



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:07 PM GMT

PDB ID : 4U26
Title : Crystal structure of the E. coli ribosome bound to dalfopristin and quinupristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-06-07
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

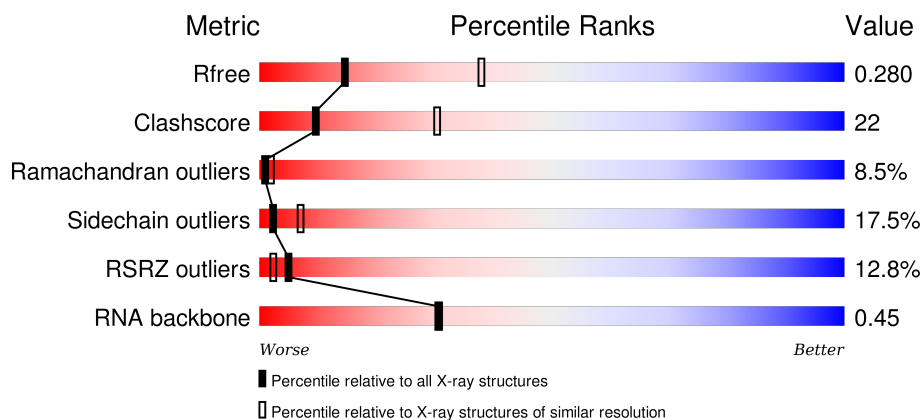
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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

Mol	Chain	Length	Quality of chain
1	AA	1539	<div> <div>14%</div> <div>34%</div> <div>50%</div> <div>15%</div> </div>
1	CA	1539	<div> <div>3%</div> <div>31%</div> <div>54%</div> <div>16%</div> </div>
2	AB	218	<div> <div>25%</div> <div>50%</div> <div>18%</div> <div>7%</div> </div>
2	CB	218	<div> <div>21%</div> <div>30%</div> <div>49%</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	
54	B6	8	
54	D6	8	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1622	-	-	-	X
55	MG	AA	1662	-	-	-	X
55	MG	AA	1669	-	-	-	X
55	MG	BA	3042	-	-	-	X
55	MG	BA	3070	-	-	-	X
55	MG	BA	3085	-	-	-	X
55	MG	BA	3106	-	-	-	X
55	MG	BA	3109	-	-	-	X
55	MG	BA	3111	-	-	-	X
55	MG	BA	3137	-	-	-	X
55	MG	BA	3146	-	-	-	X
55	MG	BA	3150	-	-	-	X
55	MG	BA	3151	-	-	-	X
55	MG	BA	3154	-	-	-	X
55	MG	BA	3178	-	-	-	X
55	MG	BA	3183	-	-	-	X
55	MG	BA	3185	-	-	-	X
55	MG	BA	3195	-	-	-	X
55	MG	CA	1615	-	-	-	X
55	MG	DA	3003	-	-	-	X
55	MG	DA	3028	-	-	-	X
55	MG	DA	3071	-	-	-	X
55	MG	DA	3072	-	-	-	X
55	MG	DA	3074	-	-	-	X
55	MG	DA	3110	-	-	-	X
55	MG	DA	3113	-	-	-	X
55	MG	DA	3116	-	-	-	X
55	MG	DA	3131	-	-	-	X
55	MG	DA	3139	-	-	-	X
55	MG	DA	3151	-	-	-	X
55	MG	DA	3153	-	-	-	X
55	MG	DA	3157	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	DOL	BA	3001	-	-	-	X
56	DOL	DA	3001	-	-	X	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 288423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

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

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

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

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

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

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

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

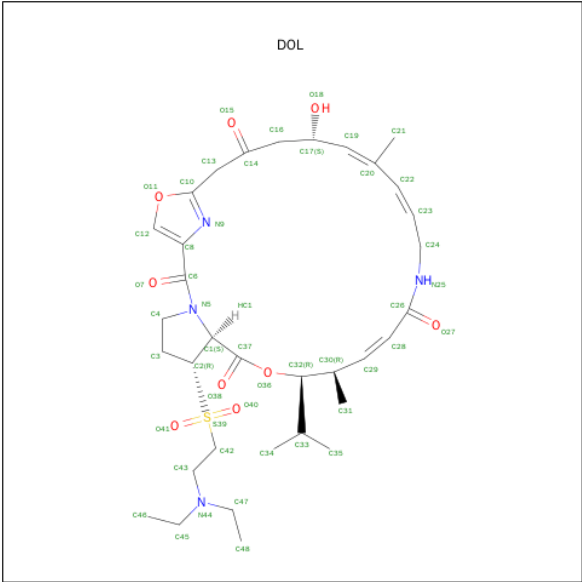
- Molecule 54 is a protein called Quinupristin.

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

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

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

- Molecule 56 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C₃₄H₅₀N₄O₉S).



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

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

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

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	194	Total	O	0	0
			194	194		
58	AE	2	Total	O	0	0
			2	2		
58	AL	1	Total	O	0	0
			1	1		
58	AN	3	Total	O	0	0
			3	3		
58	AT	2	Total	O	0	0
			2	2		

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

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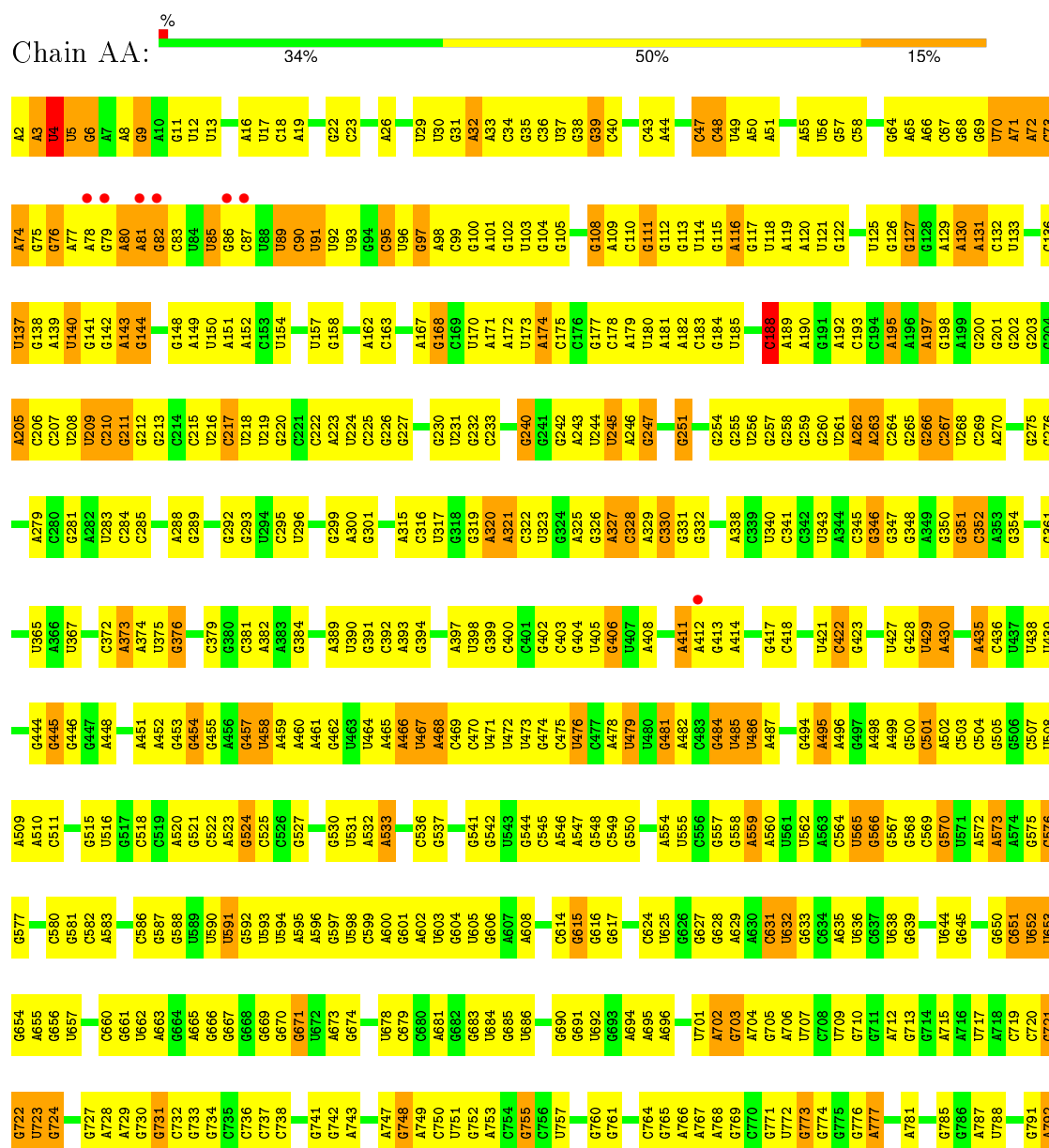
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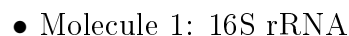
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DA	610	Total 610	O 610	0	0
58	DB	13	Total 13	O 13	0	0
58	DC	8	Total 8	O 8	0	0
58	DD	4	Total 4	O 4	0	0
58	DE	4	Total 4	O 4	0	0
58	DJ	1	Total 1	O 1	0	0
58	DL	4	Total 4	O 4	0	0
58	DN	2	Total 2	O 2	0	0
58	DS	2	Total 2	O 2	0	0
58	DT	3	Total 3	O 3	0	0
58	DU	1	Total 1	O 1	0	0
58	DV	1	Total 1	O 1	0	0
58	D2	1	Total 1	O 1	0	0
58	D3	1	Total 1	O 1	0	0
58	D4	1	Total 1	O 1	0	0

3 Residue-property plots

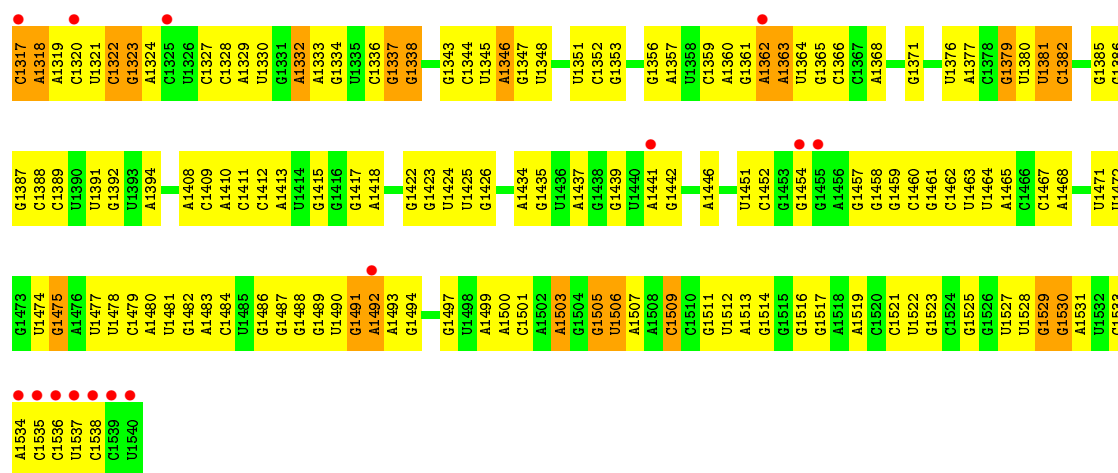
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA

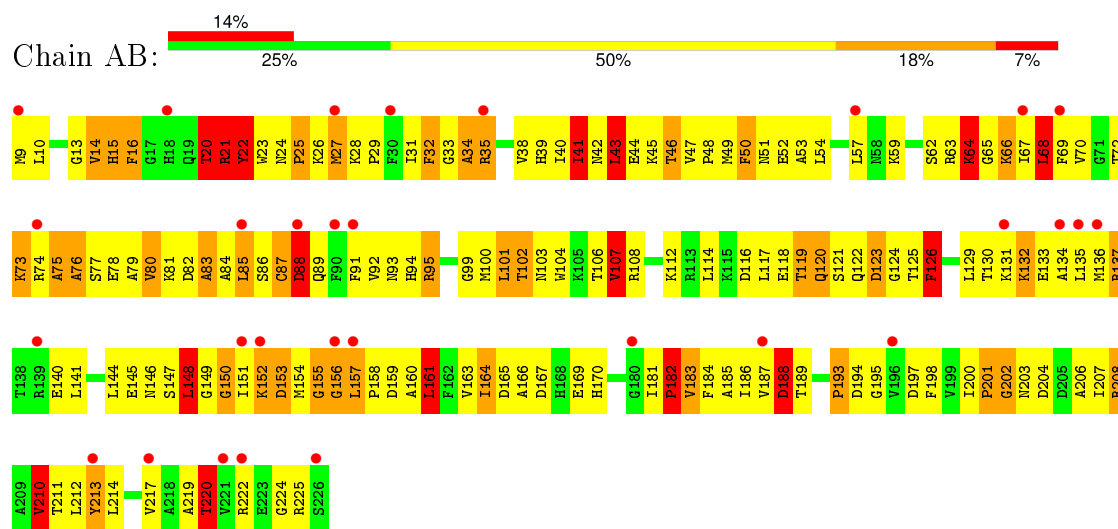




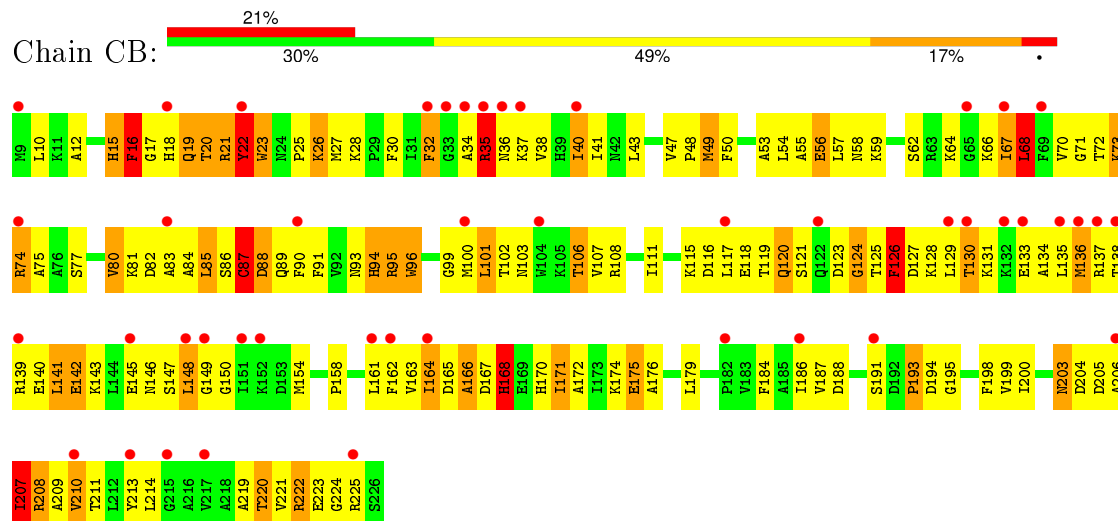
G1253	U1125	U1052	U991	C912	C839	G774	G711	A642	G567	A499	U426	A353	C271	U209
A1254	U1126	G1053	U992	A913	C840	G775	A712	A643	G568	A502	U427	G354	C210	C210
G1255	G1127	C1054	G993	A914	C841	A776	G713	U644	G569	A503	U428	C355	G276	G211
A1196	G1128	A1055	A994	A919	U842	A777	G714	U645	C502	C504	U429	A356	C277	G212
A1197	C1129	U1056	C995	A920	U843	G778	A715	G645	C505	C505	A430	G357	G278	G213
G1258	A1130	C996	A996	U921	U844	G779	A716	A649	A572	G505	A431	U358	A279	C214
G1131	U1060	U1061	C999	U922	C846	A781	U717	G650	A573	G506	A432	G359	C280	C215
G1132	G1061	U1062	A1000	G923	C847	A782	A718	G651	A574	A509	A435	G362	A281	U216
G1133	U1063	C1063	C1001	G924	C848	A783	G720	U652	C576	A510	U436	U367	A282	C217
G1134	G1064	G925	G1002	G925	C849	A784	G721	U653	C577	C511	U437	C284	U218	U218
U1135	U1065	G926	G1003	G926	U850	G785	G722	G654	C578	U512	U438	C285	C285	G220
C1136	C1066	G927	G1004	G927	C851	G786	U723	A661	A579	C513	U439	G369	C286	C221
C1137	U1067	A1067	A1005	C932	C852	A787	G724	G661	C580	C514	C440	C370	C222	C222
G1138	G1068	C853	A1006	C933	C853	A790	G725	U662	G581	G517	G445	A372	G289	A223
G1139	C1069	U1069	U1007	G933	U854	G791	A728	A663	C582	G518	G446	A373	C290	U224
C1140	U1070	C934	A935	A935	C857	A792	A729	G664	A583	C519	A451	A374	U291	G227
G1141	C1071	C1071	U1009	A936	C858	A793	G730	G665	C584	C519	A452	U375	U294	A228
G1142	G1072	U1072	U1010	A937	C859	U793	G731	G666	G585	A520	A453	G376	C295	U229
G1143	U1073	G1073	G1011	A938	C860	A794	G732	G667	C586	G524	A454	G377	U296	G230
G1144	G1074	G1074	A1012	C940	C861	G795	G733	G668	U590	G527	A455	C379	A297	U231
A1145	U1075	G1075	G1013	G945	C862	A798	G734	G669	U591	C528	A456	C391	G299	C233
A1146	C1147	G1077	A1014	G946	U863	U799	C735	G670	U591	G529	A457	G384	A300	C234
C1147	C1147	G1077	A1014	G947	C866	G800	C736	G671	U598	G530	U458	C385	G302	G237
U1148	A1080	A1081	U1015	A948	C867	G801	C737	U672	G597	G531	A459	C386	A303	A238
A1150	A1082	A1082	U1016	G949	C868	U802	G738	A673	U598	U532	A460	U387	G302	U239
A1151	U1083	C1083	G1018	C948	C869	G803	G739	A674	U603	A533	A461	G388	A306	G240
A1152	U1084	G1084	A1019	A949	C869	U804	G740	A675	G604	U534	A462	A389	A307	G241
G1153	G1085	U950	U950	U950	C870	C805	G741	U677	U605	U535	A463	U390	C308	G242
G1154	A1085	G951	A1021	G951	C871	C806	G742	U678	G606	C536	U464	G391	A309	C243
G1155	U1086	U952	A1022	U952	C872	C807	G743	C679	A607	G537	A465	C392	A243	G247
A1157	C1087	U1087	U1023	U955	C873	G809	G744	C680	A608	G538	A466	A393	C312	U244
C1158	G1088	C1088	G1024	U956	C874	C810	A746	C681	A609	G539	U467	A397	A313	A246
C1159	U1089	U1089	U1025	U957	C875	C811	G747	G682	U610	A539	A468	U398	G316	G247
U1160	C1090	C1090	G1026	U957	C876	G812	A748	G683	C611	G540	C469	U399	C248	C248
C1161	U1091	U1091	C1027	A958	C877	G813	A749	U684	C612	G541	C470	C400	U249	U249
C1162	A1092	A1092	C1028	U959	C878	A815	C750	G685	C613	G542	U471	C401	A250	G251
A1167	G1094	C1094	U1029	U960	C879	A816	G751	U686	C614	C544	U472	C402	A320	U252
U1168	U1095	U1095	C1030	G963	C880	C817	G752	A687	G615	C545	U473	C403	A321	G253
U1169	C1096	C1096	A964	A964	C881	G818	A753	G688	C616	A546	U474	G404	G332	G254
A1170	C1097	C1097	U965	U965	C882	A819	C754	C689	C617	A547	C475	U405	A327	G255
A1171	U1098	U1098	G966	C967	C883	U820	G755	C690	U619	A548	U476	U406	C328	G256
C1172	C1099	C1099	C967	C967	C884	G821	C756	G691	C620	G550	C477	U407	A329	U257
G1175	G1100	A1101	A1036	A968	C885	U822	U757	U692	A621	U551	A478	U408	C330	G258
A1176	A1101	A1101	C1037	A969	C886	C823	G758	G693	A622	U552	U479	U409	G331	G259
G1177	C1103	C1103	C1038	C970	C887	G824	A759	C623	C624	A553	U480	G410	G332	G260
G1178	G1104	G1104	G1039	G971	C888	A825	G760	A695	U625	A554	G481	A411	A337	A253
A1179	A1105	A1105	U1040	C972	C889	C826	G763	A696	C626	U555	C484	A412	C328	G254
G1180	G1106	G1106	U1041	G973	C890	U827	G764	G700	G628	C556	U485	A413	A329	G255
G1181	C1107	C1107	A1042	A974	C891	U828	G765	U701	A629	A559	U486	A414	C330	A262
G1182	G1108	G1108	G1043	A975	C892	G829	A766	A702	A630	A560	U487	A415	C331	A263
U1183	C1109	C1109	A1044	A976	C893	G832	A767	G703	C631	U561	C490	G422	G346	C264
G1184	G1114	G1114	U1045	A977	C894	U833	A768	G704	C632	U562	A485	G423	G347	G265
U1247	C1115	C1115	A1046	A978	C895	G834	A769	G705	G633	A563	A486	G424	G348	G266
G1248	A1117	A1117	G1047	C979	C896	U835	G770	A706	C634	U564	A487	G425	G349	C267
G1249	C1118	C1118	U1048	C980	C897	G836	G771	U707	A635	U565	A488	G426	G350	U268
A1187	A1117	A1117	G1049	C981	C898	G837	U772	U708	U636	U566	A489	G427	G351	G269
G1190	U1123	U1123	G1050	A983	C910	U837	U773	G710	C637	G566	A490	G428	G352	A270
A1191	G1124	G1124	C1051	A983	U911	G838	G773	G710	C637	G566	A490	G428	G352	A270



