



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:06 am GMT

PDB ID : 4U26
Title : Crystal structure of the E. coli ribosome bound to dalbavand 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28972

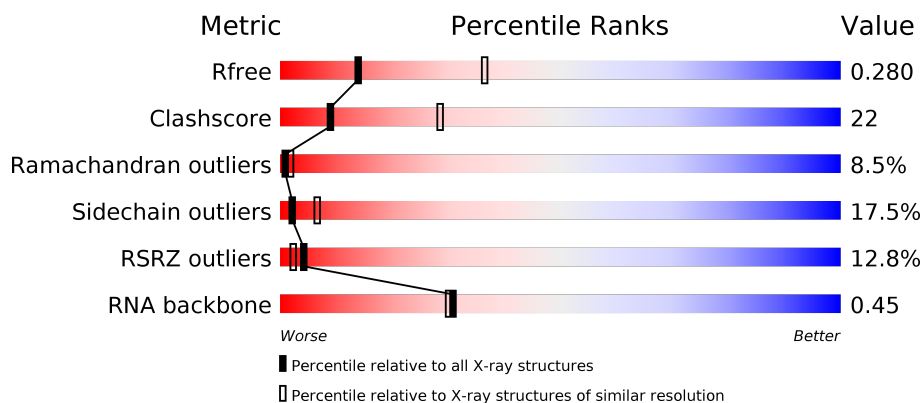
1 Overall quality at a glance

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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)
RNA backbone	2435	1007 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	AA	1539	<div> <div>34%</div> <div>51%</div> <div>15%</div> </div>
1	CA	1539	<div> <div>4%</div> <div>31%</div> <div>54%</div> <div>15%</div> </div>
2	AB	218	<div> <div>13%</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>

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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				

Continued on next page...

Continued from previous page...

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	AltCon
56	BA	1	Total 48	C 34	N 4	O 9	S 1	0	0
56	DA	1	Total 48	C 34	N 4	O 9	S 1	0	0

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

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

- Molecule 58 is water.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

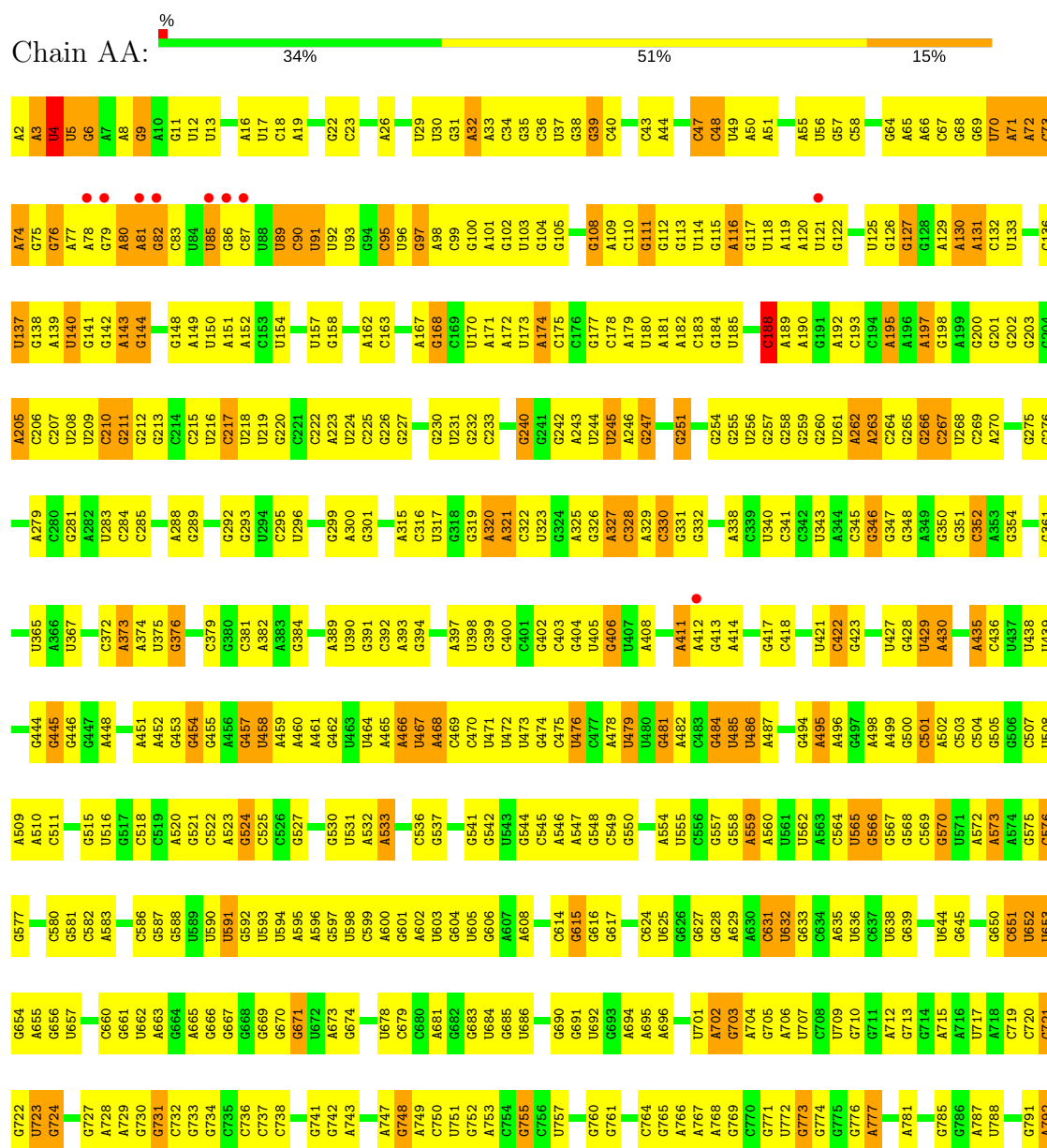
Continued from previous page...

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

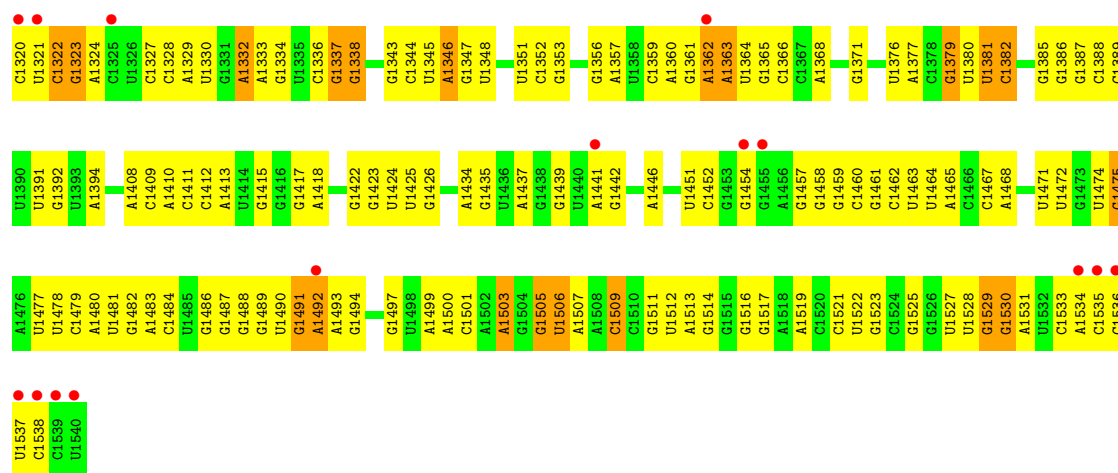
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA

