



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 3, 2024 – 04:55 PM EDT

PDB ID : 4U26  
Title : Crystal structure of the E. coli ribosome bound to dalfopristin and quinupristin.  
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.  
Deposited on : 2014-07-16  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

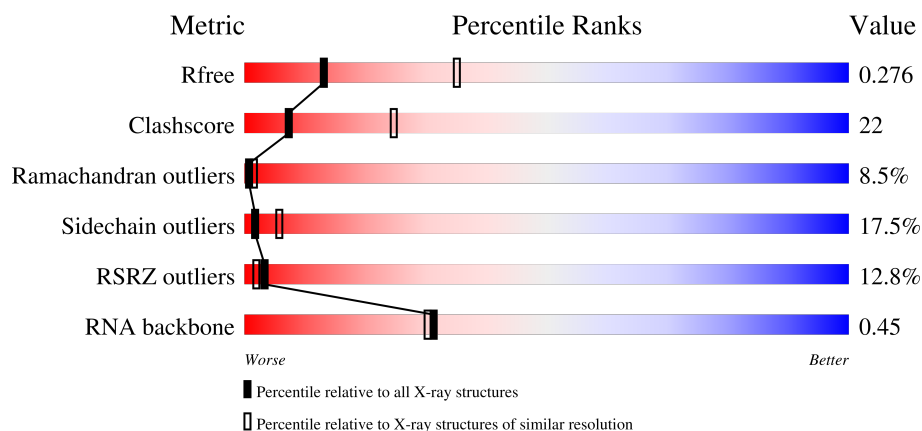
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	AA	1539	<div> <div></div> <div>34%</div> <div>50%</div> <div>15%</div> </div>
1	CA	1539	<div> <div>4%</div> <div>31%</div> <div>54%</div> <div>16%</div> </div>
2	AB	218	<div> <div>13%</div> <div>25%</div> <div>50%</div> <div>18%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	CB	218	
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	

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Mol	Chain	Length	Quality of chain
15	AO	88	
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	

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Mol	Chain	Length	Quality of chain
27	DF	177	
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	

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Mol	Chain	Length	Quality of chain
40	BS	110	
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	

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Mol	Chain	Length	Quality of chain
52	D4	38	
53	B5	228	
54	B6	8	
54	D6	8	

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
55	MG	AA	1659	-	-	-	X
55	MG	AM	201	-	-	-	X
55	MG	BA	3134	-	-	-	X
55	MG	DA	3003	-	-	-	X
55	MG	DA	3005	-	-	-	X
55	MG	DA	3026	-	-	-	X
55	MG	DA	3028	-	-	-	X
55	MG	DA	3041	-	-	-	X
55	MG	DA	3048	-	-	-	X
55	MG	DA	3056	-	-	-	X
55	MG	DA	3062	-	-	-	X
55	MG	DA	3071	-	-	-	X
55	MG	DA	3072	-	-	-	X
55	MG	DA	3077	-	-	-	X
55	MG	DA	3131	-	-	-	X
55	MG	DA	3133	-	-	-	X
55	MG	DA	3155	-	-	-	X
56	DOL	DA	3001	-	-	X	-

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 288423 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			
			780	492	146	142	0	0	0

- 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		
			753	479	137	134	3	0	0
43	DV	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- 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		
			580	359	117	103	1	0	0
44	DW	75	Total	C	N	O	S		
			569	353	113	102	1	0	0

- 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		
			625	388	129	106	2	0	0
45	DX	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

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

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

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

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

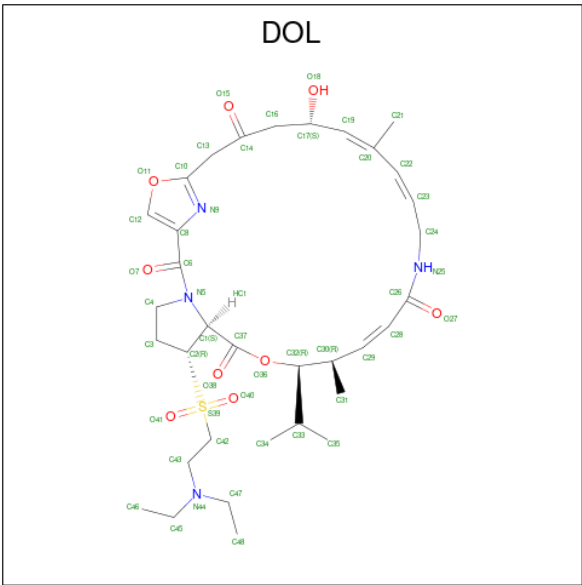
- Molecule 54 is a protein called Quinupristin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			
54	D6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	71	Total	Mg	0	0
			71	71		
55	AM	1	Total	Mg	0	0
			1	1		
55	BA	194	Total	Mg	0	0
			194	194		
55	BB	4	Total	Mg	0	0
			4	4		
55	BQ	1	Total	Mg	0	0
			1	1		
55	CA	56	Total	Mg	0	0
			56	56		
55	DA	166	Total	Mg	0	0
			166	166		
55	DB	3	Total	Mg	0	0
			3	3		
55	DQ	1	Total	Mg	0	0
			1	1		
55	D2	1	Total	Mg	0	0
			1	1		

- Molecule 56 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C<sub>34</sub>H<sub>50</sub>N<sub>4</sub>O<sub>9</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
56	BA	1	Total	C	N	O	S	0	0
			48	34	4	9	1		
56	DA	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

- 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	194	Total	O	0	0
			194	194		
58	AE	2	Total	O	0	0
			2	2		
58	AL	1	Total	O	0	0
			1	1		
58	AN	3	Total	O	0	0
			3	3		
58	AT	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AU	1	Total 1	O 1	0	0
58	BA	617	Total 617	O 617	0	0
58	BB	14	Total 14	O 14	0	0
58	BC	6	Total 6	O 6	0	0
58	BD	4	Total 4	O 4	0	0
58	BE	1	Total 1	O 1	0	0
58	BF	1	Total 1	O 1	0	0
58	BG	1	Total 1	O 1	0	0
58	BJ	1	Total 1	O 1	0	0
58	BL	7	Total 7	O 7	0	0
58	BN	5	Total 5	O 5	0	0
58	BQ	1	Total 1	O 1	0	0
58	BS	1	Total 1	O 1	0	0
58	BT	2	Total 2	O 2	0	0
58	B3	3	Total 3	O 3	0	0
58	B4	1	Total 1	O 1	0	0
58	CA	192	Total 192	O 192	0	0
58	CL	1	Total 1	O 1	0	0
58	CN	2	Total 2	O 2	0	0
58	CT	2	Total 2	O 2	0	0
58	CU	1	Total 1	O 1	0	0

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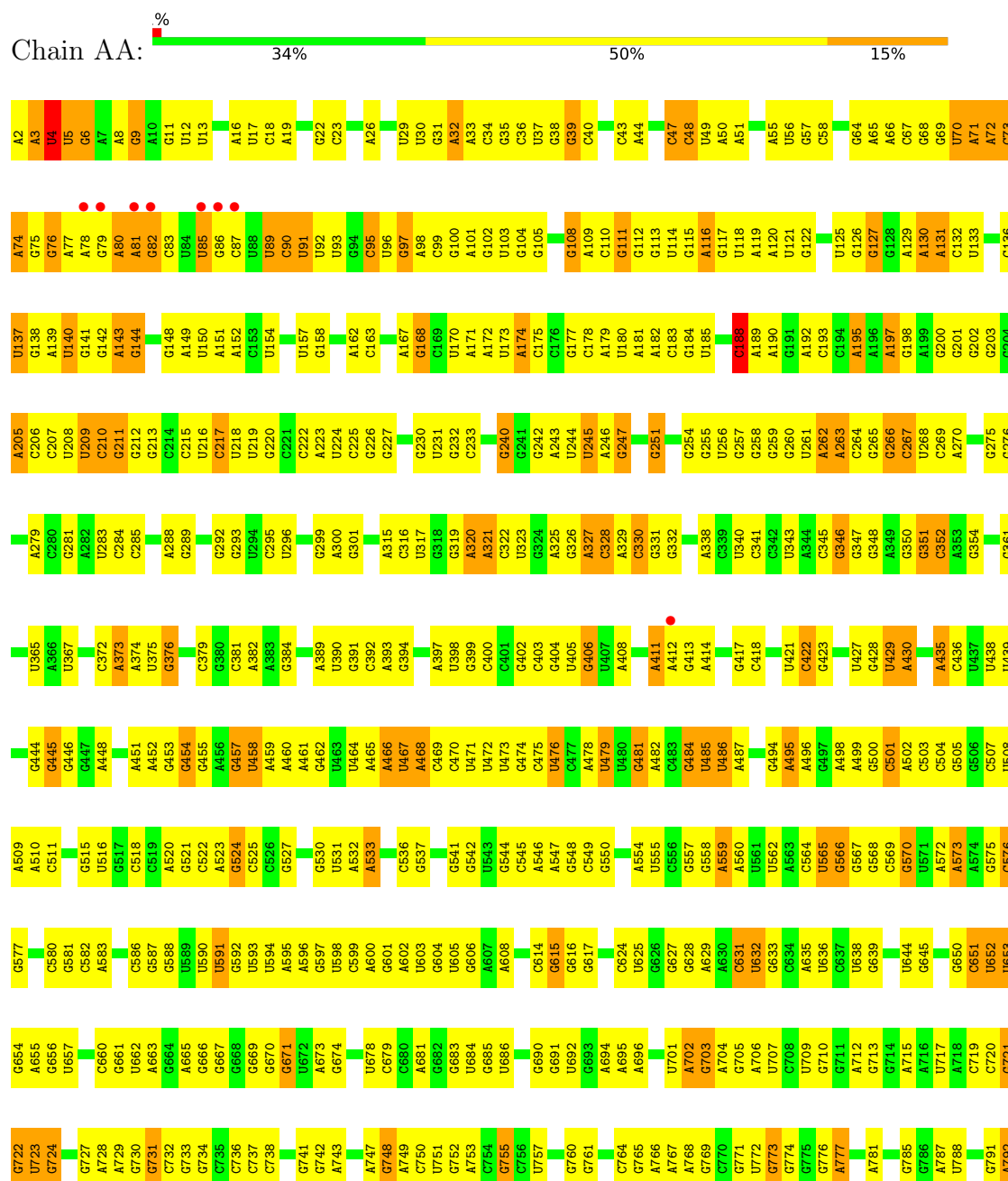
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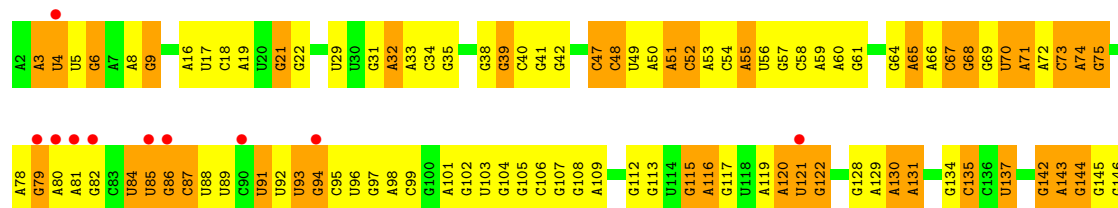
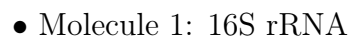
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58	DB	13	Total 13	O 13	0	0
58	DC	8	Total 8	O 8	0	0
58	DD	4	Total 4	O 4	0	0
58	DE	4	Total 4	O 4	0	0
58	DJ	1	Total 1	O 1	0	0
58	DL	4	Total 4	O 4	0	0
58	DN	2	Total 2	O 2	0	0
58	DS	2	Total 2	O 2	0	0
58	DT	3	Total 3	O 3	0	0
58	DU	1	Total 1	O 1	0	0
58	DV	1	Total 1	O 1	0	0
58	D2	1	Total 1	O 1	0	0
58	D3	1	Total 1	O 1	0	0
58	D4	1	Total 1	O 1	0	0

### 3 Residue-property plots

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

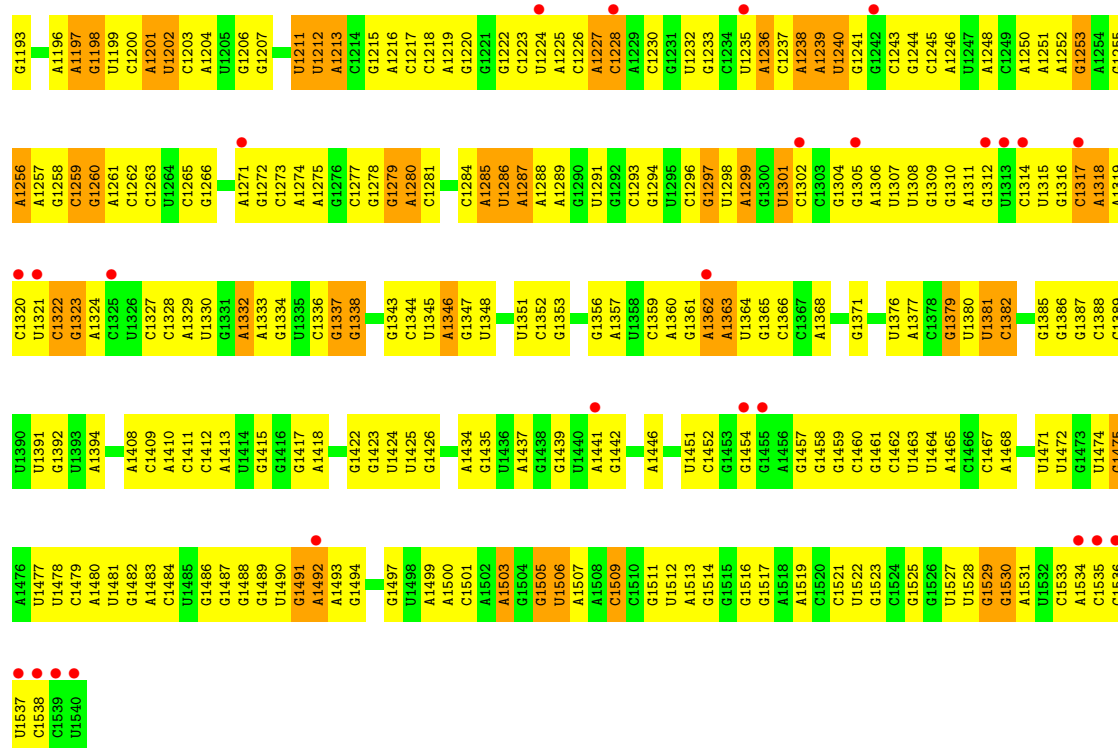
#### • Molecule 1: 16S rRNA



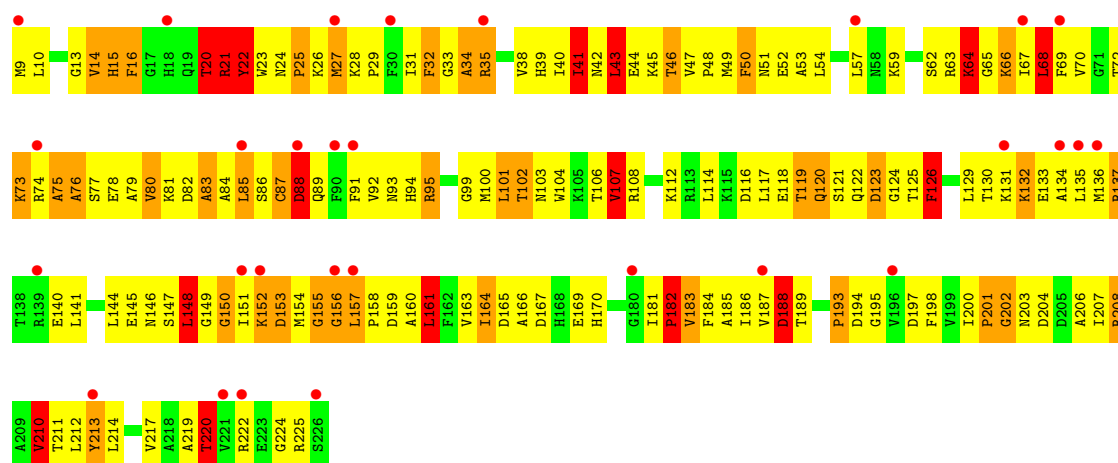


U1125	U1126	U1127	U1128	U1129	A1130	U1060	G1133	G1134	U1135	G1064	U1065	G1137	G1138	G1139	U1067	G1068	C1141	U1070	G1142	G1143	G1144	A1145	U1146	C1147	U1148	C1149	A1150	A1151	A1080	A1081	U1082	U1083	G1153	G1154	U1085	G951	U1086	G1087	G1088	G1089	C1161	C1162	U1091	A1092	A1093	G1094	U1095	C1096	C1097	G1098	G1099	G1100	A1101	A1102	G1103	G1104	A1105	G1106	C1107	G1108	G1114	A1117	U1123	G1124																	
C839	C840	G841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911									
G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838																	
G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773																			
A642	G643	U644	G645	A646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710													
U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498									
A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566														
G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637											
A642	G643	U644	G645	A646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710													
G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773																			
G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838																	
C839	C840	G841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911									
C912	A913	A914	G915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983										
U991	U992	G993	A994	A995	A996	C997	C998	A1000	C1001	G1002	G1003	A1004	A1005	G1006	C1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060													
U1052	G1053	C1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124									
G147	G148	C149	U150	A151	A152	G153	U154	U155	C156	U157	G158	G159	A160	A161	C162	C163	G164	G165	U166	U167	G168	C169	U170	U171	A172	U173	A174	C175	C176	G177	C178	U179	U180	A181	C182	C183	G184	U185	C186	G187	C188	A189	A190	G191	A192	A193	A194	A195	A196	A197	G198	G199	G200	G201	G202	G203	G204	A205	C206	C207	U208																				
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G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425									
U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498									
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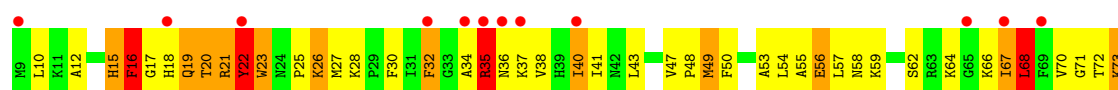


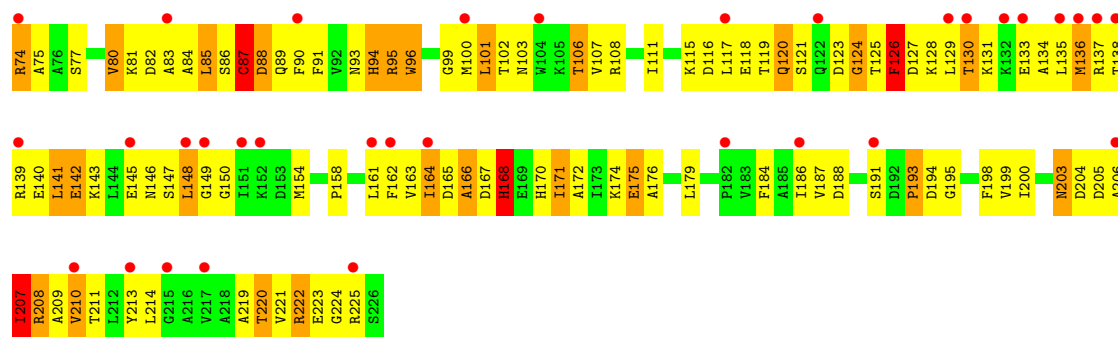


• Molecule 2: 30S ribosomal protein S2

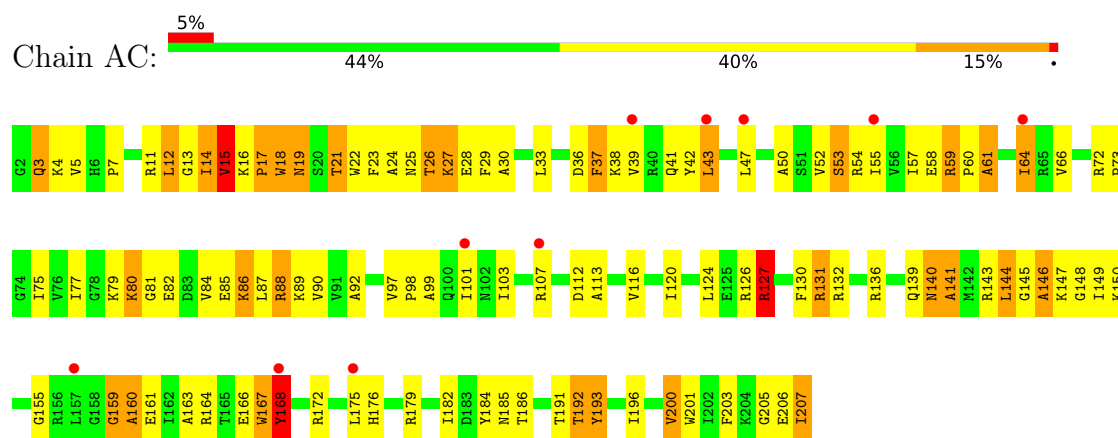


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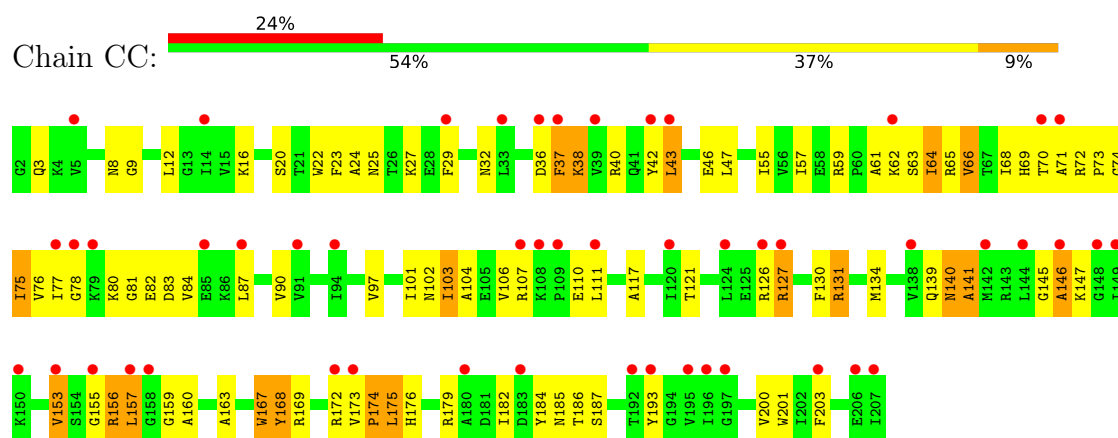




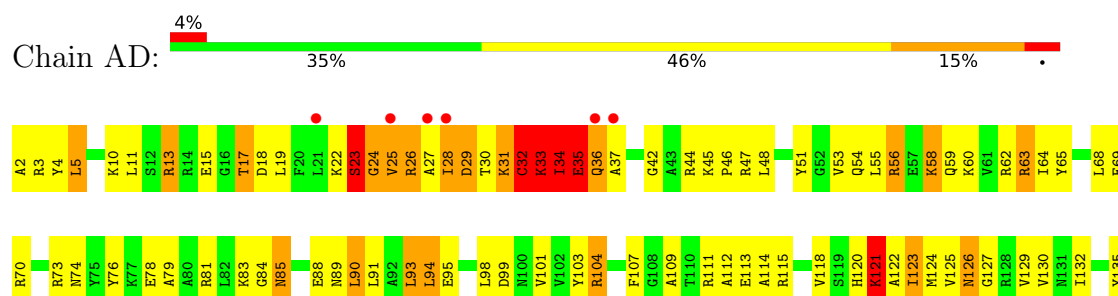
- Molecule 3: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S3

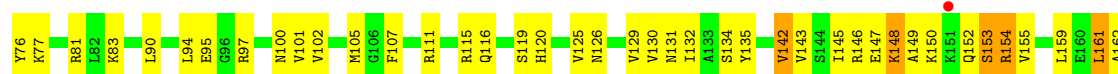
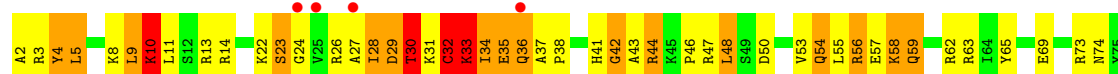


- Molecule 4: 30S ribosomal protein S4

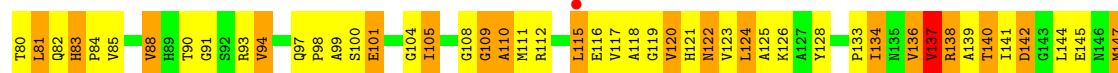
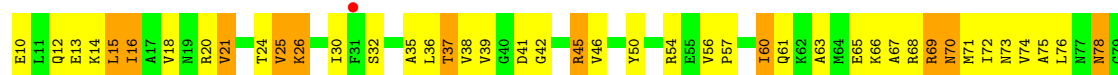




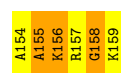
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