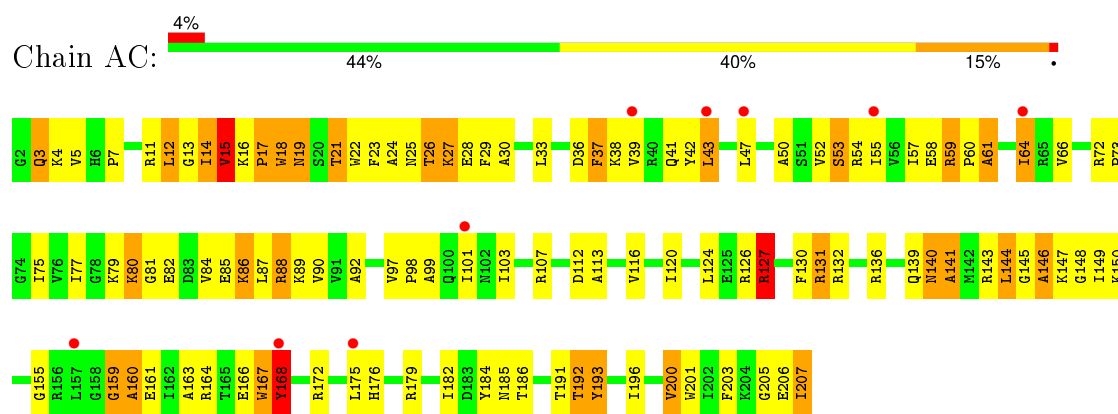
• Molecule 2: 30S ribosomal protein S2



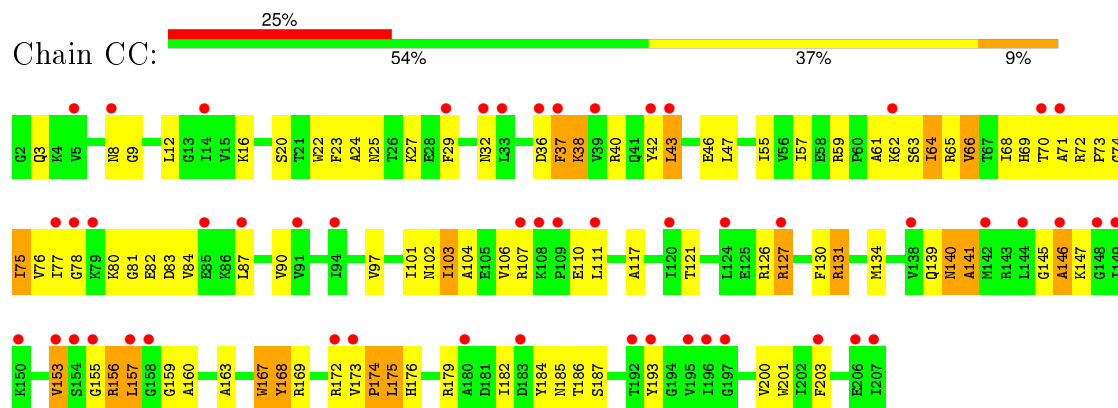
• Molecule 2: 30S ribosomal protein S2



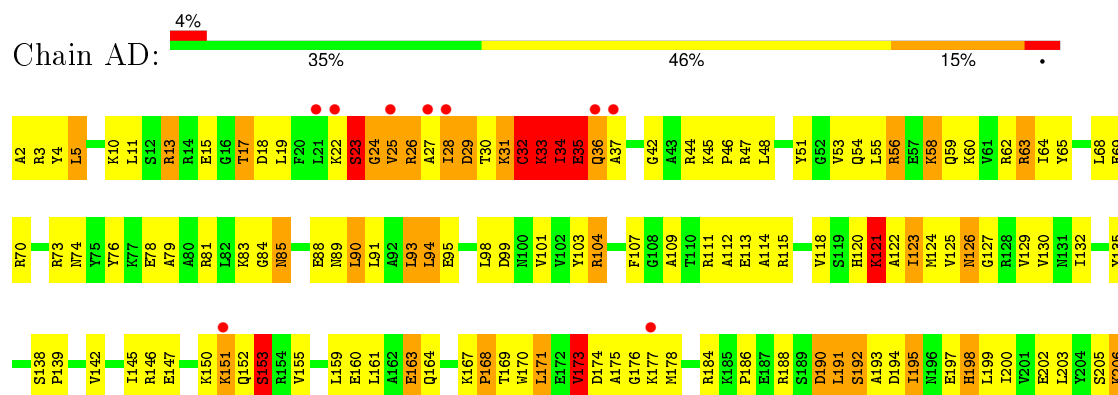
• Molecule 3: 30S ribosomal protein S3



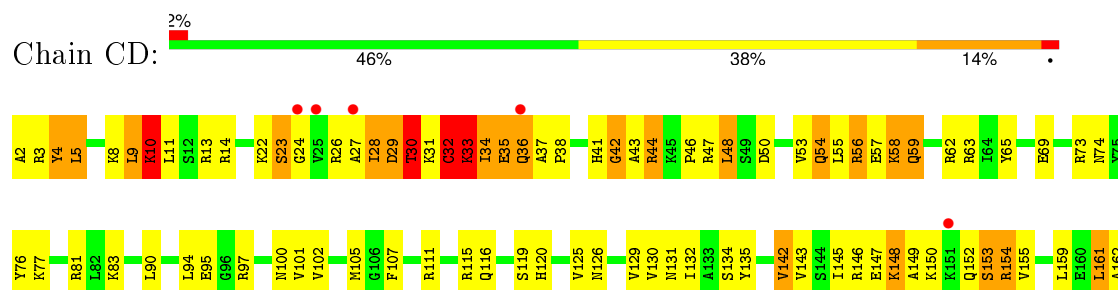
• Molecule 3: 30S ribosomal protein S3

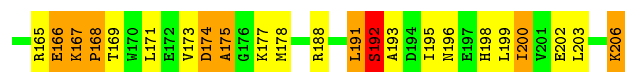


• Molecule 4: 30S ribosomal protein S4

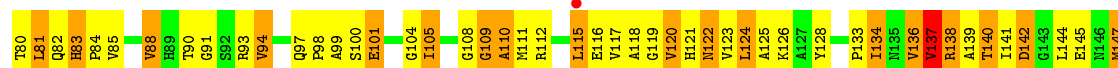
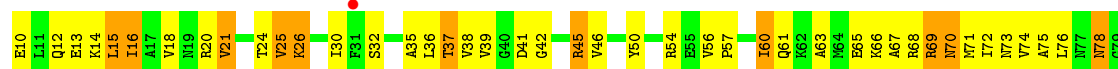


• Molecule 4: 30S ribosomal protein S4





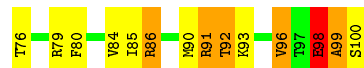
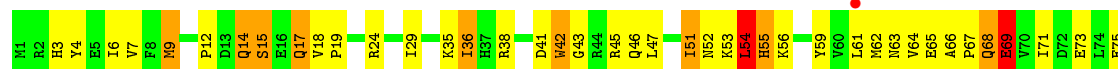
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5



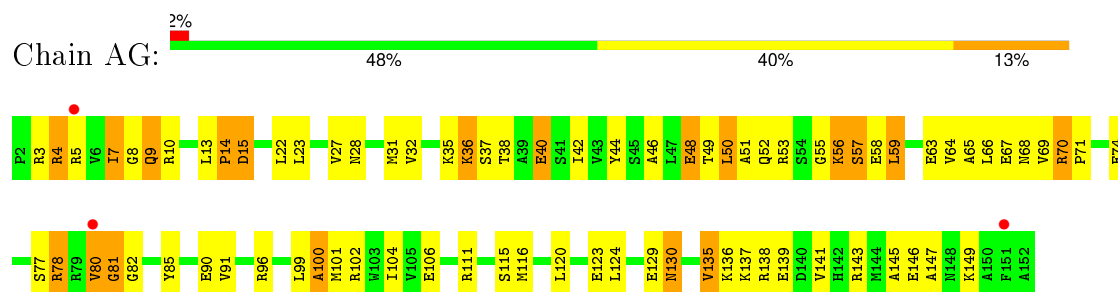
• Molecule 6: 30S ribosomal protein S6



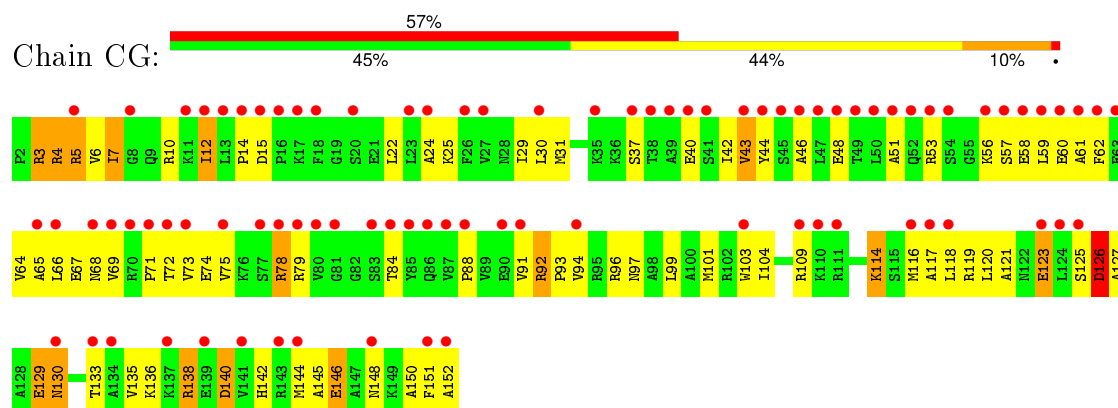
• Molecule 6: 30S ribosomal protein S6



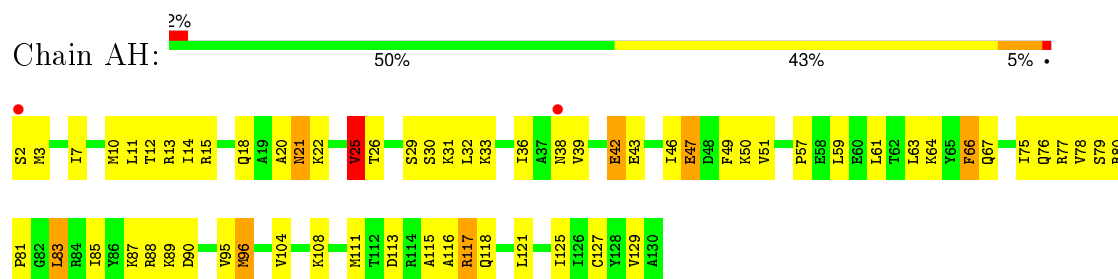
- Molecule 7: 30S ribosomal protein S7



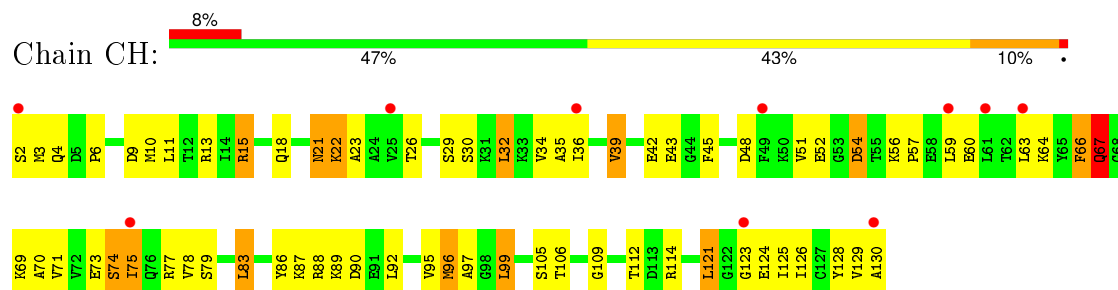
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

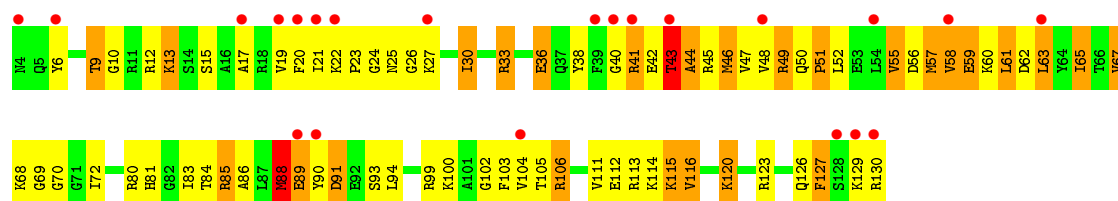


- Molecule 8: 30S ribosomal protein S8

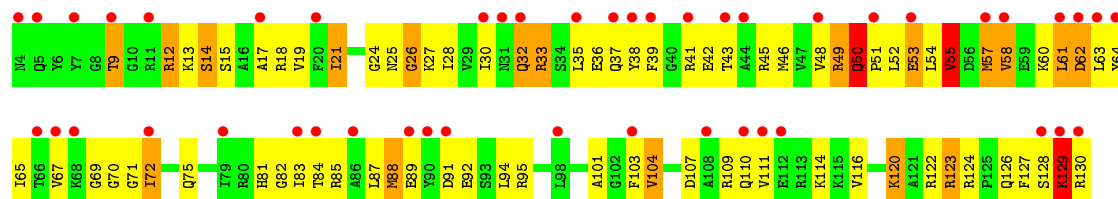
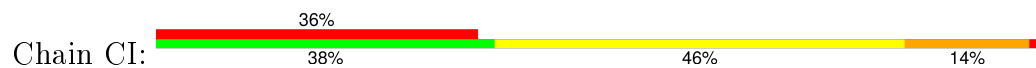


- Molecule 9: 30S ribosomal protein S9

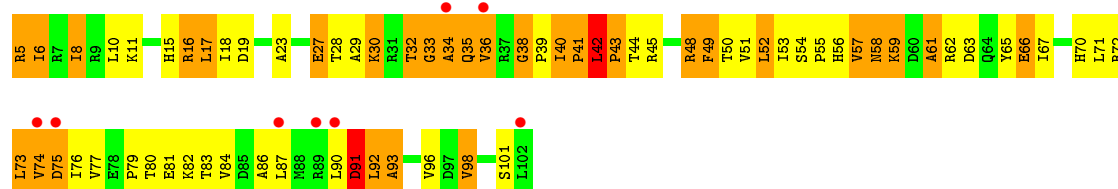




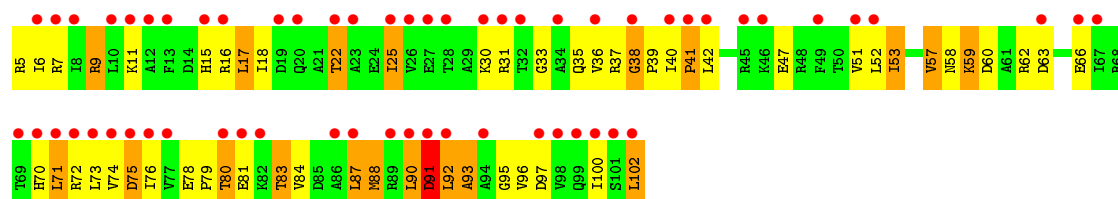
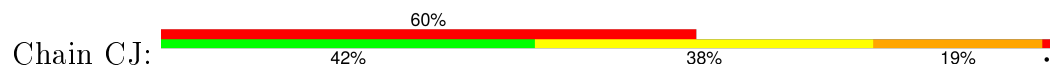
• Molecule 9: 30S ribosomal protein S9



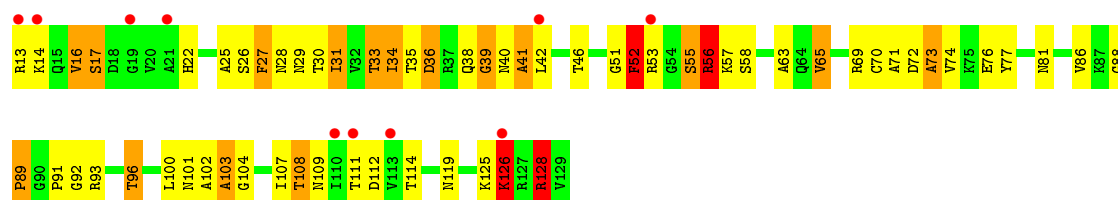
• Molecule 10: 30S ribosomal protein S10



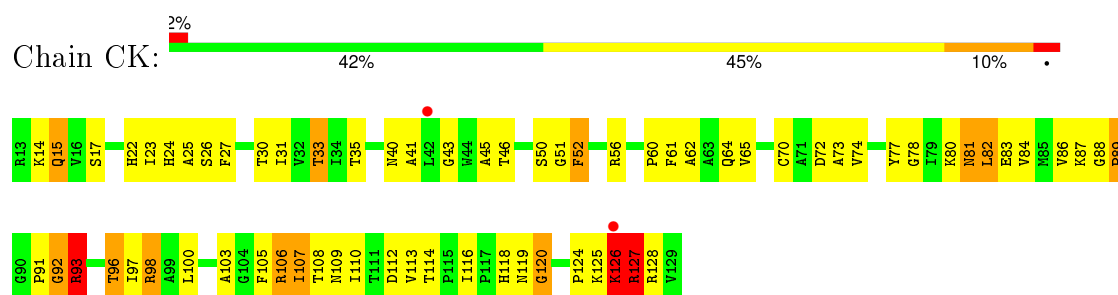
• Molecule 10: 30S ribosomal protein S10



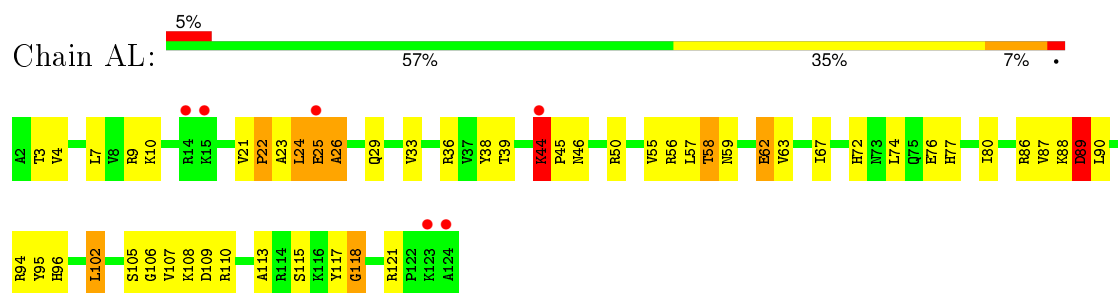
• Molecule 11: 30S ribosomal protein S11



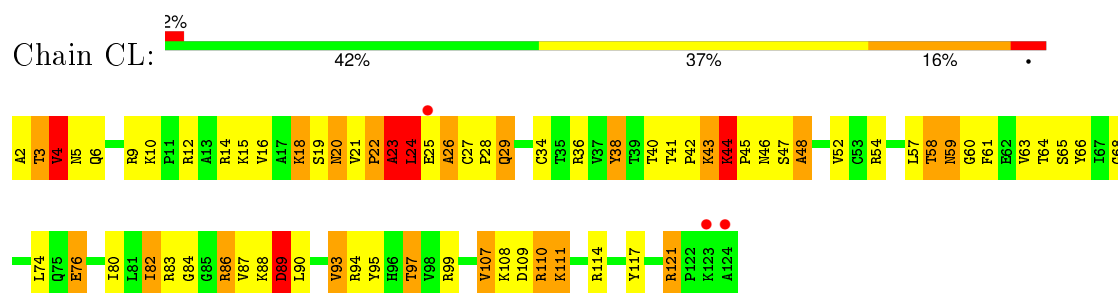
• Molecule 11: 30S ribosomal protein S11



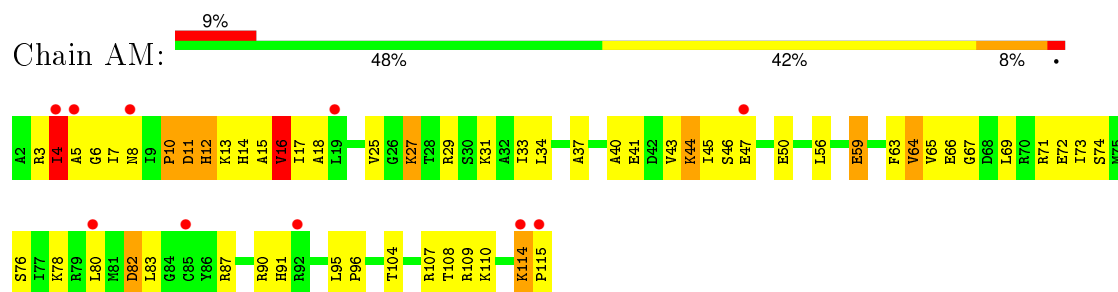
- Molecule 12: 30S ribosomal protein S12



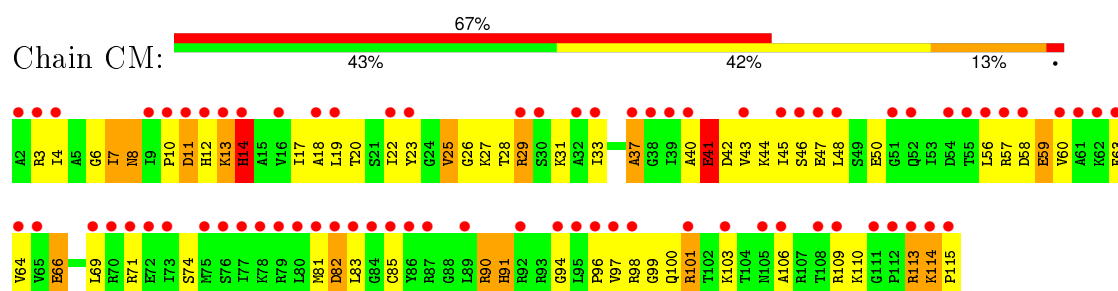
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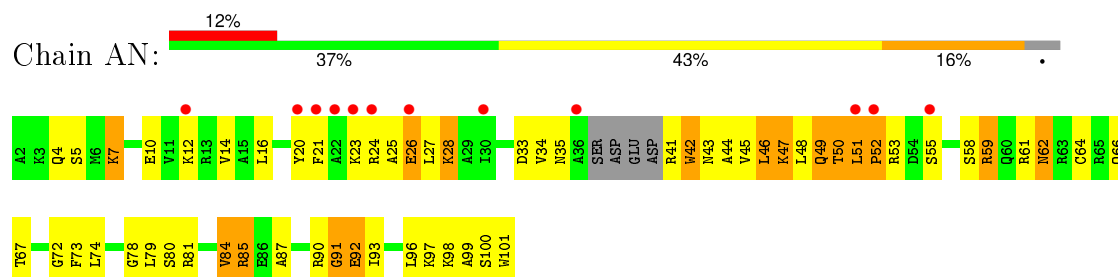
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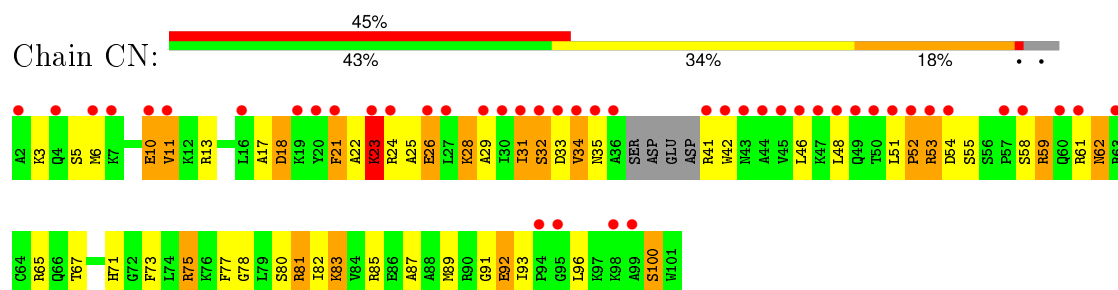
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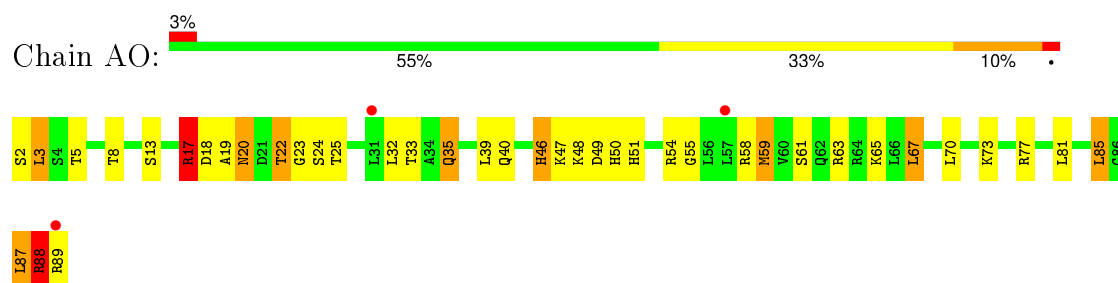
- Molecule 14: 30S ribosomal protein S14



