



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 06:48 pm BST

PDB ID : 4U25  
Title : Crystal structure of the E. coli ribosome bound to virginiamycin M1.  
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.  
Deposited on : 2014-07-16  
Resolution : 2.90 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.

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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	:	2.11
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)	:	2.11

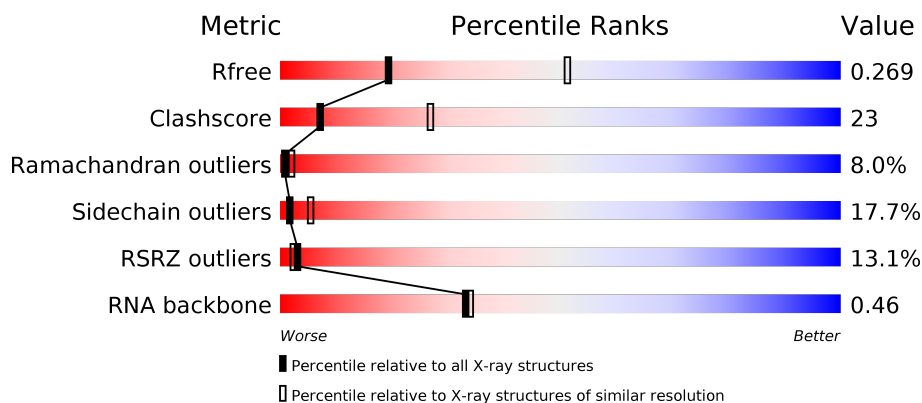
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>2%</div> <div>32%</div> <div>52%</div> <div>15%</div> </div>
1	CA	1539	<div> <div>4%</div> <div>33%</div> <div>53%</div> <div>13%</div> </div>
2	AB	218	<div> <div>14%</div> <div>20%</div> <div>50%</div> <div>23%</div> <div>6%</div> </div>
2	CB	218	<div> <div>27%</div> <div>30%</div> <div>51%</div> <div>17%</div> <div>•</div> </div>

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

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

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Mol	Chain	Length	Quality of chain
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	76	
44	DW	76	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	

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Mol	Chain	Length	Quality of chain
53	B5	228	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	1643	-	-	-	X
54	MG	AA	1657	-	-	-	X
54	MG	AA	1659	-	-	-	X
54	MG	AA	1667	-	-	-	X
54	MG	AA	1671	-	-	-	X
54	MG	BA	3016	-	-	-	X
54	MG	BA	3058	-	-	-	X
54	MG	BA	3077	-	-	-	X
54	MG	CA	1630	-	-	-	X
54	MG	CA	1656	-	-	-	X
54	MG	DA	3008	-	-	-	X
54	MG	DA	3009	-	-	-	X
54	MG	DA	3017	-	-	-	X
54	MG	DA	3027	-	-	-	X
54	MG	DA	3059	-	-	-	X
54	MG	DA	3061	-	-	-	X
54	MG	DA	3062	-	-	-	X
54	MG	DA	3063	-	-	-	X
54	MG	DA	3093	-	-	-	X
54	MG	DA	3094	-	-	-	X
54	MG	DA	3100	-	-	-	X
54	MG	DA	3114	-	-	-	X
54	MG	DA	3120	-	-	-	X
54	MG	DA	3125	-	-	-	X
54	MG	DA	3132	-	-	-	X
54	MG	DA	3134	-	-	-	X
54	MG	DA	3136	-	-	-	X
54	MG	DA	3148	-	-	-	X

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 288258 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			
15	CO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BW	76	Total	C	N	O	S	0	0	0
			580	359	117	103	1			
44	DW	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			

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

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

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

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

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

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



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

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

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

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

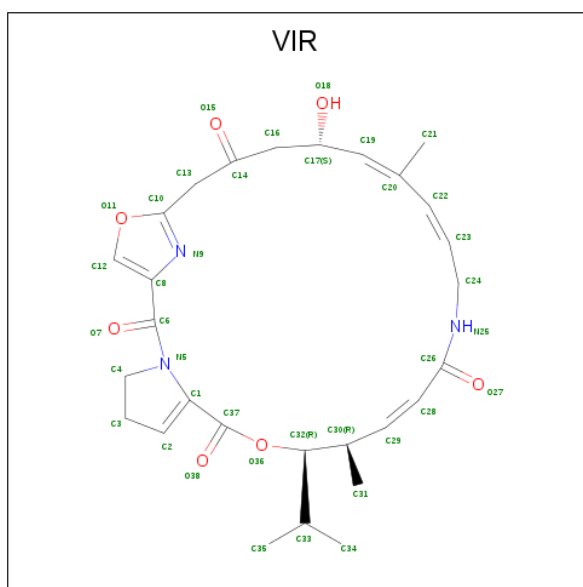
- Molecule 53 is a protein called 50S ribosomal protein L1.

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

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	4	Total	Mg	0	0
			4	4		
54	BA	193	Total	Mg	0	0
			193	193		
54	CA	56	Total	Mg	0	0
			56	56		
54	DQ	1	Total	Mg	0	0
			1	1		
54	BD	1	Total	Mg	0	0
			1	1		
54	DA	166	Total	Mg	0	0
			166	166		
54	AA	71	Total	Mg	0	0
			71	71		
54	BQ	1	Total	Mg	0	0
			1	1		
54	AN	1	Total	Mg	0	0
			1	1		
54	D2	1	Total	Mg	0	0
			1	1		
54	DB	3	Total	Mg	0	0
			3	3		

- Molecule 55 is VIRGINIAMYCIN M1 (three-letter code: VIR) (formula: C<sub>28</sub>H<sub>35</sub>N<sub>3</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BA	1	Total	C	N	O	0	0
			38	28	3	7		
55	DA	1	Total	C	N	O	0	0
			38	28	3	7		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	192	Total	O	0	0
			192	192		
57	AL	2	Total	O	0	0
			2	2		
57	AN	6	Total	O	0	0
			6	6		
57	AT	2	Total	O	0	0
			2	2		
57	AU	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BA	620	Total 620	O 620	0	0
57	BB	13	Total 13	O 13	0	0
57	BC	7	Total 7	O 7	0	0
57	BD	3	Total 3	O 3	0	0
57	BE	4	Total 4	O 4	0	0
57	BF	1	Total 1	O 1	0	0
57	BJ	1	Total 1	O 1	0	0
57	BL	5	Total 5	O 5	0	0
57	BN	3	Total 3	O 3	0	0
57	BQ	1	Total 1	O 1	0	0
57	BS	1	Total 1	O 1	0	0
57	BT	1	Total 1	O 1	0	0
57	BV	1	Total 1	O 1	0	0
57	B2	1	Total 1	O 1	0	0
57	B3	2	Total 2	O 2	0	0
57	B4	2	Total 2	O 2	0	0
57	CA	191	Total 191	O 191	0	0
57	CL	1	Total 1	O 1	0	0
57	CN	2	Total 2	O 2	0	0
57	CT	2	Total 2	O 2	0	0
57	CU	2	Total 2	O 2	0	0

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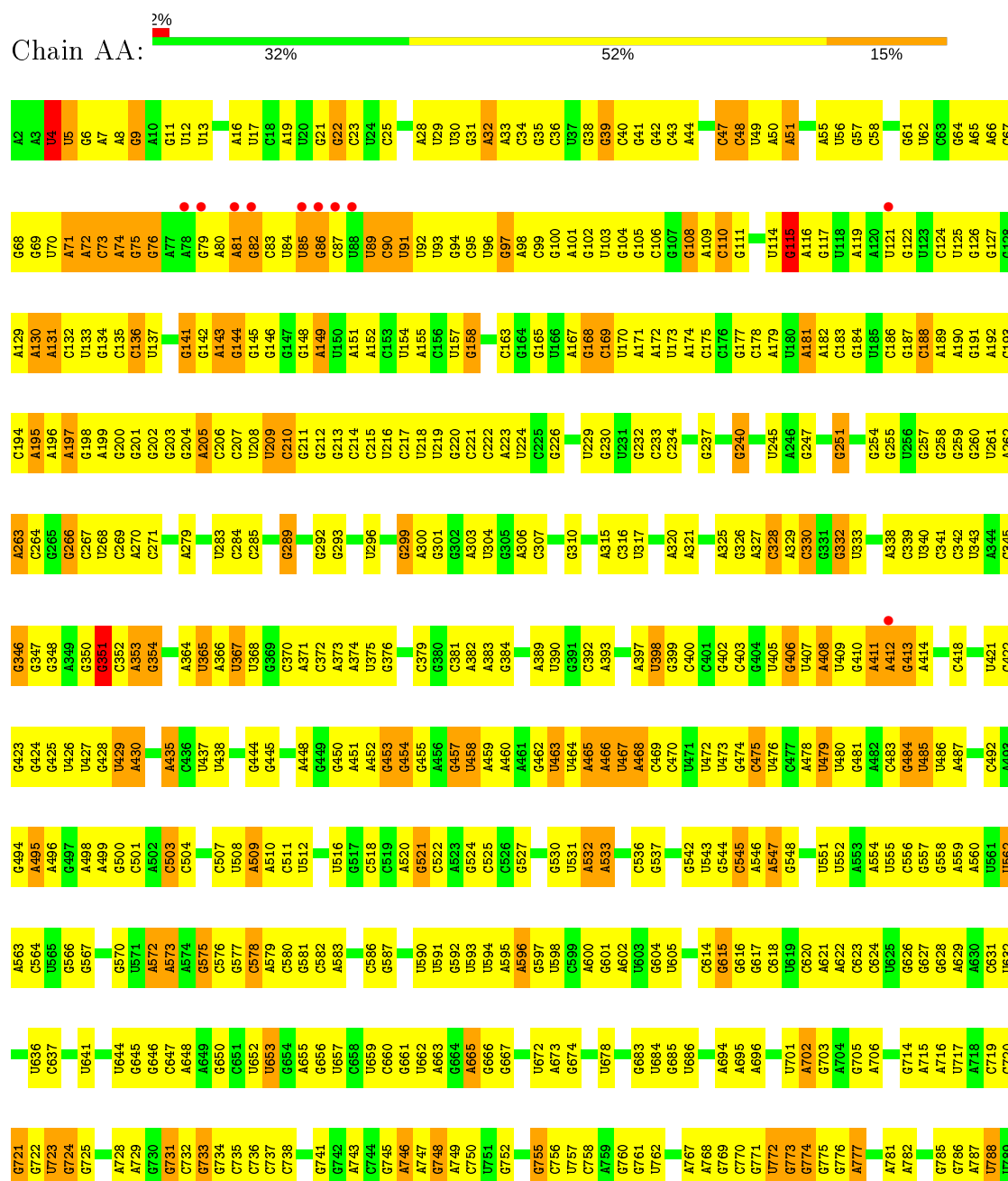
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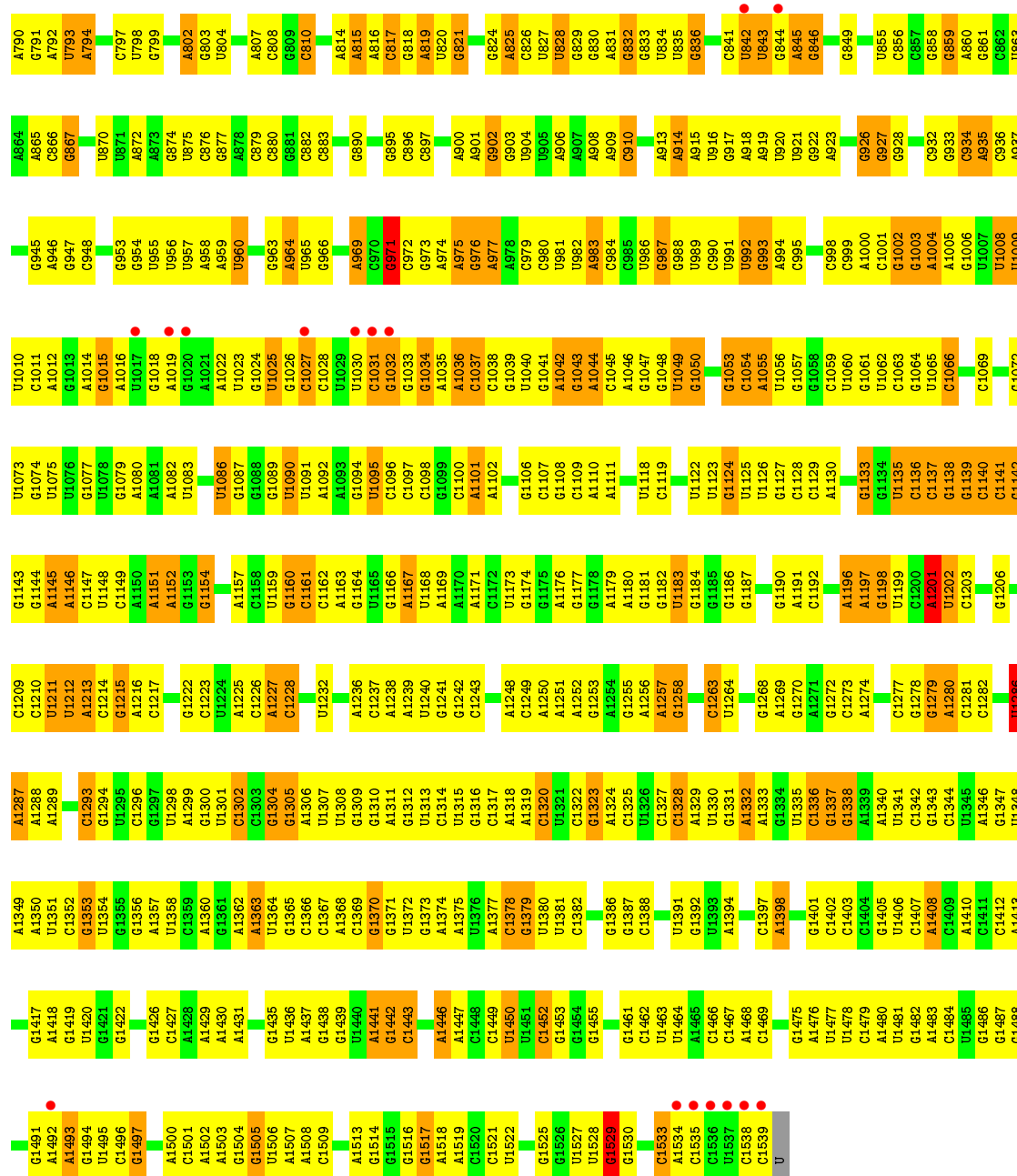
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DA	607	Total 607	O 607	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	12	Total 12	O 12	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	6	Total 6	O 6	0	0
57	DJ	1	Total 1	O 1	0	0
57	DL	4	Total 4	O 4	0	0
57	DN	2	Total 2	O 2	0	0
57	DT	1	Total 1	O 1	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D3	2	Total 2	O 2	0	0
57	D4	1	Total 1	O 1	0	0

### 3 Residue-property plots

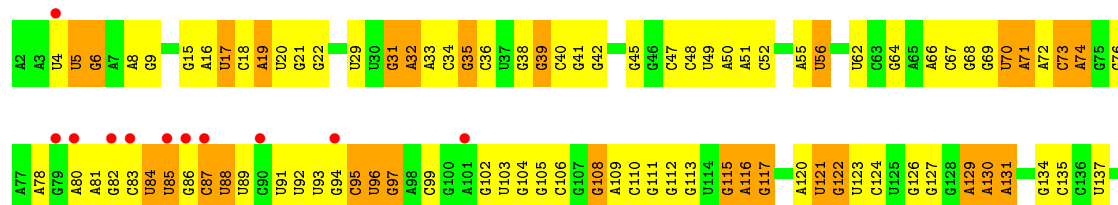
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 16S rRNA



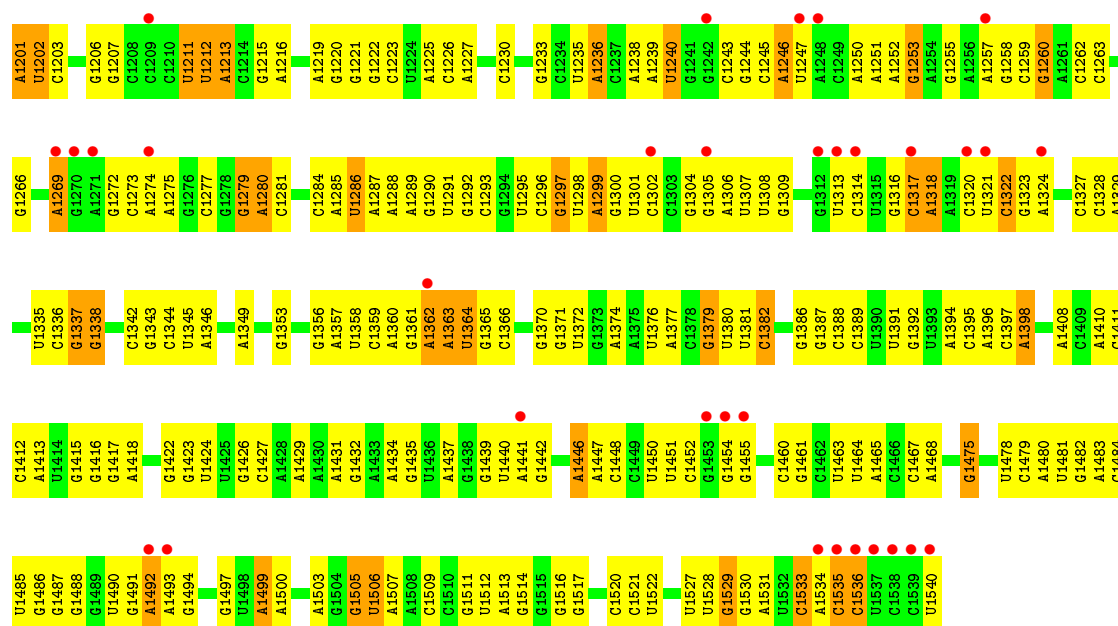


• Molecule 1: 16S rRNA

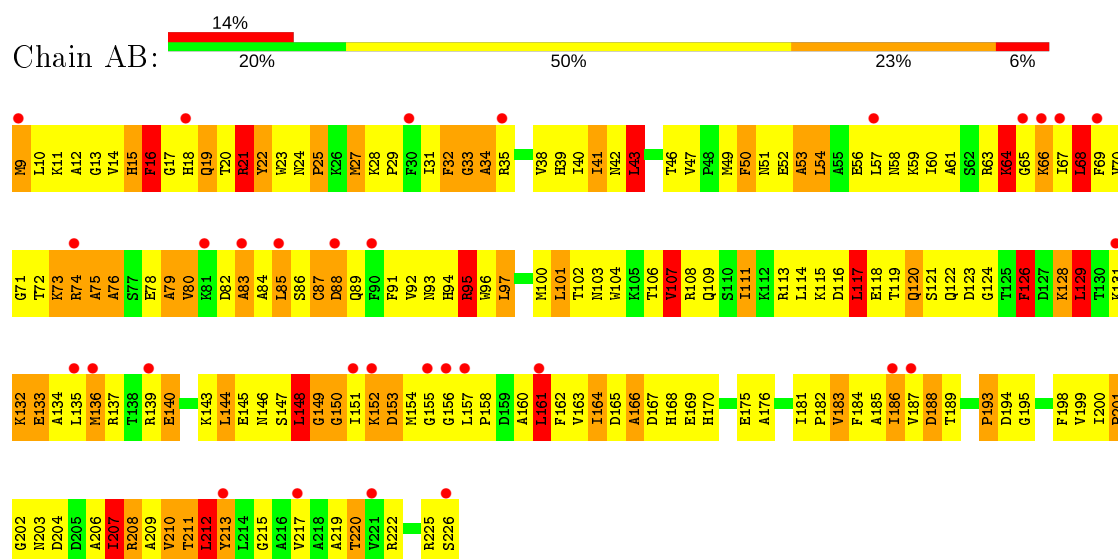


C1137	G1138	U1062	C995	G952	A782	C637	A554	U485	G413	G350	U273	G204	G142
G1139	U1065	U1066	A996	C857	C783	U638	U555	U486	A414	G351	A273	A205	A143
C1140	C1066	C1065	C998	G858	A784	G639	C556	C490	A415	C352	A274	C206	A144
G1141	C999	C999	C999	G859	A785	A642	A557	C491	C418	A353	G278	C207	G145
G1142	C1001	A1000	C934	A860	A787	C643	A559	C492	C419	C354	A279	U209	G146
G1143	C1002	A1001	A838	G861	A790	U644	A560	A493	C420	C355	C280	C210	G147
G1144	G1002	G1002	G939	C862	A791	G645	U561	G494	U421	A356	G281	G211	G148
A1145	G1003	G1072	G940	U863	A792	U722	U562	A496	C422	G357	A282	G212	U150
A1146	G941	G1073	G941	A1004	A793	U723	A563	A497	G425	U358	U283	G213	A151
C1147	G1074	G1074	G942	C866	A794	G724	C564	A498	G426	G360	C284	C214	A152
U1148	U1075	U1075	G945	G867	A795	A728	U565	A499	U427	G361	G289	C215	G153
U1149	U1007	U1007	A946	G868	A796	A729	U566	A499	U428	U154	U154	U216	U154
A1150	U1008	U1008	A947	G869	C797	G730	U567	G500	G428	A364	C290	C217	A155
A1151	U1009	U1009	G948	A872	U798	G731	U568	C501	U429	U365	U291	U218	A156
A1152	U1010	U1010	G949	G873	U799	G732	U569	A502	A430	A366	G291	U219	U157
A1155	A1014	A1014	A950	A874	U801	G733	A570	C503	A435	U367	U294	G220	G158
G1156	U1015	U1015	A951	G875	A802	G734	A571	C504	A436	U368	C295	G221	G159
A1157	G951	G951	G952	G876	G803	C735	A572	C505	U437	G369	U296	C222	A160
U1159	U1086	U1086	U955	A878	U804	C736	A573	G506	U438	C370	G297	A223	A161
G1160	U1087	U1087	U956	C879	C805	C737	A574	A509	A439	A371	A298	U224	A162
C1161	G1087	G1087	U957	C880	C806	U740	A575	C511	U440	C372	G301	G227	C163
C1162	U1088	U1088	U958	G881	A807	G741	A576	U512	A441	A374	G302	A228	G164
A1163	G1088	G1088	A958	C882	G808	G742	A577	C513	A442	A375	A303	G234	A167
U1090	U1091	U1091	A959	U884	C810	A743	A578	C514	A443	U376	G304	C234	G168
U1091	G1024	G1024	U960	G885	G812	C744	A579	C515	G444	G377	G305	G237	C169
U1092	U1025	U1025	G963	G888	U813	A747	A581	U516	A445	G378	A306	U239	U170
A1093	G1026	G1026	A964	U889	U814	G748	A582	C517	G446	C379	C307	A238	A171
G1094	C1027	C1027	A965	G890	A815	A749	A583	C518	A447	C380	C308	U239	A172
U1095	U1028	U1028	U966	G891	A816	A749	A584	C519	A448	C381	A309	G240	U173
C1096	U1029	U1029	G966	U891	A817	A749	A585	C520	A449	A382	A174	A243	A174
C1097	U1030	U1030	A967	G892	C817	A753	A586	U531	A450	A383	C312	U244	C175
C1098	U1031	U1031	A968	G893	G818	C754	A587	A532	A461	A313	A313	U245	G176
C1099	G1032	G1032	A969	U894	A819	G755	A588	C521	A455	G384	G314	G246	G177
C1100	G1033	G1033	A970	G895	U820	C756	A589	C522	A456	C385	C315	A247	C178
G1034	G1034	G1034	G971	U896	G821	U757	A600	C523	A457	C386	A316	G248	A179
A1035	A1035	A1035	C972	U897	U822	C758	A601	C524	A458	U387	C316	C249	U180
C1036	A1036	A1036	G973	U901	U823	A759	G604	U532	A460	A389	A321	U249	A181
G1103	A1037	A1037	A974	G902	C826	G760	U605	A533	A461	U390	C322	A250	A182
A1104	C1038	C1038	A975	A906	U827	G761	G606	U534	A462	G391	G323	G251	C183
C1039	G1039	G1039	G976	A907	U828	U762	A607	U535	A463	C392	G324	U252	G184
U1040	U1040	U1040	A977	A908	G829	U763	A608	A536	U464	A393	A325	G253	U185
G1041	G1041	G1041	A978	U909	G832	A765	A609	C536	A465	A397	G326	G254	C186
A1042	A1042	A1042	C979	A909	G833	A766	G618	U537	A466	U398	A327	G255	G187
G1043	G1043	G1043	C980	U910	G834	A767	U619	C540	A467	U399	C328	U256	C188
A1044	A1044	A1044	U981	A913	U834	A768	U620	A546	A468	G399	A329	G257	A189
C1045	C1045	C1045	U982	A914	U835	G769	A621	A547	C469	C400	C330	G258	A190
G1046	G1046	G1046	A983	A915	G836	A770	A622	U543	C470	G402	G331	G259	G191
G1047	G1047	G1047	C984	A915	G837	G771	A623	U544	A474	G403	G332	G260	A192
U1048	U1048	U1048	U985	A919	C840	U772	G628	G545	C475	C403	C341	U261	C193
G1124	G1124	G1124	U986	A920	C841	G773	G629	G546	A476	G404	A262	A262	C194
C1128	C1128	C1128	G987	U920	U842	A774	U625	A546	A477	U405	A263	G264	A195
C1129	G1050	G1050	G988	U921	U843	G775	U626	A547	A478	G406	U343	G265	A196
A1130	C1051	C1051	G989	G922	G844	G776	G628	C548	A479	U407	A344	G266	A197
U1052	U1052	U1052	C990	A923	A845	A777	G629	C549	U480	A408	C345	G267	G198
G1131	G1131	G1131	C991	C924	G846	G778	U632	G550	G481	U409	G346	C267	A199
C1053	C1053	C1053	U991	G925	G847	G779	U633	U551	A482	G410	G347	U268	G199
C1054	C1054	C1054	U992	G926	G848	G780	U634	U552	A483	G411	G348	U269	G202
A1055	A1055	A1055	G993	G927	G851	A781	U636	A553	G484	A412	A349	A270	G203

