100	
15	AO	88	



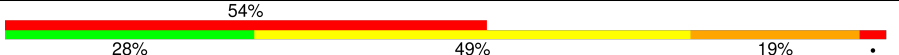
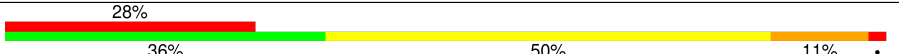


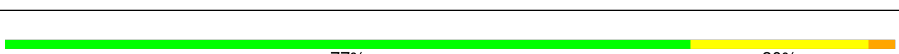
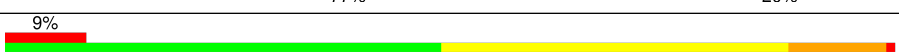

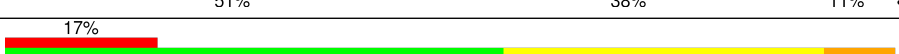
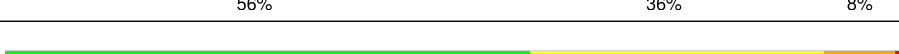
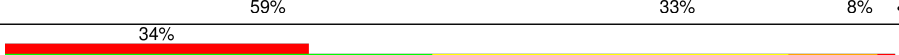
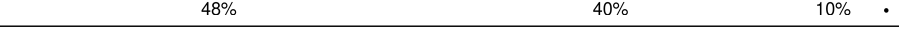
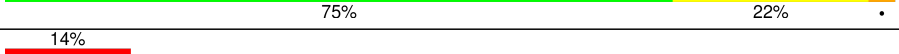


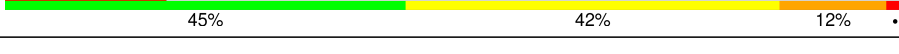


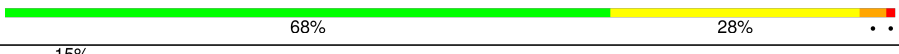
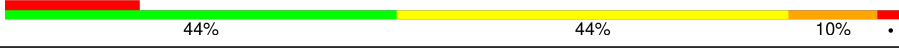
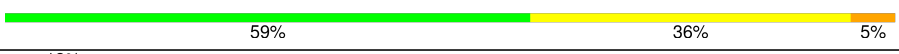



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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
27	DF	177	

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Mol	Chain	Length	Quality of chain
28	BG	176	% 
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
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	% 

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	76	
44	DW	76	
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	

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Mol	Chain	Length	Quality of chain
53	B5	228	
54	B6	7	
54	D6	7	

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
54	MHW	D6	1	-	-	X	-
55	MG	AA	1622	-	-	-	X
55	MG	AA	1635	-	-	-	X
55	MG	AA	1644	-	-	-	X
55	MG	AA	1647	-	-	-	X
55	MG	AA	1656	-	-	-	X
55	MG	AA	1670	-	-	-	X
55	MG	AA	1671	-	-	-	X
55	MG	BA	3016	-	-	-	X
55	MG	BA	3041	-	-	-	X
55	MG	BA	3058	-	-	-	X
55	MG	BA	3084	-	-	-	X
55	MG	BA	3105	-	-	-	X
55	MG	BA	3106	-	-	-	X
55	MG	BA	3109	-	-	-	X
55	MG	BA	3110	-	-	-	X
55	MG	BA	3132	-	-	-	X
55	MG	BA	3137	-	-	-	X
55	MG	BA	3147	-	-	-	X
55	MG	BA	3151	-	-	-	X
55	MG	BA	3153	-	-	-	X
55	MG	BA	3174	-	-	-	X
55	MG	BA	3177	-	-	-	X
55	MG	DA	3003	-	-	-	X
55	MG	DA	3025	-	-	-	X
55	MG	DA	3026	-	-	-	X
55	MG	DA	3042	-	-	-	X
55	MG	DA	3065	-	-	-	X
55	MG	DA	3103	-	-	-	X
55	MG	DA	3110	-	-	-	X
55	MG	DA	3114	-	-	-	X
55	MG	DA	3117	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3121	-	-	-	X
55	MG	DA	3125	-	-	-	X
55	MG	DA	3140	-	-	-	X
55	MG	DA	3153	-	-	-	X
55	MG	DA	3159	-	-	-	X
56	VIF	BA	3001	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 288396 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	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

- 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			
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			
7	CG	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
13	CM	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	96	Total	C	N	O	S	0	0	0
			774	483	160	128	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
			710	437	143	129	1			
15	CO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	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			
16	CP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
22	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
27	DF	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
			1110	699	197	213	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	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			
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	S	0	0	0
			947	604	192	151				
38	DQ	117	Total	C	N	O	S	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	S	0	0	0
			780	492	146	142				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	76	Total	C	N	O	S	0	0	0
			580	359	117	103	1			
44	DW	75	Total	C	N	O	S	0	0	0
			569	353	113	102	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 509	C 313	N 99	O 95	S 2	0	0	0
46	DY	63	Total 509	C 313	N 99	O 95	S 2	0	0	0

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

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

- 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			
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 protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

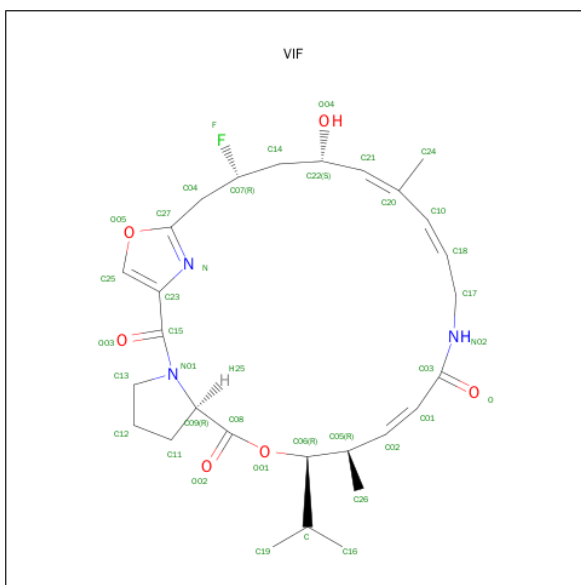
- Molecule 54 is a protein called Linopristin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	B6	7	Total	C	N	O	0	0	0
			69	50	9	10			
54	D6	7	Total	C	N	O	0	0	0
			69	50	9	10			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BB	4	Total	Mg	0	0
			4	4		
55	BA	193	Total	Mg	0	0
			193	193		
55	CA	56	Total	Mg	0	0
			56	56		
55	BD	1	Total	Mg	0	0
			1	1		
55	AA	72	Total	Mg	0	0
			72	72		
55	BQ	1	Total	Mg	0	0
			1	1		
55	DA	167	Total	Mg	0	0
			167	167		
55	D2	1	Total	Mg	0	0
			1	1		
55	DB	3	Total	Mg	0	0
			3	3		

- Molecule 56 is Flopristin (three-letter code: VIF) (formula: C₂₈H₃₈FN₃O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
56	BA	1	Total	C	F	N	O	0	0
			38	28	1	3	6		
56	DA	1	Total	C	F	N	O	0	0
			38	28	1	3	6		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	193	Total	O	0	0
			193	193		
58	AL	2	Total	O	0	0
			2	2		
58	AN	5	Total	O	0	0
			5	5		
58	AT	2	Total	O	0	0
			2	2		
58	AU	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BA	623	Total 623	O 623	0	0
58	BB	14	Total 14	O 14	0	0
58	BC	6	Total 6	O 6	0	0
58	BD	3	Total 3	O 3	0	0
58	BE	4	Total 4	O 4	0	0
58	BF	1	Total 1	O 1	0	0
58	BG	1	Total 1	O 1	0	0
58	BL	4	Total 4	O 4	0	0
58	BN	3	Total 3	O 3	0	0
58	BS	1	Total 1	O 1	0	0
58	BT	1	Total 1	O 1	0	0
58	B2	1	Total 1	O 1	0	0
58	B3	2	Total 2	O 2	0	0
58	B4	2	Total 2	O 2	0	0
58	CA	192	Total 192	O 192	0	0
58	CL	1	Total 1	O 1	0	0
58	CN	3	Total 3	O 3	0	0
58	CT	1	Total 1	O 1	0	0
58	CU	1	Total 1	O 1	0	0
58	DA	608	Total 608	O 608	0	0
58	DB	13	Total 13	O 13	0	0

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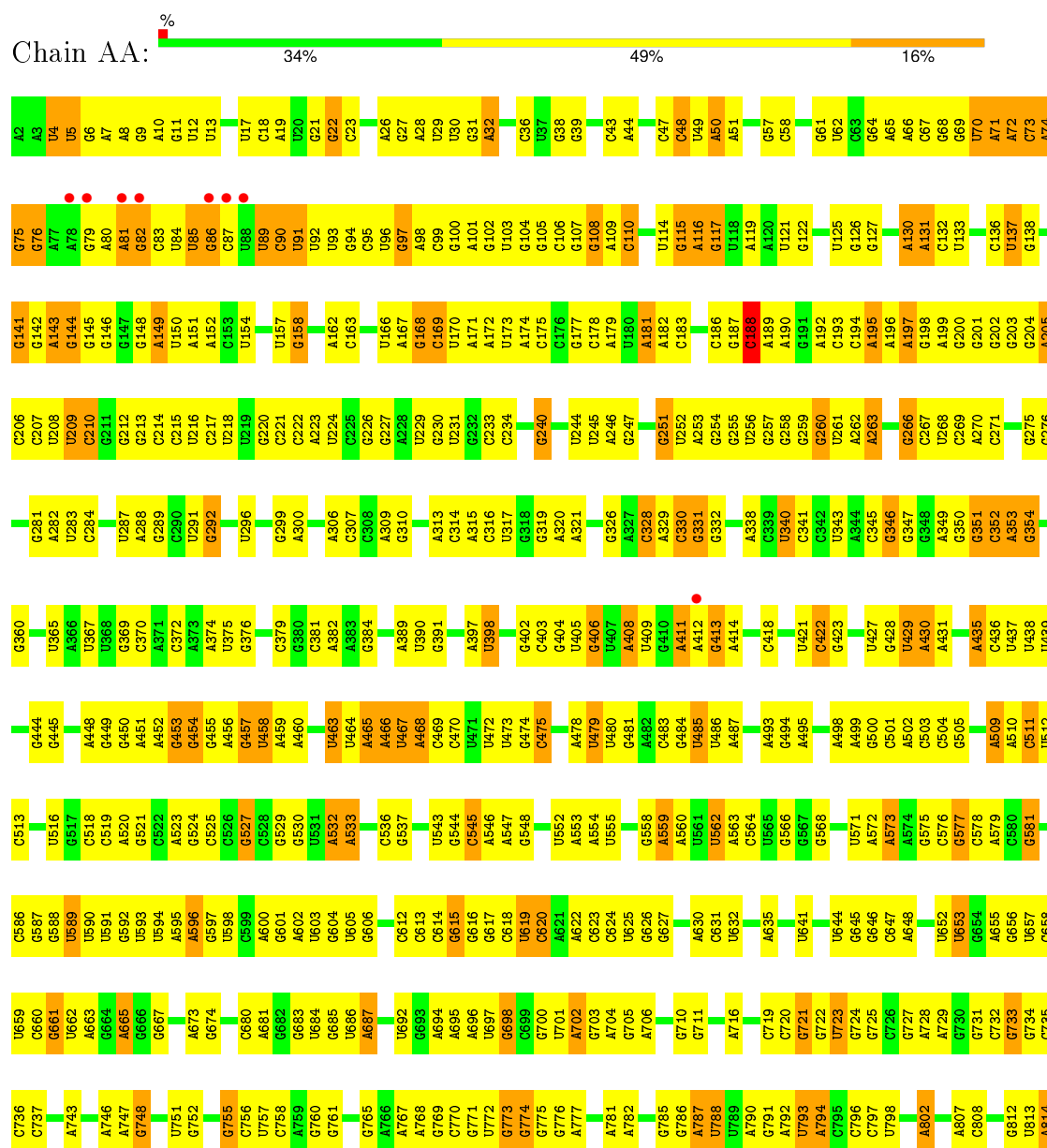
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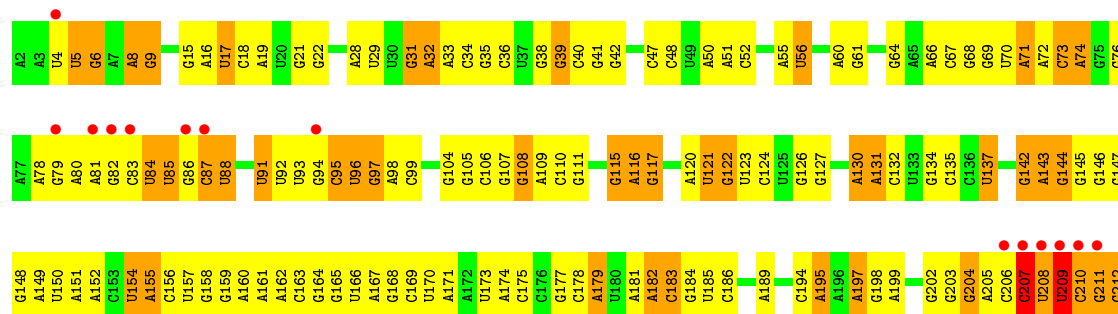
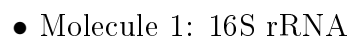
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DC	11	Total 11	O 11	0	0
58	DD	4	Total 4	O 4	0	0
58	DE	5	Total 5	O 5	0	0
58	DJ	1	Total 1	O 1	0	0
58	DL	4	Total 4	O 4	0	0
58	DN	2	Total 2	O 2	0	0
58	DT	1	Total 1	O 1	0	0
58	DU	1	Total 1	O 1	0	0
58	DV	1	Total 1	O 1	0	0
58	D0	1	Total 1	O 1	0	0
58	D2	1	Total 1	O 1	0	0
58	D3	2	Total 2	O 2	0	0
58	D4	1	Total 1	O 1	0	0

3 Residue-property plots

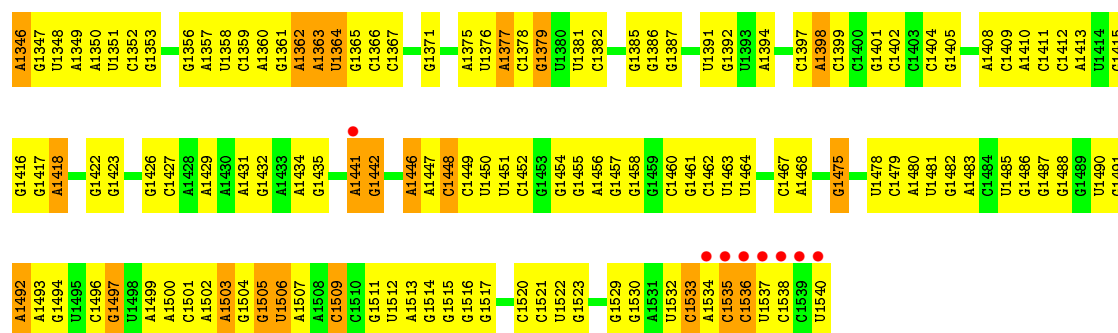
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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

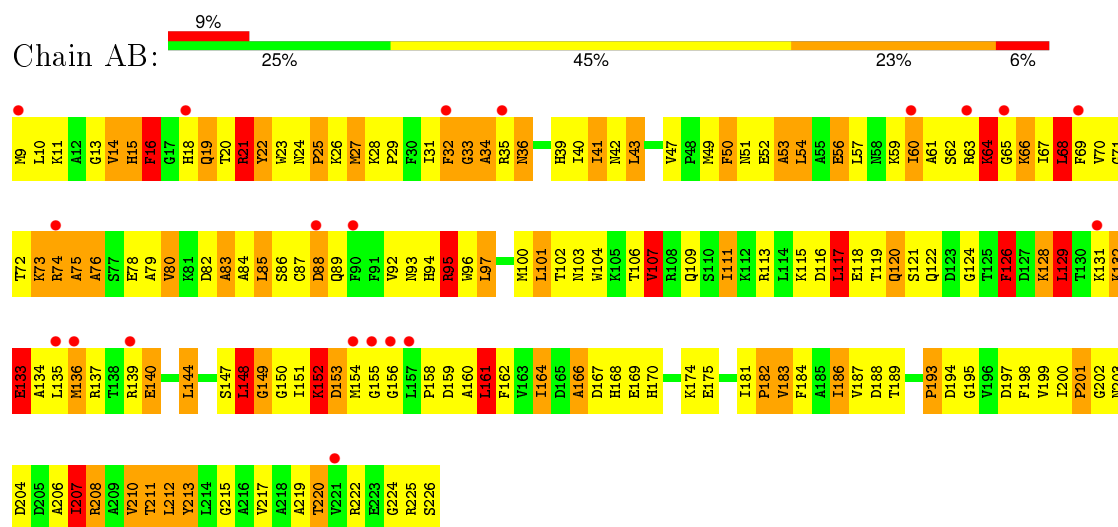




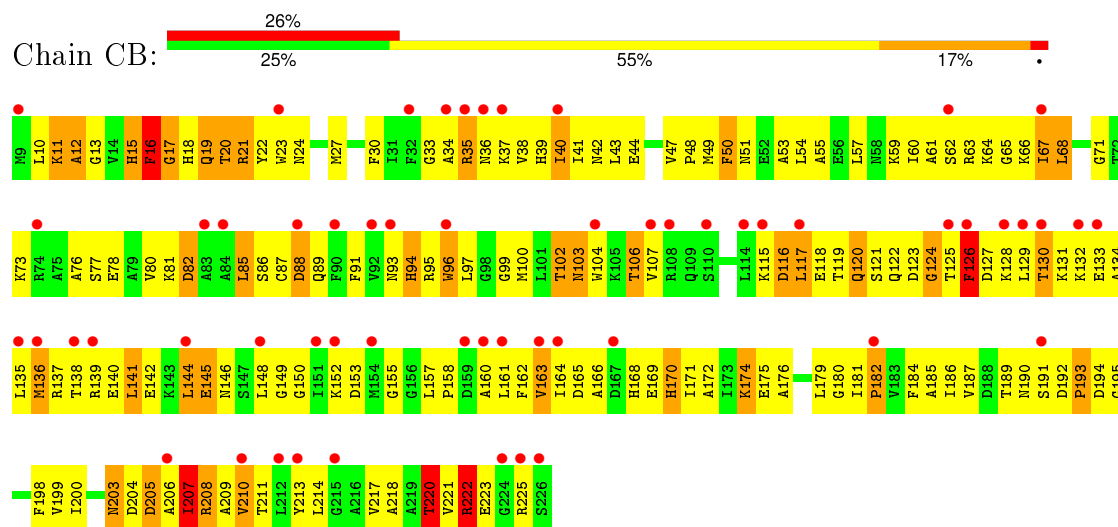
G1282	A1150	G1084	U950	G874	U801	G731	G568	C503	A432	G361	G289	G213
U1283	A1151	U1085	U1016	U875	U802	G732	U662	G504	A436	U367	C290	C214
G1284	A1152	U1086	G1018	U876	A802	G733	A663	G505	U437	U368	U291	C215
A1285	G1153	G1087	A1019	C979	G803	G734	A664	U508	U438	G369	G292	C217
U1287	A1154	G1088	G1020	C880	U804	G735	A665	A509	U439	C370	U294	U218
G1288	A1155	G1089	A1021	G881	G805	G736	G666	A509	A440	A371	C295	U219
A1288	G1156	U1090	A1022	C882	G806	G737	U671	C511	C441	C372	U296	G220
G1289	A1157	U1091	U1023	C883	A807	G738	A673	C512	G442	A373	G297	G221
U1290	G1158	A1092	U1024	U884	G808	G739	A674	C513	G443	A374	A298	C222
U1291	U1159	A1093	G1025	G885	G809	G740	A675	C514	G444	U375	G299	A223
G1292	G1160	G1094	G1026	U886	C810	G741	A676	C515	G445	G376	A300	U224
U1293	C1161	U1095	C1027	G888	C811	G742	A677	C516	G446	G377	G301	C225
G1294	C1162	C1096	A1028	A889	G812	G743	A678	C517	G447	G378	G302	G226
A1297	A1163	C1097	U1029	G890	U813	G744	A679	C518	G448	C379	G303	G227
C1296	G1159	U1098	U1030	U891	A814	G745	U678	C519	G449	G380	A306	A228
G1297	A1166	G1031	G1031	A892	A815	G746	U678	C520	G450	G381	C307	
U1298	G1167	C1032	G1032	C893	A816	G747	U679	C521	G451	A383	C308	G237
A1299	U1168	A1101	G1033	C893	C817	G748	U680	A520	A451	A384	C309	
G1300	A1169	A1102	G1034	C896	G818	G749	U681	C522	A452	A385	A309	
U1301	C1103	A1035	G1035	C897	A819	A753	G683	C523	G453	C386		G240
C1302	U1235	A1036	A1036	G898	U820	C754	G684	C525	G454	U387	C312	G241
G1303	A1171	G1105	G1037	C899	G821	G755	G685	C526	G455	U387	A313	G242
G1297	U1173	G1106	C1038	A900	U822	G756	U686	C527	G456	G388	C314	A243
G1305	G1174	C1107	G1039	A901	U822	G757	U687	C528	G457	A389	A315	U244
A1306	G1175	G1108	U1040	A902	C826	G758	U688	C529	G458	U390	C316	U245
U1307	A1176	U1041	G1041	G902	U827	A759	G689	C530	A459	G391	A246	
G1308	G1177	G1042	U1042	U905	U828	G760	G690	C531	U463	C392	G247	
G1243	A1178	G1043	G1043	A906	G829	G761	U692	C532	U463	A321	C248	
U1309	U1115	A1044	A1044	U909	G832	A766	U693	C533	U464	C322	U249	
G1244	U1116	U1117	G1045	C910	G833	G769	A695	C534	A466	U397	U250	
C1246	G1181	U1118	A1046	C910	U834	G770	A696	C535	U467	U398	G251	
A1252	G1182	U1118	G1047	A913	U834	G771	U697	C536	U468	C399	U252	
G1315	U1183	U1048	U1048	A914	G840	G772	A702	C537	C469	C400	G253	
A1254	G1184	G1049	U1049	A914	C841	U772	G703	C538	U469	C401	G254	
G1255	G1185	G1124	G1050	U913	U842	G773	A704	C539	G474	G402	U255	
A1256	G1186	U1125	U1125	A918	U843	G774	A705	C540	C475	C403	U256	
G1318	U1190	U1126	G1053	A919	U844	G775	G706	C541	C476	C330	G257	
A1319	A1191	G1127	C1054	U920	G844	G776	A707	C542	U477	C331	U258	
G1320	G1258	C1128	A1055	U921	U845	G777	U707	C543	C477	U405	G259	
U1321	C1129	G1129	A1055	G922	U846	A777	C708	C544	U478	G406		
G1322	G1193	A1130	U1062	A923	G847	G778	U709	C545	A546	U407		
A1261	U1194	G1131	U1062	C924	G847	G779	C709	C546	U479	A408		
C1262	C1195	G1132	U1065	C925	G851	G780	G710	C547	U480	U409		
A1324	A1196	G1133	C1066	G926	G852	A781	G711	C548	G481	U409		
G1266	U1197	G1134	A1067	C927	G852	A782	A712	C549	A482	G410		
U1328	G1198	U1135	G1068	U927	G858	G783	G713	C550	C483	A411		
A1329	U1199	C1136	C1069	U928	G859	G784	A714	C551	G484	A412		
U1330	C1200	G1137	U1070	C931	A860	G785	A715	C552	U485	G413		
G1331	A1201	G1138	C1071	C931	G861	G786	U716	C553	U486			
A1332	U1202	G1139	G1072	C934	G862	G787	U717	C554	A487			
G1333	C1203	C1140	U1073	U934	U863	A787	C719	C555	A493	U421		
G1334	G1204	C1141	G1074	A938	A864	G790	G720	C556	G494	G423		
U1335	U1205	C1142	U1007	C939	A865	G791	G721	C557	A495	G424		
G1336	G1207	G1143	U1008	C940	A866	A792	G722	C558	A496	G425		
A1337	C1208	A1144	U1078	C941	C867	U793	G723	C559	G497	U426		
G1338	U1209	A1145	G1079	G941	G868	A794	U724	C560	A498	U427		
G1342	U1211	C1147	A1080	G945	G869	G795	G725	C561	G500	G428		
A1343	U1212	U1148	A1081	A946	G870	C796	A728	C562	U429	U358		
G1343	U1213	C1149	U1082	A946	A872	G797	A729	C563	C501	G359		
			U1083	U946	A873	U798	C726	C564	A502	A431		