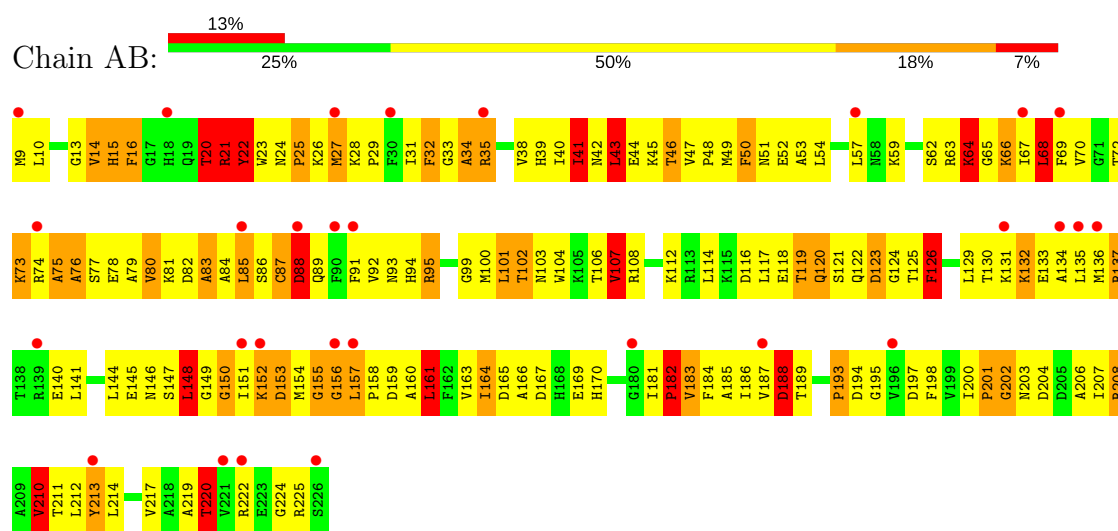




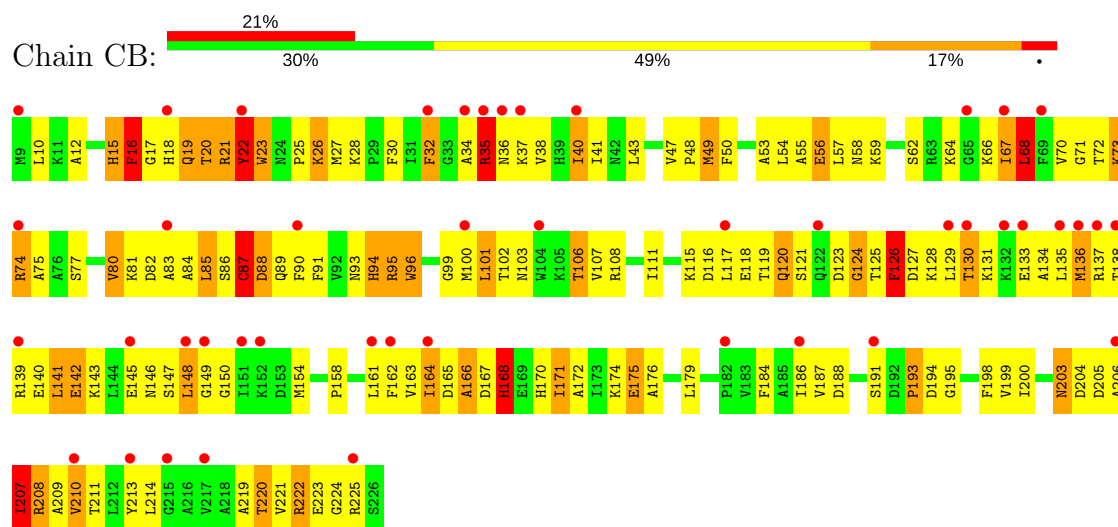




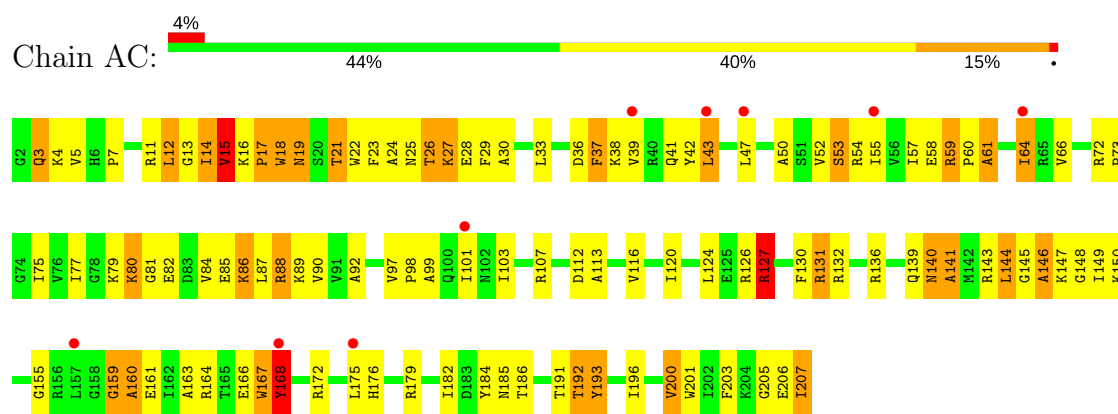
• Molecule 2: 30S ribosomal protein S2



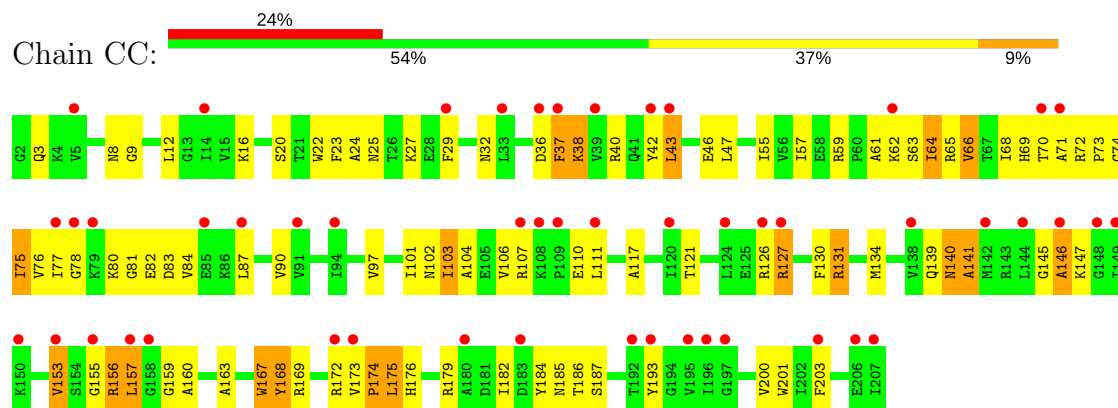
• Molecule 2: 30S ribosomal protein S2



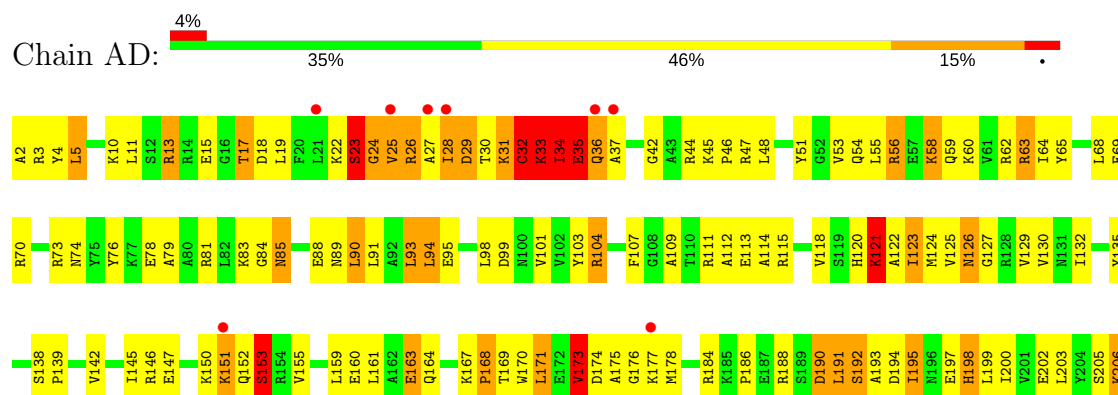
• Molecule 3: 30S ribosomal protein S3



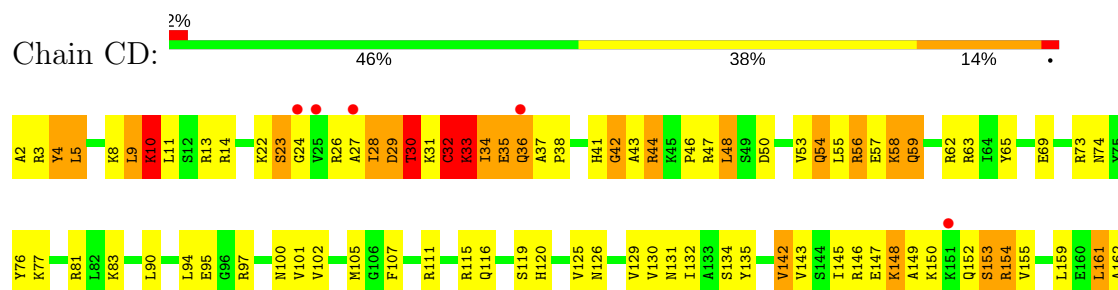
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

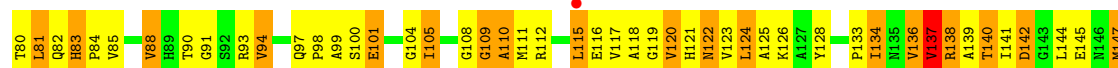


• Molecule 4: 30S ribosomal protein S4

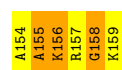