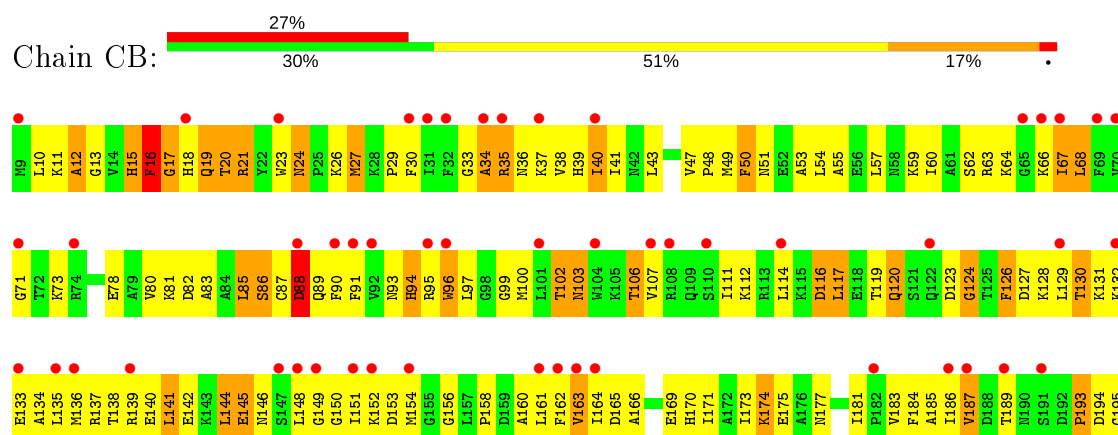




### • Molecule 2: 30S ribosomal protein S2

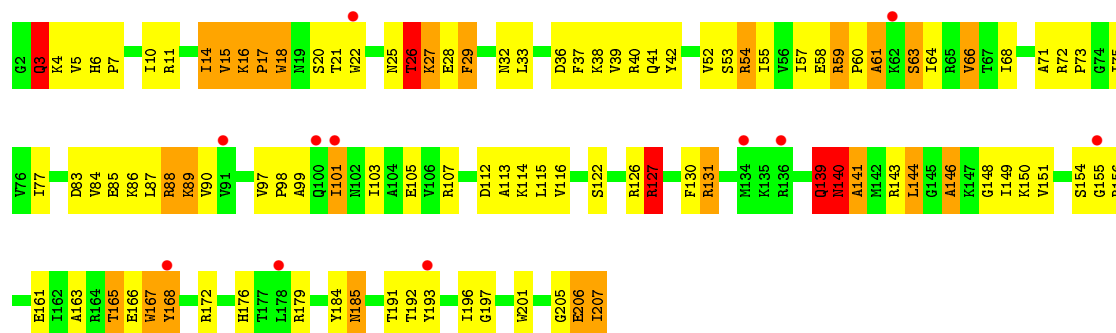


### • Molecule 2: 30S ribosomal protein S2

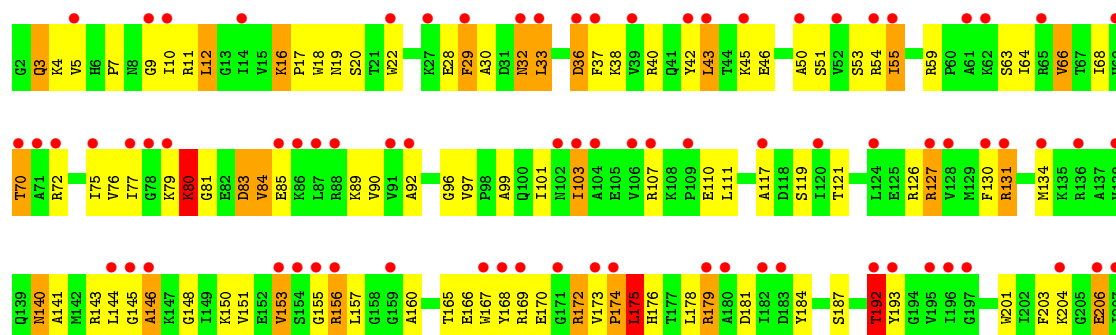
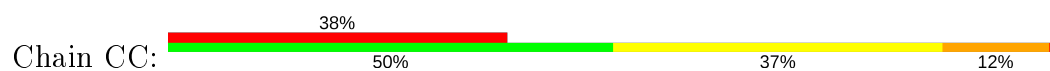




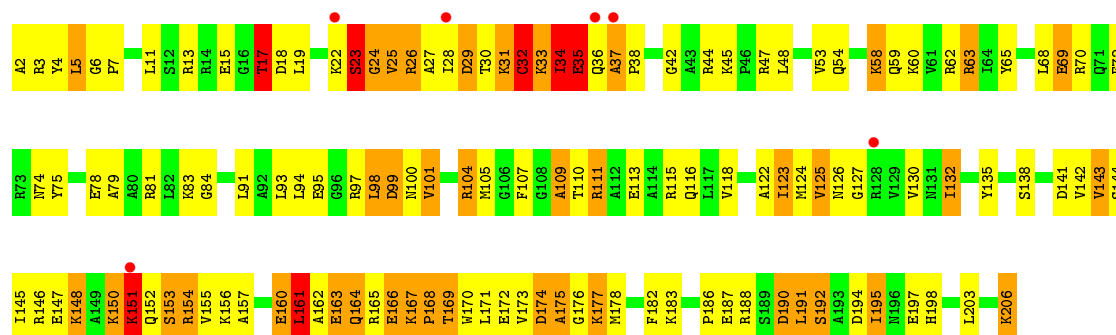
- Molecule 3: 30S ribosomal protein S3



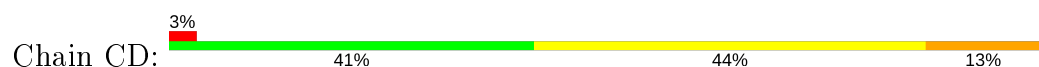
- Molecule 3: 30S ribosomal protein S3

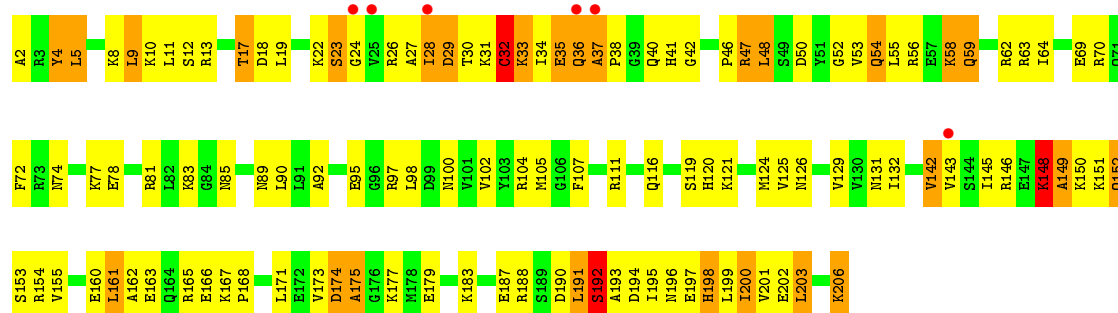


- Molecule 4: 30S ribosomal protein S4

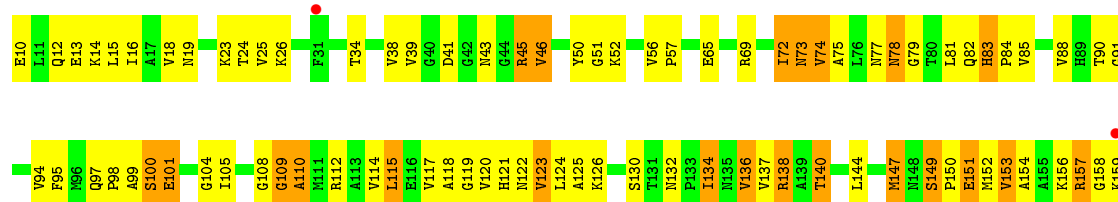


- Molecule 4: 30S ribosomal protein S4

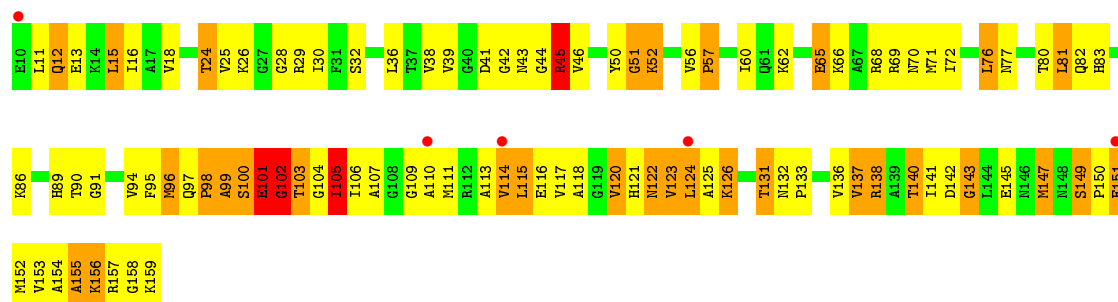




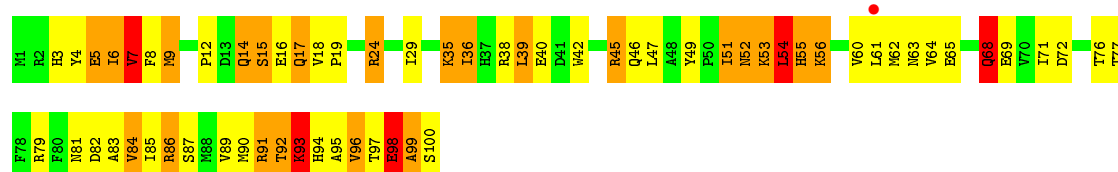
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

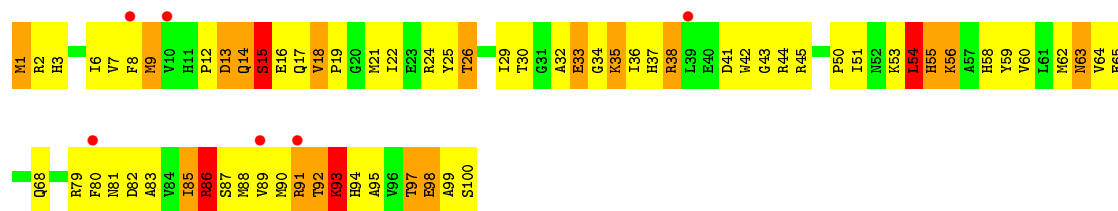


• Molecule 6: 30S ribosomal protein S6

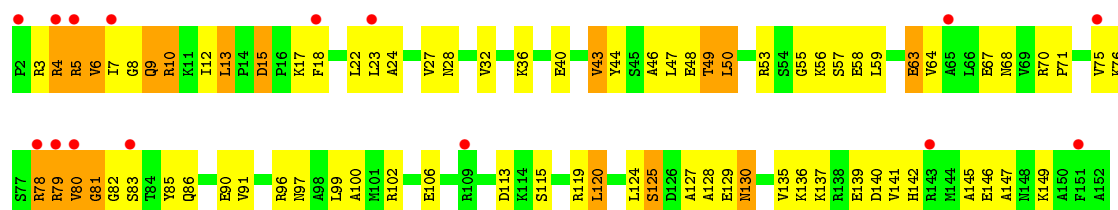


• Molecule 6: 30S ribosomal protein S6

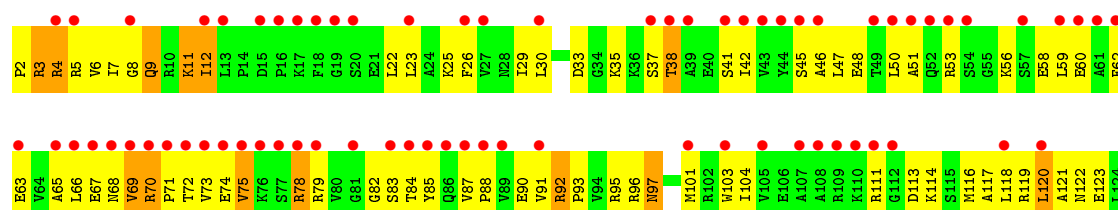




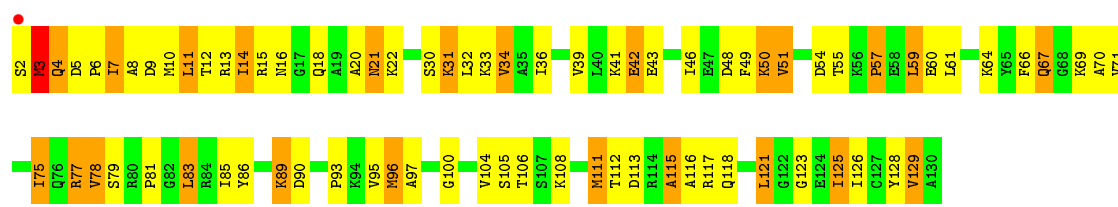
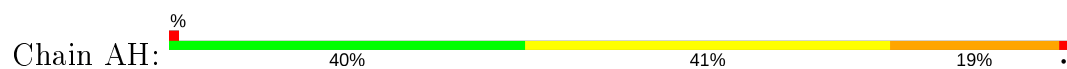
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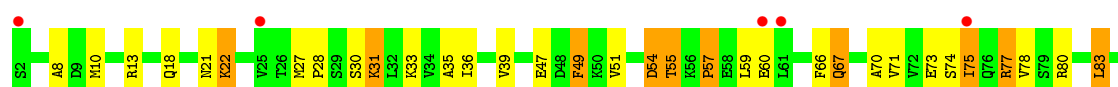
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

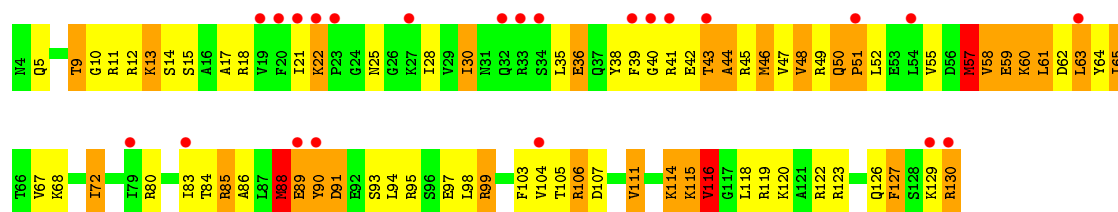


• Molecule 8: 30S ribosomal protein S8

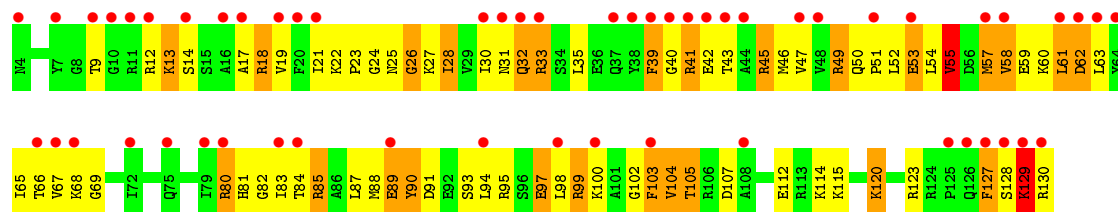
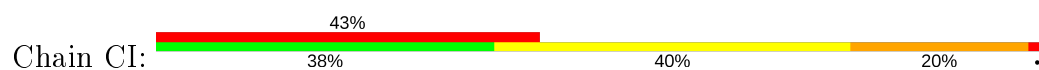




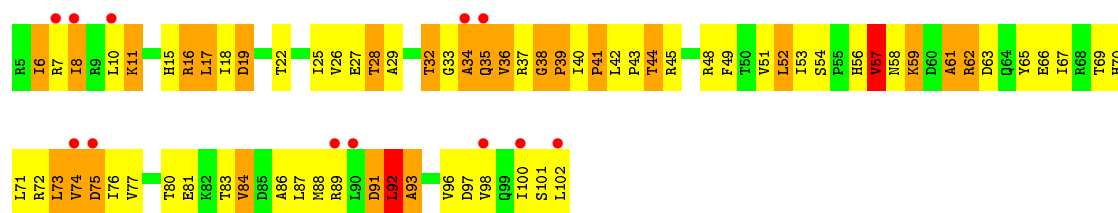
- Molecule 9: 30S ribosomal protein S9



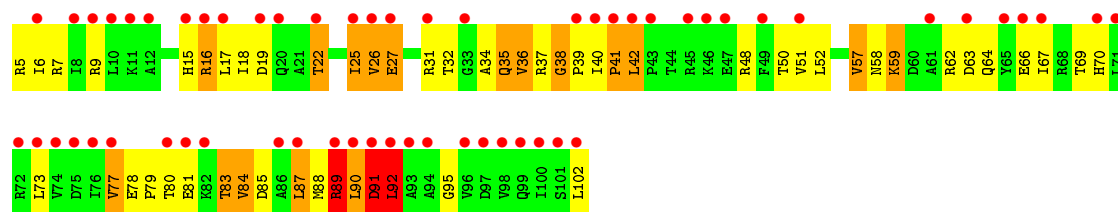
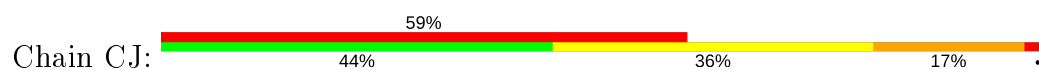
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

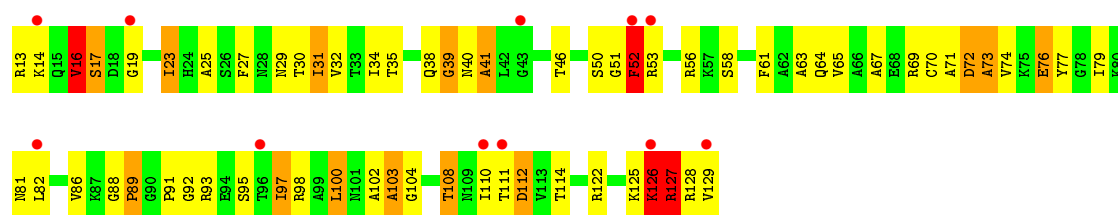


- Molecule 10: 30S ribosomal protein S10

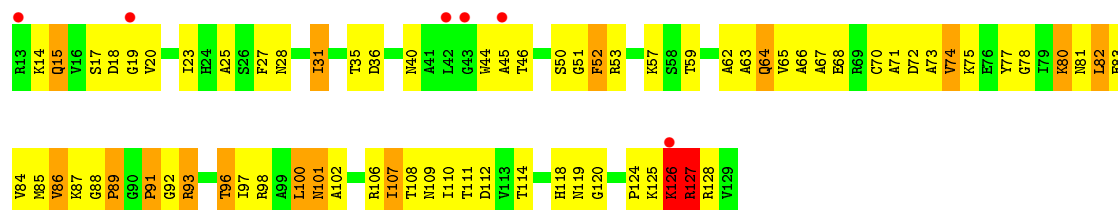


- Molecule 11: 30S ribosomal protein S11

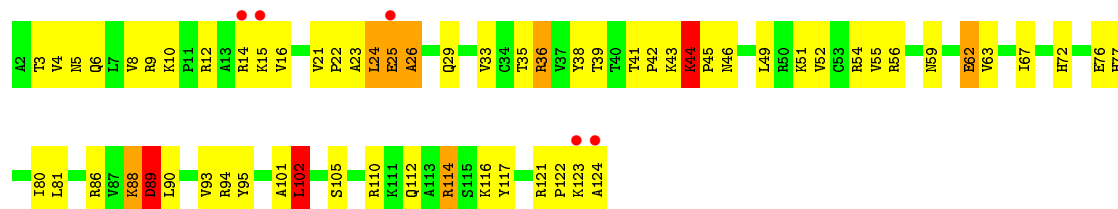




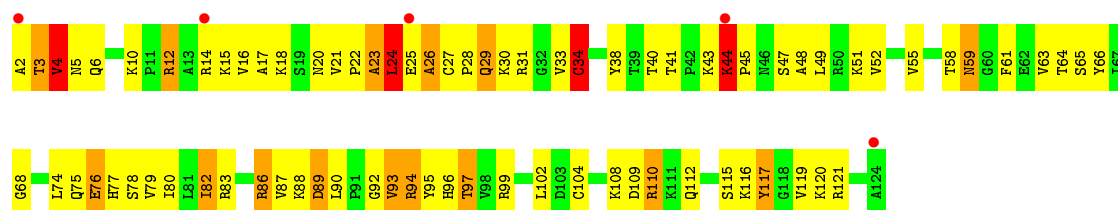
• Molecule 11: 30S ribosomal protein S11



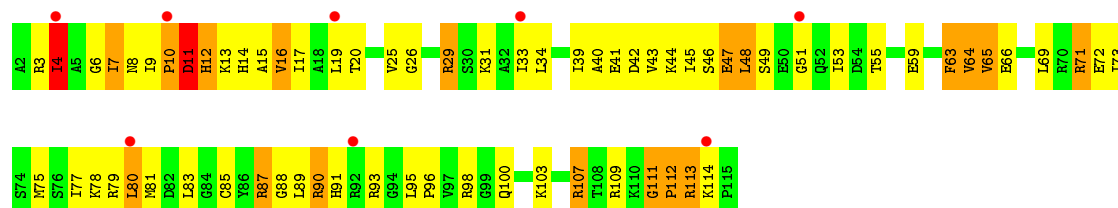
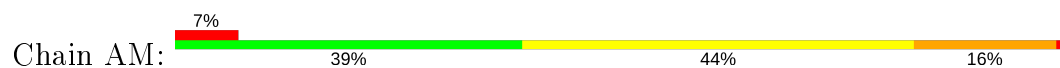
• Molecule 12: 30S ribosomal protein S12



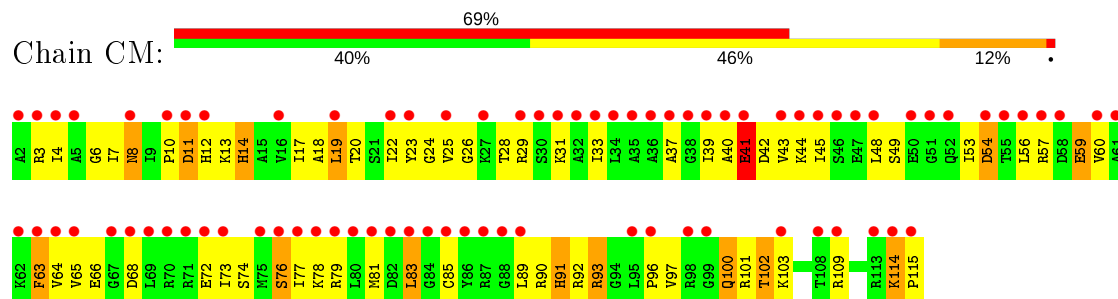
• Molecule 12: 30S ribosomal protein S12



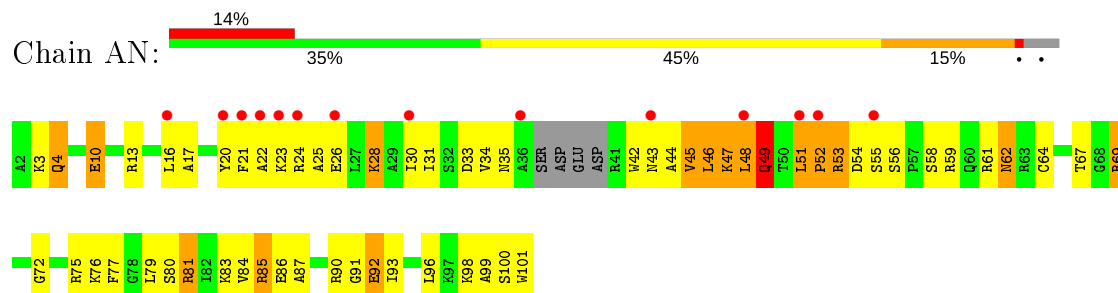
• Molecule 13: 30S ribosomal protein S13



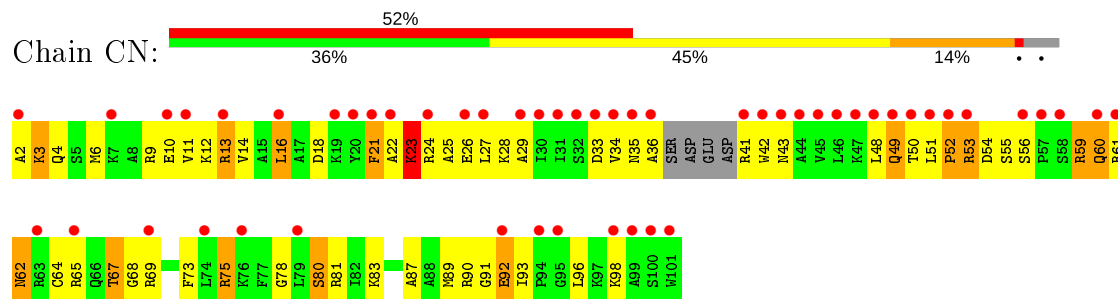
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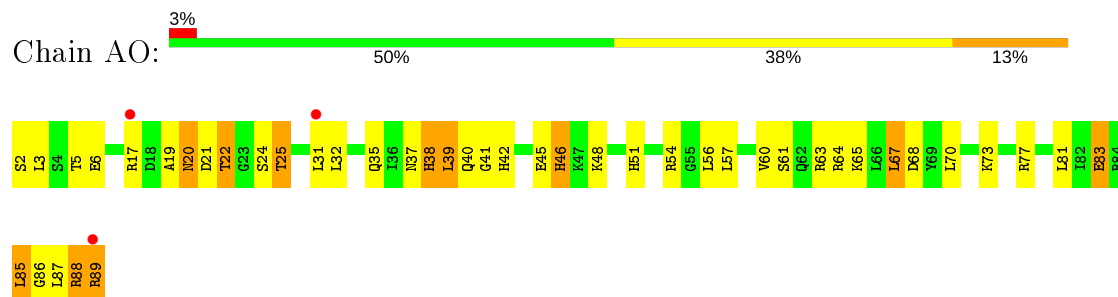
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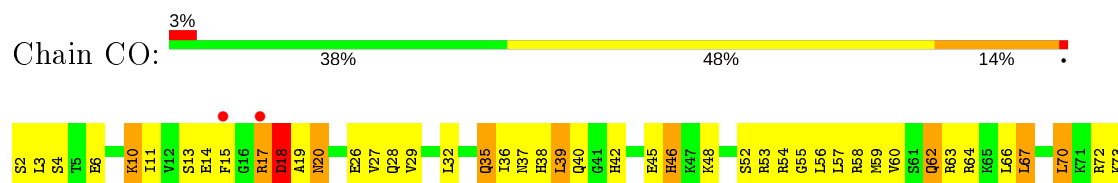
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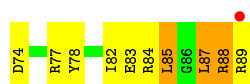