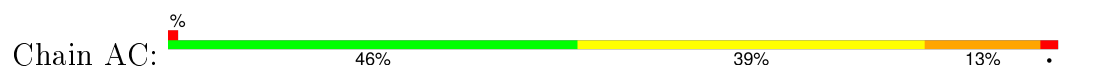
• Molecule 2: 30S ribosomal protein S2

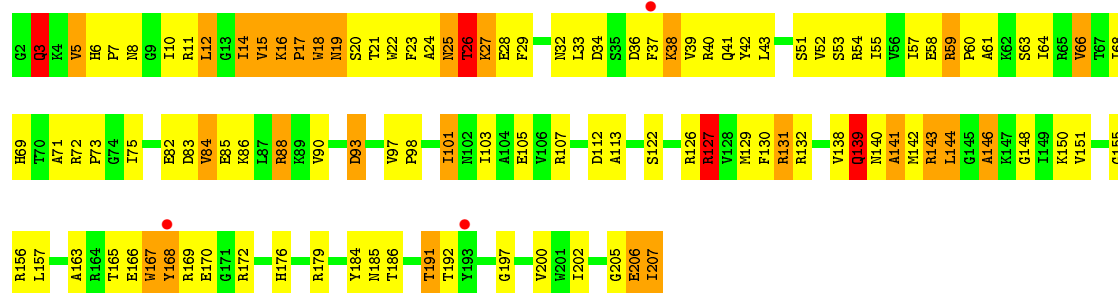


• Molecule 2: 30S ribosomal protein S2

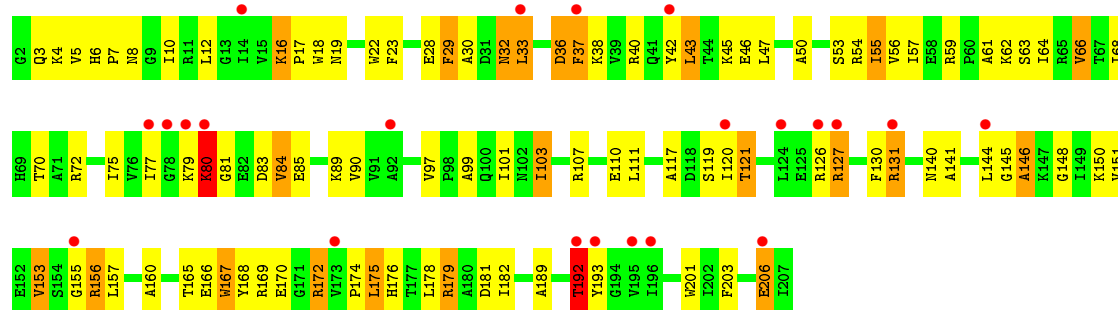


• Molecule 3: 30S ribosomal protein S3

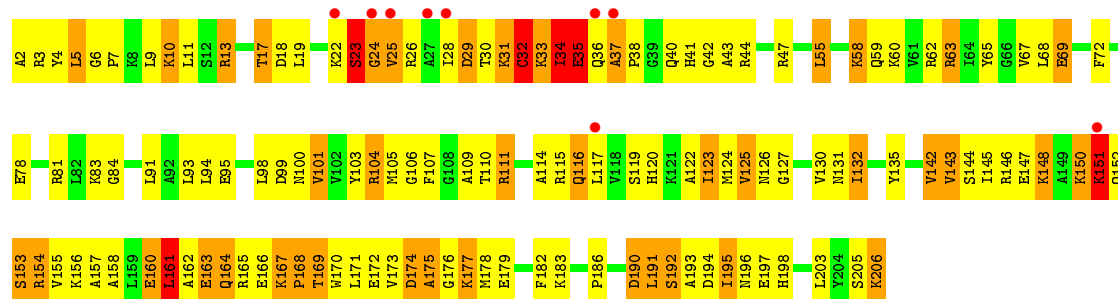




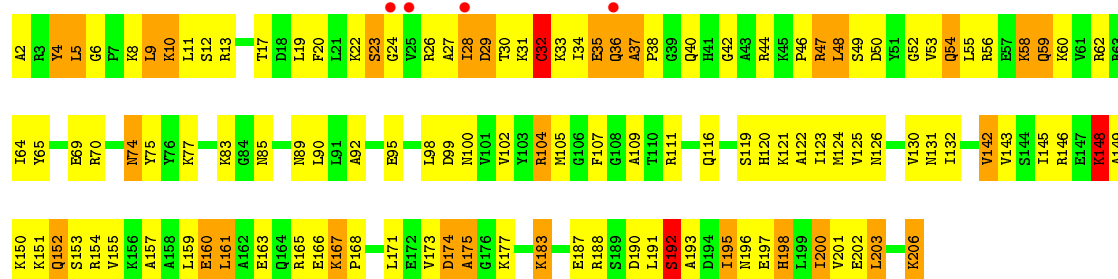
• Molecule 3: 30S ribosomal protein S3



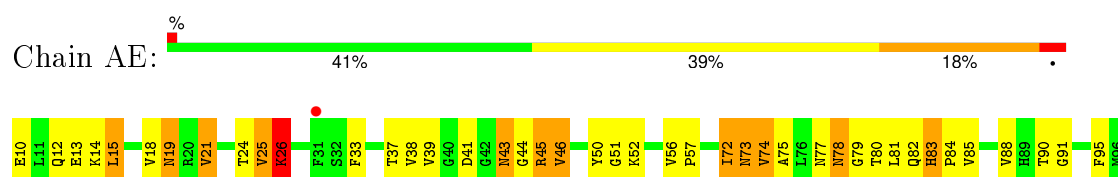
• Molecule 4: 30S ribosomal protein S4



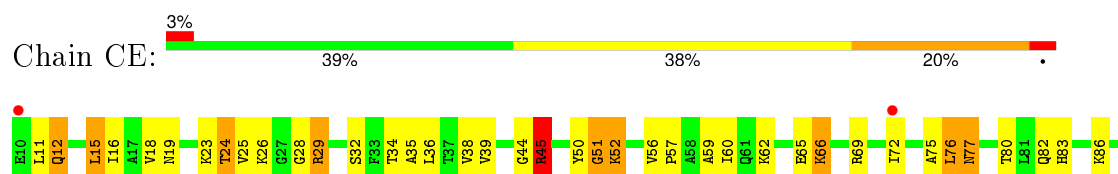
• Molecule 4: 30S ribosomal protein S4



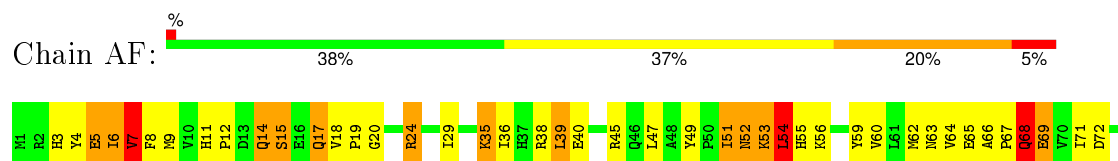
• Molecule 5: 30S ribosomal protein S5



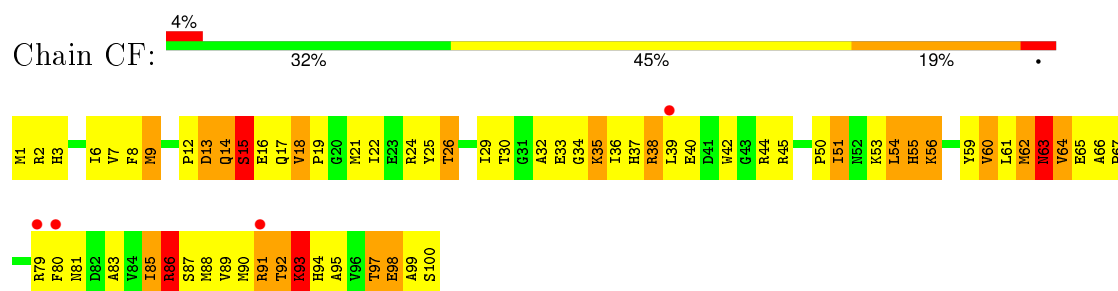
• Molecule 5: 30S ribosomal protein S5



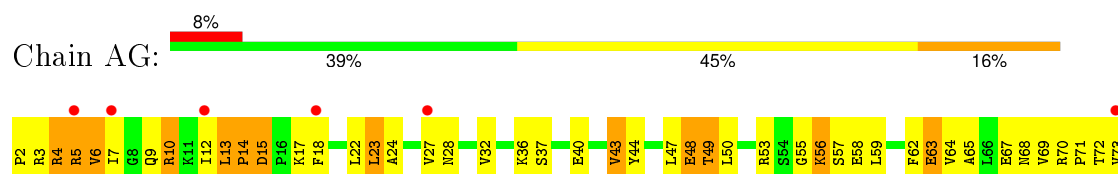
• Molecule 6: 30S ribosomal protein S6

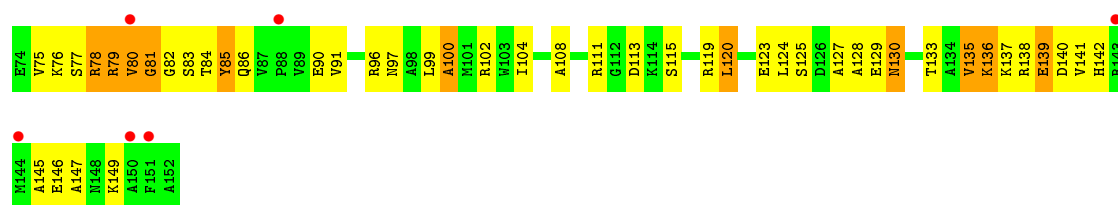


• Molecule 6: 30S ribosomal protein S6

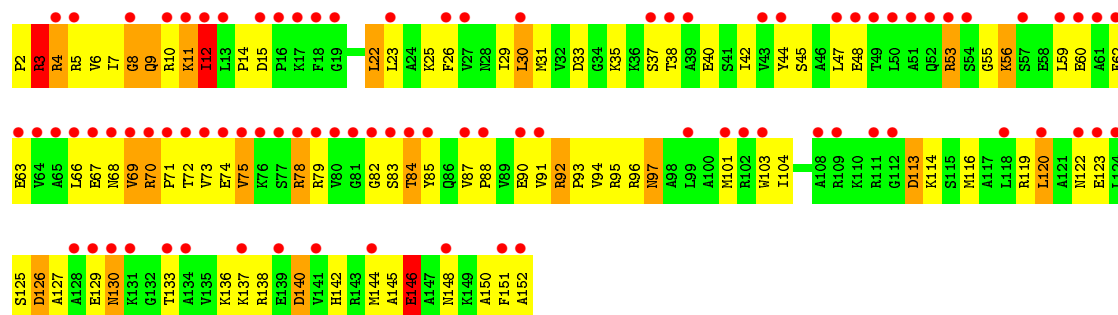
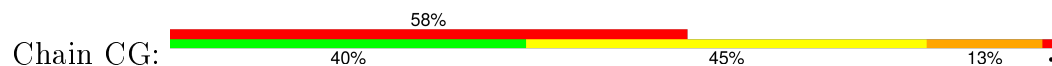


• Molecule 7: 30S ribosomal protein S7

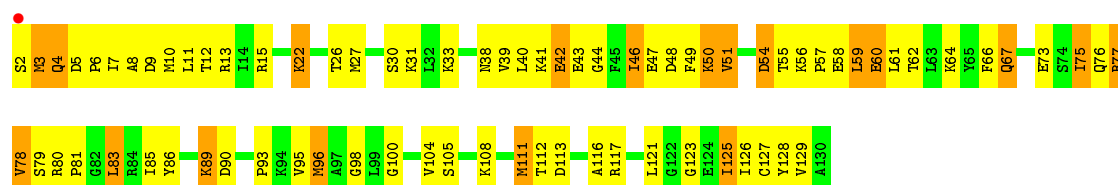




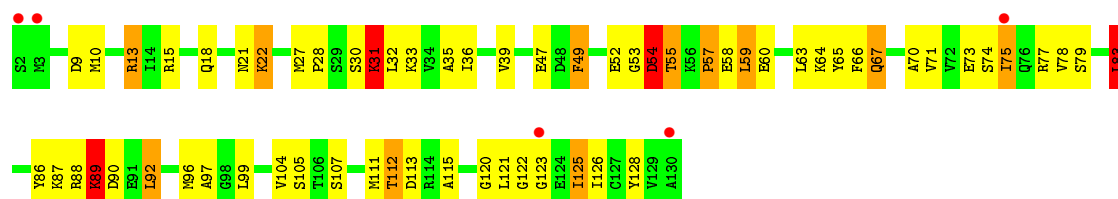
• Molecule 7: 30S ribosomal protein S7



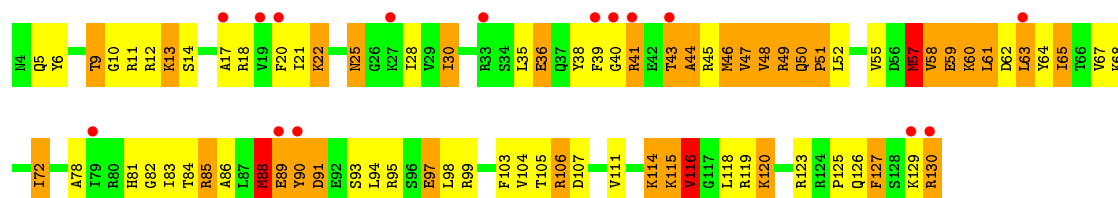
• Molecule 8: 30S ribosomal protein S8

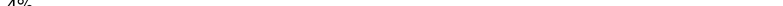


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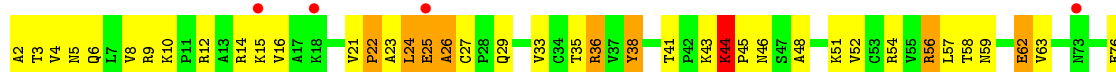
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- Chain CK: 



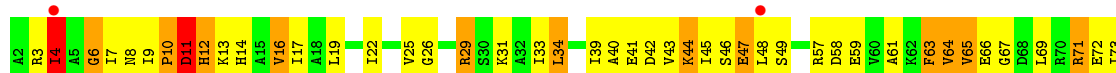
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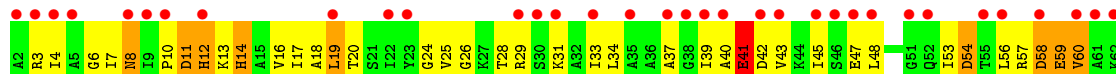
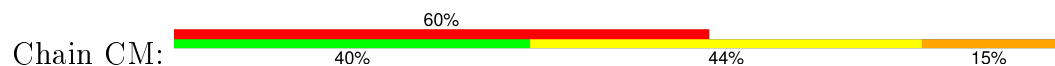
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

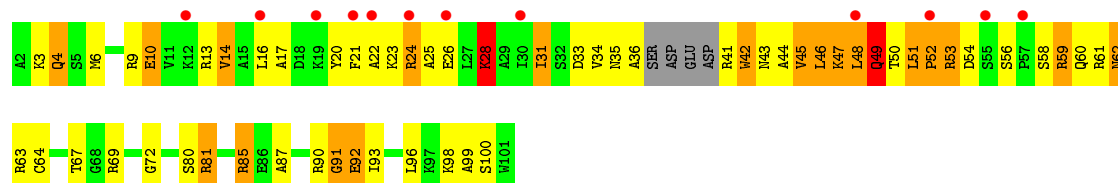


- Molecule 13: 30S ribosomal protein S13

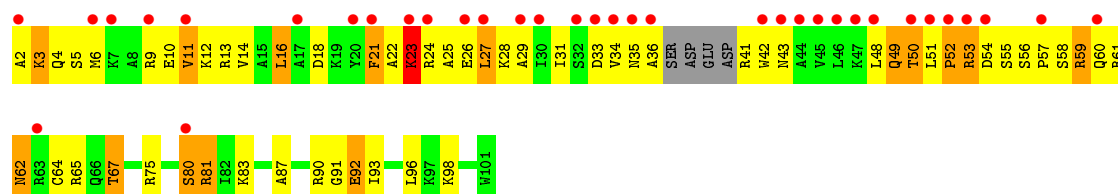


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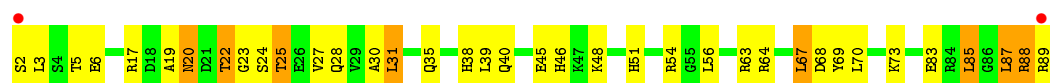




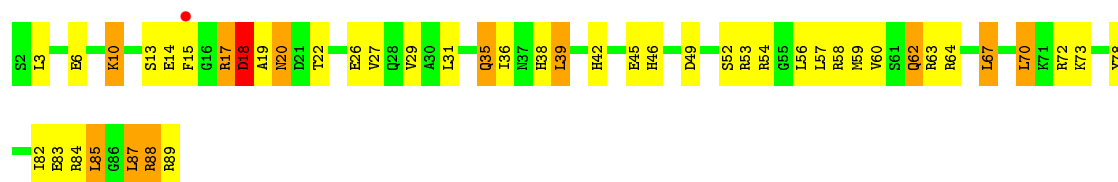
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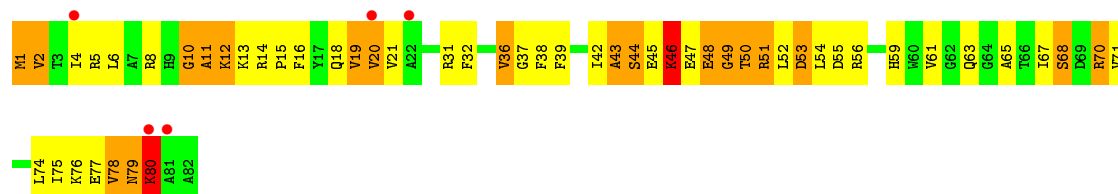
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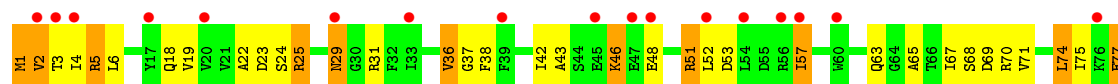
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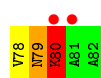


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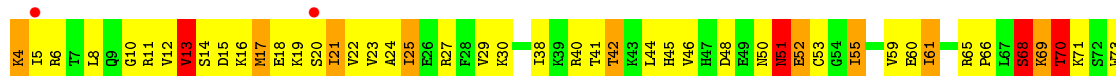


• Molecule 16: 30S ribosomal protein S16





- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



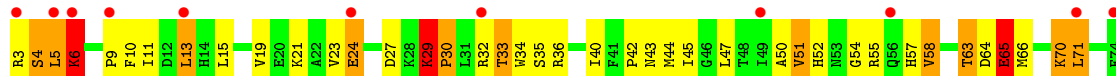
- Molecule 18: 30S ribosomal protein S18



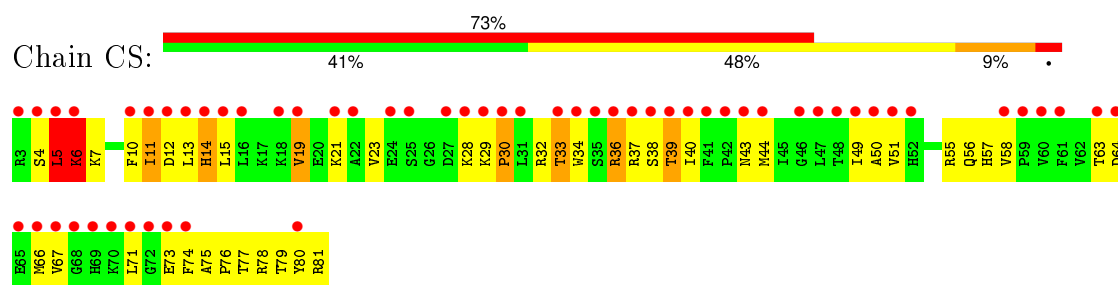
- Molecule 18: 30S ribosomal protein S18



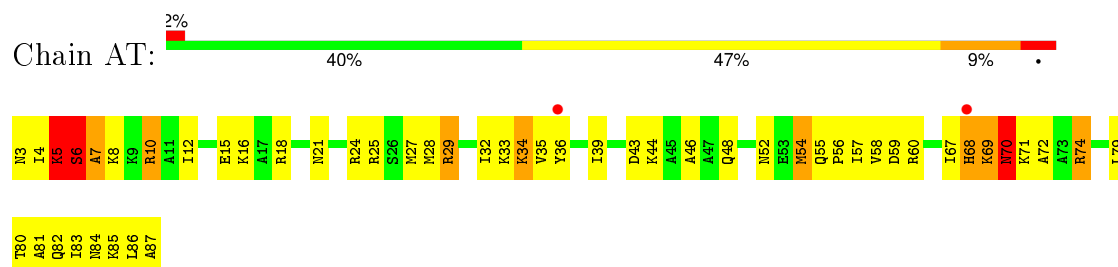
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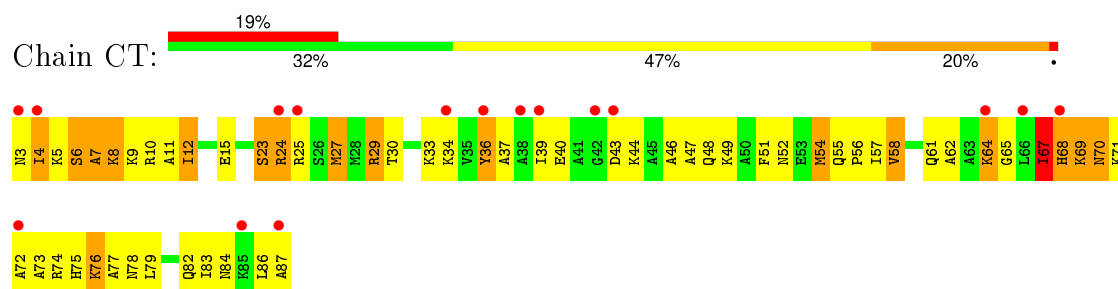
- Molecule 19: 30S ribosomal protein S19



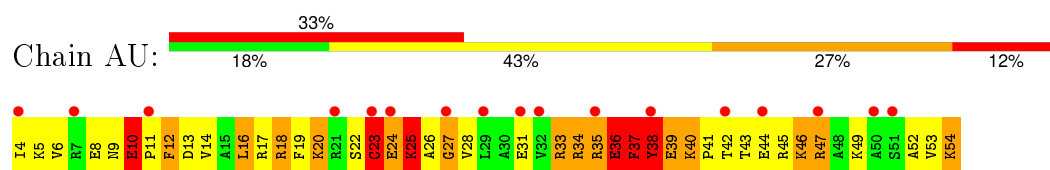
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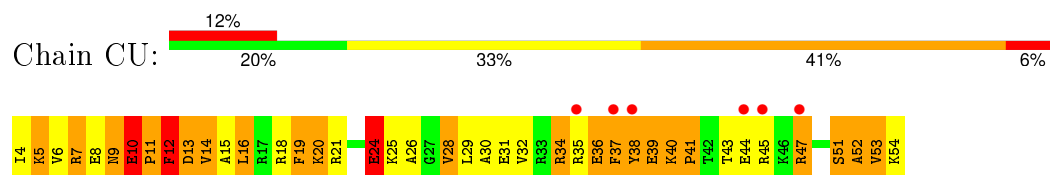
• Molecule 20: 30S ribosomal protein S20



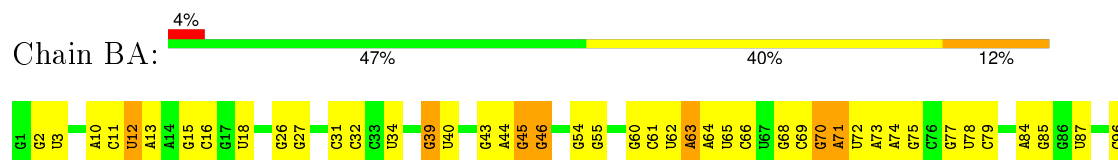
• Molecule 21: 30S ribosomal protein S21