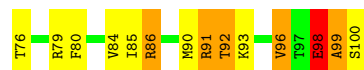
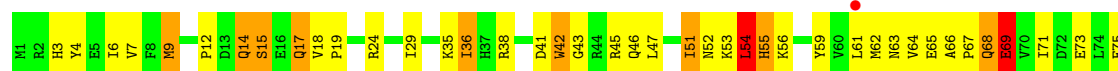
• Molecule 5: 30S ribosomal protein S5



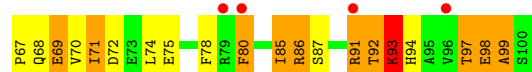
• Molecule 5: 30S ribosomal protein S5



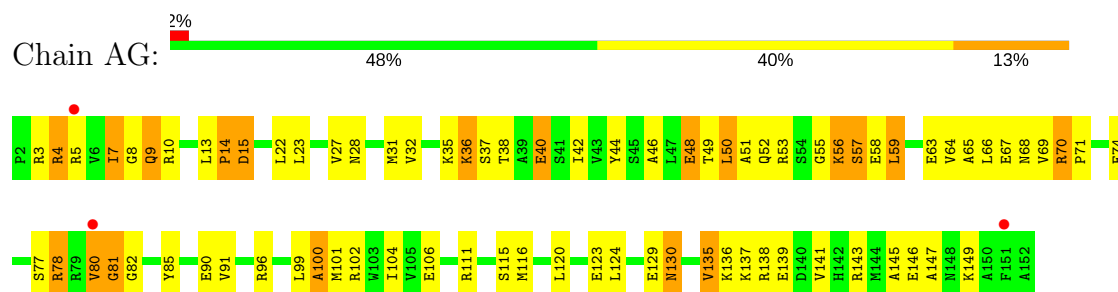
• Molecule 6: 30S ribosomal protein S6



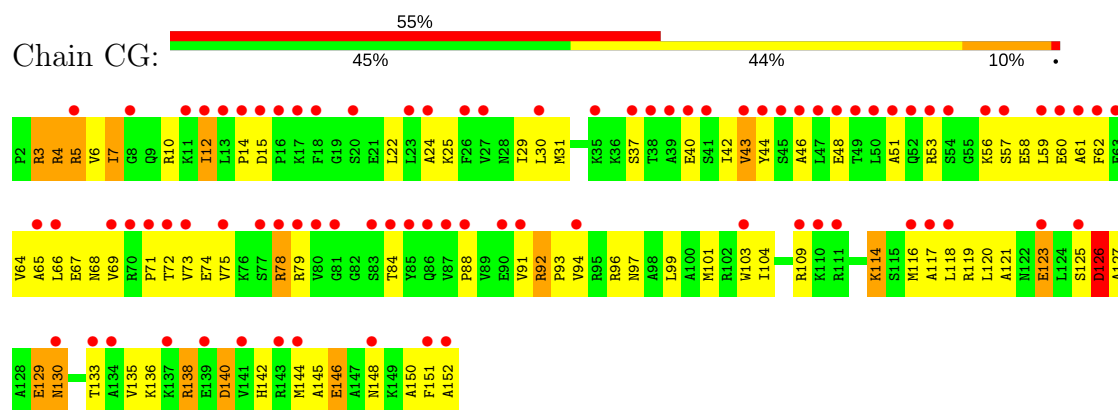
• Molecule 6: 30S ribosomal protein S6



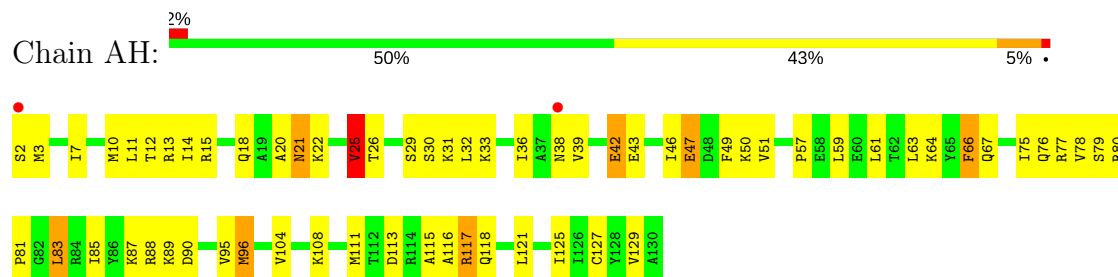
- Molecule 7: 30S ribosomal protein S7



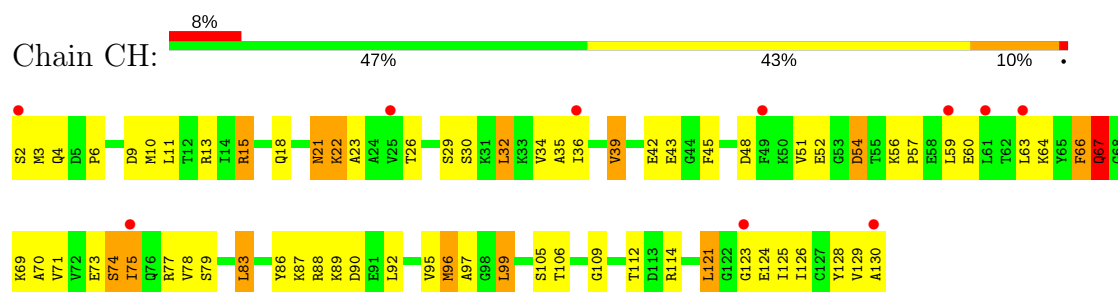
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