## Chain AO:



## Chain CO:

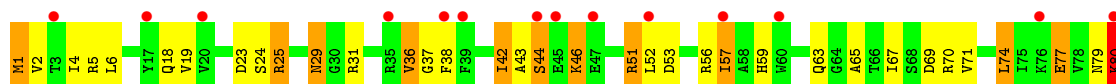




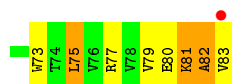
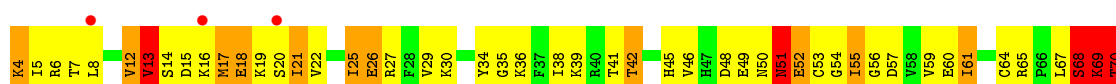
• Molecule 16: 30S ribosomal protein S16



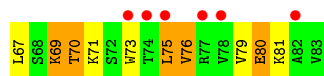
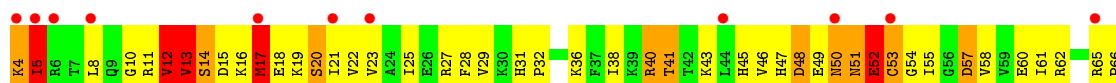
• Molecule 16: 30S ribosomal protein S16



• Molecule 17: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S17



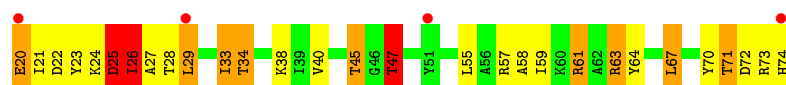
• Molecule 18: 30S ribosomal protein S18



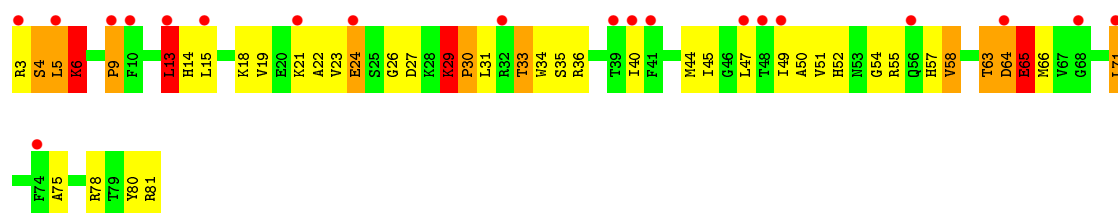




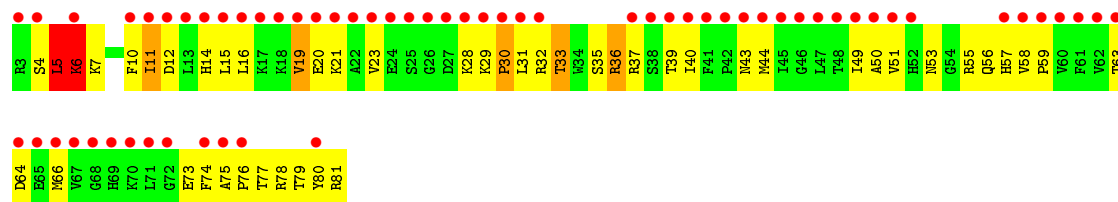
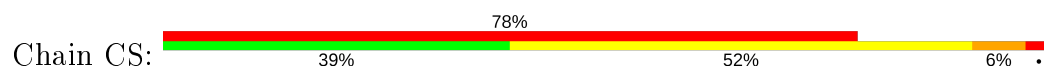
- Molecule 18: 30S ribosomal protein S18



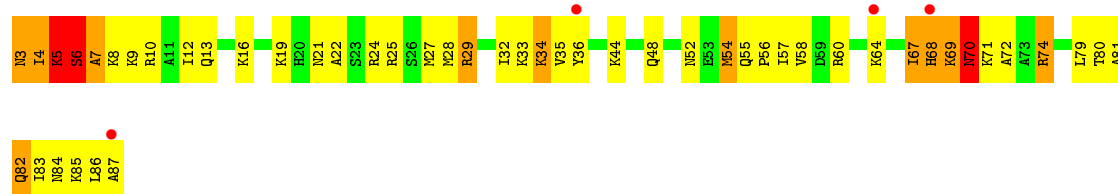
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19

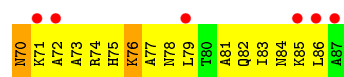


- Molecule 20: 30S ribosomal protein S20

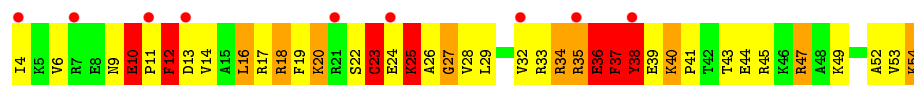


- Molecule 20: 30S ribosomal protein S20

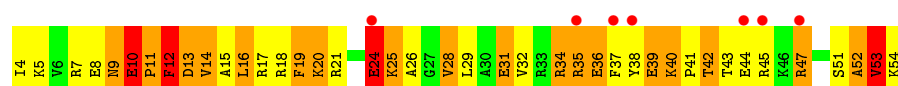
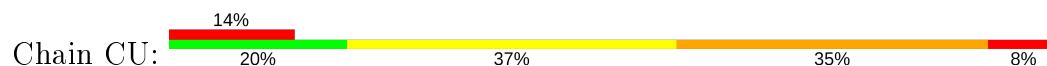




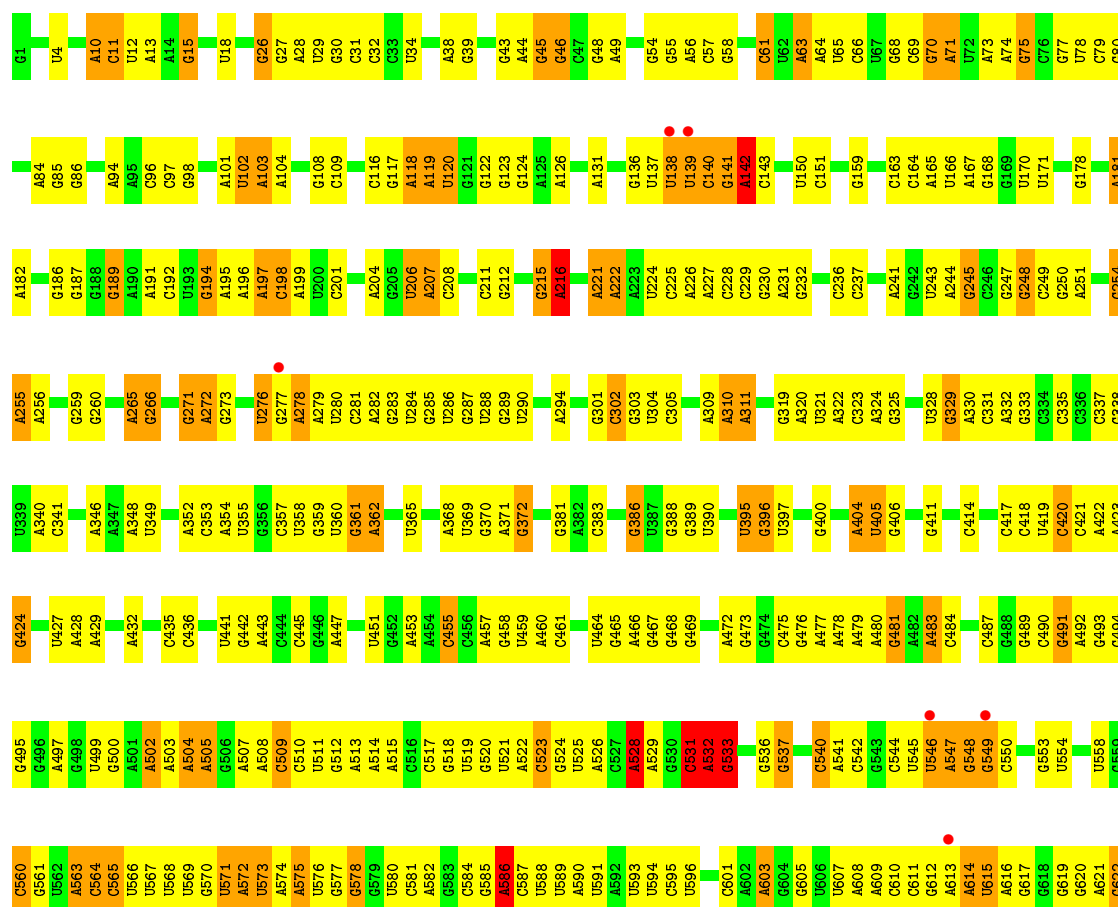
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

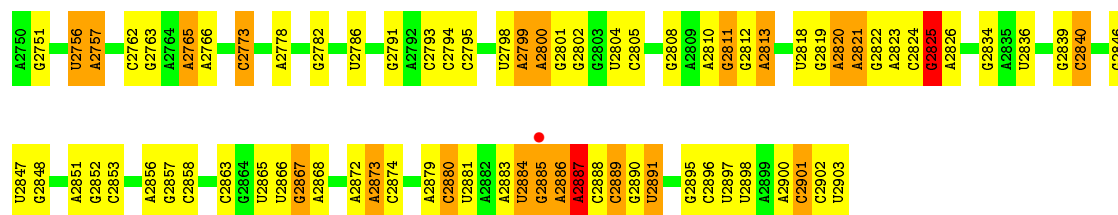


- Molecule 22: 23S rRNA



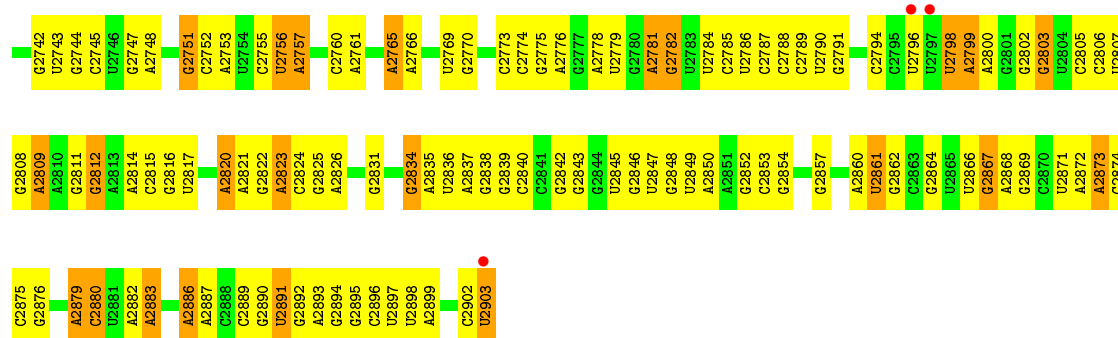
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G1658	C1574	A1496	G1423	A1353	G1280	U1203	G1137	A1073	A1000	A928	C853	G785	G704	G630
G1659	C1575	A1354		G1355	A1283	G1206	G1139	G1074	A1001		G858	A788	A705	A631
G1660	C1576	G1356	G1426	G1356	A1284	G1207	G1140	A1077	C1007	U932	G859	A789	G713	G634
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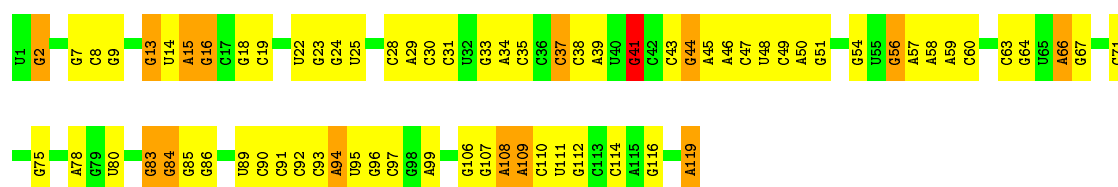
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G1564	U1478	U1478	U1412	U1478	U1412	G1368	C1305	G1245	C1178	A1096	A1032	A960	A825	A825
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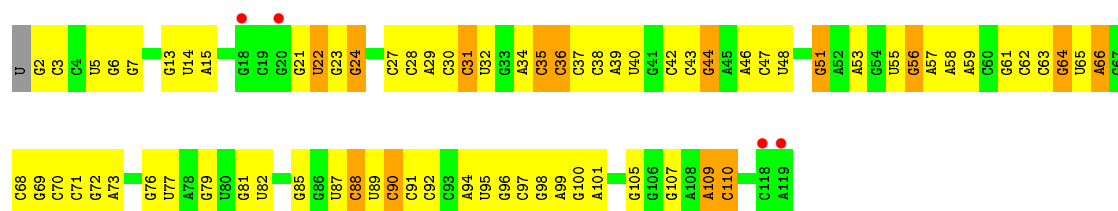
- Molecule 23: 5S rRNA

Chain BB: 39% 48% 12%



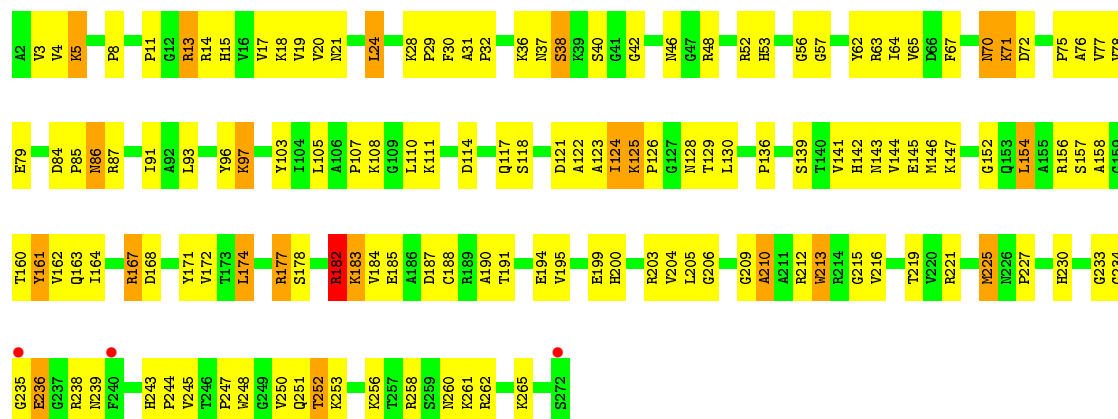
- Molecule 23: 5S rRNA

Chain DB: 3% 37% 50% 12%



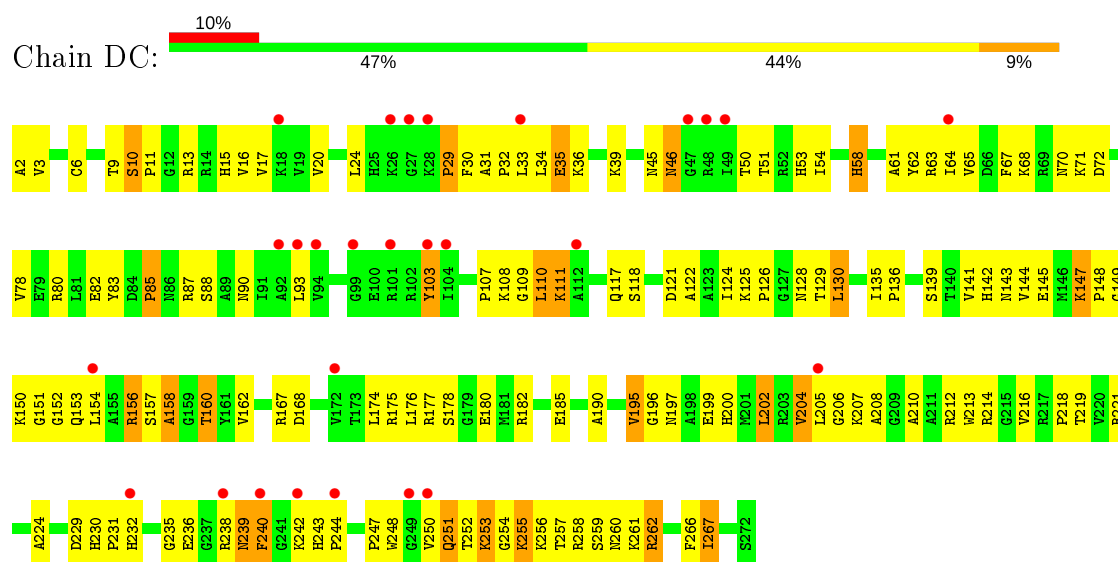
- Molecule 24: 50S ribosomal protein L2

Chain BC: 47% 45% 8%

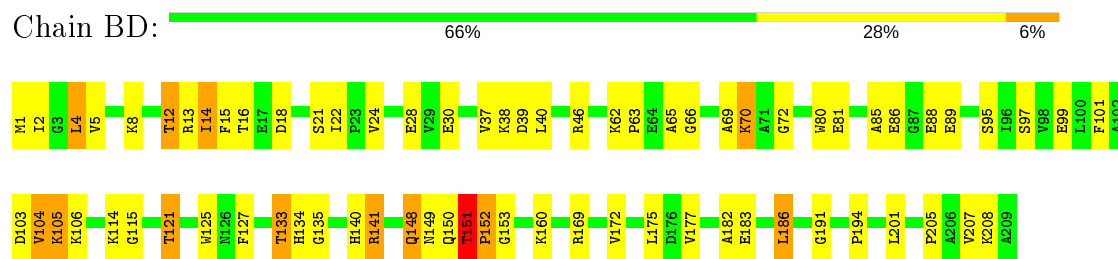


- Molecule 24: 50S ribosomal protein L2

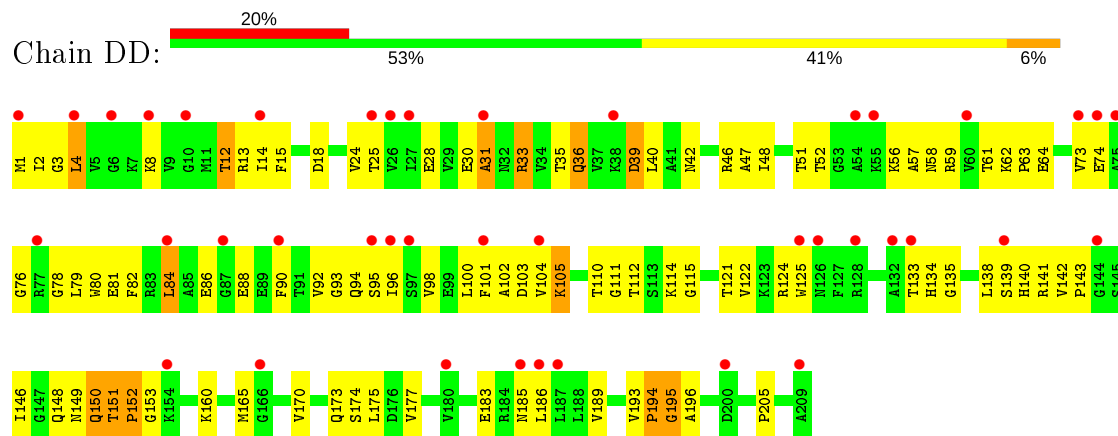




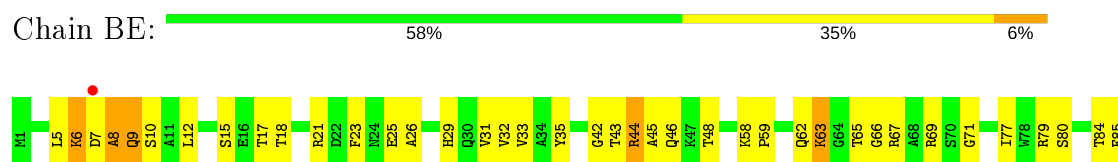
- Molecule 25: 50S ribosomal protein L3

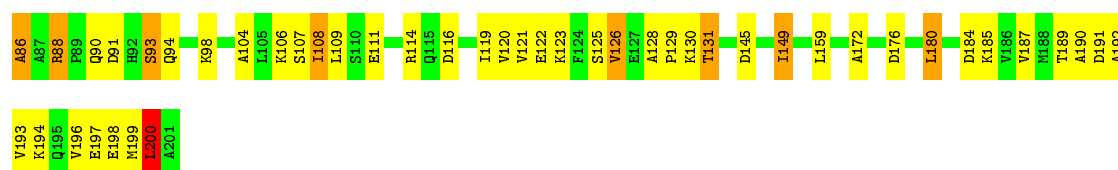


- Molecule 25: 50S ribosomal protein L3

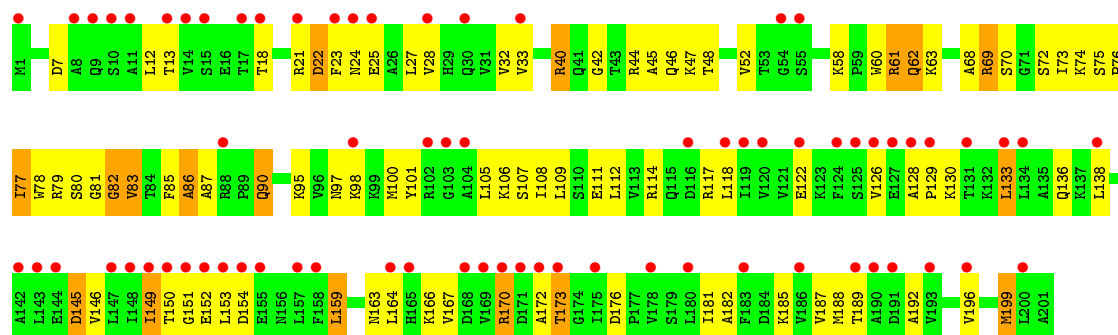
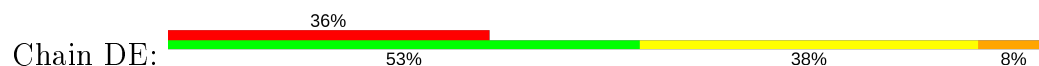


- Molecule 26: 50S ribosomal protein L4

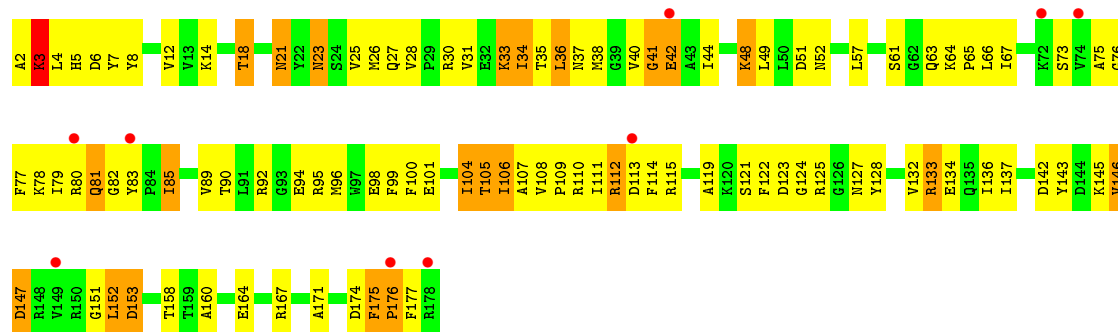
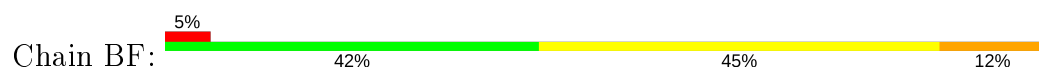




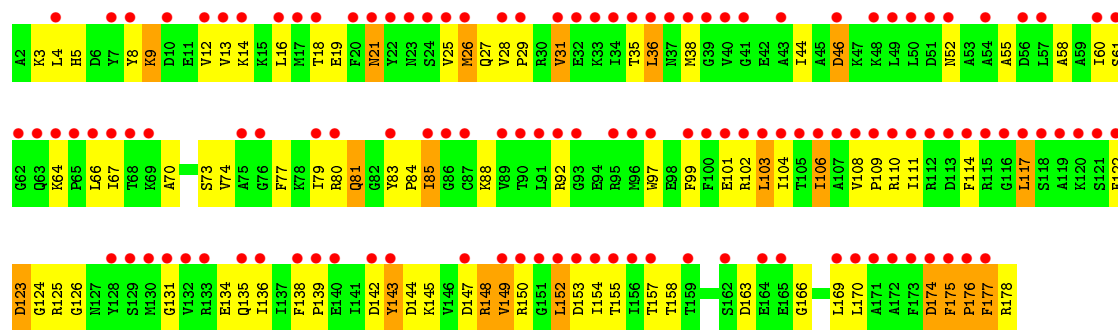
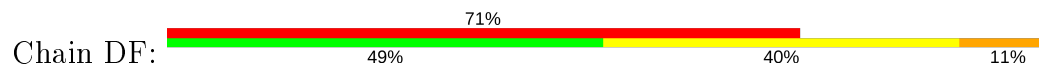
• Molecule 26: 50S ribosomal protein L4