• Molecule 21: 30S ribosomal protein S21

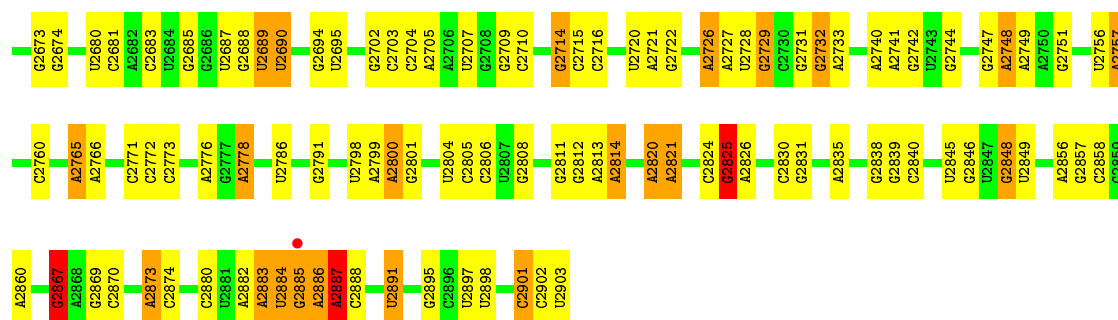


• Molecule 22: 23S rRNA

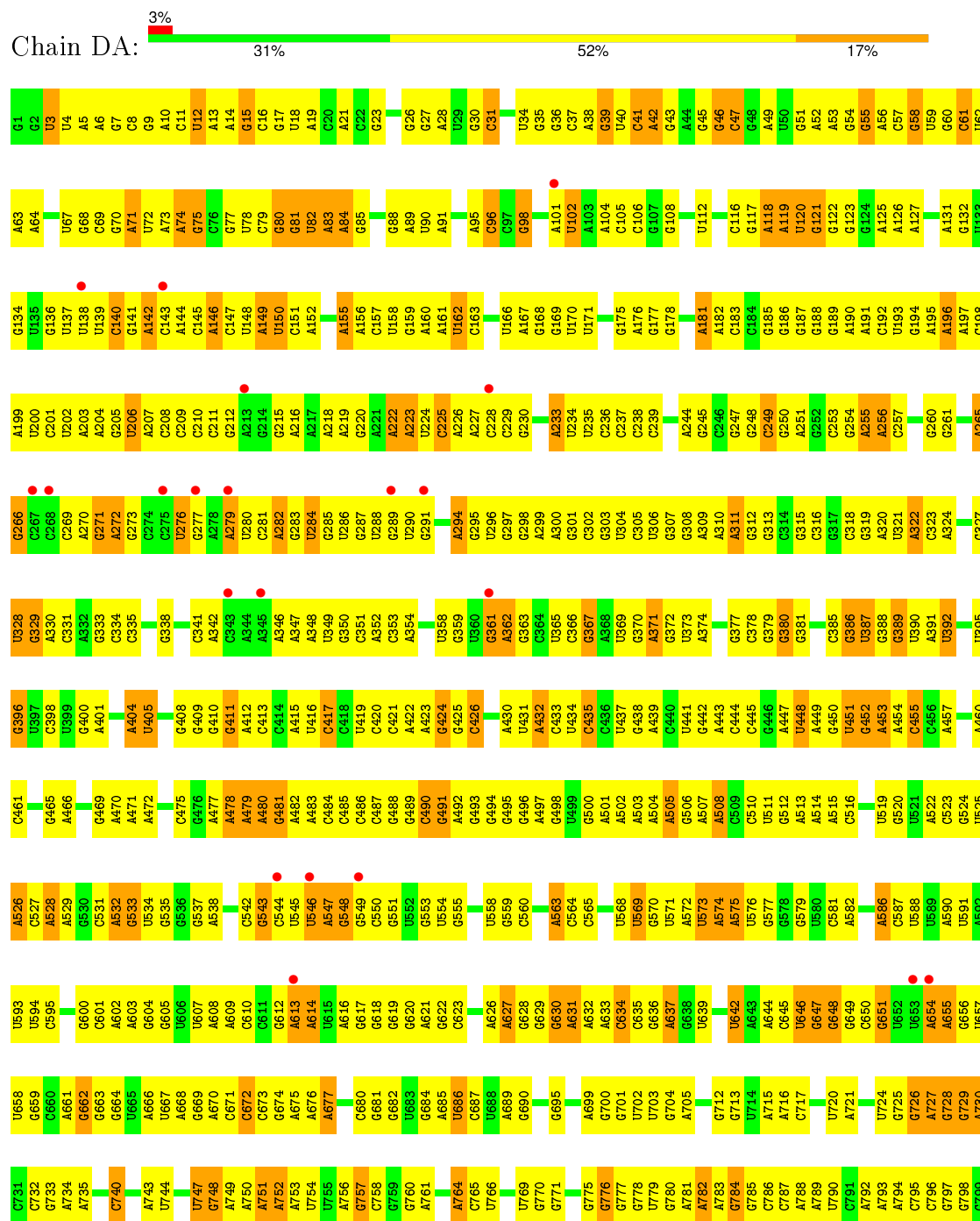


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WORLDWIDE
PDB
PROTEIN DATA BANK



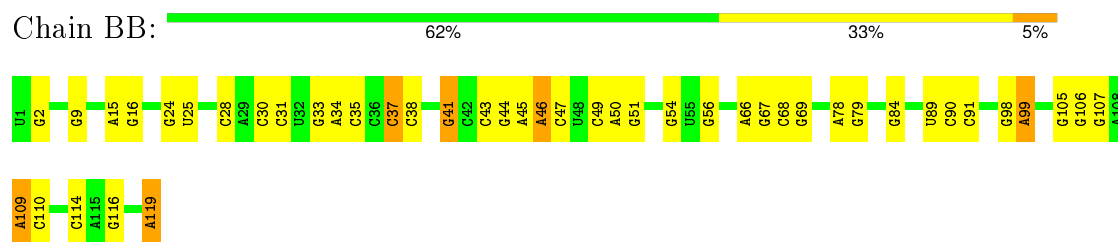
• Molecule 22: 23S rRNA



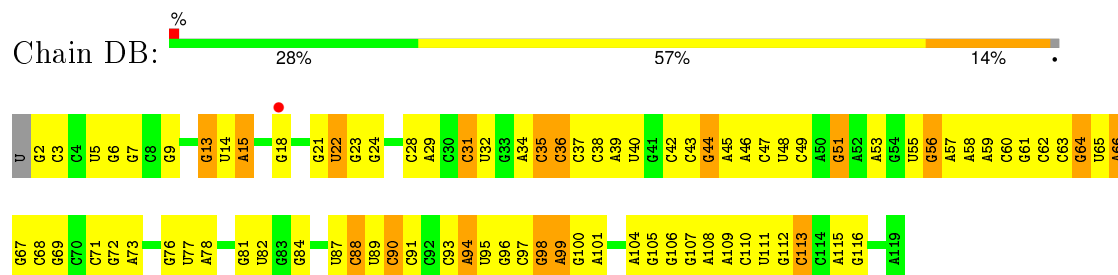
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U2882	C2814	U2684	G2685	G2602	U2533	A2448	A2378	C2306	U2167	C2103	U1943	G2022	G1862
U2883	G2815	A2750	G2686	G2603	A2534	U2449	G2379	C2307	U2168	U2105	U1951	G2023	U1865
G2884	G2816	C2752	U2687	G2608	G2535	U2452	C2380	G2308	G2229	U2106	A1952	G2024	A1866
A2885	U2817	U2753	G2688	U2609	G2536	A2453	A2381	A2309	U2230	G2107	A1953	G2025	G1867
A2887		U2754	U2689	G2610	U2537	G2454	G2382	C2310	U2231	A2170	G1954	G2026	C1868
C2888	A2820	C2755	U2690	G2613	G2542	U2457	C2385	U2312	G2232	U2172	U1955	G2027	C1869
C2889	G2821	U2756	U2691	G2614	G2543	G2458	A2386	U2313	G2233	A2173	C1956	G2028	C1870
C2890	A2822	A2757	C2692	C2611	C2538	U2459	U2387	G2314	U2234	C2174	G1957	G2029	C1871
G2891	G2823	U2758	G2693	U2612	C2539	G2458	U2388	A2315	G2235	U2175	C1958	A2030	A1870
U2891	C2824	G2759	U2694	U2613	G2542	G2459	U2389	G2316	G2236	U2176	G1959	A2031	A1872
G2892	G2825	C2760	G2695	G2614	G2543	A2461	A2390	G2317	G2237	U2177	A1960	G2032	G1873
A2893	A2826	A2761	U2696	C2615	G2544	U2462	G2391	U2320	G2238	C2178	U1963	A2033	C1874
G2894	G2834	A2762	U2697	C2620	G2545	G2464	U2392	U2321	A2241	U2179	U1964	U2034	G1875
U2895	A2835	A2763	U2698	G2624	G2546	C2465	A2393	U2322	G2242	U2180	G1965	G2037	A1876
U2896	G2836	A2766	G2699	G2625	A2547	C2466	U2394	A2323	U2243	U2181	C1966	A2038	G1877
A2897	A2837		C2704	C2626	U2548	C2467	C2394	G2324	U2244	U2182	C1967	U2039	C1878
C2902	G2838	U2769	A2705	G2627	G2549	A2468	U2402	U2325	U2245	U2183	G1968	G2040	U1880
U2903	G2839	G2770	U2706	G2628	G2550	A2469	C2403	C2326	G2246	U2184	C1969	A2042	C1881
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	G2841	G2773	G2708	G2630	U2552	U2473	A2407	U2328	G2250	U2186	U1971	G2044	U1883
	G2842	C2774	G2709	G2631	G2553	U2474	A2408	A2329	C2261	U2187	G1972	G2045	G1884
G2843	A2843	G2775	C2710	G2632	U2554	U2475	U2409	U2330	U2262	U2188	C1973	C2050	
G2844	G2844	A2776	A2711	G2633	A2555	A2476	G2410	C2331	U2263	A2126	C1974	A2052	A1889
G2845	G2845	G2777	G2712	G2634	C2556	G2481	G2413	C2332	C2264	U2192	A1978	G2055	C1893
U2847	G2846	U2778	U2713	A2635	C2557	G2482	G2414	U2333	U2265	U2193	A1981	C2056	A1899
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G2854	G2854	C2785	U2720	G2645	A2566	G2490	U2420	C2339	A2273	A2199	U1991	A2062	G1907
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A2856	A2856	C2787	C2722		U2568		G2422	G2345	G2277	C2201	U1993		A1912
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G2862	G2862	U2793	U2728	A2657	G2576	U2503	G2428	C2351	G2283	C2147	C1999	C2072	A1918
C2863	C2863	C2794	C2729	C2658	U2577	U2504	G2429	G2352	A2284	A2148	G2004	G2073	
G2864	G2864	U2795	C2730	G2659	C2578	G2505	U2430	A2353	G2285	U2149	A2005	U2074	U1923
U2865	U2865	U2796	G2731	A2660	U2580	U2506	U2431	C2354	G2286	U2150	C2006	U2075	C1924
G2866	G2866	A2797	A2732	G2661	G2581	C2507	U2432	U2355	A2287	C2151	U2007		U1925
G2867	G2867	U2800	U2733	G2662	U2582	U2511	A2433	U2356	A2288	G2152	G2008	U2079	C1926
A2868	A2868	G2801	G2734	G2663	U2583	C2512	A2434	U2357	G2289	C2153	A2009	A2080	C1927
G2869	G2869	U2802	A2735	U2584	U2584	A2513	G2435	C2358	G2290	A2154	G2010		U1928
C2870	C2870	G2803	U2736	U2585	U2585	A2514	A2436	U2359	G2291	G2155		G2083	
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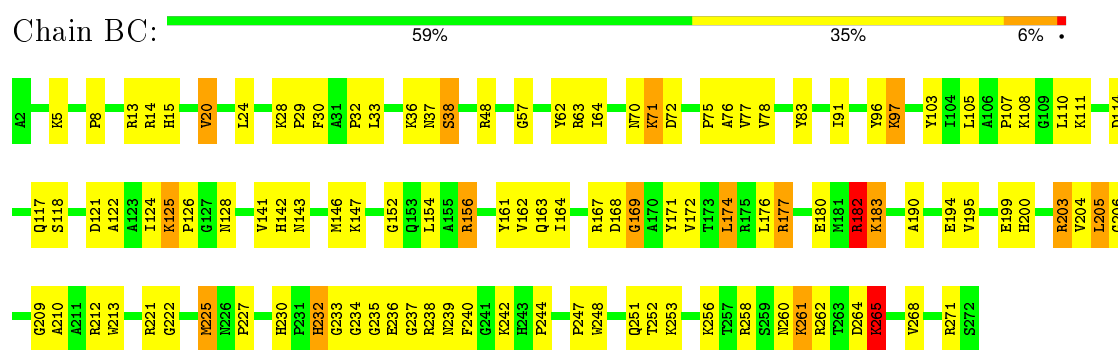
- Molecule 23: 5S rRNA



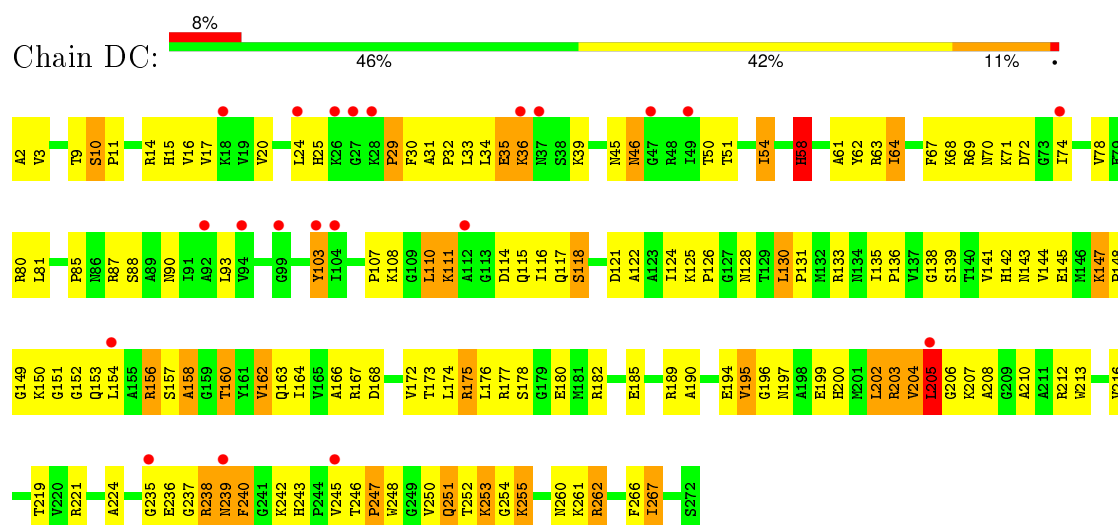
- Molecule 23: 5S rRNA



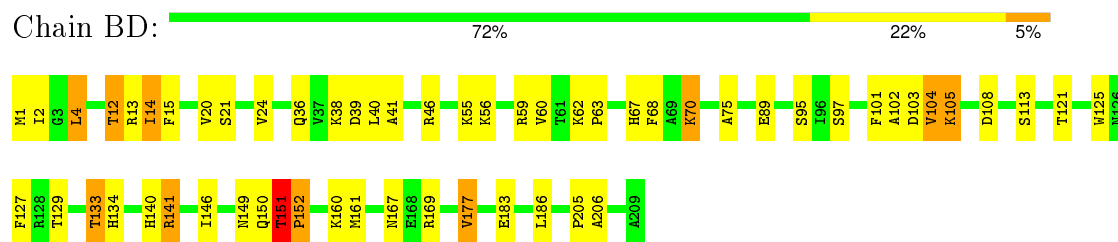
- Molecule 24: 50S ribosomal protein L2



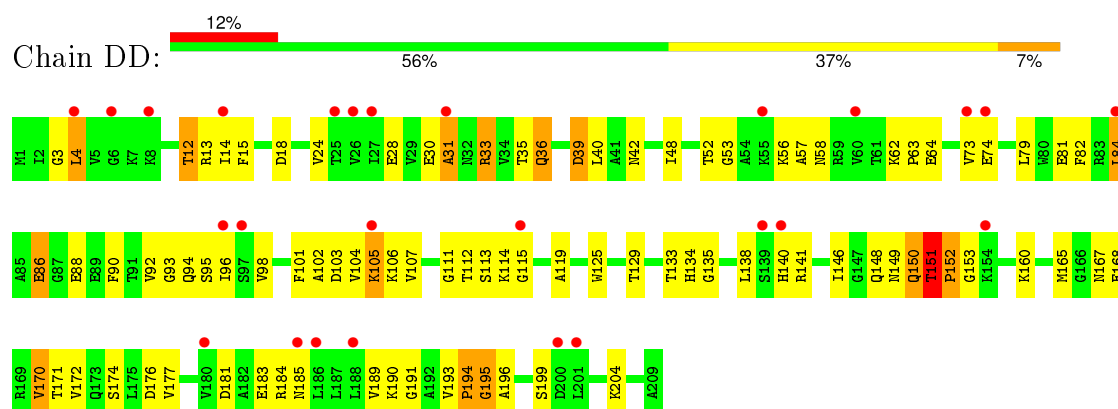
- Molecule 24: 50S ribosomal protein L2



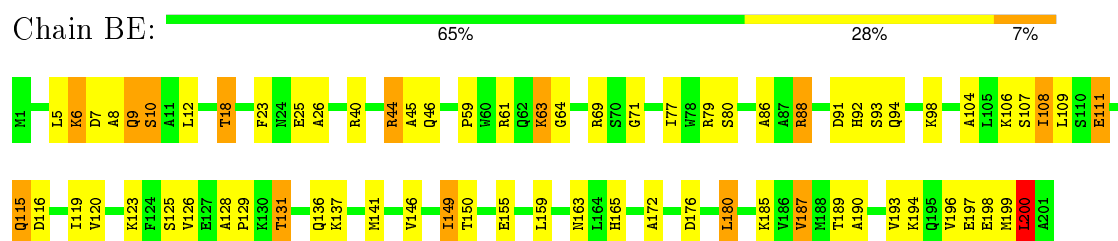
- Molecule 25: 50S ribosomal protein L3



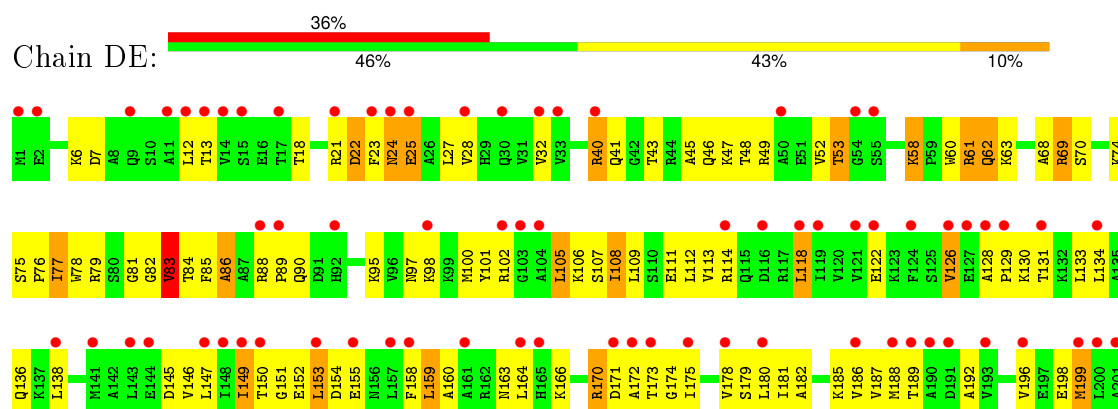
• Molecule 25: 50S ribosomal protein L3



• Molecule 26: 50S ribosomal protein L4

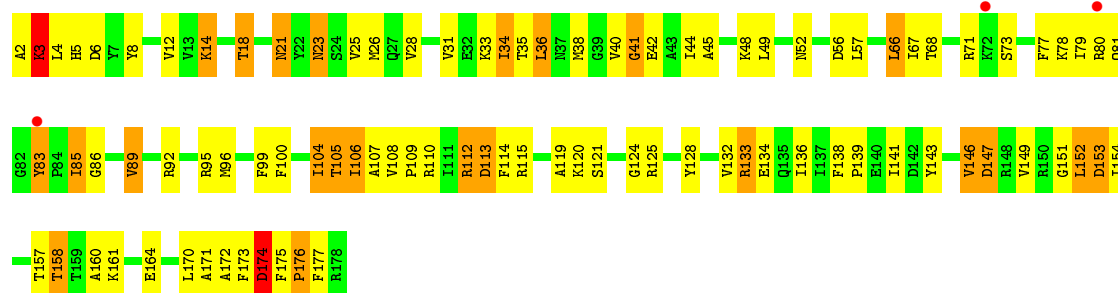


• Molecule 26: 50S ribosomal protein L4

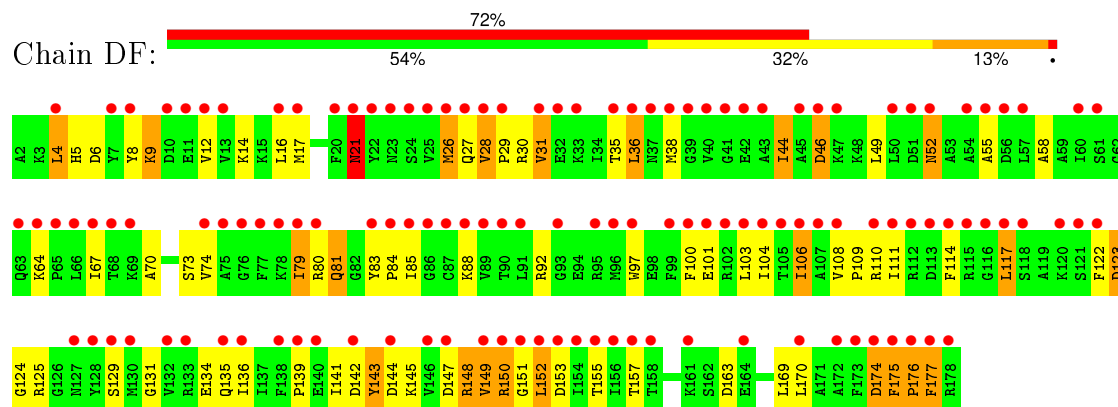


• Molecule 27: 50S ribosomal protein L5

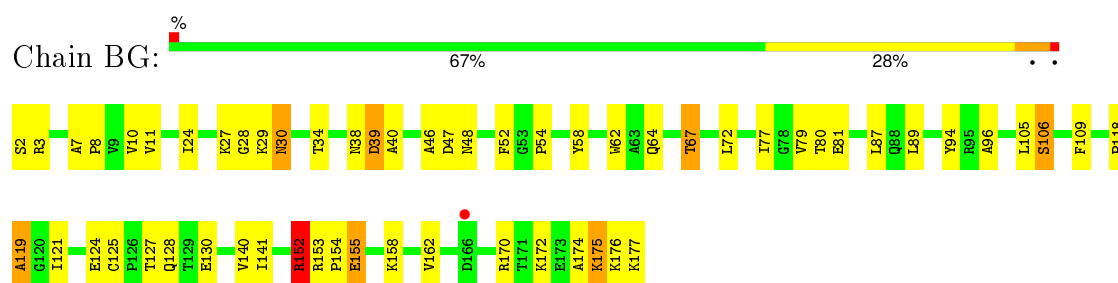




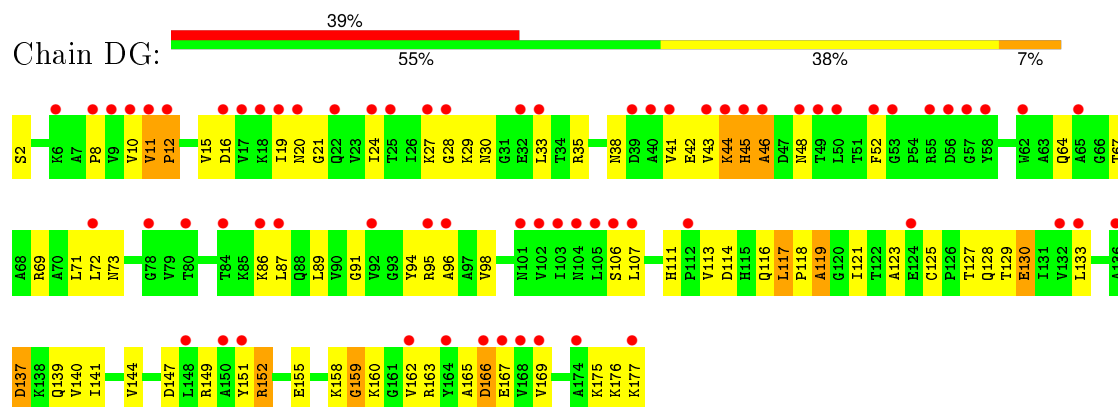
• Molecule 27: 50S ribosomal protein L5



• Molecule 28: 50S ribosomal protein L6

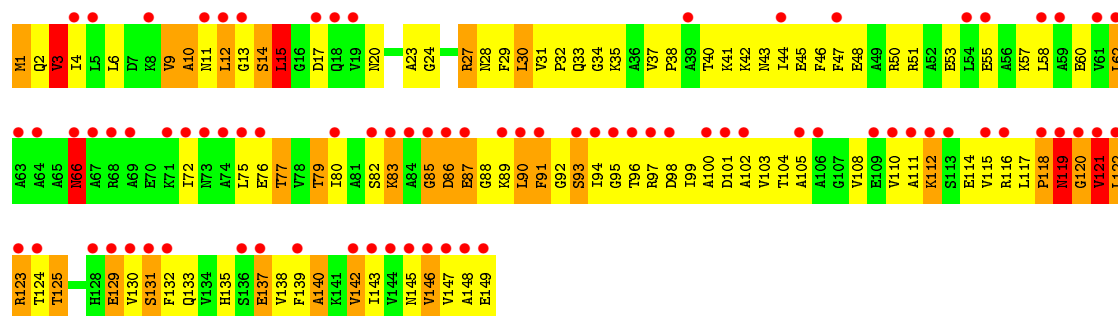


• Molecule 28: 50S ribosomal protein L6



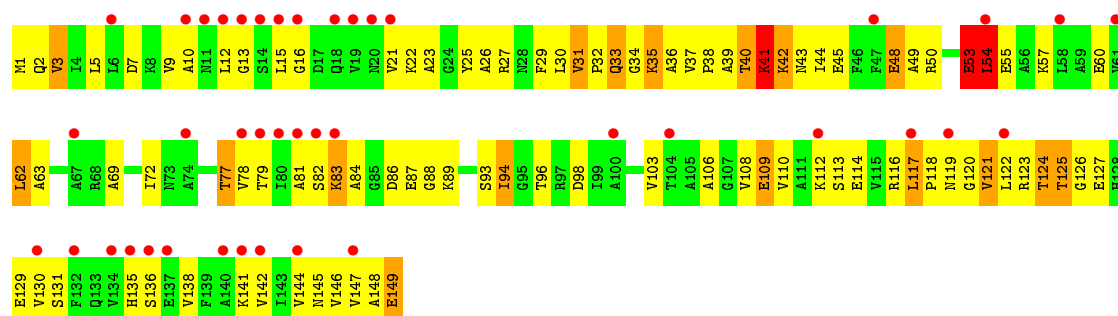
• Molecule 29: 50S ribosomal protein L9





• Molecule 29: 50S ribosomal protein L9

Chain DH: 28% 36% 50% 11%



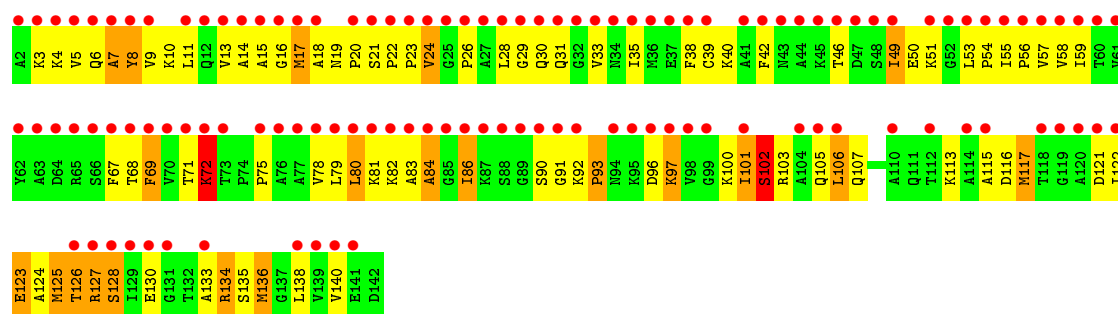
• Molecule 30: 50S ribosomal protein L11