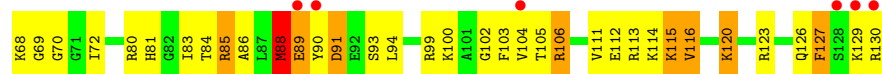
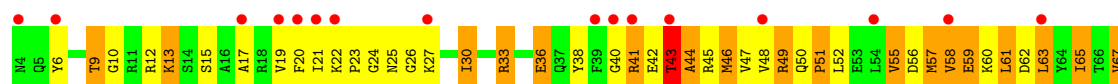


- Molecule 8: 30S ribosomal protein S8

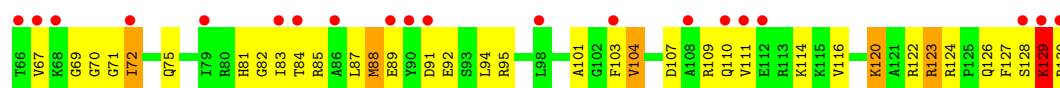
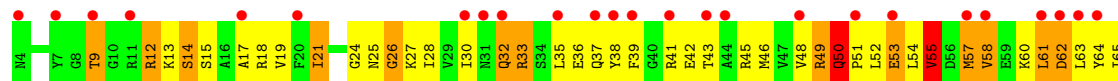


- Molecule 9: 30S ribosomal protein S9

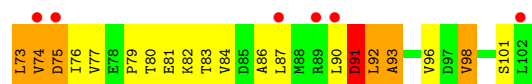
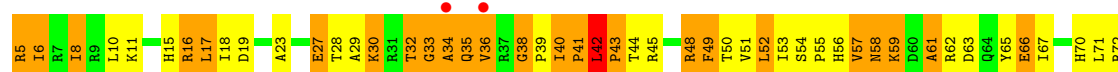




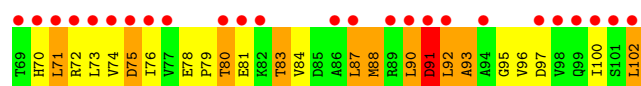
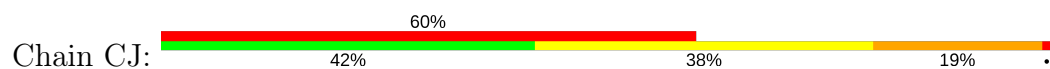
• Molecule 9: 30S ribosomal protein S9



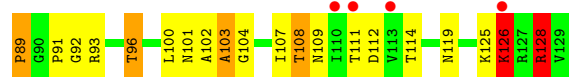
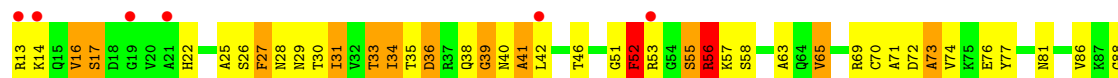
• Molecule 10: 30S ribosomal protein S10



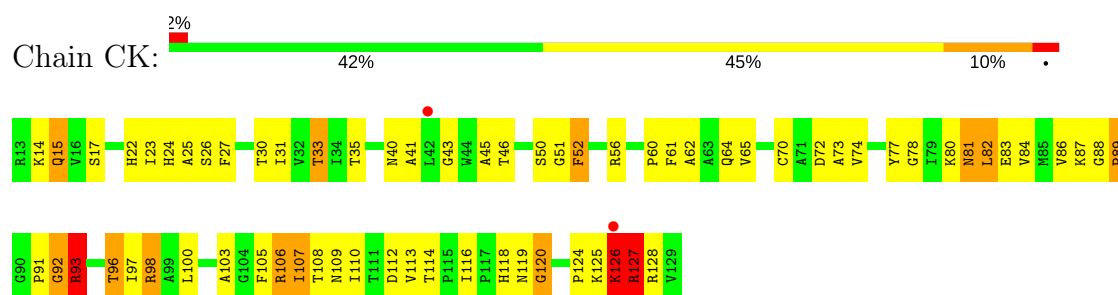
• Molecule 10: 30S ribosomal protein S10



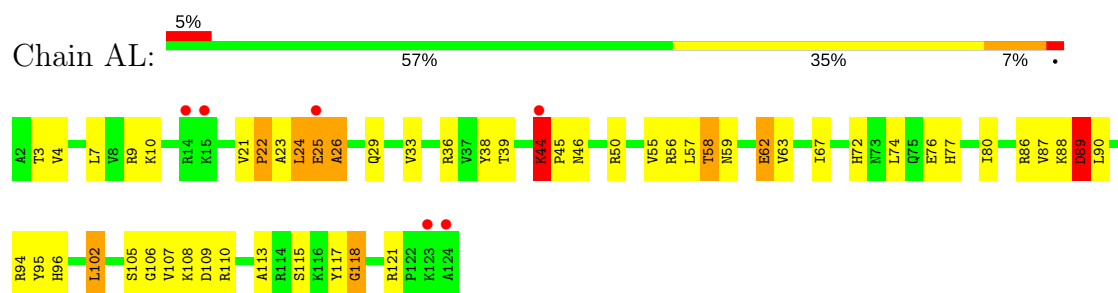
• Molecule 11: 30S ribosomal protein S11



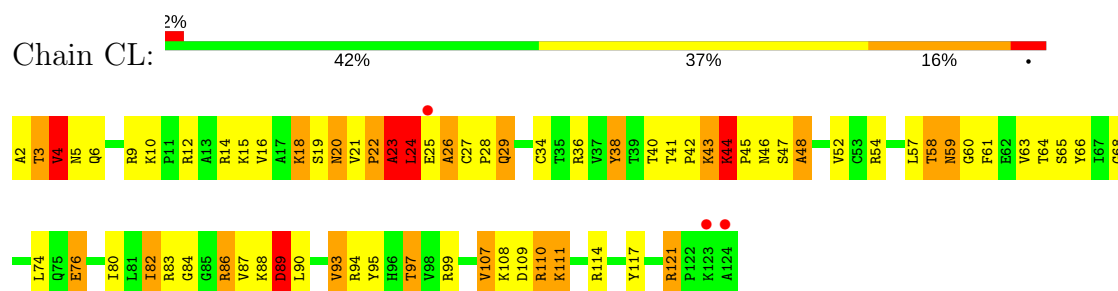
• Molecule 11: 30S ribosomal protein S11