• Molecule 27: 50S ribosomal protein L5

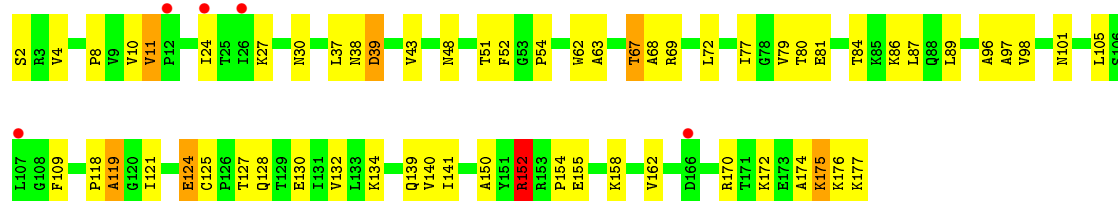


• Molecule 27: 50S ribosomal protein L5



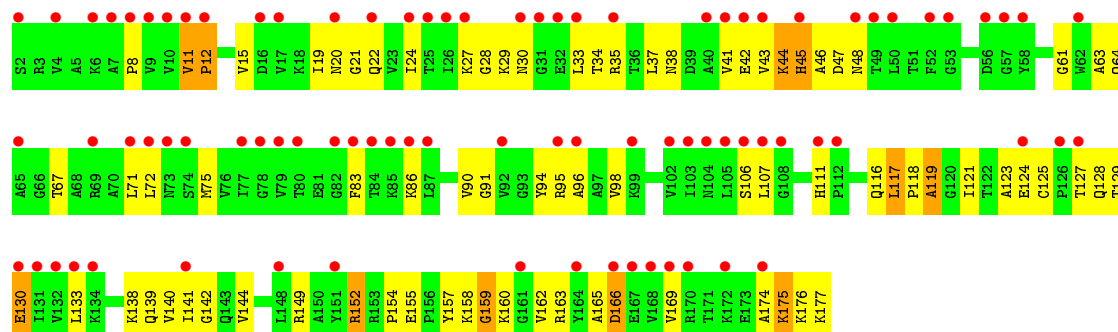
• Molecule 28: 50S ribosomal protein L6

Chain BG: 



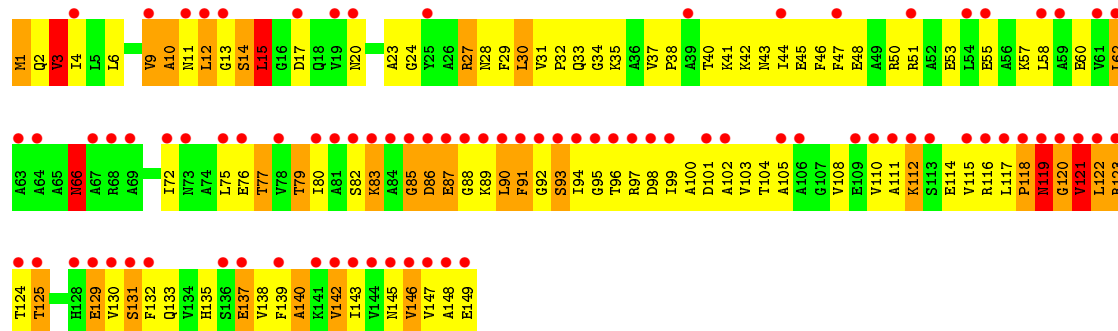
• Molecule 28: 50S ribosomal protein L6

Chain DG: 



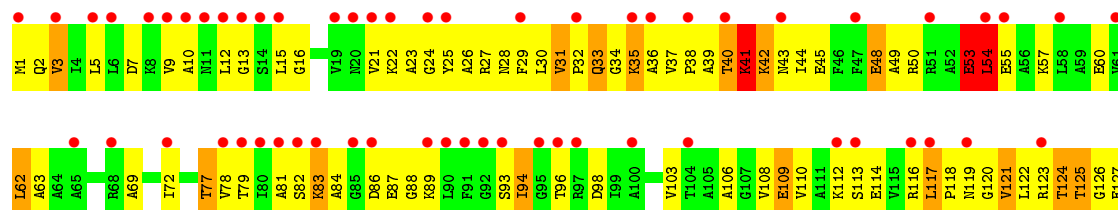
• Molecule 29: 50S ribosomal protein L9

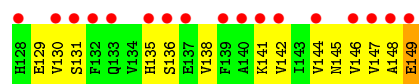
Chain BH: 



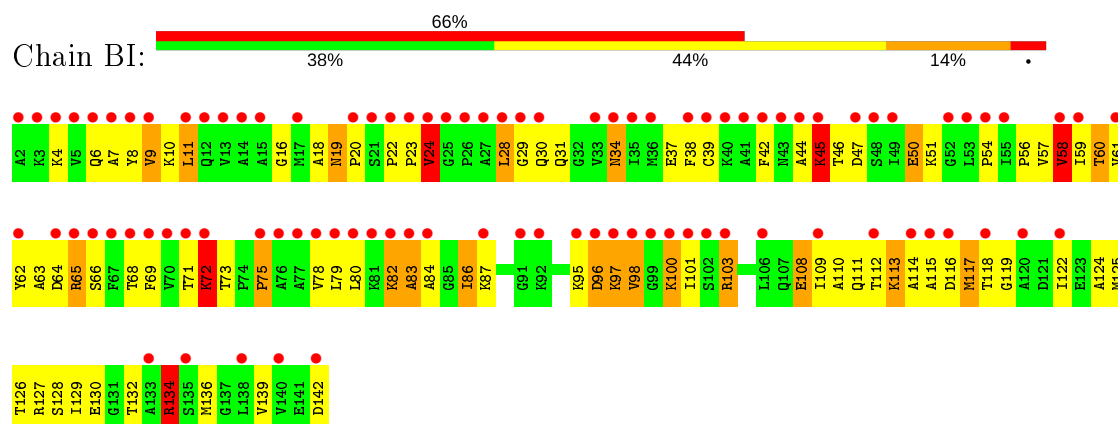
• Molecule 29: 50S ribosomal protein L9

Chain DH: 

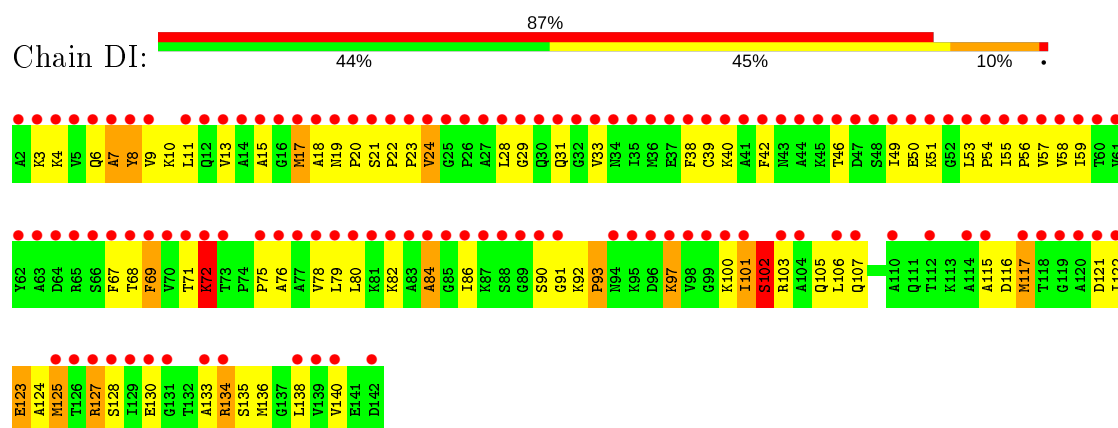




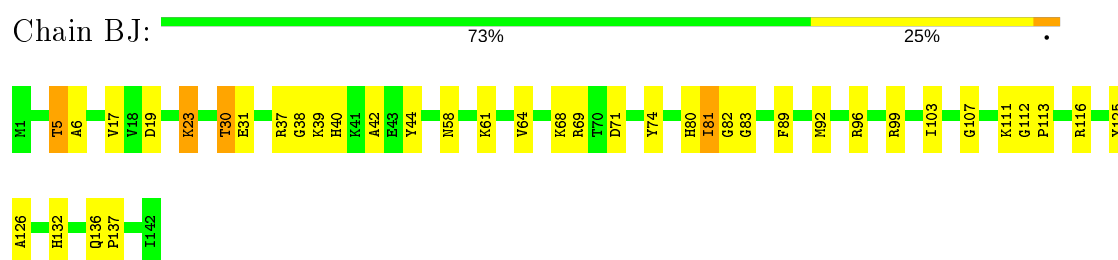
- Molecule 30: 50S ribosomal protein L11



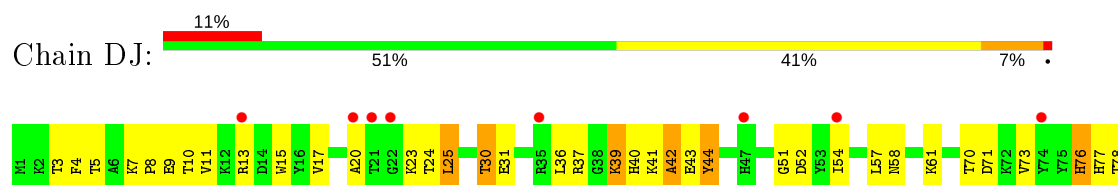
- Molecule 30: 50S ribosomal protein L11



- Molecule 31: 50S ribosomal protein L13

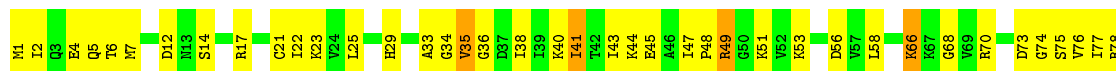


- Molecule 31: 50S ribosomal protein L13

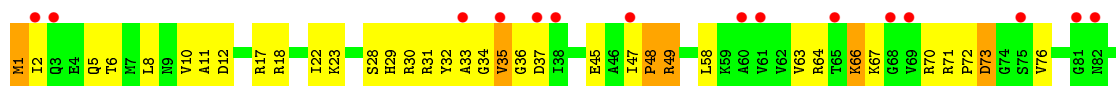




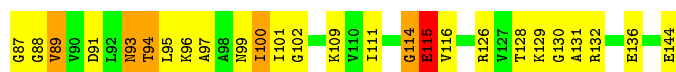
- Molecule 32: 50S ribosomal protein L14



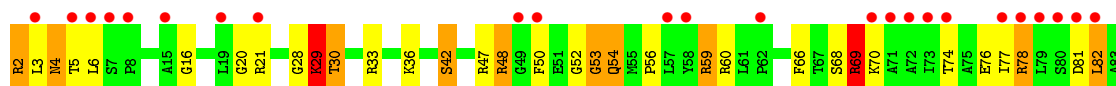
- Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15

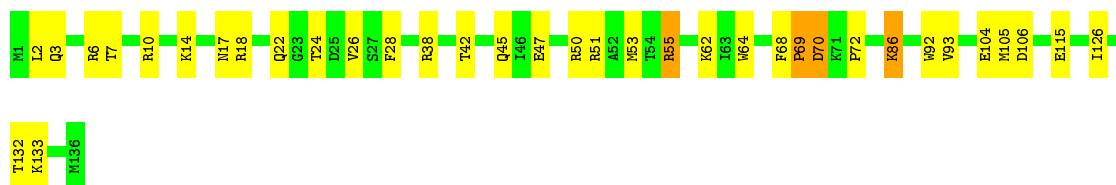


- Molecule 33: 50S ribosomal protein L15

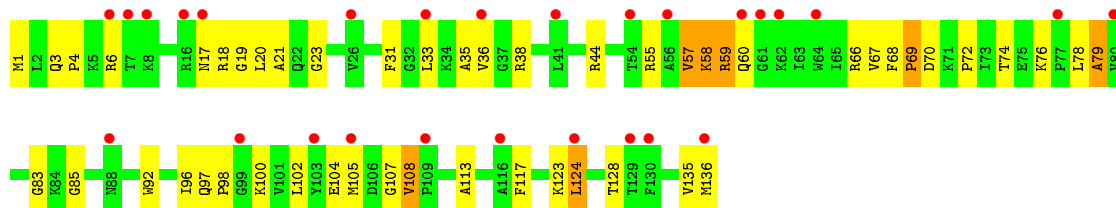


- Molecule 34: 50S ribosomal protein L16

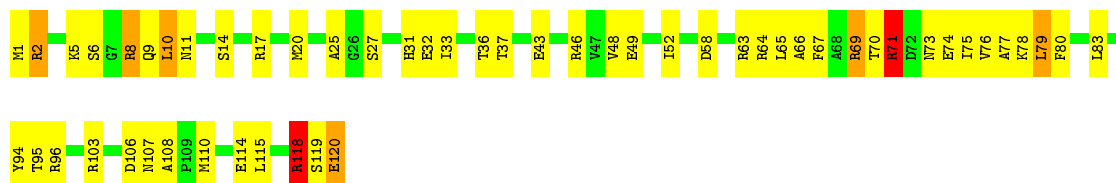




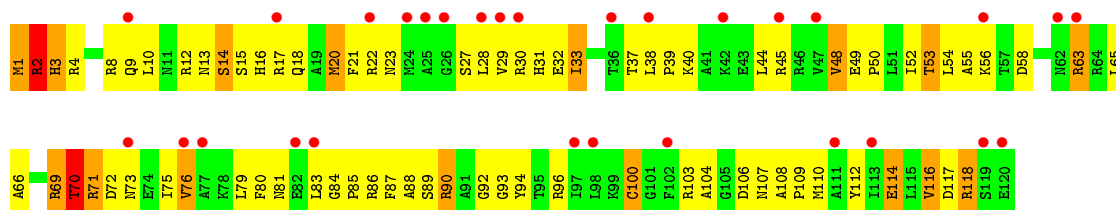
- Molecule 34: 50S ribosomal protein L16



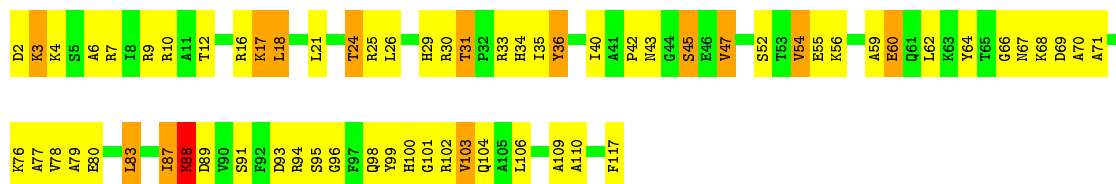
- Molecule 35: 50S ribosomal protein L17



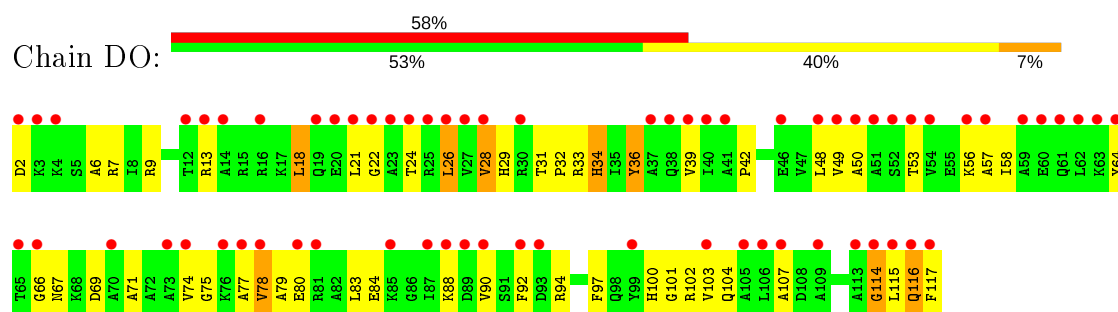
- Molecule 35: 50S ribosomal protein L17



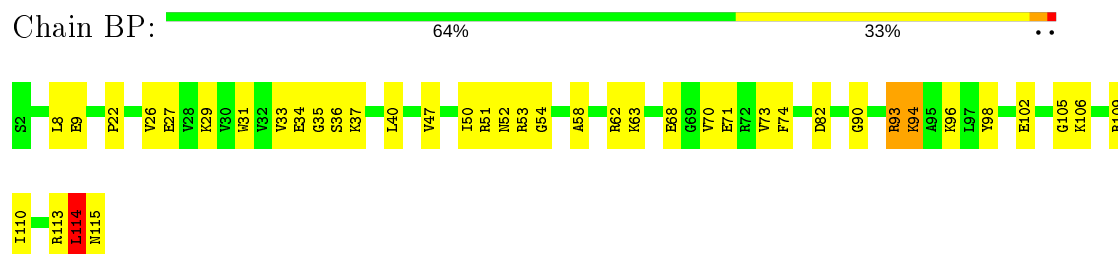
- Molecule 36: 50S ribosomal protein L18



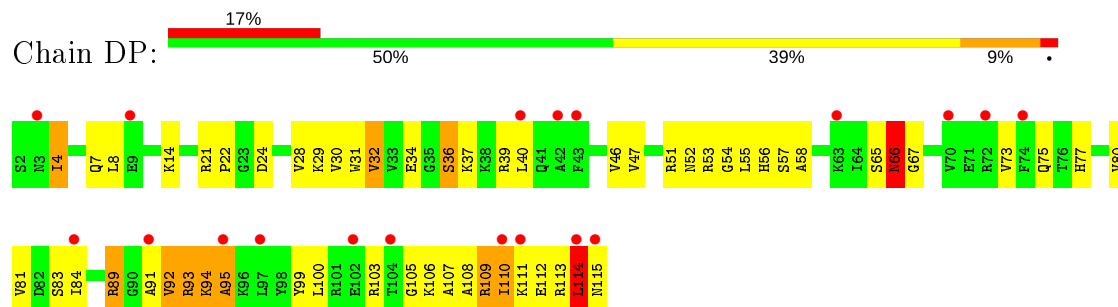
- Molecule 36: 50S ribosomal protein L18



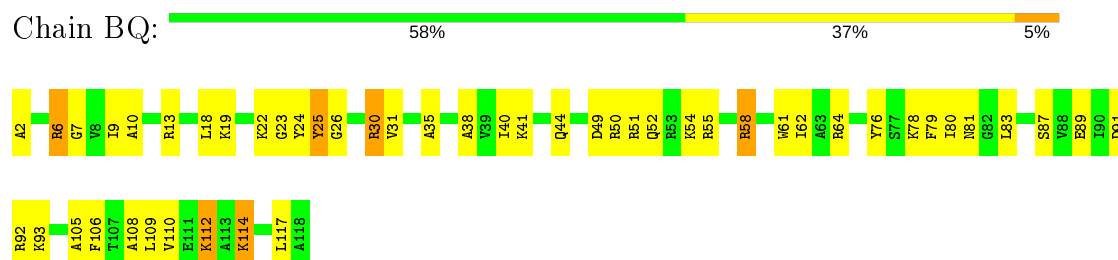
- Molecule 37: 50S ribosomal protein L19



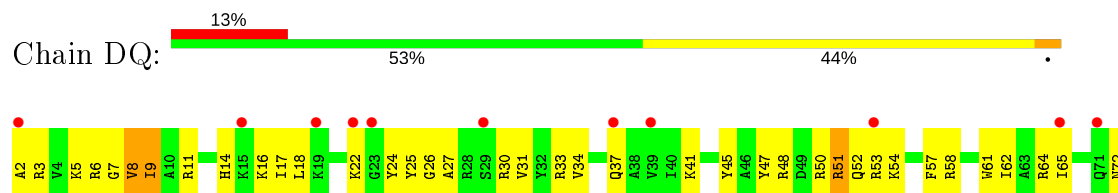
- Molecule 37: 50S ribosomal protein L19

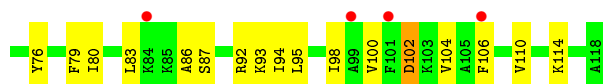


- Molecule 38: 50S ribosomal protein L20

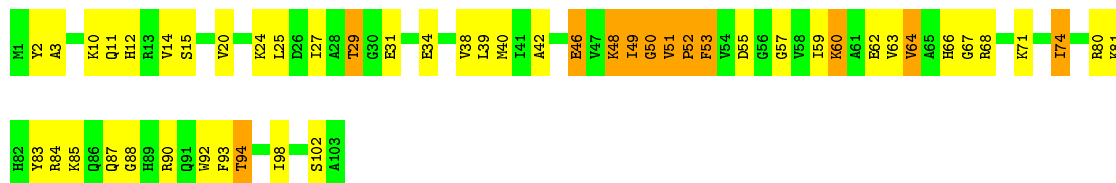


- Molecule 38: 50S ribosomal protein L20

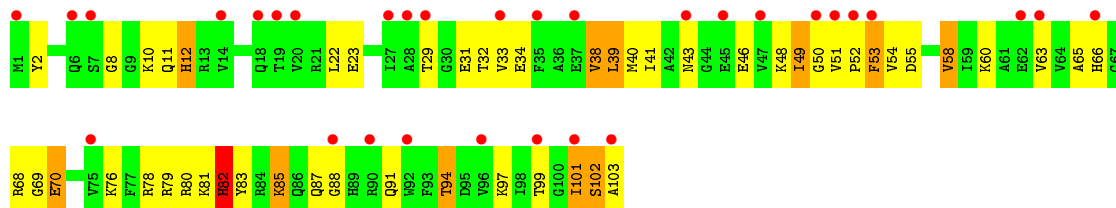




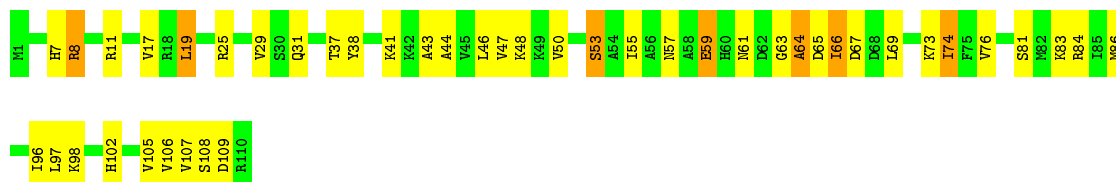
- Molecule 39: 50S ribosomal protein L21



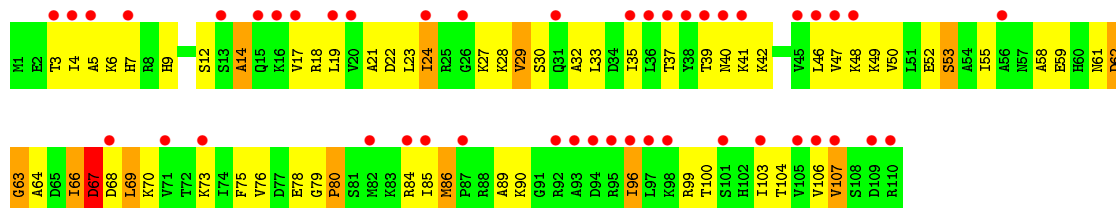
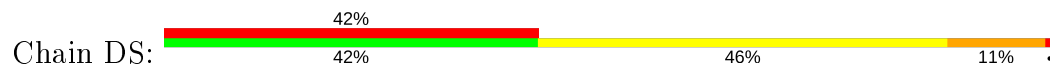
- Molecule 39: 50S ribosomal protein L21



- Molecule 40: 50S ribosomal protein L22



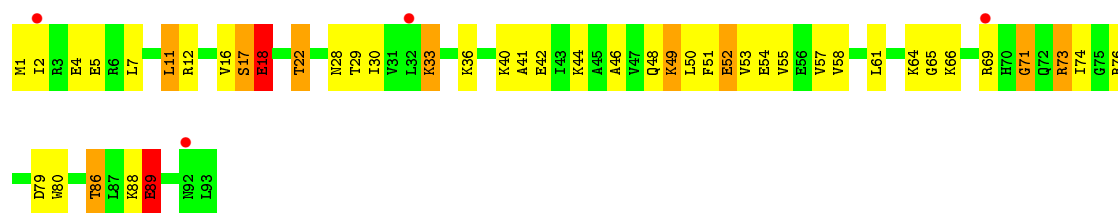
- Molecule 40: 50S ribosomal protein L22



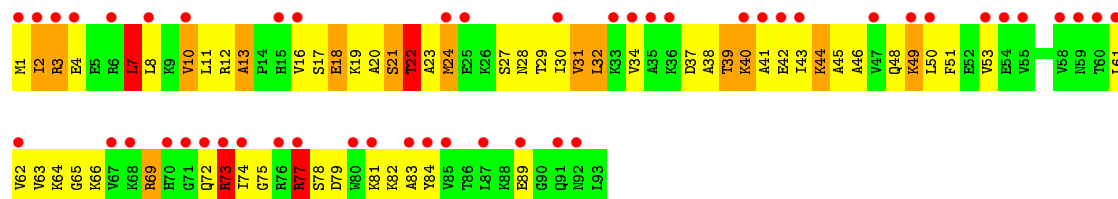
- Molecule 41: 50S ribosomal protein L23