Chain BI: 67% 31% 50% 16%

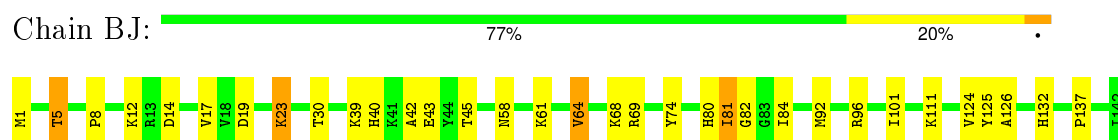


• Molecule 30: 50S ribosomal protein L11

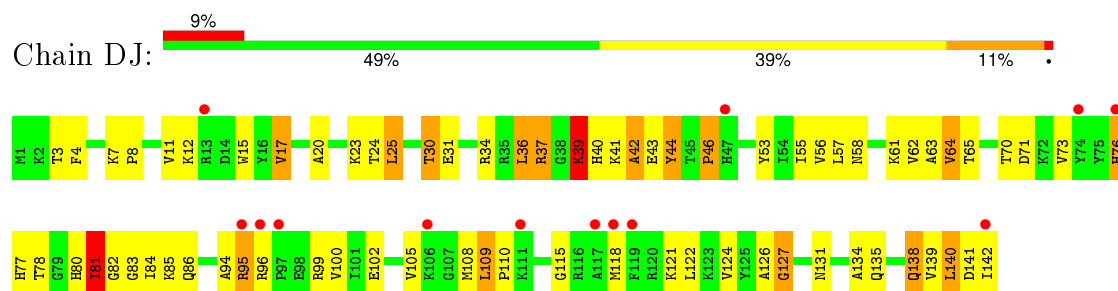
Chain DI: 82% 37% 47% 15%



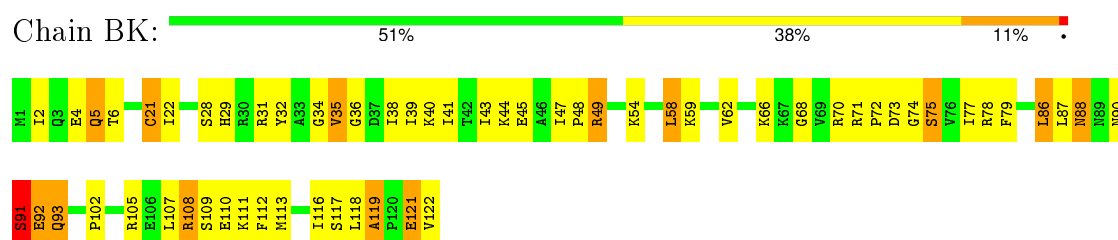
- Molecule 31: 50S ribosomal protein L13



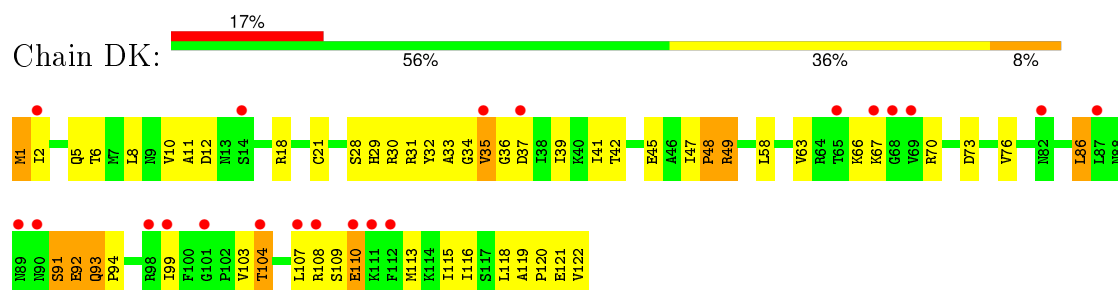
- Molecule 31: 50S ribosomal protein L13



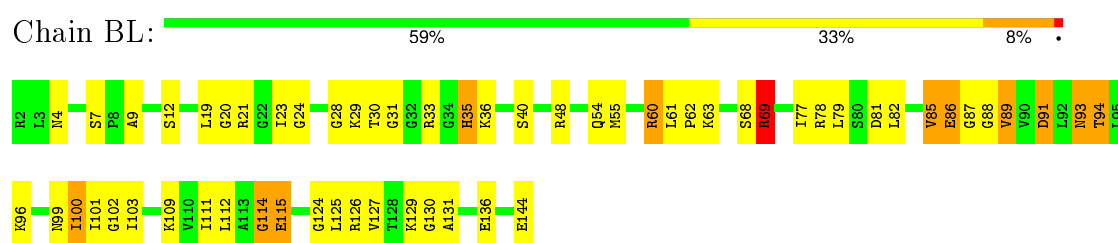
- Molecule 32: 50S ribosomal protein L14



- Molecule 32: 50S ribosomal protein L14

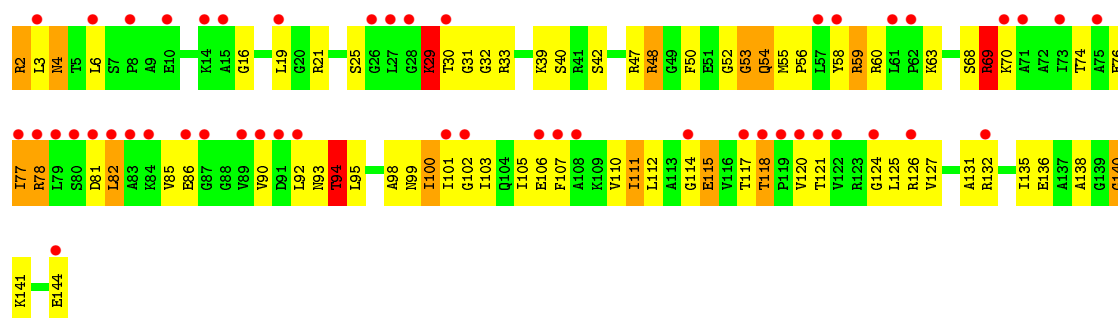


- Molecule 33: 50S ribosomal protein L15



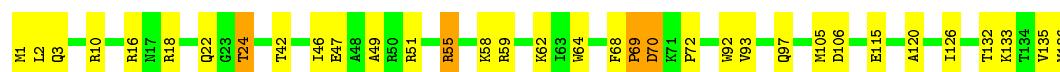
- Molecule 33: 50S ribosomal protein L15





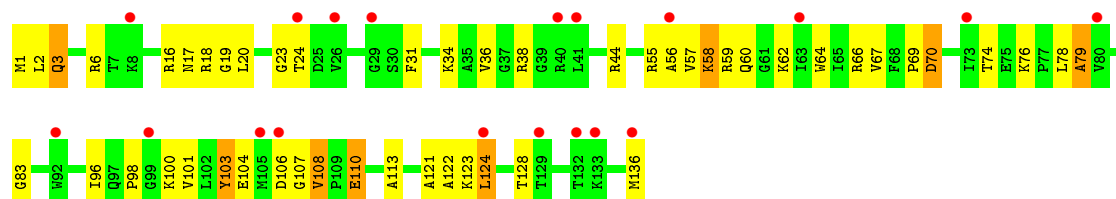
- Molecule 34: 50S ribosomal protein L16

Chain BM: 75% 22% .



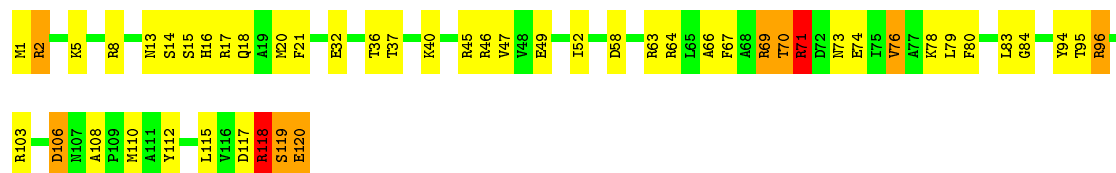
- Molecule 34: 50S ribosomal protein L16

Chain DM: 14% 63% 31% 6% .



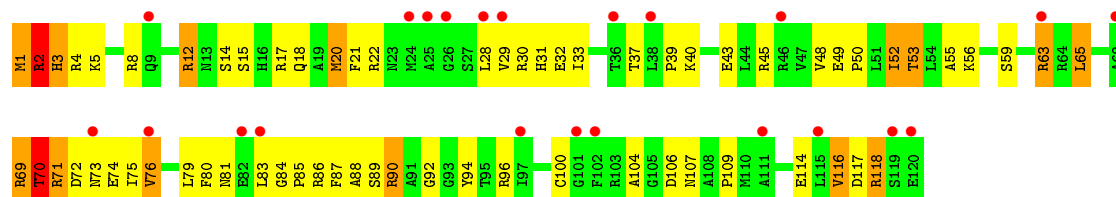
- Molecule 35: 50S ribosomal protein L17

Chain BN: 58% 33% 7% .



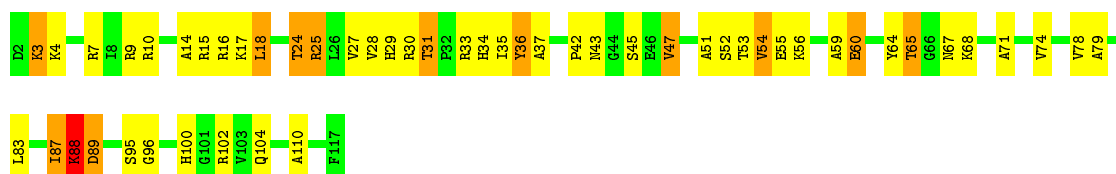
- Molecule 35: 50S ribosomal protein L17

Chain DN: 18% 45% 42% 12% .

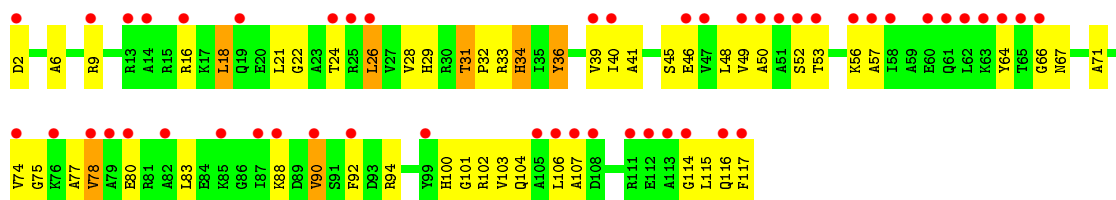
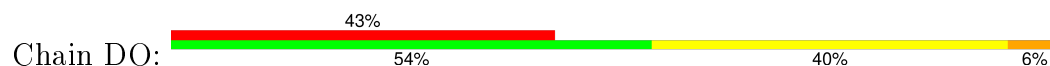


- Molecule 36: 50S ribosomal protein L18

Chain BO: 55% 34% 10% .



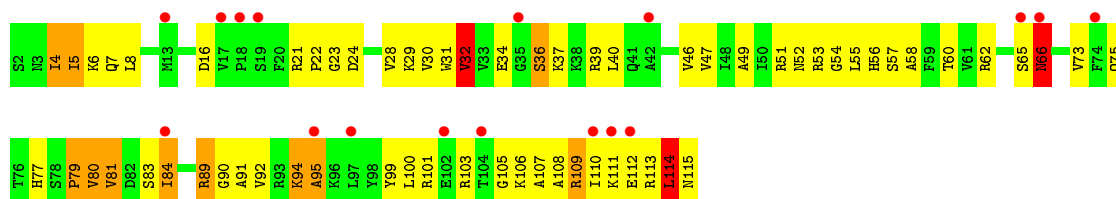
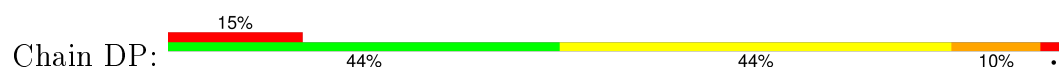
- Molecule 36: 50S ribosomal protein L18



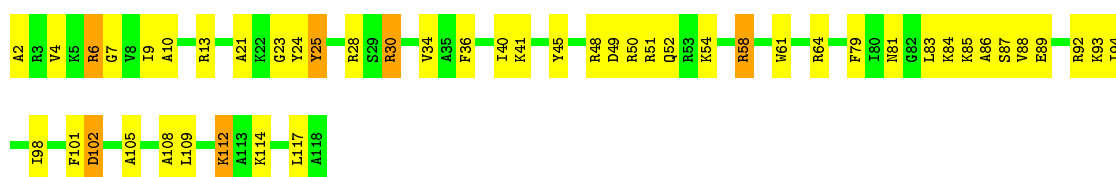
- Molecule 37: 50S ribosomal protein L19



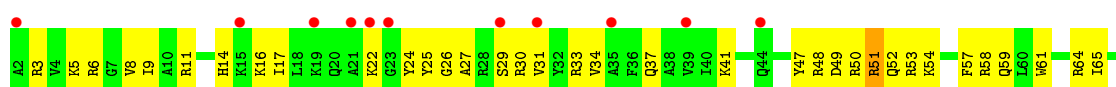
- Molecule 37: 50S ribosomal protein L19

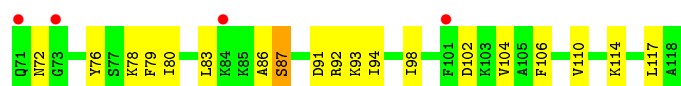


- Molecule 38: 50S ribosomal protein L20



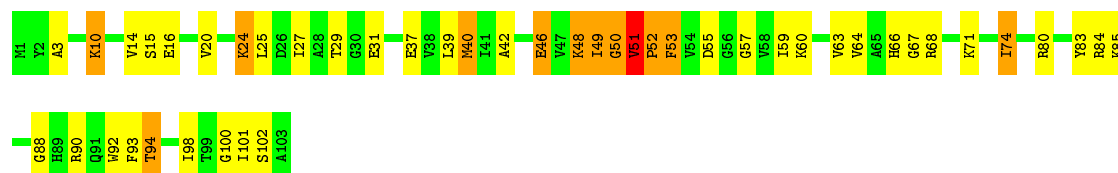
- Molecule 38: 50S ribosomal protein L20





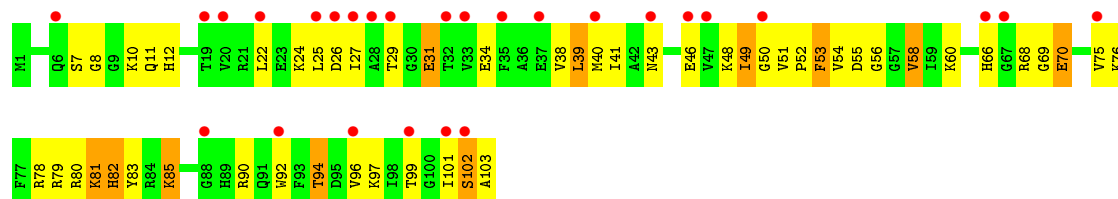
• Molecule 39: 50S ribosomal protein L21

Chain BR: 55% 33% 11%



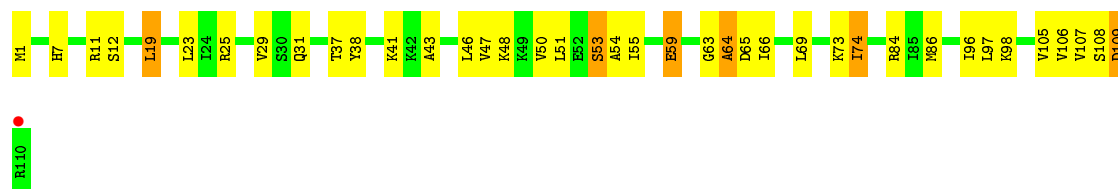
• Molecule 39: 50S ribosomal protein L21

Chain DR: 26% 50% 40% 11%



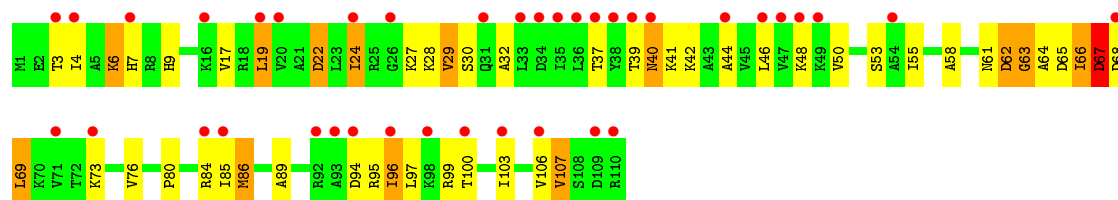
• Molecule 40: 50S ribosomal protein L22

Chain BS: 65% 30% 5%



• Molecule 40: 50S ribosomal protein L22

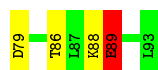
Chain DS: 35% 54% 34% 12%



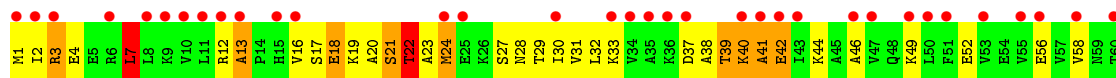
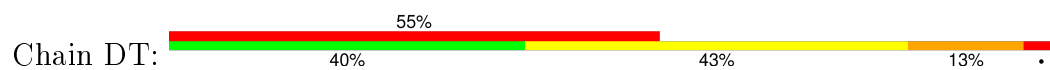
• Molecule 41: 50S ribosomal protein L23

Chain BT: 2% 54% 35% 9%

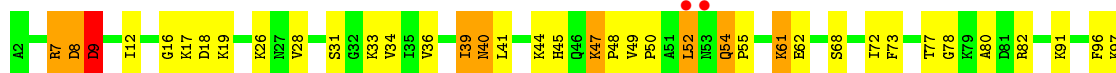




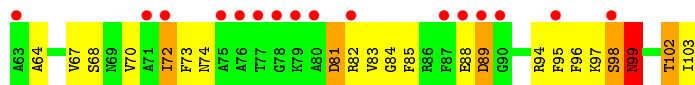
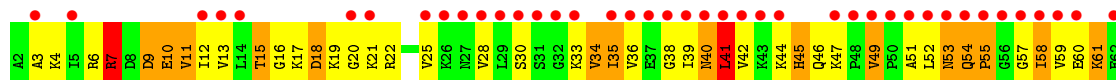
- Molecule 41: 50S ribosomal protein L23



- Molecule 42: 50S ribosomal protein L24



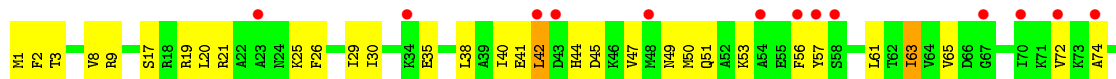
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25

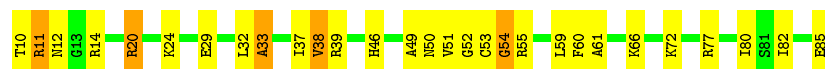


- Molecule 43: 50S ribosomal protein L25



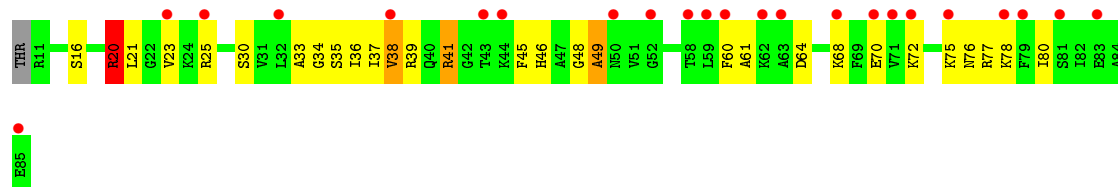
- Molecule 44: 50S ribosomal protein L27

Chain BW: 



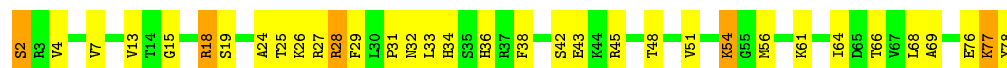
- Molecule 44: 50S ribosomal protein L27

Chain DW: 




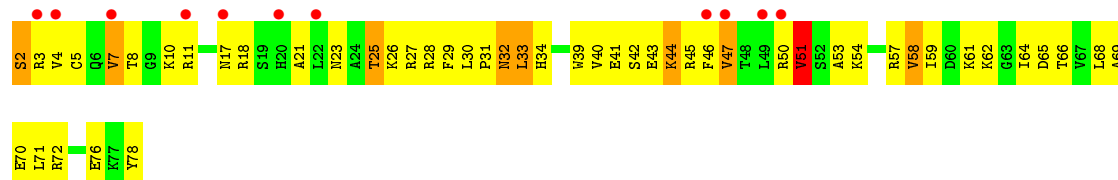
- Molecule 45: 50S ribosomal protein L28

Chain BX: 

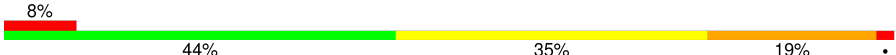


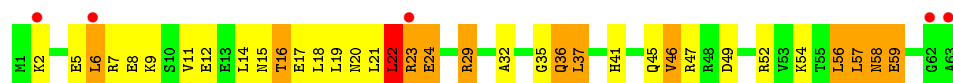
- Molecule 45: 50S ribosomal protein L28

Chain DX: 

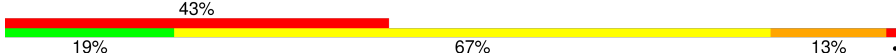


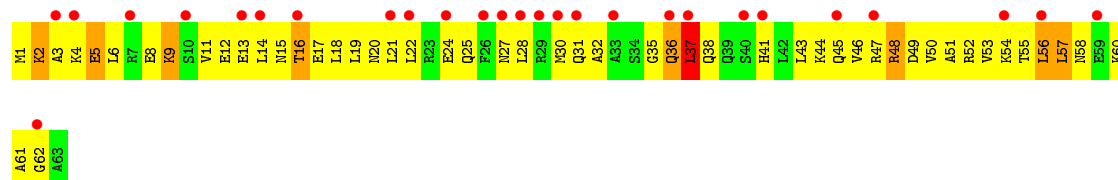
- Molecule 46: 50S ribosomal protein L29