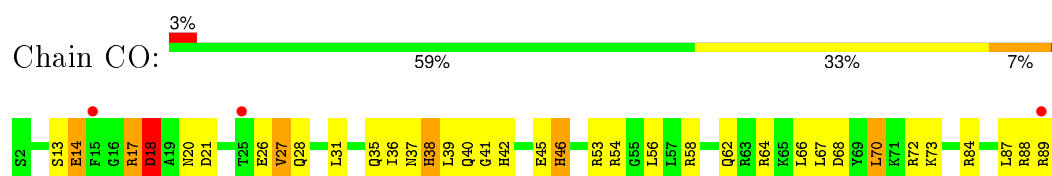
- Molecule 14: 30S ribosomal protein S14



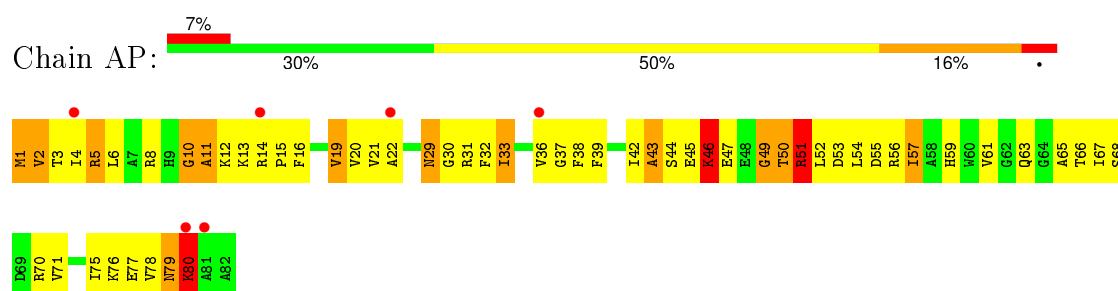
- Molecule 15: 30S ribosomal protein S15



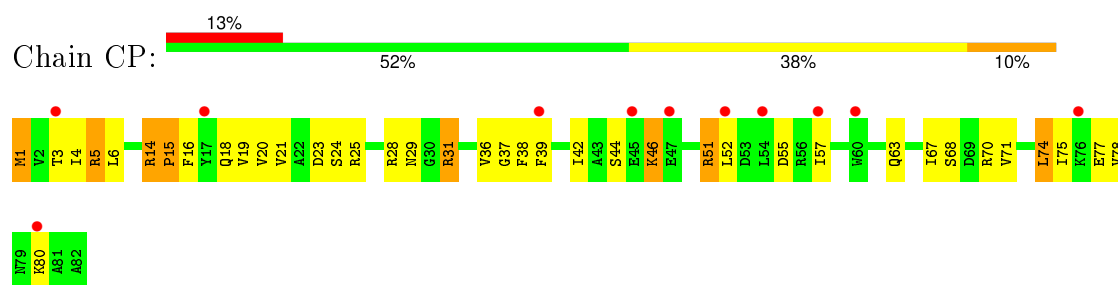
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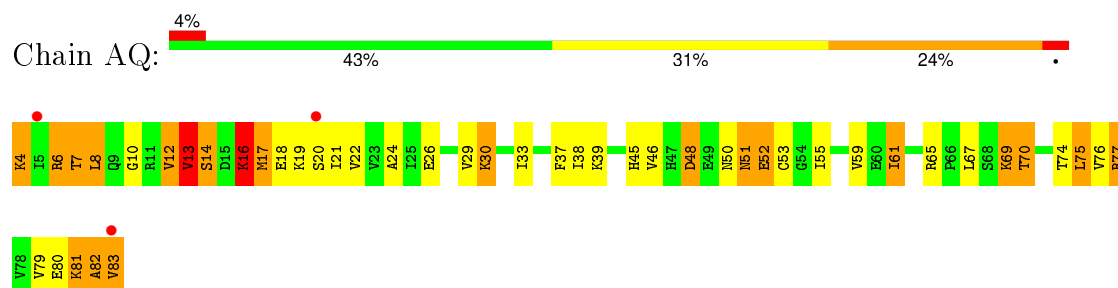
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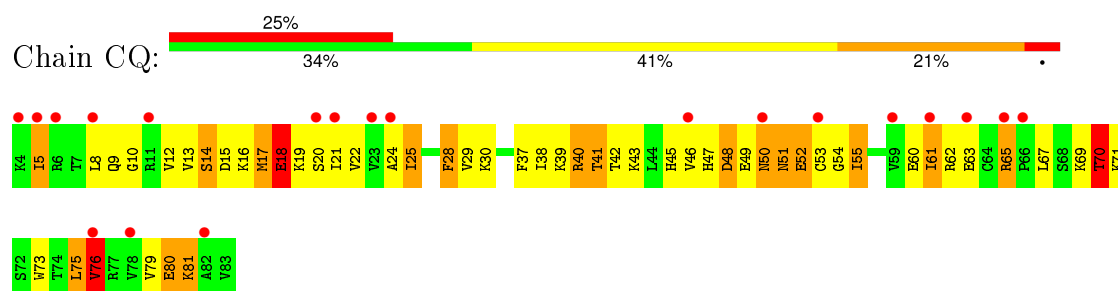
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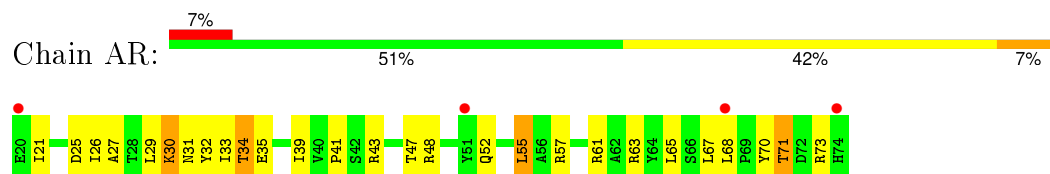
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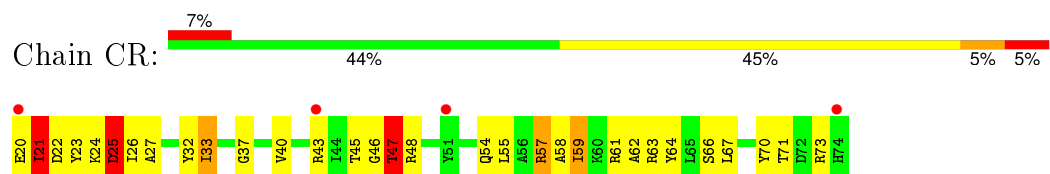
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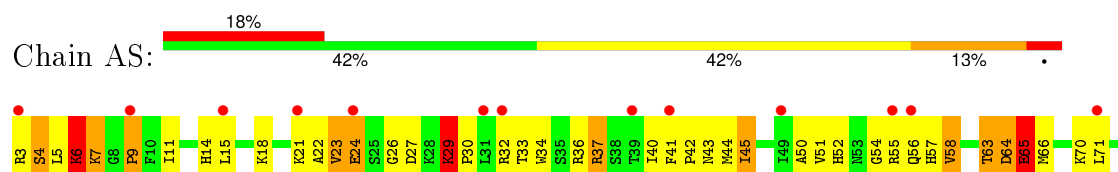
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

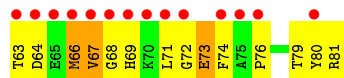
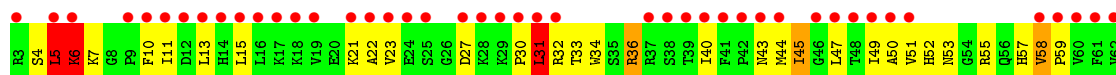
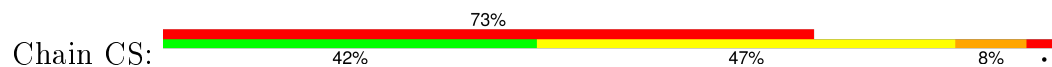


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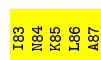
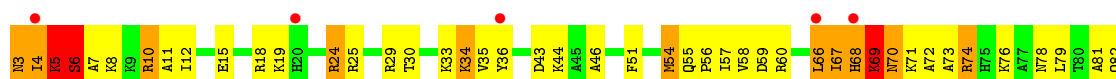




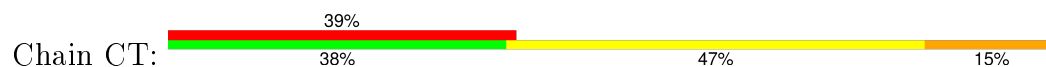
- Molecule 19: 30S ribosomal protein S19



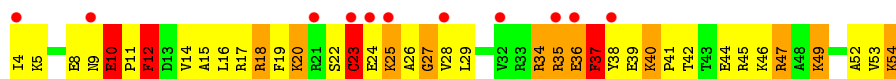
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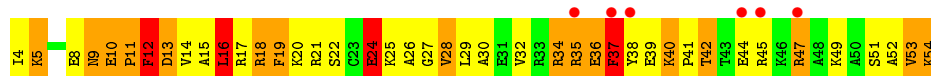
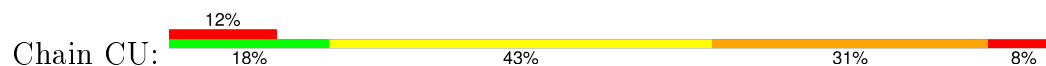
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21



- Molecule 22: 23S rRNA

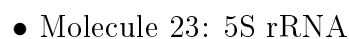




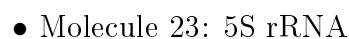


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C1376	G1250	G1315	G1187	C1110	A1046		G907	U842	G774	U702	A637	A575	C509
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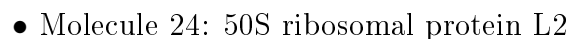
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Response	Percentage
Yes	56%
No	39%
Don't know	5%

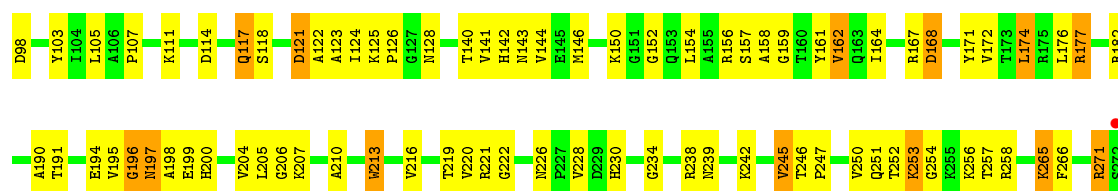


Category	Percentage
Very bad	3%
Bad	36%
Good	54%
Very good	9%

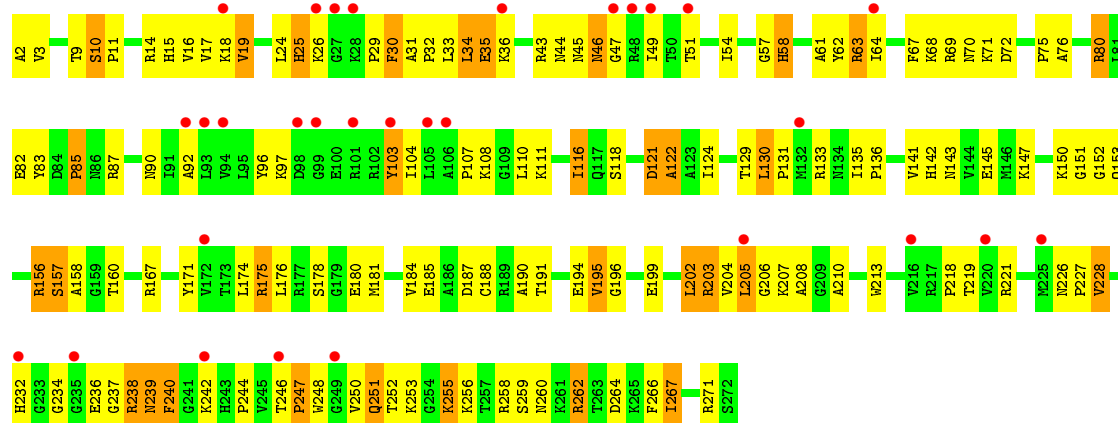


Response	Percentage
Yes	56%
No	38%
Don't know	6%

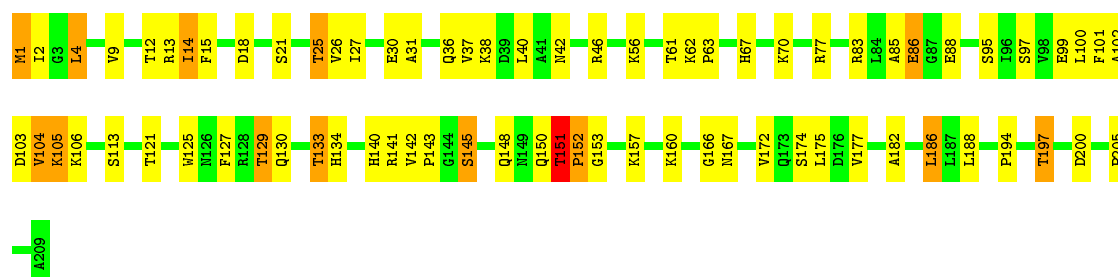




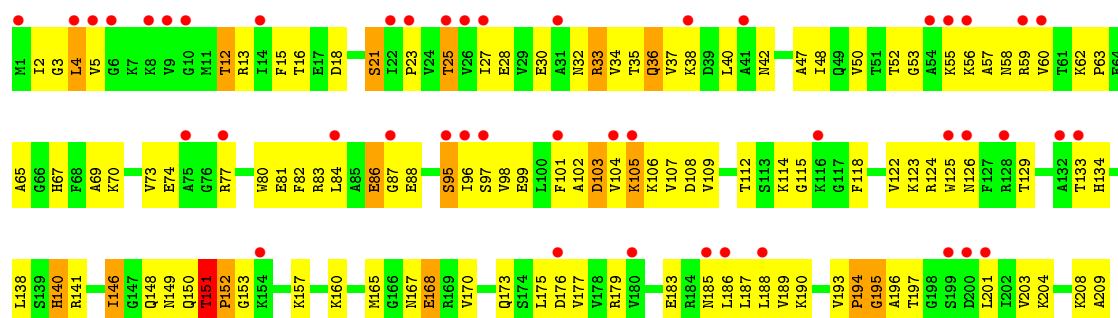
• Molecule 24: 50S ribosomal protein L2



• Molecule 25: 50S ribosomal protein L3

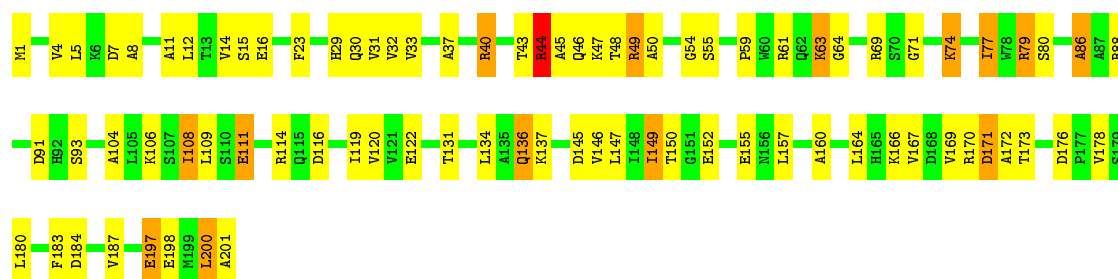


• Molecule 25: 50S ribosomal protein L3




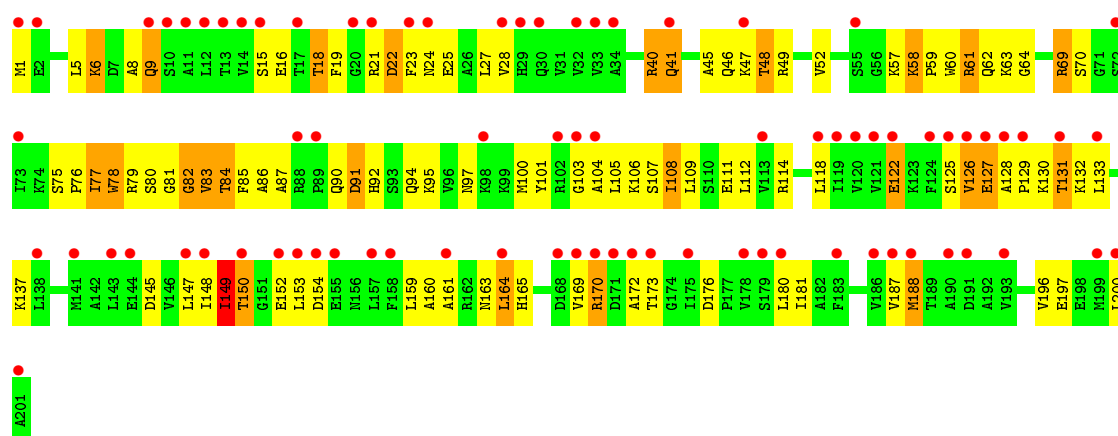
• Molecule 26: 50S ribosomal protein L4

Chain BE: 



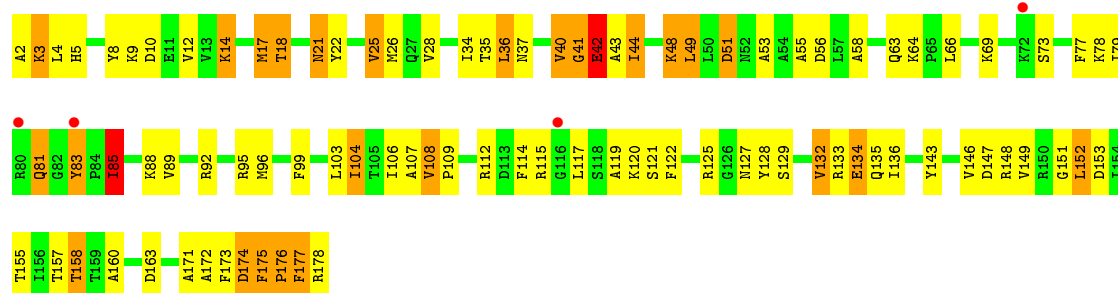
- Molecule 26: 50S ribosomal protein L4

Chain DE: 




- Molecule 27: 50S ribosomal protein L5

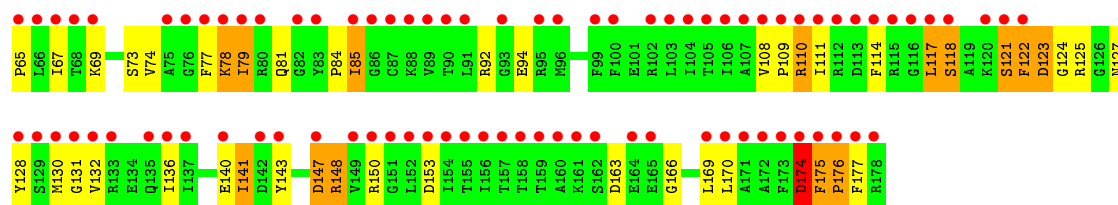
Chain BF: 



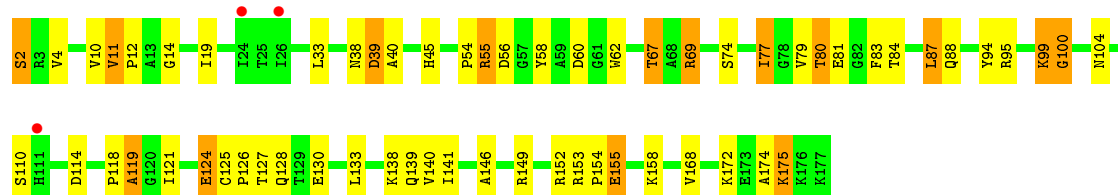
- Molecule 27: 50S ribosomal protein L5

Chain DF: 