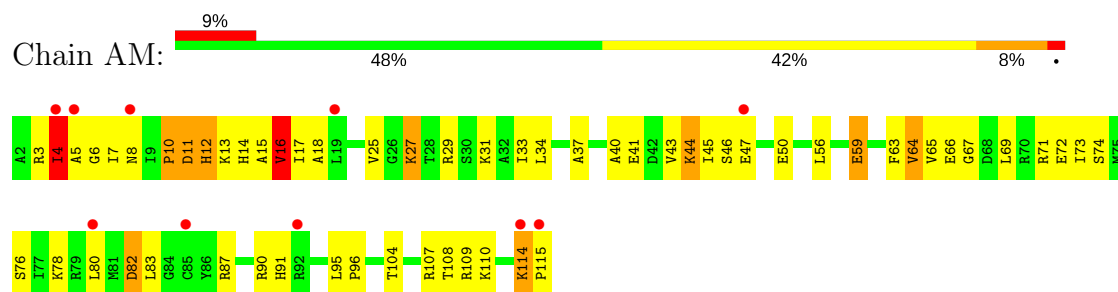
• Molecule 12: 30S ribosomal protein S12



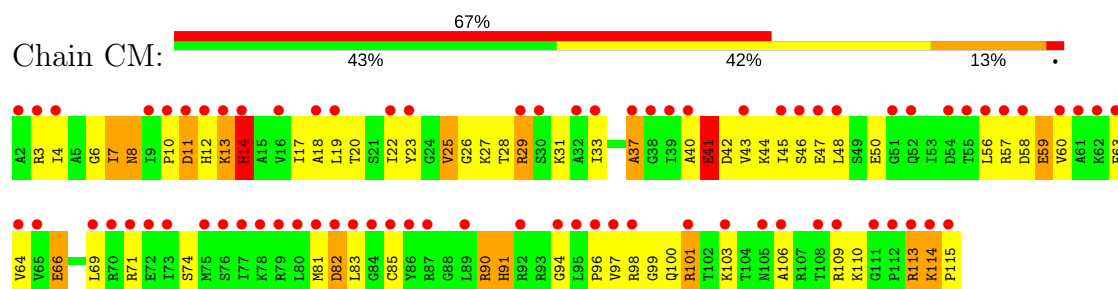
• Molecule 12: 30S ribosomal protein S12



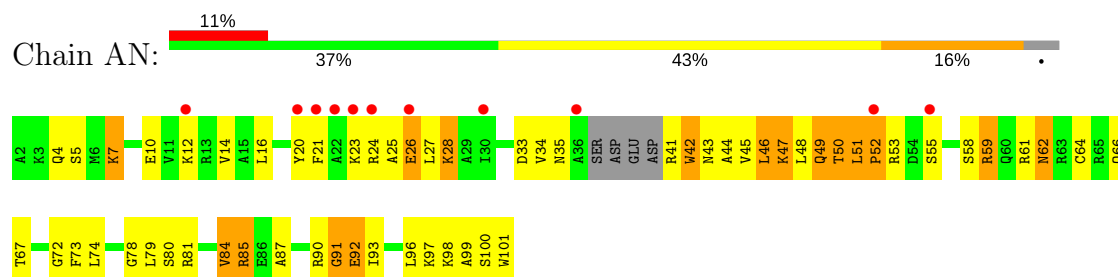
• Molecule 13: 30S ribosomal protein S13



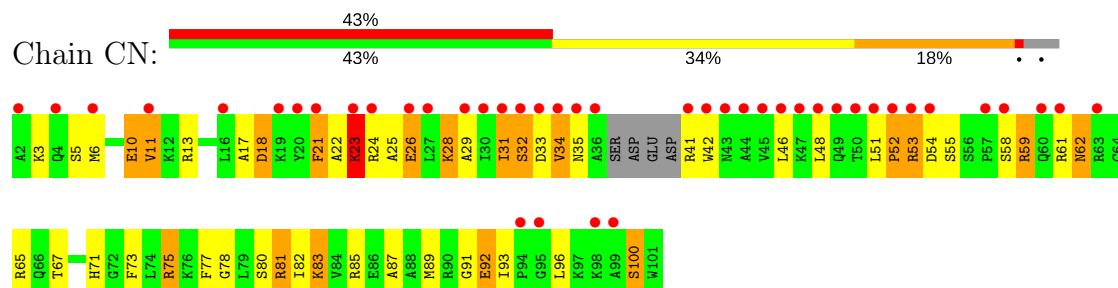
• Molecule 13: 30S ribosomal protein S13



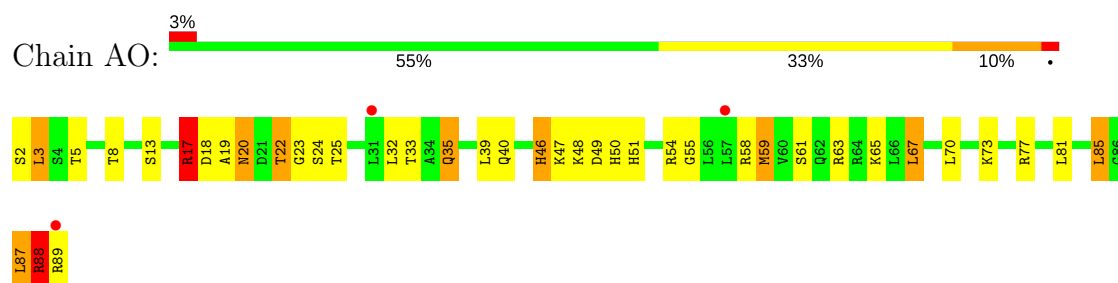
- Molecule 14: 30S ribosomal protein S14



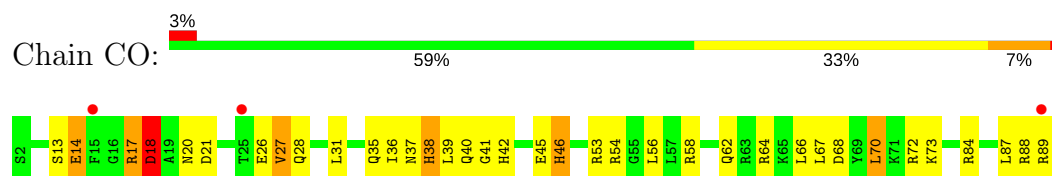
- Molecule 14: 30S ribosomal protein S14



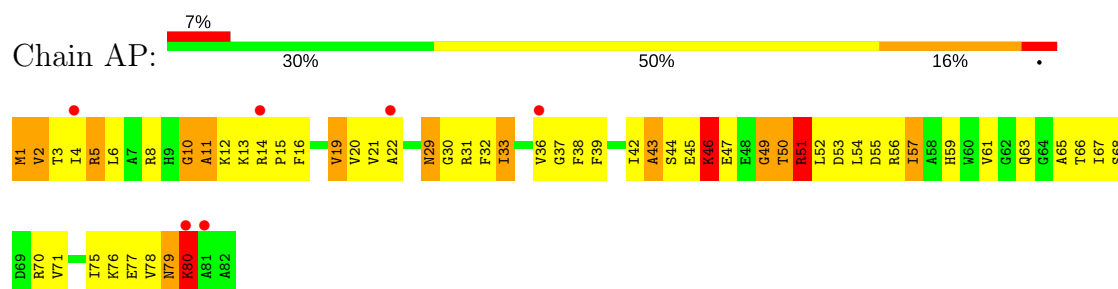
- Molecule 15: 30S ribosomal protein S15