Chain BY: 

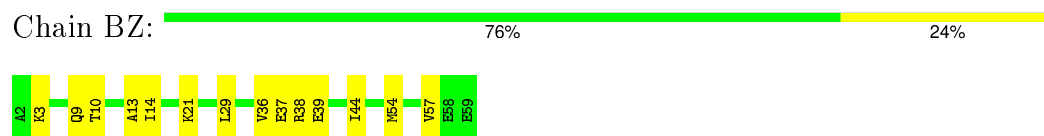


- Molecule 46: 50S ribosomal protein L29

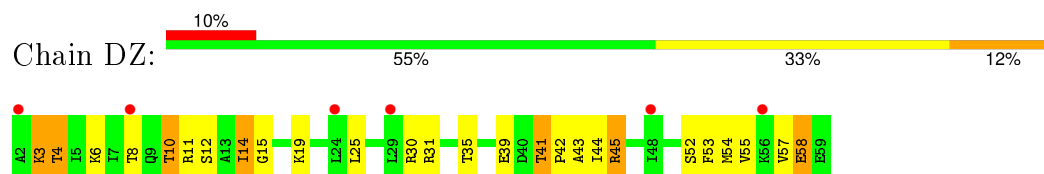
Chain DY: 



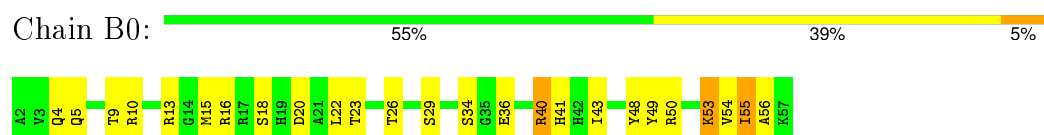
- Molecule 47: 50S ribosomal protein L30



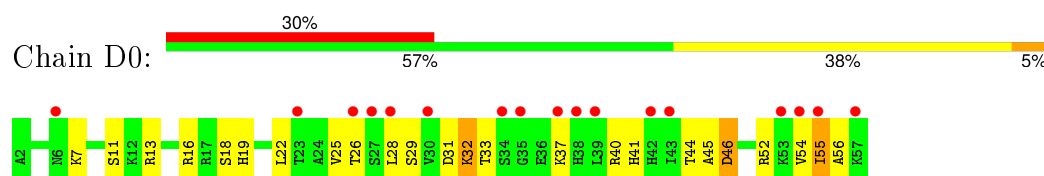
- Molecule 47: 50S ribosomal protein L30



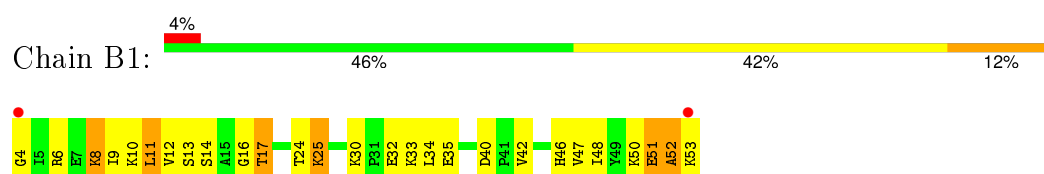
- Molecule 48: 50S ribosomal protein L32



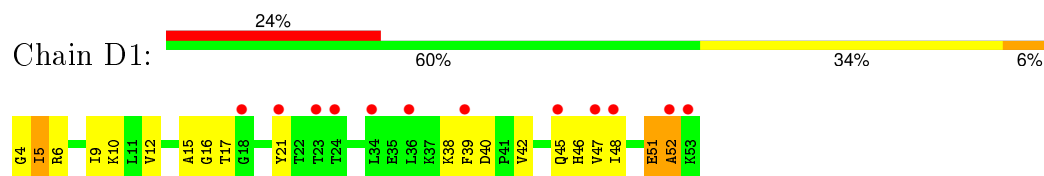
- Molecule 48: 50S ribosomal protein L32



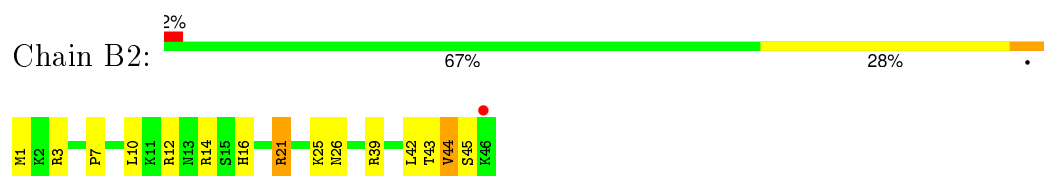
- Molecule 49: 50S ribosomal protein L33



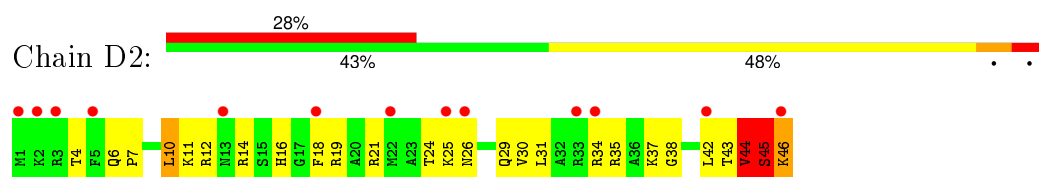
- Molecule 49: 50S ribosomal protein L33



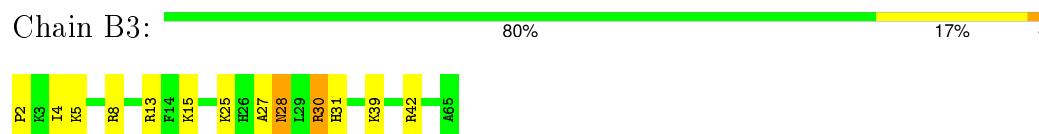
- Molecule 50: 50S ribosomal protein L34



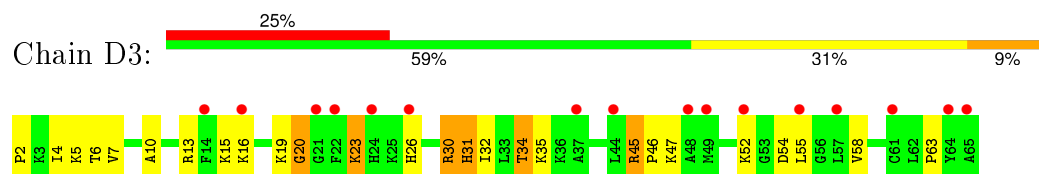
- Molecule 50: 50S ribosomal protein L34



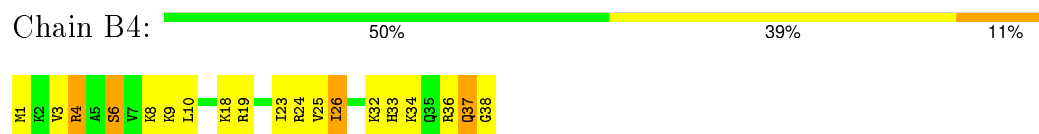
- Molecule 51: 50S ribosomal protein L35



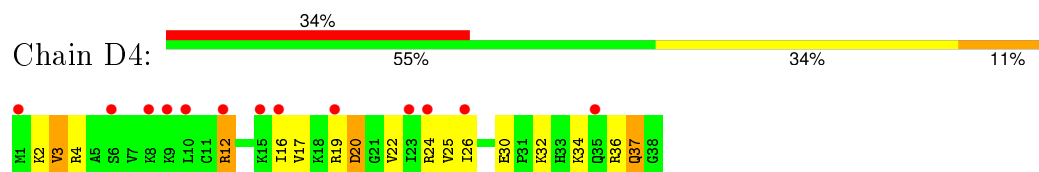
- Molecule 51: 50S ribosomal protein L35



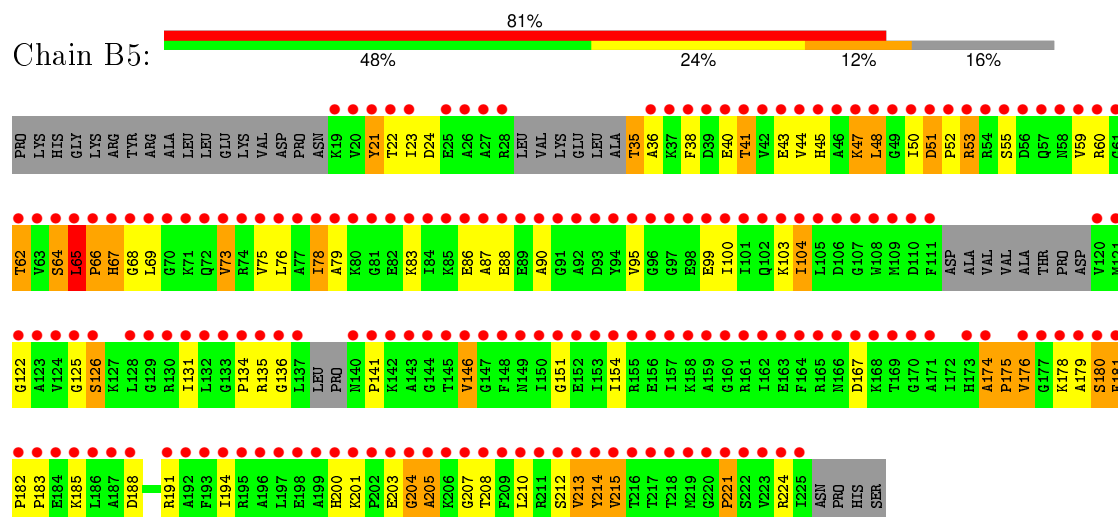
- Molecule 52: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1



- Molecule 54: Linopristin

Chain B6:  57% 43%



- Molecule 54: Linopristin

Chain D6:  71% 14% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.97Å 434.65Å 623.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.36 – 2.80 69.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.2 (69.36-2.80) 89.2 (69.36-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.215 , 0.260 0.224 , 0.269	Depositor DCC
R_{free} test set	5006 reflections (0.40%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1244949 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288396	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, VIF, DBB, MG, 04X, 004, MHW, MHU

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	0.35	0/36944	0.82	6/57632 (0.0%)
1	CA	0.29	0/36966	0.79	2/57666 (0.0%)
2	AB	0.29	0/1736	0.58	0/2338
2	CB	0.26	0/1736	0.52	0/2338
3	AC	0.28	0/1652	0.54	0/2225
3	CC	0.26	0/1652	0.50	0/2225
4	AD	0.29	0/1665	0.55	0/2227
4	CD	0.32	0/1665	0.57	0/2227
5	AE	0.32	0/1119	0.61	0/1504
5	CE	0.31	0/1119	0.64	0/1504
6	AF	0.31	0/836	0.61	1/1128 (0.1%)
6	CF	0.27	0/836	0.60	1/1128 (0.1%)
7	AG	0.26	0/1196	0.50	0/1602
7	CG	0.26	0/1196	0.50	0/1602
8	AH	0.31	0/989	0.54	0/1326
8	CH	0.26	0/989	0.50	0/1326
9	AI	0.27	0/1034	0.58	0/1375
9	CI	0.27	0/1034	0.54	0/1375
10	AJ	0.29	0/797	0.56	0/1077
10	CJ	0.27	0/797	0.55	0/1077
11	AK	0.28	0/893	0.57	0/1205
11	CK	0.28	0/893	0.58	0/1205
12	AL	0.32	0/969	0.62	0/1300
12	CL	0.30	0/969	0.61	0/1300
13	AM	0.27	0/893	0.56	0/1193
13	CM	0.26	0/893	0.55	0/1193
14	AN	0.29	0/785	0.56	0/1043
14	CN	0.25	0/785	0.48	0/1043
15	AO	0.27	0/718	0.53	0/959
15	CO	0.26	0/718	0.48	0/959
16	AP	0.30	0/659	0.58	0/884
16	CP	0.27	0/659	0.52	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.30	0/658	0.58	0/881
17	CQ	0.29	0/658	0.54	0/881
18	AR	0.27	0/463	0.53	0/621
18	CR	0.28	0/463	0.54	0/621
19	AS	0.29	0/653	0.58	0/877
19	CS	0.28	0/653	0.52	0/877
20	AT	0.30	0/671	0.56	0/888
20	CT	0.26	0/671	0.51	0/888
21	AU	0.35	0/431	0.64	0/570
21	CU	0.35	0/431	0.60	0/570
22	BA	0.60	5/69659 (0.0%)	1.01	98/108672 (0.1%)
22	DA	0.28	0/69659	0.80	8/108672 (0.0%)
23	BB	0.53	0/2850	0.95	0/4444
23	DB	0.24	0/2828	0.79	0/4410
24	BC	0.39	0/2122	0.63	1/2852 (0.0%)
24	DC	0.28	0/2122	0.54	0/2852
25	BD	0.42	0/1586	0.65	1/2134 (0.0%)
25	DD	0.28	0/1586	0.53	0/2134
26	BE	0.38	0/1571	0.60	0/2113
26	DE	0.27	0/1571	0.52	0/2113
27	BF	0.31	0/1435	0.53	0/1926
27	DF	0.26	0/1435	0.48	0/1926
28	BG	0.31	0/1343	0.57	0/1816
28	DG	0.25	0/1343	0.47	0/1816
29	BH	0.36	0/1121	0.66	1/1515 (0.1%)
29	DH	0.35	0/1121	0.56	0/1515
30	BI	0.28	0/1046	0.56	0/1410
30	DI	0.29	0/1046	0.54	0/1410
31	BJ	0.44	0/1152	0.62	0/1551
31	DJ	0.27	0/1152	0.51	0/1551
32	BK	0.44	0/948	0.66	0/1268
32	DK	0.28	0/948	0.51	0/1268
33	BL	0.40	0/1054	0.68	0/1403
33	DL	0.27	0/1054	0.57	0/1403
34	BM	0.43	0/1093	0.64	0/1460
34	DM	0.26	0/1093	0.47	0/1460
35	BN	0.46	0/974	0.68	1/1301 (0.1%)
35	DN	0.27	0/974	0.51	0/1301
36	BO	0.34	0/902	0.59	0/1209
36	DO	0.26	0/902	0.48	0/1209
37	BP	0.39	0/929	0.57	0/1242
37	DP	0.28	0/929	0.53	0/1242
38	BQ	0.48	0/960	0.68	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.27	0/960	0.48	0/1278
39	BR	0.47	0/829	0.73	1/1107 (0.1%)
39	DR	0.27	0/829	0.55	0/1107
40	BS	0.51	0/864	0.69	0/1156
40	DS	0.27	0/864	0.52	0/1156
41	BT	0.35	0/745	0.58	0/994
41	DT	0.27	0/745	0.53	0/994
42	BU	0.36	0/788	0.60	0/1051
42	DU	0.30	0/788	0.55	0/1051
43	BV	0.36	0/766	0.59	0/1025
43	DV	0.25	0/766	0.45	0/1025
44	BW	0.43	0/587	0.63	0/776
44	DW	0.26	0/576	0.48	0/762
45	BX	0.35	0/635	0.59	0/848
45	DX	0.28	0/635	0.52	0/848
46	BY	0.32	0/510	0.60	0/677
46	DY	0.26	0/510	0.54	0/677
47	BZ	0.46	0/453	0.60	0/605
47	DZ	0.26	0/453	0.52	0/605
48	B0	0.43	0/450	0.63	0/599
48	D0	0.29	0/450	0.55	0/599
49	B1	0.35	0/417	0.56	0/554
49	D1	0.27	0/417	0.48	0/554
50	B2	0.45	0/380	0.71	0/498
50	D2	0.29	0/380	0.52	0/498
51	B3	0.39	0/513	0.61	0/676
51	D3	0.26	0/513	0.48	0/676
52	B4	0.46	0/303	0.72	0/397
52	D4	0.25	0/303	0.50	0/397
53	B5	0.26	0/1145	0.50	0/1556
54	B6	4.15	4/13 (30.8%)	3.77	4/15 (26.7%)
54	D6	3.89	4/13 (30.8%)	3.55	1/15 (6.7%)
All	All	0.40	13/310652 (0.0%)	0.81	126/464396 (0.0%)

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
5	CE	0	1
6	CF	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	AK	0	1
12	AL	0	1
12	CL	0	1
21	AU	0	1
21	CU	0	1
24	BC	0	1
25	BD	0	1
25	DD	0	1
All	All	0	10

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-10.72	1.31	1.37
22	BA	984	A	N9-C4	-9.17	1.32	1.37
22	BA	1936	A	N9-C4	-7.33	1.33	1.37
22	BA	974	G	N9-C8	6.97	1.42	1.37
54	B6	2	THR	CB-OG1	-6.86	1.29	1.43

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	984	A	C2-N3-C4	-10.54	105.33	110.60
22	BA	1142	A	C2-N3-C4	-9.69	105.75	110.60
22	BA	1142	A	N3-C4-C5	9.46	133.42	126.80
22	BA	984	A	N3-C4-C5	9.37	133.36	126.80
22	BA	974	G	C4-C5-N7	9.29	114.51	110.80

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
12	AL	38	TYR	Peptide
21	AU	39	GLU	Peptide
24	BC	232	HIS	Peptide
25	BD	151	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	1047	0
1	CA	33015	0	16617	1004	0
2	AB	1705	0	1732	177	0
2	CB	1705	0	1732	125	0
3	AC	1625	0	1696	75	0
3	CC	1625	0	1696	64	0
4	AD	1643	0	1707	134	0
4	CD	1643	0	1707	121	0
5	AE	1106	0	1148	75	0
5	CE	1106	0	1148	101	0
6	AF	818	0	808	60	0
6	CF	818	0	808	56	0
7	AG	1182	0	1238	58	0
7	CG	1182	0	1238	54	0
8	AH	979	0	1031	74	0
8	CH	979	0	1031	42	0
9	AI	1022	0	1070	82	0
9	CI	1022	0	1070	70	0
10	AJ	787	0	828	69	0
10	CJ	787	0	828	59	0
11	AK	877	0	887	66	0
11	CK	877	0	887	65	0
12	AL	955	0	1016	61	0
12	CL	955	0	1016	72	0
13	AM	884	0	941	61	0
13	CM	884	0	941	49	0
14	AN	774	0	824	59	0
14	CN	774	0	824	45	0
15	AO	710	0	728	27	0
15	CO	710	0	728	31	0
16	AP	649	0	666	60	0
16	CP	649	0	666	29	0
17	AQ	649	0	691	65	0
17	CQ	649	0	691	59	0
18	AR	456	0	478	17	0
18	CR	456	0	478	40	0
19	AS	638	0	665	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	638	0	665	37	0
20	AT	665	0	714	50	0
20	CT	665	0	714	46	0
21	AU	426	0	449	49	0
21	CU	426	0	449	59	0
22	BA	62195	0	31280	1407	0
22	DA	62195	0	31280	2116	0
23	BB	2549	0	1291	30	0
23	DB	2529	0	1281	80	0
24	BC	2083	0	2154	82	0
24	DC	2083	0	2154	116	0
25	BD	1565	0	1616	52	0
25	DD	1565	0	1616	80	0
26	BE	1552	0	1619	46	0
26	DE	1552	0	1619	79	0
27	BF	1411	0	1444	89	0
27	DF	1411	0	1444	55	0
28	BG	1323	0	1371	43	0
28	DG	1323	0	1371	54	0
29	BH	1110	0	1147	151	0
29	DH	1110	0	1148	87	0
30	BI	1032	0	1085	81	0
30	DI	1032	0	1085	78	0
31	BJ	1129	0	1162	22	0
31	DJ	1129	0	1162	52	0
32	BK	939	0	1012	48	0
32	DK	939	0	1012	42	0
33	BL	1045	0	1117	55	0
33	DL	1045	0	1117	66	0
34	BM	1074	0	1157	25	0
34	DM	1074	0	1157	35	0
35	BN	961	0	1000	46	0
35	DN	961	0	1000	58	0
36	BO	892	0	923	37	0
36	DO	892	0	923	39	0
37	BP	917	0	962	28	0
37	DP	917	0	962	47	0
38	BQ	947	0	1019	39	0
38	DQ	947	0	1019	47	0
39	BR	816	0	839	56	0
39	DR	816	0	839	46	0
40	BS	857	0	922	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DS	857	0	922	40	0
41	BT	739	0	807	37	0
41	DT	739	0	807	47	0
42	BU	780	0	831	27	0
42	DU	780	0	831	64	0
43	BV	753	0	780	20	0
43	DV	753	0	780	27	0
44	BW	580	0	594	18	0
44	DW	569	0	581	25	0
45	BX	625	0	652	22	0
45	DX	625	0	652	45	0
46	BY	509	0	543	35	0
46	DY	509	0	543	45	0
47	BZ	449	0	488	9	0
47	DZ	449	0	488	13	0
48	B0	444	0	458	23	0
48	D0	444	0	458	18	0
49	B1	410	0	440	22	0
49	D1	410	0	440	11	0
50	B2	377	0	418	17	0
50	D2	377	0	418	24	0
51	B3	504	0	572	12	0
51	D3	504	0	572	27	0
52	B4	302	0	340	23	0
52	D4	302	0	340	15	0
53	B5	1142	0	865	52	0
54	B6	69	0	60	1	0
54	D6	69	0	61	20	0
55	AA	72	0	0	0	0
55	BA	193	0	0	0	0
55	BB	4	0	0	0	0
55	BD	1	0	0	0	0
55	BQ	1	0	0	0	0
55	CA	56	0	0	0	0
55	D2	1	0	0	0	0
55	DA	167	0	0	0	0
55	DB	3	0	0	0	0
56	BA	38	0	38	2	0
56	DA	38	0	37	11	0
57	B4	1	0	0	0	0
57	D4	1	0	0	0	0
58	AA	193	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	AL	2	0	0	0	0
58	AN	5	0	0	0	0
58	AT	2	0	0	0	0
58	AU	1	0	0	0	0
58	B2	1	0	0	0	0
58	B3	2	0	0	0	0
58	B4	2	0	0	0	0
58	BA	623	0	0	64	0
58	BB	14	0	0	0	0
58	BC	6	0	0	1	0
58	BD	3	0	0	2	0
58	BE	4	0	0	0	0
58	BF	1	0	0	1	0
58	BG	1	0	0	1	0
58	BL	4	0	0	2	0
58	BN	3	0	0	0	0
58	BS	1	0	0	0	0
58	BT	1	0	0	0	0
58	CA	192	0	0	21	0
58	CL	1	0	0	0	0
58	CN	3	0	0	0	0
58	CT	1	0	0	0	0
58	CU	1	0	0	1	0
58	D0	1	0	0	0	0
58	D2	1	0	0	0	0
58	D3	2	0	0	0	0
58	D4	1	0	0	0	0
58	DA	608	0	0	99	0
58	DB	13	0	0	1	0
58	DC	11	0	0	0	0
58	DD	4	0	0	2	0
58	DE	5	0	0	2	0
58	DJ	1	0	0	0	0
58	DL	4	0	0	2	0
58	DN	2	0	0	0	0
58	DT	1	0	0	0	0
58	DU	1	0	0	0	0
58	DV	1	0	0	0	0
All	All	288396	0	192983	10007	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 21.