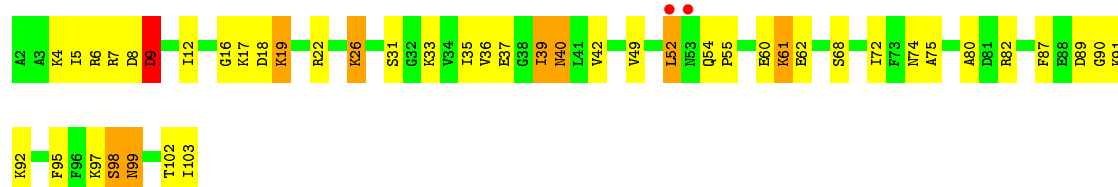




• Molecule 41: 50S ribosomal protein L23



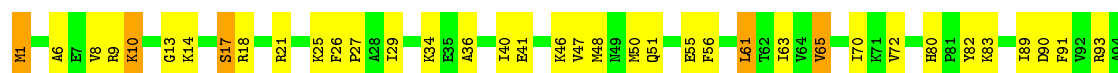
• Molecule 42: 50S ribosomal protein L24



• Molecule 42: 50S ribosomal protein L24

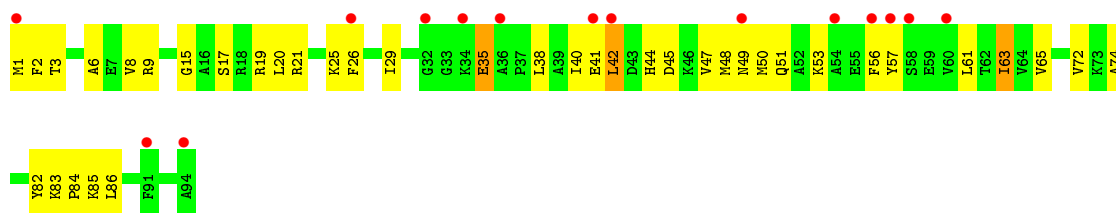


• Molecule 43: 50S ribosomal protein L25



• Molecule 43: 50S ribosomal protein L25

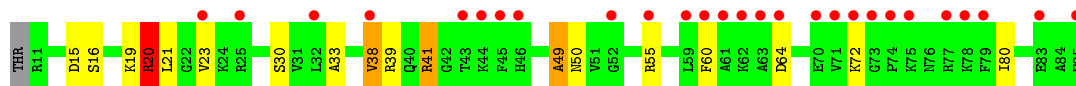
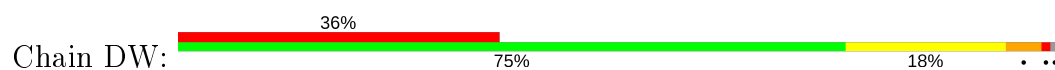




- Molecule 44: 50S ribosomal protein L27



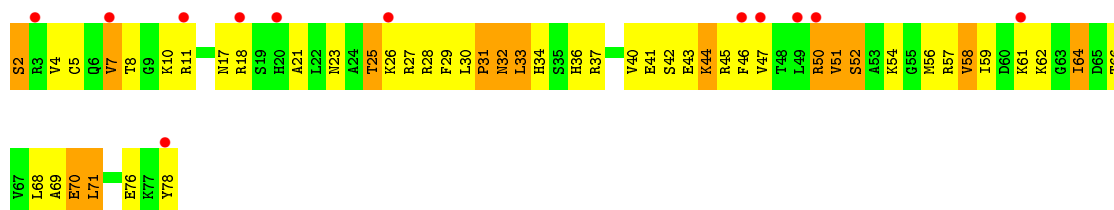
- Molecule 44: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L28



- Molecule 45: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L29

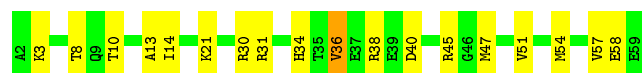


- Molecule 46: 50S ribosomal protein L29

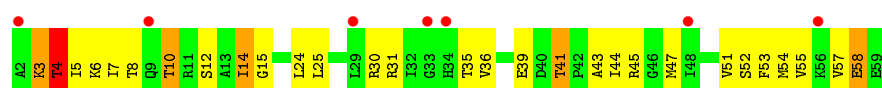




- Molecule 47: 50S ribosomal protein L30



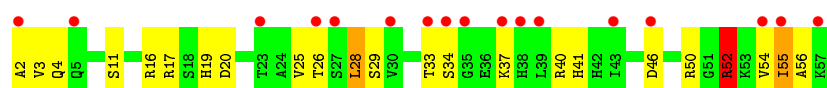
- Molecule 47: 50S ribosomal protein L30



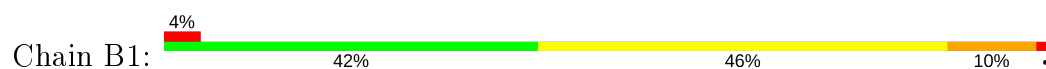
- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32



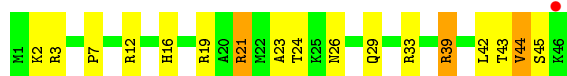
- Molecule 49: 50S ribosomal protein L33



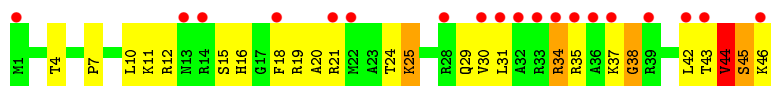
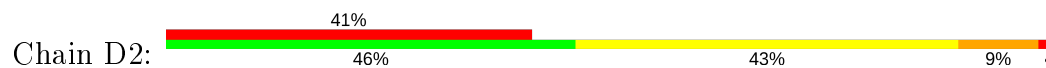
- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34



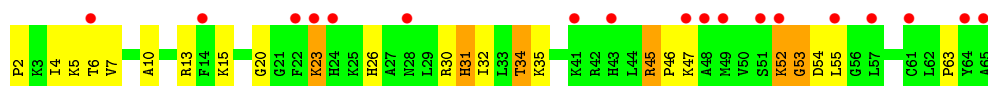
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



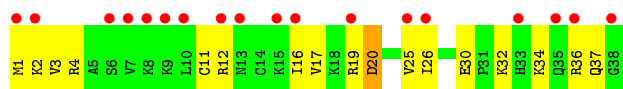
- Molecule 51: 50S ribosomal protein L35



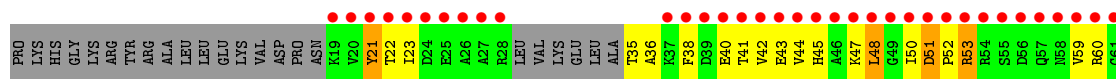
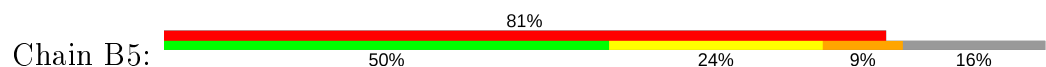
- Molecule 52: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.64Å 434.61Å 625.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.41 – 2.90 69.41 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.0 (69.41-2.90) 90.0 (69.41-2.90)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.223 , 0.265 0.229 , 0.269	Depositor DCC
$R_{free}$ test set	4560 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	288258	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 1.74% 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: VIR, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.48	0/36944	0.93	23/57632 (0.0%)
1	CA	0.41	0/36966	0.88	12/57666 (0.0%)
2	AB	0.34	0/1736	0.59	0/2338
2	CB	0.32	0/1736	0.55	0/2338
3	AC	0.35	0/1652	0.58	0/2225
3	CC	0.31	0/1652	0.51	0/2225
4	AD	0.36	0/1665	0.61	0/2227
4	CD	0.40	0/1665	0.63	0/2227
5	AE	0.38	0/1119	0.65	0/1504
5	CE	0.38	0/1119	0.69	0/1504
6	AF	0.40	0/836	0.66	1/1128 (0.1%)
6	CF	0.33	0/836	0.61	1/1128 (0.1%)
7	AG	0.34	0/1196	0.54	0/1602
7	CG	0.32	0/1196	0.51	0/1602
8	AH	0.40	0/989	0.59	0/1326
8	CH	0.31	0/989	0.54	0/1326
9	AI	0.32	0/1034	0.60	0/1375
9	CI	0.31	0/1034	0.56	0/1375
10	AJ	0.36	0/797	0.58	0/1077
10	CJ	0.32	0/797	0.55	0/1077
11	AK	0.33	0/893	0.58	0/1205
11	CK	0.35	0/893	0.60	0/1205
12	AL	0.40	0/969	0.68	0/1300
12	CL	0.37	0/969	0.66	0/1300
13	AM	0.33	0/893	0.61	0/1193
13	CM	0.32	0/893	0.56	0/1193
14	AN	0.37	0/785	0.59	0/1043
14	CN	0.30	0/785	0.49	0/1043
15	AO	0.33	0/718	0.60	0/959
15	CO	0.31	0/718	0.51	0/959
16	AP	0.38	0/659	0.62	0/884
16	CP	0.33	0/659	0.55	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.38	0/658	0.62	0/881
17	CQ	0.37	0/658	0.57	0/881
18	AR	0.33	0/463	0.54	0/621
18	CR	0.35	0/463	0.58	0/621
19	AS	0.35	0/653	0.60	0/877
19	CS	0.34	0/653	0.53	0/877
20	AT	0.39	0/671	0.60	0/888
20	CT	0.32	0/671	0.55	0/888
21	AU	0.43	0/431	0.65	0/570
21	CU	0.45	0/431	0.63	0/570
22	BA	0.82	19/69659 (0.0%)	1.28	469/108672 (0.4%)
22	DA	0.39	0/69659	0.88	19/108672 (0.0%)
23	BB	0.74	0/2850	1.25	7/4444 (0.2%)
23	DB	0.31	0/2828	0.81	0/4410
24	BC	0.52	0/2122	0.72	1/2852 (0.0%)
24	DC	0.35	0/2122	0.59	0/2852
25	BD	0.58	0/1586	0.75	1/2134 (0.0%)
25	DD	0.33	0/1586	0.55	0/2134
26	BE	0.51	0/1571	0.66	0/2113
26	DE	0.33	0/1571	0.54	0/2113
27	BF	0.41	0/1435	0.63	0/1926
27	DF	0.30	0/1435	0.48	0/1926
28	BG	0.41	0/1343	0.61	0/1816
28	DG	0.30	0/1343	0.48	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	0.36	0/1046	0.57	0/1410
30	DI	0.36	0/1046	0.53	0/1410
31	BJ	0.61	0/1152	0.73	0/1551
31	DJ	0.32	0/1152	0.55	0/1551
32	BK	0.57	0/948	0.76	1/1268 (0.1%)
32	DK	0.36	0/948	0.55	0/1268
33	BL	0.55	0/1054	0.77	0/1403
33	DL	0.32	0/1054	0.58	0/1403
34	BM	0.58	0/1093	0.75	0/1460
34	DM	0.31	0/1093	0.50	0/1460
35	BN	0.57	0/974	0.77	2/1301 (0.2%)
35	DN	0.33	0/974	0.55	0/1301
36	BO	0.48	0/902	0.67	0/1209
36	DO	0.30	0/902	0.49	0/1209
37	BP	0.54	0/929	0.67	0/1242
37	DP	0.34	0/929	0.55	0/1242
38	BQ	0.67	0/960	0.76	0/1278



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DQ	0.33	0/960	0.51	0/1278
39	BR	0.63	0/829	0.83	0/1107
39	DR	0.32	0/829	0.57	0/1107
40	BS	0.66	0/864	0.83	1/1156 (0.1%)
40	DS	0.33	0/864	0.56	0/1156
41	BT	0.48	0/745	0.65	0/994
41	DT	0.32	0/745	0.56	0/994
42	BU	0.46	0/788	0.68	0/1051
42	DU	0.37	0/788	0.56	0/1051
43	BV	0.51	0/766	0.69	0/1025
43	DV	0.28	0/766	0.45	0/1025
44	BW	0.56	0/587	0.70	0/776
44	DW	0.31	0/576	0.50	0/762
45	BX	0.46	0/635	0.65	0/848
45	DX	0.32	0/635	0.55	0/848
46	BY	0.42	0/510	0.66	0/677
46	DY	0.33	0/510	0.55	0/677
47	BZ	0.63	0/453	0.68	0/605
47	DZ	0.30	0/453	0.53	0/605
48	B0	0.58	0/450	0.72	0/599
48	D0	0.34	0/450	0.57	0/599
49	B1	0.45	0/417	0.62	0/554
49	D1	0.33	0/417	0.52	0/554
50	B2	0.57	0/380	0.80	0/498
50	D2	0.36	0/380	0.60	0/498
51	B3	0.52	0/513	0.70	0/676
51	D3	0.32	0/513	0.52	0/676
52	B4	0.57	0/303	0.74	0/397
52	D4	0.30	0/303	0.54	0/397
53	B5	0.33	0/1145	0.50	0/1556
All	All	0.54	19/310626 (0.0%)	0.94	539/464366 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	1
6	CF	0	1
11	AK	0	1
12	CL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	AU	0	1
21	CU	0	1
25	BD	0	1
All	All	0	7

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-11.58	1.30	1.37
22	BA	984	A	N9-C4	-11.48	1.30	1.37
22	BA	1936	A	N9-C4	-9.61	1.32	1.37
22	BA	528	A	N7-C5	-6.85	1.35	1.39
22	BA	752	A	N9-C4	-6.64	1.33	1.37

The worst 5 of 539 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	528	A	N1-C6-N6	15.09	127.66	118.60
22	BA	974	G	C4-C5-N7	14.38	116.55	110.80
22	BA	984	A	C2-N3-C4	-13.21	103.99	110.60
22	BA	984	A	N3-C4-C5	12.10	135.27	126.80
22	BA	1936	A	C2-N3-C4	-11.70	104.75	110.60

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
25	BD	151	THR	Peptide
5	CE	102	GLY	Peptide
6	CF	54	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	1123	4
1	CA	33015	0	16617	1084	0
2	AB	1705	0	1732	191	0
2	CB	1705	0	1732	131	0
3	AC	1625	0	1696	83	0
3	CC	1625	0	1696	69	0
4	AD	1643	0	1707	149	0
4	CD	1643	0	1707	119	0
5	AE	1106	0	1148	74	0
5	CE	1106	0	1148	112	0
6	AF	818	0	808	67	0
6	CF	818	0	808	56	0
7	AG	1182	0	1238	55	0
7	CG	1182	0	1238	65	0
8	AH	979	0	1031	68	0
8	CH	979	0	1031	41	0
9	AI	1022	0	1070	79	0
9	CI	1022	0	1070	63	0
10	AJ	787	0	828	80	0
10	CJ	787	0	828	50	0
11	AK	877	0	887	66	0
11	CK	877	0	887	67	0
12	AL	955	0	1016	66	0
12	CL	955	0	1016	77	0
13	AM	884	0	941	66	0
13	CM	884	0	941	47	0
14	AN	774	0	824	65	0
14	CN	774	0	824	48	0
15	AO	710	0	728	31	0
15	CO	710	0	728	42	0
16	AP	649	0	666	61	0
16	CP	649	0	666	28	0
17	AQ	649	0	691	70	0
17	CQ	649	0	691	53	0
18	AR	456	0	478	21	0
18	CR	456	0	478	33	0
19	AS	638	0	665	54	0
19	CS	638	0	665	36	0
20	AT	665	0	714	56	0
20	CT	665	0	714	43	0
21	AU	426	0	449	58	0
21	CU	426	0	449	54	0
22	BA	62195	0	31280	1616	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	62195	0	31280	2231	0
23	BB	2549	0	1291	52	0
23	DB	2529	0	1281	62	0
24	BC	2083	0	2154	122	0
24	DC	2083	0	2154	127	0
25	BD	1565	0	1616	66	0
25	DD	1565	0	1616	81	0
26	BE	1552	0	1619	69	0
26	DE	1552	0	1619	78	0
27	BF	1411	0	1444	94	0
27	DF	1411	0	1444	62	0
28	BG	1323	0	1371	50	0
28	DG	1323	0	1371	52	0
29	BH	1110	0	1147	154	0
29	DH	1110	0	1148	120	4
30	BI	1032	0	1085	70	0
30	DI	1032	0	1085	67	0
31	BJ	1129	0	1162	37	0
31	DJ	1129	0	1162	54	0
32	BK	939	0	1012	46	0
32	DK	939	0	1012	50	0
33	BL	1045	0	1117	61	0
33	DL	1045	0	1117	66	0
34	BM	1074	0	1157	27	0
34	DM	1074	0	1157	30	0
35	BN	961	0	1000	44	0
35	DN	961	0	1000	70	0
36	BO	892	0	923	55	0
36	DO	892	0	923	44	0
37	BP	917	0	962	31	0
37	DP	917	0	962	45	0
38	BQ	947	0	1019	49	0
38	DQ	947	0	1019	50	0
39	BR	816	0	839	71	0
39	DR	816	0	839	47	0
40	BS	857	0	922	36	0
40	DS	857	0	922	46	0
41	BT	739	0	807	41	0
41	DT	739	0	807	59	0
42	BU	780	0	831	28	0
42	DU	780	0	831	73	0
43	BV	753	0	780	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DV	753	0	780	27	0
44	BW	580	0	594	17	0
44	DW	569	0	581	16	0
45	BX	625	0	652	24	0
45	DX	625	0	652	47	0
46	BY	509	0	543	33	0
46	DY	509	0	543	45	0
47	BZ	449	0	488	10	0
47	DZ	449	0	488	18	0
48	B0	444	0	458	24	0
48	D0	444	0	458	18	0
49	B1	410	0	440	25	0
49	D1	410	0	440	16	0
50	B2	377	0	418	15	0
50	D2	377	0	418	24	0
51	B3	504	0	572	27	0
51	D3	504	0	572	20	0
52	B4	302	0	340	14	0
52	D4	302	0	342	15	0
53	B5	1142	0	865	48	0
54	AA	71	0	0	0	0
54	AN	1	0	0	0	0
54	BA	193	0	0	0	0
54	BB	4	0	0	0	0
54	BD	1	0	0	0	0
54	BQ	1	0	0	0	0
54	CA	56	0	0	0	0
54	D2	1	0	0	0	0
54	DA	166	0	0	0	0
54	DB	3	0	0	0	0
54	DQ	1	0	0	0	0
55	BA	38	0	35	5	0
55	DA	38	0	35	15	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	192	0	0	25	0
57	AL	2	0	0	0	0
57	AN	6	0	0	1	0
57	AT	2	0	0	0	0
57	AU	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B4	2	0	0	0	0
57	BA	620	0	0	65	0
57	BB	13	0	0	0	0
57	BC	7	0	0	1	0
57	BD	3	0	0	2	0
57	BE	4	0	0	0	0
57	BF	1	0	0	1	0
57	BJ	1	0	0	0	0
57	BL	5	0	0	0	0
57	BN	3	0	0	0	0
57	BQ	1	0	0	0	0
57	BS	1	0	0	0	0
57	BT	1	0	0	0	0
57	BV	1	0	0	0	0
57	CA	191	0	0	26	0
57	CL	1	0	0	0	0
57	CN	2	0	0	0	0
57	CT	2	0	0	0	0
57	CU	2	0	0	1	0
57	D2	1	0	0	1	0
57	D3	2	0	0	0	0
57	D4	1	0	0	0	0
57	DA	607	0	0	105	0
57	DB	13	0	0	0	0
57	DC	12	0	0	2	0
57	DD	4	0	0	2	0
57	DE	6	0	0	2	0
57	DJ	1	0	0	0	0
57	DL	4	0	0	1	0
57	DN	2	0	0	0	0
57	DT	1	0	0	0	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
All	All	288258	0	192859	10766	4

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 23.

The worst 5 of 10766 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1153:C:OP2	57:BA:3360:HOH:O	1.56	1.23
22:BA:621:A:OP2	57:BA:3293:HOH:O	1.57	1.23
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
29:BH:123:ARG:HH22	1:CA:367:U:P	1.69	1.15
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14

All (4) 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:AA:368:U:OP1	29:DH:93:SER:OG[4_455]	1.70	0.50
1:AA:367:U:O5'	29:DH:123:ARG:NH2[4_455]	2.02	0.18
1:AA:368:U:O4	29:DH:83:LYS:CE[4_455]	2.03	0.17
1:AA:368:U:O4	29:DH:83:LYS:CB[4_455]	2.13	0.07

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	126 (58%)	40 (18%)	50 (23%)	0	0
2	CB	216/218 (99%)	133 (62%)	52 (24%)	31 (14%)	0	0
3	AC	204/206 (99%)	149 (73%)	38 (19%)	17 (8%)	1	2
3	CC	204/206 (99%)	153 (75%)	40 (20%)	11 (5%)	2	6
4	AD	203/205 (99%)	139 (68%)	33 (16%)	31 (15%)	0	0
4	CD	203/205 (99%)	150 (74%)	31 (15%)	22 (11%)	0	1
5	AE	148/150 (99%)	104 (70%)	31 (21%)	13 (9%)	1	2
5	CE	148/150 (99%)	98 (66%)	28 (19%)	22 (15%)	0	0
6	AF	98/100 (98%)	66 (67%)	19 (19%)	13 (13%)	0	0
6	CF	98/100 (98%)	66 (67%)	16 (16%)	16 (16%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	111 (74%)	28 (19%)	10 (7%)	1	3
7	CG	149/151 (99%)	121 (81%)	20 (13%)	8 (5%)	2	6
8	AH	127/129 (98%)	91 (72%)	21 (16%)	15 (12%)	0	1
8	CH	127/129 (98%)	95 (75%)	24 (19%)	8 (6%)	1	4
9	AI	125/127 (98%)	91 (73%)	21 (17%)	13 (10%)	0	1
9	CI	125/127 (98%)	86 (69%)	28 (22%)	11 (9%)	1	2
10	AJ	96/98 (98%)	60 (62%)	15 (16%)	21 (22%)	0	0
10	CJ	96/98 (98%)	71 (74%)	13 (14%)	12 (12%)	0	0
11	AK	115/117 (98%)	84 (73%)	19 (16%)	12 (10%)	0	1
11	CK	115/117 (98%)	81 (70%)	24 (21%)	10 (9%)	1	2
12	AL	121/123 (98%)	92 (76%)	22 (18%)	7 (6%)	1	5
12	CL	121/123 (98%)	94 (78%)	12 (10%)	15 (12%)	0	1
13	AM	112/114 (98%)	81 (72%)	20 (18%)	11 (10%)	0	1
13	CM	112/114 (98%)	86 (77%)	17 (15%)	9 (8%)	1	2
14	AN	92/100 (92%)	62 (67%)	18 (20%)	12 (13%)	0	0
14	CN	92/100 (92%)	59 (64%)	18 (20%)	15 (16%)	0	0
15	AO	86/88 (98%)	65 (76%)	16 (19%)	5 (6%)	1	5
15	CO	86/88 (98%)	70 (81%)	12 (14%)	4 (5%)	2	8
16	AP	80/82 (98%)	53 (66%)	15 (19%)	12 (15%)	0	0
16	CP	80/82 (98%)	59 (74%)	16 (20%)	5 (6%)	1	4
17	AQ	78/80 (98%)	54 (69%)	15 (19%)	9 (12%)	0	1
17	CQ	78/80 (98%)	56 (72%)	11 (14%)	11 (14%)	0	0
18	AR	53/55 (96%)	43 (81%)	10 (19%)	0	100	100
18	CR	53/55 (96%)	34 (64%)	13 (24%)	6 (11%)	0	1
19	AS	77/79 (98%)	54 (70%)	12 (16%)	11 (14%)	0	0
19	CS	77/79 (98%)	60 (78%)	12 (16%)	5 (6%)	1	3
20	AT	83/85 (98%)	60 (72%)	15 (18%)	8 (10%)	0	1
20	CT	83/85 (98%)	64 (77%)	12 (14%)	7 (8%)	1	2
21	AU	49/51 (96%)	27 (55%)	9 (18%)	13 (26%)	0	0
21	CU	49/51 (96%)	26 (53%)	12 (24%)	11 (22%)	0	0
24	BC	269/271 (99%)	211 (78%)	47 (18%)	11 (4%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	204 (76%)	50 (19%)	15 (6%)	2	5
25	BD	207/209 (99%)	180 (87%)	20 (10%)	7 (3%)	3	15
25	DD	207/209 (99%)	168 (81%)	29 (14%)	10 (5%)	2	8
26	BE	199/201 (99%)	167 (84%)	26 (13%)	6 (3%)	4	17
26	DE	199/201 (99%)	160 (80%)	28 (14%)	11 (6%)	2	5
27	BF	175/177 (99%)	144 (82%)	24 (14%)	7 (4%)	3	11
27	DF	175/177 (99%)	137 (78%)	24 (14%)	14 (8%)	1	2
28	BG	174/176 (99%)	149 (86%)	20 (12%)	5 (3%)	4	18
28	DG	174/176 (99%)	136 (78%)	29 (17%)	9 (5%)	2	6
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%)	85 (61%)	36 (26%)	18 (13%)	0	0
30	DI	139/141 (99%)	82 (59%)	44 (32%)	13 (9%)	0	1
31	BJ	140/142 (99%)	129 (92%)	10 (7%)	1 (1%)	22	54
31	DJ	140/142 (99%)	118 (84%)	17 (12%)	5 (4%)	3	14
32	BK	120/122 (98%)	99 (82%)	15 (12%)	6 (5%)	2	7
32	DK	120/122 (98%)	100 (83%)	13 (11%)	7 (6%)	1	5
33	BL	141/143 (99%)	112 (79%)	22 (16%)	7 (5%)	2	7
33	DL	141/143 (99%)	99 (70%)	29 (21%)	13 (9%)	1	1
34	BM	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	10	34
34	DM	134/136 (98%)	111 (83%)	15 (11%)	8 (6%)	1	4
35	BN	118/120 (98%)	104 (88%)	10 (8%)	4 (3%)	3	15
35	DN	118/120 (98%)	94 (80%)	16 (14%)	8 (7%)	1	3
36	BO	114/116 (98%)	87 (76%)	21 (18%)	6 (5%)	2	6
36	DO	114/116 (98%)	85 (75%)	22 (19%)	7 (6%)	1	4
37	BP	112/114 (98%)	99 (88%)	9 (8%)	4 (4%)	3	14
37	DP	112/114 (98%)	84 (75%)	16 (14%)	12 (11%)	0	1
38	BQ	115/117 (98%)	109 (95%)	4 (4%)	2 (2%)	9	31
38	DQ	115/117 (98%)	101 (88%)	13 (11%)	1 (1%)	17	48
39	BR	101/103 (98%)	84 (83%)	9 (9%)	8 (8%)	1	2
39	DR	101/103 (98%)	76 (75%)	18 (18%)	7 (7%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	98 (91%)	7 (6%)	3 (3%)	5	19
40	DS	108/110 (98%)	88 (82%)	12 (11%)	8 (7%)	1	2
41	BT	91/93 (98%)	72 (79%)	13 (14%)	6 (7%)	1	3
41	DT	91/93 (98%)	52 (57%)	28 (31%)	11 (12%)	0	1
42	BU	100/102 (98%)	76 (76%)	16 (16%)	8 (8%)	1	2
42	DU	100/102 (98%)	71 (71%)	16 (16%)	13 (13%)	0	0
43	BV	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
43	DV	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	14	42
44	BW	74/76 (97%)	68 (92%)	5 (7%)	1 (1%)	11	36
44	DW	73/76 (96%)	63 (86%)	8 (11%)	2 (3%)	5	19
45	BX	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	12	37
45	DX	75/77 (97%)	55 (73%)	12 (16%)	8 (11%)	0	1
46	BY	61/63 (97%)	47 (77%)	7 (12%)	7 (12%)	0	1
46	DY	61/63 (97%)	43 (70%)	13 (21%)	5 (8%)	1	2
47	BZ	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
47	DZ	56/58 (97%)	47 (84%)	6 (11%)	3 (5%)	2	6
48	B0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	3	13
48	D0	54/56 (96%)	39 (72%)	13 (24%)	2 (4%)	3	13
49	B1	48/50 (96%)	39 (81%)	5 (10%)	4 (8%)	1	2
49	D1	48/50 (96%)	37 (77%)	8 (17%)	3 (6%)	1	4
50	B2	44/46 (96%)	40 (91%)	3 (7%)	1 (2%)	6	23
50	D2	44/46 (96%)	33 (75%)	8 (18%)	3 (7%)	1	3
51	B3	62/64 (97%)	55 (89%)	6 (10%)	1 (2%)	9	32
51	D3	62/64 (97%)	46 (74%)	13 (21%)	3 (5%)	2	8
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	19
53	B5	183/228 (80%)	97 (53%)	57 (31%)	29 (16%)	0	0
All	All	11418/11672 (98%)	8663 (76%)	1837 (16%)	918 (8%)	1	2