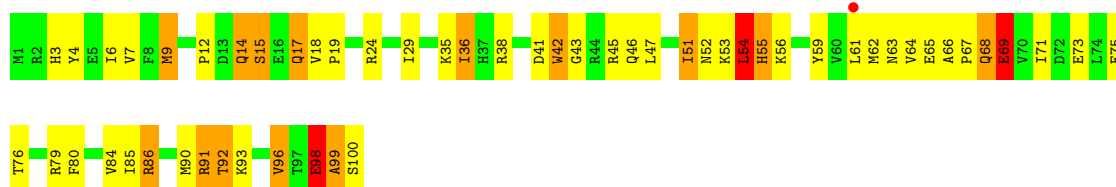


• Molecule 5: 30S ribosomal protein S5

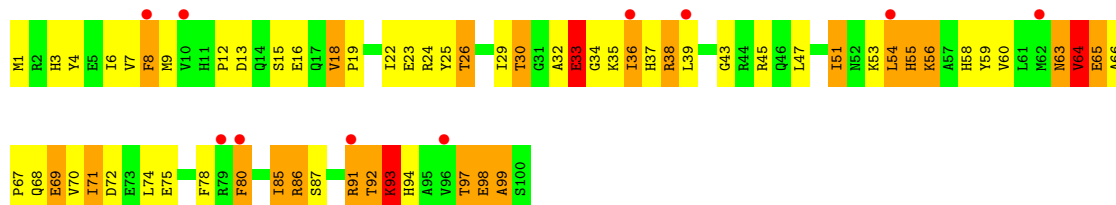


• Molecule 6: 30S ribosomal protein S6

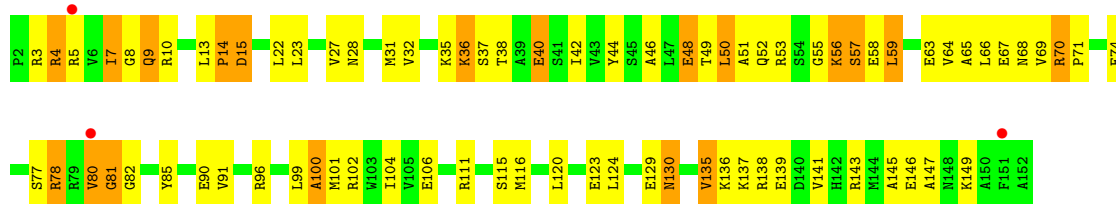




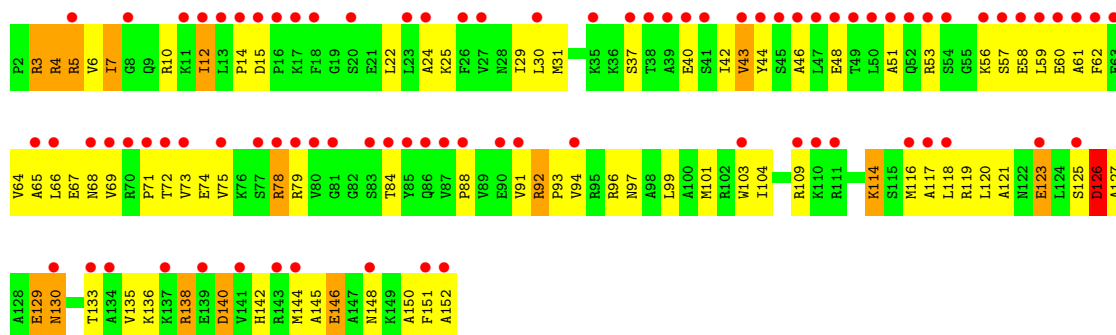
• Molecule 6: 30S ribosomal protein S6



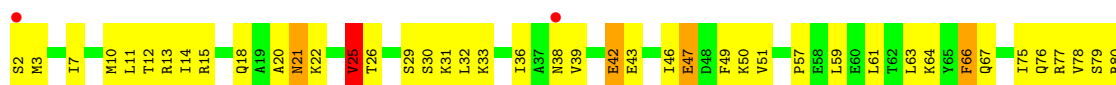
• Molecule 7: 30S ribosomal protein S7

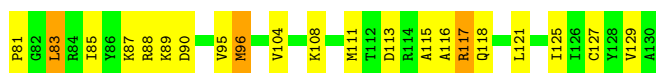


• Molecule 7: 30S ribosomal protein S7

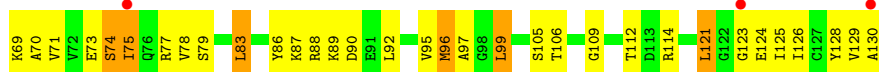
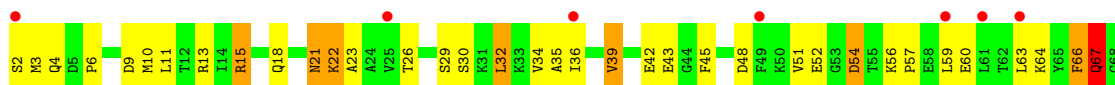


• Molecule 8: 30S ribosomal protein S8

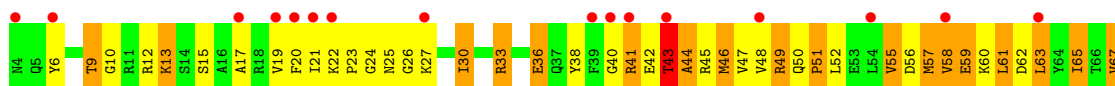




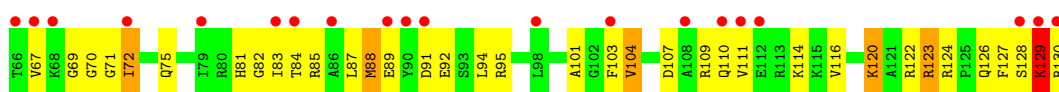
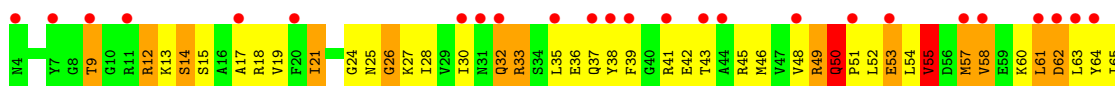
• Molecule 8: 30S ribosomal protein S8



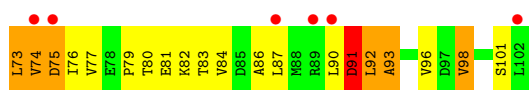
• Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9

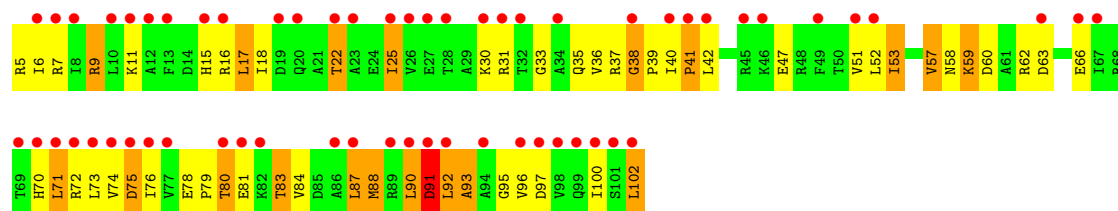


• Molecule 10: 30S ribosomal protein S10

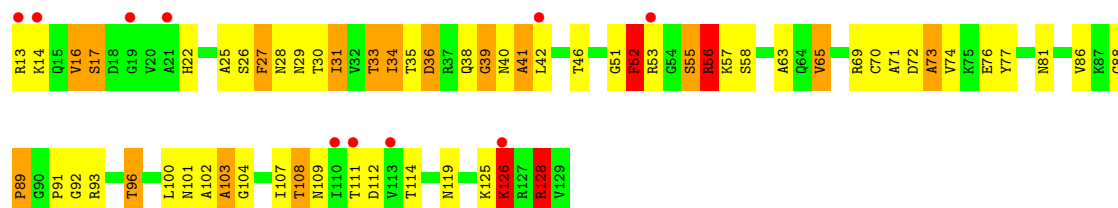


• Molecule 10: 30S ribosomal protein S10

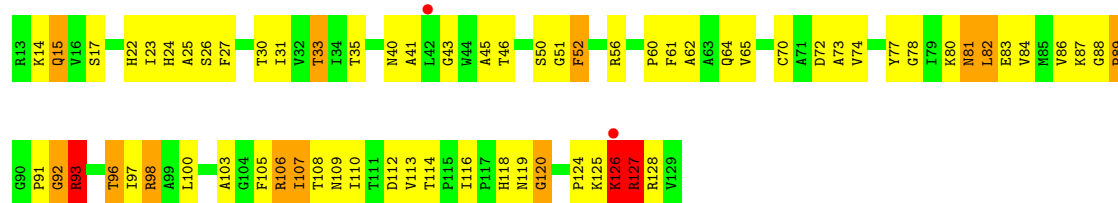
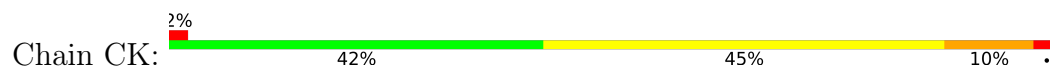




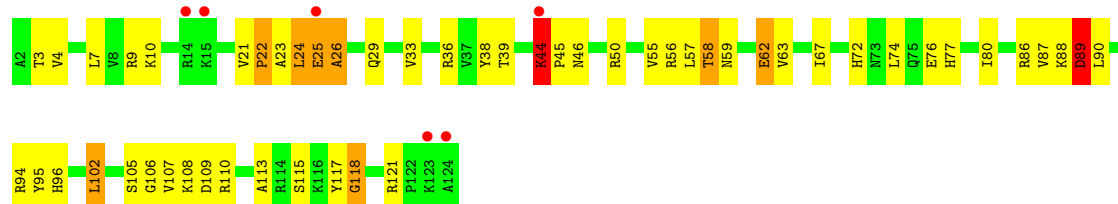
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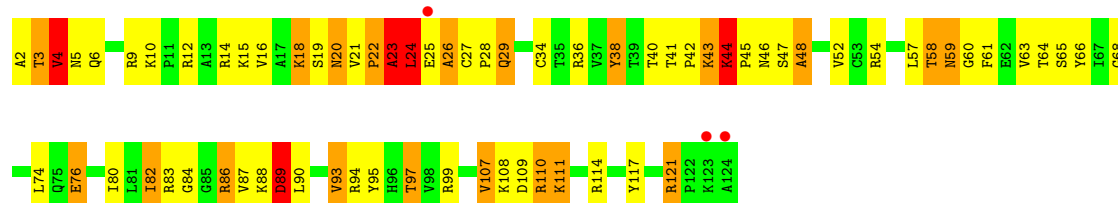
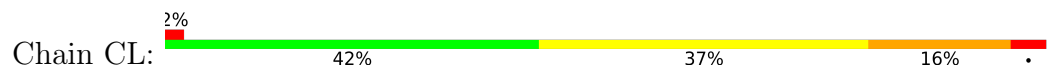
• Molecule 11: 30S ribosomal protein S11



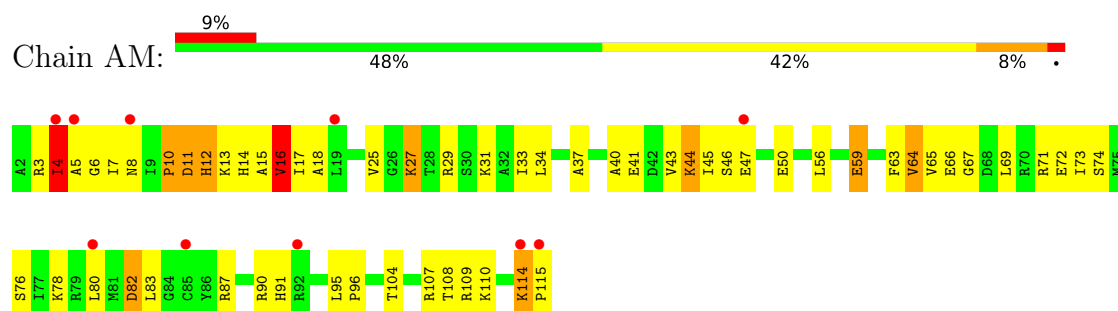
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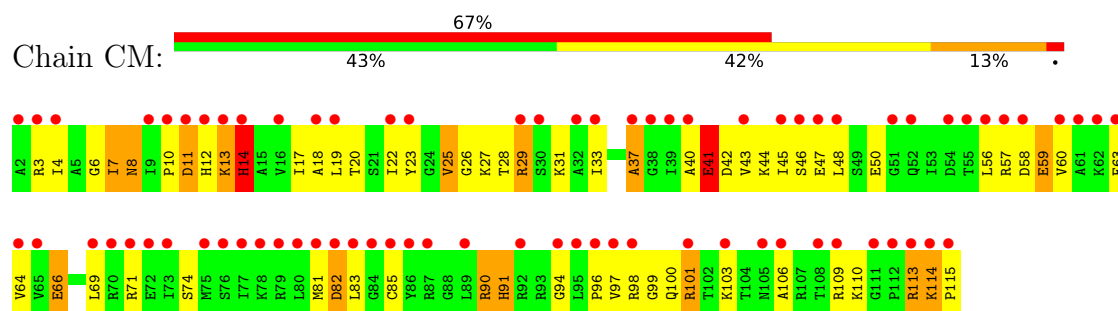
• Molecule 12: 30S ribosomal protein S12



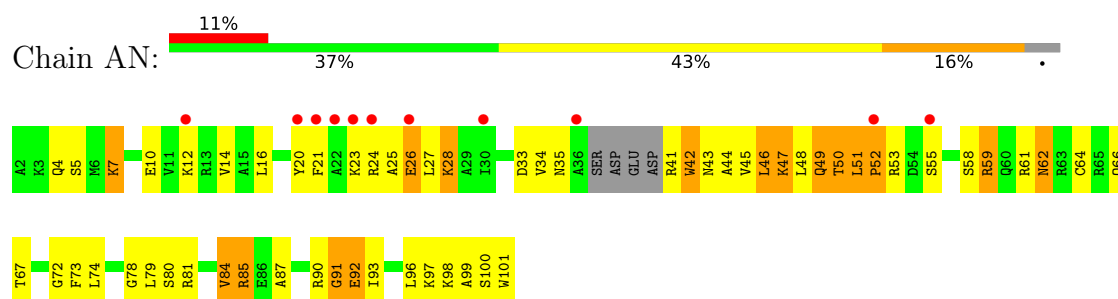
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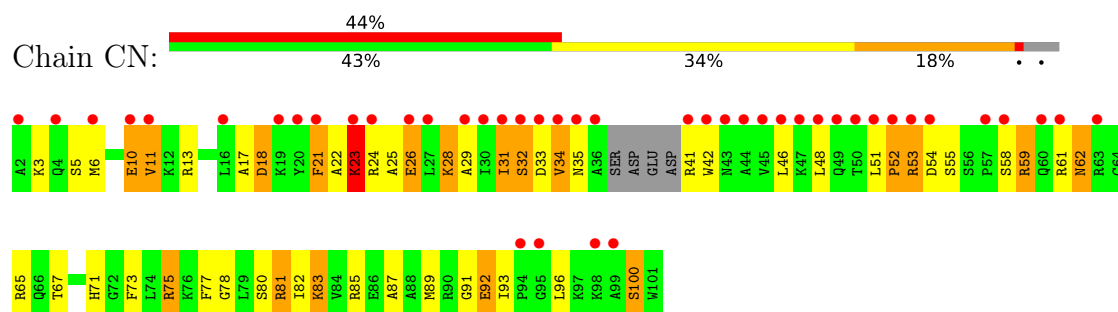
- Molecule 13: 30S ribosomal protein S13



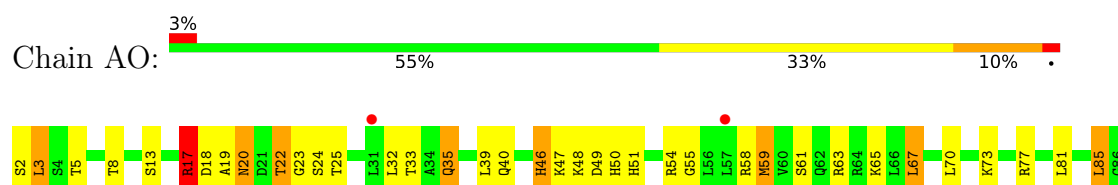
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

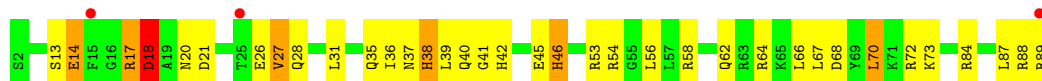


- Molecule 15: 30S ribosomal protein S15

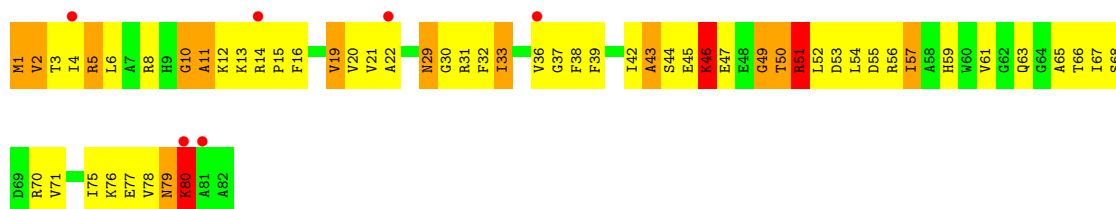




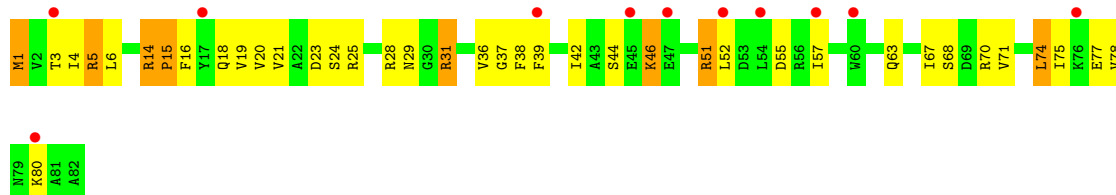
- Molecule 15: 30S ribosomal protein S15



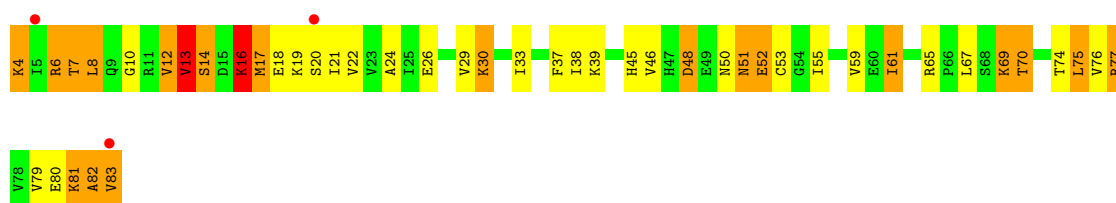
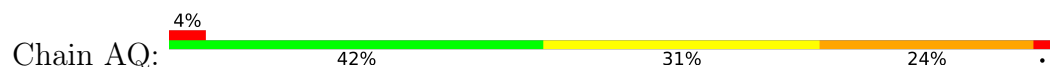
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17







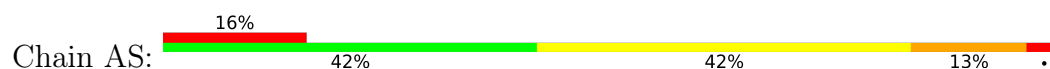
- Molecule 18: 30S ribosomal protein S18



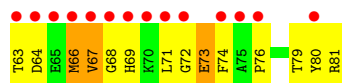
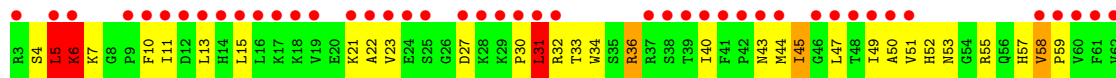
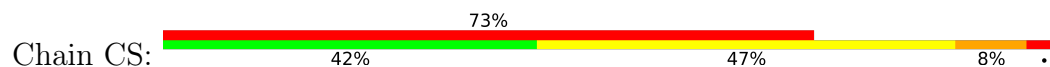
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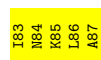
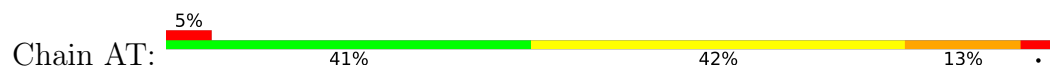
- Molecule 19: 30S ribosomal protein S19



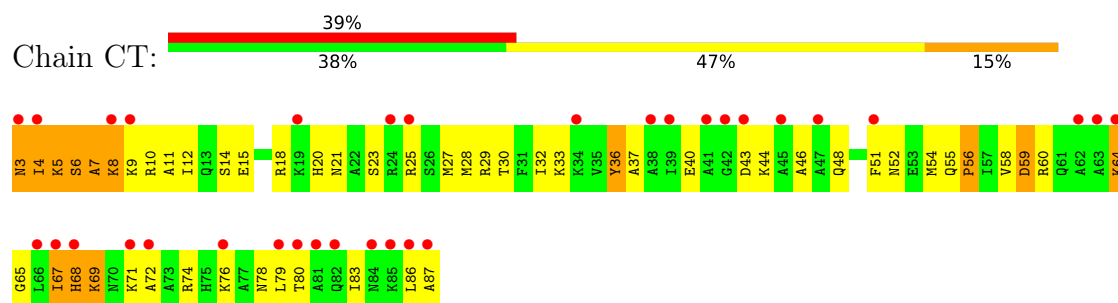
- Molecule 19: 30S ribosomal protein S19



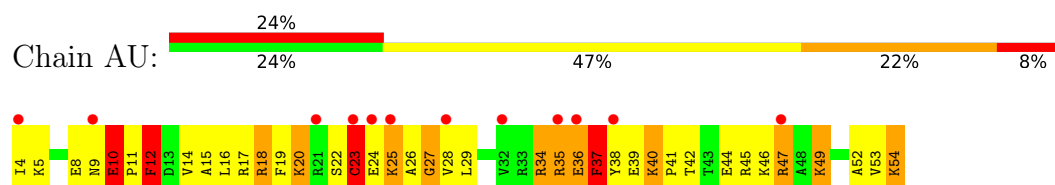
- Molecule 20: 30S ribosomal protein S20



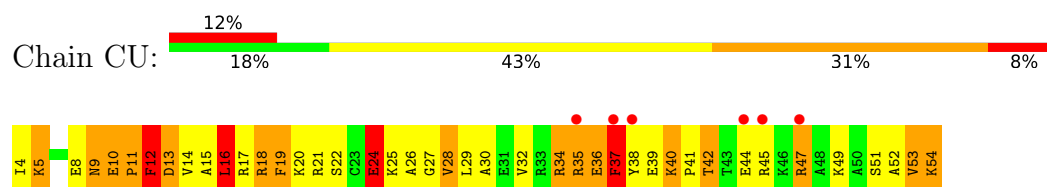
- Molecule 20: 30S ribosomal protein S20



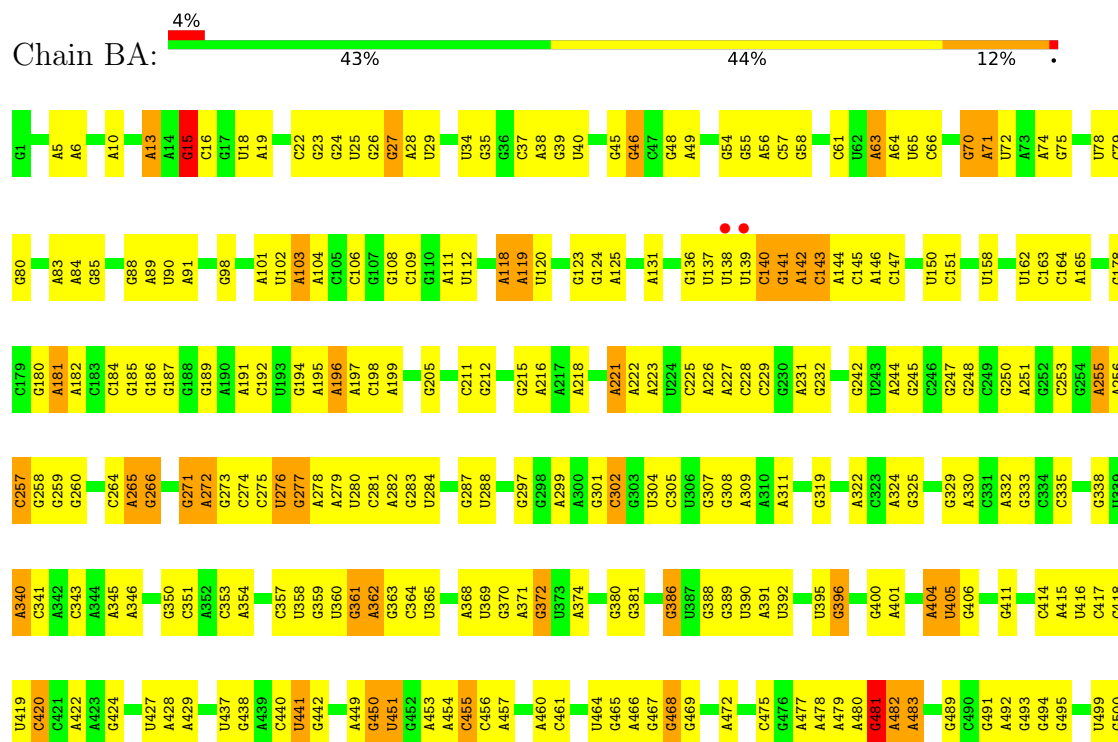
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