The worst 5 of 10007 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)
29:BH:123:ARG:HH22	1:CA:367:U:P	1.57	1.26
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14
22:BA:2498:C:OP2	58:BA:3690:HOH:O	1.65	1.12
1:AA:533:A:OP1	58:AA:1848:HOH:O	1.68	1.11

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%)	127 (59%)	39 (18%)	50 (23%)	0	0
2	CB	216/218 (99%)	137 (63%)	46 (21%)	33 (15%)	0	0
3	AC	204/206 (99%)	149 (73%)	34 (17%)	21 (10%)	1	1
3	CC	204/206 (99%)	149 (73%)	44 (22%)	11 (5%)	2	7
4	AD	203/205 (99%)	135 (66%)	38 (19%)	30 (15%)	0	0
4	CD	203/205 (99%)	150 (74%)	32 (16%)	21 (10%)	1	1
5	AE	148/150 (99%)	105 (71%)	23 (16%)	20 (14%)	0	1
5	CE	148/150 (99%)	92 (62%)	36 (24%)	20 (14%)	0	1
6	AF	98/100 (98%)	60 (61%)	25 (26%)	13 (13%)	0	1
6	CF	98/100 (98%)	66 (67%)	17 (17%)	15 (15%)	0	0
7	AG	149/151 (99%)	111 (74%)	25 (17%)	13 (9%)	1	2
7	CG	149/151 (99%)	119 (80%)	18 (12%)	12 (8%)	1	2
8	AH	127/129 (98%)	88 (69%)	32 (25%)	7 (6%)	2	6
8	CH	127/129 (98%)	102 (80%)	16 (13%)	9 (7%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AI	125/127 (98%)	89 (71%)	20 (16%)	16 (13%)	0	1
9	CI	125/127 (98%)	86 (69%)	28 (22%)	11 (9%)	1	2
10	AJ	96/98 (98%)	63 (66%)	15 (16%)	18 (19%)	0	0
10	CJ	96/98 (98%)	70 (73%)	15 (16%)	11 (12%)	0	1
11	AK	115/117 (98%)	84 (73%)	20 (17%)	11 (10%)	1	1
11	CK	115/117 (98%)	81 (70%)	25 (22%)	9 (8%)	1	2
12	AL	121/123 (98%)	92 (76%)	20 (16%)	9 (7%)	1	3
12	CL	121/123 (98%)	88 (73%)	18 (15%)	15 (12%)	0	1
13	AM	112/114 (98%)	87 (78%)	12 (11%)	13 (12%)	0	1
13	CM	112/114 (98%)	81 (72%)	23 (20%)	8 (7%)	1	3
14	AN	92/100 (92%)	58 (63%)	19 (21%)	15 (16%)	0	0
14	CN	92/100 (92%)	60 (65%)	15 (16%)	17 (18%)	0	0
15	AO	86/88 (98%)	68 (79%)	15 (17%)	3 (4%)	4	15
15	CO	86/88 (98%)	72 (84%)	10 (12%)	4 (5%)	3	9
16	AP	80/82 (98%)	54 (68%)	13 (16%)	13 (16%)	0	0
16	CP	80/82 (98%)	61 (76%)	14 (18%)	5 (6%)	2	4
17	AQ	78/80 (98%)	52 (67%)	21 (27%)	5 (6%)	2	4
17	CQ	78/80 (98%)	56 (72%)	13 (17%)	9 (12%)	0	1
18	AR	53/55 (96%)	39 (74%)	12 (23%)	2 (4%)	4	13
18	CR	53/55 (96%)	34 (64%)	12 (23%)	7 (13%)	0	1
19	AS	77/79 (98%)	50 (65%)	18 (23%)	9 (12%)	0	1
19	CS	77/79 (98%)	60 (78%)	12 (16%)	5 (6%)	1	4
20	AT	83/85 (98%)	66 (80%)	11 (13%)	6 (7%)	1	3
20	CT	83/85 (98%)	62 (75%)	16 (19%)	5 (6%)	2	5
21	AU	49/51 (96%)	28 (57%)	8 (16%)	13 (26%)	0	0
21	CU	49/51 (96%)	24 (49%)	12 (24%)	13 (26%)	0	0
24	BC	269/271 (99%)	217 (81%)	42 (16%)	10 (4%)	4	14
24	DC	269/271 (99%)	205 (76%)	47 (18%)	17 (6%)	2	4
25	BD	207/209 (99%)	180 (87%)	22 (11%)	5 (2%)	7	25
25	DD	207/209 (99%)	162 (78%)	33 (16%)	12 (6%)	2	5
26	BE	199/201 (99%)	172 (86%)	22 (11%)	5 (2%)	7	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	DE	199/201 (99%)	158 (79%)	30 (15%)	11 (6%)	2	6
27	BF	175/177 (99%)	144 (82%)	22 (13%)	9 (5%)	2	8
27	DF	175/177 (99%)	133 (76%)	29 (17%)	13 (7%)	1	3
28	BG	174/176 (99%)	150 (86%)	19 (11%)	5 (3%)	6	19
28	DG	174/176 (99%)	136 (78%)	30 (17%)	8 (5%)	3	9
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	1
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	1	1
30	BI	139/141 (99%)	82 (59%)	37 (27%)	20 (14%)	0	1
30	DI	139/141 (99%)	77 (55%)	47 (34%)	15 (11%)	0	1
31	BJ	140/142 (99%)	125 (89%)	14 (10%)	1 (1%)	26	62
31	DJ	140/142 (99%)	119 (85%)	13 (9%)	8 (6%)	2	6
32	BK	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	1	4
32	DK	120/122 (98%)	94 (78%)	19 (16%)	7 (6%)	2	5
33	BL	141/143 (99%)	110 (78%)	25 (18%)	6 (4%)	3	10
33	DL	141/143 (99%)	96 (68%)	33 (23%)	12 (8%)	1	2
34	BM	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	13	40
34	DM	134/136 (98%)	108 (81%)	18 (13%)	8 (6%)	2	5
35	BN	118/120 (98%)	106 (90%)	9 (8%)	3 (2%)	7	24
35	DN	118/120 (98%)	97 (82%)	13 (11%)	8 (7%)	1	4
36	BO	114/116 (98%)	93 (82%)	18 (16%)	3 (3%)	7	22
36	DO	114/116 (98%)	87 (76%)	20 (18%)	7 (6%)	2	5
37	BP	112/114 (98%)	100 (89%)	7 (6%)	5 (4%)	3	10
37	DP	112/114 (98%)	84 (75%)	15 (13%)	13 (12%)	0	1
38	BQ	115/117 (98%)	111 (96%)	1 (1%)	3 (3%)	7	22
38	DQ	115/117 (98%)	97 (84%)	16 (14%)	2 (2%)	11	36
39	BR	101/103 (98%)	86 (85%)	6 (6%)	9 (9%)	1	2
39	DR	101/103 (98%)	74 (73%)	20 (20%)	7 (7%)	1	3
40	BS	108/110 (98%)	95 (88%)	10 (9%)	3 (3%)	6	21
40	DS	108/110 (98%)	84 (78%)	16 (15%)	8 (7%)	1	3
41	BT	91/93 (98%)	72 (79%)	13 (14%)	6 (7%)	1	4
41	DT	91/93 (98%)	54 (59%)	23 (25%)	14 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BU	100/102 (98%)	79 (79%)	12 (12%)	9 (9%)	1	2
42	DU	100/102 (98%)	68 (68%)	19 (19%)	13 (13%)	0	1
43	BV	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
43	DV	92/94 (98%)	77 (84%)	13 (14%)	2 (2%)	8	28
44	BW	74/76 (97%)	69 (93%)	2 (3%)	3 (4%)	3	11
44	DW	73/76 (96%)	64 (88%)	7 (10%)	2 (3%)	6	21
45	BX	75/77 (97%)	70 (93%)	4 (5%)	1 (1%)	15	44
45	DX	75/77 (97%)	52 (69%)	16 (21%)	7 (9%)	1	1
46	BY	61/63 (97%)	42 (69%)	13 (21%)	6 (10%)	1	1
46	DY	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	4
47	BZ	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
47	DZ	56/58 (97%)	48 (86%)	5 (9%)	3 (5%)	2	7
48	B0	54/56 (96%)	43 (80%)	9 (17%)	2 (4%)	4	14
48	D0	54/56 (96%)	36 (67%)	15 (28%)	3 (6%)	2	6
49	B1	48/50 (96%)	37 (77%)	9 (19%)	2 (4%)	3	11
49	D1	48/50 (96%)	37 (77%)	8 (17%)	3 (6%)	2	4
50	B2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	8	26
50	D2	44/46 (96%)	35 (80%)	7 (16%)	2 (4%)	3	10
51	B3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	12	38
51	D3	62/64 (97%)	46 (74%)	14 (23%)	2 (3%)	5	17
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	21
53	B5	183/228 (80%)	100 (55%)	50 (27%)	33 (18%)	0	0
54	B6	2/7 (29%)	2 (100%)	0	0	100	100
54	D6	2/7 (29%)	0	1 (50%)	1 (50%)	0	0
All	All	11422/11686 (98%)	8617 (75%)	1868 (16%)	937 (8%)	1	2

5 of 937 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	21	ARG
2	AB	22	TYR

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Mol	Chain	Res	Type
2	AB	25	PRO
2	AB	34	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%)	134 (74%)	46 (26%)	0	2
2	CB	180/180 (100%)	131 (73%)	49 (27%)	0	1
3	AC	170/170 (100%)	128 (75%)	42 (25%)	1	2
3	CC	170/170 (100%)	136 (80%)	34 (20%)	1	5
4	AD	172/172 (100%)	135 (78%)	37 (22%)	1	3
4	CD	172/172 (100%)	140 (81%)	32 (19%)	2	6
5	AE	113/113 (100%)	82 (73%)	31 (27%)	0	1
5	CE	113/113 (100%)	86 (76%)	27 (24%)	1	2
6	AF	87/87 (100%)	64 (74%)	23 (26%)	0	1
6	CF	87/87 (100%)	63 (72%)	24 (28%)	0	1
7	AG	124/124 (100%)	91 (73%)	33 (27%)	0	1
7	CG	124/124 (100%)	86 (69%)	38 (31%)	0	1
8	AH	104/104 (100%)	84 (81%)	20 (19%)	2	5
8	CH	104/104 (100%)	82 (79%)	22 (21%)	1	4
9	AI	105/105 (100%)	71 (68%)	34 (32%)	0	1
9	CI	105/105 (100%)	73 (70%)	32 (30%)	0	1
10	AJ	86/86 (100%)	65 (76%)	21 (24%)	1	2
10	CJ	86/86 (100%)	68 (79%)	18 (21%)	1	4
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	3
11	CK	90/90 (100%)	65 (72%)	25 (28%)	0	1
12	AL	103/103 (100%)	86 (84%)	17 (16%)	3	8
12	CL	103/103 (100%)	81 (79%)	22 (21%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AM	92/92 (100%)	70 (76%)	22 (24%)	1	2
13	CM	92/92 (100%)	66 (72%)	26 (28%)	0	1
14	AN	79/83 (95%)	64 (81%)	15 (19%)	2	5
14	CN	79/83 (95%)	67 (85%)	12 (15%)	3	10
15	AO	75/76 (99%)	61 (81%)	14 (19%)	2	6
15	CO	75/76 (99%)	59 (79%)	16 (21%)	1	4
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	3
16	CP	65/65 (100%)	49 (75%)	16 (25%)	1	2
17	AQ	74/74 (100%)	53 (72%)	21 (28%)	0	1
17	CQ	74/74 (100%)	49 (66%)	25 (34%)	0	0
18	AR	48/48 (100%)	36 (75%)	12 (25%)	1	2
18	CR	48/48 (100%)	38 (79%)	10 (21%)	1	4
19	AS	70/70 (100%)	56 (80%)	14 (20%)	1	5
19	CS	70/70 (100%)	57 (81%)	13 (19%)	2	6
20	AT	65/65 (100%)	49 (75%)	16 (25%)	1	2
20	CT	65/65 (100%)	48 (74%)	17 (26%)	0	1
21	AU	44/44 (100%)	25 (57%)	19 (43%)	0	0
21	CU	44/44 (100%)	27 (61%)	17 (39%)	0	0
24	BC	216/216 (100%)	189 (88%)	27 (12%)	6	17
24	DC	216/216 (100%)	180 (83%)	36 (17%)	3	8
25	BD	164/164 (100%)	152 (93%)	12 (7%)	17	44
25	DD	164/164 (100%)	147 (90%)	17 (10%)	9	25
26	BE	165/165 (100%)	139 (84%)	26 (16%)	3	9
26	DE	165/165 (100%)	135 (82%)	30 (18%)	2	6
27	BF	148/148 (100%)	114 (77%)	34 (23%)	1	3
27	DF	148/148 (100%)	123 (83%)	25 (17%)	2	7
28	BG	137/137 (100%)	125 (91%)	12 (9%)	12	35
28	DG	137/137 (100%)	117 (85%)	20 (15%)	4	11
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	3
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	3
30	BI	109/109 (100%)	76 (70%)	33 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	DI	109/109 (100%)	78 (72%)	31 (28%)	0	1
31	BJ	116/116 (100%)	103 (89%)	13 (11%)	7	22
31	DJ	116/116 (100%)	96 (83%)	20 (17%)	2	7
32	BK	103/103 (100%)	90 (87%)	13 (13%)	5	17
32	DK	103/103 (100%)	96 (93%)	7 (7%)	20	49
33	BL	102/102 (100%)	88 (86%)	14 (14%)	4	13
33	DL	102/102 (100%)	85 (83%)	17 (17%)	3	8
34	BM	109/109 (100%)	101 (93%)	8 (7%)	17	44
34	DM	109/109 (100%)	100 (92%)	9 (8%)	14	38
35	BN	100/100 (100%)	89 (89%)	11 (11%)	8	23
35	DN	100/100 (100%)	78 (78%)	22 (22%)	1	3
36	BO	86/86 (100%)	68 (79%)	18 (21%)	1	4
36	DO	86/86 (100%)	73 (85%)	13 (15%)	3	10
37	BP	99/99 (100%)	90 (91%)	9 (9%)	12	33
37	DP	99/99 (100%)	84 (85%)	15 (15%)	3	10
38	BQ	89/89 (100%)	81 (91%)	8 (9%)	12	34
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	4	11
39	BR	84/84 (100%)	73 (87%)	11 (13%)	5	15
39	DR	84/84 (100%)	66 (79%)	18 (21%)	1	3
40	BS	93/93 (100%)	80 (86%)	13 (14%)	4	13
40	DS	93/93 (100%)	81 (87%)	12 (13%)	5	16
41	BT	80/80 (100%)	65 (81%)	15 (19%)	2	6
41	DT	80/80 (100%)	65 (81%)	15 (19%)	2	6
42	BU	83/83 (100%)	70 (84%)	13 (16%)	3	9
42	DU	83/83 (100%)	65 (78%)	18 (22%)	1	3
43	BV	78/78 (100%)	69 (88%)	9 (12%)	7	21
43	DV	78/78 (100%)	64 (82%)	14 (18%)	2	6
44	BW	57/58 (98%)	52 (91%)	5 (9%)	12	35
44	DW	56/58 (97%)	51 (91%)	5 (9%)	12	34
45	BX	67/67 (100%)	55 (82%)	12 (18%)	2	6
45	DX	67/67 (100%)	54 (81%)	13 (19%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BY	55/55 (100%)	47 (86%)	8 (14%)	4	11
46	DY	55/55 (100%)	40 (73%)	15 (27%)	0	1
47	BZ	48/48 (100%)	45 (94%)	3 (6%)	22	53
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	4
48	B0	47/47 (100%)	43 (92%)	4 (8%)	13	36
48	D0	47/47 (100%)	43 (92%)	4 (8%)	13	36
49	B1	45/45 (100%)	40 (89%)	5 (11%)	8	23
49	D1	45/45 (100%)	40 (89%)	5 (11%)	8	23
50	B2	38/38 (100%)	34 (90%)	4 (10%)	8	24
50	D2	38/38 (100%)	30 (79%)	8 (21%)	1	4
51	B3	51/51 (100%)	48 (94%)	3 (6%)	24	57
51	D3	51/51 (100%)	44 (86%)	7 (14%)	4	13
52	B4	34/34 (100%)	27 (79%)	7 (21%)	1	4
52	D4	34/34 (100%)	29 (85%)	5 (15%)	4	11
53	B5	61/180 (34%)	46 (75%)	15 (25%)	1	2
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7602 (81%)	1788 (19%)	2	5

5 of 1788 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BX	45	ARG
5	CE	137	VAL
39	DR	85	LYS
49	B1	46	HIS
2	CB	213	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
36	BO	100	HIS
2	CB	15	HIS
46	DY	15	ASN
39	BR	89	HIS

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Mol	Chain	Res	Type
40	BS	15	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	344 (22%)	12 (0%)
1	CA	1538/1539 (99%)	340 (22%)	9 (0%)
22	BA	2895/2903 (99%)	542 (18%)	21 (0%)
22	DA	2895/2903 (99%)	673 (23%)	28 (0%)
23	BB	118/119 (99%)	19 (16%)	0
23	DB	117/119 (98%)	24 (20%)	0
All	All	9100/9122 (99%)	1942 (21%)	70 (0%)

5 of 1942 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	13	U

5 of 70 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2583	G
1	CA	1201	A
22	DA	2225	A
22	BA	2873	A
1	CA	209	U

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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
54	MHW	B6	1	54	9,9,10	3.14	4 (44%)	8,11,13	2.14	5 (62%)
54	DBB	B6	3	54	4,5,6	0.37	0	3,5,7	4.99	1 (33%)
54	MHU	B6	5	54	13,15,16	2.87	8 (61%)	15,19,21	2.17	1 (6%)
54	04X	B6	6	54	12,16,17	1.75	2 (16%)	11,20,22	4.91	6 (54%)
54	004	B6	7	54	9,10,11	4.09	6 (66%)	10,12,14	1.85	1 (10%)
54	MHW	D6	1	54	9,9,10	3.11	4 (44%)	8,11,13	2.07	4 (50%)
54	DBB	D6	3	54	4,5,6	0.63	0	3,5,7	5.48	2 (66%)
54	MHU	D6	5	54	13,15,16	2.84	7 (53%)	15,19,21	1.82	1 (6%)
54	04X	D6	6	54	12,16,17	1.37	2 (16%)	11,20,22	5.06	7 (63%)
54	004	D6	7	54	9,10,11	3.32	6 (66%)	10,12,14	2.01	2 (20%)

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
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	B6	3	54	-	0/2/4/6	0/0/0/0
54	MHU	B6	5	54	-	0/8/12/14	0/1/1/1
54	04X	B6	6	54	-	0/4/24/26	0/2/2/2
54	004	B6	7	54	-	0/4/6/8	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	D6	3	54	-	0/2/4/6	0/0/0/0
54	MHU	D6	5	54	-	0/8/12/14	0/1/1/1
54	04X	D6	6	54	-	0/4/24/26	0/2/2/2
54	004	D6	7	54	-	0/4/6/8	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-9.16	1.43	1.52
54	D6	7	004	CB-CA	-6.05	1.46	1.52
54	B6	1	MHW	CA-N	-6.00	1.27	1.35
54	D6	1	MHW	CA-N	-5.83	1.27	1.35
54	D6	1	MHW	CG2-CB	-5.11	1.30	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	3	DBB	O-C-CA	-9.12	101.73	125.49
54	B6	3	DBB	O-C-CA	-8.36	103.73	125.49
54	B6	5	MHU	O-C-CA	-7.27	106.23	125.44
54	D6	5	MHU	O-C-CA	-6.15	109.21	125.44
54	D6	6	04X	C2-C1-N1	-4.78	102.88	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	B6	1	MHW	1	0
54	D6	1	MHW	6	0
54	D6	3	DBB	2	0
54	D6	5	MHU	5	0
54	D6	6	04X	4	0
54	D6	7	004	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 502 ligands modelled in this entry, 500 are monoatomic - leaving 2 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	$\# Z > 2$
56	VIF	BA	3001	-	35,40,40	2.64	13 (37%)	41,55,55	1.96	14 (34%)
56	VIF	DA	3001	-	35,40,40	2.58	13 (37%)	41,55,55	1.95	13 (31%)

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
56	VIF	BA	3001	-	-	0/42/58/58	0/1/3/3
56	VIF	DA	3001	-	-	0/42/58/58	0/1/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BA	3001	VIF	F-C07	-6.45	1.25	1.41
56	DA	3001	VIF	F-C07	-6.07	1.26	1.41
56	BA	3001	VIF	O01-C06	-4.60	1.37	1.44
56	BA	3001	VIF	C11-C09	-4.46	1.43	1.53
56	DA	3001	VIF	O01-C06	-4.36	1.38	1.44

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DA	3001	VIF	C18-C10-C20	-5.86	116.82	125.75
56	BA	3001	VIF	C18-C10-C20	-4.14	119.44	125.75
56	BA	3001	VIF	C07-C14-C22	-3.96	108.39	113.87
56	DA	3001	VIF	C17-C18-C10	-3.85	114.05	125.31
56	BA	3001	VIF	O03-C15-N01	-3.35	116.90	121.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BA	3001	VIF	2	0
56	DA	3001	VIF	11	0