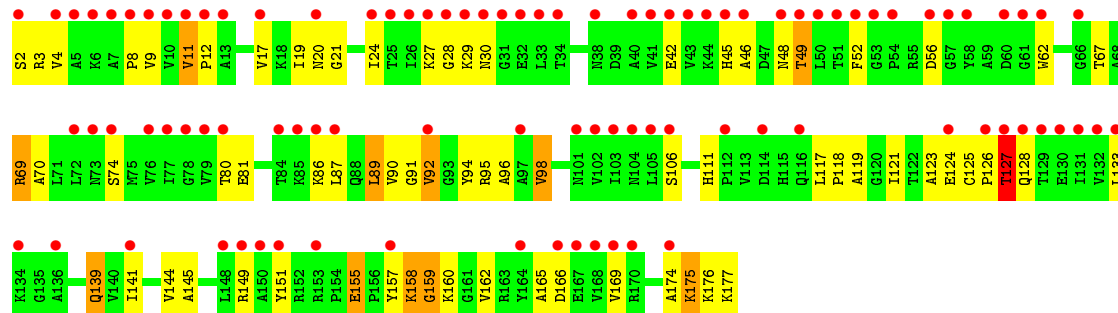




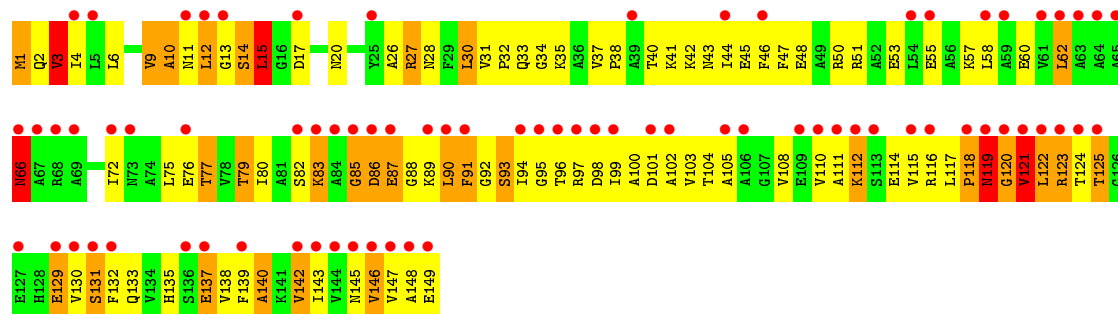
• Molecule 28: 50S ribosomal protein L6



• Molecule 28: 50S ribosomal protein L6

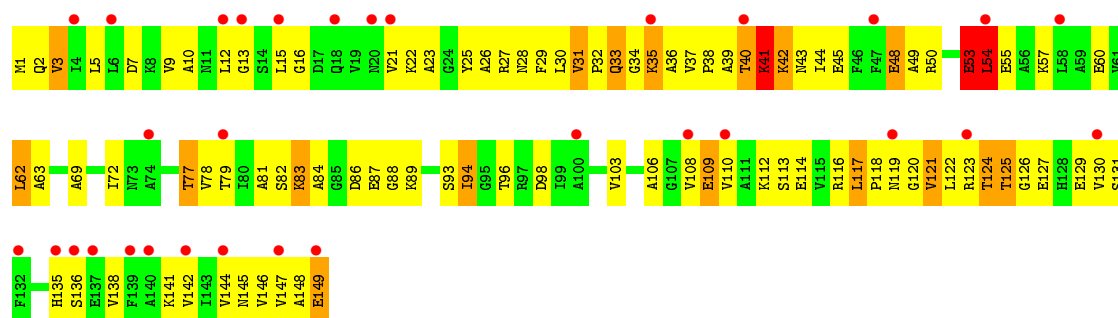


• Molecule 29: 50S ribosomal protein L9

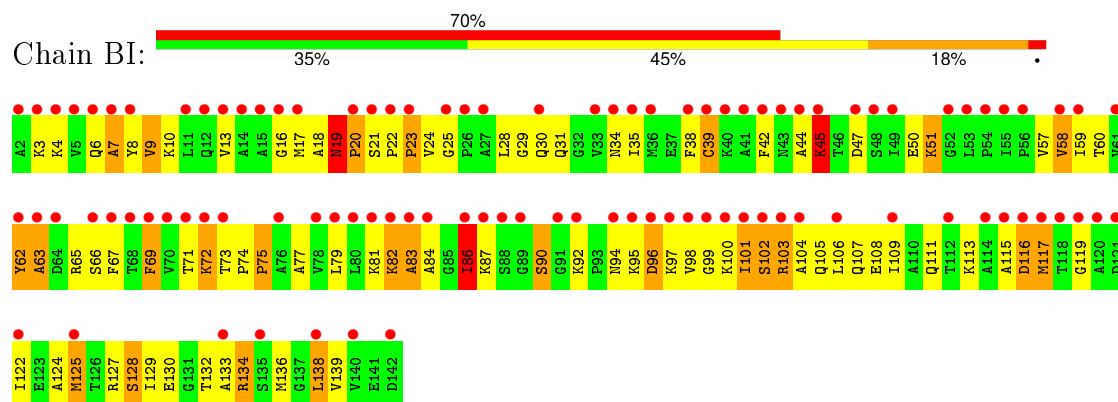


• Molecule 29: 50S ribosomal protein L9

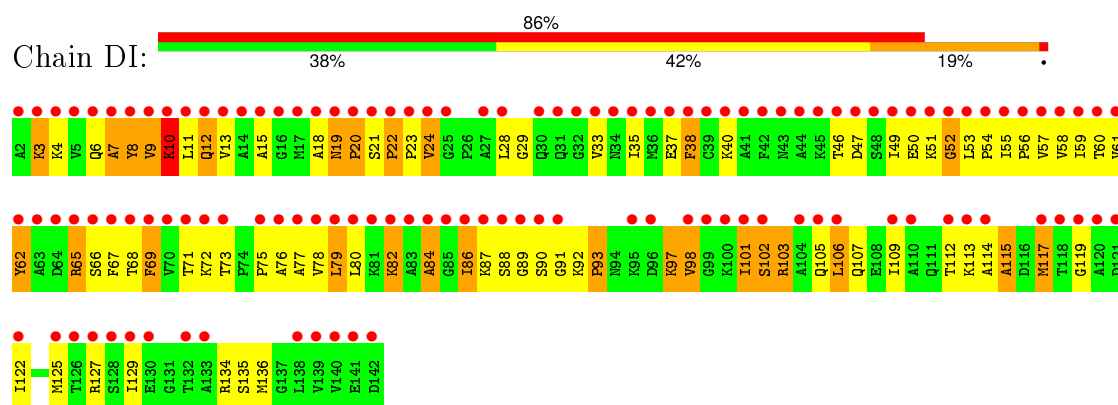




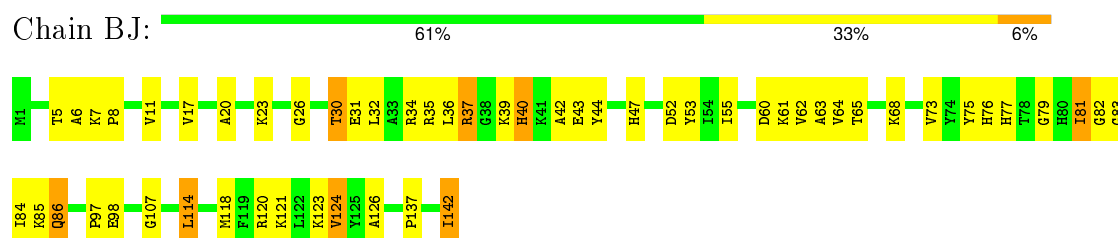
- Molecule 30: 50S ribosomal protein L11



- Molecule 30: 50S ribosomal protein L11

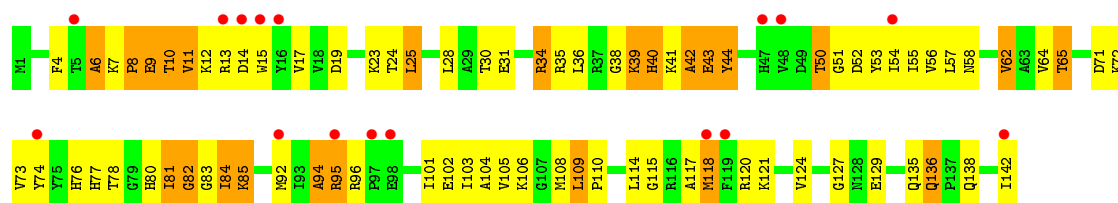


- Molecule 31: 50S ribosomal protein L13



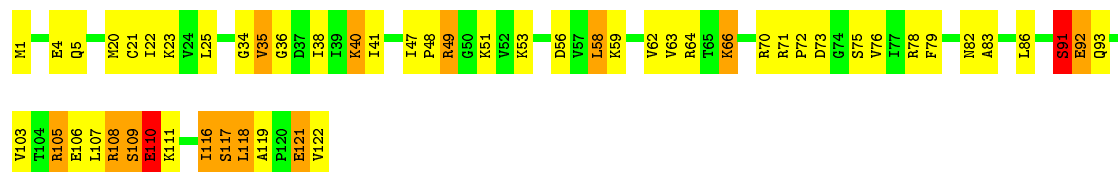
- Molecule 31: 50S ribosomal protein L13





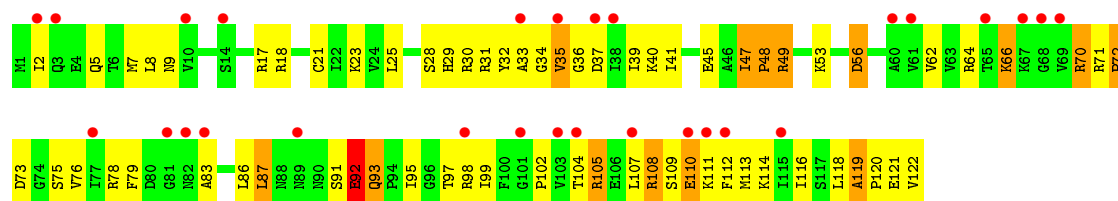
• Molecule 32: 50S ribosomal protein L14

Chain BK: 56% 32% 11% .



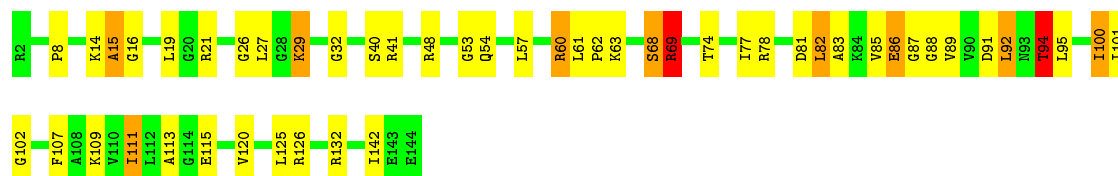
• Molecule 32: 50S ribosomal protein L14

Chain DK: 23% 45% 43% 11% .



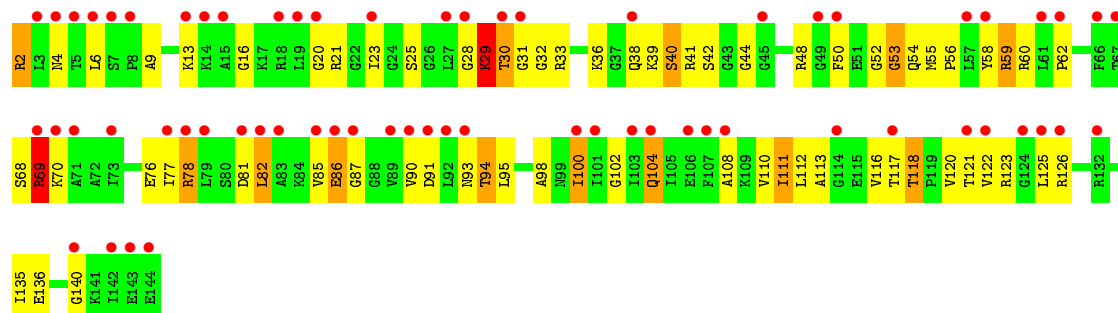
• Molecule 33: 50S ribosomal protein L15

Chain BL: 65% 27% 6% .

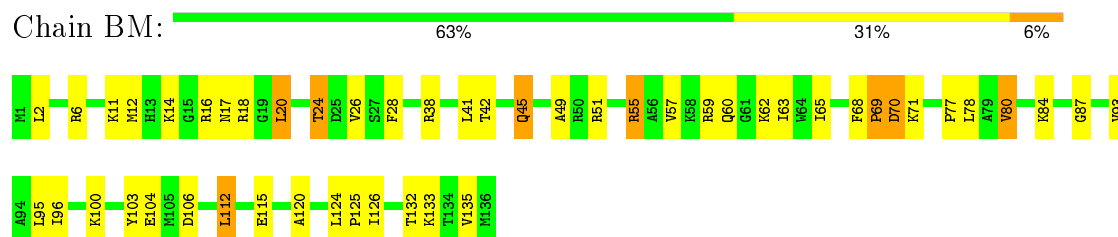


• Molecule 33: 50S ribosomal protein L15

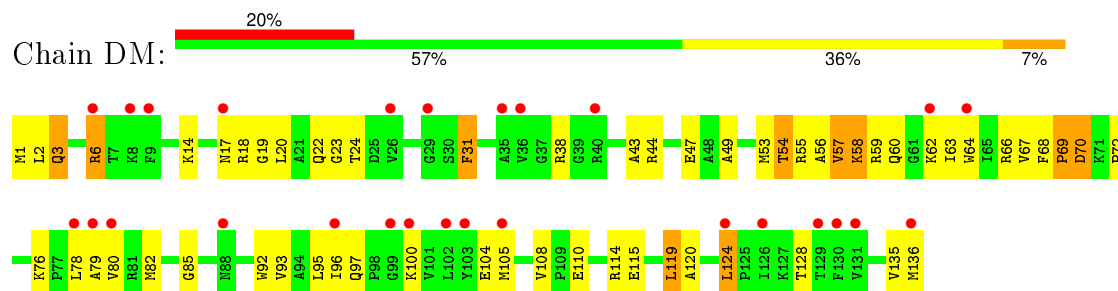
Chain DL: 45% 50% 39% 9% .



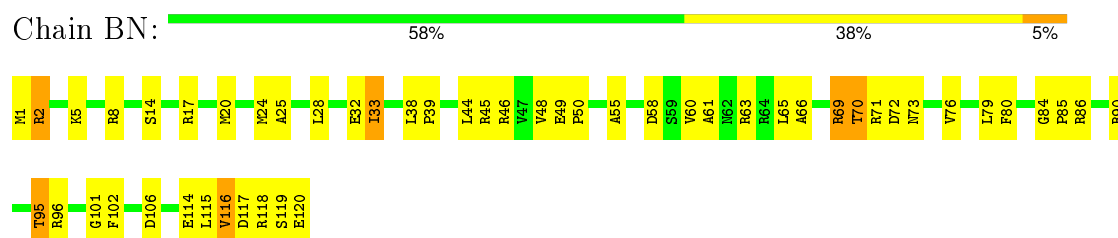
- Molecule 34: 50S ribosomal protein L16



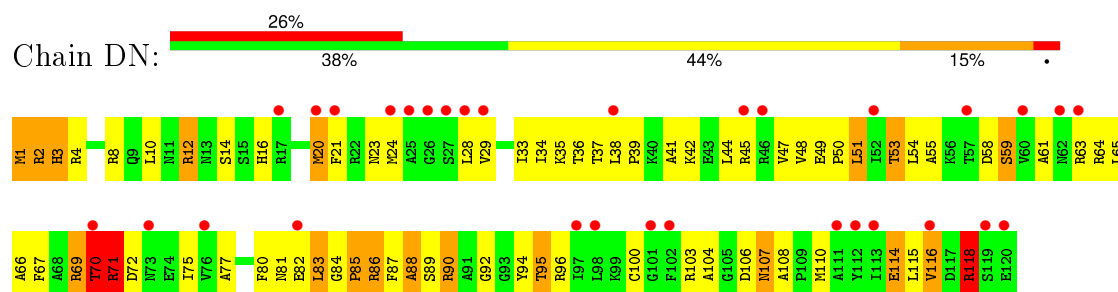
- Molecule 34: 50S ribosomal protein L16



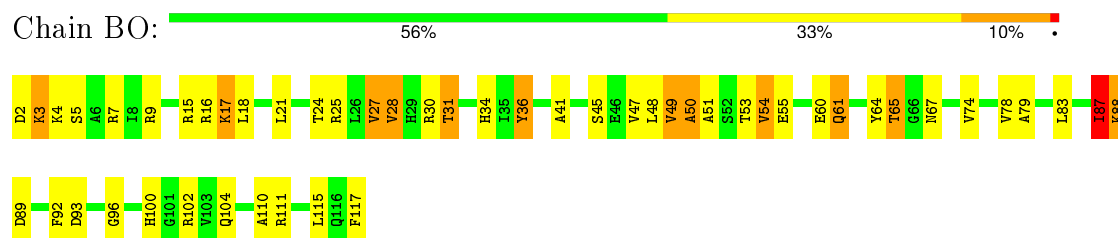
- Molecule 35: 50S ribosomal protein L17



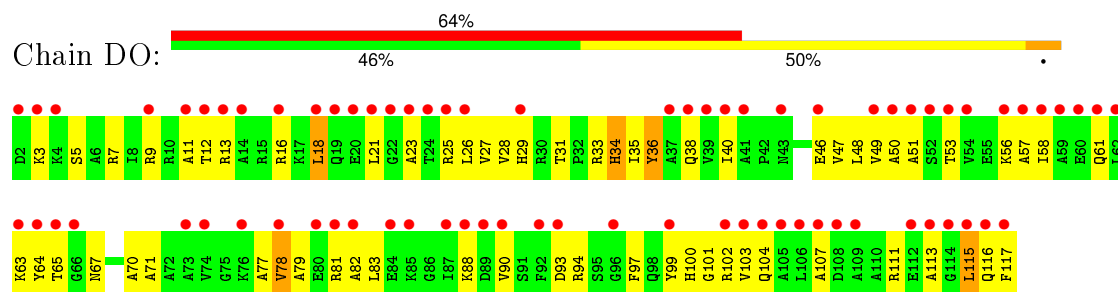
- Molecule 35: 50S ribosomal protein L17



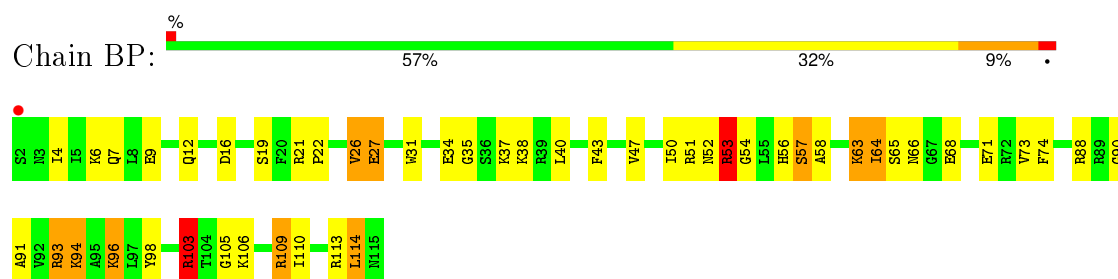
- Molecule 36: 50S ribosomal protein L18



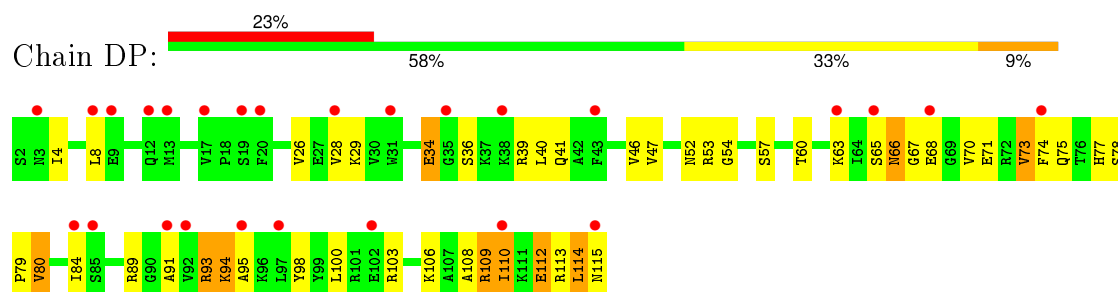
- Molecule 36: 50S ribosomal protein L18



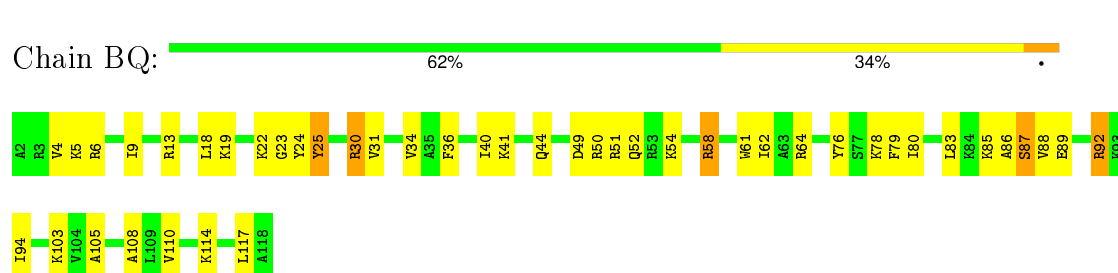
- Molecule 37: 50S ribosomal protein L19



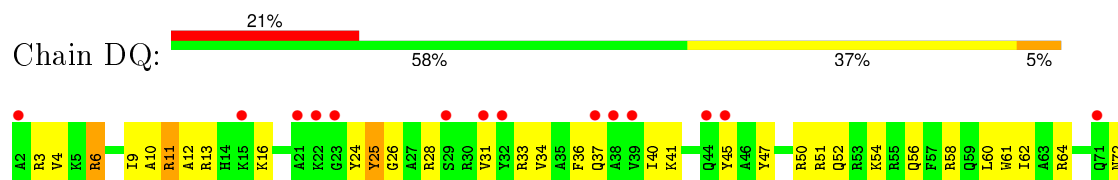
- Molecule 37: 50S ribosomal protein L19

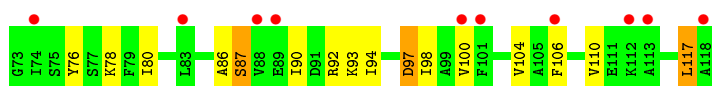


- Molecule 38: 50S ribosomal protein L20



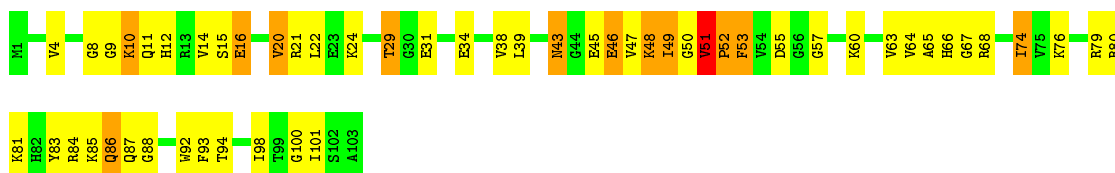
- Molecule 38: 50S ribosomal protein L20





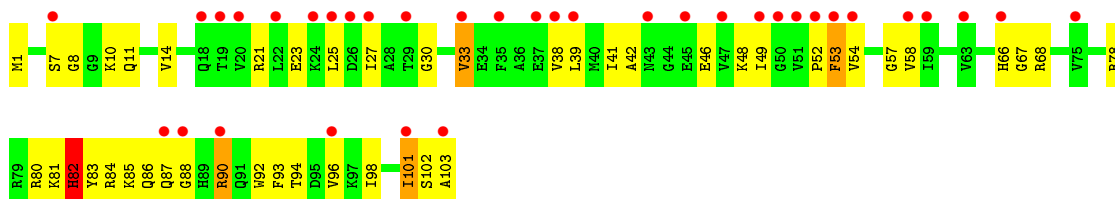
• Molecule 39: 50S ribosomal protein L21

Chain BR: 48% 40% 12%



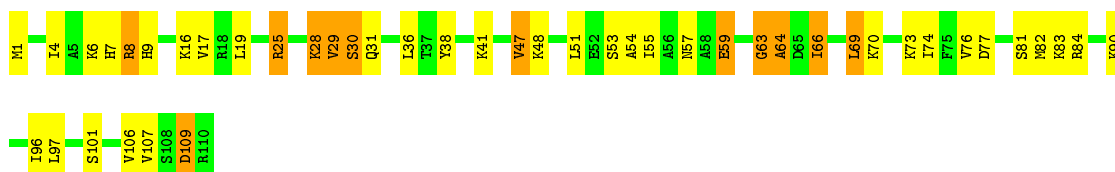
• Molecule 39: 50S ribosomal protein L21