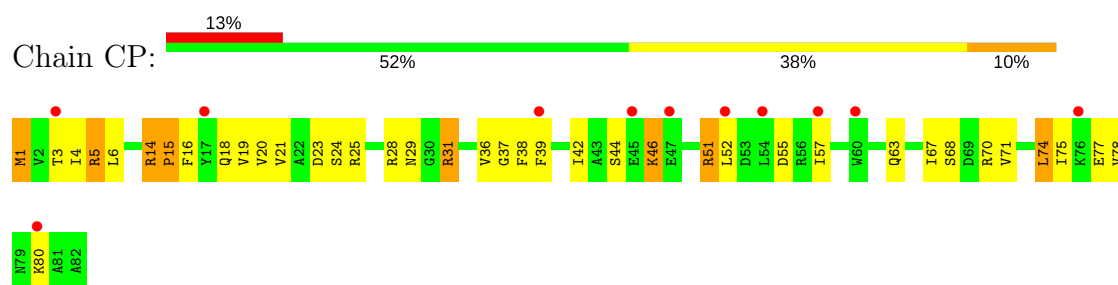
- Molecule 15: 30S ribosomal protein S15



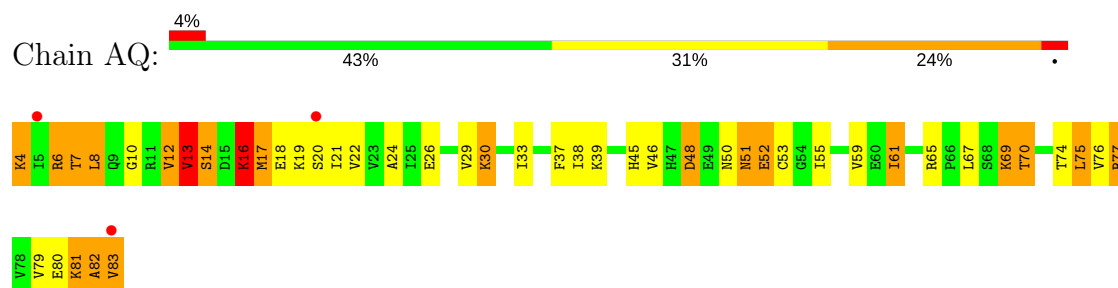
- Molecule 16: 30S ribosomal protein S16



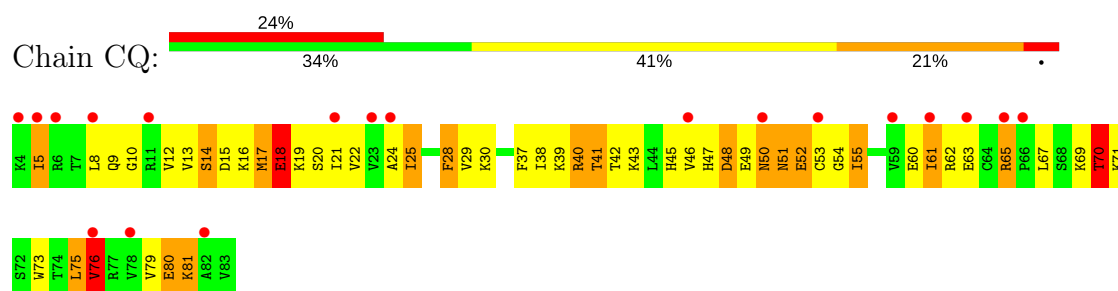
- Molecule 16: 30S ribosomal protein S16



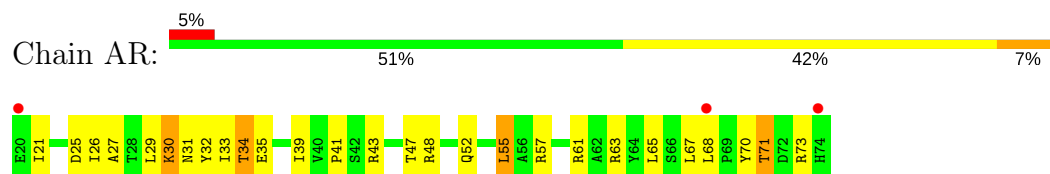
- Molecule 17: 30S ribosomal protein S17



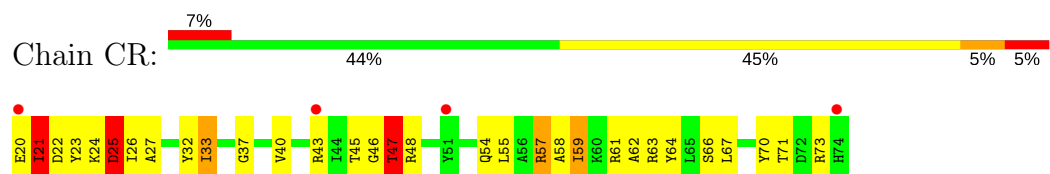
- Molecule 17: 30S ribosomal protein S17



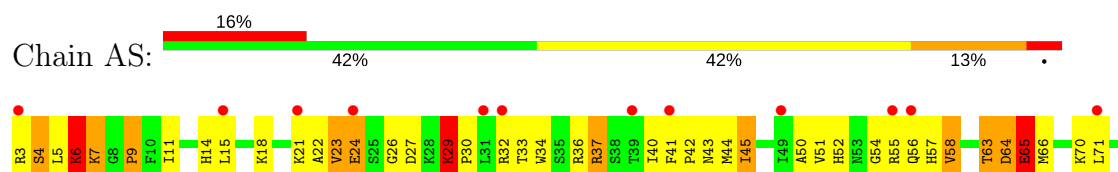
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

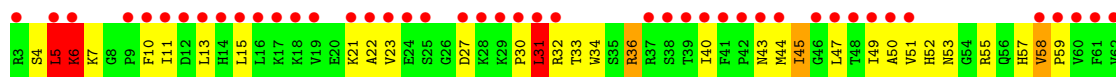
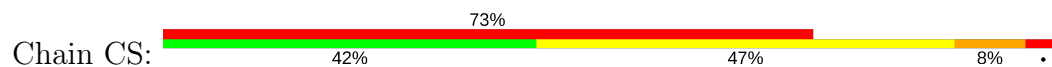


- Molecule 19: 30S ribosomal protein S19

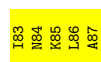




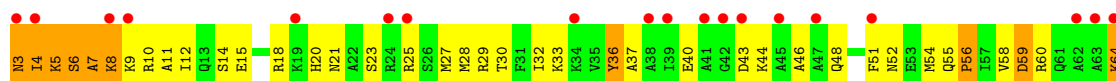
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



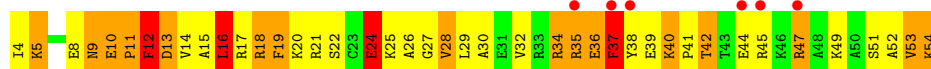
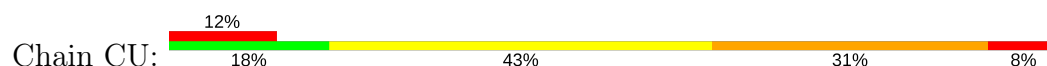
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