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	1538/1539 (99%)	-0.17	22 (1%) 78 69	13, 50, 135, 180	0
1	CA	1539/1539 (100%)	0.04	49 (3%) 51 39	27, 70, 145, 177	0
2	AB	218/218 (100%)	0.67	20 (9%) 11 5	38, 73, 99, 121	0
2	CB	218/218 (100%)	1.08	57 (26%) 1 0	61, 87, 107, 125	0
3	AC	206/206 (100%)	-0.06	3 (1%) 76 68	33, 57, 78, 93	0
3	CC	206/206 (100%)	0.71	22 (10%) 8 4	48, 78, 95, 105	0
4	AD	205/205 (100%)	0.18	9 (4%) 38 26	32, 55, 79, 105	0
4	CD	205/205 (100%)	-0.15	4 (1%) 68 58	18, 38, 64, 88	0
5	AE	150/150 (100%)	0.00	2 (1%) 79 71	30, 49, 79, 102	0
5	CE	150/150 (100%)	0.12	4 (2%) 58 45	32, 56, 82, 104	0
6	AF	100/100 (100%)	-0.14	1 (1%) 84 77	34, 58, 73, 86	0
6	CF	100/100 (100%)	-0.03	4 (4%) 42 30	44, 74, 93, 105	0
7	AG	151/151 (100%)	0.35	12 (7%) 15 8	54, 77, 96, 102	0
7	CG	151/151 (100%)	2.47	87 (57%) 0 0	81, 100, 109, 114	0
8	AH	129/129 (100%)	-0.11	1 (0%) 87 81	27, 48, 66, 76	0
8	CH	129/129 (100%)	0.18	5 (3%) 43 31	49, 65, 80, 90	0
9	AI	127/127 (100%)	0.89	15 (11%) 6 3	43, 73, 96, 109	0
9	CI	127/127 (100%)	1.41	36 (28%) 1 0	71, 93, 110, 122	0
10	AJ	98/98 (100%)	0.40	6 (6%) 25 15	40, 64, 92, 122	0
10	CJ	98/98 (100%)	2.21	47 (47%) 0 0	72, 93, 111, 125	0
11	AK	117/117 (100%)	0.57	11 (9%) 11 5	27, 65, 91, 115	0
11	CK	117/117 (100%)	0.15	5 (4%) 39 27	39, 66, 79, 93	0
12	AL	123/123 (100%)	0.06	6 (4%) 33 22	18, 35, 65, 96	0
12	CL	123/123 (100%)	0.24	6 (4%) 33 22	38, 52, 78, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.18	5 (4%) 38 26	45, 68, 92, 102	0
13	CM	114/114 (100%)	2.64	68 (59%) 0 0	96, 108, 116, 119	0
14	AN	96/100 (96%)	0.73	12 (12%) 5 2	37, 58, 94, 103	0
14	CN	96/100 (96%)	1.93	35 (36%) 0 0	69, 94, 111, 120	0
15	AO	88/88 (100%)	0.03	2 (2%) 64 52	28, 51, 65, 90	0
15	CO	88/88 (100%)	0.08	1 (1%) 82 74	40, 62, 80, 98	0
16	AP	82/82 (100%)	0.29	5 (6%) 25 15	31, 47, 85, 101	0
16	CP	82/82 (100%)	1.02	19 (23%) 1 1	44, 61, 87, 105	0
17	AQ	80/80 (100%)	0.26	3 (3%) 44 32	27, 49, 77, 122	0
17	CQ	80/80 (100%)	0.99	14 (17%) 2 1	44, 75, 97, 102	0
18	AR	55/55 (100%)	-0.13	2 (3%) 46 34	39, 52, 78, 108	0
18	CR	55/55 (100%)	0.10	3 (5%) 29 18	42, 55, 79, 111	0
19	AS	79/79 (100%)	0.73	11 (13%) 4 2	52, 68, 89, 102	0
19	CS	79/79 (100%)	3.64	58 (73%) 0 0	89, 108, 118, 124	0
20	AT	85/85 (100%)	0.34	2 (2%) 62 50	34, 48, 70, 103	0
20	CT	85/85 (100%)	1.15	16 (18%) 2 1	55, 73, 91, 97	0
21	AU	51/51 (100%)	1.35	17 (33%) 0 0	48, 74, 95, 106	0
21	CU	51/51 (100%)	0.68	6 (11%) 6 3	45, 71, 96, 105	0
22	BA	2897/2903 (99%)	0.06	105 (3%) 46 34	0, 13, 130, 195	0
22	DA	2897/2903 (99%)	0.20	88 (3%) 54 41	40, 82, 145, 181	0
23	BB	119/119 (100%)	-0.33	0 100 100	2, 23, 49, 85	0
23	DB	118/119 (99%)	0.07	1 (0%) 87 81	66, 112, 133, 143	0
24	BC	271/271 (100%)	-0.25	0 100 100	3, 19, 36, 51	0
24	DC	271/271 (100%)	0.50	21 (7%) 16 8	43, 61, 77, 89	0
25	BD	209/209 (100%)	-0.34	0 100 100	0, 10, 34, 68	0
25	DD	209/209 (100%)	0.78	26 (12%) 5 2	49, 68, 83, 96	0
26	BE	201/201 (100%)	-0.35	0 100 100	1, 23, 54, 90	0
26	DE	201/201 (100%)	1.43	72 (35%) 0 0	42, 84, 100, 108	0
27	BF	177/177 (100%)	0.03	3 (1%) 73 63	20, 41, 78, 90	0
27	DF	177/177 (100%)	2.99	127 (71%) 0 0	90, 107, 119, 125	0
28	BG	176/176 (100%)	-0.14	1 (0%) 90 86	17, 37, 62, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	1.84	68 (38%) 0 0	72, 93, 105, 114	0
29	BH	149/149 (100%)	3.17	81 (54%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.36	41 (27%) 1 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.43	94 (66%) 0 0	90, 111, 122, 133	0
30	DI	141/141 (100%)	4.74	116 (82%) 0 0	101, 117, 127, 130	0
31	BJ	142/142 (100%)	-0.42	0 100 100	1, 6, 22, 36	0
31	DJ	142/142 (100%)	0.55	13 (9%) 11 5	50, 66, 79, 96	0
32	BK	122/122 (100%)	-0.48	0 100 100	4, 12, 32, 67	0
32	DK	122/122 (100%)	0.94	21 (17%) 2 1	46, 63, 82, 97	0
33	BL	143/143 (100%)	-0.30	0 100 100	1, 18, 43, 74	0
33	DL	143/143 (100%)	1.63	49 (34%) 0 0	46, 79, 94, 113	0
34	BM	136/136 (100%)	-0.45	0 100 100	1, 9, 29, 84	0
34	DM	136/136 (100%)	0.81	19 (13%) 4 2	45, 69, 82, 101	0
35	BN	120/120 (100%)	-0.35	0 100 100	2, 7, 16, 52	0
35	DN	120/120 (100%)	1.02	22 (18%) 2 1	56, 75, 88, 114	0
36	BO	116/116 (100%)	-0.29	0 100 100	13, 24, 42, 50	0
36	DO	116/116 (100%)	1.85	50 (43%) 0 0	80, 94, 105, 114	0
37	BP	114/114 (100%)	-0.36	0 100 100	6, 18, 42, 64	0
37	DP	114/114 (100%)	0.76	17 (14%) 3 2	57, 69, 86, 91	0
38	BQ	117/117 (100%)	-0.35	0 100 100	1, 4, 13, 31	0
38	DQ	117/117 (100%)	0.64	15 (12%) 5 2	52, 67, 78, 82	0
39	BR	103/103 (100%)	-0.42	0 100 100	0, 11, 33, 66	0
39	DR	103/103 (100%)	1.39	27 (26%) 1 0	51, 77, 88, 99	0
40	BS	110/110 (100%)	-0.36	1 (0%) 85 79	1, 4, 21, 80	0
40	DS	110/110 (100%)	1.63	38 (34%) 0 0	57, 74, 89, 100	0
41	BT	93/93 (100%)	0.04	2 (2%) 65 54	8, 26, 75, 103	0
41	DT	93/93 (100%)	2.49	51 (54%) 0 0	66, 85, 103, 117	0
42	BU	102/102 (100%)	-0.29	2 (1%) 68 58	12, 28, 63, 92	0
42	DU	102/102 (100%)	2.97	57 (55%) 0 0	75, 90, 109, 118	0
43	BV	94/94 (100%)	-0.44	0 100 100	5, 19, 41, 53	0
43	DV	94/94 (100%)	0.90	15 (15%) 3 1	69, 84, 95, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.32	0 100 100	4, 12, 27, 54	0
44	DW	75/76 (98%)	1.56	23 (30%) 1 0	60, 80, 90, 105	0
45	BX	77/77 (100%)	-0.30	0 100 100	6, 24, 51, 73	0
45	DX	77/77 (100%)	0.71	11 (14%) 4 2	51, 71, 84, 87	0
46	BY	63/63 (100%)	0.16	5 (7%) 15 8	20, 40, 73, 93	0
46	DY	63/63 (100%)	1.95	27 (42%) 0 0	78, 94, 100, 105	0
47	BZ	58/58 (100%)	-0.29	0 100 100	2, 6, 23, 42	0
47	DZ	58/58 (100%)	0.60	6 (10%) 9 4	58, 71, 81, 94	0
48	B0	56/56 (100%)	-0.35	0 100 100	0, 9, 36, 68	0
48	D0	56/56 (100%)	1.49	17 (30%) 1 0	56, 78, 92, 102	0
49	B1	50/50 (100%)	-0.15	2 (4%) 42 30	17, 29, 49, 77	0
49	D1	50/50 (100%)	1.49	12 (24%) 1 1	69, 84, 93, 103	0
50	B2	46/46 (100%)	-0.23	1 (2%) 65 54	3, 9, 16, 88	0
50	D2	46/46 (100%)	1.46	13 (28%) 1 0	56, 68, 79, 102	0
51	B3	64/64 (100%)	-0.24	0 100 100	4, 9, 16, 31	0
51	D3	64/64 (100%)	1.09	16 (25%) 1 0	57, 71, 80, 81	0
52	B4	38/38 (100%)	-0.23	0 100 100	8, 16, 35, 52	0
52	D4	38/38 (100%)	1.52	13 (34%) 0 0	58, 75, 87, 101	0
53	B5	191/228 (83%)	5.83	184 (96%) 0 0	99, 115, 127, 135	0
54	B6	2/7 (28%)	-0.24	0 100 100	1, 1, 1, 1	0
54	D6	2/7 (28%)	0.50	0 100 100	47, 47, 47, 57	0
All	All	20738/20808 (99%)	0.47	2286 (11%) 7 3	0, 63, 120, 195	0