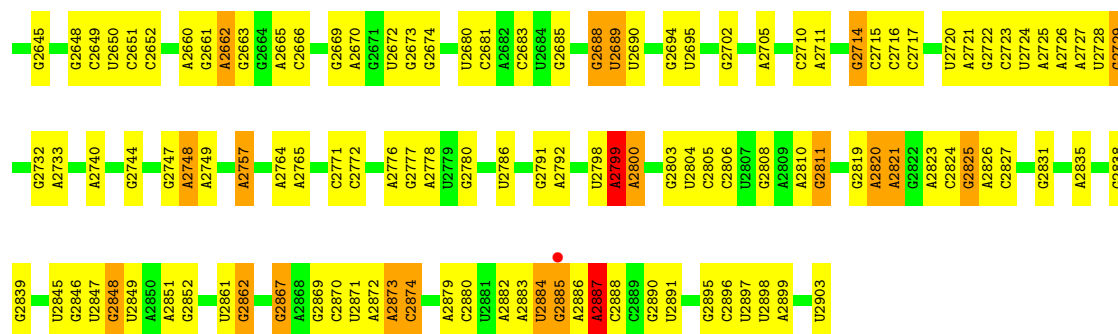


- Molecule 22: 23S rRNA

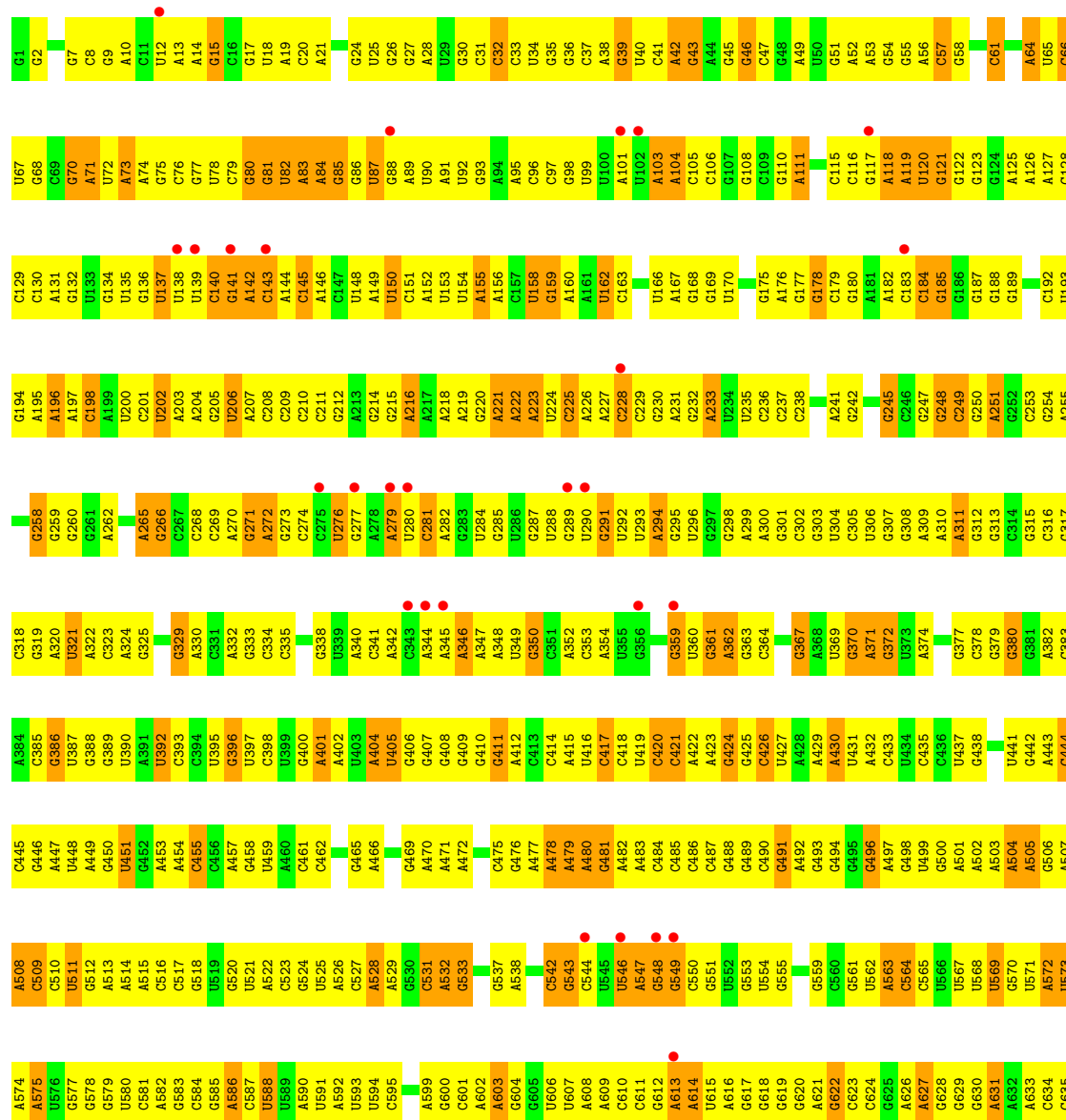




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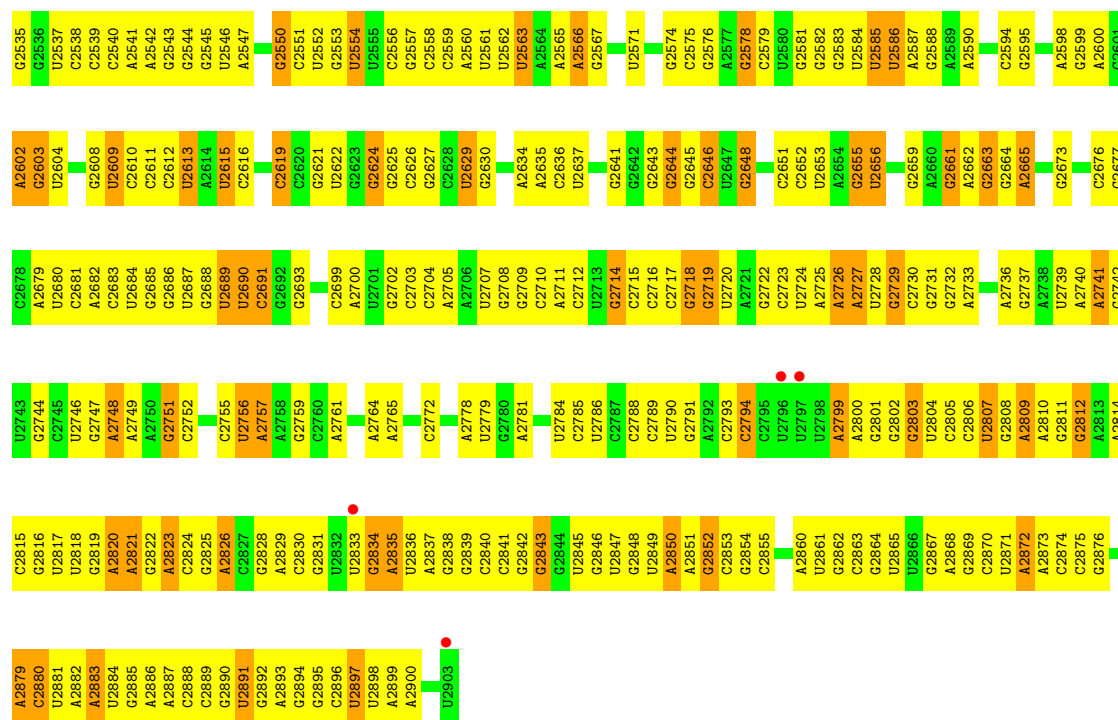


• Molecule 22: 23S rRNA



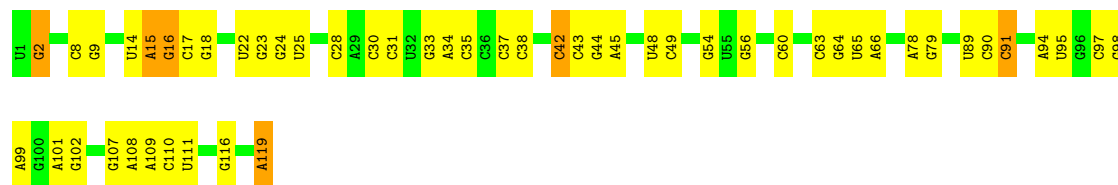


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G2490	G2293	C2354	G2293	G2224	A2163	C2091	G2023	A1960	A1890	G1817	G1752	U1603
C2420	G2294	G2355	G2294	A2225	C2164	G2092	G2024	G1961	A1891	U1818	G1753	A1604
		U2356		C2226	C2165	G2093	G2025	G1962	C1892	A1819	A1754	C1605
U2492		G2357	A2297	A2227	U2166	A2094	U2026	G1963	C1893	U1820	G1674	
		A2358	A2298		U2167			C1964	C1894			C1675
A2497	C2359	C2359	U2299	G2230	C2168	C2103		A1966	C1895			A1676
C2498	G2360	C2360	C2300	U2231	A2169	C2104	A2030	G1967	C1896	G1826		C1606
G2499	G2361	C2361	C2301	U2232	A2170	U2105	A2031	G1968	C1897	U1827	A1677	C1607
U2500	C2362		U2302	U2233	C2171	U2106	G2032	A1969	C1898	G1828	A1678	A1608
C2501			G2303	G2234	U2172	G2107	A2033	G1970	C1899	G1829	A1759	A1609
C2502			G2304	G2235	A2173	A2108	U2034	U1971	U1898	C1830	G1682	A1610
A2503			U2305	U2236	C2174	U2109	G2035	G1972	A1899	G1831	U1683	C1611
U2504	G2366		U2306	G2237	C2175	G2110	C2036	G1973	A1900	C1832	U1684	C1612
G2505	G2367			G2238	A2176	U2111	A2037	C1974		C1833	U1688	G1613
			G2307	G2239	C2177	U2112	G2038	G1975		U1834	A1614	C1615
A2435			G2308	G2240	C2178	U2113	U2039	U1976		G1835	U1692	A1616
G2436	G2370		A2309	A2241	U2180	A2114	G2040	A1977		C1836	U1693	C1617
G2437	U2372		C2310	G2242	C2179	G2115	A2041	A1978		C1837	G1767	C1618
U2438	G2373		U2311	U2243	U2181	G2116	A2042	U1979		C1838	G1768	G1619
C2440	C2374		U2312	U2244	U2182	A2117	C2043	G1980		G1839	U1769	
U2441	G2375		U2313	U2245	U2183	U2118	C2044	A1981				G1620
C2442	A2376		A2314	U2246	A2184	A2119	C2045	U1982		C1843	A1773	U1621
G2443	A2377		G2315	G2246	U2185	G2120		G1983		C1844	C1774	G1622
A2516	A2378		G2316		U2186	G2121	G2048	G1984		G1845	C1775	G1623
C2517	G2379		A2317	G2250	U2187	U2122	G2049	C1985		G1846	G1707	U1624
A2518	C2380		G2318	G2251	U2188	G2123	C2050	C1986		A1847	U1709	C1625
A2519	A2381		G2319	G2252	U2189	G2124	A2051	A1987		G1849	G1710	A1626
G2520	G2382		U2320	G2253	G2190	G2125	A2052	G1988		U1780		G1627
U2449	C2383		U2321	C2254	A2191	A2126	G2053	G1989		U1781		G1628
C2521	U2384		A2322		U2192	G2127	A2054	C1990		U1782		
	C2385		G2323	C2258	U2193	G2128	C2055	U1991		A1701		A1634
G2525	A2451		U2324		U2194	C2129	G2056	G1992		A1716		
G2526	C2452		G2325	C2261	U2195	C2130	G2057	U1993		A1717		
C2527	A2453		C2326	U2262	C2196	U2131	G2058	U1994		G1718		C1638
U2528	G2454		A2327	C2263	U2197	U2132	A2059	C1995		A1722		A1640
G2529			G2328	C2264	A2198	G2133	A2060	U1996		G1723		A1641
A2530			A2328	U2265	A2199	A2134	C2061	C1997		U1725		
G2531	U2457		U2329	U2266	G2300			C1998				
A2458	G2458		A2459	A2266								
G2532	U2460											