Chain DR: 34% 55% 40%



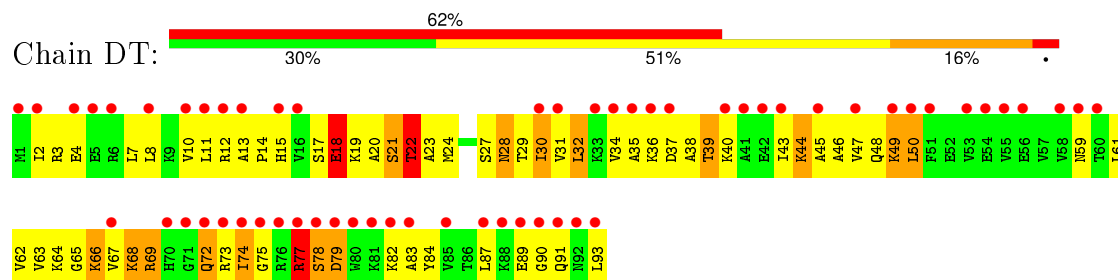
• Molecule 40: 50S ribosomal protein L22

Chain BS: 59% 30% 11%

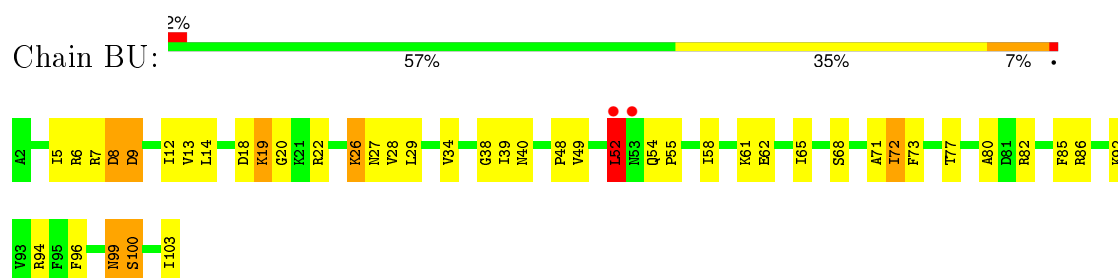




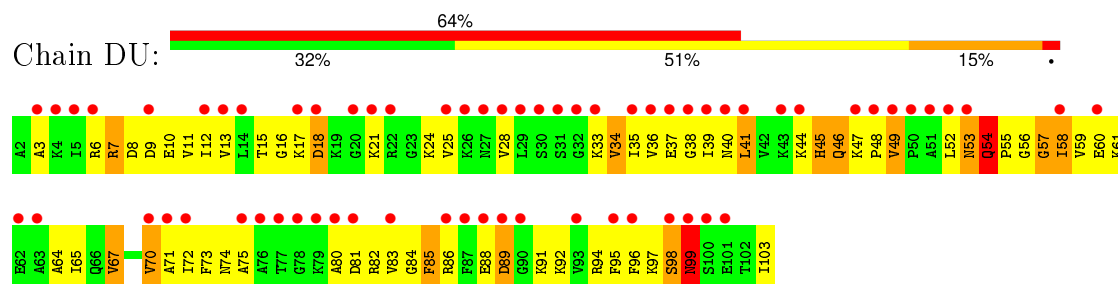
• Molecule 41: 50S ribosomal protein L23



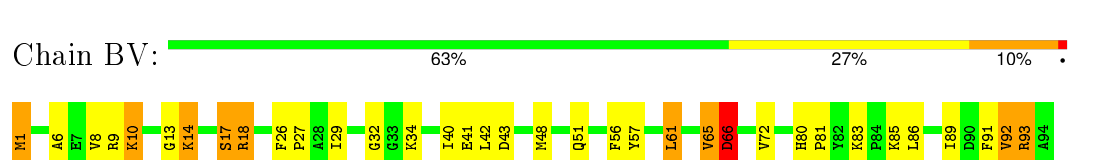
• Molecule 42: 50S ribosomal protein L24



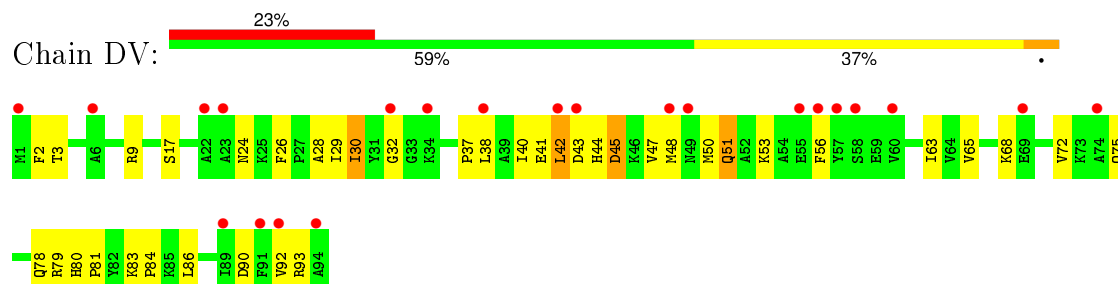
• Molecule 42: 50S ribosomal protein L24



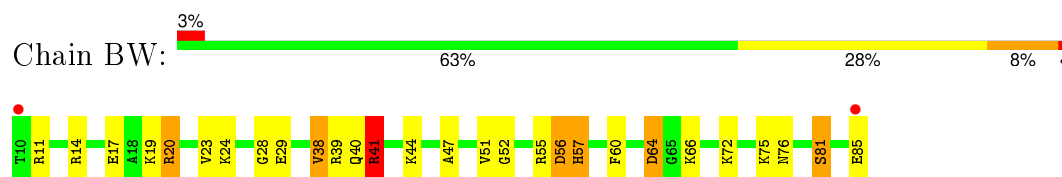
• Molecule 43: 50S ribosomal protein L25



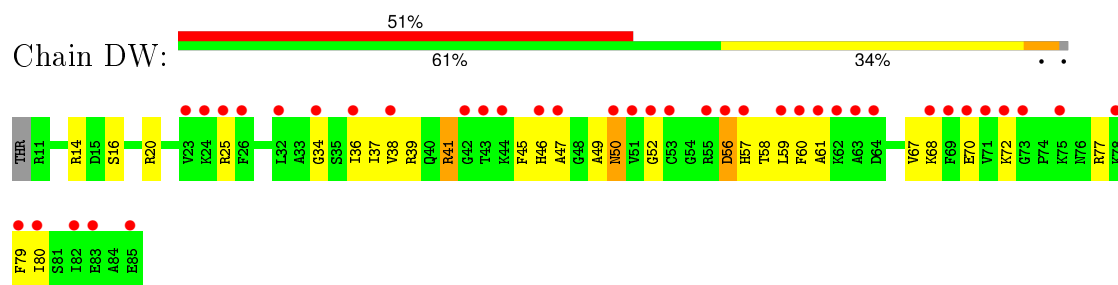
• Molecule 43: 50S ribosomal protein L25



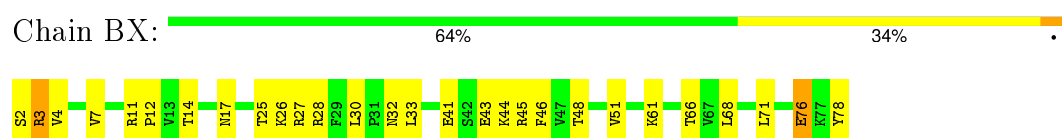
- Molecule 44: 50S ribosomal protein L27



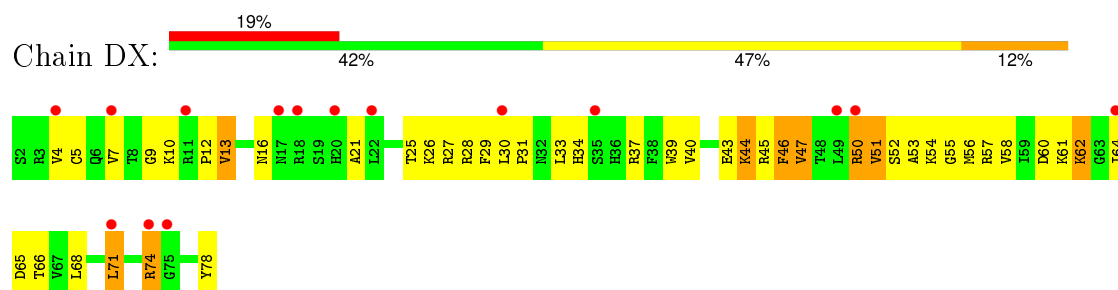
- Molecule 44: 50S ribosomal protein L27



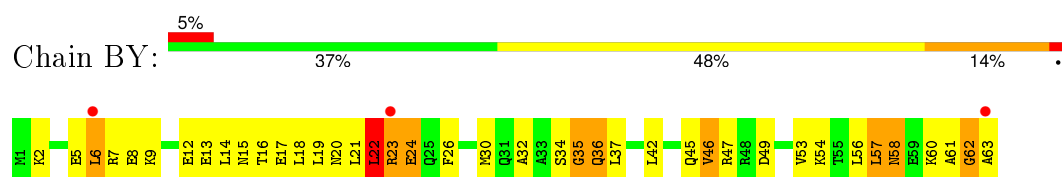
- Molecule 45: 50S ribosomal protein L28



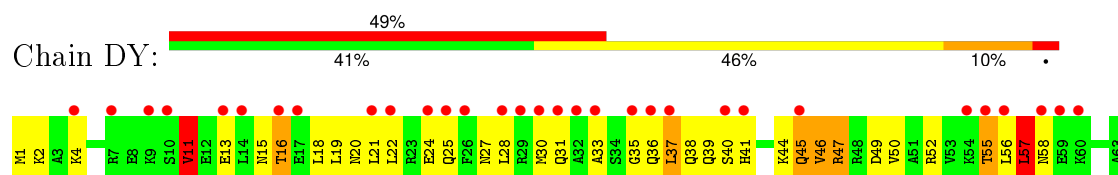
- Molecule 45: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29



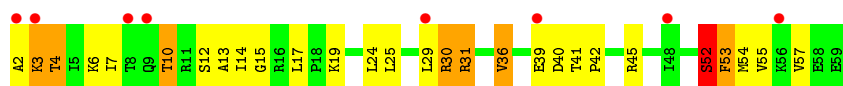
- Molecule 47: 50S ribosomal protein L30

Chain BZ:  69% 29% .



- Molecule 47: 50S ribosomal protein L30

Chain DZ:  14% 52% 34% 12% .



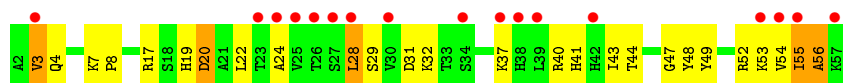
- Molecule 48: 50S ribosomal protein L32

Chain B0:  48% 43% 9%



- Molecule 48: 50S ribosomal protein L32

Chain D0:  30% 54% 38% 9%



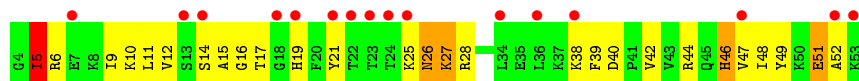
- Molecule 49: 50S ribosomal protein L33

Chain B1:  2% 54% 36% 8% .




- Molecule 49: 50S ribosomal protein L33

Chain D1:  32% 46% 44% 8% .

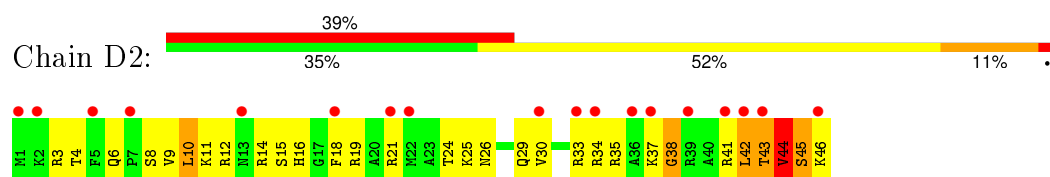


- Molecule 50: 50S ribosomal protein L34

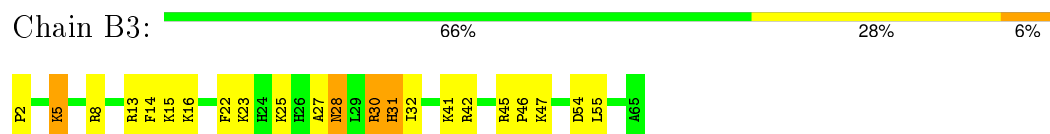
Chain B2:  2% 70% 26% .



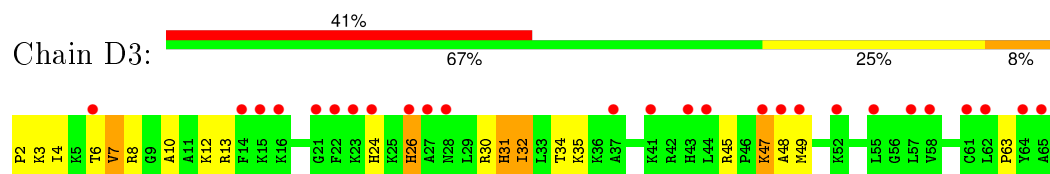
- Molecule 50: 50S ribosomal protein L34



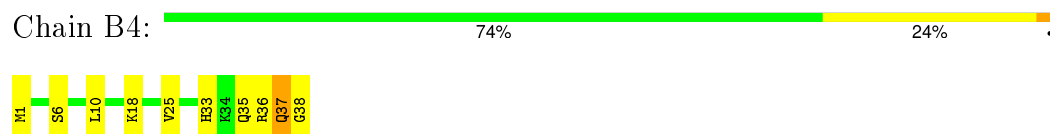
- Molecule 51: 50S ribosomal protein L35



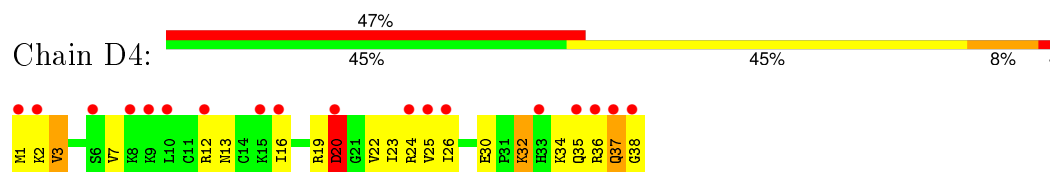
- Molecule 51: 50S ribosomal protein L35



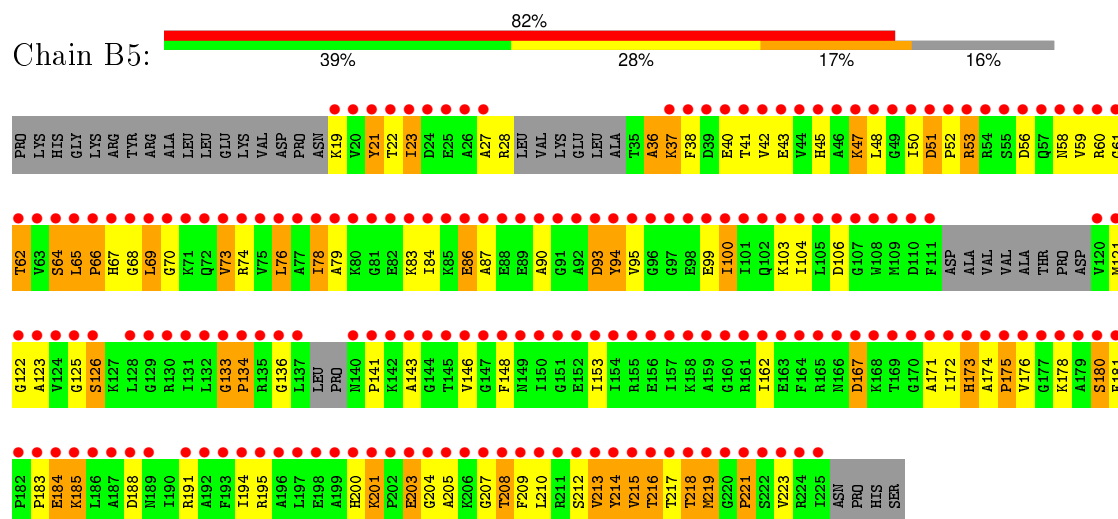
- Molecule 52: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1

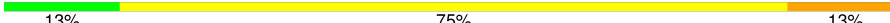


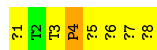
- Molecule 54: Quinupristin

Chain B6:  63% 38%



- Molecule 54: Quinupristin

Chain D6:  13% 75% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.26Å 432.34Å 621.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.08 – 2.80 69.08 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (69.08-2.80) 94.1 (69.08-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1160)	Depositor
R, R_{free}	0.225 , 0.271 0.234 , 0.280	Depositor DCC
R_{free} test set	5217 reflections (0.40%)	DCC
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 1296566 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288423	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.34	0/36944	0.80	3/57632 (0.0%)
1	CA	0.28	0/36966	0.78	1/57666 (0.0%)
2	AB	0.28	0/1736	0.56	0/2338
2	CB	0.26	0/1736	0.50	0/2338
3	AC	0.28	0/1652	0.53	0/2225
3	CC	0.25	0/1652	0.48	0/2225
4	AD	0.29	0/1665	0.55	0/2227
4	CD	0.31	0/1665	0.55	0/2227
5	AE	0.31	0/1119	0.61	0/1504
5	CE	0.29	0/1119	0.59	0/1504
6	AF	0.30	0/836	0.55	0/1128
6	CF	0.27	0/836	0.57	1/1128 (0.1%)
7	AG	0.26	0/1196	0.48	0/1602
7	CG	0.25	0/1196	0.49	0/1602
8	AH	0.31	0/989	0.50	0/1326
8	CH	0.25	0/989	0.48	0/1326
9	AI	0.26	0/1034	0.54	0/1375
9	CI	0.26	0/1034	0.52	0/1375
10	AJ	0.29	0/797	0.55	0/1077
10	CJ	0.25	0/797	0.50	0/1077
11	AK	0.29	0/893	0.63	1/1205 (0.1%)
11	CK	0.26	0/893	0.52	0/1205
12	AL	0.31	0/969	0.58	0/1300
12	CL	0.29	0/969	0.60	0/1300
13	AM	0.27	0/893	0.55	0/1193
13	CM	0.26	0/893	0.50	0/1193
14	AN	0.28	0/785	0.55	0/1043
14	CN	0.25	0/785	0.46	0/1043
15	AO	0.28	0/718	0.53	0/959
15	CO	0.26	0/718	0.46	0/959
16	AP	0.30	0/659	0.66	1/884 (0.1%)
16	CP	0.27	0/659	0.49	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.30	0/658	0.58	0/881
17	CQ	0.28	0/658	0.51	0/881
18	AR	0.26	0/463	0.53	0/621
18	CR	0.26	0/463	0.49	0/621
19	AS	0.27	0/653	0.50	0/877
19	CS	0.27	0/653	0.54	0/877
20	AT	0.31	0/671	0.55	0/888
20	CT	0.25	0/671	0.50	0/888
21	AU	0.36	0/431	0.62	0/570
21	CU	0.33	0/431	0.56	0/570
22	BA	0.59	5/69659 (0.0%)	0.99	92/108672 (0.1%)
22	DA	0.27	0/69659	0.79	4/108672 (0.0%)
23	BB	0.52	0/2850	0.93	0/4444
23	DB	0.23	0/2828	0.76	0/4410
24	BC	0.38	0/2122	0.60	0/2852
24	DC	0.27	0/2122	0.52	0/2852
25	BD	0.42	0/1586	0.63	1/2134 (0.0%)
25	DD	0.26	0/1586	0.51	0/2134
26	BE	0.37	0/1571	0.60	0/2113
26	DE	0.26	0/1571	0.51	0/2113
27	BF	0.30	0/1435	0.52	0/1926
27	DF	0.24	0/1435	0.46	0/1926
28	BG	0.30	0/1343	0.53	0/1816
28	DG	0.25	0/1343	0.46	0/1816
29	BH	0.36	0/1121	0.66	1/1515 (0.1%)
29	DH	0.35	0/1121	0.56	0/1515
30	BI	0.29	0/1046	0.54	0/1410
30	DI	0.28	0/1046	0.52	0/1410
31	BJ	0.42	0/1152	0.58	0/1551
31	DJ	0.25	0/1152	0.51	0/1551
32	BK	0.41	0/948	0.64	0/1268
32	DK	0.27	0/948	0.51	0/1268
33	BL	0.39	0/1054	0.64	0/1403
33	DL	0.26	0/1054	0.51	0/1403
34	BM	0.42	0/1093	0.63	0/1460
34	DM	0.25	0/1093	0.46	0/1460
35	BN	0.43	0/974	0.68	0/1301
35	DN	0.27	0/974	0.56	1/1301 (0.1%)
36	BO	0.34	0/902	0.55	0/1209
36	DO	0.24	0/902	0.45	0/1209
37	BP	0.42	0/929	0.69	2/1242 (0.2%)
37	DP	0.26	0/929	0.47	0/1242
38	BQ	0.50	0/960	0.66	0/1278

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	CF	0	1
11	AK	0	1

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

All (5) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
25	BD	151	THR	Peptide
6	CF	54	LEU	Peptide
12	CL	23	ALA	Peptide
12	CL	24	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	962	0
1	CA	33015	0	16617	1107	1
2	AB	1705	0	1732	164	0
2	CB	1705	0	1732	135	0
3	AC	1625	0	1696	78	0
3	CC	1625	0	1696	69	0
4	AD	1643	0	1707	116	0
4	CD	1643	0	1707	116	0
5	AE	1106	0	1148	88	0
5	CE	1106	0	1148	99	0
6	AF	818	0	808	47	0
6	CF	818	0	808	60	0
7	AG	1182	0	1238	58	0
7	CG	1182	0	1238	66	0
8	AH	979	0	1031	49	0
8	CH	979	0	1031	52	0
9	AI	1022	0	1070	87	0
9	CI	1022	0	1070	66	0
10	AJ	787	0	828	81	0
10	CJ	787	0	828	56	0
11	AK	877	0	887	68	0
11	CK	877	0	887	55	0
12	AL	955	0	1016	44	0
12	CL	955	0	1016	74	0
13	AM	884	0	941	44	0
13	CM	884	0	941	51	0
14	AN	774	0	824	58	0
14	CN	774	0	824	51	0
15	AO	710	0	728	31	0
15	CO	710	0	728	29	0
16	AP	649	0	666	53	0
16	CP	649	0	666	36	0
17	AQ	649	0	691	63	0
17	CQ	649	0	691	53	0
18	AR	456	0	478	17	0
18	CR	456	0	478	25	0
19	AS	638	0	665	39	0
19	CS	638	0	665	42	0
20	AT	665	0	714	65	0
20	CT	665	0	714	46	0
21	AU	426	0	449	52	0
21	CU	426	0	449	53	0
22	BA	62195	0	31280	1486	0