5 of 918 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE

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Mol	Chain	Res	Type
2	AB	21	ARG
2	AB	22	TYR
2	AB	34	ALA
2	AB	64	LYS

### 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%)	133 (74%)	47 (26%)	0	1
2	CB	180/180 (100%)	140 (78%)	40 (22%)	1	3
3	AC	170/170 (100%)	134 (79%)	36 (21%)	1	3
3	CC	170/170 (100%)	136 (80%)	34 (20%)	1	4
4	AD	172/172 (100%)	136 (79%)	36 (21%)	1	3
4	CD	172/172 (100%)	145 (84%)	27 (16%)	2	8
5	AE	113/113 (100%)	87 (77%)	26 (23%)	1	2
5	CE	113/113 (100%)	87 (77%)	26 (23%)	1	2
6	AF	87/87 (100%)	61 (70%)	26 (30%)	0	1
6	CF	87/87 (100%)	62 (71%)	25 (29%)	0	1
7	AG	124/124 (100%)	95 (77%)	29 (23%)	1	2
7	CG	124/124 (100%)	89 (72%)	35 (28%)	0	1
8	AH	104/104 (100%)	87 (84%)	17 (16%)	2	7
8	CH	104/104 (100%)	84 (81%)	20 (19%)	1	4
9	AI	105/105 (100%)	71 (68%)	34 (32%)	0	0
9	CI	105/105 (100%)	77 (73%)	28 (27%)	0	1
10	AJ	86/86 (100%)	69 (80%)	17 (20%)	1	4
10	CJ	86/86 (100%)	67 (78%)	19 (22%)	1	3
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	3
11	CK	90/90 (100%)	68 (76%)	22 (24%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	87 (84%)	16 (16%)	2	8
12	CL	103/103 (100%)	83 (81%)	20 (19%)	1	4
13	AM	92/92 (100%)	72 (78%)	20 (22%)	1	3
13	CM	92/92 (100%)	71 (77%)	21 (23%)	1	2
14	AN	79/83 (95%)	64 (81%)	15 (19%)	1	4
14	CN	79/83 (95%)	65 (82%)	14 (18%)	2	5
15	AO	75/76 (99%)	61 (81%)	14 (19%)	1	5
15	CO	75/76 (99%)	58 (77%)	17 (23%)	1	2
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	2
16	CP	65/65 (100%)	51 (78%)	14 (22%)	1	3
17	AQ	74/74 (100%)	52 (70%)	22 (30%)	0	1
17	CQ	74/74 (100%)	50 (68%)	24 (32%)	0	0
18	AR	48/48 (100%)	37 (77%)	11 (23%)	1	2
18	CR	48/48 (100%)	37 (77%)	11 (23%)	1	2
19	AS	70/70 (100%)	58 (83%)	12 (17%)	2	6
19	CS	70/70 (100%)	59 (84%)	11 (16%)	2	8
20	AT	65/65 (100%)	50 (77%)	15 (23%)	1	2
20	CT	65/65 (100%)	48 (74%)	17 (26%)	0	1
21	AU	44/44 (100%)	26 (59%)	18 (41%)	0	0
21	CU	44/44 (100%)	25 (57%)	19 (43%)	0	0
24	BC	216/216 (100%)	184 (85%)	32 (15%)	3	9
24	DC	216/216 (100%)	185 (86%)	31 (14%)	3	9
25	BD	164/164 (100%)	152 (93%)	12 (7%)	14	38
25	DD	164/164 (100%)	146 (89%)	18 (11%)	6	19
26	BE	165/165 (100%)	142 (86%)	23 (14%)	3	10
26	DE	165/165 (100%)	142 (86%)	23 (14%)	3	10
27	BF	148/148 (100%)	121 (82%)	27 (18%)	1	5
27	DF	148/148 (100%)	124 (84%)	24 (16%)	2	7
28	BG	137/137 (100%)	127 (93%)	10 (7%)	14	38
28	DG	137/137 (100%)	121 (88%)	16 (12%)	5	16
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	2
30	BI	109/109 (100%)	80 (73%)	29 (27%)	0	1
30	DI	109/109 (100%)	84 (77%)	25 (23%)	1	2
31	BJ	116/116 (100%)	111 (96%)	5 (4%)	29	62
31	DJ	116/116 (100%)	101 (87%)	15 (13%)	4	13
32	BK	103/103 (100%)	91 (88%)	12 (12%)	5	16
32	DK	103/103 (100%)	96 (93%)	7 (7%)	16	42
33	BL	102/102 (100%)	88 (86%)	14 (14%)	3	11
33	DL	102/102 (100%)	89 (87%)	13 (13%)	4	13
34	BM	109/109 (100%)	102 (94%)	7 (6%)	17	45
34	DM	109/109 (100%)	101 (93%)	8 (7%)	14	38
35	BN	100/100 (100%)	90 (90%)	10 (10%)	7	23
35	DN	100/100 (100%)	80 (80%)	20 (20%)	1	4
36	BO	86/86 (100%)	70 (81%)	16 (19%)	1	5
36	DO	86/86 (100%)	73 (85%)	13 (15%)	3	9
37	BP	99/99 (100%)	91 (92%)	8 (8%)	11	33
37	DP	99/99 (100%)	84 (85%)	15 (15%)	3	8
38	BQ	89/89 (100%)	81 (91%)	8 (9%)	9	29
38	DQ	89/89 (100%)	78 (88%)	11 (12%)	4	14
39	BR	84/84 (100%)	72 (86%)	12 (14%)	3	10
39	DR	84/84 (100%)	68 (81%)	16 (19%)	1	4
40	BS	93/93 (100%)	80 (86%)	13 (14%)	3	10
40	DS	93/93 (100%)	80 (86%)	13 (14%)	3	10
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%)	73 (88%)	10 (12%)	5	15
42	DU	83/83 (100%)	66 (80%)	17 (20%)	1	3
43	BV	78/78 (100%)	69 (88%)	9 (12%)	5	17
43	DV	78/78 (100%)	65 (83%)	13 (17%)	2	6
44	BW	57/58 (98%)	50 (88%)	7 (12%)	4	14
44	DW	56/58 (97%)	51 (91%)	5 (9%)	9	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	56 (84%)	11 (16%)	2	7
45	DX	67/67 (100%)	54 (81%)	13 (19%)	1	4
46	BY	55/55 (100%)	47 (86%)	8 (14%)	3	9
46	DY	55/55 (100%)	45 (82%)	10 (18%)	1	5
47	BZ	48/48 (100%)	44 (92%)	4 (8%)	11	32
47	DZ	48/48 (100%)	37 (77%)	11 (23%)	1	2
48	B0	47/47 (100%)	41 (87%)	6 (13%)	4	13
48	D0	47/47 (100%)	43 (92%)	4 (8%)	10	31
49	B1	45/45 (100%)	38 (84%)	7 (16%)	2	8
49	D1	45/45 (100%)	41 (91%)	4 (9%)	9	29
50	B2	38/38 (100%)	33 (87%)	5 (13%)	4	12
50	D2	38/38 (100%)	31 (82%)	7 (18%)	1	5
51	B3	51/51 (100%)	48 (94%)	3 (6%)	19	49
51	D3	51/51 (100%)	44 (86%)	7 (14%)	3	11
52	B4	34/34 (100%)	28 (82%)	6 (18%)	2	5
52	D4	34/34 (100%)	30 (88%)	4 (12%)	5	16
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1	3
All	All	9386/9518 (99%)	7728 (82%)	1658 (18%)	2	5

5 of 1658 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BX	18	ARG
5	CE	115	LEU
39	DR	85	LYS
48	B0	18	SER
2	CB	163	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	CC	176	HIS
8	CH	18	GLN
46	DY	41	HIS
4	CD	74	ASN

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Mol	Chain	Res	Type
4	CD	198	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	321 (20%)	13 (0%)
1	CA	1538/1539 (99%)	312 (20%)	8 (0%)
22	BA	2895/2903 (99%)	513 (17%)	22 (0%)
22	DA	2895/2903 (99%)	635 (21%)	23 (0%)
23	BB	118/119 (99%)	18 (15%)	0
23	DB	117/119 (98%)	22 (18%)	0
All	All	9100/9122 (99%)	1821 (20%)	66 (0%)

5 of 1821 RNA backbone outliers are listed below:

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

5 of 66 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2211	A
1	CA	115	G
22	DA	2286	G
22	BA	2282	G
22	BA	2756	U

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	$\# Z  > 2$
55	VIR	BA	3001	-	34,40,40	3.45	12 (35%)	36,55,55	3.55	19 (52%)
55	VIR	DA	3001	-	34,40,40	3.42	12 (35%)	36,55,55	3.29	14 (38%)

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
55	VIR	BA	3001	-	-	15/42/58/58	0/2/3/3
55	VIR	DA	3001	-	-	17/42/58/58	0/2/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BA	3001	VIR	C28-C29	9.76	1.55	1.32
55	DA	3001	VIR	C28-C29	9.47	1.54	1.32
55	BA	3001	VIR	C22-C23	9.35	1.56	1.32
55	DA	3001	VIR	C22-C23	9.13	1.55	1.32
55	DA	3001	VIR	C26-N25	6.85	1.49	1.34

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	3001	VIR	C23-C22-C20	-9.51	111.52	125.89
55	BA	3001	VIR	C23-C22-C20	-8.91	112.42	125.89
55	BA	3001	VIR	O36-C37-C1	7.69	119.90	110.53
55	BA	3001	VIR	C37-C1-N5	-7.46	113.59	123.15
55	DA	3001	VIR	O36-C37-C1	7.40	119.54	110.53



There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	BA	3001	VIR	C2-C1-C37-O36
55	BA	3001	VIR	C17-C19-C20-C21
55	BA	3001	VIR	C20-C22-C23-C24
55	BA	3001	VIR	O7-C6-N5-C4
55	DA	3001	VIR	C17-C19-C20-C21

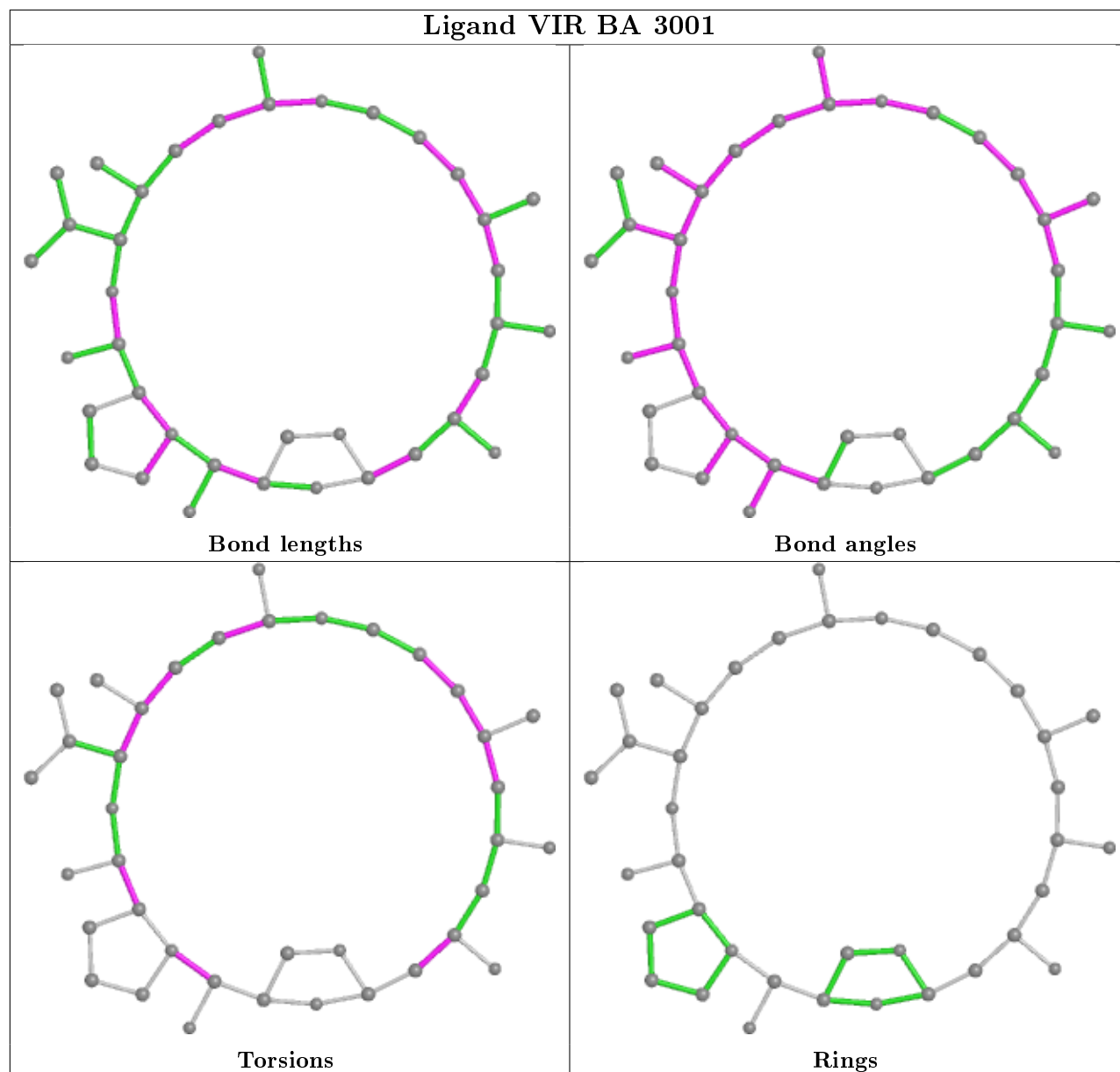
There are no ring outliers.

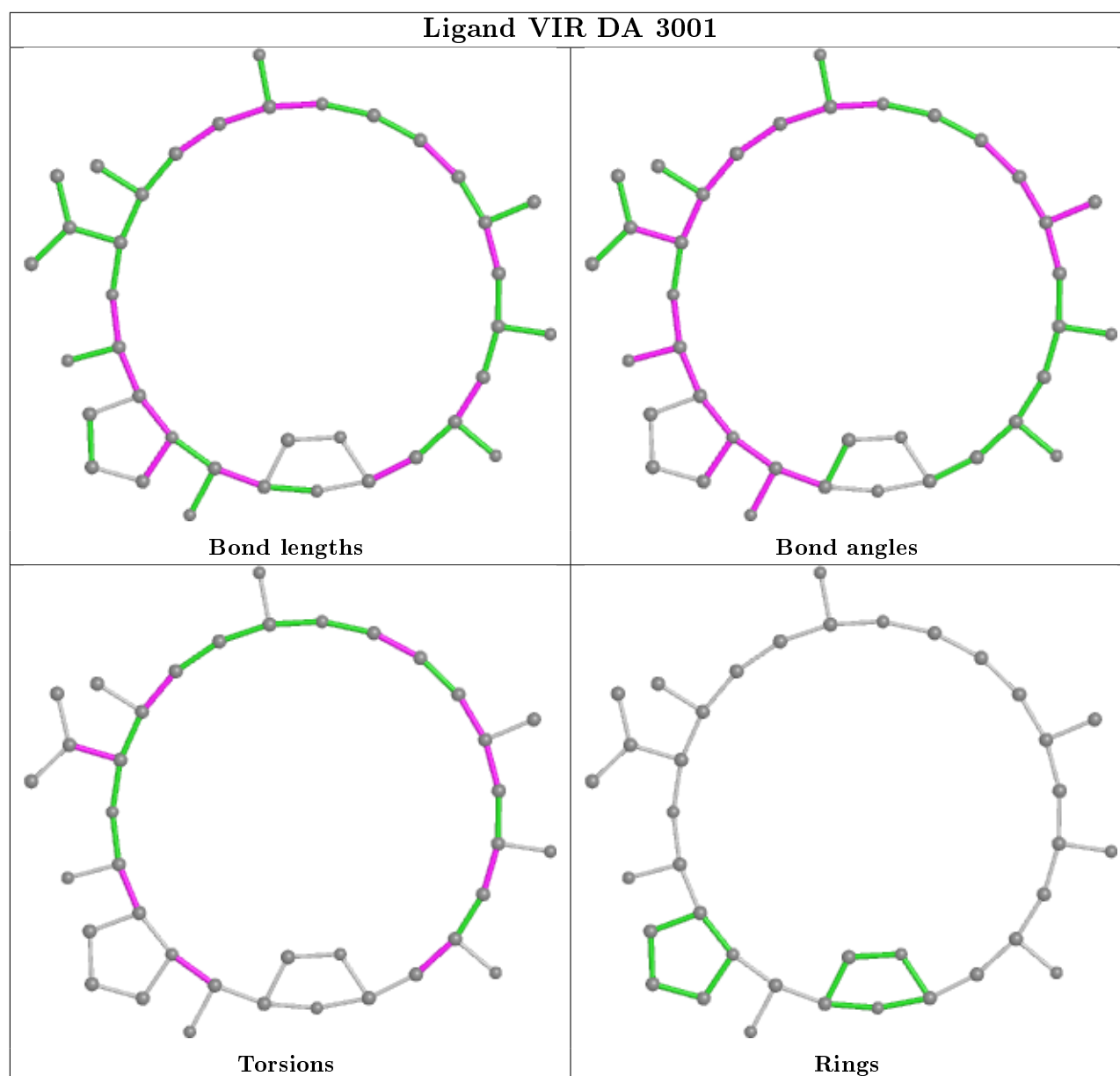
2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	BA	3001	VIR	5	0
55	DA	3001	VIR	15	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.

## Ligand VIR BA 3001





## 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%)	-0.15	26 (1%) 70 69	12, 51, 134, 181	0
1	CA	1539/1539 (100%)	0.17	68 (4%) 34 30	25, 70, 145, 177	0
2	AB	218/218 (100%)	1.00	31 (14%) 2 2	38, 75, 100, 123	0
2	CB	218/218 (100%)	1.22	58 (26%) 0 0	61, 87, 107, 126	0
3	AC	206/206 (100%)	0.25	11 (5%) 26 22	35, 57, 78, 93	0
3	CC	206/206 (100%)	1.62	78 (37%) 0 0	51, 80, 95, 105	0
4	AD	205/205 (100%)	0.32	6 (2%) 51 47	33, 56, 78, 104	0
4	CD	205/205 (100%)	0.02	6 (2%) 51 47	17, 38, 63, 87	0
5	AE	150/150 (100%)	0.08	2 (1%) 77 77	32, 48, 79, 101	0
5	CE	150/150 (100%)	0.25	5 (3%) 46 41	30, 56, 82, 103	0
6	AF	100/100 (100%)	-0.11	1 (1%) 82 82	34, 57, 73, 87	0
6	CF	100/100 (100%)	0.30	6 (6%) 21 18	45, 74, 94, 105	0
7	AG	151/151 (100%)	0.63	15 (9%) 7 5	54, 77, 96, 103	0
7	CG	151/151 (100%)	2.65	85 (56%) 0 0	82, 101, 110, 115	0
8	AH	129/129 (100%)	0.19	1 (0%) 86 86	31, 49, 66, 75	0
8	CH	129/129 (100%)	0.45	7 (5%) 25 22	50, 65, 81, 92	0
9	AI	127/127 (100%)	0.99	23 (18%) 1 1	44, 74, 96, 110	0
9	CI	127/127 (100%)	2.15	55 (43%) 0 0	73, 94, 111, 122	0
10	AJ	98/98 (100%)	0.71	12 (12%) 4 3	39, 66, 92, 122	0
10	CJ	98/98 (100%)	2.91	58 (59%) 0 0	71, 95, 111, 126	0
11	AK	117/117 (100%)	0.62	11 (9%) 8 6	26, 65, 92, 117	0
11	CK	117/117 (100%)	0.43	6 (5%) 28 24	38, 67, 80, 92	0
12	AL	123/123 (100%)	0.18	5 (4%) 37 32	21, 35, 64, 98	0
12	CL	123/123 (100%)	0.42	5 (4%) 37 32	36, 52, 78, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/114 (100%)	0.50	8 (7%) 16 12	48, 69, 94, 103	0
13	CM	114/114 (100%)	3.03	79 (69%) 0 0	97, 109, 118, 119	0
14	AN	96/100 (96%)	0.74	14 (14%) 2 1	41, 61, 94, 103	0
14	CN	96/100 (96%)	2.57	52 (54%) 0 0	70, 95, 113, 120	0
15	AO	88/88 (100%)	0.24	3 (3%) 45 40	28, 51, 65, 89	0
15	CO	88/88 (100%)	0.26	3 (3%) 45 40	40, 63, 81, 98	0
16	AP	82/82 (100%)	0.68	7 (8%) 10 8	33, 47, 85, 101	0
16	CP	82/82 (100%)	1.19	16 (19%) 1 0	44, 61, 89, 106	0
17	AQ	80/80 (100%)	0.28	4 (5%) 28 25	28, 52, 77, 122	0
17	CQ	80/80 (100%)	1.10	17 (21%) 0 0	44, 76, 98, 103	0
18	AR	55/55 (100%)	0.12	3 (5%) 25 21	39, 52, 79, 108	0
18	CR	55/55 (100%)	0.35	4 (7%) 15 11	39, 55, 79, 111	0
19	AS	79/79 (100%)	0.99	20 (25%) 0 0	54, 69, 89, 101	0
19	CS	79/79 (100%)	4.42	62 (78%) 0 0	90, 110, 119, 125	0
20	AT	85/85 (100%)	0.56	4 (4%) 31 28	35, 48, 71, 101	0
20	CT	85/85 (100%)	1.60	27 (31%) 0 0	55, 74, 92, 99	0
21	AU	51/51 (100%)	1.05	9 (17%) 1 1	46, 75, 97, 106	0
21	CU	51/51 (100%)	0.67	7 (13%) 3 2	45, 72, 97, 105	0
22	BA	2897/2903 (99%)	0.07	113 (3%) 39 35	1, 15, 131, 195	0
22	DA	2897/2903 (99%)	0.32	127 (4%) 34 30	40, 82, 146, 181	0
23	BB	119/119 (100%)	-0.36	0 100 100	3, 25, 52, 85	0
23	DB	118/119 (99%)	0.14	4 (3%) 45 40	67, 112, 133, 144	0
24	BC	271/271 (100%)	-0.16	3 (1%) 80 80	5, 21, 36, 54	0
24	DC	271/271 (100%)	0.70	27 (9%) 7 5	43, 62, 77, 90	0
25	BD	209/209 (100%)	-0.26	0 100 100	1, 11, 35, 68	0
25	DD	209/209 (100%)	1.00	41 (19%) 1 0	49, 68, 84, 96	0
26	BE	201/201 (100%)	-0.27	1 (0%) 91 91	1, 23, 53, 91	0
26	DE	201/201 (100%)	1.64	72 (35%) 0 0	46, 85, 102, 109	0
27	BF	177/177 (100%)	0.30	9 (5%) 28 24	24, 43, 77, 90	0
27	DF	177/177 (100%)	3.28	126 (71%) 0 0	91, 108, 120, 126	0
28	BG	176/176 (100%)	0.11	5 (2%) 53 49	17, 38, 62, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DG	176/176 (100%)	2.14	85 (48%) 0 0	72, 94, 106, 116	0
29	BH	149/149 (100%)	3.51	86 (57%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	2.15	75 (50%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.69	93 (65%) 0 0	90, 112, 122, 133	0
30	DI	141/141 (100%)	4.98	123 (87%) 0 0	102, 119, 129, 132	0
31	BJ	142/142 (100%)	-0.36	0 100 100	2, 7, 21, 37	0
31	DJ	142/142 (100%)	0.82	15 (10%) 6 4	50, 66, 79, 94	0
32	BK	122/122 (100%)	-0.36	0 100 100	4, 13, 32, 69	0
32	DK	122/122 (100%)	1.19	28 (22%) 0 0	47, 64, 83, 97	0
33	BL	143/143 (100%)	-0.20	0 100 100	1, 19, 44, 73	0
33	DL	143/143 (100%)	1.76	49 (34%) 0 0	46, 80, 95, 115	0
34	BM	136/136 (100%)	-0.31	0 100 100	2, 11, 31, 83	0
34	DM	136/136 (100%)	1.03	27 (19%) 1 0	42, 69, 82, 101	0
35	BN	120/120 (100%)	-0.34	0 100 100	3, 8, 19, 53	0
35	DN	120/120 (100%)	1.42	29 (24%) 0 0	56, 76, 89, 116	0
36	BO	116/116 (100%)	-0.18	0 100 100	12, 27, 45, 52	0
36	DO	116/116 (100%)	2.47	67 (57%) 0 0	81, 95, 105, 115	0
37	BP	114/114 (100%)	-0.30	0 100 100	7, 18, 43, 66	0
37	DP	114/114 (100%)	0.94	19 (16%) 1 1	58, 70, 85, 93	0
38	BQ	117/117 (100%)	-0.26	0 100 100	1, 4, 15, 30	0
38	DQ	117/117 (100%)	0.95	15 (12%) 3 2	54, 67, 79, 83	0
39	BR	103/103 (100%)	-0.35	0 100 100	1, 13, 33, 67	0
39	DR	103/103 (100%)	1.47	31 (30%) 0 0	52, 78, 88, 99	0
40	BS	110/110 (100%)	-0.29	0 100 100	1, 5, 24, 79	0
40	DS	110/110 (100%)	1.87	46 (41%) 0 0	57, 75, 89, 101	0
41	BT	93/93 (100%)	0.22	4 (4%) 35 31	8, 26, 75, 104	0
41	DT	93/93 (100%)	2.65	49 (52%) 0 0	68, 87, 103, 119	0
42	BU	102/102 (100%)	-0.20	2 (1%) 65 63	14, 29, 63, 92	0
42	DU	102/102 (100%)	3.29	64 (62%) 0 0	75, 92, 111, 120	0
43	BV	94/94 (100%)	-0.22	0 100 100	6, 20, 41, 55	0
43	DV	94/94 (100%)	0.88	15 (15%) 1 1	70, 85, 96, 104	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	1 (1%) 77 77	7, 13, 29, 53	0
44	DW	75/76 (98%)	1.78	27 (36%) 0 0	61, 80, 90, 104	0
45	BX	77/77 (100%)	-0.27	0 100 100	7, 23, 51, 72	0
45	DX	77/77 (100%)	0.91	12 (15%) 2 1	52, 70, 84, 88	0
46	BY	63/63 (100%)	0.15	3 (4%) 30 27	21, 39, 72, 94	0
46	DY	63/63 (100%)	1.57	23 (36%) 0 0	78, 95, 102, 106	0
47	BZ	58/58 (100%)	-0.21	0 100 100	1, 8, 24, 41	0
47	DZ	58/58 (100%)	0.72	7 (12%) 4 3	58, 71, 82, 95	0
48	B0	56/56 (100%)	-0.30	0 100 100	1, 12, 36, 69	0
48	D0	56/56 (100%)	1.49	17 (30%) 0 0	58, 79, 92, 102	0
49	B1	50/50 (100%)	-0.05	2 (4%) 38 33	18, 29, 48, 76	0
49	D1	50/50 (100%)	1.43	13 (26%) 0 0	70, 86, 94, 105	0
50	B2	46/46 (100%)	-0.20	1 (2%) 62 59	4, 9, 15, 86	0
50	D2	46/46 (100%)	1.96	19 (41%) 0 0	55, 69, 80, 102	0
51	B3	64/64 (100%)	-0.18	0 100 100	5, 10, 20, 33	0
51	D3	64/64 (100%)	1.37	18 (28%) 0 0	58, 71, 79, 82	0
52	B4	38/38 (100%)	-0.05	0 100 100	9, 18, 37, 53	0
52	D4	38/38 (100%)	2.10	18 (47%) 0 0	59, 75, 87, 101	0
53	B5	191/228 (83%)	6.79	184 (96%) 0 0	101, 117, 128, 136	0
All	All	20734/20794 (99%)	0.63	2715 (13%) 3 2	1, 63, 121, 195	0