The worst 5 of 2286 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	21.2
29	BH	97	ARG	15.6
30	DI	3	LYS	14.4
30	DI	2	ALA	14.0
30	DI	60	THR	13.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
54	04X	B6	6	15/16	0.97	0.14	-	1,3,15,15	0
54	04X	D6	6	15/16	0.94	0.15	-	46,56,70,73	0
54	004	B6	7	10/11	0.97	0.21	-	0,0,1,2	0
54	MHW	D6	1	9/10	0.92	0.19	-	36,47,54,54	0
54	DBB	D6	3	6/7	0.94	0.28	-	45,52,56,63	0
54	MHW	B6	1	9/10	0.97	0.16	-	0,1,2,9	0
54	MHU	B6	5	15/16	0.97	0.21	-	0,1,3,6	0
54	MHU	D6	5	15/16	0.87	0.27	-	45,56,65,65	0
54	004	D6	7	10/11	0.95	0.18	-	40,51,56,56	0
54	DBB	B6	3	6/7	0.97	0.19	-	0,1,1,4	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
55	MG	DA	3117	1/1	0.92	0.57	40.28	73,73,73,73	0
55	MG	AA	1671	1/1	0.91	0.47	30.80	47,47,47,47	0
55	MG	BA	3137	1/1	0.87	0.69	26.12	66,66,66,66	0
55	MG	BA	3016	1/1	0.77	0.36	17.25	59,59,59,59	0
55	MG	DA	3121	1/1	0.87	0.27	11.18	78,78,78,78	0
55	MG	BA	3041	1/1	0.94	0.38	10.35	2,2,2,2	0
55	MG	BA	3132	1/1	0.96	0.28	9.61	50,50,50,50	0
55	MG	AA	1644	1/1	0.83	0.52	9.31	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3025	1/1	0.84	0.39	8.60	56,56,56,56	0
55	MG	BA	3151	1/1	0.83	0.24	8.60	49,49,49,49	0
55	MG	AA	1670	1/1	0.83	0.34	8.00	56,56,56,56	0
55	MG	BA	3084	1/1	0.80	0.24	7.35	49,49,49,49	0
55	MG	BA	3106	1/1	0.97	0.26	7.22	0,0,0,0	0
55	MG	BA	3058	1/1	0.83	0.25	7.15	45,45,45,45	0
55	MG	DA	3003	1/1	0.73	0.29	6.74	92,92,92,92	0
55	MG	AA	1647	1/1	0.82	0.25	6.41	58,58,58,58	0
55	MG	DA	3159	1/1	0.91	0.38	6.32	61,61,61,61	0
55	MG	BA	3153	1/1	0.96	0.28	6.21	11,11,11,11	0
55	MG	DA	3103	1/1	0.95	0.31	5.66	83,83,83,83	0
55	MG	BA	3110	1/1	0.97	0.22	5.48	0,0,0,0	0
55	MG	BA	3109	1/1	0.98	0.20	5.44	1,1,1,1	0
55	MG	AA	1635	1/1	0.94	0.19	5.40	65,65,65,65	0
55	MG	AA	1656	1/1	0.93	0.23	5.29	36,36,36,36	0
55	MG	DA	3125	1/1	0.82	0.45	5.26	92,92,92,92	0
55	MG	DA	3042	1/1	0.47	0.33	5.09	68,68,68,68	0
55	MG	DA	3114	1/1	0.55	0.29	4.74	80,80,80,80	0
55	MG	BA	3174	1/1	0.81	0.22	4.46	27,27,27,27	0
55	MG	BA	3147	1/1	0.93	0.19	4.18	39,39,39,39	0
55	MG	DA	3140	1/1	0.97	0.29	4.03	28,28,28,28	0
55	MG	AA	1622	1/1	0.98	0.20	3.75	17,17,17,17	0
55	MG	DA	3065	1/1	0.94	0.21	3.58	43,43,43,43	0
55	MG	DA	3110	1/1	0.80	0.23	3.08	48,48,48,48	0
55	MG	BA	3105	1/1	0.96	0.19	2.89	0,0,0,0	0
55	MG	DA	3026	1/1	0.88	0.24	2.73	67,67,67,67	0
56	VIF	BA	3001	38/38	0.97	0.20	2.51	0,2,7,10	0
55	MG	BA	3177	1/1	0.90	0.19	2.50	29,29,29,29	0
55	MG	DA	3153	1/1	0.78	0.34	2.21	62,62,62,62	0
55	MG	BA	3035	1/1	0.97	0.19	1.35	47,47,47,47	0
56	VIF	DA	3001	38/38	0.94	0.23	1.33	34,47,57,61	0
55	MG	BA	3170	1/1	0.90	0.15	1.31	33,33,33,33	0
55	MG	BA	3050	1/1	0.92	0.19	1.06	6,6,6,6	0
55	MG	DA	3096	1/1	0.84	0.18	1.04	75,75,75,75	0
55	MG	DA	3064	1/1	0.87	0.19	0.97	48,48,48,48	0
55	MG	DA	3009	1/1	0.93	0.20	0.87	81,81,81,81	0
55	MG	CA	1635	1/1	0.79	0.25	0.84	120,120,120,120	0
55	MG	DA	3070	1/1	0.86	0.19	0.69	86,86,86,86	0
55	MG	DA	3106	1/1	0.94	0.20	0.67	72,72,72,72	0
55	MG	BA	3165	1/1	0.96	0.17	0.64	5,5,5,5	0
55	MG	DA	3116	1/1	0.85	0.34	0.60	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3069	1/1	0.97	0.18	0.52	0,0,0,0	0
55	MG	DA	3109	1/1	0.89	0.17	0.50	50,50,50,50	0
55	MG	BA	3131	1/1	0.96	0.19	0.45	0,0,0,0	0
55	MG	BA	3014	1/1	0.95	0.19	0.43	0,0,0,0	0
55	MG	BA	3019	1/1	0.97	0.15	0.39	12,12,12,12	0
55	MG	BA	3097	1/1	0.95	0.16	0.10	5,5,5,5	0
55	MG	DA	3130	1/1	0.94	0.18	-0.12	39,39,39,39	0
55	MG	BA	3018	1/1	0.94	0.17	-0.26	0,0,0,0	0
55	MG	CA	1630	1/1	0.47	0.21	-0.41	105,105,105,105	0
55	MG	BA	3023	1/1	0.98	0.17	-0.52	0,0,0,0	0
55	MG	BA	3080	1/1	0.92	0.14	-0.52	17,17,17,17	0
55	MG	AA	1632	1/1	0.90	0.11	-0.64	54,54,54,54	0
55	MG	DA	3020	1/1	0.71	0.19	-0.64	83,83,83,83	0
55	MG	DA	3099	1/1	0.95	0.16	-0.65	50,50,50,50	0
57	ZN	B4	101	1/1	1.00	0.14	-0.77	24,24,24,24	0
55	MG	BA	3037	1/1	0.78	0.15	-0.77	35,35,35,35	0
55	MG	CA	1614	1/1	0.89	0.09	-0.78	49,49,49,49	0
57	ZN	D4	101	1/1	0.99	0.10	-0.85	86,86,86,86	0
55	MG	DA	3079	1/1	0.86	0.12	-0.88	92,92,92,92	0
55	MG	BA	3187	1/1	0.94	0.13	-0.89	25,25,25,25	0
55	MG	DA	3044	1/1	0.96	0.13	-0.99	47,47,47,47	0
55	MG	AA	1663	1/1	0.92	0.13	-1.03	41,41,41,41	0
55	MG	DA	3133	1/1	0.85	0.11	-1.12	53,53,53,53	0
55	MG	DA	3050	1/1	0.88	0.15	-1.16	83,83,83,83	0
55	MG	AA	1607	1/1	0.90	0.14	-1.17	41,41,41,41	0
55	MG	BA	3013	1/1	0.97	0.17	-1.20	0,0,0,0	0
55	MG	DB	202	1/1	0.85	0.08	-1.21	65,65,65,65	0
55	MG	DA	3029	1/1	0.89	0.12	-1.24	65,65,65,65	0
55	MG	BA	3159	1/1	0.89	0.14	-1.28	21,21,21,21	0
55	MG	AA	1641	1/1	0.97	0.14	-1.35	15,15,15,15	0
55	MG	DA	3111	1/1	0.92	0.15	-1.36	43,43,43,43	0
55	MG	DA	3051	1/1	0.95	0.13	-1.52	54,54,54,54	0
55	MG	BA	3063	1/1	0.93	0.17	-1.59	6,6,6,6	0
55	MG	BA	3025	1/1	0.99	0.15	-1.60	0,0,0,0	0
55	MG	CA	1632	1/1	0.72	0.12	-1.63	74,74,74,74	0
55	MG	CA	1603	1/1	0.98	0.12	-1.63	36,36,36,36	0
55	MG	BA	3066	1/1	0.95	0.14	-1.66	1,1,1,1	0
55	MG	AA	1630	1/1	0.84	0.13	-1.68	63,63,63,63	0
55	MG	DA	3095	1/1	0.88	0.12	-1.75	80,80,80,80	0
55	MG	DA	3013	1/1	0.96	0.16	-1.76	34,34,34,34	0
55	MG	BA	3056	1/1	0.97	0.14	-1.77	29,29,29,29	0
55	MG	AA	1642	1/1	0.98	0.15	-1.79	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3163	1/1	0.96	0.12	-1.80	31,31,31,31	0
55	MG	DA	3137	1/1	0.38	0.11	-1.83	88,88,88,88	0
55	MG	BB	201	1/1	0.98	0.08	-1.85	29,29,29,29	0
55	MG	BA	3024	1/1	0.95	0.14	-1.88	4,4,4,4	0
55	MG	CA	1610	1/1	0.93	0.10	-1.90	64,64,64,64	0
55	MG	BA	3135	1/1	0.95	0.15	-1.91	2,2,2,2	0
55	MG	DA	3135	1/1	0.85	0.11	-1.94	53,53,53,53	0
55	MG	DA	3080	1/1	0.70	0.10	-2.01	101,101,101,101	0
55	MG	DA	3023	1/1	0.96	0.13	-2.04	42,42,42,42	0
55	MG	BA	3152	1/1	0.94	0.15	-2.11	18,18,18,18	0
55	MG	DA	3024	1/1	0.92	0.07	-2.17	61,61,61,61	0
55	MG	AA	1617	1/1	0.97	0.04	-2.18	51,51,51,51	0
55	MG	BA	3133	1/1	0.82	0.07	-2.23	37,37,37,37	0
55	MG	AA	1616	1/1	0.78	0.12	-2.34	50,50,50,50	0
55	MG	DA	3083	1/1	0.94	0.12	-2.37	49,49,49,49	0
55	MG	BA	3036	1/1	0.97	0.14	-2.47	0,0,0,0	0
55	MG	BA	3029	1/1	0.97	0.15	-2.47	2,2,2,2	0
55	MG	BA	3108	1/1	0.98	0.14	-2.59	9,9,9,9	0
55	MG	DA	3048	1/1	0.91	0.09	-2.63	53,53,53,53	0
55	MG	DA	3081	1/1	0.93	0.12	-2.76	84,84,84,84	0
55	MG	DA	3131	1/1	0.94	0.07	-2.79	67,67,67,67	0
55	MG	DA	3107	1/1	0.77	0.14	-3.18	48,48,48,48	0
55	MG	BA	3033	1/1	0.96	0.15	-3.30	4,4,4,4	0
55	MG	AA	1612	1/1	0.89	0.14	-3.41	37,37,37,37	0
55	MG	CA	1621	1/1	0.56	0.07	-3.44	71,71,71,71	0
55	MG	BA	3054	1/1	0.91	0.15	-3.60	2,2,2,2	0
55	MG	DA	3018	1/1	0.90	0.15	-3.68	51,51,51,51	0
55	MG	DA	3040	1/1	0.89	0.14	-3.77	60,60,60,60	0
55	MG	DA	3052	1/1	0.93	0.09	-3.77	49,49,49,49	0
55	MG	DA	3060	1/1	0.97	0.10	-3.79	43,43,43,43	0
55	MG	DA	3006	1/1	0.72	0.11	-3.82	98,98,98,98	0
55	MG	BA	3098	1/1	0.98	0.14	-3.83	2,2,2,2	0
55	MG	BA	3155	1/1	0.96	0.16	-3.89	26,26,26,26	0
55	MG	AA	1604	1/1	0.93	0.05	-3.96	58,58,58,58	0
55	MG	CA	1612	1/1	0.96	0.07	-4.13	44,44,44,44	0
55	MG	DA	3055	1/1	0.80	0.10	-4.41	41,41,41,41	0
55	MG	DB	201	1/1	0.86	0.06	-4.44	97,97,97,97	0
55	MG	DA	3067	1/1	0.93	0.08	-4.45	42,42,42,42	0
55	MG	AA	1606	1/1	0.95	0.10	-4.48	41,41,41,41	0
55	MG	CA	1617	1/1	0.77	0.09	-4.52	40,40,40,40	0
55	MG	AA	1613	1/1	0.88	0.11	-4.66	30,30,30,30	0
55	MG	AA	1629	1/1	0.99	0.05	-4.89	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3075	1/1	0.90	0.09	-5.01	63,63,63,63	0
55	MG	CA	1601	1/1	0.90	0.10	-5.27	45,45,45,45	0
55	MG	BA	3003	1/1	0.68	0.11	-5.34	23,23,23,23	0
55	MG	BA	3161	1/1	0.98	0.13	-5.44	13,13,13,13	0
55	MG	AA	1618	1/1	0.98	0.09	-5.77	41,41,41,41	0
55	MG	CA	1640	1/1	0.96	0.08	-5.81	31,31,31,31	0
55	MG	CA	1607	1/1	0.94	0.09	-6.03	47,47,47,47	0
55	MG	BA	3051	1/1	0.98	0.08	-6.03	5,5,5,5	0
55	MG	BA	3130	1/1	0.99	0.15	-6.44	0,0,0,0	0
55	MG	BA	3121	1/1	0.89	0.07	-6.47	7,7,7,7	0
55	MG	BA	3009	1/1	0.98	0.14	-7.34	5,5,5,5	0
55	MG	AA	1625	1/1	0.96	0.11	-7.69	33,33,33,33	0
55	MG	AA	1609	1/1	0.92	0.09	-7.77	35,35,35,35	0
55	MG	AA	1633	1/1	0.96	0.10	-7.78	41,41,41,41	0
55	MG	BA	3117	1/1	0.97	0.10	-7.80	3,3,3,3	0
55	MG	BA	3022	1/1	0.96	0.16	-7.98	0,0,0,0	0
55	MG	CA	1626	1/1	0.83	0.06	-7.98	43,43,43,43	0
55	MG	CA	1619	1/1	0.92	0.09	-8.47	40,40,40,40	0
55	MG	CA	1616	1/1	0.96	0.11	-8.50	33,33,33,33	0
55	MG	BA	3074	1/1	0.89	0.13	-8.82	14,14,14,14	0
55	MG	BA	3006	1/1	0.82	0.08	-8.98	51,51,51,51	0
55	MG	BA	3111	1/1	0.94	0.08	-9.07	24,24,24,24	0
55	MG	BA	3094	1/1	0.93	0.06	-10.05	30,30,30,30	0
55	MG	BA	3119	1/1	0.90	0.09	-10.15	14,14,14,14	0
55	MG	BA	3059	1/1	0.95	0.05	-10.65	13,13,13,13	0
55	MG	BA	3072	1/1	0.95	0.08	-11.55	23,23,23,23	0
55	MG	BA	3028	1/1	0.97	0.06	-12.19	15,15,15,15	0
55	MG	DA	3073	1/1	0.75	0.09	-12.21	72,72,72,72	0
55	MG	CA	1615	1/1	0.66	0.09	-12.44	55,55,55,55	0
55	MG	BA	3071	1/1	0.98	0.09	-12.83	5,5,5,5	0
55	MG	DA	3168	1/1	0.92	0.10	-	47,47,47,47	0
55	MG	DA	3068	1/1	0.87	0.10	-	47,47,47,47	0
55	MG	DA	3054	1/1	0.92	0.12	-	41,41,41,41	0
55	MG	BA	3091	1/1	0.93	0.10	-	23,23,23,23	0
55	MG	AA	1652	1/1	0.84	0.36	-	56,56,56,56	0
55	MG	DA	3155	1/1	0.96	0.15	-	45,45,45,45	0
55	MG	DA	3037	1/1	0.93	0.09	-	54,54,54,54	0
55	MG	CA	1650	1/1	0.78	0.26	-	44,44,44,44	0
55	MG	BA	3169	1/1	0.95	0.09	-	34,34,34,34	0
55	MG	BA	3020	1/1	0.86	0.18	-	8,8,8,8	0
55	MG	BA	3150	1/1	0.91	0.14	-	45,45,45,45	0
55	MG	BA	3149	1/1	0.92	0.15	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1666	1/1	0.89	0.57	-	41,41,41,41	0
55	MG	CA	1638	1/1	0.73	0.18	-	84,84,84,84	0
55	MG	DA	3144	1/1	0.97	0.21	-	30,30,30,30	0
55	MG	DA	3082	1/1	0.95	0.08	-	66,66,66,66	0
55	MG	BA	3095	1/1	0.94	0.06	-	20,20,20,20	0
55	MG	BA	3114	1/1	0.97	0.22	-	0,0,0,0	0
55	MG	CA	1622	1/1	0.85	0.10	-	51,51,51,51	0
55	MG	DA	3091	1/1	0.88	0.06	-	76,76,76,76	0
55	MG	DA	3146	1/1	0.78	0.08	-	84,84,84,84	0
55	MG	BA	3124	1/1	0.97	0.15	-	5,5,5,5	0
55	MG	DA	3129	1/1	0.98	0.14	-	75,75,75,75	0
55	MG	DA	3034	1/1	0.88	0.11	-	62,62,62,62	0
55	MG	BA	3082	1/1	0.98	0.17	-	0,0,0,0	0
55	MG	DA	3061	1/1	0.58	0.17	-	80,80,80,80	0
55	MG	CA	1641	1/1	0.91	0.44	-	67,67,67,67	0
55	MG	DA	3078	1/1	0.95	0.23	-	83,83,83,83	0
55	MG	BA	3103	1/1	0.89	0.11	-	13,13,13,13	0
55	MG	BA	3160	1/1	0.92	0.22	-	29,29,29,29	0
55	MG	BA	3175	1/1	0.97	0.13	-	33,33,33,33	0
55	MG	CA	1654	1/1	0.93	0.24	-	58,58,58,58	0
55	MG	DA	3138	1/1	0.78	0.44	-	52,52,52,52	0
55	MG	DA	3093	1/1	0.48	0.43	-	101,101,101,101	0
55	MG	BB	203	1/1	0.95	0.06	-	15,15,15,15	0
55	MG	BA	3062	1/1	0.88	0.83	-	57,57,57,57	0
55	MG	AA	1657	1/1	0.98	0.21	-	46,46,46,46	0
55	MG	CA	1623	1/1	0.97	0.10	-	35,35,35,35	0
55	MG	DA	3049	1/1	0.28	0.28	-	109,109,109,109	0
55	MG	BA	3073	1/1	0.92	0.18	-	2,2,2,2	0
55	MG	BA	3044	1/1	0.92	0.04	-	19,19,19,19	0
55	MG	AA	1636	1/1	0.89	0.09	-	42,42,42,42	0
55	MG	DA	3094	1/1	0.55	0.14	-	93,93,93,93	0
55	MG	DA	3127	1/1	0.90	0.15	-	86,86,86,86	0
55	MG	DA	3143	1/1	0.93	0.20	-	39,39,39,39	0
55	MG	DA	3036	1/1	0.86	0.08	-	70,70,70,70	0
55	MG	BA	3168	1/1	0.86	0.23	-	35,35,35,35	0
55	MG	DA	3008	1/1	0.72	0.41	-	100,100,100,100	0
55	MG	CA	1644	1/1	0.95	0.48	-	55,55,55,55	0
55	MG	AA	1653	1/1	0.71	0.28	-	51,51,51,51	0
55	MG	AA	1624	1/1	0.88	0.09	-	35,35,35,35	0
55	MG	DA	3012	1/1	0.88	0.20	-	74,74,74,74	0
55	MG	BA	3179	1/1	0.94	0.20	-	34,34,34,34	0
55	MG	DA	3166	1/1	0.92	0.20	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1628	1/1	0.72	0.24	-	98,98,98,98	0
55	MG	DA	3071	1/1	0.85	0.08	-	96,96,96,96	0
55	MG	BA	3191	1/1	0.93	0.16	-	20,20,20,20	0
55	MG	BA	3143	1/1	0.99	0.30	-	14,14,14,14	0
55	MG	BA	3052	1/1	0.96	0.15	-	3,3,3,3	0
55	MG	DA	3105	1/1	0.94	0.08	-	67,67,67,67	0
55	MG	AA	1640	1/1	0.94	0.05	-	45,45,45,45	0
55	MG	AA	1668	1/1	0.80	0.20	-	58,58,58,58	0
55	MG	AA	1626	1/1	0.93	0.15	-	19,19,19,19	0
55	MG	DA	3058	1/1	0.61	0.17	-	73,73,73,73	0
55	MG	DA	3021	1/1	0.85	0.08	-	64,64,64,64	0
55	MG	DA	3098	1/1	0.89	0.14	-	73,73,73,73	0
55	MG	AA	1638	1/1	0.81	0.06	-	77,77,77,77	0
55	MG	CA	1649	1/1	0.50	0.18	-	71,71,71,71	0
55	MG	DA	3139	1/1	0.91	0.43	-	49,49,49,49	0
55	MG	BA	3078	1/1	0.92	0.08	-	31,31,31,31	0
55	MG	CA	1625	1/1	0.82	0.13	-	43,43,43,43	0
55	MG	DA	3092	1/1	0.84	0.10	-	77,77,77,77	0
55	MG	AA	1660	1/1	0.70	1.01	-	70,70,70,70	0
55	MG	BA	3031	1/1	0.98	0.15	-	2,2,2,2	0
55	MG	DA	3142	1/1	0.93	0.27	-	40,40,40,40	0
55	MG	CA	1642	1/1	0.96	0.24	-	29,29,29,29	0
55	MG	CA	1637	1/1	0.90	0.11	-	64,64,64,64	0
55	MG	BA	3047	1/1	0.91	0.15	-	9,9,9,9	0
55	MG	DA	3005	1/1	0.39	0.28	-	94,94,94,94	0
55	MG	AA	1603	1/1	0.97	0.13	-	48,48,48,48	0
55	MG	BA	3034	1/1	0.96	0.21	-	0,0,0,0	0
55	MG	DA	3045	1/1	0.36	0.26	-	95,95,95,95	0
55	MG	BA	3088	1/1	0.91	0.15	-	37,37,37,37	0
55	MG	DA	3038	1/1	0.93	0.08	-	75,75,75,75	0
55	MG	AA	1658	1/1	0.72	0.44	-	72,72,72,72	0
55	MG	AA	1611	1/1	0.99	0.10	-	19,19,19,19	0
55	MG	BA	3007	1/1	0.98	0.09	-	17,17,17,17	0
55	MG	BA	3085	1/1	0.95	0.08	-	16,16,16,16	0
55	MG	BA	3005	1/1	0.93	0.08	-	42,42,42,42	0
55	MG	AA	1605	1/1	0.86	0.15	-	33,33,33,33	0
55	MG	BA	3027	1/1	0.96	0.09	-	4,4,4,4	0
55	MG	DA	3041	1/1	0.84	0.11	-	92,92,92,92	0
55	MG	CA	1653	1/1	0.97	0.10	-	42,42,42,42	0
55	MG	AA	1623	1/1	0.92	0.07	-	46,46,46,46	0
55	MG	BA	3176	1/1	0.96	0.11	-	13,13,13,13	0
55	MG	DA	3164	1/1	0.93	0.21	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1608	1/1	0.99	0.18	-	16,16,16,16	0
55	MG	DA	3090	1/1	0.89	0.18	-	80,80,80,80	0
55	MG	CA	1608	1/1	0.92	0.13	-	63,63,63,63	0
55	MG	DA	3057	1/1	0.75	0.27	-	88,88,88,88	0
55	MG	DA	3085	1/1	0.85	0.08	-	78,78,78,78	0
55	MG	AA	1621	1/1	0.95	0.06	-	35,35,35,35	0
55	MG	CA	1636	1/1	0.79	0.20	-	113,113,113,113	0
55	MG	BA	3089	1/1	0.79	0.09	-	22,22,22,22	0
55	MG	BA	3158	1/1	0.96	0.20	-	15,15,15,15	0
55	MG	DA	3163	1/1	0.93	0.42	-	71,71,71,71	0
55	MG	BA	3164	1/1	0.99	0.31	-	19,19,19,19	0
55	MG	BA	3060	1/1	0.92	0.12	-	9,9,9,9	0
55	MG	DA	3115	1/1	0.96	0.11	-	51,51,51,51	0
55	MG	DA	3112	1/1	0.75	0.08	-	70,70,70,70	0
55	MG	BA	3183	1/1	0.99	0.21	-	24,24,24,24	0
55	MG	BA	3076	1/1	0.94	0.17	-	4,4,4,4	0
55	MG	DA	3149	1/1	0.63	0.26	-	54,54,54,54	0
55	MG	DA	3124	1/1	0.91	0.16	-	51,51,51,51	0
55	MG	BA	3126	1/1	0.95	0.15	-	4,4,4,4	0
55	MG	DA	3043	1/1	0.72	0.10	-	82,82,82,82	0
55	MG	BA	3118	1/1	0.96	0.13	-	1,1,1,1	0
55	MG	CA	1624	1/1	0.86	0.11	-	47,47,47,47	0
55	MG	BA	3039	1/1	0.96	0.14	-	0,0,0,0	0
55	MG	CA	1648	1/1	0.98	0.21	-	30,30,30,30	0
55	MG	BA	3167	1/1	0.96	0.12	-	21,21,21,21	0
55	MG	DA	3101	1/1	0.45	0.27	-	78,78,78,78	0
55	MG	AA	1610	1/1	0.93	0.19	-	63,63,63,63	0
55	MG	DA	3123	1/1	0.97	0.17	-	37,37,37,37	0
55	MG	DA	3069	1/1	0.88	0.08	-	60,60,60,60	0
55	MG	BA	3099	1/1	0.55	0.37	-	64,64,64,64	0
55	MG	BA	3065	1/1	0.88	0.17	-	0,0,0,0	0
55	MG	DA	3014	1/1	0.68	0.16	-	80,80,80,80	0
55	MG	CA	1652	1/1	0.93	0.07	-	62,62,62,62	0
55	MG	AA	1615	1/1	0.97	0.07	-	50,50,50,50	0
55	MG	BA	3180	1/1	0.92	0.23	-	40,40,40,40	0
55	MG	BA	3102	1/1	0.82	0.19	-	10,10,10,10	0
55	MG	AA	1662	1/1	0.79	0.55	-	47,47,47,47	0
55	MG	BA	3101	1/1	0.97	0.09	-	2,2,2,2	0
55	MG	AA	1654	1/1	0.96	0.23	-	30,30,30,30	0
55	MG	AA	1643	1/1	0.97	0.12	-	25,25,25,25	0
55	MG	BA	3120	1/1	0.94	0.18	-	32,32,32,32	0
55	MG	DA	3031	1/1	0.94	0.07	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3070	1/1	0.88	0.07	-	50,50,50,50	0
55	MG	BA	3083	1/1	0.87	0.13	-	20,20,20,20	0
55	MG	DA	3089	1/1	0.89	0.07	-	78,78,78,78	0
55	MG	BA	3055	1/1	0.88	0.12	-	6,6,6,6	0
55	MG	DA	3154	1/1	0.75	0.34	-	70,70,70,70	0
55	MG	CA	1631	1/1	0.89	0.14	-	92,92,92,92	0
55	MG	AA	1665	1/1	0.91	0.07	-	48,48,48,48	0
55	MG	BA	3145	1/1	0.87	0.39	-	41,41,41,41	0
55	MG	BA	3081	1/1	0.81	0.12	-	16,16,16,16	0
55	MG	AA	1627	1/1	0.86	0.13	-	58,58,58,58	0
55	MG	DA	3019	1/1	0.75	0.17	-	85,85,85,85	0
55	MG	DA	3122	1/1	0.97	0.08	-	44,44,44,44	0
55	MG	BA	3049	1/1	0.82	0.07	-	13,13,13,13	0
55	MG	DA	3056	1/1	0.84	0.07	-	66,66,66,66	0
55	MG	BA	3182	1/1	0.91	0.21	-	20,20,20,20	0
55	MG	DA	3084	1/1	0.91	0.20	-	72,72,72,72	0
55	MG	DA	3161	1/1	0.88	0.19	-	49,49,49,49	0
55	MG	BA	3141	1/1	0.93	0.18	-	26,26,26,26	0
55	MG	AA	1672	1/1	0.75	0.47	-	49,49,49,49	0
55	MG	BA	3128	1/1	0.97	0.13	-	0,0,0,0	0
55	MG	DA	3004	1/1	0.86	0.10	-	65,65,65,65	0
55	MG	CA	1651	1/1	0.86	0.30	-	50,50,50,50	0
55	MG	BA	3043	1/1	0.94	0.14	-	11,11,11,11	0
55	MG	AA	1651	1/1	0.86	0.25	-	40,40,40,40	0
55	MG	BA	3021	1/1	0.97	0.07	-	2,2,2,2	0
55	MG	BA	3125	1/1	0.94	0.14	-	20,20,20,20	0
55	MG	BA	3123	1/1	0.97	0.20	-	0,0,0,0	0
55	MG	DA	3157	1/1	0.85	0.49	-	63,63,63,63	0
55	MG	BA	3173	1/1	0.85	0.20	-	32,32,32,32	0
55	MG	DA	3113	1/1	0.76	0.61	-	77,77,77,77	0
55	MG	DA	3087	1/1	0.91	0.10	-	69,69,69,69	0
55	MG	BA	3194	1/1	0.98	0.08	-	32,32,32,32	0
55	MG	BA	3142	1/1	0.98	0.39	-	5,5,5,5	0
55	MG	BA	3100	1/1	0.81	0.09	-	14,14,14,14	0
55	MG	CA	1643	1/1	0.94	0.24	-	56,56,56,56	0
55	MG	BA	3154	1/1	0.85	0.17	-	34,34,34,34	0
55	MG	DA	3027	1/1	0.58	0.99	-	96,96,96,96	0
55	MG	BA	3140	1/1	0.97	0.36	-	3,3,3,3	0
55	MG	BA	3186	1/1	0.90	0.14	-	32,32,32,32	0
55	MG	DA	3010	1/1	0.91	0.09	-	68,68,68,68	0
55	MG	BA	3002	1/1	0.78	0.07	-	15,15,15,15	0
55	MG	DA	3158	1/1	0.90	0.19	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3017	1/1	0.57	0.13	-	84,84,84,84	0
55	MG	BB	202	1/1	0.96	0.10	-	2,2,2,2	0
55	MG	BA	3122	1/1	0.94	0.08	-	39,39,39,39	0
55	MG	CA	1634	1/1	0.95	0.10	-	52,52,52,52	0
55	MG	AA	1631	1/1	0.92	0.10	-	48,48,48,48	0
55	MG	CA	1655	1/1	0.86	0.13	-	51,51,51,51	0
55	MG	AA	1669	1/1	0.91	0.32	-	51,51,51,51	0
55	MG	BA	3192	1/1	0.96	0.22	-	34,34,34,34	0
55	MG	DA	3039	1/1	0.95	0.13	-	63,63,63,63	0
55	MG	BA	3048	1/1	0.66	0.11	-	53,53,53,53	0
55	MG	DA	3151	1/1	0.88	0.27	-	49,49,49,49	0
55	MG	BA	3017	1/1	0.98	0.06	-	1,1,1,1	0
55	MG	DA	3100	1/1	0.76	0.32	-	81,81,81,81	0
55	MG	DA	3066	1/1	0.94	0.15	-	39,39,39,39	0
55	MG	AA	1620	1/1	0.95	0.07	-	59,59,59,59	0
55	MG	BA	3162	1/1	0.97	0.13	-	37,37,37,37	0
55	MG	BA	3087	1/1	0.97	0.20	-	1,1,1,1	0
55	MG	CA	1629	1/1	0.60	0.08	-	80,80,80,80	0
55	MG	BA	3090	1/1	0.95	0.14	-	1,1,1,1	0
55	MG	BA	3093	1/1	0.96	0.04	-	38,38,38,38	0
55	MG	BA	3115	1/1	0.91	0.14	-	17,17,17,17	0
55	MG	DA	3022	1/1	0.74	0.13	-	62,62,62,62	0
55	MG	CA	1606	1/1	0.94	0.15	-	70,70,70,70	0
55	MG	CA	1633	1/1	0.85	0.34	-	78,78,78,78	0
55	MG	BA	3190	1/1	0.87	0.21	-	39,39,39,39	0
55	MG	AA	1639	1/1	0.89	0.06	-	60,60,60,60	0
55	MG	BA	3092	1/1	0.92	0.04	-	55,55,55,55	0
55	MG	CA	1618	1/1	0.97	0.12	-	45,45,45,45	0
55	MG	CA	1639	1/1	0.94	0.09	-	49,49,49,49	0
55	MG	BA	3053	1/1	0.90	0.12	-	6,6,6,6	0
55	MG	BA	3038	1/1	0.93	0.25	-	0,0,0,0	0
55	MG	BD	301	1/1	0.96	0.17	-	27,27,27,27	0
55	MG	CA	1611	1/1	0.96	0.21	-	82,82,82,82	0
55	MG	BA	3046	1/1	0.99	0.12	-	2,2,2,2	0
55	MG	BA	3079	1/1	0.89	0.08	-	37,37,37,37	0
55	MG	DA	3059	1/1	0.77	0.23	-	70,70,70,70	0
55	MG	DA	3011	1/1	0.86	0.08	-	60,60,60,60	0
55	MG	DA	3134	1/1	0.71	0.64	-	100,100,100,100	0
55	MG	AA	1637	1/1	0.96	0.11	-	16,16,16,16	0
55	MG	DA	3072	1/1	0.43	0.16	-	80,80,80,80	0
55	MG	BA	3193	1/1	0.93	0.15	-	42,42,42,42	0
55	MG	DA	3033	1/1	0.80	0.16	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3136	1/1	0.85	0.11	-	34,34,34,34	0
55	MG	BA	3011	1/1	0.98	0.18	-	1,1,1,1	0
55	MG	AA	1648	1/1	0.97	0.11	-	57,57,57,57	0
55	MG	DA	3165	1/1	0.62	0.51	-	68,68,68,68	0
55	MG	DA	3086	1/1	0.85	0.08	-	72,72,72,72	0
55	MG	DB	203	1/1	0.78	0.07	-	83,83,83,83	0
55	MG	DA	3088	1/1	0.94	0.07	-	52,52,52,52	0
55	MG	BA	3077	1/1	0.81	0.25	-	61,61,61,61	0
55	MG	CA	1604	1/1	0.72	0.07	-	89,89,89,89	0
55	MG	BA	3138	1/1	0.94	0.38	-	4,4,4,4	0
55	MG	DA	3032	1/1	0.88	0.10	-	63,63,63,63	0
55	MG	BA	3156	1/1	0.92	0.23	-	23,23,23,23	0
55	MG	DA	3007	1/1	0.67	0.21	-	101,101,101,101	0
55	MG	DA	3102	1/1	0.94	0.08	-	58,58,58,58	0
55	MG	BA	3139	1/1	0.99	0.40	-	0,0,0,0	0
55	MG	AA	1614	1/1	0.81	0.12	-	55,55,55,55	0
55	MG	DA	3118	1/1	0.95	0.10	-	66,66,66,66	0
55	MG	BA	3026	1/1	0.86	0.13	-	36,36,36,36	0
55	MG	DA	3074	1/1	0.77	0.11	-	68,68,68,68	0
55	MG	BA	3185	1/1	0.94	0.25	-	25,25,25,25	0
55	MG	BA	3057	1/1	0.95	0.06	-	3,3,3,3	0
55	MG	BA	3189	1/1	0.81	0.27	-	44,44,44,44	0
55	MG	CA	1620	1/1	0.93	0.04	-	65,65,65,65	0
55	MG	DA	3097	1/1	0.84	0.15	-	51,51,51,51	0
55	MG	BA	3184	1/1	0.98	0.17	-	10,10,10,10	0
55	MG	DA	3152	1/1	0.94	0.16	-	47,47,47,47	0
55	MG	DA	3132	1/1	0.55	0.42	-	89,89,89,89	0
55	MG	AA	1664	1/1	0.88	0.33	-	42,42,42,42	0
55	MG	BA	3061	1/1	0.93	0.25	-	28,28,28,28	0
55	MG	BA	3107	1/1	0.99	0.24	-	0,0,0,0	0
55	MG	BA	3129	1/1	0.94	0.14	-	5,5,5,5	0
55	MG	BA	3067	1/1	0.98	0.17	-	1,1,1,1	0
55	MG	DA	3015	1/1	0.95	0.05	-	44,44,44,44	0
55	MG	CA	1645	1/1	0.95	0.19	-	40,40,40,40	0
55	MG	AA	1661	1/1	0.91	0.11	-	53,53,53,53	0
55	MG	BA	3032	1/1	0.92	0.08	-	5,5,5,5	0
55	MG	DA	3053	1/1	0.98	0.07	-	45,45,45,45	0
55	MG	DA	3126	1/1	0.87	0.16	-	59,59,59,59	0
55	MG	AA	1634	1/1	0.89	0.12	-	42,42,42,42	0
55	MG	BA	3045	1/1	0.95	0.10	-	21,21,21,21	0
55	MG	BA	3010	1/1	0.97	0.13	-	0,0,0,0	0
55	MG	BA	3171	1/1	0.87	0.21	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1645	1/1	0.83	0.37	-	53,53,53,53	0
55	MG	BA	3157	1/1	0.90	0.27	-	27,27,27,27	0
55	MG	BA	3030	1/1	0.95	0.05	-	12,12,12,12	0
55	MG	DA	3141	1/1	0.91	0.37	-	41,41,41,41	0
55	MG	BA	3064	1/1	0.98	0.20	-	0,0,0,0	0
55	MG	CA	1647	1/1	0.81	0.22	-	45,45,45,45	0
55	MG	BA	3075	1/1	0.87	0.07	-	29,29,29,29	0
55	MG	BA	3134	1/1	0.94	0.34	-	47,47,47,47	0
55	MG	BA	3127	1/1	0.98	0.20	-	6,6,6,6	0
55	MG	BA	3004	1/1	0.92	0.12	-	25,25,25,25	0
55	MG	BB	204	1/1	0.96	0.39	-	21,21,21,21	0
55	MG	BA	3172	1/1	0.93	0.17	-	32,32,32,32	0
55	MG	DA	3120	1/1	0.44	0.31	-	97,97,97,97	0
55	MG	CA	1656	1/1	0.78	0.75	-	53,53,53,53	0
55	MG	D2	101	1/1	0.70	0.12	-	77,77,77,77	0
55	MG	CA	1646	1/1	0.67	0.33	-	65,65,65,65	0
55	MG	DA	3046	1/1	0.90	0.10	-	77,77,77,77	0
55	MG	BA	3086	1/1	0.89	0.11	-	5,5,5,5	0
55	MG	AA	1646	1/1	0.99	0.16	-	55,55,55,55	0
55	MG	DA	3167	1/1	0.89	0.40	-	43,43,43,43	0
55	MG	AA	1655	1/1	0.92	0.25	-	45,45,45,45	0
55	MG	DA	3162	1/1	0.93	0.12	-	35,35,35,35	0
55	MG	DA	3076	1/1	0.82	0.16	-	70,70,70,70	0
55	MG	AA	1602	1/1	0.91	0.10	-	46,46,46,46	0
55	MG	BA	3096	1/1	0.99	0.05	-	10,10,10,10	0
55	MG	BA	3112	1/1	0.84	0.17	-	8,8,8,8	0
55	MG	AA	1659	1/1	0.95	0.31	-	61,61,61,61	0
55	MG	BA	3068	1/1	0.95	0.20	-	0,0,0,0	0
55	MG	AA	1649	1/1	0.81	0.18	-	46,46,46,46	0
55	MG	BA	3104	1/1	0.95	0.06	-	18,18,18,18	0
55	MG	BA	3008	1/1	0.94	0.04	-	22,22,22,22	0
55	MG	DA	3136	1/1	0.72	0.27	-	84,84,84,84	0
55	MG	BA	3015	1/1	0.91	0.12	-	6,6,6,6	0
55	MG	BA	3116	1/1	0.96	0.22	-	50,50,50,50	0
55	MG	BA	3148	1/1	0.86	0.46	-	24,24,24,24	0
55	MG	DA	3028	1/1	0.74	0.23	-	83,83,83,83	0
55	MG	DA	3147	1/1	0.96	0.10	-	60,60,60,60	0
55	MG	DA	3047	1/1	0.78	0.10	-	80,80,80,80	0
55	MG	DA	3104	1/1	0.82	0.15	-	67,67,67,67	0
55	MG	BA	3040	1/1	0.97	0.17	-	3,3,3,3	0
55	MG	BQ	201	1/1	0.98	0.26	-	1,1,1,1	0
55	MG	DA	3145	1/1	0.90	0.38	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1605	1/1	0.73	0.17	-	88,88,88,88	0
55	MG	BA	3144	1/1	0.99	0.28	-	8,8,8,8	0
55	MG	DA	3119	1/1	0.97	0.07	-	46,46,46,46	0
55	MG	CA	1613	1/1	0.96	0.11	-	24,24,24,24	0
55	MG	DA	3128	1/1	0.76	0.13	-	71,71,71,71	0
55	MG	DA	3077	1/1	0.98	0.13	-	65,65,65,65	0
55	MG	AA	1667	1/1	0.76	0.36	-	54,54,54,54	0
55	MG	DA	3016	1/1	0.69	0.42	-	78,78,78,78	0
55	MG	DA	3156	1/1	0.90	0.11	-	42,42,42,42	0
55	MG	BA	3188	1/1	0.97	0.17	-	16,16,16,16	0
55	MG	AA	1619	1/1	0.96	0.16	-	37,37,37,37	0
55	MG	AA	1628	1/1	0.98	0.05	-	35,35,35,35	0
55	MG	DA	3160	1/1	0.87	0.11	-	74,74,74,74	0
55	MG	AA	1601	1/1	0.88	0.07	-	41,41,41,41	0
55	MG	BA	3042	1/1	0.98	0.14	-	11,11,11,11	0
55	MG	BA	3113	1/1	0.97	0.08	-	13,13,13,13	0
55	MG	DA	3063	1/1	0.61	0.75	-	93,93,93,93	0
55	MG	CA	1609	1/1	0.78	0.11	-	77,77,77,77	0
55	MG	DA	3150	1/1	0.71	0.20	-	61,61,61,61	0
55	MG	DA	3148	1/1	0.71	0.14	-	58,58,58,58	0
55	MG	DA	3108	1/1	0.80	0.12	-	72,72,72,72	0
55	MG	CA	1602	1/1	0.82	0.15	-	69,69,69,69	0
55	MG	BA	3166	1/1	0.93	0.17	-	36,36,36,36	0
55	MG	DA	3035	1/1	0.98	0.09	-	41,41,41,41	0
55	MG	AA	1650	1/1	0.90	0.16	-	37,37,37,37	0
55	MG	DA	3062	1/1	0.92	1.19	-	104,104,104,104	0
55	MG	DA	3002	1/1	0.87	0.08	-	65,65,65,65	0
55	MG	BA	3146	1/1	0.96	0.26	-	15,15,15,15	0
55	MG	BA	3012	1/1	0.98	0.09	-	25,25,25,25	0
55	MG	CA	1627	1/1	0.90	0.11	-	76,76,76,76	0
55	MG	BA	3181	1/1	0.96	0.18	-	19,19,19,19	0
55	MG	BA	3178	1/1	0.94	0.14	-	13,13,13,13	0
55	MG	DA	3030	1/1	0.78	0.18	-	72,72,72,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.