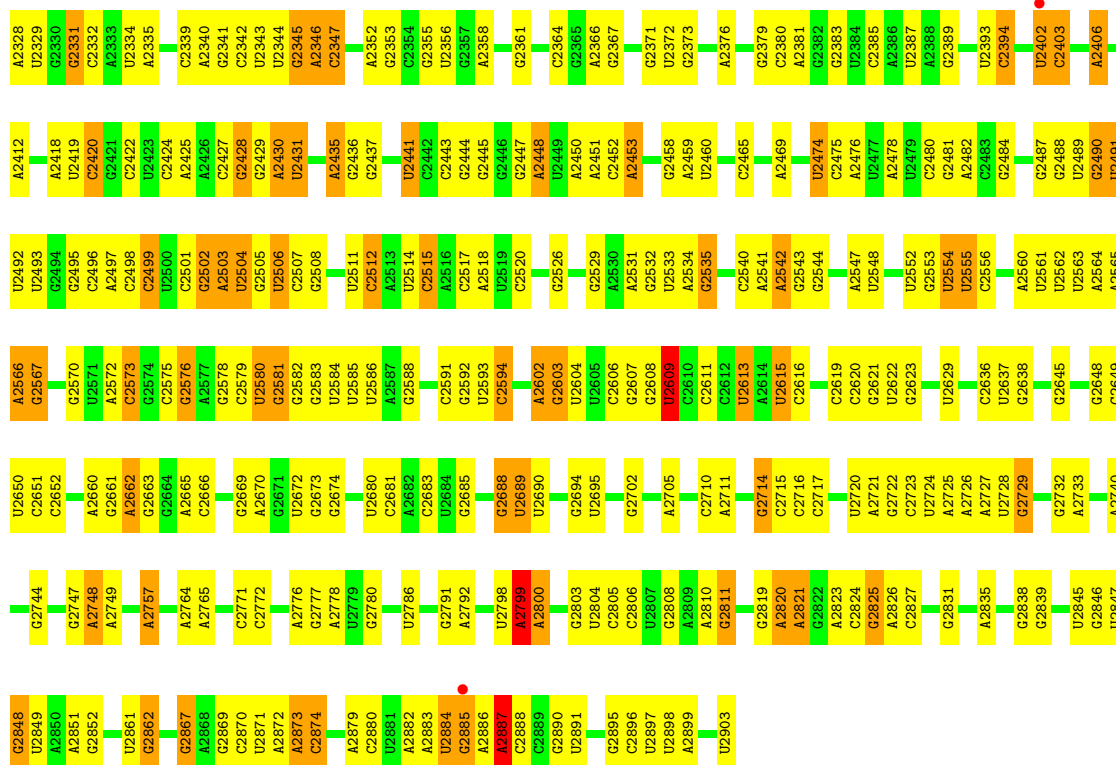
- Molecule 21: 30S ribosomal protein S21