The worst 5 of 2715 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DI	2	ALA	27.5
53	B5	208	THR	23.4
53	B5	207	GLY	21.7
53	B5	111	PHE	20.1
22	BA	2184	A	17.7

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	DA	3134	1/1	-0.06	1.03	105,105,105,105	0
54	MG	DA	3045	1/1	0.12	0.40	102,102,102,102	0
54	MG	DA	3027	1/1	0.24	1.06	98,98,98,98	0
54	MG	DA	3136	1/1	0.25	0.50	90,90,90,90	0
54	MG	CA	1611	1/1	0.26	0.21	85,85,85,85	0
54	MG	DA	3078	1/1	0.30	0.37	89,89,89,89	0
54	MG	CA	1630	1/1	0.32	0.49	111,111,111,111	0
54	MG	AA	1659	1/1	0.33	2.11	77,77,77,77	0
54	MG	DA	3114	1/1	0.34	0.79	85,85,85,85	0
54	MG	CA	1636	1/1	0.36	0.23	118,118,118,118	0
54	MG	DA	3093	1/1	0.36	0.60	108,108,108,108	0
54	MG	DA	3005	1/1	0.38	0.36	96,96,96,96	0
54	MG	AA	1667	1/1	0.39	1.40	66,66,66,66	0
54	MG	DA	3057	1/1	0.41	0.31	87,87,87,87	0
54	MG	CA	1656	1/1	0.43	0.55	55,55,55,55	0
54	MG	CA	1646	1/1	0.43	0.35	66,66,66,66	0
54	MG	DA	3148	1/1	0.47	0.45	58,58,58,58	0
54	MG	AA	1614	1/1	0.47	0.14	66,66,66,66	0
54	MG	DA	3061	1/1	0.48	0.54	85,85,85,85	0
54	MG	DA	3062	1/1	0.49	2.55	110,110,110,110	0
54	MG	DA	3096	1/1	0.51	0.33	86,86,86,86	0
54	MG	BA	3048	1/1	0.55	0.15	50,50,50,50	0
54	MG	DA	3017	1/1	0.57	0.49	90,90,90,90	0
54	MG	DA	3149	1/1	0.57	0.24	63,63,63,63	0
54	MG	DA	3101	1/1	0.58	0.21	81,81,81,81	0
54	MG	CA	1641	1/1	0.59	0.38	69,69,69,69	0
54	MG	BA	3077	1/1	0.59	0.64	74,74,74,74	0
54	MG	DA	3063	1/1	0.62	0.61	95,95,95,95	0
54	MG	DA	3094	1/1	0.63	0.51	101,101,101,101	0
54	MG	CA	1633	1/1	0.65	0.30	81,81,81,81	0
54	MG	CA	1638	1/1	0.65	0.21	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3071	1/1	0.66	0.11	97,97,97,97	0
54	MG	DQ	201	1/1	0.67	0.33	53,53,53,53	0
54	MG	DA	3128	1/1	0.67	0.11	67,67,67,67	0
54	MG	DA	3159	1/1	0.68	0.14	68,68,68,68	0
54	MG	CA	1605	1/1	0.68	0.30	91,91,91,91	0
54	MG	DA	3059	1/1	0.68	0.41	79,79,79,79	0
54	MG	DA	3014	1/1	0.69	0.19	80,80,80,80	0
54	MG	DA	3072	1/1	0.70	0.27	81,81,81,81	0
54	MG	CA	1621	1/1	0.70	0.09	69,69,69,69	0
54	MG	CA	1635	1/1	0.71	0.20	123,123,123,123	0
54	MG	CA	1602	1/1	0.71	0.08	79,79,79,79	0
54	MG	DA	3132	1/1	0.71	0.86	93,93,93,93	0
54	MG	DA	3008	1/1	0.71	0.42	104,104,104,104	0
54	MG	AA	1644	1/1	0.72	0.23	50,50,50,50	0
54	MG	DA	3121	1/1	0.72	0.16	83,83,83,83	0
54	MG	CA	1644	1/1	0.72	0.38	54,54,54,54	0
54	MG	DA	3041	1/1	0.72	0.15	89,89,89,89	0
54	MG	AA	1634	1/1	0.73	0.38	74,74,74,74	0
54	MG	BA	3058	1/1	0.73	0.50	50,50,50,50	0
54	MG	AA	1657	1/1	0.74	0.49	68,68,68,68	0
54	MG	DA	3099	1/1	0.74	0.12	62,62,62,62	0
54	MG	CA	1628	1/1	0.74	0.17	99,99,99,99	0
54	MG	AA	1637	1/1	0.74	0.08	79,79,79,79	0
54	MG	CA	1629	1/1	0.74	0.12	85,85,85,85	0
54	MG	DA	3030	1/1	0.75	0.13	70,70,70,70	0
54	MG	DA	3100	1/1	0.75	0.41	83,83,83,83	0
54	MG	DA	3042	1/1	0.75	0.39	64,64,64,64	0
54	MG	DA	3080	1/1	0.75	0.07	99,99,99,99	0
54	MG	BA	3081	1/1	0.75	0.11	19,19,19,19	0
54	MG	CA	1650	1/1	0.75	0.19	46,46,46,46	0
54	MG	DA	3043	1/1	0.76	0.18	84,84,84,84	0
54	MG	DA	3046	1/1	0.76	0.12	78,78,78,78	0
54	MG	CA	1615	1/1	0.76	0.14	57,57,57,57	0
54	MG	AA	1671	1/1	0.76	0.90	56,56,56,56	0
54	MG	DA	3113	1/1	0.76	0.28	74,74,74,74	0
54	MG	DA	3028	1/1	0.76	0.15	87,87,87,87	0
54	MG	CA	1609	1/1	0.76	0.13	82,82,82,82	0
54	MG	DA	3120	1/1	0.76	0.58	102,102,102,102	0
54	MG	DA	3025	1/1	0.77	0.18	54,54,54,54	0
54	MG	BA	3026	1/1	0.77	0.22	35,35,35,35	0
54	MG	DA	3070	1/1	0.77	0.13	82,82,82,82	0
54	MG	BA	3037	1/1	0.77	0.13	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3016	1/1	0.77	0.34	75,75,75,75	0
54	MG	DA	3036	1/1	0.77	0.15	78,78,78,78	0
54	MG	CA	1622	1/1	0.77	0.10	50,50,50,50	0
54	MG	DA	3125	1/1	0.77	0.58	92,92,92,92	0
54	MG	DA	3075	1/1	0.77	0.13	64,64,64,64	0
54	MG	DA	3047	1/1	0.78	0.14	78,78,78,78	0
54	MG	CA	1631	1/1	0.78	0.22	97,97,97,97	0
54	MG	DA	3009	1/1	0.78	0.40	82,82,82,82	0
54	MG	DA	3089	1/1	0.78	0.10	77,77,77,77	0
54	MG	BA	3016	1/1	0.78	0.53	65,65,65,65	0
54	MG	DA	3087	1/1	0.78	0.12	70,70,70,70	0
54	MG	DA	3049	1/1	0.78	0.21	108,108,108,108	0
54	MG	DA	3097	1/1	0.78	0.07	62,62,62,62	0
54	MG	AA	1635	1/1	0.78	0.27	53,53,53,53	0
54	MG	DA	3104	1/1	0.79	0.15	67,67,67,67	0
54	MG	AA	1629	1/1	0.79	0.11	65,65,65,65	0
54	MG	AA	1643	1/1	0.79	1.29	61,61,61,61	0
54	MG	DA	3110	1/1	0.79	0.29	46,46,46,46	0
54	MG	DA	3020	1/1	0.79	0.26	87,87,87,87	0
54	MG	DA	3012	1/1	0.79	0.14	74,74,74,74	0
54	MG	DA	3127	1/1	0.80	0.24	81,81,81,81	0
54	MG	BA	3099	1/1	0.80	0.28	55,55,55,55	0
54	MG	DA	3018	1/1	0.80	0.11	59,59,59,59	0
54	MG	AA	1648	1/1	0.80	0.38	49,49,49,49	0
54	MG	DA	3141	1/1	0.80	0.37	40,40,40,40	0
54	MG	DA	3076	1/1	0.80	0.10	65,65,65,65	0
54	MG	DA	3137	1/1	0.80	0.11	88,88,88,88	0
54	MG	D2	101	1/1	0.80	0.22	78,78,78,78	0
54	MG	DA	3029	1/1	0.81	0.37	74,74,74,74	0
54	MG	BA	3041	1/1	0.81	0.37	2,2,2,2	0
54	MG	CA	1637	1/1	0.81	0.15	66,66,66,66	0
54	MG	DA	3158	1/1	0.81	0.25	56,56,56,56	0
54	MG	AA	1623	1/1	0.81	0.11	39,39,39,39	0
54	MG	DB	201	1/1	0.81	0.12	101,101,101,101	0
54	MG	BA	3085	1/1	0.81	0.21	30,30,30,30	0
54	MG	BA	3134	1/1	0.82	0.34	47,47,47,47	0
54	MG	DA	3164	1/1	0.82	0.67	67,67,67,67	0
54	MG	DA	3084	1/1	0.82	0.11	68,68,68,68	0
54	MG	DA	3162	1/1	0.82	0.26	67,67,67,67	0
54	MG	DA	3074	1/1	0.82	0.29	66,66,66,66	0
54	MG	CA	1624	1/1	0.82	0.08	49,49,49,49	0
54	MG	DA	3103	1/1	0.82	0.14	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1649	1/1	0.82	0.11	68,68,68,68	0
54	MG	BA	3053	1/1	0.83	0.12	8,8,8,8	0
54	MG	DA	3146	1/1	0.83	0.21	62,62,62,62	0
54	MG	BA	3083	1/1	0.83	0.14	23,23,23,23	0
54	MG	DA	3153	1/1	0.83	0.34	61,61,61,61	0
54	MG	DA	3024	1/1	0.83	0.07	65,65,65,65	0
54	MG	DA	3033	1/1	0.83	0.25	76,76,76,76	0
54	MG	AA	1661	1/1	0.83	0.44	43,43,43,43	0
54	MG	DA	3007	1/1	0.83	0.20	104,104,104,104	0
54	MG	DA	3161	1/1	0.83	0.21	35,35,35,35	0
54	MG	DA	3133	1/1	0.83	0.34	72,72,72,72	0
54	MG	AA	1651	1/1	0.83	0.36	52,52,52,52	0
54	MG	BA	3124	1/1	0.83	0.15	18,18,18,18	0
54	MG	BA	3154	1/1	0.83	0.63	33,33,33,33	0
54	MG	BA	3063	1/1	0.83	0.17	9,9,9,9	0
54	MG	BA	3089	1/1	0.84	0.15	28,28,28,28	0
54	MG	DA	3003	1/1	0.84	0.49	95,95,95,95	0
54	MG	BA	3167	1/1	0.84	0.20	35,35,35,35	0
54	MG	DA	3073	1/1	0.84	0.20	74,74,74,74	0
54	MG	AA	1646	1/1	0.84	0.28	53,53,53,53	0
54	MG	BA	3084	1/1	0.84	0.23	41,41,41,41	0
54	MG	BA	3074	1/1	0.84	0.17	22,22,22,22	0
54	MG	CA	1608	1/1	0.84	0.11	61,61,61,61	0
54	MG	AA	1619	1/1	0.84	0.07	61,61,61,61	0
54	MG	DA	3054	1/1	0.84	0.12	36,36,36,36	0
54	MG	DA	3157	1/1	0.84	0.22	49,49,49,49	0
54	MG	DB	202	1/1	0.85	0.13	61,61,61,61	0
54	MG	BA	3174	1/1	0.85	0.17	21,21,21,21	0
54	MG	DA	3048	1/1	0.85	0.13	61,61,61,61	0
54	MG	CA	1655	1/1	0.85	0.12	44,44,44,44	0
54	MG	CA	1606	1/1	0.85	0.09	68,68,68,68	0
54	MG	BA	3120	1/1	0.85	0.19	39,39,39,39	0
54	MG	AA	1602	1/1	0.85	0.31	55,55,55,55	0
54	MG	AA	1605	1/1	0.85	0.15	28,28,28,28	0
54	MG	DA	3050	1/1	0.85	0.31	89,89,89,89	0
54	MG	CA	1618	1/1	0.86	0.15	38,38,38,38	0
54	MG	BA	3043	1/1	0.86	0.15	2,2,2,2	0
54	MG	AA	1610	1/1	0.86	0.29	69,69,69,69	0
54	MG	CA	1619	1/1	0.86	0.11	41,41,41,41	0
54	MG	DA	3085	1/1	0.86	0.16	83,83,83,83	0
54	MG	BA	3088	1/1	0.86	0.12	35,35,35,35	0
54	MG	DA	3107	1/1	0.86	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3059	1/1	0.86	0.06	17,17,17,17	0
54	MG	DA	3160	1/1	0.86	0.19	44,44,44,44	0
54	MG	DA	3112	1/1	0.86	0.13	73,73,73,73	0
54	MG	BA	3056	1/1	0.86	0.40	53,53,53,53	0
54	MG	CA	1617	1/1	0.86	0.11	36,36,36,36	0
54	MG	DA	3109	1/1	0.86	0.17	48,48,48,48	0
54	MG	DA	3156	1/1	0.87	0.25	64,64,64,64	0
54	MG	CA	1614	1/1	0.87	0.09	48,48,48,48	0
54	MG	DA	3064	1/1	0.87	0.12	47,47,47,47	0
54	MG	AA	1660	1/1	0.87	0.14	51,51,51,51	0
54	MG	BA	3166	1/1	0.87	0.25	40,40,40,40	0
54	MG	DA	3142	1/1	0.87	0.24	41,41,41,41	0
54	MG	BA	3055	1/1	0.87	0.13	13,13,13,13	0
54	MG	BA	3125	1/1	0.87	0.39	36,36,36,36	0
54	MG	DA	3129	1/1	0.87	0.11	81,81,81,81	0
54	MG	DA	3163	1/1	0.87	0.27	59,59,59,59	0
54	MG	DA	3111	1/1	0.87	0.19	41,41,41,41	0
54	MG	BA	3095	1/1	0.88	0.12	30,30,30,30	0
54	MG	DA	3106	1/1	0.88	0.19	73,73,73,73	0
54	MG	DA	3138	1/1	0.88	0.61	46,46,46,46	0
54	MG	AN	201	1/1	0.88	0.18	60,60,60,60	0
54	MG	DA	3002	1/1	0.88	0.19	64,64,64,64	0
54	MG	DA	3117	1/1	0.88	0.46	73,73,73,73	0
54	MG	DA	3058	1/1	0.88	0.13	75,75,75,75	0
54	MG	AA	1639	1/1	0.88	0.09	53,53,53,53	0
54	MG	DA	3004	1/1	0.88	0.09	69,69,69,69	0
54	MG	CA	1627	1/1	0.88	0.18	80,80,80,80	0
54	MG	AA	1665	1/1	0.88	0.24	37,37,37,37	0
54	MG	BA	3024	1/1	0.88	0.15	1,1,1,1	0
54	MG	CA	1642	1/1	0.89	0.20	26,26,26,26	0
54	MG	DA	3006	1/1	0.89	0.07	99,99,99,99	0
54	MG	DA	3092	1/1	0.89	0.09	79,79,79,79	0
54	MG	DA	3086	1/1	0.89	0.18	83,83,83,83	0
54	MG	AA	1652	1/1	0.89	0.15	55,55,55,55	0
54	MG	AA	1618	1/1	0.89	0.40	54,54,54,54	0
54	MG	AA	1620	1/1	0.89	0.07	37,37,37,37	0
54	MG	DA	3152	1/1	0.89	0.27	60,60,60,60	0
54	MG	DA	3150	1/1	0.89	0.23	42,42,42,42	0
54	MG	BA	3080	1/1	0.89	0.13	22,22,22,22	0
54	MG	AA	1638	1/1	0.89	0.08	61,61,61,61	0
54	MG	AA	1631	1/1	0.89	0.12	47,47,47,47	0
54	MG	BA	3017	1/1	0.89	0.18	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3015	1/1	0.89	0.08	14,14,14,14	0
54	MG	DA	3091	1/1	0.89	0.08	78,78,78,78	0
54	MG	DA	3167	1/1	0.89	0.14	47,47,47,47	0
54	MG	AA	1601	1/1	0.89	0.14	56,56,56,56	0
54	MG	BA	3045	1/1	0.89	0.12	20,20,20,20	0
54	MG	DA	3037	1/1	0.89	0.14	59,59,59,59	0
54	MG	BA	3160	1/1	0.89	0.19	21,21,21,21	0
54	MG	BA	3114	1/1	0.89	0.17	0,0,0,0	0
54	MG	DA	3026	1/1	0.89	0.20	67,67,67,67	0
54	MG	BA	3020	1/1	0.89	0.21	2,2,2,2	0
54	MG	BA	3150	1/1	0.89	0.22	41,41,41,41	0
54	MG	AA	1666	1/1	0.89	0.27	43,43,43,43	0
54	MG	DA	3145	1/1	0.90	0.09	80,80,80,80	0
54	MG	DA	3135	1/1	0.90	0.12	54,54,54,54	0
54	MG	DA	3039	1/1	0.90	0.12	65,65,65,65	0
54	MG	DA	3116	1/1	0.90	0.20	95,95,95,95	0
54	MG	DA	3124	1/1	0.90	0.11	54,54,54,54	0
54	MG	DA	3011	1/1	0.90	0.13	57,57,57,57	0
54	MG	BA	3060	1/1	0.90	0.13	19,19,19,19	0
54	MG	BA	3190	1/1	0.90	0.21	43,43,43,43	0
54	MG	DA	3079	1/1	0.90	0.07	96,96,96,96	0
54	MG	CA	1651	1/1	0.90	0.38	50,50,50,50	0
54	MG	AA	1632	1/1	0.90	0.10	39,39,39,39	0
54	MG	BA	3136	1/1	0.90	0.13	39,39,39,39	0
54	MG	BA	3159	1/1	0.90	0.15	21,21,21,21	0
54	MG	CA	1626	1/1	0.90	0.11	52,52,52,52	0
54	MG	CA	1654	1/1	0.90	0.15	56,56,56,56	0
54	MG	BA	3092	1/1	0.90	0.06	53,53,53,53	0
54	MG	DA	3055	1/1	0.90	0.10	50,50,50,50	0
54	MG	BA	3003	1/1	0.90	0.09	23,23,23,23	0
54	MG	CA	1623	1/1	0.90	0.14	45,45,45,45	0
54	MG	BA	3032	1/1	0.90	0.09	6,6,6,6	0
54	MG	BA	3189	1/1	0.90	0.26	38,38,38,38	0
54	MG	AA	1640	1/1	0.90	0.14	21,21,21,21	0
54	MG	BA	3187	1/1	0.90	0.11	30,30,30,30	0
54	MG	AA	1670	1/1	0.90	0.39	40,40,40,40	0
54	MG	AA	1626	1/1	0.90	0.28	56,56,56,56	0
54	MG	CA	1639	1/1	0.90	0.11	52,52,52,52	0
54	MG	DA	3034	1/1	0.90	0.06	64,64,64,64	0
54	MG	BA	3062	1/1	0.91	0.55	52,52,52,52	0
54	MG	CA	1648	1/1	0.91	0.20	25,25,25,25	0
54	MG	DA	3082	1/1	0.91	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3013	1/1	0.91	0.13	45,45,45,45	0
54	MG	AA	1668	1/1	0.91	0.07	36,36,36,36	0
54	MG	BA	3103	1/1	0.91	0.11	8,8,8,8	0
54	MG	AA	1604	1/1	0.91	0.05	55,55,55,55	0
54	MG	BA	3157	1/1	0.91	0.20	20,20,20,20	0
54	MG	BA	3005	1/1	0.91	0.06	45,45,45,45	0
54	MG	DA	3066	1/1	0.91	0.10	32,32,32,32	0
54	MG	DA	3065	1/1	0.91	0.19	49,49,49,49	0
54	MG	DA	3139	1/1	0.91	0.42	49,49,49,49	0
54	MG	DA	3032	1/1	0.91	0.12	61,61,61,61	0
54	MG	CA	1645	1/1	0.91	0.16	42,42,42,42	0
54	MG	DA	3095	1/1	0.91	0.26	84,84,84,84	0
54	MG	BA	3008	1/1	0.91	0.11	32,32,32,32	0
54	MG	BA	3079	1/1	0.91	0.05	41,41,41,41	0
54	MG	BA	3191	1/1	0.91	0.25	22,22,22,22	0
54	MG	DA	3165	1/1	0.91	0.21	56,56,56,56	0
54	MG	AA	1669	1/1	0.91	0.20	56,56,56,56	0
54	MG	BA	3104	1/1	0.91	0.09	12,12,12,12	0
54	MG	BA	3004	1/1	0.91	0.13	27,27,27,27	0
54	MG	CA	1601	1/1	0.91	0.12	35,35,35,35	0
54	MG	BA	3171	1/1	0.91	0.14	16,16,16,16	0
54	MG	AA	1616	1/1	0.91	0.12	47,47,47,47	0
54	MG	BA	3145	1/1	0.91	0.61	37,37,37,37	0
54	MG	CA	1625	1/1	0.91	0.14	22,22,22,22	0
54	MG	BB	201	1/1	0.92	0.09	36,36,36,36	0
54	MG	AA	1663	1/1	0.92	0.25	33,33,33,33	0
54	MG	DA	3108	1/1	0.92	0.08	74,74,74,74	0
54	MG	DA	3060	1/1	0.92	0.12	41,41,41,41	0
54	MG	AA	1664	1/1	0.92	0.15	51,51,51,51	0
54	MG	AA	1628	1/1	0.92	0.12	53,53,53,53	0
54	MG	CA	1604	1/1	0.92	0.12	88,88,88,88	0
54	MG	BA	3137	1/1	0.92	0.28	60,60,60,60	0
54	MG	BA	3141	1/1	0.92	0.13	22,22,22,22	0
54	MG	DA	3069	1/1	0.92	0.17	53,53,53,53	0
54	MG	BA	3028	1/1	0.92	0.11	16,16,16,16	0
54	MG	BA	3116	1/1	0.92	0.15	48,48,48,48	0
54	MG	DA	3044	1/1	0.92	0.08	57,57,57,57	0
54	MG	DA	3131	1/1	0.92	0.13	69,69,69,69	0
54	MG	DA	3038	1/1	0.92	0.04	77,77,77,77	0
54	MG	DA	3115	1/1	0.92	0.11	48,48,48,48	0
54	MG	DA	3118	1/1	0.92	0.07	71,71,71,71	0
54	MG	DB	203	1/1	0.92	0.08	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3105	1/1	0.92	0.07	67,67,67,67	0
54	MG	DA	3102	1/1	0.92	0.07	64,64,64,64	0
54	MG	DA	3088	1/1	0.92	0.03	61,61,61,61	0
54	MG	BA	3168	1/1	0.92	0.22	19,19,19,19	0
54	MG	DA	3068	1/1	0.92	0.08	51,51,51,51	0
54	MG	AA	1607	1/1	0.92	0.07	51,51,51,51	0
54	MG	DA	3119	1/1	0.92	0.07	50,50,50,50	0
55	VIR	DA	3001	38/38	0.92	0.28	27,39,47,53	0
54	MG	BA	3193	1/1	0.93	0.18	34,34,34,34	0
54	MG	DA	3051	1/1	0.93	0.07	60,60,60,60	0
54	MG	BA	3132	1/1	0.93	0.20	44,44,44,44	0
54	MG	BA	3155	1/1	0.93	0.30	18,18,18,18	0
54	MG	BA	3031	1/1	0.93	0.14	3,3,3,3	0
54	MG	BA	3135	1/1	0.93	0.13	1,1,1,1	0
54	MG	BB	203	1/1	0.93	0.07	11,11,11,11	0
54	MG	DA	3031	1/1	0.93	0.24	65,65,65,65	0
54	MG	BA	3044	1/1	0.93	0.07	21,21,21,21	0
54	MG	CA	1632	1/1	0.93	0.24	77,77,77,77	0
54	MG	DA	3081	1/1	0.93	0.11	83,83,83,83	0
54	MG	BA	3173	1/1	0.93	0.14	33,33,33,33	0
54	MG	DA	3019	1/1	0.93	0.20	84,84,84,84	0
54	MG	AA	1658	1/1	0.93	0.67	65,65,65,65	0
54	MG	DA	3040	1/1	0.93	0.21	57,57,57,57	0
54	MG	BA	3123	1/1	0.93	0.19	0,0,0,0	0
54	MG	BA	3122	1/1	0.93	0.09	26,26,26,26	0
54	MG	BA	3119	1/1	0.93	0.07	12,12,12,12	0
54	MG	BA	3133	1/1	0.93	0.13	27,27,27,27	0
54	MG	CA	1653	1/1	0.93	0.06	40,40,40,40	0
54	MG	AA	1612	1/1	0.93	0.12	43,43,43,43	0
54	MG	DA	3126	1/1	0.93	0.15	57,57,57,57	0
54	MG	AA	1650	1/1	0.93	0.20	42,42,42,42	0
54	MG	AA	1630	1/1	0.93	0.17	53,53,53,53	0
54	MG	BA	3115	1/1	0.94	0.14	21,21,21,21	0
54	MG	BA	3151	1/1	0.94	0.27	33,33,33,33	0
54	MG	BA	3093	1/1	0.94	0.08	33,33,33,33	0
54	MG	AA	1649	1/1	0.94	0.13	26,26,26,26	0
54	MG	DA	3010	1/1	0.94	0.09	71,71,71,71	0
54	MG	DA	3154	1/1	0.94	0.23	42,42,42,42	0
54	MG	BA	3018	1/1	0.94	0.12	0,0,0,0	0
54	MG	AA	1622	1/1	0.94	0.20	51,51,51,51	0
54	MG	BA	3178	1/1	0.94	0.23	12,12,12,12	0
54	MG	DA	3067	1/1	0.94	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3147	1/1	0.94	0.08	51,51,51,51	0
54	MG	DA	3056	1/1	0.94	0.09	61,61,61,61	0
54	MG	BA	3102	1/1	0.94	0.10	9,9,9,9	0
54	MG	BA	3002	1/1	0.94	0.06	15,15,15,15	0
54	MG	BA	3076	1/1	0.94	0.14	12,12,12,12	0
54	MG	DA	3053	1/1	0.94	0.05	53,53,53,53	0
54	MG	AA	1609	1/1	0.94	0.07	46,46,46,46	0
54	MG	DA	3144	1/1	0.94	0.15	63,63,63,63	0
54	MG	BA	3147	1/1	0.94	0.19	42,42,42,42	0
54	MG	DA	3122	1/1	0.94	0.10	39,39,39,39	0
54	MG	BD	301	1/1	0.94	0.11	34,34,34,34	0
54	MG	BA	3109	1/1	0.94	0.19	1,1,1,1	0
54	MG	BA	3111	1/1	0.94	0.08	24,24,24,24	0
54	MG	BA	3127	1/1	0.94	0.16	9,9,9,9	0
54	MG	BA	3075	1/1	0.94	0.09	19,19,19,19	0
54	MG	CA	1610	1/1	0.94	0.10	63,63,63,63	0
54	MG	BA	3047	1/1	0.94	0.13	4,4,4,4	0
54	MG	BA	3009	1/1	0.94	0.16	3,3,3,3	0
54	MG	BA	3100	1/1	0.94	0.08	8,8,8,8	0
54	MG	BA	3177	1/1	0.94	0.52	37,37,37,37	0
54	MG	DA	3083	1/1	0.94	0.07	54,54,54,54	0
54	MG	BA	3014	1/1	0.94	0.17	0,0,0,0	0
54	MG	DA	3090	1/1	0.94	0.31	81,81,81,81	0
54	MG	CA	1603	1/1	0.95	0.14	36,36,36,36	0
54	MG	BA	3096	1/1	0.95	0.08	5,5,5,5	0
54	MG	BA	3101	1/1	0.95	0.10	5,5,5,5	0
54	MG	DA	3155	1/1	0.95	0.12	42,42,42,42	0
54	MG	CA	1647	1/1	0.95	0.10	42,42,42,42	0
54	MG	BA	3176	1/1	0.95	0.07	17,17,17,17	0
54	MG	BA	3086	1/1	0.95	0.14	10,10,10,10	0
54	MG	DA	3015	1/1	0.95	0.08	46,46,46,46	0
54	MG	CA	1634	1/1	0.95	0.10	50,50,50,50	0
54	MG	BA	3078	1/1	0.95	0.10	21,21,21,21	0
54	MG	CA	1640	1/1	0.95	0.11	31,31,31,31	0
54	MG	CA	1607	1/1	0.95	0.09	56,56,56,56	0
54	MG	BA	3049	1/1	0.95	0.07	11,11,11,11	0
54	MG	AA	1655	1/1	0.95	0.15	37,37,37,37	0
54	MG	BA	3090	1/1	0.95	0.07	3,3,3,3	0
54	MG	BA	3131	1/1	0.95	0.18	2,2,2,2	0
54	MG	BA	3182	1/1	0.95	0.15	21,21,21,21	0
54	MG	BA	3164	1/1	0.95	0.29	15,15,15,15	0
54	MG	DA	3140	1/1	0.95	0.34	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3169	1/1	0.95	0.10	24,24,24,24	0
54	MG	DA	3098	1/1	0.95	0.19	71,71,71,71	0
54	MG	BA	3163	1/1	0.95	0.16	29,29,29,29	0
54	MG	BA	3113	1/1	0.95	0.13	14,14,14,14	0
54	MG	AA	1603	1/1	0.95	0.16	49,49,49,49	0
54	MG	AA	1625	1/1	0.95	0.16	19,19,19,19	0
54	MG	BA	3188	1/1	0.95	0.12	6,6,6,6	0
54	MG	BA	3162	1/1	0.95	0.12	32,32,32,32	0
54	MG	BB	202	1/1	0.95	0.07	8,8,8,8	0
54	MG	CA	1643	1/1	0.96	0.19	56,56,56,56	0
54	MG	DA	3166	1/1	0.96	0.33	37,37,37,37	0
54	MG	CA	1652	1/1	0.96	0.07	65,65,65,65	0
54	MG	DA	3022	1/1	0.96	0.19	56,56,56,56	0
54	MG	DA	3021	1/1	0.96	0.19	56,56,56,56	0
54	MG	DA	3023	1/1	0.96	0.08	50,50,50,50	0
54	MG	DA	3151	1/1	0.96	0.08	45,45,45,45	0
54	MG	AA	1627	1/1	0.96	0.07	39,39,39,39	0
54	MG	BA	3061	1/1	0.96	0.41	48,48,48,48	0
54	MG	BA	3143	1/1	0.96	0.33	15,15,15,15	0
54	MG	BA	3069	1/1	0.96	0.15	7,7,7,7	0
54	MG	BA	3180	1/1	0.96	0.13	31,31,31,31	0
54	MG	BA	3040	1/1	0.96	0.15	0,0,0,0	0
54	MG	AA	1653	1/1	0.96	0.18	21,21,21,21	0
54	MG	AA	1621	1/1	0.96	0.21	16,16,16,16	0
54	MG	BA	3146	1/1	0.96	0.19	6,6,6,6	0
54	MG	CA	1620	1/1	0.96	0.05	59,59,59,59	0
54	MG	BA	3022	1/1	0.96	0.17	1,1,1,1	0
54	MG	BA	3042	1/1	0.96	0.16	11,11,11,11	0
54	MG	BA	3033	1/1	0.96	0.15	6,6,6,6	0
54	MG	BA	3098	1/1	0.96	0.10	3,3,3,3	0
54	MG	CA	1613	1/1	0.96	0.16	15,15,15,15	0
54	MG	BA	3153	1/1	0.96	0.25	6,6,6,6	0
54	MG	BA	3158	1/1	0.96	0.15	16,16,16,16	0
54	MG	BA	3006	1/1	0.96	0.08	47,47,47,47	0
54	MG	BA	3108	1/1	0.96	0.15	9,9,9,9	0
54	MG	BA	3172	1/1	0.96	0.09	26,26,26,26	0
54	MG	BA	3121	1/1	0.96	0.09	4,4,4,4	0
54	MG	BA	3181	1/1	0.96	0.20	31,31,31,31	0
54	MG	BA	3152	1/1	0.96	0.10	14,14,14,14	0
54	MG	CA	1616	1/1	0.96	0.14	34,34,34,34	0
54	MG	BA	3021	1/1	0.96	0.07	9,9,9,9	0
54	MG	BA	3106	1/1	0.96	0.18	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3140	1/1	0.96	0.35	1,1,1,1	0
54	MG	BA	3051	1/1	0.96	0.12	4,4,4,4	0
54	MG	BA	3072	1/1	0.96	0.06	13,13,13,13	0
54	MG	DA	3052	1/1	0.96	0.07	35,35,35,35	0
54	MG	AA	1654	1/1	0.96	0.21	42,42,42,42	0
54	MG	BA	3091	1/1	0.96	0.11	21,21,21,21	0
54	MG	BA	3156	1/1	0.96	0.17	21,21,21,21	0
54	MG	BA	3070	1/1	0.96	0.15	59,59,59,59	0
54	MG	BA	3110	1/1	0.96	0.20	2,2,2,2	0
54	MG	BA	3025	1/1	0.96	0.12	3,3,3,3	0
55	VIR	BA	3001	38/38	0.97	0.23	3,15,28,31	0
54	MG	AA	1642	1/1	0.97	0.06	23,23,23,23	0
54	MG	BA	3066	1/1	0.97	0.08	3,3,3,3	0
54	MG	BA	3161	1/1	0.97	0.09	11,11,11,11	0
54	MG	BA	3065	1/1	0.97	0.14	0,0,0,0	0
54	MG	DA	3130	1/1	0.97	0.18	37,37,37,37	0
54	MG	AA	1662	1/1	0.97	0.25	51,51,51,51	0
54	MG	BA	3175	1/1	0.97	0.11	20,20,20,20	0
54	MG	BA	3007	1/1	0.97	0.08	17,17,17,17	0
54	MG	BA	3057	1/1	0.97	0.12	6,6,6,6	0
54	MG	CA	1612	1/1	0.97	0.07	43,43,43,43	0
54	MG	BA	3023	1/1	0.97	0.14	2,2,2,2	0
54	MG	AA	1615	1/1	0.97	0.04	63,63,63,63	0
54	MG	BA	3186	1/1	0.97	0.09	23,23,23,23	0
54	MG	BA	3030	1/1	0.97	0.12	14,14,14,14	0
54	MG	DA	3077	1/1	0.97	0.11	62,62,62,62	0
54	MG	BA	3126	1/1	0.97	0.16	1,1,1,1	0
54	MG	BA	3117	1/1	0.97	0.14	2,2,2,2	0
54	MG	AA	1617	1/1	0.97	0.09	33,33,33,33	0
54	MG	BA	3128	1/1	0.97	0.07	9,9,9,9	0
54	MG	BA	3112	1/1	0.97	0.10	7,7,7,7	0
54	MG	BA	3142	1/1	0.97	0.35	0,0,0,0	0
54	MG	AA	1624	1/1	0.97	0.07	32,32,32,32	0
54	MG	DA	3143	1/1	0.97	0.10	32,32,32,32	0
54	MG	BA	3094	1/1	0.97	0.08	21,21,21,21	0
54	MG	AA	1608	1/1	0.97	0.13	18,18,18,18	0
54	MG	BA	3170	1/1	0.97	0.07	23,23,23,23	0
54	MG	BA	3067	1/1	0.97	0.13	1,1,1,1	0
54	MG	AA	1641	1/1	0.97	0.15	22,22,22,22	0
54	MG	AA	1606	1/1	0.97	0.12	35,35,35,35	0
54	MG	BA	3046	1/1	0.97	0.08	5,5,5,5	0
54	MG	BA	3165	1/1	0.97	0.17	2,2,2,2	0