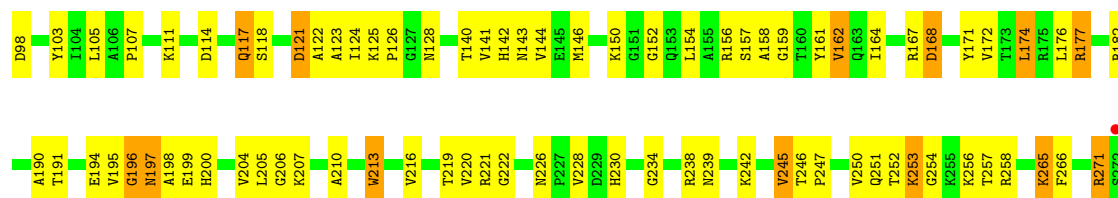


• Molecule 23: 5S rRNA

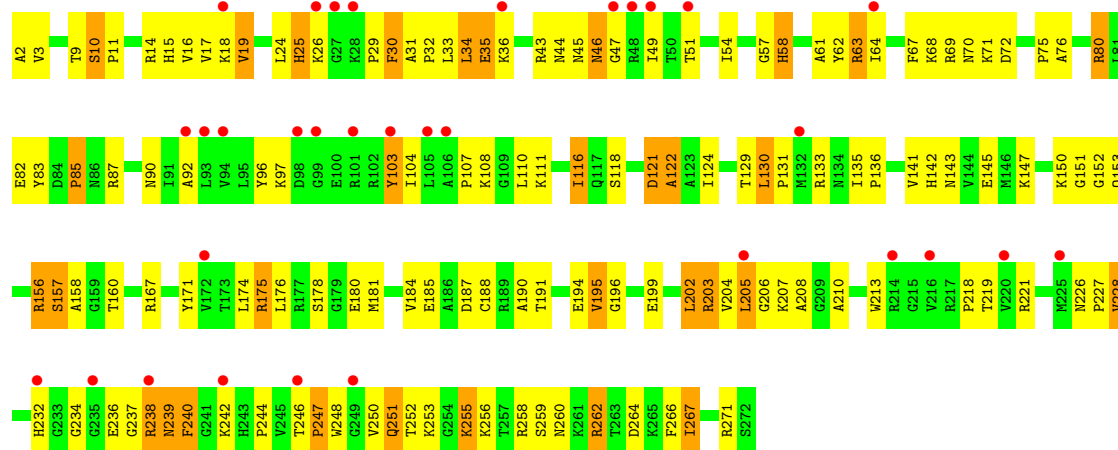
Chain BB: 56% 39% 5%



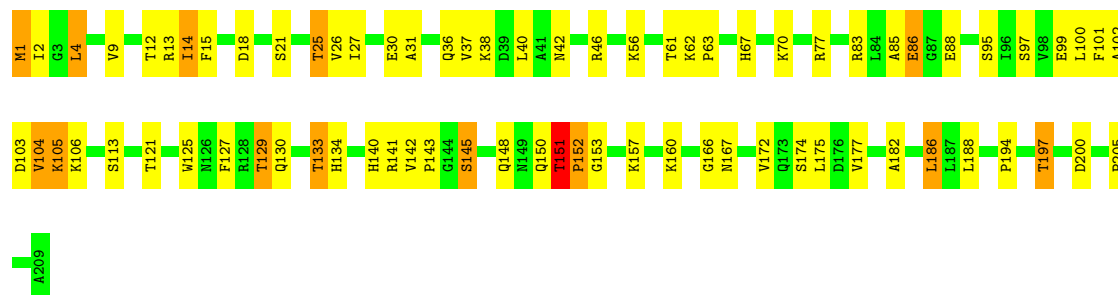




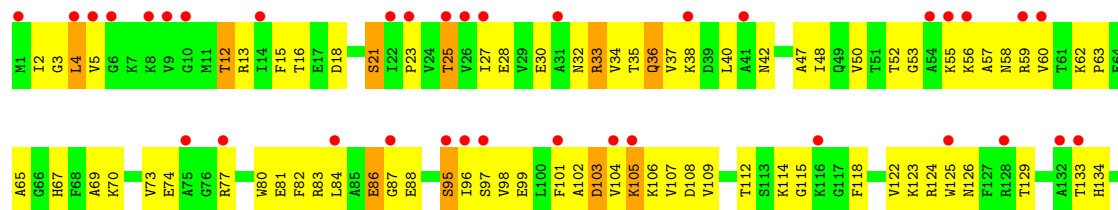
• Molecule 24: 50S ribosomal protein L2

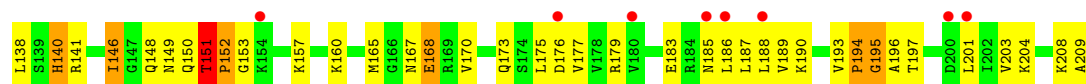


• Molecule 25: 50S ribosomal protein L3



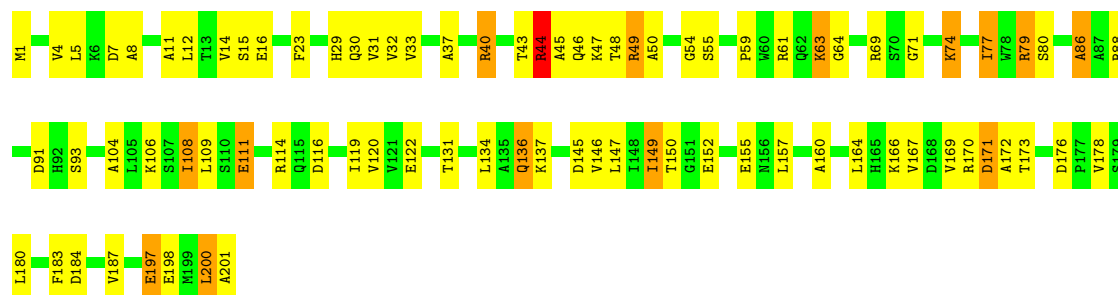
• Molecule 25: 50S ribosomal protein L3





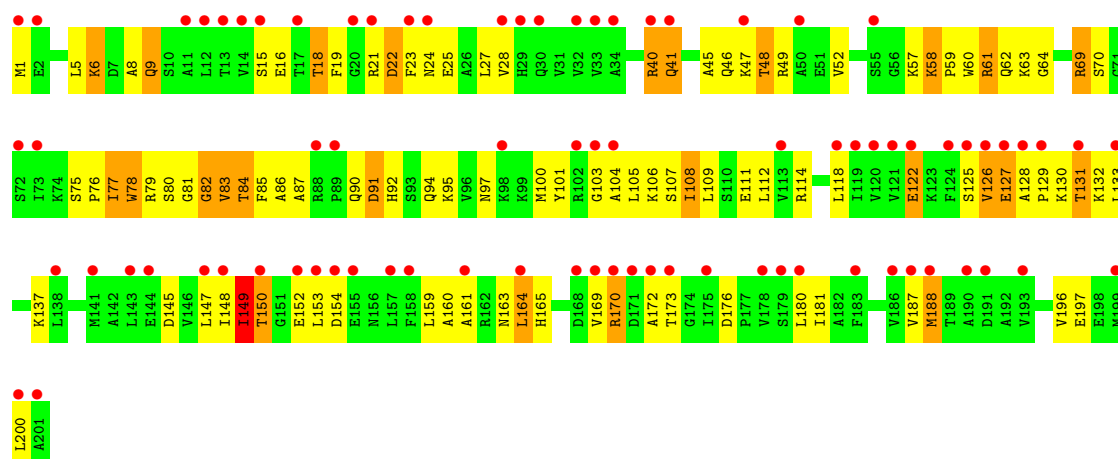
• Molecule 26: 50S ribosomal protein L4

Chain BE: 59% 34% 7%



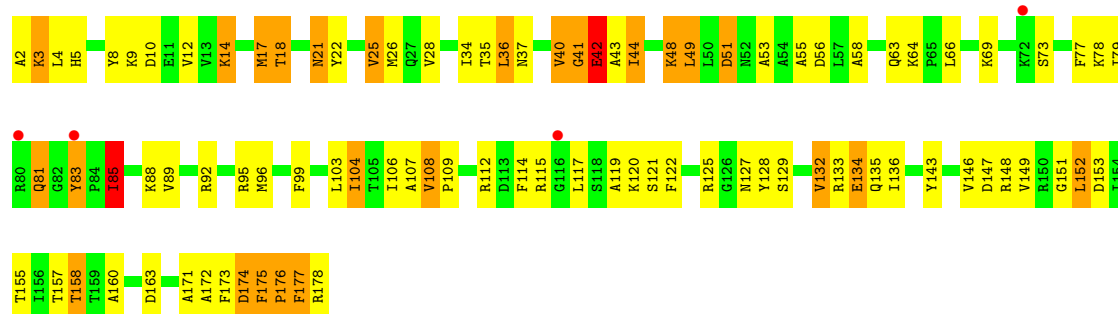
• Molecule 26: 50S ribosomal protein L4

Chain DE: 40% 49% 38% 12%

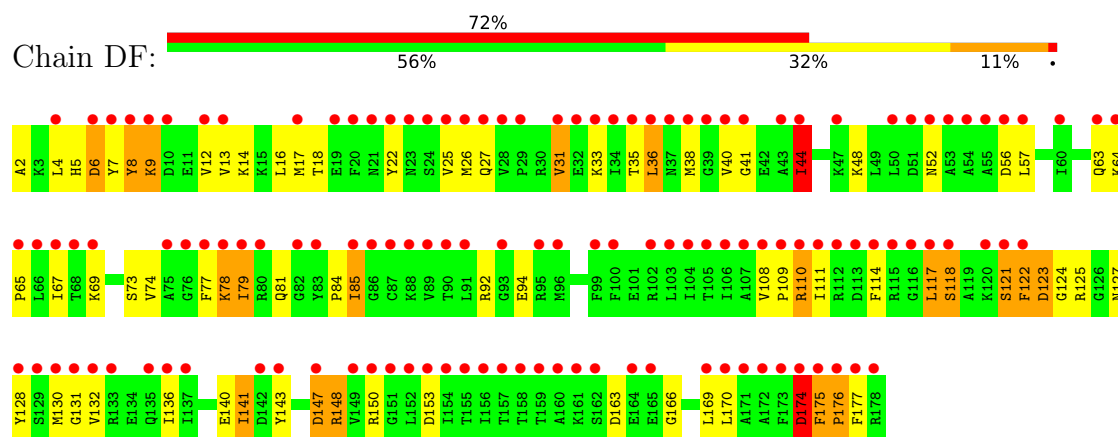


• Molecule 27: 50S ribosomal protein L5

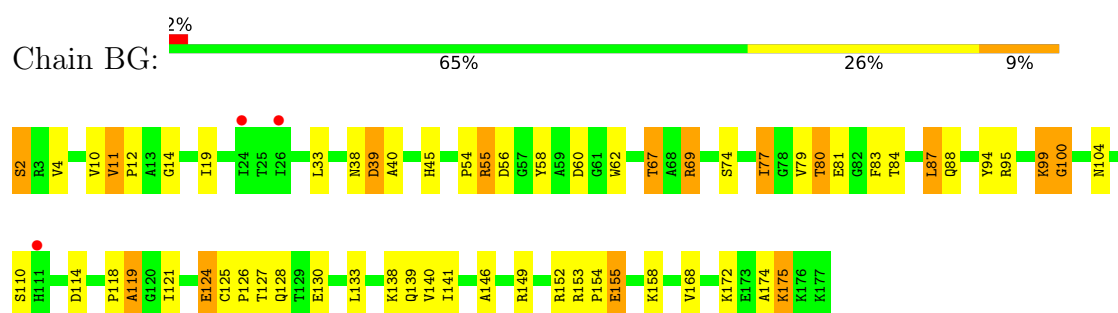
Chain BF: 2% 47% 37% 14%



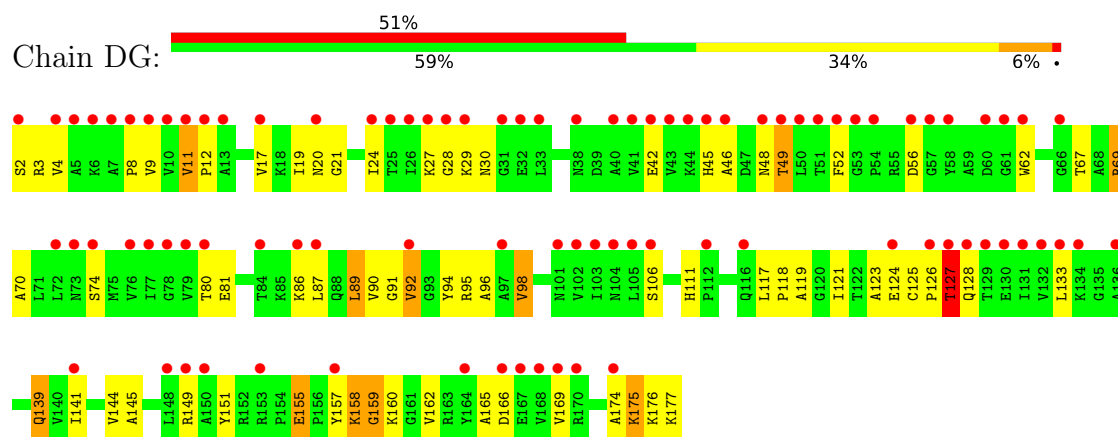
• Molecule 27: 50S ribosomal protein L5



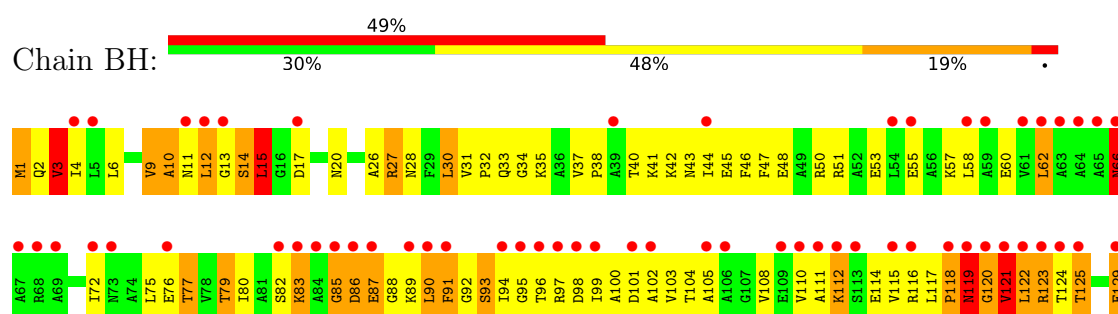
• Molecule 28: 50S ribosomal protein L6

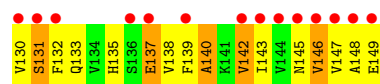


• Molecule 28: 50S ribosomal protein L6

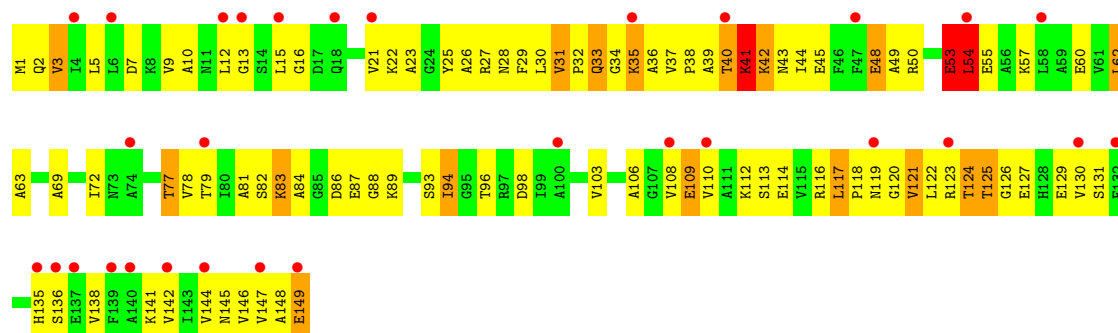


• Molecule 29: 50S ribosomal protein L9

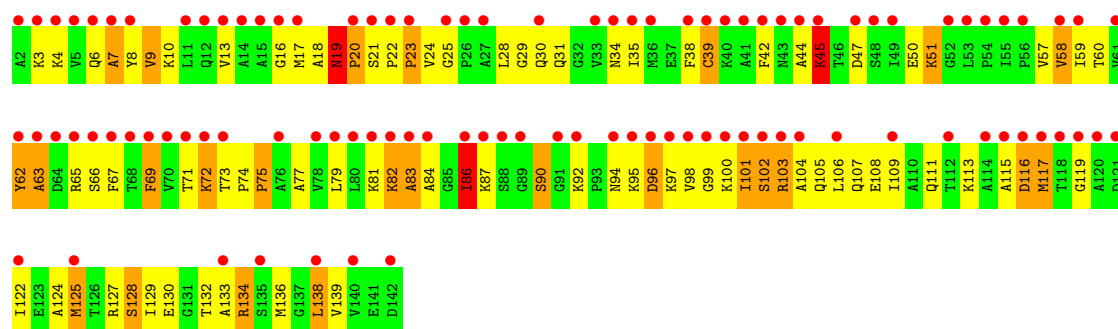




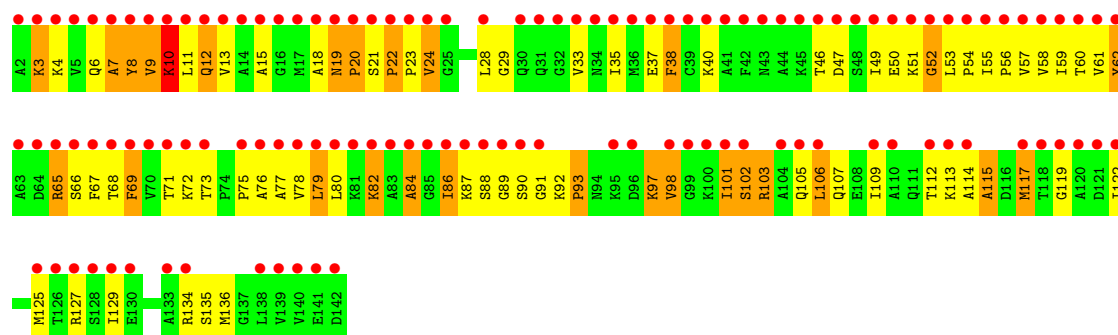
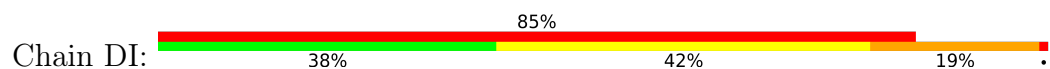
• Molecule 29: 50S ribosomal protein L9



• Molecule 30: 50S ribosomal protein L11

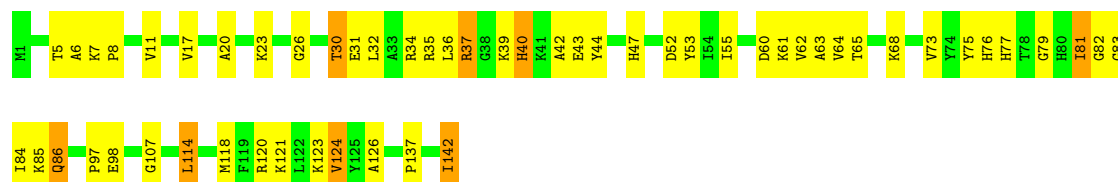


• Molecule 30: 50S ribosomal protein L11

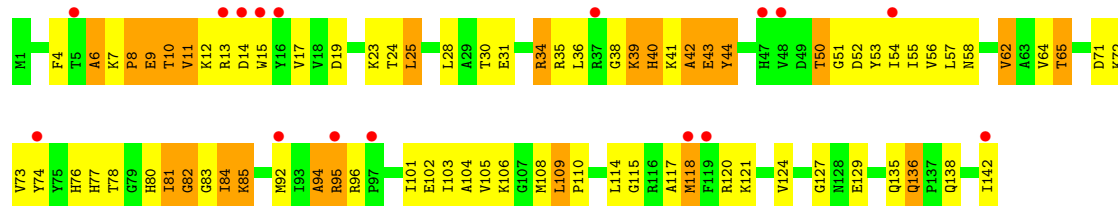
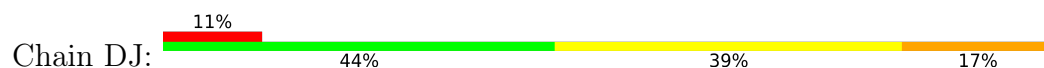


• Molecule 31: 50S ribosomal protein L13





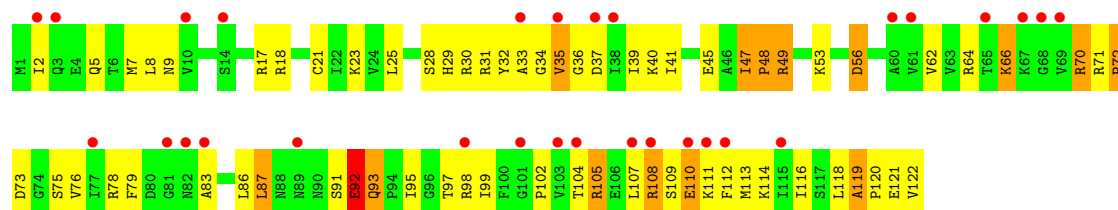
- Molecule 31: 50S ribosomal protein L13



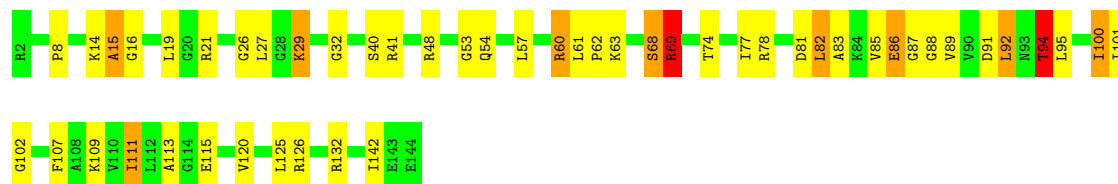
- Molecule 32: 50S ribosomal protein L14



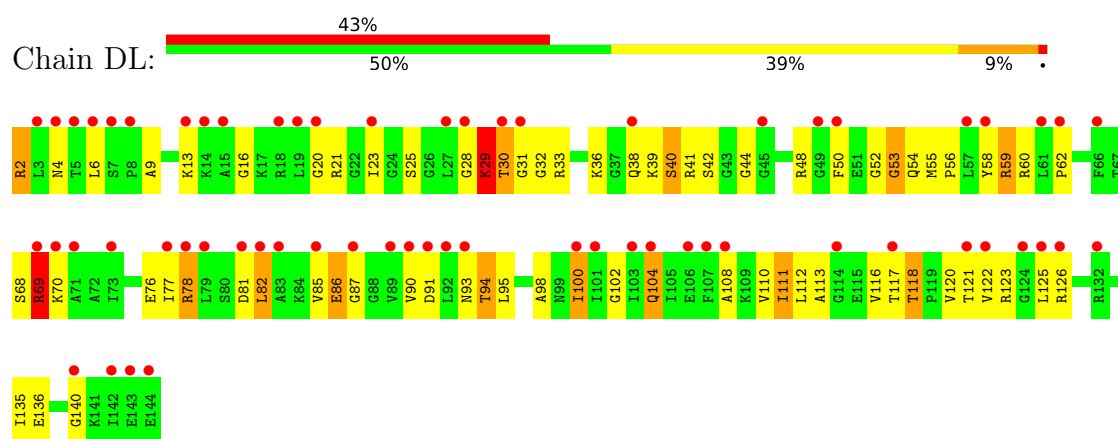
- Molecule 32: 50S ribosomal protein L14



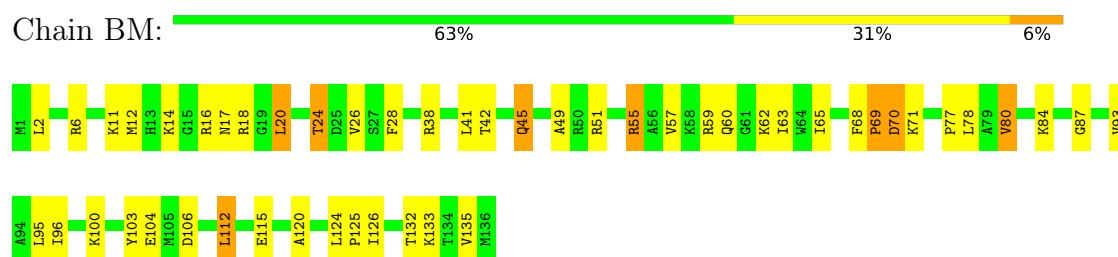
- Molecule 33: 50S ribosomal protein L15



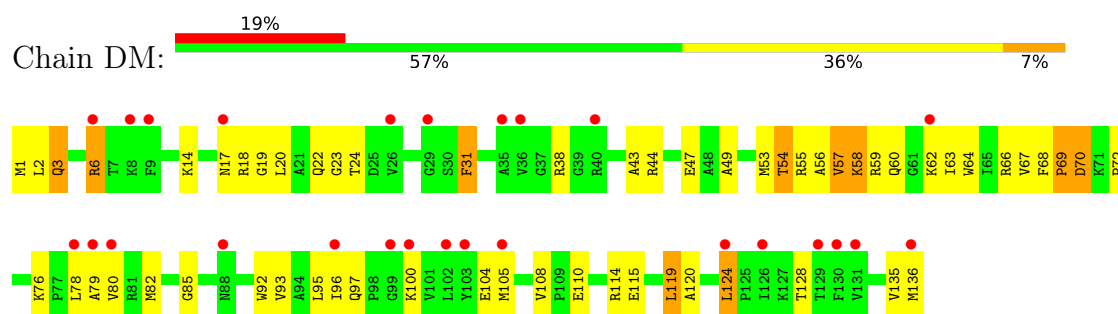
- Molecule 33: 50S ribosomal protein L15



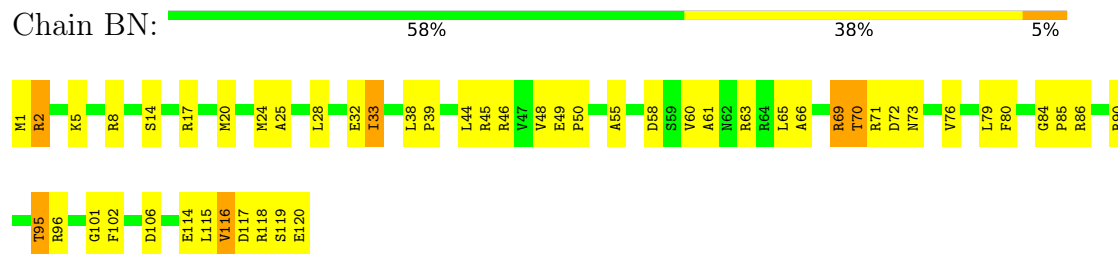
- Molecule 34: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L16

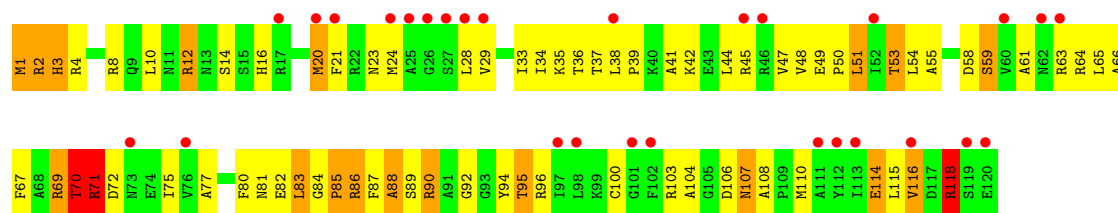


- Molecule 35: 50S ribosomal protein L17

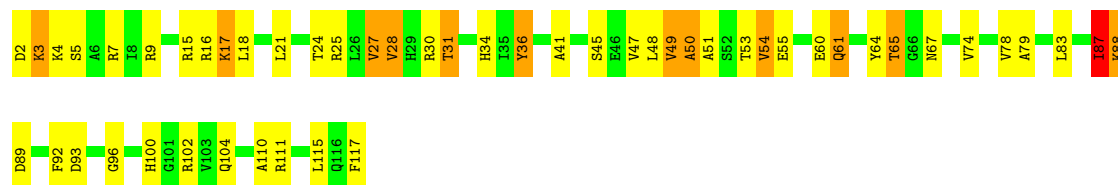


- Molecule 35: 50S ribosomal protein L17

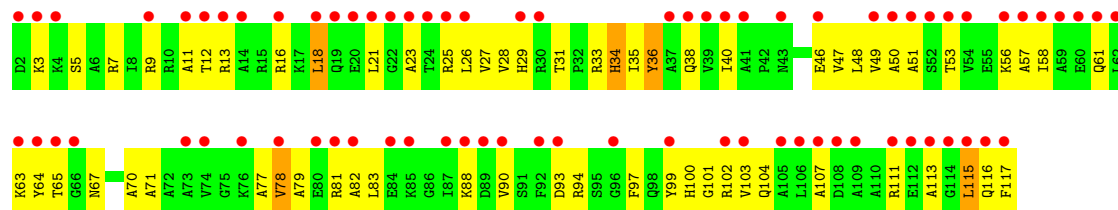




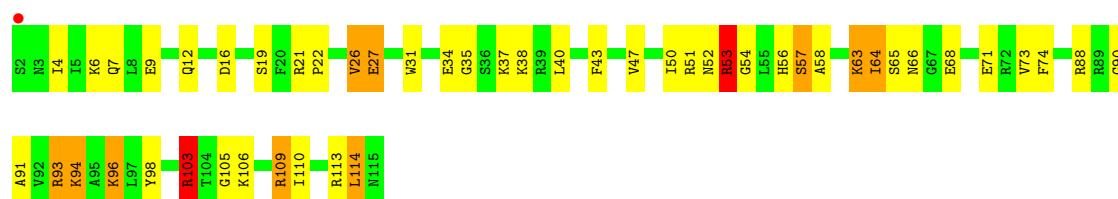
• Molecule 36: 50S ribosomal protein L18



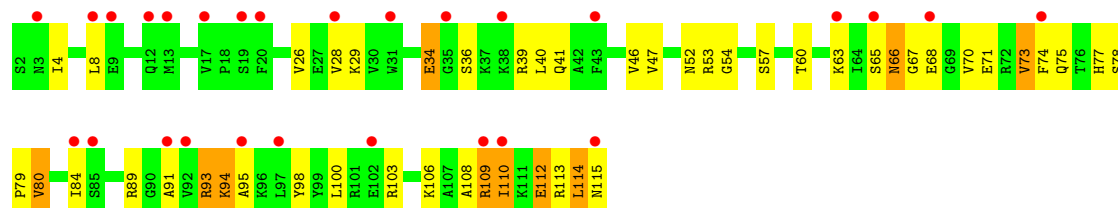
• Molecule 36: 50S ribosomal protein L18



• Molecule 37: 50S ribosomal protein L19

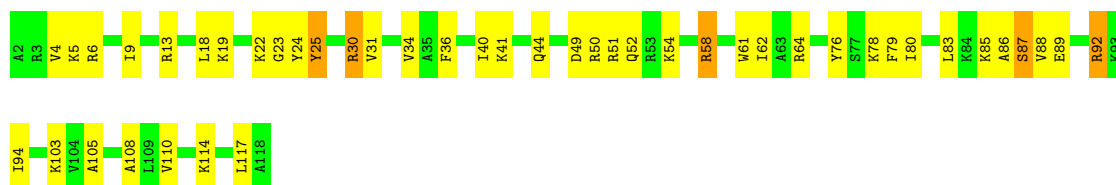


• Molecule 37: 50S ribosomal protein L19



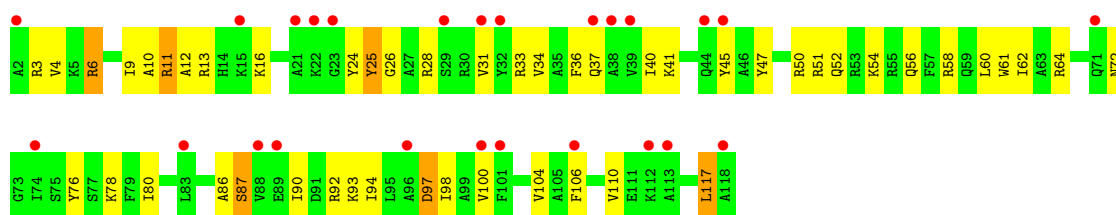
- Molecule 38: 50S ribosomal protein L20

Chain BQ:  62% 34% .



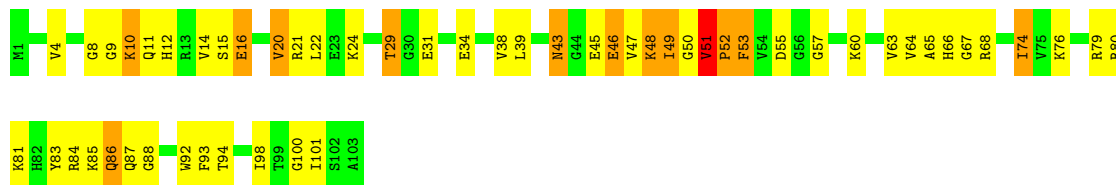
- Molecule 38: 50S ribosomal protein L20

Chain DQ:  21% 58% 37% 5%



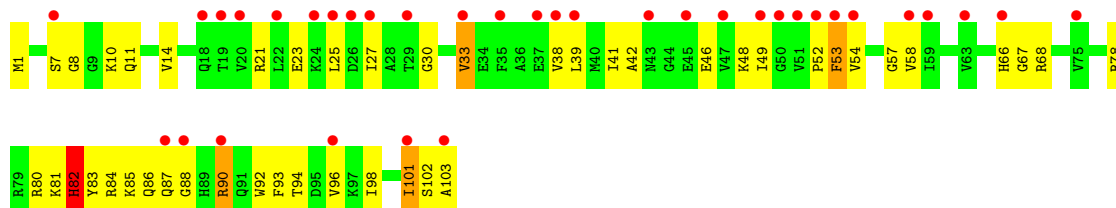
- Molecule 39: 50S ribosomal protein L21

Chain BR:  48% 40% 12% .



- Molecule 39: 50S ribosomal protein L21

Chain DR:  34% 55% 40% . .



- Molecule 40: 50S ribosomal protein L22

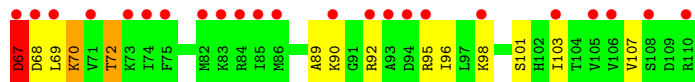
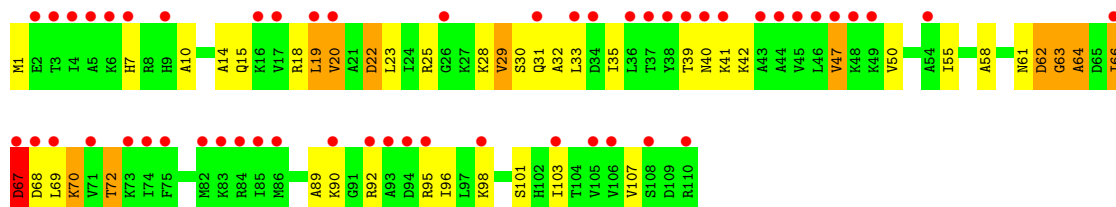
Chain BS:  59% 30% 11%







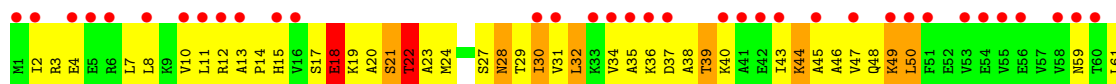
- Molecule 40: 50S ribosomal protein L22



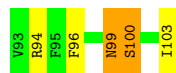
- Molecule 41: 50S ribosomal protein L23



- Molecule 41: 50S ribosomal protein L23

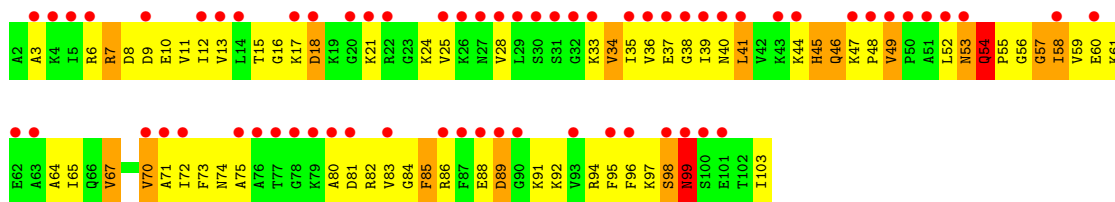


- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24





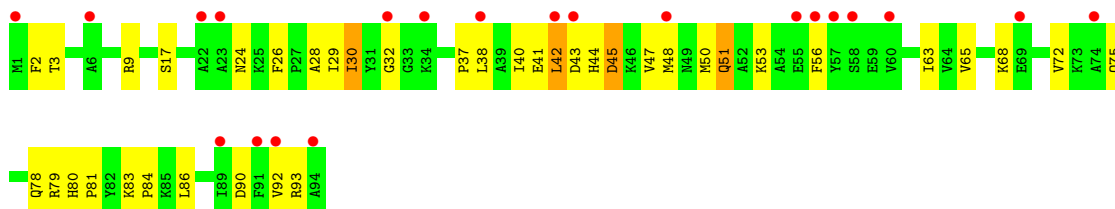
• Molecule 43: 50S ribosomal protein L25

Chain BV: 63% 27% 10% .



• Molecule 43: 50S ribosomal protein L25

Chain DV: 22% 59% 37% .



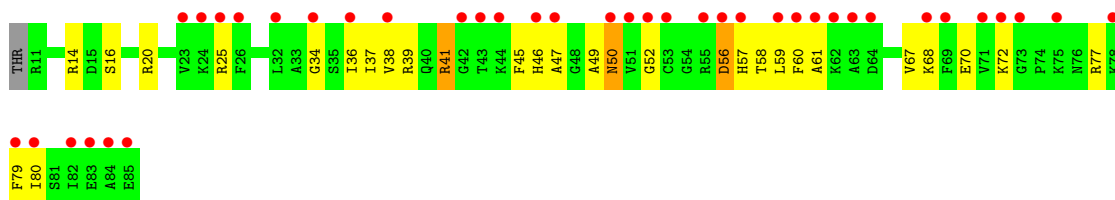
• Molecule 44: 50S ribosomal protein L27

Chain BW: 3% 63% 28% 8% .



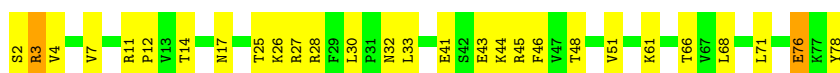
• Molecule 44: 50S ribosomal protein L27

Chain DW: 51% 61% 34% .