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

The worst 5 of 10587 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
22:BA:730:A:OP2	58:BA:3693:HOH:O	1.58	1.21
1:AA:533:A:OP1	58:AA:1848:HOH:O	1.65	1.15
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14
22:BA:2498:C:OP2	58:BA:3684:HOH:O	1.64	1.13

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

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

5.3 Torsion angles ⓘ

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BE	199/201 (99%)	165 (83%)	30 (15%)	4 (2%)	9	30
26	DE	199/201 (99%)	154 (77%)	27 (14%)	18 (9%)	1	2
27	BF	175/177 (99%)	142 (81%)	24 (14%)	9 (5%)	2	8
27	DF	175/177 (99%)	135 (77%)	27 (15%)	13 (7%)	1	3
28	BG	174/176 (99%)	148 (85%)	16 (9%)	10 (6%)	2	6
28	DG	174/176 (99%)	127 (73%)	36 (21%)	11 (6%)	2	4
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	1
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	1	1
30	BI	139/141 (99%)	78 (56%)	37 (27%)	24 (17%)	0	0
30	DI	139/141 (99%)	82 (59%)	38 (27%)	19 (14%)	0	1
31	BJ	140/142 (99%)	125 (89%)	14 (10%)	1 (1%)	26	62
31	DJ	140/142 (99%)	104 (74%)	23 (16%)	13 (9%)	1	1
32	BK	120/122 (98%)	97 (81%)	14 (12%)	9 (8%)	1	3
32	DK	120/122 (98%)	95 (79%)	15 (12%)	10 (8%)	1	2
33	BL	141/143 (99%)	112 (79%)	21 (15%)	8 (6%)	2	6
33	DL	141/143 (99%)	98 (70%)	31 (22%)	12 (8%)	1	2
34	BM	134/136 (98%)	120 (90%)	11 (8%)	3 (2%)	8	28
34	DM	134/136 (98%)	112 (84%)	17 (13%)	5 (4%)	4	14
35	BN	118/120 (98%)	95 (80%)	21 (18%)	2 (2%)	11	36
35	DN	118/120 (98%)	90 (76%)	18 (15%)	10 (8%)	1	2
36	BO	114/116 (98%)	96 (84%)	14 (12%)	4 (4%)	4	15
36	DO	114/116 (98%)	82 (72%)	24 (21%)	8 (7%)	1	3
37	BP	112/114 (98%)	99 (88%)	8 (7%)	5 (4%)	3	10
37	DP	112/114 (98%)	88 (79%)	18 (16%)	6 (5%)	2	7
38	BQ	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	21	55
38	DQ	115/117 (98%)	92 (80%)	22 (19%)	1 (1%)	21	55
39	BR	101/103 (98%)	81 (80%)	10 (10%)	10 (10%)	1	1
39	DR	101/103 (98%)	72 (71%)	23 (23%)	6 (6%)	2	5
40	BS	108/110 (98%)	94 (87%)	10 (9%)	4 (4%)	4	14
40	DS	108/110 (98%)	83 (77%)	17 (16%)	8 (7%)	1	3
41	BT	91/93 (98%)	74 (81%)	9 (10%)	8 (9%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	DT	91/93 (98%)	53 (58%)	28 (31%)	10 (11%)	0	1
42	BU	100/102 (98%)	77 (77%)	19 (19%)	4 (4%)	4	12
42	DU	100/102 (98%)	69 (69%)	19 (19%)	12 (12%)	0	1
43	BV	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	17	50
43	DV	92/94 (98%)	76 (83%)	14 (15%)	2 (2%)	8	28
44	BW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	6	21
44	DW	73/76 (96%)	61 (84%)	12 (16%)	0	100	100
45	BX	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	15	44
45	DX	75/77 (97%)	58 (77%)	12 (16%)	5 (7%)	1	4
46	BY	61/63 (97%)	43 (70%)	10 (16%)	8 (13%)	0	1
46	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	2
47	BZ	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
47	DZ	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	1	2
48	B0	54/56 (96%)	46 (85%)	4 (7%)	4 (7%)	1	3
48	D0	54/56 (96%)	37 (68%)	12 (22%)	5 (9%)	1	1
49	B1	48/50 (96%)	40 (83%)	4 (8%)	4 (8%)	1	2
49	D1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	2
50	B2	44/46 (96%)	37 (84%)	5 (11%)	2 (4%)	3	10
50	D2	44/46 (96%)	34 (77%)	6 (14%)	4 (9%)	1	2
51	B3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	12	38
51	D3	62/64 (97%)	52 (84%)	6 (10%)	4 (6%)	1	4
52	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	6	21
52	D4	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2	6
53	B5	183/228 (80%)	87 (48%)	53 (29%)	43 (24%)	0	0
54	B6	2/8 (25%)	2 (100%)	0	0	100	100
54	D6	2/8 (25%)	0	2 (100%)	0	100	100
All	All	11422/11688 (98%)	8528 (75%)	1918 (17%)	976 (8%)	1	2

5 of 976 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
2	AB	22	TYR
2	AB	25	PRO
2	AB	34	ALA

5.3.2 Protein sidechains ⓘ

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	103/103 (100%)	82 (80%)	21 (20%)	1	4
13	AM	92/92 (100%)	74 (80%)	18 (20%)	1	5
13	CM	92/92 (100%)	75 (82%)	17 (18%)	2	6
14	AN	79/83 (95%)	64 (81%)	15 (19%)	2	5
14	CN	79/83 (95%)	70 (89%)	9 (11%)	7	21
15	AO	75/76 (99%)	63 (84%)	12 (16%)	3	9
15	CO	75/76 (99%)	65 (87%)	10 (13%)	5	14
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	3
16	CP	65/65 (100%)	54 (83%)	11 (17%)	2	7
17	AQ	74/74 (100%)	50 (68%)	24 (32%)	0	1
17	CQ	74/74 (100%)	51 (69%)	23 (31%)	0	1
18	AR	48/48 (100%)	38 (79%)	10 (21%)	1	4
18	CR	48/48 (100%)	38 (79%)	10 (21%)	1	4
19	AS	70/70 (100%)	55 (79%)	15 (21%)	1	3
19	CS	70/70 (100%)	58 (83%)	12 (17%)	2	7
20	AT	65/65 (100%)	51 (78%)	14 (22%)	1	3
20	CT	65/65 (100%)	57 (88%)	8 (12%)	6	18
21	AU	44/44 (100%)	29 (66%)	15 (34%)	0	0
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0	0
24	BC	216/216 (100%)	189 (88%)	27 (12%)	6	17
24	DC	216/216 (100%)	197 (91%)	19 (9%)	12	35
25	BD	164/164 (100%)	148 (90%)	16 (10%)	10	28
25	DD	164/164 (100%)	145 (88%)	19 (12%)	7	20
26	BE	165/165 (100%)	136 (82%)	29 (18%)	2	7
26	DE	165/165 (100%)	137 (83%)	28 (17%)	2	7
27	BF	148/148 (100%)	116 (78%)	32 (22%)	1	3
27	DF	148/148 (100%)	119 (80%)	29 (20%)	1	5
28	BG	137/137 (100%)	118 (86%)	19 (14%)	4	13
28	DG	137/137 (100%)	114 (83%)	23 (17%)	2	8
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	3
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BI	109/109 (100%)	82 (75%)	27 (25%)	1	2
30	DI	109/109 (100%)	80 (73%)	29 (27%)	0	1
31	BJ	116/116 (100%)	105 (90%)	11 (10%)	11	30
31	DJ	116/116 (100%)	94 (81%)	22 (19%)	2	5
32	BK	103/103 (100%)	89 (86%)	14 (14%)	5	14
32	DK	103/103 (100%)	90 (87%)	13 (13%)	5	17
33	BL	102/102 (100%)	91 (89%)	11 (11%)	8	23
33	DL	102/102 (100%)	86 (84%)	16 (16%)	3	9
34	BM	109/109 (100%)	99 (91%)	10 (9%)	11	32
34	DM	109/109 (100%)	95 (87%)	14 (13%)	5	16
35	BN	100/100 (100%)	94 (94%)	6 (6%)	24	56
35	DN	100/100 (100%)	76 (76%)	24 (24%)	1	2
36	BO	86/86 (100%)	65 (76%)	21 (24%)	1	2
36	DO	86/86 (100%)	70 (81%)	16 (19%)	2	6
37	BP	99/99 (100%)	81 (82%)	18 (18%)	2	6
37	DP	99/99 (100%)	90 (91%)	9 (9%)	12	33
38	BQ	89/89 (100%)	78 (88%)	11 (12%)	6	17
38	DQ	89/89 (100%)	78 (88%)	11 (12%)	6	17
39	BR	84/84 (100%)	74 (88%)	10 (12%)	6	19
39	DR	84/84 (100%)	76 (90%)	8 (10%)	11	30
40	BS	93/93 (100%)	76 (82%)	17 (18%)	2	6
40	DS	93/93 (100%)	83 (89%)	10 (11%)	8	23
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	11
41	DT	80/80 (100%)	66 (82%)	14 (18%)	2	7
42	BU	83/83 (100%)	72 (87%)	11 (13%)	5	14
42	DU	83/83 (100%)	68 (82%)	15 (18%)	2	6
43	BV	78/78 (100%)	63 (81%)	15 (19%)	2	5
43	DV	78/78 (100%)	65 (83%)	13 (17%)	3	8
44	BW	57/58 (98%)	47 (82%)	10 (18%)	2	7
44	DW	56/58 (97%)	50 (89%)	6 (11%)	8	24
45	BX	67/67 (100%)	61 (91%)	6 (9%)	12	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DX	67/67 (100%)	58 (87%)	9 (13%)	5	14
46	BY	55/55 (100%)	50 (91%)	5 (9%)	12	33
46	DY	55/55 (100%)	43 (78%)	12 (22%)	1	3
47	BZ	48/48 (100%)	41 (85%)	7 (15%)	4	11
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	4
48	B0	47/47 (100%)	42 (89%)	5 (11%)	8	24
48	D0	47/47 (100%)	43 (92%)	4 (8%)	13	36
49	B1	45/45 (100%)	42 (93%)	3 (7%)	20	50
49	D1	45/45 (100%)	39 (87%)	6 (13%)	5	14
50	B2	38/38 (100%)	34 (90%)	4 (10%)	8	24
50	D2	38/38 (100%)	31 (82%)	7 (18%)	2	6
51	B3	51/51 (100%)	45 (88%)	6 (12%)	6	19
51	D3	51/51 (100%)	46 (90%)	5 (10%)	10	28
52	B4	34/34 (100%)	32 (94%)	2 (6%)	24	57
52	D4	34/34 (100%)	26 (76%)	8 (24%)	1	2
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1	4
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7747 (82%)	1643 (18%)	2	7

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

Mol	Chain	Res	Type
42	BU	72	ILE
4	CD	155	VAL
39	DR	41	ILE
44	BW	39	ARG
2	CB	43	LEU

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

Mol	Chain	Res	Type
5	CE	122	ASN
17	CQ	31	HIS
49	D1	26	ASN

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Mol	Chain	Res	Type
7	CG	97	ASN
15	CO	42	HIS

5.3.3 RNA ⓘ

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

5 of 1985 RNA backbone outliers are listed below:

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

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2873	A
1	CA	1279	G
22	DA	2326	C
1	CA	85	U
1	CA	484	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	MHW	B6	1	54	9,9,10	1.42	1 (11%)	8,11,13	2.63	3 (37%)
54	DBB	B6	3	54	4,5,6	1.24	0	3,5,7	2.10	2 (66%)
54	MHU	B6	5	54	13,15,16	1.78	3 (23%)	15,19,21	1.00	1 (6%)
54	MHV	B6	6	54	7,9,10	1.51	1 (14%)	8,11,13	3.46	4 (50%)
54	004	B6	7	54	9,10,11	1.59	1 (11%)	10,12,14	2.37	3 (30%)
54	MHW	D6	1	54	9,9,10	1.64	1 (11%)	8,11,13	2.90	2 (25%)
54	DBB	D6	3	54	4,5,6	1.10	0	3,5,7	1.54	1 (33%)
54	MHU	D6	5	54	13,15,16	1.62	3 (23%)	15,19,21	1.20	2 (13%)
54	MHV	D6	6	54	7,9,10	1.15	0	8,11,13	3.32	5 (62%)
54	004	D6	7	54	9,10,11	0.77	0	10,12,14	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	B6	3	54	-	0/2/4/6	0/0/0/0
54	MHU	B6	5	54	-	0/8/12/14	0/1/1/1
54	MHV	B6	6	54	-	0/1/12/14	0/1/1/1
54	004	B6	7	54	-	0/4/6/8	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	D6	3	54	-	0/2/4/6	0/0/0/0
54	MHU	D6	5	54	-	0/8/12/14	0/1/1/1
54	MHV	D6	6	54	-	0/1/12/14	0/1/1/1
54	004	D6	7	54	-	0/4/6/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-4.56	1.48	1.52
54	B6	6	MHV	CB-CG	-2.76	1.45	1.50
54	D6	5	MHU	CD2-CE2	2.02	1.42	1.38
54	D6	5	MHU	CB-CG	2.07	1.56	1.51
54	B6	5	MHU	CB-CG	2.11	1.56	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	MHV	CD2-CE-N	-5.70	98.62	109.82
54	B6	6	MHV	CD2-CE-N	-5.22	99.55	109.82
54	D6	1	MHW	CG2-CD-CE	-4.67	111.66	118.90
54	B6	6	MHV	OD1-CG-CB	-4.51	116.26	121.98
54	B6	7	004	CB-CA-N	-4.22	102.59	112.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 502 ligands modelled in this entry, 500 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	DOL	BA	3001	-	43,50,50	3.20	15 (34%)	50,70,70	3.24	13 (26%)
56	DOL	DA	3001	-	43,50,50	3.18	13 (30%)	50,70,70	3.07	12 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	DOL	BA	3001	-	-	0/58/77/77	0/1/3/3
56	DOL	DA	3001	-	-	0/58/77/77	0/1/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BA	3001	DOL	C1-C2	-7.67	1.43	1.55
56	DA	3001	DOL	C1-C2	-6.65	1.45	1.55
56	BA	3001	DOL	O36-C32	-3.50	1.39	1.44
56	BA	3001	DOL	C16-C17	-3.20	1.49	1.54
56	DA	3001	DOL	C16-C17	-3.14	1.49	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DA	3001	DOL	O40-S39-O41	-18.11	100.57	117.98
56	BA	3001	DOL	O40-S39-O41	-17.18	101.47	117.98
56	DA	3001	DOL	C4-N5-C1	-5.65	106.22	112.39
56	BA	3001	DOL	O7-C6-N5	-4.61	115.16	121.52
56	BA	3001	DOL	C23-C22-C20	-4.49	118.91	125.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 40 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.12	19 (1%) 81 73	10, 49, 132, 182	0
1	CA	1539/1539 (100%)	0.17	49 (3%) 51 39	22, 70, 146, 178	0
2	AB	218/218 (100%)	0.82	30 (13%) 4 2	36, 73, 100, 117	0
2	CB	218/218 (100%)	1.07	46 (21%) 1 1	57, 86, 108, 121	0
3	AC	206/206 (100%)	0.16	9 (4%) 38 26	33, 57, 78, 95	0
3	CC	206/206 (100%)	1.20	52 (25%) 1 0	55, 80, 96, 107	0
4	AD	205/205 (100%)	0.37	9 (4%) 38 26	31, 56, 79, 99	0
4	CD	205/205 (100%)	-0.02	5 (2%) 62 50	13, 35, 60, 82	0
5	AE	150/150 (100%)	0.11	2 (1%) 79 71	26, 47, 78, 93	0
5	CE	150/150 (100%)	0.19	1 (0%) 89 84	25, 52, 84, 104	0
6	AF	100/100 (100%)	-0.16	1 (1%) 84 77	32, 54, 73, 77	0
6	CF	100/100 (100%)	0.54	10 (10%) 9 4	41, 74, 92, 103	0
7	AG	151/151 (100%)	0.26	3 (1%) 68 58	51, 75, 92, 100	0
7	CG	151/151 (100%)	2.58	86 (56%) 0 0	82, 106, 114, 118	0
8	AH	129/129 (100%)	0.19	2 (1%) 74 66	29, 46, 67, 79	0
8	CH	129/129 (100%)	0.46	10 (7%) 16 8	46, 64, 80, 94	0
9	AI	127/127 (100%)	0.95	22 (17%) 2 1	40, 74, 98, 107	0
9	CI	127/127 (100%)	1.86	46 (36%) 0 0	79, 96, 112, 121	0
10	AJ	98/98 (100%)	0.65	8 (8%) 14 7	38, 66, 86, 116	0
10	CJ	98/98 (100%)	2.74	59 (60%) 0 0	72, 97, 115, 123	0
11	AK	117/117 (100%)	0.49	10 (8%) 13 6	25, 61, 89, 119	0
11	CK	117/117 (100%)	0.24	2 (1%) 73 63	35, 68, 79, 90	0
12	AL	123/123 (100%)	0.16	6 (4%) 33 22	20, 34, 65, 97	0
12	CL	123/123 (100%)	0.33	3 (2%) 62 50	30, 50, 74, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.42	10 (8%) 12 6	47, 69, 91, 103	0
13	CM	114/114 (100%)	3.16	76 (66%) 0 0	93, 113, 122, 125	0
14	AN	96/100 (96%)	0.69	12 (12%) 5 2	36, 60, 96, 105	0
14	CN	96/100 (96%)	2.18	45 (46%) 0 0	70, 96, 115, 122	0
15	AO	88/88 (100%)	0.37	3 (3%) 49 36	29, 47, 64, 91	0
15	CO	88/88 (100%)	0.34	3 (3%) 49 36	36, 64, 80, 102	0
16	AP	82/82 (100%)	0.70	6 (7%) 18 10	34, 47, 83, 109	0
16	CP	82/82 (100%)	0.99	11 (13%) 4 2	45, 62, 91, 112	0
17	AQ	80/80 (100%)	0.28	3 (3%) 44 32	27, 48, 75, 111	0
17	CQ	80/80 (100%)	1.17	20 (25%) 1 0	42, 77, 97, 99	0
18	AR	55/55 (100%)	0.22	4 (7%) 18 10	40, 52, 77, 102	0
18	CR	55/55 (100%)	0.29	4 (7%) 18 10	36, 54, 78, 108	0
19	AS	79/79 (100%)	0.72	14 (17%) 2 1	54, 70, 88, 97	0
19	CS	79/79 (100%)	4.01	58 (73%) 0 0	95, 114, 122, 128	0
20	AT	85/85 (100%)	0.44	5 (5%) 26 16	35, 48, 68, 96	0
20	CT	85/85 (100%)	1.83	33 (38%) 0 0	53, 78, 96, 101	0
21	AU	51/51 (100%)	1.27	11 (21%) 1 1	41, 74, 95, 105	0
21	CU	51/51 (100%)	0.69	6 (11%) 6 3	42, 69, 98, 102	0
22	BA	2897/2903 (99%)	0.15	101 (3%) 48 35	0, 14, 129, 195	0
22	DA	2897/2903 (99%)	0.40	109 (3%) 44 32	41, 85, 148, 181	0
23	BB	119/119 (100%)	-0.31	0 100 100	2, 23, 46, 81	0
23	DB	118/119 (99%)	0.23	4 (3%) 49 36	69, 115, 134, 142	0
24	BC	271/271 (100%)	-0.17	1 (0%) 93 90	2, 18, 35, 55	0
24	DC	271/271 (100%)	0.75	30 (11%) 7 3	46, 64, 77, 95	0
25	BD	209/209 (100%)	-0.24	0 100 100	0, 9, 34, 65	0
25	DD	209/209 (100%)	1.19	46 (22%) 1 1	53, 72, 87, 97	0
26	BE	201/201 (100%)	-0.29	0 100 100	1, 23, 54, 88	0
26	DE	201/201 (100%)	1.89	80 (39%) 0 0	52, 89, 105, 113	0
27	BF	177/177 (100%)	0.20	4 (2%) 64 52	21, 40, 74, 88	0
27	DF	177/177 (100%)	3.32	129 (72%) 0 0	94, 113, 124, 131	0
28	BG	176/176 (100%)	0.05	3 (1%) 73 63	15, 35, 58, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	2.26	94 (53%) 0 0	78, 96, 110, 121	0
29	BH	149/149 (100%)	3.05	76 (51%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.20	31 (20%) 1 1	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.63	99 (70%) 0 0	89, 116, 126, 134	0
30	DI	141/141 (100%)	4.91	121 (85%) 0 0	105, 124, 135, 142	0
31	BJ	142/142 (100%)	-0.26	0 100 100	1, 6, 26, 35	0
31	DJ	142/142 (100%)	0.85	16 (11%) 7 3	49, 69, 83, 91	0
32	BK	122/122 (100%)	-0.33	0 100 100	3, 11, 28, 60	0
32	DK	122/122 (100%)	1.14	28 (22%) 1 1	48, 66, 84, 95	0
33	BL	143/143 (100%)	-0.12	0 100 100	1, 18, 42, 65	0
33	DL	143/143 (100%)	1.97	64 (44%) 0 0	43, 87, 98, 115	0
34	BM	136/136 (100%)	-0.37	0 100 100	1, 10, 24, 85	0
34	DM	136/136 (100%)	1.03	27 (19%) 1 1	44, 70, 85, 99	0
35	BN	120/120 (100%)	-0.23	0 100 100	2, 7, 17, 65	0
35	DN	120/120 (100%)	1.31	31 (25%) 1 0	58, 78, 92, 112	0
36	BO	116/116 (100%)	-0.20	0 100 100	14, 24, 42, 54	0
36	DO	116/116 (100%)	2.80	74 (63%) 0 0	85, 99, 110, 117	0
37	BP	114/114 (100%)	-0.21	1 (0%) 85 79	6, 16, 41, 71	0
37	DP	114/114 (100%)	1.09	26 (22%) 1 1	61, 74, 86, 94	0
38	BQ	117/117 (100%)	-0.30	0 100 100	0, 3, 12, 30	0
38	DQ	117/117 (100%)	1.16	24 (20%) 1 1	55, 70, 81, 89	0
39	BR	103/103 (100%)	-0.29	0 100 100	0, 11, 31, 56	0
39	DR	103/103 (100%)	1.70	35 (33%) 0 0	57, 80, 92, 103	0
40	BS	110/110 (100%)	-0.22	0 100 100	1, 4, 21, 68	0
40	DS	110/110 (100%)	2.15	54 (49%) 0 0	60, 79, 94, 105	0
41	BT	93/93 (100%)	0.20	3 (3%) 51 39	10, 24, 68, 99	0
41	DT	93/93 (100%)	2.73	58 (62%) 0 0	73, 91, 106, 115	0
42	BU	102/102 (100%)	-0.21	2 (1%) 68 58	10, 25, 58, 77	0
42	DU	102/102 (100%)	3.26	65 (63%) 0 0	77, 95, 109, 120	0
43	BV	94/94 (100%)	-0.26	0 100 100	4, 18, 39, 52	0
43	DV	94/94 (100%)	1.16	22 (23%) 1 1	72, 86, 98, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.13	2 (2%) 59 47	4, 11, 27, 57	0
44	DW	75/76 (98%)	2.05	39 (52%) 0 0	58, 83, 93, 104	0
45	BX	77/77 (100%)	-0.22	0 100 100	8, 22, 48, 68	0
45	DX	77/77 (100%)	1.13	15 (19%) 1 1	47, 72, 87, 91	0
46	BY	63/63 (100%)	0.25	3 (4%) 34 23	18, 38, 71, 94	0
46	DY	63/63 (100%)	1.99	31 (49%) 0 0	81, 99, 106, 109	0
47	BZ	58/58 (100%)	-0.21	0 100 100	2, 6, 25, 34	0
47	DZ	58/58 (100%)	0.85	8 (13%) 4 2	60, 73, 85, 103	0
48	B0	56/56 (100%)	-0.29	0 100 100	0, 7, 33, 60	0
48	D0	56/56 (100%)	1.51	17 (30%) 1 0	51, 82, 95, 103	0
49	B1	50/50 (100%)	-0.22	1 (2%) 68 58	13, 25, 49, 57	0
49	D1	50/50 (100%)	1.77	16 (32%) 1 0	73, 89, 94, 106	0
50	B2	46/46 (100%)	-0.12	1 (2%) 65 54	4, 8, 15, 79	0
50	D2	46/46 (100%)	1.94	18 (39%) 0 0	58, 72, 86, 101	0
51	B3	64/64 (100%)	-0.17	0 100 100	4, 9, 17, 29	0
51	D3	64/64 (100%)	1.73	26 (40%) 0 0	60, 75, 84, 94	0
52	B4	38/38 (100%)	-0.12	0 100 100	5, 15, 29, 52	0
52	D4	38/38 (100%)	2.27	18 (47%) 0 0	62, 77, 88, 98	0
53	B5	191/228 (83%)	6.32	186 (97%) 0 0	100, 121, 133, 141	0
54	B6	2/8 (25%)	0.49	0 100 100	1, 1, 1, 1	0
54	D6	2/8 (25%)	-0.01	0 100 100	46, 46, 46, 51	0
All	All	20738/20810 (99%)	0.64	2653 (12%) 5 2	0, 63, 124, 195	0