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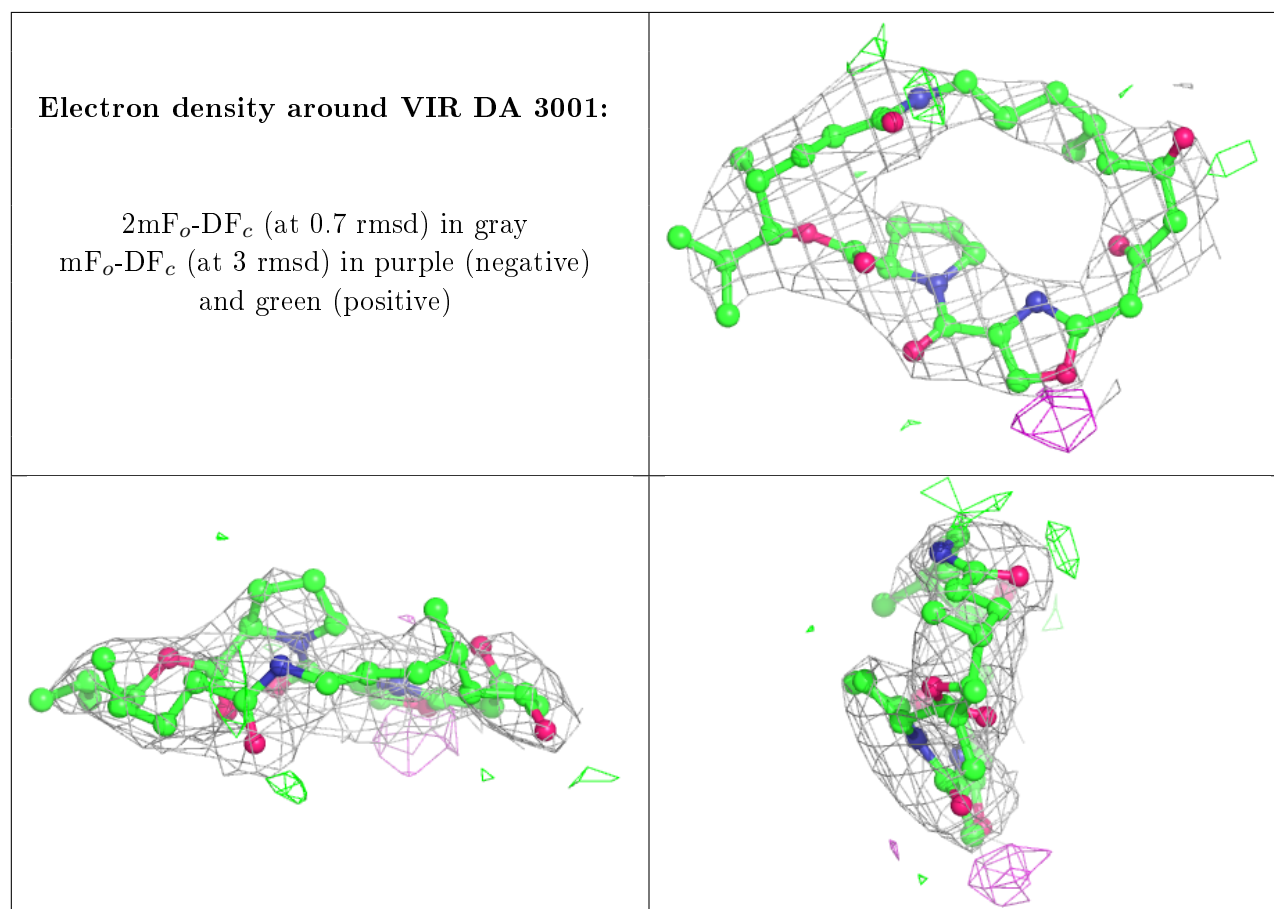
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1633	1/1	0.97	0.14	38,38,38,38	0
54	MG	BA	3129	1/1	0.98	0.16	3,3,3,3	0
54	MG	BA	3179	1/1	0.98	0.10	37,37,37,37	0
54	MG	BA	3010	1/1	0.98	0.10	0,0,0,0	0
54	MG	BA	3039	1/1	0.98	0.15	0,0,0,0	0
54	MG	BA	3050	1/1	0.98	0.18	4,4,4,4	0
54	MG	DA	3035	1/1	0.98	0.06	43,43,43,43	0
54	MG	AA	1613	1/1	0.98	0.06	26,26,26,26	0
54	MG	BA	3068	1/1	0.98	0.21	0,0,0,0	0
54	MG	DA	3123	1/1	0.98	0.17	38,38,38,38	0
54	MG	BA	3138	1/1	0.98	0.43	7,7,7,7	0
54	MG	BA	3027	1/1	0.98	0.10	3,3,3,3	0
54	MG	BA	3013	1/1	0.98	0.16	0,0,0,0	0
54	MG	BA	3184	1/1	0.98	0.21	11,11,11,11	0
54	MG	BA	3130	1/1	0.98	0.14	0,0,0,0	0
54	MG	BA	3183	1/1	0.98	0.18	26,26,26,26	0
54	MG	AA	1645	1/1	0.98	0.19	58,58,58,58	0
54	MG	BB	204	1/1	0.98	0.33	6,6,6,6	0
54	MG	BA	3073	1/1	0.98	0.12	2,2,2,2	0
54	MG	BA	3149	1/1	0.98	0.11	26,26,26,26	0
54	MG	BQ	201	1/1	0.98	0.17	0,0,0,0	0
54	MG	BA	3082	1/1	0.98	0.17	0,0,0,0	0
54	MG	BA	3118	1/1	0.98	0.10	5,5,5,5	0
54	MG	BA	3034	1/1	0.98	0.20	0,0,0,0	0
54	MG	BA	3097	1/1	0.98	0.12	2,2,2,2	0
54	MG	BA	3029	1/1	0.98	0.16	0,0,0,0	0
54	MG	BA	3194	1/1	0.98	0.06	28,28,28,28	0
54	MG	BA	3012	1/1	0.98	0.09	9,9,9,9	0
54	MG	BA	3035	1/1	0.98	0.34	44,44,44,44	0
54	MG	BA	3054	1/1	0.98	0.12	2,2,2,2	0
54	MG	BA	3139	1/1	0.98	0.41	3,3,3,3	0
54	MG	BA	3148	1/1	0.98	0.48	28,28,28,28	0
54	MG	BA	3019	1/1	0.98	0.11	15,15,15,15	0
54	MG	BA	3107	1/1	0.98	0.23	1,1,1,1	0
54	MG	BA	3087	1/1	0.98	0.17	2,2,2,2	0
54	MG	AA	1656	1/1	0.99	0.11	37,37,37,37	0
54	MG	BA	3144	1/1	0.99	0.18	12,12,12,12	0
54	MG	AA	1636	1/1	0.99	0.12	11,11,11,11	0
54	MG	BA	3064	1/1	0.99	0.16	1,1,1,1	0
54	MG	BA	3192	1/1	0.99	0.15	17,17,17,17	0
54	MG	BA	3036	1/1	0.99	0.11	2,2,2,2	0
54	MG	BA	3071	1/1	0.99	0.08	6,6,6,6	0

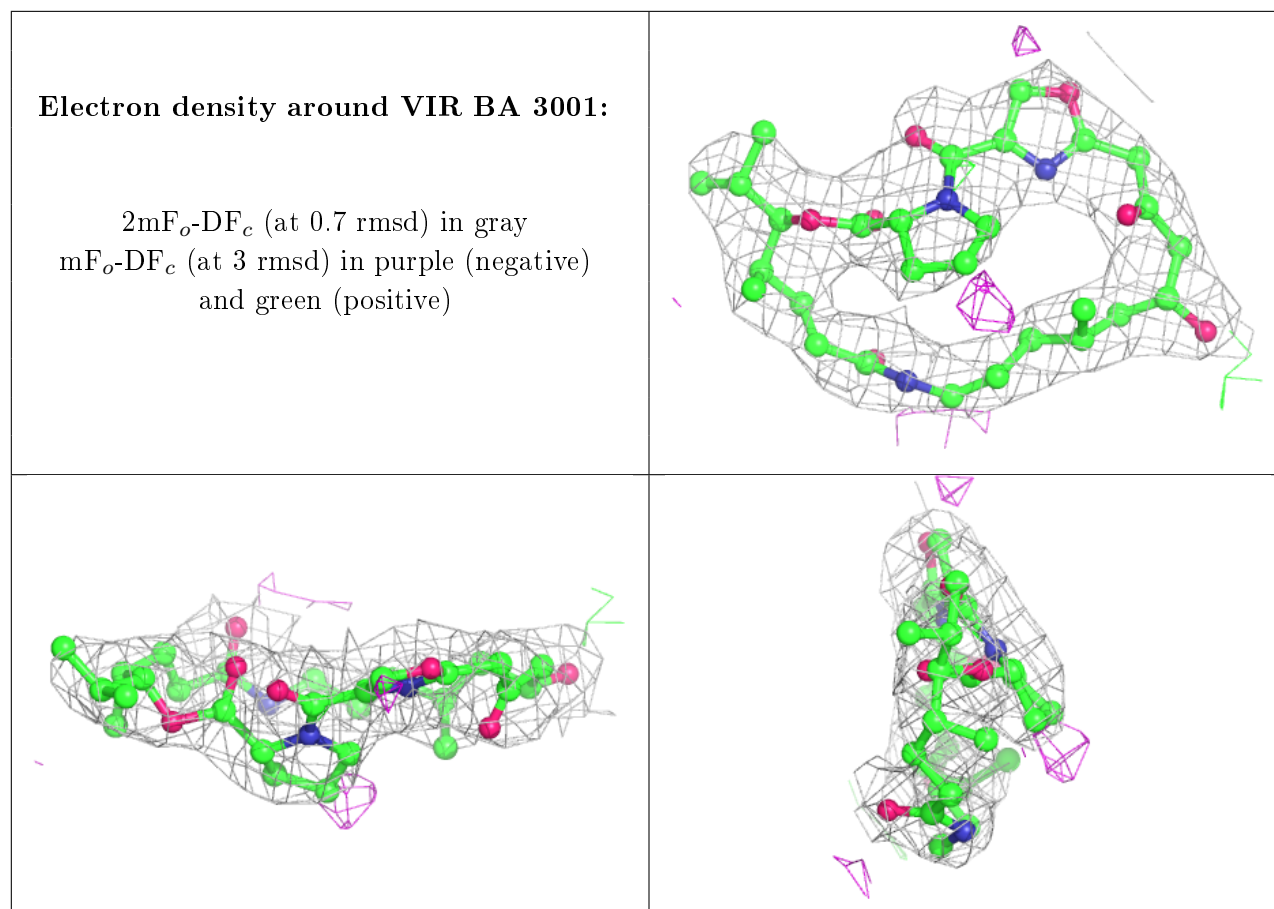
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1647	1/1	0.99	0.08	54,54,54,54	0
54	MG	BA	3011	1/1	0.99	0.12	0,0,0,0	0
54	MG	BA	3052	1/1	0.99	0.12	8,8,8,8	0
54	MG	BA	3185	1/1	0.99	0.20	13,13,13,13	0
54	MG	AA	1611	1/1	0.99	0.11	12,12,12,12	0
56	ZN	B4	101	1/1	0.99	0.12	29,29,29,29	0
56	ZN	D4	101	1/1	0.99	0.10	84,84,84,84	0
54	MG	BA	3105	1/1	0.99	0.21	0,0,0,0	0
54	MG	BA	3038	1/1	0.99	0.19	0,0,0,0	0

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.