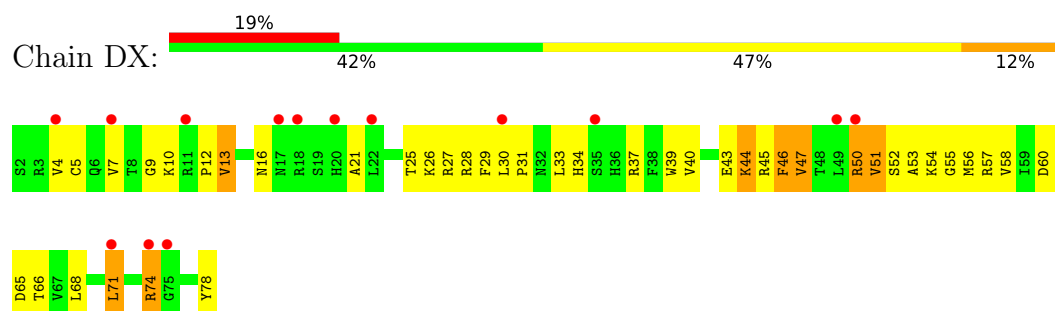


• Molecule 45: 50S ribosomal protein L28

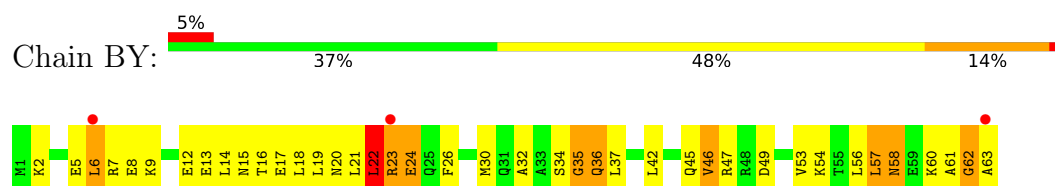
Chain BX: 64% 34% .



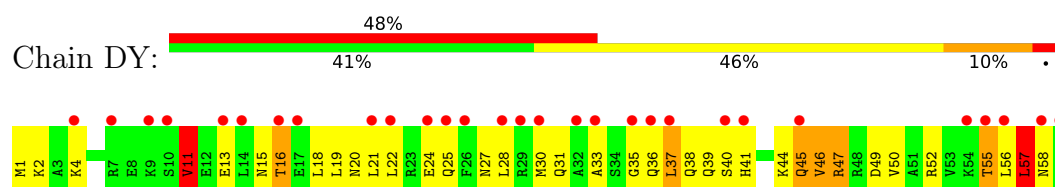
- Molecule 45: 50S ribosomal protein L28



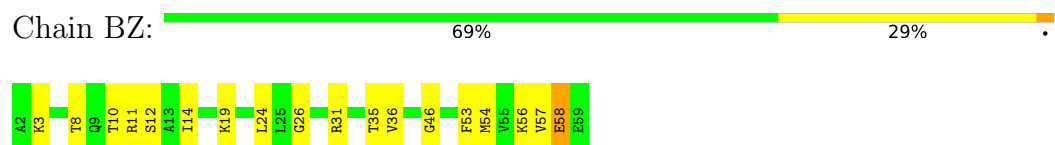
- Molecule 46: 50S ribosomal protein L29



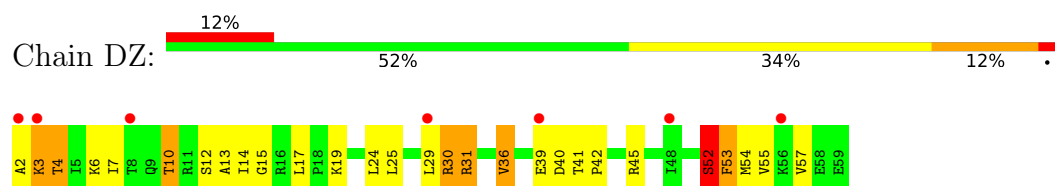
- Molecule 46: 50S ribosomal protein L29



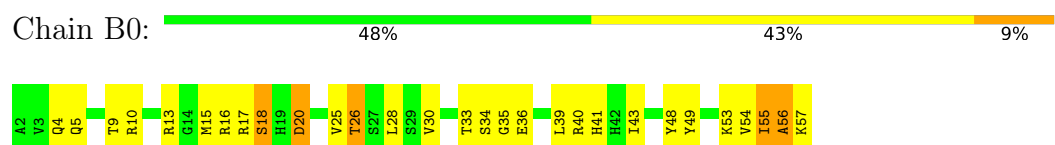
- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30

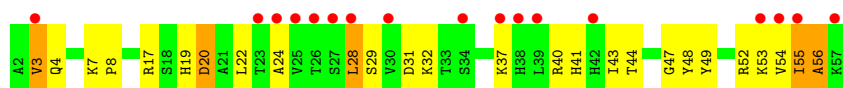


- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32

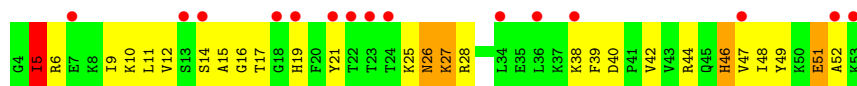




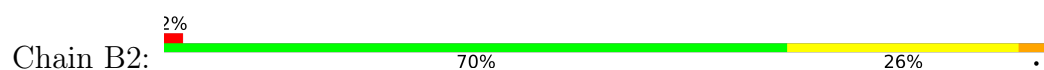
- Molecule 49: 50S ribosomal protein L33



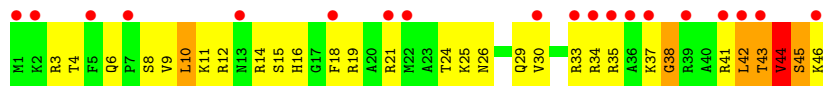
- Molecule 49: 50S ribosomal protein L33



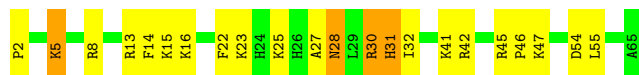
- Molecule 50: 50S ribosomal protein L34



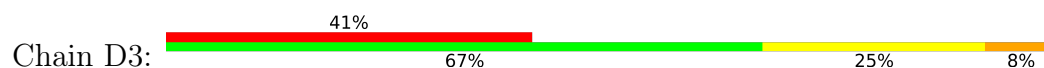
- Molecule 50: 50S ribosomal protein L34




- Molecule 51: 50S ribosomal protein L35

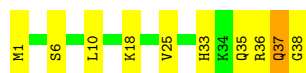


- Molecule 51: 50S ribosomal protein L35



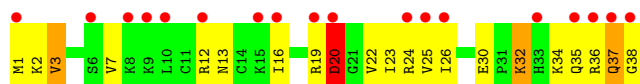
- Molecule 52: 50S ribosomal protein L36

Chain B4:  74% 24% .

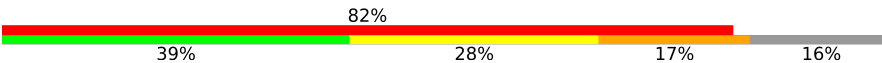


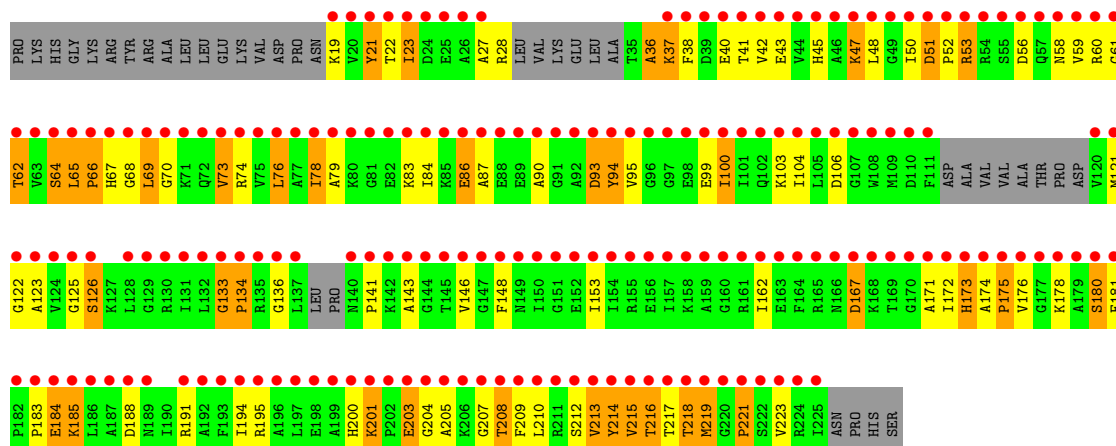
- Molecule 52: 50S ribosomal protein L36

Chain D4:  47% 45% 8% .



- Molecule 53: 50S ribosomal protein L1

Chain B5:  82% 39% 28% 17% 16%



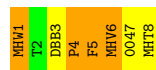
- Molecule 54: Quinupristin

Chain B6:  12% 75% 12%



- Molecule 54: Quinupristin

Chain D6:  12% 38% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.26Å 432.34Å 621.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.08 – 2.80 69.08 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (69.08-2.80) 94.1 (69.08-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1160)	Depositor
R, $R_{free}$	0.225 , 0.271 0.230 , 0.276	Depositor DCC
$R_{free}$ test set	5217 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	288423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MHW, 004, MHV, MG, DOL, ZN, DBB, MHU, MHT

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	0.34	0/36944	0.80	3/57632 (0.0%)
1	CA	0.28	0/36966	0.78	1/57666 (0.0%)
2	AB	0.28	0/1736	0.56	0/2338
2	CB	0.26	0/1736	0.50	0/2338
3	AC	0.28	0/1652	0.53	0/2225
3	CC	0.25	0/1652	0.48	0/2225
4	AD	0.29	0/1665	0.55	0/2227
4	CD	0.31	0/1665	0.55	0/2227
5	AE	0.31	0/1119	0.61	0/1504
5	CE	0.29	0/1119	0.59	0/1504
6	AF	0.30	0/836	0.55	0/1128
6	CF	0.27	0/836	0.57	1/1128 (0.1%)
7	AG	0.26	0/1196	0.48	0/1602
7	CG	0.25	0/1196	0.49	0/1602
8	AH	0.31	0/989	0.50	0/1326
8	CH	0.25	0/989	0.48	0/1326
9	AI	0.26	0/1034	0.54	0/1375
9	CI	0.26	0/1034	0.52	0/1375
10	AJ	0.29	0/797	0.55	0/1077
10	CJ	0.25	0/797	0.50	0/1077
11	AK	0.29	0/893	0.63	1/1205 (0.1%)
11	CK	0.26	0/893	0.52	0/1205
12	AL	0.31	0/969	0.58	0/1300
12	CL	0.29	0/969	0.60	0/1300
13	AM	0.27	0/893	0.55	0/1193
13	CM	0.26	0/893	0.50	0/1193
14	AN	0.28	0/785	0.55	0/1043
14	CN	0.25	0/785	0.46	0/1043
15	AO	0.28	0/718	0.53	0/959
15	CO	0.26	0/718	0.46	0/959
16	AP	0.30	0/659	0.66	1/884 (0.1%)
16	CP	0.27	0/659	0.49	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	0.28	0/658	0.51	0/881
18	AR	0.26	0/463	0.53	0/621
18	CR	0.26	0/463	0.49	0/621
19	AS	0.27	0/653	0.50	0/877
19	CS	0.27	0/653	0.54	0/877
20	AT	0.31	0/671	0.55	0/888
20	CT	0.25	0/671	0.50	0/888
21	AU	0.36	0/431	0.62	0/570
21	CU	0.33	0/431	0.56	0/570
22	BA	0.59	5/69659 (0.0%)	0.99	92/108672 (0.1%)
22	DA	0.27	0/69659	0.79	4/108672 (0.0%)
23	BB	0.52	0/2850	0.93	0/4444
23	DB	0.23	0/2828	0.76	0/4410
24	BC	0.38	0/2122	0.60	0/2852
24	DC	0.27	0/2122	0.52	0/2852
25	BD	0.42	0/1586	0.63	1/2134 (0.0%)
25	DD	0.26	0/1586	0.51	0/2134
26	BE	0.37	0/1571	0.60	0/2113
26	DE	0.26	0/1571	0.51	0/2113
27	BF	0.30	0/1435	0.52	0/1926
27	DF	0.24	0/1435	0.46	0/1926
28	BG	0.30	0/1343	0.53	0/1816
28	DG	0.25	0/1343	0.46	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	0.29	0/1046	0.54	0/1410
30	DI	0.28	0/1046	0.52	0/1410
31	BJ	0.42	0/1152	0.58	0/1551
31	DJ	0.25	0/1152	0.51	0/1551
32	BK	0.41	0/948	0.64	0/1268
32	DK	0.27	0/948	0.51	0/1268
33	BL	0.39	0/1054	0.64	0/1403
33	DL	0.26	0/1054	0.51	0/1403
34	BM	0.42	0/1093	0.63	0/1460
34	DM	0.25	0/1093	0.46	0/1460
35	BN	0.43	0/974	0.68	0/1301
35	DN	0.27	0/974	0.56	1/1301 (0.1%)
36	BO	0.34	0/902	0.55	0/1209
36	DO	0.24	0/902	0.45	0/1209
37	BP	0.42	0/929	0.69	2/1242 (0.2%)
37	DP	0.26	0/929	0.47	0/1242
38	BQ	0.50	0/960	0.66	0/1278



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DQ	0.26	0/960	0.47	0/1278
39	BR	0.47	0/829	0.73	1/1107 (0.1%)
39	DR	0.25	0/829	0.50	0/1107
40	BS	0.51	0/864	0.64	0/1156
40	DS	0.26	0/864	0.50	0/1156
41	BT	0.36	0/745	0.60	0/994
41	DT	0.25	0/745	0.49	0/994
42	BU	0.36	0/788	0.57	0/1051
42	DU	0.28	0/788	0.52	0/1051
43	BV	0.37	0/766	0.58	0/1025
43	DV	0.24	0/766	0.44	0/1025
44	BW	0.44	0/587	0.71	2/776 (0.3%)
44	DW	0.25	0/576	0.47	0/762
45	BX	0.34	0/635	0.57	0/848
45	DX	0.28	0/635	0.53	0/848
46	BY	0.32	0/510	0.63	0/677
46	DY	0.25	0/510	0.50	0/677
47	BZ	0.43	0/453	0.61	0/605
47	DZ	0.26	0/453	0.48	0/605
48	B0	0.44	0/450	0.64	0/599
48	D0	0.27	0/450	0.50	0/599
49	B1	0.37	0/417	0.53	0/554
49	D1	0.28	0/417	0.49	0/554
50	B2	0.44	0/380	0.69	0/498
50	D2	0.28	0/380	0.51	0/498
51	B3	0.38	0/513	0.57	0/676
51	D3	0.25	0/513	0.44	0/676
52	B4	0.43	0/303	0.63	0/397
52	D4	0.25	0/303	0.49	0/397
53	B5	0.25	0/1145	0.49	0/1556
54	B6	1.77	0/13	2.40	1/15 (6.7%)
54	D6	1.44	0/13	2.02	1/15 (6.7%)
All	All	0.39	5/310652 (0.0%)	0.79	113/464396 (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
6	CF	0	1
11	AK	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	CL	0	2
25	BD	0	1
25	DD	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	984	A	N9-C4	-8.33	1.32	1.37
22	BA	1142	A	N9-C4	-7.64	1.33	1.37
22	BA	1936	A	N9-C4	-7.63	1.33	1.37
22	BA	528	A	N9-C4	-7.62	1.33	1.37
22	BA	528	A	N3-C4	-5.47	1.31	1.34

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	974	G	C4-C5-N7	10.83	115.13	110.80
22	BA	974	G	C6-C5-N7	-10.21	124.27	130.40
25	BD	151	THR	C-N-CD	-9.98	98.64	120.60
22	BA	984	A	C2-N3-C4	-9.95	105.62	110.60
22	BA	974	G	C5-N7-C8	-9.65	99.48	104.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
25	BD	151	THR	Peptide
6	CF	54	LEU	Peptide
12	CL	23	ALA	Peptide
12	CL	24	LEU	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	962	0
1	CA	33015	0	16617	1107	1
2	AB	1705	0	1732	164	0
2	CB	1705	0	1732	135	0
3	AC	1625	0	1696	78	0
3	CC	1625	0	1696	69	0
4	AD	1643	0	1707	116	0
4	CD	1643	0	1707	116	0
5	AE	1106	0	1148	88	0
5	CE	1106	0	1148	99	0
6	AF	818	0	808	47	0
6	CF	818	0	808	60	0
7	AG	1182	0	1238	58	0
7	CG	1182	0	1238	66	0
8	AH	979	0	1031	49	0
8	CH	979	0	1031	52	0
9	AI	1022	0	1070	87	0
9	CI	1022	0	1070	66	0
10	AJ	787	0	828	81	0
10	CJ	787	0	828	56	0
11	AK	877	0	887	68	0
11	CK	877	0	887	55	0
12	AL	955	0	1016	44	0
12	CL	955	0	1016	74	0
13	AM	884	0	941	44	0
13	CM	884	0	941	51	0
14	AN	774	0	824	58	0
14	CN	774	0	824	51	0
15	AO	710	0	728	31	0
15	CO	710	0	728	29	0
16	AP	649	0	666	53	0
16	CP	649	0	666	36	0
17	AQ	649	0	691	63	0
17	CQ	649	0	691	53	0
18	AR	456	0	478	17	0
18	CR	456	0	478	25	0
19	AS	638	0	665	39	0
19	CS	638	0	665	42	0
20	AT	665	0	714	65	0
20	CT	665	0	714	46	0
21	AU	426	0	449	52	0
21	CU	426	0	449	53	0
22	BA	62195	0	31280	1486	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	62195	0	31280	2451	1
23	BB	2549	0	1291	37	0
23	DB	2529	0	1281	66	0
24	BC	2083	0	2154	102	0
24	DC	2083	0	2154	128	0
25	BD	1565	0	1616	66	0
25	DD	1565	0	1616	97	0
26	BE	1552	0	1619	67	0
26	DE	1552	0	1619	91	0
27	BF	1411	0	1444	84	0
27	DF	1411	0	1444	54	0
28	BG	1323	0	1371	41	0
28	DG	1323	0	1371	42	0
29	BH	1110	0	1147	139	0
29	DH	1110	0	1148	87	0
30	BI	1032	0	1085	76	0
30	DI	1032	0	1085	85	0
31	BJ	1129	0	1162	48	0
31	DJ	1129	0	1162	62	0
32	BK	939	0	1012	45	0
32	DK	939	0	1012	53	0
33	BL	1045	0	1117	54	0
33	DL	1045	0	1117	75	0
34	BM	1074	0	1157	43	0
34	DM	1074	0	1157	41	0
35	BN	961	0	1000	39	0
35	DN	961	0	1000	71	0
36	BO	892	0	923	38	0
36	DO	892	0	923	41	0
37	BP	917	0	962	45	0
37	DP	917	0	962	42	0
38	BQ	947	0	1019	39	0
38	DQ	947	0	1019	47	0
39	BR	816	0	839	66	0
39	DR	816	0	839	36	0
40	BS	857	0	922	33	0
40	DS	857	0	922	37	0
41	BT	739	0	807	41	0
41	DT	739	0	807	60	0
42	BU	780	0	831	37	0
42	DU	780	0	831	68	0
43	BV	753	0	780	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DV	753	0	780	21	0
44	BW	580	0	594	20	0
44	DW	569	0	581	23	0
45	BX	625	0	652	15	0
45	DX	625	0	652	46	0
46	BY	509	0	543	34	0
46	DY	509	0	543	26	0
47	BZ	449	0	488	9	0
47	DZ	449	0	488	24	0
48	B0	444	0	458	27	0
48	D0	444	0	458	23	0
49	B1	410	0	440	19	0
49	D1	410	0	440	22	0
50	B2	377	0	418	10	0
50	D2	377	0	418	31	0
51	B3	504	0	572	28	0
51	D3	504	0	572	22	0
52	B4	302	0	340	7	0
52	D4	302	0	340	15	0
53	B5	1142	0	865	69	0
54	B6	73	0	64	3	0
54	D6	73	0	65	12	0
55	AA	71	0	0	0	0
55	AM	1	0	0	0	0
55	BA	194	0	0	0	0
55	BB	4	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	166	0	0	0	0
55	DB	3	0	0	0	0
55	DQ	1	0	0	0	0
56	BA	48	0	50	15	0
56	DA	48	0	50	25	0
57	B4	1	0	0	0	0
57	D4	1	0	0	0	0
58	AA	194	0	0	18	0
58	AE	2	0	0	0	0
58	AL	1	0	0	0	0
58	AN	3	0	0	0	0
58	AT	2	0	0	0	0
58	AU	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	B3	3	0	0	0	0
58	B4	1	0	0	0	0
58	BA	617	0	0	66	0
58	BB	14	0	0	1	0
58	BC	6	0	0	1	0
58	BD	4	0	0	2	0
58	BE	1	0	0	0	0
58	BF	1	0	0	1	0
58	BG	1	0	0	1	0
58	BJ	1	0	0	0	0
58	BL	7	0	0	0	0
58	BN	5	0	0	0	0
58	BQ	1	0	0	0	0
58	BS	1	0	0	0	0
58	BT	2	0	0	0	0
58	CA	192	0	0	12	0
58	CL	1	0	0	0	0
58	CN	2	0	0	0	0
58	CT	2	0	0	0	0
58	CU	1	0	0	1	0
58	D2	1	0	0	1	0
58	D3	1	0	0	0	0
58	D4	1	0	0	0	0
58	DA	610	0	0	84	0
58	DB	13	0	0	1	0
58	DC	8	0	0	1	0
58	DD	4	0	0	2	0
58	DE	4	0	0	0	0
58	DJ	1	0	0	0	0
58	DL	4	0	0	1	0
58	DN	2	0	0	0	0
58	DS	2	0	0	0	0
58	DT	3	0	0	1	0
58	DU	1	0	0	0	0
58	DV	1	0	0	0	0
All	All	288423	0	193016	10587	1

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 22.