The worst 5 of 2653 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	25.6
53	B5	55	SER	20.3
53	B5	207	GLY	16.3
10	AJ	102	LEU	16.2
22	BA	2184	A	16.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	DA	3131	1/1	0.64	1.04	53.93	99,99,99,99	0
55	MG	BA	3178	1/1	0.86	0.68	39.48	30,30,30,30	0
55	MG	DA	3072	1/1	0.76	0.52	28.42	90,90,90,90	0
55	MG	BA	3185	1/1	0.92	0.30	23.32	16,16,16,16	0
55	MG	DA	3116	1/1	0.92	0.36	17.28	76,76,76,76	0
55	MG	BA	3195	1/1	0.91	0.57	16.32	23,23,23,23	0
55	MG	DA	3028	1/1	0.61	0.87	15.62	103,103,103,103	0
55	MG	BA	3042	1/1	0.92	0.38	14.72	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1669	1/1	0.93	0.42	13.72	51,51,51,51	0
55	MG	DA	3071	1/1	0.63	0.49	13.07	92,92,92,92	0
55	MG	BA	3137	1/1	0.81	0.42	12.77	49,49,49,49	0
55	MG	CA	1615	1/1	0.86	0.30	11.06	58,58,58,58	0
55	MG	AA	1662	1/1	0.80	0.38	10.91	57,57,57,57	0
55	MG	DA	3151	1/1	0.85	0.52	9.59	59,59,59,59	0
55	MG	DA	3157	1/1	0.86	0.30	9.40	58,58,58,58	0
55	MG	DA	3003	1/1	0.80	0.47	8.66	99,99,99,99	0
55	MG	DA	3074	1/1	0.89	0.34	6.80	77,77,77,77	0
55	MG	BA	3151	1/1	0.82	0.28	6.45	12,12,12,12	0
55	MG	DA	3139	1/1	0.99	0.33	6.29	30,30,30,30	0
55	MG	BA	3183	1/1	0.97	0.21	4.83	12,12,12,12	0
55	MG	BA	3070	1/1	0.96	0.21	3.74	0,0,0,0	0
55	MG	AA	1622	1/1	0.98	0.20	3.62	16,16,16,16	0
55	MG	DA	3113	1/1	0.52	0.29	3.61	66,66,66,66	0
55	MG	BA	3085	1/1	0.93	0.21	3.57	27,27,27,27	0
55	MG	DA	3153	1/1	0.84	0.26	3.40	53,53,53,53	0
55	MG	BA	3150	1/1	0.94	0.20	3.29	37,37,37,37	0
56	DOL	DA	3001	48/48	0.88	0.26	2.84	26,45,58,63	0
55	MG	BA	3106	1/1	0.98	0.20	2.82	16,16,16,16	0
55	MG	BA	3146	1/1	0.82	0.19	2.73	30,30,30,30	0
55	MG	BA	3111	1/1	0.97	0.20	2.72	6,6,6,6	0
55	MG	BA	3109	1/1	0.98	0.19	2.67	12,12,12,12	0
56	DOL	BA	3001	48/48	0.96	0.21	2.63	0,3,25,36	0
55	MG	BA	3154	1/1	0.86	0.33	2.51	25,25,25,25	0
55	MG	DA	3110	1/1	0.89	0.22	2.07	33,33,33,33	0
55	MG	DA	3109	1/1	0.95	0.22	1.89	42,42,42,42	0
55	MG	DA	3097	1/1	0.81	0.25	1.87	91,91,91,91	0
55	MG	DA	3154	1/1	0.85	0.17	1.86	40,40,40,40	0
55	MG	DA	3064	1/1	0.73	0.20	1.72	48,48,48,48	0
55	MG	BA	3018	1/1	0.97	0.20	1.46	0,0,0,0	0
55	MG	BA	3110	1/1	0.96	0.20	1.27	3,3,3,3	0
55	MG	DA	3009	1/1	0.81	0.37	1.19	90,90,90,90	0
55	MG	BA	3067	1/1	0.97	0.17	1.09	0,0,0,0	0
55	MG	DA	3102	1/1	0.94	0.22	1.03	62,62,62,62	0
55	MG	DA	3063	1/1	0.97	0.22	0.97	54,54,54,54	0
55	MG	BA	3013	1/1	0.93	0.21	0.96	0,0,0,0	0
55	MG	DA	3025	1/1	0.87	0.26	0.96	69,69,69,69	0
55	MG	AA	1630	1/1	0.89	0.18	0.85	73,73,73,73	0
55	MG	DA	3049	1/1	0.88	0.24	0.73	84,84,84,84	0
55	MG	BA	3107	1/1	0.98	0.19	0.57	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1630	1/1	0.48	0.35	0.50	120,120,120,120	0
55	MG	BA	3049	1/1	0.76	0.13	0.38	44,44,44,44	0
55	MG	BA	3152	1/1	0.92	0.19	0.34	6,6,6,6	0
55	MG	AA	1654	1/1	0.92	0.13	0.20	43,43,43,43	0
55	MG	DA	3108	1/1	0.79	0.17	0.10	59,59,59,59	0
55	MG	BA	3131	1/1	0.92	0.18	0.06	1,1,1,1	0
55	MG	BA	3014	1/1	0.96	0.18	-0.06	0,0,0,0	0
55	MG	BA	3024	1/1	0.96	0.17	-0.07	0,0,0,0	0
55	MG	BA	3064	1/1	0.89	0.19	-0.20	5,5,5,5	0
55	MG	BA	3055	1/1	0.98	0.17	-0.22	0,0,0,0	0
55	MG	BA	3117	1/1	0.97	0.17	-0.30	1,1,1,1	0
55	MG	CA	1646	1/1	0.82	0.24	-0.35	92,92,92,92	0
55	MG	DA	3129	1/1	0.84	0.18	-0.36	45,45,45,45	0
55	MG	DA	3019	1/1	0.69	0.18	-0.37	107,107,107,107	0
55	MG	DA	3132	1/1	0.88	0.19	-0.43	54,54,54,54	0
55	MG	AA	1641	1/1	0.91	0.15	-0.52	19,19,19,19	0
55	MG	DA	3036	1/1	0.88	0.15	-0.61	62,62,62,62	0
55	MG	DA	3105	1/1	0.91	0.18	-0.64	80,80,80,80	0
55	MG	AA	1629	1/1	0.91	0.14	-0.68	61,61,61,61	0
55	MG	BA	3051	1/1	0.90	0.17	-0.69	6,6,6,6	0
55	MG	DA	3094	1/1	0.84	0.19	-0.71	84,84,84,84	0
55	MG	BA	3113	1/1	0.92	0.17	-0.76	22,22,22,22	0
55	MG	DA	3078	1/1	0.68	0.13	-0.80	106,106,106,106	0
55	MG	BA	3006	1/1	0.91	0.14	-0.83	50,50,50,50	0
55	MG	DA	3027	1/1	0.62	0.17	-0.84	91,91,91,91	0
55	MG	DA	3042	1/1	0.54	0.19	-0.85	87,87,87,87	0
55	MG	DA	3115	1/1	0.80	0.19	-0.87	111,111,111,111	0
55	MG	CA	1603	1/1	0.85	0.15	-0.89	44,44,44,44	0
55	MG	CA	1631	1/1	0.73	0.13	-0.95	95,95,95,95	0
55	MG	CA	1640	1/1	0.90	0.14	-0.97	26,26,26,26	0
55	MG	DA	3145	1/1	0.86	0.17	-0.98	71,71,71,71	0
55	MG	AA	1632	1/1	0.88	0.10	-0.99	55,55,55,55	0
55	MG	BA	3038	1/1	0.77	0.17	-1.00	42,42,42,42	0
55	MG	AA	1642	1/1	0.96	0.15	-1.00	23,23,23,23	0
55	MG	DA	3024	1/1	0.87	0.16	-1.06	46,46,46,46	0
55	MG	DB	202	1/1	0.87	0.11	-1.10	66,66,66,66	0
57	ZN	D4	101	1/1	0.98	0.09	-1.10	87,87,87,87	0
55	MG	BA	3177	1/1	0.98	0.17	-1.11	17,17,17,17	0
55	MG	BA	3019	1/1	0.98	0.12	-1.29	11,11,11,11	0
55	MG	DA	3136	1/1	0.74	0.16	-1.33	91,91,91,91	0
55	MG	DA	3134	1/1	0.73	0.14	-1.36	58,58,58,58	0
55	MG	CA	1614	1/1	0.91	0.08	-1.40	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3013	1/1	0.73	0.16	-1.44	44,44,44,44	0
55	MG	AA	1607	1/1	0.94	0.09	-1.48	44,44,44,44	0
55	MG	DA	3093	1/1	0.47	0.11	-1.50	86,86,86,86	0
55	MG	DA	3130	1/1	0.93	0.10	-1.53	81,81,81,81	0
55	MG	CA	1632	1/1	0.69	0.12	-1.61	73,73,73,73	0
55	MG	DA	3080	1/1	0.85	0.15	-1.62	95,95,95,95	0
55	MG	DA	3079	1/1	0.94	0.13	-1.67	96,96,96,96	0
55	MG	BA	3164	1/1	0.94	0.14	-1.68	4,4,4,4	0
55	MG	BA	3075	1/1	0.82	0.16	-1.70	29,29,29,29	0
55	MG	DA	3043	1/1	0.95	0.13	-1.72	66,66,66,66	0
55	MG	CA	1635	1/1	0.53	0.13	-1.76	124,124,124,124	0
55	MG	BA	3115	1/1	0.94	0.12	-1.84	20,20,20,20	0
55	MG	DA	3098	1/1	0.72	0.16	-1.84	66,66,66,66	0
55	MG	BB	201	1/1	0.96	0.10	-1.87	20,20,20,20	0
55	MG	AA	1617	1/1	0.93	0.12	-1.93	52,52,52,52	0
55	MG	CA	1634	1/1	0.96	0.13	-1.96	49,49,49,49	0
57	ZN	B4	101	1/1	0.98	0.10	-1.97	33,33,33,33	0
55	MG	BA	3081	1/1	0.91	0.12	-2.13	24,24,24,24	0
55	MG	BA	3158	1/1	0.97	0.12	-2.15	19,19,19,19	0
55	MG	BA	3133	1/1	0.92	0.10	-2.18	32,32,32,32	0
55	MG	BA	3066	1/1	0.92	0.15	-2.23	0,0,0,0	0
55	MG	DA	3051	1/1	0.95	0.09	-2.26	28,28,28,28	0
55	MG	DA	3047	1/1	0.85	0.13	-2.28	73,73,73,73	0
55	MG	BA	3174	1/1	0.92	0.12	-2.30	12,12,12,12	0
55	MG	DA	3035	1/1	0.94	0.09	-2.62	79,79,79,79	0
55	MG	DA	3106	1/1	0.91	0.14	-2.77	52,52,52,52	0
55	MG	BA	3103	1/1	0.81	0.17	-2.77	0,0,0,0	0
55	MG	DB	201	1/1	0.73	0.06	-2.90	116,116,116,116	0
55	MG	DA	3120	1/1	0.82	0.11	-3.02	79,79,79,79	0
55	MG	DA	3096	1/1	0.90	0.08	-3.13	57,57,57,57	0
55	MG	BA	3026	1/1	0.96	0.15	-3.13	3,3,3,3	0
55	MG	AA	1616	1/1	0.94	0.12	-3.18	50,50,50,50	0
55	MG	CA	1622	1/1	0.92	0.13	-3.37	51,51,51,51	0
55	MG	DA	3018	1/1	0.96	0.11	-3.40	60,60,60,60	0
55	MG	DA	3006	1/1	0.80	0.13	-3.42	93,93,93,93	0
55	MG	BA	3095	1/1	0.96	0.09	-3.43	21,21,21,21	0
55	MG	AA	1606	1/1	0.92	0.11	-3.65	44,44,44,44	0
55	MG	DA	3050	1/1	0.90	0.10	-3.66	56,56,56,56	0
55	MG	AA	1633	1/1	0.96	0.12	-3.84	30,30,30,30	0
55	MG	BA	3121	1/1	0.93	0.12	-3.90	3,3,3,3	0
55	MG	BA	3162	1/1	0.98	0.07	-3.91	36,36,36,36	0
55	MG	BA	3098	1/1	0.92	0.12	-3.96	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3023	1/1	0.91	0.05	-4.01	69,69,69,69	0
55	MG	DA	3022	1/1	0.81	0.10	-4.14	52,52,52,52	0
55	MG	BA	3135	1/1	0.96	0.14	-4.20	2,2,2,2	0
55	MG	DA	3054	1/1	0.91	0.10	-4.53	55,55,55,55	0
55	MG	CA	1610	1/1	0.89	0.10	-4.53	63,63,63,63	0
55	MG	DA	3059	1/1	0.96	0.10	-4.59	51,51,51,51	0
55	MG	CA	1616	1/1	0.91	0.10	-4.86	37,37,37,37	0
55	MG	AA	1613	1/1	0.88	0.09	-4.89	24,24,24,24	0
55	MG	CA	1612	1/1	0.96	0.05	-4.90	40,40,40,40	0
55	MG	CA	1607	1/1	0.92	0.08	-4.99	54,54,54,54	0
55	MG	BA	3099	1/1	0.98	0.12	-5.03	4,4,4,4	0
55	MG	AA	1604	1/1	0.97	0.06	-5.05	48,48,48,48	0
55	MG	BA	3052	1/1	0.97	0.06	-5.17	11,11,11,11	0
55	MG	BA	3025	1/1	0.94	0.10	-5.28	2,2,2,2	0
55	MG	CA	1619	1/1	0.94	0.10	-5.32	33,33,33,33	0
55	MG	CA	1617	1/1	0.76	0.12	-5.40	39,39,39,39	0
55	MG	AA	1618	1/1	0.93	0.08	-5.44	37,37,37,37	0
55	MG	BA	3023	1/1	0.96	0.14	-5.52	1,1,1,1	0
55	MG	BA	3073	1/1	0.97	0.07	-5.62	7,7,7,7	0
55	MG	BA	3040	1/1	0.89	0.15	-6.34	0,0,0,0	0
55	MG	CA	1601	1/1	0.85	0.09	-6.41	39,39,39,39	0
55	MG	BA	3130	1/1	0.95	0.12	-6.74	0,0,0,0	0
55	MG	BA	3009	1/1	0.96	0.09	-7.09	4,4,4,4	0
55	MG	BA	3187	1/1	0.92	0.06	-7.12	33,33,33,33	0
55	MG	BA	3160	1/1	0.94	0.10	-7.19	10,10,10,10	0
55	MG	AA	1609	1/1	0.88	0.08	-7.77	36,36,36,36	0
55	MG	BA	3003	1/1	0.91	0.06	-7.81	17,17,17,17	0
55	MG	BA	3029	1/1	0.96	0.08	-8.19	21,21,21,21	0
55	MG	BA	3119	1/1	0.82	0.07	-8.21	20,20,20,20	0
55	MG	BA	3132	1/1	0.91	0.09	-8.40	23,23,23,23	0
55	MG	DA	3069	1/1	0.90	0.10	-8.70	79,79,79,79	0
55	MG	AA	1625	1/1	0.92	0.07	-8.74	47,47,47,47	0
55	MG	AA	1611	1/1	0.97	0.09	-9.01	21,21,21,21	0
55	MG	DA	3066	1/1	0.90	0.07	-9.12	47,47,47,47	0
55	MG	BA	3112	1/1	0.90	0.08	-9.39	20,20,20,20	0
55	MG	BA	3034	1/1	0.93	0.10	-9.55	6,6,6,6	0
55	MG	BA	3010	1/1	0.97	0.11	-10.12	0,0,0,0	0
55	MG	BA	3060	1/1	0.97	0.05	-10.33	15,15,15,15	0
55	MG	BA	3015	1/1	0.91	0.07	-10.69	2,2,2,2	0
55	MG	CA	1626	1/1	0.82	0.07	-12.25	48,48,48,48	0
55	MG	BA	3072	1/1	0.97	0.08	-16.96	3,3,3,3	0
55	MG	DA	3111	1/1	0.18	0.32	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3142	1/1	0.93	0.26	-	33,33,33,33	0
55	MG	BA	3079	1/1	0.93	0.09	-	22,22,22,22	0
55	MG	AA	1640	1/1	0.95	0.09	-	36,36,36,36	0
55	MG	DA	3031	1/1	0.88	0.08	-	69,69,69,69	0
55	MG	D2	101	1/1	0.65	0.15	-	83,83,83,83	0
55	MG	DA	3026	1/1	0.43	0.48	-	101,101,101,101	0
55	MG	BA	3092	1/1	0.88	0.10	-	19,19,19,19	0
55	MG	BA	3083	1/1	0.97	0.17	-	0,0,0,0	0
55	MG	BA	3190	1/1	0.93	0.10	-	31,31,31,31	0
55	MG	BA	3159	1/1	0.94	0.22	-	14,14,14,14	0
55	MG	AA	1602	1/1	0.90	0.13	-	46,46,46,46	0
55	MG	BA	3179	1/1	0.88	0.33	-	26,26,26,26	0
55	MG	BA	3084	1/1	0.94	0.05	-	6,6,6,6	0
55	MG	DA	3101	1/1	0.93	0.09	-	57,57,57,57	0
55	MG	BA	3017	1/1	0.95	0.06	-	2,2,2,2	0
55	MG	DA	3163	1/1	0.77	0.33	-	54,54,54,54	0
55	MG	AA	1655	1/1	0.96	0.11	-	35,35,35,35	0
55	MG	BA	3094	1/1	0.95	0.05	-	31,31,31,31	0
55	MG	CA	1636	1/1	0.50	0.14	-	126,126,126,126	0
55	MG	CA	1653	1/1	0.94	0.09	-	52,52,52,52	0
55	MG	BB	202	1/1	0.87	0.10	-	16,16,16,16	0
55	MG	AA	1615	1/1	0.97	0.06	-	47,47,47,47	0
55	MG	DA	3004	1/1	0.91	0.11	-	76,76,76,76	0
55	MG	CA	1633	1/1	0.93	0.32	-	64,64,64,64	0
55	MG	DA	3041	1/1	0.38	0.42	-	68,68,68,68	0
55	MG	BA	3008	1/1	0.91	0.14	-	37,37,37,37	0
55	MG	CA	1606	1/1	0.64	0.19	-	89,89,89,89	0
55	MG	CA	1602	1/1	0.73	0.11	-	88,88,88,88	0
55	MG	BA	3166	1/1	0.93	0.17	-	19,19,19,19	0
55	MG	CA	1644	1/1	0.96	0.15	-	42,42,42,42	0
55	MG	BA	3156	1/1	0.89	0.28	-	19,19,19,19	0
55	MG	AA	1636	1/1	0.98	0.09	-	27,27,27,27	0
55	MG	DA	3090	1/1	0.65	0.14	-	90,90,90,90	0
55	MG	CA	1641	1/1	0.94	0.68	-	73,73,73,73	0
55	MG	DA	3140	1/1	0.93	0.43	-	43,43,43,43	0
55	MG	DA	3008	1/1	0.86	0.26	-	100,100,100,100	0
55	MG	BA	3176	1/1	0.96	0.10	-	20,20,20,20	0
55	MG	AA	1645	1/1	0.98	0.13	-	42,42,42,42	0
55	MG	DA	3053	1/1	0.94	0.11	-	40,40,40,40	0
55	MG	BA	3046	1/1	0.83	0.09	-	17,17,17,17	0
55	MG	BA	3074	1/1	0.96	0.18	-	1,1,1,1	0
55	MG	AA	1671	1/1	0.88	0.52	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1656	1/1	0.98	0.14	-	43,43,43,43	0
55	MG	BA	3102	1/1	0.88	0.10	-	7,7,7,7	0
55	MG	BA	3090	1/1	0.55	0.10	-	19,19,19,19	0
55	MG	DA	3156	1/1	0.97	0.19	-	41,41,41,41	0
55	MG	BA	3045	1/1	0.95	0.08	-	9,9,9,9	0
55	MG	BA	3184	1/1	0.97	0.20	-	6,6,6,6	0
55	MG	BB	204	1/1	0.89	0.37	-	16,16,16,16	0
55	MG	CA	1654	1/1	0.87	0.36	-	56,56,56,56	0
55	MG	DA	3056	1/1	0.78	0.41	-	93,93,93,93	0
55	MG	BA	3171	1/1	0.90	0.20	-	24,24,24,24	0
55	MG	AA	1610	1/1	0.93	0.23	-	65,65,65,65	0
55	MG	BA	3097	1/1	0.98	0.07	-	4,4,4,4	0
55	MG	DA	3087	1/1	0.91	0.09	-	54,54,54,54	0
55	MG	DA	3062	1/1	0.51	0.61	-	82,82,82,82	0
55	MG	DA	3100	1/1	0.36	0.21	-	77,77,77,77	0
55	MG	DA	3086	1/1	0.97	0.10	-	76,76,76,76	0
55	MG	BA	3020	1/1	0.95	0.09	-	22,22,22,22	0
55	MG	BA	3126	1/1	0.93	0.12	-	6,6,6,6	0
55	MG	CA	1656	1/1	0.87	0.36	-	54,54,54,54	0
55	MG	CA	1627	1/1	0.61	0.20	-	89,89,89,89	0
55	MG	DA	3052	1/1	0.88	0.07	-	56,56,56,56	0
55	MG	DA	3114	1/1	0.83	0.14	-	65,65,65,65	0
55	MG	AA	1652	1/1	0.79	0.19	-	49,49,49,49	0
55	MG	BA	3048	1/1	0.99	0.15	-	8,8,8,8	0
55	MG	DA	3159	1/1	0.91	0.30	-	43,43,43,43	0