The worst 5 of 10587 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:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
22:BA:730:A:OP2	58:BA:3693:HOH:O	1.58	1.21
1:AA:533:A:OP1	58:AA:1848:HOH:O	1.65	1.15
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14
22:BA:2498:C:OP2	58:BA:3684:HOH:O	1.64	1.13

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:204:G:OP1	22:DA:289:G:O2'[3_545]	2.12	0.08

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	126 (58%)	45 (21%)	45 (21%)	0	0
2	CB	216/218 (99%)	140 (65%)	51 (24%)	25 (12%)	0	1
3	AC	204/206 (99%)	148 (72%)	35 (17%)	21 (10%)	0	1
3	CC	204/206 (99%)	154 (76%)	39 (19%)	11 (5%)	2	5
4	AD	203/205 (99%)	137 (68%)	39 (19%)	27 (13%)	0	0
4	CD	203/205 (99%)	152 (75%)	32 (16%)	19 (9%)	0	1
5	AE	148/150 (99%)	102 (69%)	27 (18%)	19 (13%)	0	1
5	CE	148/150 (99%)	100 (68%)	33 (22%)	15 (10%)	0	1
6	AF	98/100 (98%)	73 (74%)	15 (15%)	10 (10%)	0	1
6	CF	98/100 (98%)	68 (69%)	15 (15%)	15 (15%)	0	0
7	AG	149/151 (99%)	107 (72%)	29 (20%)	13 (9%)	1	1
7	CG	149/151 (99%)	119 (80%)	22 (15%)	8 (5%)	2	5
8	AH	127/129 (98%)	90 (71%)	28 (22%)	9 (7%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CH	127/129 (98%)	98 (77%)	19 (15%)	10 (8%)	1	2
9	AI	125/127 (98%)	87 (70%)	24 (19%)	14 (11%)	0	1
9	CI	125/127 (98%)	89 (71%)	18 (14%)	18 (14%)	0	0
10	AJ	96/98 (98%)	64 (67%)	11 (12%)	21 (22%)	0	0
10	CJ	96/98 (98%)	73 (76%)	11 (12%)	12 (12%)	0	1
11	AK	115/117 (98%)	81 (70%)	17 (15%)	17 (15%)	0	0
11	CK	115/117 (98%)	82 (71%)	24 (21%)	9 (8%)	1	2
12	AL	121/123 (98%)	91 (75%)	21 (17%)	9 (7%)	1	2
12	CL	121/123 (98%)	92 (76%)	18 (15%)	11 (9%)	1	1
13	AM	112/114 (98%)	81 (72%)	21 (19%)	10 (9%)	1	1
13	CM	112/114 (98%)	80 (71%)	18 (16%)	14 (12%)	0	1
14	AN	92/100 (92%)	61 (66%)	21 (23%)	10 (11%)	0	1
14	CN	92/100 (92%)	58 (63%)	20 (22%)	14 (15%)	0	0
15	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	2
15	CO	86/88 (98%)	64 (74%)	17 (20%)	5 (6%)	1	4
16	AP	80/82 (98%)	55 (69%)	15 (19%)	10 (12%)	0	1
16	CP	80/82 (98%)	59 (74%)	13 (16%)	8 (10%)	0	1
17	AQ	78/80 (98%)	53 (68%)	18 (23%)	7 (9%)	1	1
17	CQ	78/80 (98%)	56 (72%)	15 (19%)	7 (9%)	1	1
18	AR	53/55 (96%)	42 (79%)	11 (21%)	0	100	100
18	CR	53/55 (96%)	37 (70%)	12 (23%)	4 (8%)	1	2
19	AS	77/79 (98%)	57 (74%)	11 (14%)	9 (12%)	0	1
19	CS	77/79 (98%)	55 (71%)	11 (14%)	11 (14%)	0	0
20	AT	83/85 (98%)	59 (71%)	19 (23%)	5 (6%)	1	4
20	CT	83/85 (98%)	62 (75%)	12 (14%)	9 (11%)	0	1
21	AU	49/51 (96%)	26 (53%)	8 (16%)	15 (31%)	0	0
21	CU	49/51 (96%)	21 (43%)	16 (33%)	12 (24%)	0	0
24	BC	269/271 (99%)	218 (81%)	39 (14%)	12 (4%)	2	8
24	DC	269/271 (99%)	196 (73%)	48 (18%)	25 (9%)	0	1
25	BD	207/209 (99%)	180 (87%)	21 (10%)	6 (3%)	4	15
25	DD	207/209 (99%)	153 (74%)	43 (21%)	11 (5%)	2	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BE	199/201 (99%)	165 (83%)	30 (15%)	4 (2%)	7	24
26	DE	199/201 (99%)	154 (77%)	27 (14%)	18 (9%)	1	1
27	BF	175/177 (99%)	142 (81%)	24 (14%)	9 (5%)	2	6
27	DF	175/177 (99%)	135 (77%)	27 (15%)	13 (7%)	1	2
28	BG	174/176 (99%)	148 (85%)	16 (9%)	10 (6%)	1	5
28	DG	174/176 (99%)	127 (73%)	36 (21%)	11 (6%)	1	3
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	0
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	0	1
30	BI	139/141 (99%)	78 (56%)	37 (27%)	24 (17%)	0	0
30	DI	139/141 (99%)	82 (59%)	38 (27%)	19 (14%)	0	0
31	BJ	140/142 (99%)	125 (89%)	14 (10%)	1 (1%)	22	53
31	DJ	140/142 (99%)	104 (74%)	23 (16%)	13 (9%)	0	1
32	BK	120/122 (98%)	97 (81%)	14 (12%)	9 (8%)	1	2
32	DK	120/122 (98%)	95 (79%)	15 (12%)	10 (8%)	1	2
33	BL	141/143 (99%)	112 (79%)	21 (15%)	8 (6%)	1	5
33	DL	141/143 (99%)	98 (70%)	31 (22%)	12 (8%)	1	1
34	BM	134/136 (98%)	120 (90%)	11 (8%)	3 (2%)	6	22
34	DM	134/136 (98%)	112 (84%)	17 (13%)	5 (4%)	3	11
35	BN	118/120 (98%)	95 (80%)	21 (18%)	2 (2%)	9	29
35	DN	118/120 (98%)	90 (76%)	18 (15%)	10 (8%)	1	1
36	BO	114/116 (98%)	96 (84%)	14 (12%)	4 (4%)	3	12
36	DO	114/116 (98%)	82 (72%)	24 (21%)	8 (7%)	1	3
37	BP	112/114 (98%)	99 (88%)	8 (7%)	5 (4%)	2	8
37	DP	112/114 (98%)	88 (79%)	18 (16%)	6 (5%)	2	5
38	BQ	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	17	46
38	DQ	115/117 (98%)	92 (80%)	22 (19%)	1 (1%)	17	46
39	BR	101/103 (98%)	81 (80%)	10 (10%)	10 (10%)	0	1
39	DR	101/103 (98%)	72 (71%)	23 (23%)	6 (6%)	1	4
40	BS	108/110 (98%)	94 (87%)	10 (9%)	4 (4%)	3	11
40	DS	108/110 (98%)	83 (77%)	17 (16%)	8 (7%)	1	2
41	BT	91/93 (98%)	74 (81%)	9 (10%)	8 (9%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	DT	91/93 (98%)	53 (58%)	28 (31%)	10 (11%)	0	1
42	BU	100/102 (98%)	77 (77%)	19 (19%)	4 (4%)	3	9
42	DU	100/102 (98%)	69 (69%)	19 (19%)	12 (12%)	0	1
43	BV	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	14	41
43	DV	92/94 (98%)	76 (83%)	14 (15%)	2 (2%)	6	22
44	BW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	5	17
44	DW	73/76 (96%)	61 (84%)	12 (16%)	0	100	100
45	BX	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	12	36
45	DX	75/77 (97%)	58 (77%)	12 (16%)	5 (7%)	1	3
46	BY	61/63 (97%)	43 (70%)	10 (16%)	8 (13%)	0	1
46	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	2
47	BZ	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
47	DZ	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	1	1
48	B0	54/56 (96%)	46 (85%)	4 (7%)	4 (7%)	1	2
48	D0	54/56 (96%)	37 (68%)	12 (22%)	5 (9%)	0	1
49	B1	48/50 (96%)	40 (83%)	4 (8%)	4 (8%)	1	2
49	D1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	2
50	B2	44/46 (96%)	37 (84%)	5 (11%)	2 (4%)	2	8
50	D2	44/46 (96%)	34 (77%)	6 (14%)	4 (9%)	1	1
51	B3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	9	31
51	D3	62/64 (97%)	52 (84%)	6 (10%)	4 (6%)	1	3
52	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	17
52	D4	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2	5
53	B5	183/228 (80%)	87 (48%)	53 (29%)	43 (24%)	0	0
54	B6	2/8 (25%)	2 (100%)	0	0	100	100
54	D6	2/8 (25%)	0	2 (100%)	0	100	100
All	All	11422/11688 (98%)	8528 (75%)	1918 (17%)	976 (8%)	1	1

5 of 976 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	20	THR

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Mol	Chain	Res	Type
2	AB	22	TYR
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%)	132 (73%)	48 (27%)	0	1
2	CB	180/180 (100%)	130 (72%)	50 (28%)	0	1
3	AC	170/170 (100%)	135 (79%)	35 (21%)	1	3
3	CC	170/170 (100%)	144 (85%)	26 (15%)	2	8
4	AD	172/172 (100%)	139 (81%)	33 (19%)	1	4
4	CD	172/172 (100%)	143 (83%)	29 (17%)	2	6
5	AE	113/113 (100%)	84 (74%)	29 (26%)	0	1
5	CE	113/113 (100%)	86 (76%)	27 (24%)	0	2
6	AF	87/87 (100%)	69 (79%)	18 (21%)	1	3
6	CF	87/87 (100%)	61 (70%)	26 (30%)	0	1
7	AG	124/124 (100%)	101 (82%)	23 (18%)	1	5
7	CG	124/124 (100%)	99 (80%)	25 (20%)	1	4
8	AH	104/104 (100%)	84 (81%)	20 (19%)	1	4
8	CH	104/104 (100%)	82 (79%)	22 (21%)	1	3
9	AI	105/105 (100%)	77 (73%)	28 (27%)	0	1
9	CI	105/105 (100%)	88 (84%)	17 (16%)	2	7
10	AJ	86/86 (100%)	67 (78%)	19 (22%)	1	3
10	CJ	86/86 (100%)	68 (79%)	18 (21%)	1	3
11	AK	90/90 (100%)	76 (84%)	14 (16%)	2	8
11	CK	90/90 (100%)	71 (79%)	19 (21%)	1	3
12	AL	103/103 (100%)	89 (86%)	14 (14%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	103/103 (100%)	82 (80%)	21 (20%)	1	4
13	AM	92/92 (100%)	74 (80%)	18 (20%)	1	4
13	CM	92/92 (100%)	75 (82%)	17 (18%)	1	5
14	AN	79/83 (95%)	64 (81%)	15 (19%)	1	4
14	CN	79/83 (95%)	70 (89%)	9 (11%)	5	18
15	AO	75/76 (99%)	63 (84%)	12 (16%)	2	7
15	CO	75/76 (99%)	65 (87%)	10 (13%)	4	12
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	2
16	CP	65/65 (100%)	54 (83%)	11 (17%)	2	6
17	AQ	74/74 (100%)	50 (68%)	24 (32%)	0	0
17	CQ	74/74 (100%)	51 (69%)	23 (31%)	0	0
18	AR	48/48 (100%)	38 (79%)	10 (21%)	1	3
18	CR	48/48 (100%)	38 (79%)	10 (21%)	1	3
19	AS	70/70 (100%)	55 (79%)	15 (21%)	1	3
19	CS	70/70 (100%)	58 (83%)	12 (17%)	2	6
20	AT	65/65 (100%)	51 (78%)	14 (22%)	1	3
20	CT	65/65 (100%)	57 (88%)	8 (12%)	4	15
21	AU	44/44 (100%)	29 (66%)	15 (34%)	0	0
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0	0
24	BC	216/216 (100%)	189 (88%)	27 (12%)	4	14
24	DC	216/216 (100%)	197 (91%)	19 (9%)	10	29
25	BD	164/164 (100%)	148 (90%)	16 (10%)	8	24
25	DD	164/164 (100%)	145 (88%)	19 (12%)	5	17
26	BE	165/165 (100%)	136 (82%)	29 (18%)	2	5
26	DE	165/165 (100%)	137 (83%)	28 (17%)	2	6
27	BF	148/148 (100%)	116 (78%)	32 (22%)	1	3
27	DF	148/148 (100%)	119 (80%)	29 (20%)	1	4
28	BG	137/137 (100%)	118 (86%)	19 (14%)	3	11
28	DG	137/137 (100%)	114 (83%)	23 (17%)	2	6
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	2
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BI	109/109 (100%)	82 (75%)	27 (25%)	0	2
30	DI	109/109 (100%)	80 (73%)	29 (27%)	0	1
31	BJ	116/116 (100%)	105 (90%)	11 (10%)	8	25
31	DJ	116/116 (100%)	94 (81%)	22 (19%)	1	4
32	BK	103/103 (100%)	89 (86%)	14 (14%)	3	11
32	DK	103/103 (100%)	90 (87%)	13 (13%)	4	14
33	BL	102/102 (100%)	91 (89%)	11 (11%)	6	19
33	DL	102/102 (100%)	86 (84%)	16 (16%)	2	8
34	BM	109/109 (100%)	99 (91%)	10 (9%)	9	27
34	DM	109/109 (100%)	95 (87%)	14 (13%)	4	13
35	BN	100/100 (100%)	94 (94%)	6 (6%)	19	48
35	DN	100/100 (100%)	76 (76%)	24 (24%)	0	2
36	BO	86/86 (100%)	65 (76%)	21 (24%)	0	2
36	DO	86/86 (100%)	70 (81%)	16 (19%)	1	5
37	BP	99/99 (100%)	81 (82%)	18 (18%)	1	5
37	DP	99/99 (100%)	90 (91%)	9 (9%)	9	27
38	BQ	89/89 (100%)	78 (88%)	11 (12%)	4	14
38	DQ	89/89 (100%)	78 (88%)	11 (12%)	4	14
39	BR	84/84 (100%)	74 (88%)	10 (12%)	5	16
39	DR	84/84 (100%)	76 (90%)	8 (10%)	8	25
40	BS	93/93 (100%)	76 (82%)	17 (18%)	1	5
40	DS	93/93 (100%)	83 (89%)	10 (11%)	6	19
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	9
41	DT	80/80 (100%)	66 (82%)	14 (18%)	2	6
42	BU	83/83 (100%)	72 (87%)	11 (13%)	4	12
42	DU	83/83 (100%)	68 (82%)	15 (18%)	1	5
43	BV	78/78 (100%)	63 (81%)	15 (19%)	1	4
43	DV	78/78 (100%)	65 (83%)	13 (17%)	2	6
44	BW	57/58 (98%)	47 (82%)	10 (18%)	2	6
44	DW	56/58 (97%)	50 (89%)	6 (11%)	6	20
45	BX	67/67 (100%)	61 (91%)	6 (9%)	9	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DX	67/67 (100%)	58 (87%)	9 (13%)	4	12
46	BY	55/55 (100%)	50 (91%)	5 (9%)	9	27
46	DY	55/55 (100%)	43 (78%)	12 (22%)	1	3
47	BZ	48/48 (100%)	41 (85%)	7 (15%)	3	9
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	3
48	B0	47/47 (100%)	42 (89%)	5 (11%)	6	20
48	D0	47/47 (100%)	43 (92%)	4 (8%)	10	31
49	B1	45/45 (100%)	42 (93%)	3 (7%)	16	43
49	D1	45/45 (100%)	39 (87%)	6 (13%)	4	12
50	B2	38/38 (100%)	34 (90%)	4 (10%)	7	20
50	D2	38/38 (100%)	31 (82%)	7 (18%)	1	5
51	B3	51/51 (100%)	45 (88%)	6 (12%)	5	16
51	D3	51/51 (100%)	46 (90%)	5 (10%)	8	24
52	B4	34/34 (100%)	32 (94%)	2 (6%)	19	49
52	D4	34/34 (100%)	26 (76%)	8 (24%)	1	2
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1	3
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%)	7747 (82%)	1643 (18%)	2	6

5 of 1643 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	CD	200	ILE
16	CP	55	ASP
46	DY	49	ASP
5	CE	153	VAL
4	CD	192	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
24	DC	251	GLN
39	DR	89	HIS
25	DD	140	HIS

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Mol	Chain	Res	Type
29	DH	128	HIS
42	DU	74	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	324 (21%)	11 (0%)
1	CA	1538/1539 (99%)	342 (22%)	10 (0%)
22	BA	2895/2903 (99%)	579 (20%)	24 (0%)
22	DA	2895/2903 (99%)	704 (24%)	32 (1%)
23	BB	118/119 (99%)	16 (13%)	0
23	DB	117/119 (98%)	20 (17%)	0
All	All	9100/9122 (99%)	1985 (21%)	77 (0%)

5 of 1985 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	3	A
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	DA	1514	G
22	DA	2326	C
22	DA	1847	A
22	DA	2157	G
22	DA	2756	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	D6	1	54	9,9,10	1.95	1 (11%)	10,11,13	3.07	4 (40%)
54	MHV	D6	6	54	7,9,10	1.19	0	7,11,13	3.21	4 (57%)
54	MHW	B6	1	54	9,9,10	1.64	1 (11%)	10,11,13	2.86	4 (40%)
54	004	B6	7	54	9,10,11	1.52	1 (11%)	9,12,14	2.03	3 (33%)
54	DBB	B6	3	54	4,5,6	1.31	0	1,5,7	2.61	1 (100%)
54	MHU	B6	5	54	14,15,16	1.80	3 (21%)	18,19,21	1.27	3 (16%)
54	MHV	B6	6	54	7,9,10	1.59	1 (14%)	7,11,13	3.44	4 (57%)
54	MHU	D6	5	54	14,15,16	1.63	3 (21%)	18,19,21	1.15	2 (11%)
54	DBB	D6	3	54	4,5,6	1.18	0	1,5,7	1.37	0
54	004	D6	7	54	9,10,11	0.78	0	9,12,14	0.60	0

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	D6	1	54	-	0/2/2/4	0/1/1/1
54	MHV	D6	6	54	-	0/1/12/14	0/1/1/1
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	004	B6	7	54	-	1/4/6/8	0/1/1/1
54	DBB	B6	3	54	-	1/3/4/6	-
54	MHU	B6	5	54	-	0/9/12/14	0/1/1/1
54	MHV	B6	6	54	-	0/1/12/14	0/1/1/1
54	MHU	D6	5	54	-	0/9/12/14	0/1/1/1
54	DBB	D6	3	54	-	0/3/4/6	-
54	004	D6	7	54	-	2/4/6/8	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	1	MHW	CA-C	5.22	1.54	1.48
54	B6	5	MHU	CZ-NZ	5.22	1.49	1.37
54	D6	5	MHU	CZ-NZ	4.69	1.48	1.37
54	B6	7	004	CB-CA	-4.30	1.48	1.52
54	B6	1	MHW	CA-C	3.99	1.52	1.48

The worst 5 of 25 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	1	MHW	CD-CE-N	6.55	134.13	123.43
54	B6	1	MHW	CD-CE-N	5.89	133.04	123.43
54	B6	6	MHV	CD2-CG-CB	5.52	124.11	115.89
54	D6	6	MHV	CD2-CE-N	-5.22	98.62	110.03
54	D6	6	MHV	CD2-CG-CB	5.13	123.53	115.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	B6	3	DBB	N-CA-CB-CG
54	D6	7	004	C-CA-CB-CG1
54	D6	7	004	C-CA-CB-CG2
54	B6	7	004	C-CA-CB-CG1

There are no ring outliers.

6 monomers are involved in 11 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	DOL	BA	3001	-	43,50,50	2.86	13 (30%)	51,70,70	2.88	14 (27%)
56	DOL	DA	3001	-	43,50,50	2.90	13 (30%)	51,70,70	2.81	13 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	DOL	BA	3001	-	-	18/58/77/77	0/2/3/3
56	DOL	DA	3001	-	-	10/58/77/77	0/2/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DA	3001	DOL	O15-C14	9.27	1.37	1.21
56	BA	3001	DOL	O15-C14	8.90	1.36	1.21
56	DA	3001	DOL	C22-C23	8.04	1.53	1.32
56	BA	3001	DOL	C22-C23	7.76	1.52	1.32
56	DA	3001	DOL	O38-C37	6.42	1.37	1.21

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DA	3001	DOL	O40-S39-O41	-15.45	100.57	118.19
56	BA	3001	DOL	O40-S39-O41	-14.66	101.47	118.19
56	BA	3001	DOL	C8-C6-N5	6.55	127.31	119.76
56	BA	3001	DOL	C29-C28-C26	-5.90	107.93	122.69
56	DA	3001	DOL	C4-N5-C1	-5.06	106.22	112.45

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

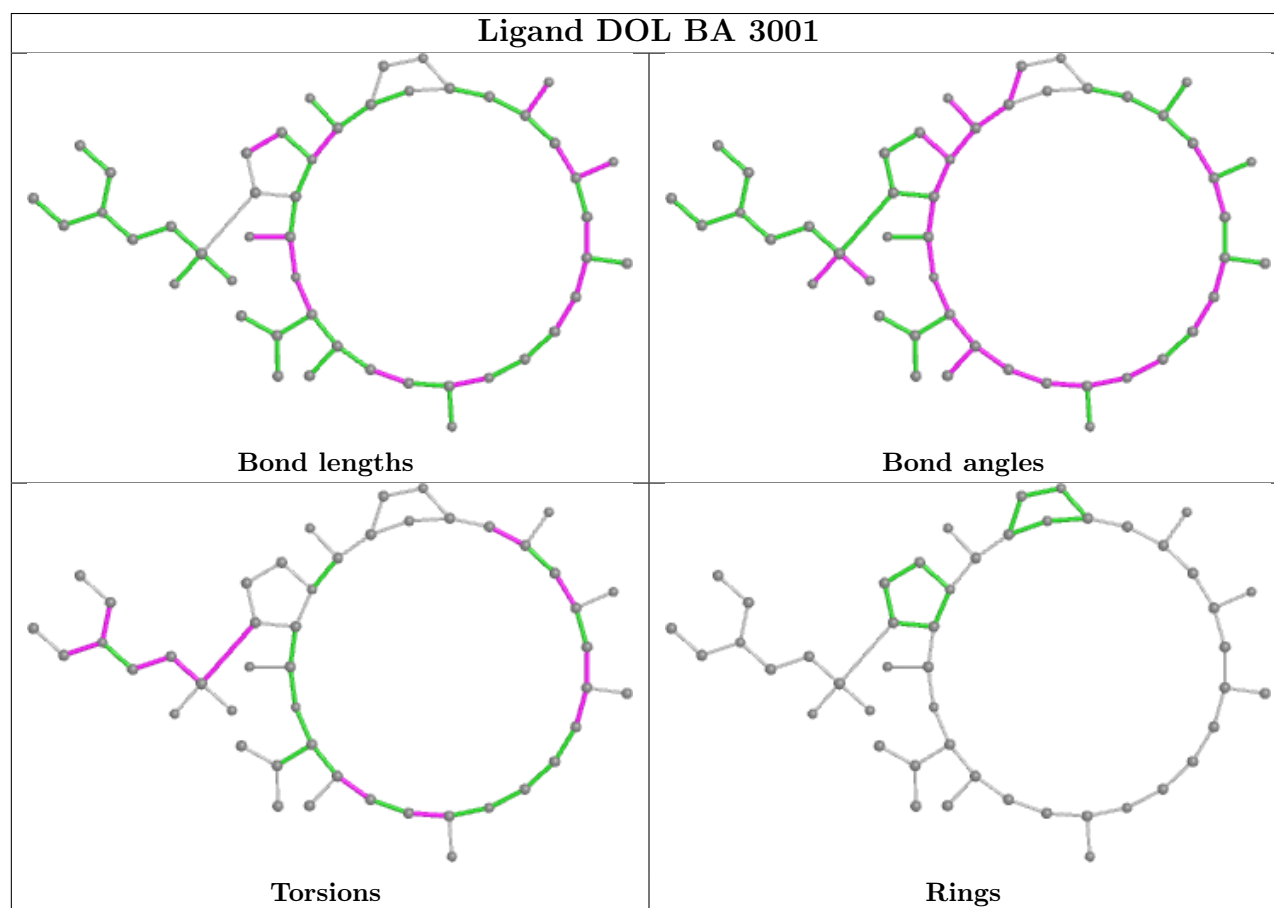
Mol	Chain	Res	Type	Atoms
56	BA	3001	DOL	C1-C2-S39-O40
56	BA	3001	DOL	C1-C2-S39-C42
56	BA	3001	DOL	S39-C42-C43-N44
56	BA	3001	DOL	C14-C16-C17-O18
56	BA	3001	DOL	C17-C19-C20-C22

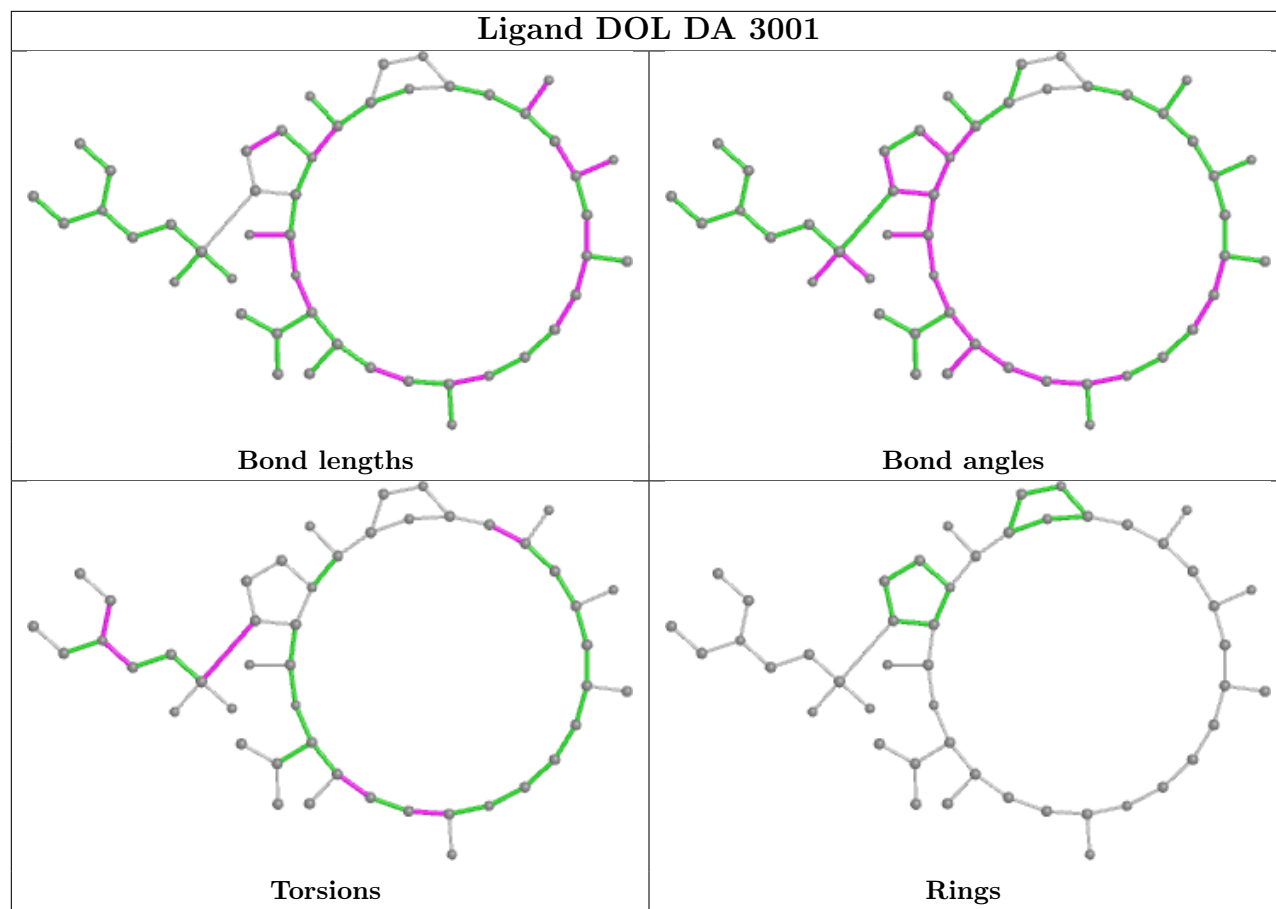
There are no ring outliers.

2 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BA	3001	DOL	15	0
56	DA	3001	DOL	25	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1538/1539 (99%)	-0.16	22 (1%) 75 70	10, 49, 132, 182	0
1	CA	1539/1539 (100%)	0.16	55 (3%) 42 32	22, 70, 146, 178	0
2	AB	218/218 (100%)	0.80	29 (13%) 3 2	36, 73, 100, 117	0
2	CB	218/218 (100%)	1.05	45 (20%) 1 0	57, 86, 108, 121	0
3	AC	206/206 (100%)	0.15	10 (4%) 29 20	33, 57, 78, 95	0
3	CC	206/206 (100%)	1.19	50 (24%) 0 0	55, 80, 96, 107	0
4	AD	205/205 (100%)	0.36	8 (3%) 39 29	31, 56, 79, 99	0
4	CD	205/205 (100%)	-0.03	5 (2%) 59 49	13, 35, 60, 82	0
5	AE	150/150 (100%)	0.10	2 (1%) 77 72	26, 47, 78, 93	0
5	CE	150/150 (100%)	0.18	1 (0%) 87 84	25, 52, 84, 104	0
6	AF	100/100 (100%)	-0.18	1 (1%) 82 77	32, 54, 73, 77	0
6	CF	100/100 (100%)	0.53	10 (10%) 7 4	41, 74, 92, 103	0
7	AG	151/151 (100%)	0.26	3 (1%) 65 56	51, 75, 92, 100	0
7	CG	151/151 (100%)	2.56	85 (56%) 0 0	82, 106, 114, 118	0
8	AH	129/129 (100%)	0.18	2 (1%) 72 66	29, 46, 67, 79	0
8	CH	129/129 (100%)	0.45	10 (7%) 13 7	46, 64, 80, 94	0
9	AI	127/127 (100%)	0.93	22 (17%) 1 1	40, 74, 98, 107	0
9	CI	127/127 (100%)	1.84	45 (35%) 0 0	79, 96, 112, 121	0
10	AJ	98/98 (100%)	0.64	7 (7%) 16 9	38, 66, 86, 116	0
10	CJ	98/98 (100%)	2.70	59 (60%) 0 0	72, 97, 115, 123	0
11	AK	117/117 (100%)	0.49	10 (8%) 10 5	25, 60, 89, 119	0
11	CK	117/117 (100%)	0.23	2 (1%) 70 63	35, 68, 79, 90	0
12	AL	123/123 (100%)	0.15	6 (4%) 29 20	20, 34, 65, 97	0
12	CL	123/123 (100%)	0.32	3 (2%) 59 49	30, 50, 74, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/114 (100%)	0.42	10 (8%) 10 5	47, 69, 91, 103	0
13	CM	114/114 (100%)	3.11	76 (66%) 0 0	93, 113, 122, 125	0
14	AN	96/100 (96%)	0.67	11 (11%) 4 2	36, 60, 96, 105	0
14	CN	96/100 (96%)	2.16	44 (45%) 0 0	70, 96, 115, 122	0
15	AO	88/88 (100%)	0.35	3 (3%) 45 35	29, 47, 64, 91	0
15	CO	88/88 (100%)	0.32	3 (3%) 45 35	36, 64, 80, 102	0
16	AP	82/82 (100%)	0.69	6 (7%) 15 8	34, 47, 83, 109	0
16	CP	82/82 (100%)	0.98	11 (13%) 3 1	45, 62, 91, 112	0
17	AQ	80/80 (100%)	0.26	3 (3%) 40 30	27, 48, 75, 111	0
17	CQ	80/80 (100%)	1.14	19 (23%) 0 0	42, 77, 97, 99	0
18	AR	55/55 (100%)	0.22	3 (5%) 25 16	40, 52, 77, 102	0
18	CR	55/55 (100%)	0.28	4 (7%) 15 8	36, 54, 78, 108	0
19	AS	79/79 (100%)	0.70	13 (16%) 1 1	54, 70, 88, 97	0
19	CS	79/79 (100%)	3.96	58 (73%) 0 0	95, 114, 122, 128	0
20	AT	85/85 (100%)	0.43	4 (4%) 31 22	35, 48, 68, 96	0
20	CT	85/85 (100%)	1.81	33 (38%) 0 0	53, 78, 96, 101	0
21	AU	51/51 (100%)	1.26	12 (23%) 0 0	41, 74, 95, 105	0
21	CU	51/51 (100%)	0.68	6 (11%) 4 2	42, 69, 98, 102	0
22	BA	2897/2903 (99%)	0.14	106 (3%) 41 31	0, 14, 129, 195	0
22	DA	2897/2903 (99%)	0.40	129 (4%) 33 23	41, 85, 148, 181	0
23	BB	119/119 (100%)	-0.36	0 100 100	2, 23, 46, 81	0
23	DB	118/119 (99%)	0.19	4 (3%) 45 35	69, 115, 134, 142	0
24	BC	271/271 (100%)	-0.18	1 (0%) 92 91	2, 18, 35, 55	0
24	DC	271/271 (100%)	0.73	32 (11%) 4 2	46, 64, 77, 95	0
25	BD	209/209 (100%)	-0.25	0 100 100	0, 9, 34, 65	0
25	DD	209/209 (100%)	1.16	44 (21%) 1 0	53, 72, 87, 97	0
26	BE	201/201 (100%)	-0.30	0 100 100	1, 23, 54, 88	0
26	DE	201/201 (100%)	1.86	80 (39%) 0 0	52, 89, 105, 113	0
27	BF	177/177 (100%)	0.19	4 (2%) 60 51	21, 40, 74, 88	0
27	DF	177/177 (100%)	3.27	128 (72%) 0 0	94, 113, 124, 131	0
28	BG	176/176 (100%)	0.04	3 (1%) 70 63	15, 35, 58, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DG	176/176 (100%)	2.22	89 (50%) 0 0	78, 96, 110, 121	0
29	BH	149/149 (100%)	3.01	73 (48%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.18	30 (20%) 1 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.56	100 (70%) 0 0	89, 116, 126, 134	0
30	DI	141/141 (100%)	4.83	120 (85%) 0 0	105, 124, 135, 142	0
31	BJ	142/142 (100%)	-0.27	0 100 100	1, 6, 26, 35	0
31	DJ	142/142 (100%)	0.84	16 (11%) 5 3	49, 69, 83, 91	0
32	BK	122/122 (100%)	-0.34	0 100 100	3, 11, 28, 60	0
32	DK	122/122 (100%)	1.12	29 (23%) 0 0	48, 66, 84, 95	0
33	BL	143/143 (100%)	-0.13	0 100 100	1, 18, 42, 65	0
33	DL	143/143 (100%)	1.95	62 (43%) 0 0	43, 87, 98, 115	0
34	BM	136/136 (100%)	-0.38	0 100 100	1, 10, 24, 85	0
34	DM	136/136 (100%)	1.01	26 (19%) 1 1	44, 70, 85, 99	0
35	BN	120/120 (100%)	-0.25	0 100 100	2, 7, 17, 65	0
35	DN	120/120 (100%)	1.29	28 (23%) 0 0	58, 78, 92, 112	0
36	BO	116/116 (100%)	-0.21	0 100 100	14, 24, 42, 54	0
36	DO	116/116 (100%)	2.77	75 (64%) 0 0	85, 99, 110, 117	0
37	BP	114/114 (100%)	-0.22	1 (0%) 84 80	6, 16, 41, 71	0
37	DP	114/114 (100%)	1.07	27 (23%) 0 0	61, 74, 86, 94	0
38	BQ	117/117 (100%)	-0.31	0 100 100	0, 3, 12, 30	0
38	DQ	117/117 (100%)	1.15	25 (21%) 0 0	55, 70, 81, 89	0
39	BR	103/103 (100%)	-0.29	0 100 100	0, 11, 31, 56	0
39	DR	103/103 (100%)	1.66	35 (33%) 0 0	57, 80, 92, 103	0
40	BS	110/110 (100%)	-0.22	0 100 100	1, 4, 21, 68	0
40	DS	110/110 (100%)	2.12	53 (48%) 0 0	60, 79, 94, 105	0
41	BT	93/93 (100%)	0.19	3 (3%) 47 37	10, 24, 68, 98	0
41	DT	93/93 (100%)	2.71	57 (61%) 0 0	73, 91, 106, 115	0
42	BU	102/102 (100%)	-0.22	2 (1%) 65 56	10, 25, 58, 77	0
42	DU	102/102 (100%)	3.20	65 (63%) 0 0	77, 95, 109, 120	0
43	BV	94/94 (100%)	-0.27	0 100 100	4, 18, 39, 52	0
43	DV	94/94 (100%)	1.14	21 (22%) 0 0	72, 86, 98, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BW	76/76 (100%)	-0.15	2 (2%) 56 46	4, 11, 27, 57	0
44	DW	75/76 (98%)	2.04	39 (52%) 0 0	58, 83, 93, 104	0
45	BX	77/77 (100%)	-0.24	0 100 100	8, 22, 48, 68	0
45	DX	77/77 (100%)	1.11	15 (19%) 1 0	47, 72, 87, 91	0
46	BY	63/63 (100%)	0.23	3 (4%) 30 21	18, 38, 71, 94	0
46	DY	63/63 (100%)	1.95	30 (47%) 0 0	81, 99, 106, 109	0
47	BZ	58/58 (100%)	-0.22	0 100 100	2, 6, 25, 34	0
47	DZ	58/58 (100%)	0.83	7 (12%) 4 2	60, 73, 85, 103	0
48	B0	56/56 (100%)	-0.30	0 100 100	0, 7, 33, 60	0
48	D0	56/56 (100%)	1.49	17 (30%) 0 0	51, 82, 95, 103	0
49	B1	50/50 (100%)	-0.23	1 (2%) 65 56	13, 25, 49, 57	0
49	D1	50/50 (100%)	1.73	15 (30%) 0 0	73, 89, 94, 106	0
50	B2	46/46 (100%)	-0.14	1 (2%) 62 52	4, 8, 15, 79	0
50	D2	46/46 (100%)	1.94	19 (41%) 0 0	58, 72, 86, 101	0
51	B3	64/64 (100%)	-0.18	0 100 100	4, 9, 17, 29	0
51	D3	64/64 (100%)	1.69	26 (40%) 0 0	60, 75, 84, 94	0
52	B4	38/38 (100%)	-0.13	0 100 100	5, 15, 29, 52	0
52	D4	38/38 (100%)	2.23	18 (47%) 0 0	62, 77, 88, 98	0
53	B5	191/228 (83%)	6.24	186 (97%) 0 0	100, 121, 133, 141	0
54	B6	2/8 (25%)	0.45	0 100 100	1, 1, 1, 1	0
54	D6	2/8 (25%)	-0.02	0 100 100	46, 46, 46, 51	0
All	All	20738/20810 (99%)	0.62	2658 (12%) 3 2	0, 63, 124, 195	0

The worst 5 of 2658 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	25.2
53	B5	55	SER	19.9
22	BA	2101	A	17.4
22	BA	2184	A	17.4
53	B5	207	GLY	16.3



## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MHW	D6	1	9/10	0.87	0.20	40,52,59,59	0
54	DBB	D6	3	6/7	0.91	0.30	36,38,47,51	0
54	MHU	D6	5	15/16	0.92	0.32	44,54,60,61	0
54	MHW	B6	1	9/10	0.94	0.18	0,0,2,9	0
54	MHV	D6	6	9/10	0.94	0.14	45,51,58,60	0
54	004	D6	7	10/11	0.94	0.21	42,47,58,59	0
54	MHU	B6	5	15/16	0.96	0.20	0,0,1,2	0
54	DBB	B6	3	6/7	0.96	0.19	0,1,1,2	0
54	004	B6	7	10/11	0.97	0.23	0,0,2,3	0
54	MHV	B6	6	9/10	0.97	0.16	0,0,1,1	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3111	1/1	0.18	0.32	107,107,107,107	0
55	MG	DA	3048	1/1	0.20	0.44	127,127,127,127	0
55	MG	DA	3135	1/1	0.24	0.32	101,101,101,101	0
55	MG	DA	3084	1/1	0.35	0.23	105,105,105,105	0
55	MG	DA	3100	1/1	0.36	0.20	77,77,77,77	0
55	MG	DA	3041	1/1	0.38	0.42	68,68,68,68	0
55	MG	DA	3017	1/1	0.38	0.25	98,98,98,98	0
55	MG	DA	3026	1/1	0.43	0.48	101,101,101,101	0
55	MG	DA	3093	1/1	0.46	0.11	86,86,86,86	0
55	MG	BA	3134	1/1	0.46	0.42	54,54,54,54	0
55	MG	CA	1630	1/1	0.48	0.36	120,120,120,120	0
55	MG	AA	1619	1/1	0.50	0.31	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3062	1/1	0.51	0.61	82,82,82,82	0
55	MG	CA	1636	1/1	0.51	0.14	126,126,126,126	0
55	MG	DA	3148	1/1	0.51	0.29	65,65,65,65	0
55	MG	DA	3113	1/1	0.52	0.29	66,66,66,66	0
55	MG	DA	3144	1/1	0.52	0.10	68,68,68,68	0
55	MG	DA	3133	1/1	0.52	0.78	100,100,100,100	0
55	MG	DA	3045	1/1	0.53	0.12	94,94,94,94	0
55	MG	DA	3042	1/1	0.54	0.19	87,87,87,87	0
55	MG	DA	3057	1/1	0.54	0.29	95,95,95,95	0
55	MG	CA	1635	1/1	0.54	0.13	124,124,124,124	0
55	MG	BA	3090	1/1	0.55	0.10	19,19,19,19	0
55	MG	DA	3099	1/1	0.57	0.38	86,86,86,86	0
55	MG	DA	3075	1/1	0.57	0.16	91,91,91,91	0
55	MG	DA	3067	1/1	0.59	0.13	58,58,58,58	0
55	MG	DA	3029	1/1	0.59	0.22	73,73,73,73	0
55	MG	BA	3100	1/1	0.60	0.28	52,52,52,52	0
55	MG	DA	3028	1/1	0.61	0.87	103,103,103,103	0
55	MG	CA	1627	1/1	0.61	0.20	89,89,89,89	0
55	MG	AA	1614	1/1	0.61	0.22	69,69,69,69	0
55	MG	CA	1608	1/1	0.61	0.22	84,84,84,84	0
55	MG	DA	3027	1/1	0.62	0.17	91,91,91,91	0
55	MG	DA	3071	1/1	0.63	0.49	92,92,92,92	0
55	MG	CA	1606	1/1	0.64	0.19	89,89,89,89	0
55	MG	DA	3002	1/1	0.64	0.10	78,78,78,78	0
55	MG	DA	3127	1/1	0.64	0.15	71,71,71,71	0
55	MG	DA	3131	1/1	0.64	1.04	99,99,99,99	0
55	MG	DA	3090	1/1	0.65	0.14	90,90,90,90	0
55	MG	DA	3070	1/1	0.65	0.17	108,108,108,108	0
55	MG	DA	3010	1/1	0.65	0.12	80,80,80,80	0
55	MG	D2	101	1/1	0.65	0.15	83,83,83,83	0
55	MG	CA	1629	1/1	0.66	0.12	91,91,91,91	0
55	MG	DA	3126	1/1	0.67	0.23	80,80,80,80	0
55	MG	AA	1658	1/1	0.67	0.35	62,62,62,62	0
55	MG	AA	1665	1/1	0.67	0.40	37,37,37,37	0
55	MG	AA	1639	1/1	0.67	0.07	65,65,65,65	0
55	MG	DA	3078	1/1	0.68	0.14	106,106,106,106	0
55	MG	CA	1632	1/1	0.69	0.12	73,73,73,73	0
55	MG	DA	3077	1/1	0.69	0.70	113,113,113,113	0
55	MG	DA	3019	1/1	0.69	0.18	107,107,107,107	0
55	MG	DA	3034	1/1	0.69	0.16	69,69,69,69	0
55	MG	DQ	201	1/1	0.69	0.30	45,45,45,45	0
55	MG	DA	3103	1/1	0.69	0.24	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3044	1/1	0.70	0.40	112,112,112,112	0
55	MG	DA	3155	1/1	0.71	0.45	62,62,62,62	0
55	MG	CA	1602	1/1	0.72	0.11	88,88,88,88	0
55	MG	DA	3088	1/1	0.72	0.10	74,74,74,74	0
55	MG	DA	3060	1/1	0.72	0.31	77,77,77,77	0
55	MG	DA	3012	1/1	0.72	0.10	73,73,73,73	0
55	MG	DA	3098	1/1	0.72	0.16	66,66,66,66	0
55	MG	AA	1620	1/1	0.73	0.12	69,69,69,69	0
55	MG	DA	3134	1/1	0.73	0.14	58,58,58,58	0
55	MG	DB	201	1/1	0.73	0.06	116,116,116,116	0
55	MG	DA	3064	1/1	0.73	0.20	48,48,48,48	0
55	MG	DA	3013	1/1	0.73	0.16	44,44,44,44	0
55	MG	AA	1648	1/1	0.74	0.20	47,47,47,47	0
55	MG	CA	1631	1/1	0.74	0.13	95,95,95,95	0
55	MG	DA	3136	1/1	0.74	0.16	91,91,91,91	0
55	MG	BA	3050	1/1	0.74	0.07	27,27,27,27	0
55	MG	DA	3147	1/1	0.74	0.39	54,54,54,54	0
55	MG	DA	3005	1/1	0.75	0.43	102,102,102,102	0
55	MG	BA	3186	1/1	0.75	0.30	29,29,29,29	0
55	MG	CA	1617	1/1	0.76	0.12	39,39,39,39	0
55	MG	BA	3093	1/1	0.76	0.09	58,58,58,58	0
55	MG	DA	3037	1/1	0.76	0.08	93,93,93,93	0
55	MG	AA	1651	1/1	0.76	0.32	61,61,61,61	0
55	MG	CA	1605	1/1	0.76	0.19	86,86,86,86	0
55	MG	BA	3049	1/1	0.76	0.13	44,44,44,44	0
55	MG	BA	3153	1/1	0.76	0.23	31,31,31,31	0
55	MG	DA	3046	1/1	0.76	0.16	62,62,62,62	0
55	MG	DA	3072	1/1	0.76	0.52	90,90,90,90	0
55	MG	DA	3163	1/1	0.77	0.32	54,54,54,54	0
55	MG	DA	3125	1/1	0.77	0.22	62,62,62,62	0
55	MG	AA	1626	1/1	0.77	0.17	23,23,23,23	0
55	MG	BA	3038	1/1	0.77	0.16	42,42,42,42	0
55	MG	DA	3107	1/1	0.78	0.16	75,75,75,75	0
55	MG	BA	3167	1/1	0.78	0.18	25,25,25,25	0
55	MG	DA	3056	1/1	0.78	0.41	93,93,93,93	0
55	MG	DB	203	1/1	0.78	0.08	85,85,85,85	0
55	MG	DA	3121	1/1	0.78	0.10	52,52,52,52	0
55	MG	AA	1659	1/1	0.78	0.76	50,50,50,50	0
55	MG	AM	201	1/1	0.79	0.86	62,62,62,62	0
55	MG	AA	1652	1/1	0.79	0.19	49,49,49,49	0
55	MG	AA	1635	1/1	0.79	0.17	66,66,66,66	0
55	MG	AA	1667	1/1	0.79	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3057	1/1	0.79	0.35	73,73,73,73	0
55	MG	BA	3058	1/1	0.79	0.29	15,15,15,15	0
55	MG	DA	3108	1/1	0.79	0.17	59,59,59,59	0
55	MG	DA	3003	1/1	0.79	0.47	99,99,99,99	0
55	MG	BA	3077	1/1	0.79	0.17	8,8,8,8	0
55	MG	AA	1657	1/1	0.80	0.63	64,64,64,64	0
55	MG	DA	3152	1/1	0.80	0.29	52,52,52,52	0
55	MG	CA	1621	1/1	0.80	0.09	64,64,64,64	0
55	MG	DA	3115	1/1	0.80	0.19	111,111,111,111	0
55	MG	DA	3006	1/1	0.80	0.13	93,93,93,93	0
55	MG	AA	1662	1/1	0.80	0.38	57,57,57,57	0
55	MG	BA	3059	1/1	0.80	0.25	38,38,38,38	0
55	MG	CA	1609	1/1	0.80	0.15	89,89,89,89	0
55	MG	DA	3073	1/1	0.81	0.11	60,60,60,60	0
55	MG	DA	3097	1/1	0.81	0.25	91,91,91,91	0
55	MG	CA	1638	1/1	0.81	0.10	76,76,76,76	0
55	MG	DA	3149	1/1	0.81	0.29	35,35,35,35	0
55	MG	DA	3009	1/1	0.81	0.37	90,90,90,90	0
55	MG	DA	3022	1/1	0.81	0.10	52,52,52,52	0
55	MG	BA	3137	1/1	0.81	0.42	49,49,49,49	0
55	MG	BA	3103	1/1	0.81	0.17	0,0,0,0	0
55	MG	DA	3089	1/1	0.81	0.33	83,83,83,83	0
55	MG	AA	1601	1/1	0.81	0.09	58,58,58,58	0
55	MG	DA	3092	1/1	0.81	0.58	113,113,113,113	0
55	MG	BA	3075	1/1	0.82	0.16	29,29,29,29	0
55	MG	CA	1646	1/1	0.82	0.24	92,92,92,92	0
55	MG	BA	3119	1/1	0.82	0.07	20,20,20,20	0
55	MG	BA	3180	1/1	0.82	0.19	32,32,32,32	0
55	MG	BA	3146	1/1	0.82	0.19	30,30,30,30	0
55	MG	BA	3189	1/1	0.82	0.24	45,45,45,45	0
55	MG	DA	3120	1/1	0.82	0.11	79,79,79,79	0
55	MG	BA	3151	1/1	0.82	0.27	12,12,12,12	0
55	MG	CA	1626	1/1	0.82	0.08	48,48,48,48	0
55	MG	DA	3033	1/1	0.83	0.10	71,71,71,71	0
55	MG	DA	3129	1/1	0.83	0.18	45,45,45,45	0
55	MG	CA	1637	1/1	0.83	0.10	64,64,64,64	0
55	MG	DA	3114	1/1	0.83	0.14	65,65,65,65	0
55	MG	BA	3021	1/1	0.83	0.19	1,1,1,1	0
55	MG	DA	3038	1/1	0.83	0.13	63,63,63,63	0
55	MG	DA	3091	1/1	0.83	0.09	77,77,77,77	0
55	MG	DA	3040	1/1	0.83	0.18	83,83,83,83	0
55	MG	AA	1628	1/1	0.83	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3054	1/1	0.84	0.09	9,9,9,9	0
55	MG	BA	3089	1/1	0.84	0.07	33,33,33,33	0
55	MG	CA	1655	1/1	0.84	0.10	44,44,44,44	0
55	MG	DA	3016	1/1	0.84	0.14	62,62,62,62	0
55	MG	DA	3153	1/1	0.84	0.26	53,53,53,53	0
55	MG	AA	1644	1/1	0.84	0.39	44,44,44,44	0
55	MG	BA	3046	1/1	0.84	0.09	17,17,17,17	0
55	MG	DA	3094	1/1	0.84	0.18	84,84,84,84	0
55	MG	AA	1638	1/1	0.84	0.10	87,87,87,87	0
55	MG	CA	1603	1/1	0.84	0.15	44,44,44,44	0
55	MG	AA	1623	1/1	0.84	0.05	46,46,46,46	0
55	MG	DA	3047	1/1	0.85	0.13	73,73,73,73	0
55	MG	BA	3170	1/1	0.85	0.35	38,38,38,38	0
55	MG	BA	3016	1/1	0.85	0.43	58,58,58,58	0
55	MG	DA	3145	1/1	0.85	0.17	71,71,71,71	0
55	MG	DA	3119	1/1	0.85	0.44	106,106,106,106	0
55	MG	AA	1631	1/1	0.85	0.10	46,46,46,46	0
55	MG	BA	3069	1/1	0.85	0.15	4,4,4,4	0
55	MG	DA	3151	1/1	0.85	0.52	59,59,59,59	0
55	MG	DA	3124	1/1	0.85	0.23	89,89,89,89	0
55	MG	DA	3080	1/1	0.85	0.15	95,95,95,95	0
55	MG	DA	3154	1/1	0.85	0.17	40,40,40,40	0
55	MG	CA	1601	1/1	0.85	0.09	39,39,39,39	0
55	MG	BA	3120	1/1	0.85	0.20	37,37,37,37	0
55	MG	DA	3104	1/1	0.85	0.08	79,79,79,79	0
55	MG	CA	1624	1/1	0.85	0.10	45,45,45,45	0
55	MG	BA	3027	1/1	0.85	0.34	46,46,46,46	0
55	MG	CA	1604	1/1	0.85	0.13	95,95,95,95	0
55	MG	CA	1654	1/1	0.86	0.36	56,56,56,56	0
55	MG	BA	3104	1/1	0.86	0.17	17,17,17,17	0
55	MG	BA	3178	1/1	0.86	0.68	30,30,30,30	0
55	MG	AA	1605	1/1	0.86	0.22	23,23,23,23	0
55	MG	CA	1615	1/1	0.86	0.30	58,58,58,58	0
55	MG	DA	3039	1/1	0.86	0.18	57,57,57,57	0
55	MG	BA	3154	1/1	0.86	0.33	25,25,25,25	0
55	MG	DA	3157	1/1	0.86	0.30	58,58,58,58	0
55	MG	DA	3061	1/1	0.86	1.12	96,96,96,96	0
55	MG	DA	3143	1/1	0.86	0.24	60,60,60,60	0
55	MG	DA	3008	1/1	0.86	0.26	100,100,100,100	0
55	MG	AA	1612	1/1	0.86	0.10	47,47,47,47	0
55	MG	CA	1651	1/1	0.86	0.30	44,44,44,44	0
55	MG	DA	3024	1/1	0.87	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3025	1/1	0.87	0.26	69,69,69,69	0
55	MG	BB	202	1/1	0.87	0.10	16,16,16,16	0
55	MG	AA	1661	1/1	0.87	0.29	29,29,29,29	0
55	MG	DA	3081	1/1	0.87	0.10	60,60,60,60	0
55	MG	CA	1656	1/1	0.87	0.37	54,54,54,54	0
55	MG	AA	1613	1/1	0.87	0.09	24,24,24,24	0
55	MG	DA	3165	1/1	0.87	0.22	42,42,42,42	0
55	MG	CA	1628	1/1	0.87	0.18	98,98,98,98	0
55	MG	DB	202	1/1	0.87	0.11	66,66,66,66	0
55	MG	BA	3125	1/1	0.87	0.54	37,37,37,37	0
55	MG	AA	1671	1/1	0.87	0.52	59,59,59,59	0
55	MG	AA	1664	1/1	0.87	0.14	49,49,49,49	0
55	MG	DA	3112	1/1	0.88	1.38	104,104,104,104	0
55	MG	AA	1650	1/1	0.88	0.32	36,36,36,36	0
55	MG	DA	3036	1/1	0.88	0.15	62,62,62,62	0
55	MG	AA	1670	1/1	0.88	0.29	33,33,33,33	0
55	MG	BA	3102	1/1	0.88	0.10	7,7,7,7	0
55	MG	AA	1634	1/1	0.88	0.13	35,35,35,35	0
55	MG	AA	1643	1/1	0.88	0.14	28,28,28,28	0
55	MG	BA	3004	1/1	0.88	0.11	26,26,26,26	0
55	MG	BA	3082	1/1	0.88	0.11	6,6,6,6	0
55	MG	BA	3179	1/1	0.88	0.33	26,26,26,26	0
55	MG	AA	1609	1/1	0.88	0.08	36,36,36,36	0
55	MG	AA	1632	1/1	0.88	0.10	55,55,55,55	0
55	MG	DA	3160	1/1	0.88	0.24	43,43,43,43	0
55	MG	BA	3092	1/1	0.88	0.10	19,19,19,19	0
55	MG	DA	3132	1/1	0.88	0.18	54,54,54,54	0
55	MG	DA	3031	1/1	0.88	0.08	69,69,69,69	0
55	MG	DA	3049	1/1	0.88	0.25	84,84,84,84	0
55	MG	DA	3052	1/1	0.88	0.07	56,56,56,56	0
55	MG	BA	3141	1/1	0.88	0.15	17,17,17,17	0
55	MG	DA	3138	1/1	0.88	0.35	40,40,40,40	0
56	DOL	DA	3001	48/48	0.88	0.26	26,45,58,63	0
55	MG	DA	3020	1/1	0.89	0.15	54,54,54,54	0
55	MG	DA	3117	1/1	0.89	0.09	67,67,67,67	0
55	MG	AA	1630	1/1	0.89	0.18	73,73,73,73	0
55	MG	BA	3064	1/1	0.89	0.19	5,5,5,5	0
55	MG	BA	3114	1/1	0.89	0.17	0,0,0,0	0
55	MG	BA	3157	1/1	0.89	0.19	24,24,24,24	0
55	MG	AA	1637	1/1	0.89	0.10	15,15,15,15	0
55	MG	DA	3074	1/1	0.89	0.33	77,77,77,77	0
55	MG	BA	3191	1/1	0.89	0.23	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1649	1/1	0.89	0.18	52,52,52,52	0
55	MG	DA	3011	1/1	0.89	0.08	75,75,75,75	0
55	MG	CA	1650	1/1	0.89	0.22	35,35,35,35	0
55	MG	BA	3040	1/1	0.89	0.15	0,0,0,0	0
55	MG	DA	3110	1/1	0.89	0.23	33,33,33,33	0
55	MG	DA	3014	1/1	0.89	0.14	73,73,73,73	0
55	MG	BB	204	1/1	0.89	0.37	16,16,16,16	0
55	MG	DA	3137	1/1	0.89	0.42	47,47,47,47	0
55	MG	CA	1610	1/1	0.89	0.10	63,63,63,63	0
55	MG	DA	3141	1/1	0.89	0.27	40,40,40,40	0
55	MG	CA	1613	1/1	0.89	0.14	19,19,19,19	0
55	MG	AA	1660	1/1	0.90	0.22	51,51,51,51	0
55	MG	BA	3002	1/1	0.90	0.06	18,18,18,18	0
55	MG	DA	3146	1/1	0.90	0.10	43,43,43,43	0
55	MG	BA	3169	1/1	0.90	0.16	35,35,35,35	0
55	MG	DA	3066	1/1	0.90	0.07	47,47,47,47	0
55	MG	BA	3112	1/1	0.90	0.08	20,20,20,20	0
55	MG	DA	3069	1/1	0.90	0.09	79,79,79,79	0
55	MG	DA	3096	1/1	0.90	0.08	57,57,57,57	0
55	MG	BA	3171	1/1	0.90	0.20	24,24,24,24	0
55	MG	BA	3076	1/1	0.90	0.07	14,14,14,14	0
55	MG	DA	3007	1/1	0.90	0.44	121,121,121,121	0
55	MG	CA	1640	1/1	0.90	0.14	26,26,26,26	0
55	MG	BA	3051	1/1	0.90	0.17	6,6,6,6	0
55	MG	CA	1647	1/1	0.90	0.11	41,41,41,41	0
55	MG	CA	1648	1/1	0.90	0.20	22,22,22,22	0
55	MG	AA	1602	1/1	0.90	0.13	46,46,46,46	0
55	MG	BA	3182	1/1	0.90	0.25	33,33,33,33	0
55	MG	BA	3087	1/1	0.90	0.13	4,4,4,4	0
55	MG	DA	3058	1/1	0.90	1.10	109,109,109,109	0
55	MG	DA	3085	1/1	0.90	0.12	67,67,67,67	0
55	MG	BA	3156	1/1	0.90	0.28	19,19,19,19	0
55	MG	BA	3116	1/1	0.91	0.26	34,34,34,34	0
55	MG	DA	3065	1/1	0.91	0.12	36,36,36,36	0
55	MG	CA	1616	1/1	0.91	0.10	37,37,37,37	0
55	MG	BA	3193	1/1	0.91	0.15	38,38,38,38	0
55	MG	DA	3068	1/1	0.91	0.13	65,65,65,65	0
55	MG	BA	3195	1/1	0.91	0.56	23,23,23,23	0
55	MG	DA	3015	1/1	0.91	0.06	55,55,55,55	0
55	MG	DA	3105	1/1	0.91	0.18	80,80,80,80	0
55	MG	DA	3106	1/1	0.91	0.14	52,52,52,52	0
55	MG	BA	3006	1/1	0.91	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3008	1/1	0.91	0.14	37,37,37,37	0
55	MG	BA	3168	1/1	0.91	0.12	35,35,35,35	0
55	MG	BA	3015	1/1	0.91	0.07	2,2,2,2	0
55	MG	DA	3021	1/1	0.91	0.18	63,63,63,63	0
55	MG	DA	3150	1/1	0.91	0.20	56,56,56,56	0
55	MG	BA	3132	1/1	0.91	0.09	23,23,23,23	0
55	MG	AA	1629	1/1	0.91	0.14	61,61,61,61	0
55	MG	BA	3003	1/1	0.91	0.06	17,17,17,17	0
55	MG	AA	1641	1/1	0.91	0.15	19,19,19,19	0
55	MG	DA	3050	1/1	0.91	0.10	56,56,56,56	0
55	MG	BA	3078	1/1	0.91	0.72	79,79,79,79	0
55	MG	DA	3159	1/1	0.91	0.30	43,43,43,43	0
55	MG	DA	3087	1/1	0.91	0.09	54,54,54,54	0
55	MG	DA	3123	1/1	0.91	0.12	57,57,57,57	0
55	MG	DA	3164	1/1	0.91	0.18	57,57,57,57	0
55	MG	DA	3054	1/1	0.91	0.10	55,55,55,55	0
55	MG	BA	3081	1/1	0.91	0.12	24,24,24,24	0
55	MG	BA	3033	1/1	0.91	0.12	11,11,11,11	0
55	MG	DA	3030	1/1	0.91	0.24	60,60,60,60	0
55	MG	BA	3005	1/1	0.91	0.07	34,34,34,34	0
55	MG	DA	3032	1/1	0.91	0.26	68,68,68,68	0
55	MG	CA	1614	1/1	0.91	0.08	50,50,50,50	0
55	MG	CA	1622	1/1	0.92	0.13	51,51,51,51	0
55	MG	DA	3004	1/1	0.92	0.11	76,76,76,76	0
55	MG	BA	3071	1/1	0.92	0.07	60,60,60,60	0
55	MG	BA	3098	1/1	0.92	0.12	2,2,2,2	0
55	MG	AA	1654	1/1	0.92	0.14	43,43,43,43	0
55	MG	AA	1625	1/1	0.92	0.07	47,47,47,47	0
55	MG	BA	3152	1/1	0.92	0.19	6,6,6,6	0
55	MG	AA	1606	1/1	0.92	0.11	44,44,44,44	0
55	MG	AA	1603	1/1	0.92	0.10	44,44,44,44	0
55	MG	BA	3042	1/1	0.92	0.38	0,0,0,0	0
55	MG	BA	3113	1/1	0.92	0.17	22,22,22,22	0
55	MG	AA	1666	1/1	0.92	0.19	46,46,46,46	0
55	MG	BA	3086	1/1	0.92	0.07	14,14,14,14	0
55	MG	BA	3063	1/1	0.92	0.45	31,31,31,31	0
55	MG	CA	1639	1/1	0.92	0.10	43,43,43,43	0
55	MG	DA	3116	1/1	0.92	0.36	76,76,76,76	0
55	MG	DA	3082	1/1	0.92	0.13	60,60,60,60	0
55	MG	CA	1607	1/1	0.92	0.08	54,54,54,54	0
55	MG	BA	3047	1/1	0.92	0.10	4,4,4,4	0
55	MG	DA	3158	1/1	0.92	0.19	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3066	1/1	0.92	0.15	0,0,0,0	0
55	MG	BA	3174	1/1	0.92	0.12	12,12,12,12	0
55	MG	DA	3023	1/1	0.92	0.05	69,69,69,69	0
55	MG	BA	3127	1/1	0.92	0.12	9,9,9,9	0
55	MG	BA	3131	1/1	0.92	0.18	1,1,1,1	0
55	MG	BA	3091	1/1	0.92	0.09	3,3,3,3	0
55	MG	BA	3133	1/1	0.92	0.10	32,32,32,32	0
55	MG	AA	1646	1/1	0.92	0.20	49,49,49,49	0
55	MG	DA	3095	1/1	0.92	0.41	91,91,91,91	0
55	MG	CA	1620	1/1	0.92	0.06	61,61,61,61	0
55	MG	BA	3187	1/1	0.92	0.06	33,33,33,33	0
55	MG	DA	3101	1/1	0.93	0.09	57,57,57,57	0
55	MG	BA	3155	1/1	0.93	0.21	20,20,20,20	0
55	MG	AA	1669	1/1	0.93	0.42	51,51,51,51	0
55	MG	DA	3140	1/1	0.93	0.43	43,43,43,43	0
55	MG	BA	3121	1/1	0.93	0.12	3,3,3,3	0
55	MG	DA	3142	1/1	0.93	0.26	33,33,33,33	0
55	MG	BA	3166	1/1	0.93	0.17	19,19,19,19	0
55	MG	CA	1633	1/1	0.93	0.32	64,64,64,64	0
55	MG	AA	1663	1/1	0.93	0.22	48,48,48,48	0
55	MG	BA	3126	1/1	0.93	0.12	6,6,6,6	0
55	MG	BA	3030	1/1	0.93	0.14	9,9,9,9	0
55	MG	BA	3031	1/1	0.93	0.07	14,14,14,14	0
55	MG	AA	1610	1/1	0.93	0.23	65,65,65,65	0
55	MG	BA	3173	1/1	0.93	0.14	27,27,27,27	0
55	MG	CA	1643	1/1	0.93	0.24	50,50,50,50	0
55	MG	BA	3056	1/1	0.93	0.08	5,5,5,5	0
55	MG	BA	3034	1/1	0.93	0.10	6,6,6,6	0
55	MG	BA	3136	1/1	0.93	0.12	21,21,21,21	0
55	MG	DA	3053	1/1	0.93	0.11	40,40,40,40	0
55	MG	BA	3079	1/1	0.93	0.09	22,22,22,22	0
55	MG	BA	3181	1/1	0.93	0.20	24,24,24,24	0
55	MG	AA	1617	1/1	0.93	0.12	52,52,52,52	0
55	MG	CA	1652	1/1	0.93	0.11	83,83,83,83	0
55	MG	DA	3161	1/1	0.93	0.11	57,57,57,57	0
55	MG	BA	3185	1/1	0.93	0.30	16,16,16,16	0
55	MG	BA	3013	1/1	0.93	0.21	0,0,0,0	0
55	MG	BA	3149	1/1	0.93	0.12	38,38,38,38	0
55	MG	DA	3130	1/1	0.93	0.10	81,81,81,81	0
55	MG	BA	3085	1/1	0.93	0.22	27,27,27,27	0
55	MG	BA	3190	1/1	0.93	0.10	31,31,31,31	0
55	MG	AA	1627	1/1	0.93	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1618	1/1	0.93	0.08	37,37,37,37	0
55	MG	BA	3065	1/1	0.93	0.14	0,0,0,0	0
55	MG	AA	1616	1/1	0.94	0.12	50,50,50,50	0
55	MG	BA	3140	1/1	0.94	0.39	0,0,0,0	0
55	MG	BA	3043	1/1	0.94	0.13	16,16,16,16	0
55	MG	DA	3079	1/1	0.94	0.13	96,96,96,96	0
55	MG	BA	3084	1/1	0.94	0.05	6,6,6,6	0
55	MG	CA	1625	1/1	0.94	0.15	22,22,22,22	0
55	MG	AA	1607	1/1	0.94	0.09	44,44,44,44	0
55	MG	CA	1653	1/1	0.94	0.09	52,52,52,52	0
55	MG	BA	3150	1/1	0.94	0.20	37,37,37,37	0
55	MG	BA	3025	1/1	0.94	0.10	2,2,2,2	0
55	MG	DA	3055	1/1	0.94	0.13	72,72,72,72	0
55	MG	AA	1649	1/1	0.94	0.14	32,32,32,32	0
55	MG	BA	3130	1/1	0.94	0.12	0,0,0,0	0
55	MG	BA	3039	1/1	0.94	0.27	0,0,0,0	0
55	MG	AA	1668	1/1	0.94	0.13	29,29,29,29	0
55	MG	BA	3053	1/1	0.94	0.14	2,2,2,2	0
55	MG	BA	3115	1/1	0.94	0.12	20,20,20,20	0
55	MG	BA	3159	1/1	0.94	0.22	14,14,14,14	0
55	MG	BA	3160	1/1	0.94	0.10	10,10,10,10	0
55	MG	DA	3035	1/1	0.94	0.09	79,79,79,79	0
55	MG	BA	3164	1/1	0.94	0.14	4,4,4,4	0
55	MG	BA	3165	1/1	0.94	0.30	43,43,43,43	0
55	MG	BA	3080	1/1	0.94	0.07	39,39,39,39	0
55	MG	DA	3167	1/1	0.94	0.29	100,100,100,100	0
55	MG	CA	1641	1/1	0.94	0.68	73,73,73,73	0
55	MG	DA	3102	1/1	0.94	0.22	62,62,62,62	0
55	MG	CA	1642	1/1	0.94	0.25	25,25,25,25	0
55	MG	BA	3192	1/1	0.94	0.21	22,22,22,22	0
55	MG	CA	1645	1/1	0.94	0.20	32,32,32,32	0
55	MG	CA	1619	1/1	0.94	0.10	33,33,33,33	0
55	MG	AA	1608	1/1	0.95	0.14	17,17,17,17	0
55	MG	AA	1653	1/1	0.95	0.17	28,28,28,28	0
55	MG	AA	1640	1/1	0.95	0.09	36,36,36,36	0
55	MG	BA	3094	1/1	0.95	0.05	31,31,31,31	0
55	MG	BA	3045	1/1	0.95	0.08	9,9,9,9	0
55	MG	BA	3061	1/1	0.95	0.35	30,30,30,30	0
55	MG	DA	3118	1/1	0.95	0.08	60,60,60,60	0
55	MG	CA	1611	1/1	0.95	0.29	90,90,90,90	0
55	MG	BA	3062	1/1	0.95	0.36	50,50,50,50	0
55	MG	AA	1655	1/1	0.95	0.11	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1624	1/1	0.95	0.04	41,41,41,41	0
55	MG	BA	3188	1/1	0.95	0.14	10,10,10,10	0
55	MG	BA	3017	1/1	0.95	0.06	2,2,2,2	0
55	MG	BA	3161	1/1	0.95	0.17	31,31,31,31	0
55	MG	BA	3035	1/1	0.95	0.18	0,0,0,0	0
55	MG	BA	3036	1/1	0.95	0.12	11,11,11,11	0
55	MG	DA	3043	1/1	0.95	0.13	66,66,66,66	0
55	MG	BA	3138	1/1	0.95	0.45	1,1,1,1	0
55	MG	BA	3088	1/1	0.95	0.23	2,2,2,2	0
55	MG	BA	3020	1/1	0.95	0.09	22,22,22,22	0
55	MG	BB	203	1/1	0.95	0.06	7,7,7,7	0
55	MG	DA	3166	1/1	0.95	0.09	41,41,41,41	0
55	MG	BA	3145	1/1	0.95	0.29	28,28,28,28	0
55	MG	BA	3118	1/1	0.95	0.12	1,1,1,1	0
55	MG	BA	3148	1/1	0.95	0.12	29,29,29,29	0
55	MG	DA	3051	1/1	0.95	0.09	28,28,28,28	0
55	MG	DA	3109	1/1	0.95	0.22	42,42,42,42	0
55	MG	BA	3172	1/1	0.95	0.17	31,31,31,31	0
55	MG	AA	1647	1/1	0.95	0.12	48,48,48,48	0
55	MG	CA	1612	1/1	0.96	0.05	40,40,40,40	0
55	MG	BA	3135	1/1	0.96	0.14	2,2,2,2	0
55	MG	BA	3023	1/1	0.96	0.14	1,1,1,1	0
55	MG	BA	3024	1/1	0.96	0.17	0,0,0,0	0
55	MG	BA	3012	1/1	0.96	0.05	14,14,14,14	0
55	MG	CA	1644	1/1	0.96	0.15	42,42,42,42	0
55	MG	DA	3018	1/1	0.96	0.12	60,60,60,60	0
55	MG	BA	3026	1/1	0.96	0.15	3,3,3,3	0
55	MG	CA	1618	1/1	0.96	0.11	37,37,37,37	0
55	MG	AA	1633	1/1	0.96	0.12	30,30,30,30	0
55	MG	DA	3083	1/1	0.96	0.10	69,69,69,69	0
55	MG	BA	3029	1/1	0.96	0.08	21,21,21,21	0
55	MG	BA	3095	1/1	0.96	0.09	21,21,21,21	0
55	MG	BB	201	1/1	0.96	0.10	20,20,20,20	0
55	MG	CA	1623	1/1	0.96	0.16	50,50,50,50	0
55	MG	BA	3147	1/1	0.96	0.31	9,9,9,9	0
55	MG	BA	3014	1/1	0.96	0.18	0,0,0,0	0
55	MG	DA	3122	1/1	0.96	0.15	41,41,41,41	0
55	MG	BA	3122	1/1	0.96	0.04	18,18,18,18	0
55	MG	BA	3124	1/1	0.96	0.09	11,11,11,11	0
55	MG	DA	3059	1/1	0.96	0.10	51,51,51,51	0
55	MG	BA	3009	1/1	0.96	0.09	4,4,4,4	0
55	MG	BA	3175	1/1	0.96	0.11	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3128	1/1	0.96	0.08	80,80,80,80	0
55	MG	BA	3176	1/1	0.96	0.10	20,20,20,20	0
55	MG	BA	3101	1/1	0.96	0.07	1,1,1,1	0
55	MG	BA	3070	1/1	0.96	0.21	0,0,0,0	0
55	MG	BA	3044	1/1	0.96	0.14	3,3,3,3	0
55	MG	CA	1634	1/1	0.96	0.13	49,49,49,49	0
55	MG	BA	3074	1/1	0.96	0.18	1,1,1,1	0
55	MG	BA	3108	1/1	0.96	0.24	0,0,0,0	0
55	MG	BA	3110	1/1	0.96	0.20	3,3,3,3	0
56	DOL	BA	3001	48/48	0.96	0.21	0,3,25,36	0
55	MG	BA	3022	1/1	0.96	0.08	2,2,2,2	0
55	MG	BA	3111	1/1	0.97	0.20	6,6,6,6	0
55	MG	DA	3086	1/1	0.97	0.10	76,76,76,76	0
55	MG	BA	3072	1/1	0.97	0.08	3,3,3,3	0
55	MG	BA	3183	1/1	0.97	0.21	12,12,12,12	0
55	MG	BA	3184	1/1	0.97	0.20	6,6,6,6	0
55	MG	BA	3158	1/1	0.97	0.12	19,19,19,19	0
55	MG	BA	3073	1/1	0.97	0.07	7,7,7,7	0
55	MG	DA	3063	1/1	0.97	0.22	54,54,54,54	0
55	MG	BA	3037	1/1	0.97	0.17	0,0,0,0	0
55	MG	BA	3060	1/1	0.97	0.06	15,15,15,15	0
55	MG	BA	3163	1/1	0.97	0.33	15,15,15,15	0
55	MG	AA	1615	1/1	0.97	0.06	47,47,47,47	0
55	MG	DA	3156	1/1	0.97	0.19	41,41,41,41	0
55	MG	BA	3117	1/1	0.97	0.17	1,1,1,1	0
55	MG	BA	3007	1/1	0.97	0.09	22,22,22,22	0
55	MG	AA	1611	1/1	0.97	0.09	21,21,21,21	0
55	MG	BA	3142	1/1	0.97	0.43	2,2,2,2	0
55	MG	BA	3052	1/1	0.97	0.06	11,11,11,11	0
55	MG	BA	3032	1/1	0.97	0.16	4,4,4,4	0
55	MG	AA	1604	1/1	0.97	0.06	48,48,48,48	0
55	MG	BA	3123	1/1	0.97	0.16	0,0,0,0	0
55	MG	DA	3076	1/1	0.97	0.12	69,69,69,69	0
55	MG	BQ	201	1/1	0.97	0.20	3,3,3,3	0
55	MG	BA	3067	1/1	0.97	0.17	0,0,0,0	0
55	MG	BA	3083	1/1	0.97	0.17	0,0,0,0	0
55	MG	BA	3068	1/1	0.97	0.17	0,0,0,0	0
55	MG	BA	3010	1/1	0.97	0.11	0,0,0,0	0
55	MG	BA	3129	1/1	0.97	0.19	4,4,4,4	0
55	MG	BA	3018	1/1	0.97	0.20	0,0,0,0	0
55	MG	AA	1642	1/1	0.97	0.15	23,23,23,23	0
55	MG	BA	3109	1/1	0.98	0.19	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1636	1/1	0.98	0.08	27,27,27,27	0
55	MG	BA	3041	1/1	0.98	0.18	6,6,6,6	0
55	MG	BA	3128	1/1	0.98	0.10	0,0,0,0	0
55	MG	BA	3096	1/1	0.98	0.07	11,11,11,11	0
55	MG	BA	3097	1/1	0.98	0.07	4,4,4,4	0
55	MG	AA	1622	1/1	0.98	0.20	16,16,16,16	0
55	MG	BA	3099	1/1	0.98	0.12	4,4,4,4	0
55	MG	BA	3194	1/1	0.98	0.07	8,8,8,8	0
55	MG	BA	3028	1/1	0.98	0.08	5,5,5,5	0
55	MG	DA	3162	1/1	0.98	0.21	38,38,38,38	0
55	MG	AA	1656	1/1	0.98	0.15	43,43,43,43	0
55	MG	AA	1621	1/1	0.98	0.08	39,39,39,39	0
55	MG	BA	3055	1/1	0.98	0.17	0,0,0,0	0
55	MG	BA	3177	1/1	0.98	0.17	17,17,17,17	0
55	MG	AA	1645	1/1	0.98	0.12	42,42,42,42	0
55	MG	BA	3105	1/1	0.98	0.10	4,4,4,4	0
55	MG	BA	3139	1/1	0.98	0.37	0,0,0,0	0
55	MG	BA	3106	1/1	0.98	0.20	16,16,16,16	0
55	MG	BA	3107	1/1	0.98	0.19	0,0,0,0	0
55	MG	BA	3162	1/1	0.98	0.07	36,36,36,36	0
55	MG	BA	3019	1/1	0.98	0.12	11,11,11,11	0
55	MG	BA	3144	1/1	0.98	0.26	15,15,15,15	0
57	ZN	B4	101	1/1	0.98	0.10	33,33,33,33	0
57	ZN	D4	101	1/1	0.98	0.10	87,87,87,87	0
55	MG	BA	3143	1/1	0.99	0.36	12,12,12,12	0
55	MG	BA	3011	1/1	0.99	0.15	1,1,1,1	0
55	MG	DA	3139	1/1	0.99	0.33	30,30,30,30	0
55	MG	BA	3048	1/1	0.99	0.15	8,8,8,8	0

## 6.5 Other polymers

There are no such residues in this entry.