55	MG	AA	1644	1/1	0.84	0.40	-	44,44,44,44	0
55	MG	BA	3142	1/1	0.97	0.43	-	2,2,2,2	0
55	MG	DA	3158	1/1	0.93	0.19	-	70,70,70,70	0
55	MG	CA	1643	1/1	0.93	0.24	-	50,50,50,50	0
55	MG	BA	3108	1/1	0.96	0.24	-	0,0,0,0	0
55	MG	AA	1665	1/1	0.67	0.40	-	37,37,37,37	0
55	MG	BA	3012	1/1	0.96	0.05	-	14,14,14,14	0
55	MG	BA	3116	1/1	0.91	0.26	-	34,34,34,34	0
55	MG	BA	3168	1/1	0.92	0.12	-	35,35,35,35	0
55	MG	DA	3146	1/1	0.90	0.10	-	43,43,43,43	0
55	MG	BA	3054	1/1	0.84	0.08	-	9,9,9,9	0
55	MG	DA	3038	1/1	0.83	0.13	-	63,63,63,63	0
55	MG	DA	3014	1/1	0.89	0.14	-	73,73,73,73	0
55	MG	AA	1658	1/1	0.67	0.35	-	62,62,62,62	0
55	MG	DA	3164	1/1	0.90	0.17	-	57,57,57,57	0
55	MG	BA	3175	1/1	0.96	0.11	-	27,27,27,27	0
55	MG	BA	3191	1/1	0.89	0.23	-	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1650	1/1	0.88	0.32	-	36,36,36,36	0
55	MG	BA	3105	1/1	0.98	0.10	-	4,4,4,4	0
55	MG	DB	203	1/1	0.78	0.08	-	85,85,85,85	0
55	MG	DA	3089	1/1	0.81	0.33	-	83,83,83,83	0
55	MG	BA	3065	1/1	0.93	0.14	-	0,0,0,0	0
55	MG	AA	1659	1/1	0.78	0.77	-	50,50,50,50	0
55	MG	BA	3129	1/1	0.97	0.19	-	4,4,4,4	0
55	MG	DA	3007	1/1	0.91	0.44	-	121,121,121,121	0
55	MG	DA	3037	1/1	0.76	0.08	-	93,93,93,93	0
55	MG	DA	3020	1/1	0.89	0.15	-	54,54,54,54	0
55	MG	AA	1639	1/1	0.66	0.07	-	65,65,65,65	0
55	MG	BA	3061	1/1	0.95	0.35	-	30,30,30,30	0
55	MG	BA	3136	1/1	0.93	0.12	-	21,21,21,21	0
55	MG	DA	3048	1/1	0.20	0.44	-	127,127,127,127	0
55	MG	DA	3112	1/1	0.88	1.38	-	104,104,104,104	0
55	MG	BA	3173	1/1	0.93	0.14	-	27,27,27,27	0
55	MG	BA	3144	1/1	0.98	0.26	-	15,15,15,15	0
55	MG	CA	1649	1/1	0.89	0.18	-	52,52,52,52	0
55	MG	BA	3082	1/1	0.88	0.11	-	6,6,6,6	0
55	MG	BA	3030	1/1	0.93	0.14	-	9,9,9,9	0
55	MG	BA	3096	1/1	0.98	0.07	-	11,11,11,11	0
55	MG	BA	3002	1/1	0.90	0.06	-	18,18,18,18	0
55	MG	DA	3103	1/1	0.69	0.24	-	73,73,73,73	0
55	MG	CA	1613	1/1	0.89	0.14	-	19,19,19,19	0
55	MG	DA	3121	1/1	0.78	0.10	-	52,52,52,52	0
55	MG	BA	3180	1/1	0.82	0.19	-	32,32,32,32	0
55	MG	BA	3039	1/1	0.94	0.27	-	0,0,0,0	0
55	MG	BA	3068	1/1	0.97	0.17	-	0,0,0,0	0
55	MG	BA	3036	1/1	0.95	0.12	-	11,11,11,11	0
55	MG	CA	1637	1/1	0.83	0.09	-	64,64,64,64	0
55	MG	BA	3192	1/1	0.94	0.21	-	22,22,22,22	0
55	MG	AA	1620	1/1	0.73	0.12	-	69,69,69,69	0
55	MG	DA	3165	1/1	0.87	0.23	-	42,42,42,42	0
55	MG	AA	1661	1/1	0.87	0.29	-	29,29,29,29	0
55	MG	DA	3002	1/1	0.64	0.10	-	78,78,78,78	0
55	MG	DA	3128	1/1	0.96	0.08	-	80,80,80,80	0
55	MG	CA	1655	1/1	0.84	0.10	-	44,44,44,44	0
55	MG	BA	3022	1/1	0.96	0.08	-	2,2,2,2	0
55	MG	DA	3011	1/1	0.89	0.08	-	75,75,75,75	0
55	MG	DA	3040	1/1	0.83	0.18	-	83,83,83,83	0
55	MG	CA	1625	1/1	0.94	0.15	-	22,22,22,22	0
55	MG	DA	3160	1/1	0.88	0.24	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3100	1/1	0.60	0.27	-	52,52,52,52	0
55	MG	DA	3148	1/1	0.51	0.29	-	65,65,65,65	0
55	MG	DQ	201	1/1	0.69	0.30	-	45,45,45,45	0
55	MG	CA	1609	1/1	0.80	0.15	-	89,89,89,89	0
55	MG	DA	3155	1/1	0.71	0.45	-	62,62,62,62	0
55	MG	AA	1603	1/1	0.92	0.10	-	44,44,44,44	0
55	MG	CA	1652	1/1	0.93	0.11	-	83,83,83,83	0
55	MG	BA	3053	1/1	0.94	0.14	-	2,2,2,2	0
55	MG	BA	3101	1/1	0.96	0.07	-	1,1,1,1	0
55	MG	AA	1649	1/1	0.94	0.14	-	32,32,32,32	0
55	MG	DA	3065	1/1	0.91	0.12	-	36,36,36,36	0
55	MG	BA	3047	1/1	0.92	0.10	-	4,4,4,4	0
55	MG	DA	3077	1/1	0.69	0.70	-	113,113,113,113	0
55	MG	CA	1642	1/1	0.94	0.25	-	25,25,25,25	0
55	MG	DA	3067	1/1	0.59	0.13	-	58,58,58,58	0
55	MG	BA	3145	1/1	0.95	0.29	-	28,28,28,28	0
55	MG	DA	3034	1/1	0.69	0.16	-	69,69,69,69	0
55	MG	BA	3182	1/1	0.90	0.25	-	33,33,33,33	0
55	MG	DA	3122	1/1	0.96	0.15	-	41,41,41,41	0
55	MG	BA	3080	1/1	0.94	0.07	-	39,39,39,39	0
55	MG	BA	3167	1/1	0.78	0.18	-	25,25,25,25	0
55	MG	BA	3161	1/1	0.95	0.17	-	31,31,31,31	0
55	MG	DA	3081	1/1	0.87	0.10	-	60,60,60,60	0
55	MG	CA	1648	1/1	0.91	0.20	-	22,22,22,22	0
55	MG	DA	3044	1/1	0.69	0.40	-	112,112,112,112	0
55	MG	BA	3037	1/1	0.97	0.17	-	0,0,0,0	0
55	MG	AA	1646	1/1	0.92	0.20	-	49,49,49,49	0
55	MG	BA	3125	1/1	0.87	0.55	-	37,37,37,37	0
55	MG	BA	3078	1/1	0.91	0.72	-	79,79,79,79	0
55	MG	AA	1651	1/1	0.76	0.33	-	61,61,61,61	0
55	MG	DA	3133	1/1	0.52	0.76	-	100,100,100,100	0
55	MG	BA	3063	1/1	0.92	0.44	-	31,31,31,31	0
55	MG	DA	3088	1/1	0.72	0.10	-	74,74,74,74	0
55	MG	BA	3093	1/1	0.76	0.09	-	58,58,58,58	0
55	MG	CA	1604	1/1	0.85	0.13	-	95,95,95,95	0
55	MG	BA	3032	1/1	0.97	0.16	-	4,4,4,4	0
55	MG	DA	3117	1/1	0.89	0.09	-	67,67,67,67	0
55	MG	DA	3029	1/1	0.59	0.22	-	73,73,73,73	0
55	MG	DA	3017	1/1	0.38	0.25	-	98,98,98,98	0
55	MG	DA	3143	1/1	0.86	0.24	-	60,60,60,60	0
55	MG	AA	1666	1/1	0.92	0.19	-	46,46,46,46	0
55	MG	CA	1623	1/1	0.96	0.17	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1645	1/1	0.94	0.20	-	32,32,32,32	0
55	MG	BA	3138	1/1	0.95	0.45	-	1,1,1,1	0
55	MG	CA	1620	1/1	0.92	0.06	-	61,61,61,61	0
55	MG	BA	3193	1/1	0.91	0.15	-	38,38,38,38	0
55	MG	CA	1638	1/1	0.81	0.10	-	76,76,76,76	0
55	MG	BA	3071	1/1	0.92	0.07	-	60,60,60,60	0
55	MG	DA	3061	1/1	0.86	1.12	-	96,96,96,96	0
55	MG	DA	3033	1/1	0.82	0.10	-	71,71,71,71	0
55	MG	AA	1643	1/1	0.88	0.14	-	28,28,28,28	0
55	MG	DA	3107	1/1	0.78	0.16	-	75,75,75,75	0
55	MG	AA	1605	1/1	0.86	0.22	-	23,23,23,23	0
55	MG	DA	3152	1/1	0.80	0.29	-	52,52,52,52	0
55	MG	DA	3084	1/1	0.36	0.23	-	105,105,105,105	0
55	MG	BA	3118	1/1	0.95	0.12	-	1,1,1,1	0
55	MG	BA	3011	1/1	0.99	0.15	-	1,1,1,1	0
55	MG	BA	3170	1/1	0.85	0.35	-	38,38,38,38	0
55	MG	BA	3104	1/1	0.86	0.17	-	17,17,17,17	0
55	MG	BA	3059	1/1	0.80	0.25	-	38,38,38,38	0
55	MG	AA	1670	1/1	0.88	0.29	-	33,33,33,33	0
55	MG	AA	1668	1/1	0.94	0.13	-	29,29,29,29	0
55	MG	DA	3091	1/1	0.83	0.09	-	77,77,77,77	0
55	MG	BA	3089	1/1	0.84	0.07	-	33,33,33,33	0
55	MG	AA	1614	1/1	0.61	0.22	-	69,69,69,69	0
55	MG	AA	1667	1/1	0.80	0.19	-	49,49,49,49	0
55	MG	DA	3083	1/1	0.96	0.09	-	69,69,69,69	0
55	MG	BA	3091	1/1	0.92	0.09	-	3,3,3,3	0
55	MG	BA	3035	1/1	0.95	0.18	-	0,0,0,0	0
55	MG	BA	3148	1/1	0.95	0.12	-	29,29,29,29	0
55	MG	BA	3088	1/1	0.95	0.23	-	2,2,2,2	0
55	MG	CA	1605	1/1	0.77	0.19	-	86,86,86,86	0
55	MG	DA	3030	1/1	0.91	0.24	-	60,60,60,60	0
55	MG	BA	3124	1/1	0.96	0.09	-	11,11,11,11	0
55	MG	DA	3068	1/1	0.91	0.14	-	65,65,65,65	0
55	MG	BA	3165	1/1	0.94	0.30	-	43,43,43,43	0
55	MG	DA	3015	1/1	0.92	0.06	-	55,55,55,55	0
55	MG	BA	3123	1/1	0.97	0.16	-	0,0,0,0	0
55	MG	DA	3118	1/1	0.95	0.08	-	60,60,60,60	0
55	MG	BA	3077	1/1	0.79	0.17	-	8,8,8,8	0
55	MG	BA	3056	1/1	0.92	0.08	-	5,5,5,5	0
55	MG	BA	3027	1/1	0.85	0.34	-	46,46,46,46	0
55	MG	DA	3123	1/1	0.91	0.12	-	57,57,57,57	0
55	MG	AA	1619	1/1	0.50	0.31	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3125	1/1	0.77	0.22	-	62,62,62,62	0
55	MG	BA	3186	1/1	0.75	0.29	-	29,29,29,29	0
55	MG	BA	3044	1/1	0.96	0.14	-	3,3,3,3	0
55	MG	DA	3124	1/1	0.84	0.23	-	89,89,89,89	0
55	MG	DA	3082	1/1	0.92	0.13	-	60,60,60,60	0
55	MG	DA	3162	1/1	0.98	0.21	-	38,38,38,38	0
55	MG	DA	3070	1/1	0.66	0.17	-	108,108,108,108	0
55	MG	BA	3127	1/1	0.92	0.12	-	9,9,9,9	0
55	MG	BA	3155	1/1	0.93	0.21	-	20,20,20,20	0
55	MG	BA	3120	1/1	0.85	0.20	-	37,37,37,37	0
55	MG	DA	3012	1/1	0.72	0.10	-	73,73,73,73	0
55	MG	BA	3128	1/1	0.98	0.10	-	0,0,0,0	0
55	MG	DA	3060	1/1	0.72	0.31	-	77,77,77,77	0
55	MG	BA	3139	1/1	0.98	0.37	-	0,0,0,0	0
55	MG	BA	3028	1/1	0.98	0.08	-	5,5,5,5	0
55	MG	AA	1648	1/1	0.74	0.20	-	47,47,47,47	0
55	MG	DA	3076	1/1	0.97	0.12	-	69,69,69,69	0
55	MG	BA	3033	1/1	0.91	0.12	-	11,11,11,11	0
55	MG	CA	1611	1/1	0.95	0.29	-	90,90,90,90	0
55	MG	AA	1664	1/1	0.87	0.14	-	49,49,49,49	0
55	MG	BA	3153	1/1	0.76	0.23	-	31,31,31,31	0
55	MG	BA	3086	1/1	0.92	0.06	-	14,14,14,14	0
55	MG	BA	3043	1/1	0.94	0.13	-	16,16,16,16	0
55	MG	BA	3134	1/1	0.46	0.42	-	54,54,54,54	0
55	MG	BA	3021	1/1	0.83	0.19	-	1,1,1,1	0
55	MG	BA	3140	1/1	0.94	0.39	-	0,0,0,0	0
55	MG	CA	1618	1/1	0.96	0.11	-	37,37,37,37	0
55	MG	AA	1627	1/1	0.92	0.09	-	37,37,37,37	0
55	MG	DA	3137	1/1	0.89	0.41	-	47,47,47,47	0
55	MG	AA	1637	1/1	0.89	0.10	-	15,15,15,15	0
55	MG	DA	3141	1/1	0.89	0.27	-	40,40,40,40	0
55	MG	DA	3126	1/1	0.67	0.23	-	80,80,80,80	0
55	MG	DA	3150	1/1	0.91	0.20	-	56,56,56,56	0
55	MG	DA	3058	1/1	0.90	1.10	-	109,109,109,109	0
55	MG	BA	3050	1/1	0.74	0.07	-	27,27,27,27	0
55	MG	CA	1608	1/1	0.61	0.22	-	84,84,84,84	0
55	MG	CA	1639	1/1	0.92	0.10	-	43,43,43,43	0
55	MG	AA	1621	1/1	0.98	0.08	-	39,39,39,39	0
55	MG	BA	3194	1/1	0.98	0.07	-	8,8,8,8	0
55	MG	DA	3104	1/1	0.85	0.08	-	79,79,79,79	0
55	MG	BA	3004	1/1	0.88	0.11	-	26,26,26,26	0
55	MG	DA	3032	1/1	0.91	0.26	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1623	1/1	0.84	0.05	-	46,46,46,46	0
55	MG	DA	3138	1/1	0.88	0.35	-	40,40,40,40	0
55	MG	AA	1663	1/1	0.93	0.22	-	48,48,48,48	0
55	MG	AA	1660	1/1	0.90	0.22	-	51,51,51,51	0
55	MG	BA	3016	1/1	0.85	0.43	-	58,58,58,58	0
55	MG	AA	1657	1/1	0.80	0.62	-	64,64,64,64	0
55	MG	DA	3149	1/1	0.81	0.29	-	35,35,35,35	0
55	MG	AA	1626	1/1	0.77	0.17	-	23,23,23,23	0
55	MG	BA	3147	1/1	0.96	0.32	-	9,9,9,9	0
55	MG	AA	1624	1/1	0.95	0.04	-	41,41,41,41	0
55	MG	BA	3087	1/1	0.90	0.13	-	4,4,4,4	0
55	MG	AA	1653	1/1	0.95	0.17	-	28,28,28,28	0
55	MG	DA	3039	1/1	0.86	0.18	-	57,57,57,57	0
55	MG	BA	3181	1/1	0.93	0.20	-	24,24,24,24	0
55	MG	DA	3144	1/1	0.53	0.10	-	68,68,68,68	0
55	MG	DA	3016	1/1	0.84	0.14	-	62,62,62,62	0
55	MG	CA	1647	1/1	0.90	0.11	-	41,41,41,41	0
55	MG	DA	3075	1/1	0.57	0.16	-	91,91,91,91	0
55	MG	BA	3076	1/1	0.90	0.07	-	14,14,14,14	0
55	MG	AA	1612	1/1	0.86	0.10	-	47,47,47,47	0
55	MG	DA	3085	1/1	0.90	0.12	-	67,67,67,67	0
55	MG	DA	3010	1/1	0.65	0.12	-	80,80,80,80	0
55	MG	BA	3031	1/1	0.93	0.07	-	14,14,14,14	0
55	MG	DA	3135	1/1	0.24	0.32	-	101,101,101,101	0
55	MG	CA	1624	1/1	0.85	0.10	-	45,45,45,45	0
55	MG	BA	3057	1/1	0.79	0.35	-	73,73,73,73	0
55	MG	AA	1647	1/1	0.95	0.12	-	48,48,48,48	0
55	MG	CA	1650	1/1	0.89	0.22	-	35,35,35,35	0
55	MG	DA	3045	1/1	0.53	0.12	-	94,94,94,94	0
55	MG	DA	3166	1/1	0.95	0.09	-	41,41,41,41	0
55	MG	BA	3041	1/1	0.98	0.18	-	6,6,6,6	0
55	MG	AA	1628	1/1	0.84	0.10	-	48,48,48,48	0
55	MG	AM	201	1/1	0.79	0.86	-	62,62,62,62	0
55	MG	DA	3092	1/1	0.81	0.59	-	113,113,113,113	0
55	MG	AA	1631	1/1	0.85	0.10	-	46,46,46,46	0
55	MG	DA	3099	1/1	0.56	0.38	-	86,86,86,86	0
55	MG	DA	3167	1/1	0.94	0.29	-	100,100,100,100	0
55	MG	DA	3005	1/1	0.75	0.43	-	102,102,102,102	0
55	MG	DA	3161	1/1	0.93	0.11	-	57,57,57,57	0
55	MG	BA	3189	1/1	0.82	0.24	-	45,45,45,45	0
55	MG	AA	1635	1/1	0.79	0.17	-	66,66,66,66	0
55	MG	DA	3046	1/1	0.76	0.16	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3021	1/1	0.91	0.19	-	63,63,63,63	0
55	MG	DA	3119	1/1	0.85	0.43	-	106,106,106,106	0
55	MG	AA	1608	1/1	0.95	0.14	-	17,17,17,17	0
55	MG	BB	203	1/1	0.95	0.06	-	7,7,7,7	0
55	MG	BA	3143	1/1	0.99	0.36	-	12,12,12,12	0
55	MG	BA	3058	1/1	0.79	0.29	-	15,15,15,15	0
55	MG	CA	1628	1/1	0.87	0.18	-	98,98,98,98	0
55	MG	BA	3069	1/1	0.85	0.15	-	4,4,4,4	0
55	MG	BA	3169	1/1	0.90	0.17	-	35,35,35,35	0
55	MG	CA	1629	1/1	0.66	0.12	-	91,91,91,91	0
55	MG	BA	3141	1/1	0.88	0.15	-	17,17,17,17	0
55	MG	DA	3073	1/1	0.80	0.11	-	60,60,60,60	0
55	MG	BA	3157	1/1	0.89	0.19	-	24,24,24,24	0
55	MG	BA	3172	1/1	0.95	0.17	-	31,31,31,31	0
55	MG	BA	3007	1/1	0.97	0.09	-	22,22,22,22	0
55	MG	DA	3055	1/1	0.94	0.13	-	72,72,72,72	0
55	MG	CA	1621	1/1	0.80	0.09	-	64,64,64,64	0
55	MG	BA	3114	1/1	0.89	0.17	-	0,0,0,0	0
55	MG	DA	3095	1/1	0.92	0.41	-	91,91,91,91	0
55	MG	BA	3122	1/1	0.96	0.05	-	18,18,18,18	0
55	MG	AA	1638	1/1	0.84	0.10	-	87,87,87,87	0
55	MG	BA	3005	1/1	0.92	0.07	-	34,34,34,34	0
55	MG	BA	3163	1/1	0.97	0.33	-	15,15,15,15	0
55	MG	DA	3057	1/1	0.54	0.29	-	95,95,95,95	0
55	MG	BA	3062	1/1	0.95	0.36	-	50,50,50,50	0
55	MG	AA	1601	1/1	0.81	0.09	-	58,58,58,58	0
55	MG	BQ	201	1/1	0.97	0.20	-	3,3,3,3	0
55	MG	AA	1634	1/1	0.88	0.13	-	35,35,35,35	0
55	MG	DA	3127	1/1	0.64	0.15	-	71,71,71,71	0
55	MG	DA	3147	1/1	0.74	0.40	-	54,54,54,54	0
55	MG	BA	3188	1/1	0.95	0.14	-	10,10,10,10	0
55	MG	CA	1651	1/1	0.86	0.30	-	44,44,44,44	0
55	MG	BA	3149	1/1	0.93	0.12	-	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.