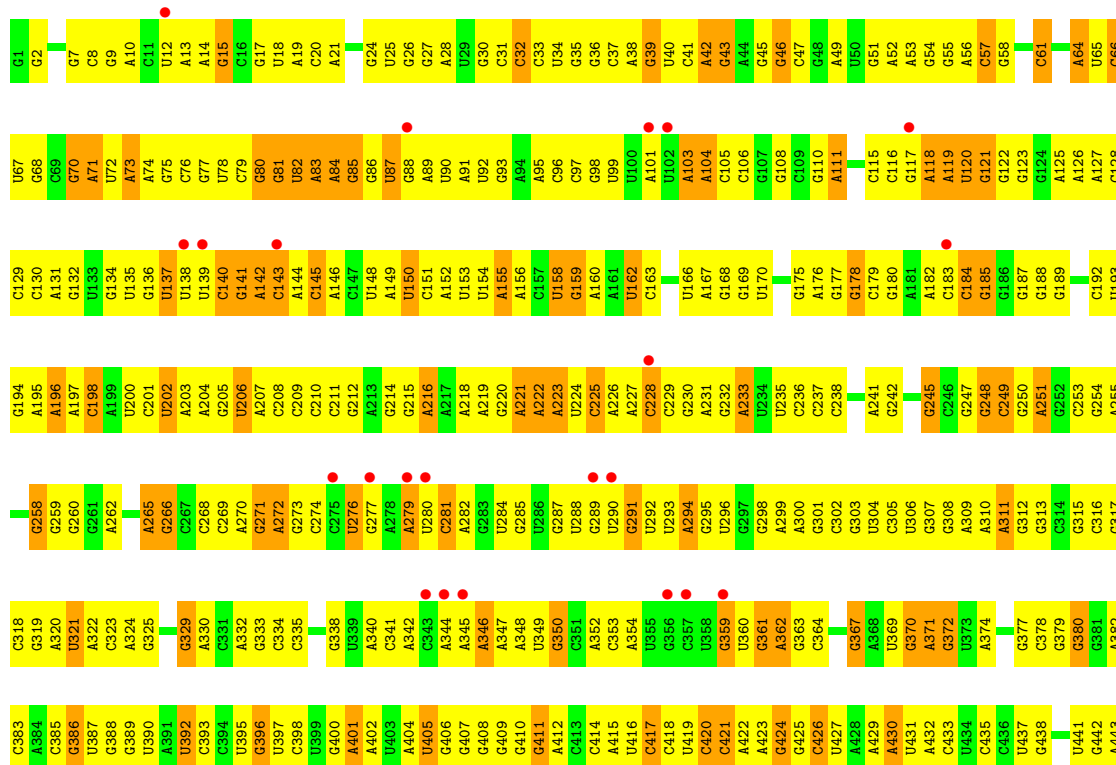
- Molecule 22: 23S rRNA



U2262	A2183	G2123	C1967	G1906	G1830	A1755	C1675	G1587	A1504	G1435	A1359	G1283	A1189
C2263	A2184	G2124	G1968	G1909	G1831	U1758	A1676	U1588	C1507	G1436	G1360	A1284	G1190
C2264	U2185	G2125	A1969	C1910	C1832	A1759	A1677	U1589	A1508	C1437	A1365	A1285	G1191
	G2186	A2052	A1970	G1910	C1833	U1760		A1590	U1680	U1438	A1366	A1286	A1194
A2267	U2187	G2127	U1971	U1911	U1834	C1760	G1681	C1592	G1510	U1440	A1367	A1287	G1195
A2268	U2188	G2128	G1972	A1912	G1835	C1761	G1682	A1593	G1511	U1441		G1288	C1196
C2269	U2189	G2055	G1975	A1913	C1838		U1683	U1594	C1512	U1442	G1371	C1289	
A2270	G2056	G2057	G1976	U1914	G1839	C1764	U1684	C1595	G1513	U1443			U1199
G2271	U2058	A2059	G1980	U1915	G1840	C1768	C1685	A1596	G1514	U1444	U1294	C1200	
C2272	A2060	A1981	A1916	U1917	U1841	U1769		A1597	A1515	G1450	A1374		
A2273	U1982	U1982	A1918	A1918	G1842		U1688		G1451	G1375		G1206	
A2274	A2062	A2062	A1919	A1919	G1843	A1773	U1689	U1602	C1452	A1301	A1300	G1207	
C2275	C2063	C2063	C1985	C1920	C1844	G1774		A1603	A1453	G1376	A1302		
	C2064	C2064	C1986	G1921	G1845	G1776		C1604	A1528	G1377	A1303	G1218	
A2278	C2065	C2065	G1922	G1922	G1846		G1695	C1605	G1529	A1378	A1304		
G2279	G2069	G2069	U1991	U1923	A1847	U1779	G1696	C1606	G1531	U1379	C1305	U1224	
C2280	U2075	U2075	G1992	C1924	A1848	U1780	G1697	C1607	A1532	U1380		U1225	
A2281	C2072	C2072	U1993	C1925	G1849	A1780	U1698	A1608	C1533	G1381		G1226	
G2282			C1994	U1926	G1850	U1781	G1699	A1609	U1534	G1382	G1309		
C2283	C2143	C2143	U1995	U1927	U1851	U1782	A1700	A1610	U1535	A1383			
	U2075	U2075	C1996	A1928	U1852	A1783	C1708	G1613	C1536	A1385	U1313	A1230	
G2286	C2144	C2144	A1998	G1930	A1853	U1784	U1709	U1618	G1537	U1464	U1316	G1232	
A2287	U2077	U2077	C2006	U1931	U1856	A1785			U1538	U1465	U1317	C1233	
	C2078	C2078	A2009	A1932	G1857	U1786	U1717	G1628	G1540	U1467	U1318	U1234	
U2291	U2085	U2085	C2001	G1933	A1866	A1789	U1712	G1622	C1541	U1468	C1319	G1235	
U2292	C2150	C2150	C1934	U1940	G1867	C1790	A1713	G1623	U1542	U1469	C1320	G1236	
C2293	U2087	U2087	G1935	C1941	U1872	U1797	U1720	U1636	G1554	A1469	A1321	G1237	
G2294	G2087	G2087	A1936	C1942	C1874	G1792	G1715	A1637	G1543	A1470	C1322	G1238	
C2295			C2006	U1943	G1875	U1798	A1722	C1638	G1555	C1480	C1330	G1239	
U2296	U2092	U2092	A2009	U1944	A1876	C1800			C1556	U1481	U1409	U1240	
A2297	C2093	C2093	A2009	G1945	A1877	A1801	U1729	G1645	C1557	G1482	G1410	G1250	
C2298	U2094	U2094	A2013	U1946	A1878	A1802	C1730	U1646	G1560	G1483	U1411	G1251	
	A2097	A2097	A2014	C1947	U1880	A1805	G1731	U1647	G1563	U1484	U1412	C1252	
G2302	U2098	U2098	A2015	G1948	C1881	A1808	C1732	U1648	U1564	U1485	A1413	G1253	
C2303	U2099	U2099	U2016	G1949	U1882	A1808	G1733	G1649	C1564	U1486	C1414	A1254	
G2304	G2100	G2100	U2017	G1950	U1883		U1734	A1650	C1565	U1487	U1415	A1255	
U2305	C2101	C2101	G2018	U1951	G1884	A1808	A1736	G1651	C1565	C1488	G1416	G1256	
C2306	A2101	A2101	A2018	A1952	A1885	G1813	U1736	A1652	A1569	U1489	C1417		
G2307	G2102	G2102	A2019	U1946	C1886	C1816	G1737	A1653	A1570	A1490	G1418	G1259	
C2308	A2103	A2103	A2020	G1948	C1887	A1817	U1738	G1658	A1571	G1491	A1419	A1260	
A2309	C2104	C2104	C2021	G1948	U1888	C1818	A1739		C1493	G1492	A1420	G1267	
C2310	U2105	U2105	U2022	G1950	A1889	U1818	G1740		C1494	A1494	G1421	G1268	
A2311	U2106	U2106	C2023	U1951	A1890	A1819		A1665	C1575	A1495	G1422	U1267	
G2312	G2107	G2107	G2024	U1952	A1891	U1820	A1744	G1666	C1576	U1496	G1423	C1269	
C2313	G2108	G2108	G2029	A1952	C1893	A1821	U1745	U1667	C1577	U1497		C1270	
A2314	U2109	U2109	A2030	G1954	C1894	C1822	A1746	A1668	U1578	C1498	G1429	A1271	
G2315	G2110	G2110	A2031	U1955	C1895	G1823	U1747	C1499	A1579	C1499	G1430	A1272	
C2316	U2111	U2111	G2032	U1956	C1896	G1824	C1748		A1583	G1500	A1431	G1275	
A2317	G2112	G2112	A2033	C1957	A1897	U1827	A1749		U1584	A1502	G1432	A1276	
G2318	U2113	U2113	U2034	C1958	A1900	G1828	G1750		C1585	A1503	A1433	G1277	
C2319	A2114	A2114	G2035	U1959	C1893	A1829	A1754		A1586				
U2320	G2115	G2115	G2036	A1960	C1894								
A2321	A2116	A2116	A2037	C1961	C1895								
C2322	U2117	U2117	G2038	C1962	A1899								
U2323	G2118	G2118	G2040	C1963	A1900								
G2324	C2119	C2119	U2041	G1964	A1901								
A2325	U2120	U2120	A2042	C1965	A1901								
C2326	G2121	G2121	G2043	A1966									
A2327	U2122	U2122											

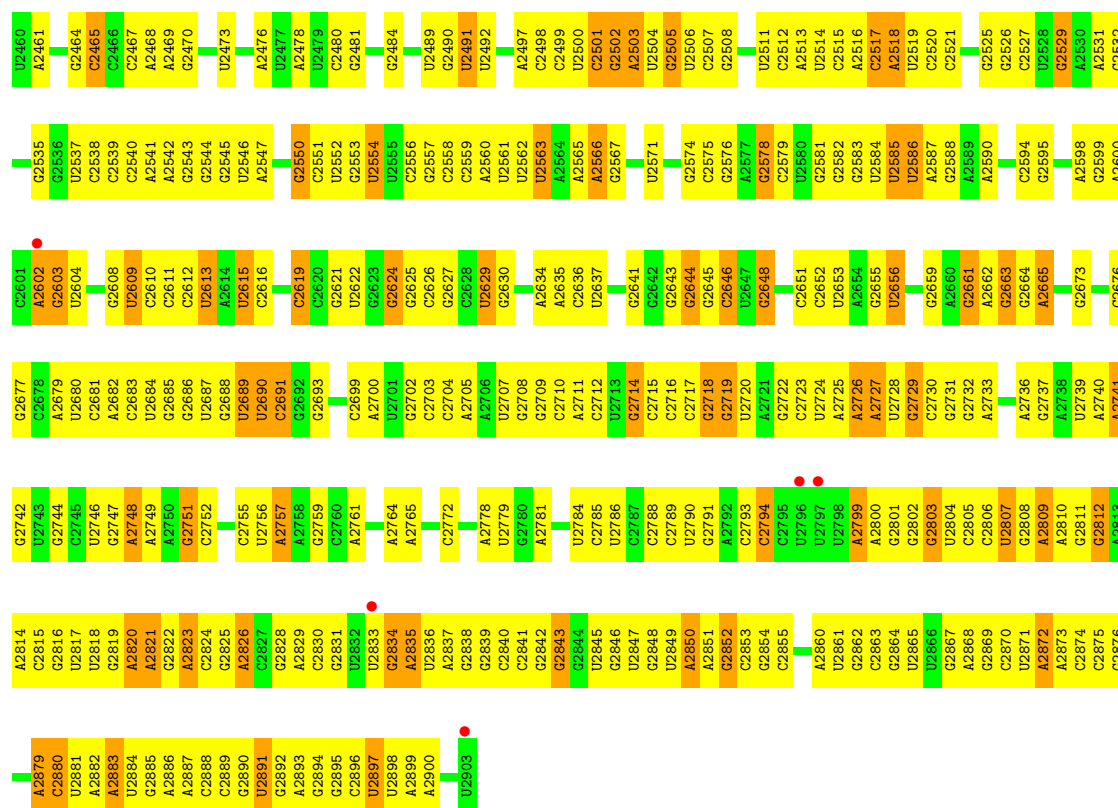


• Molecule 22: 23S rRNA

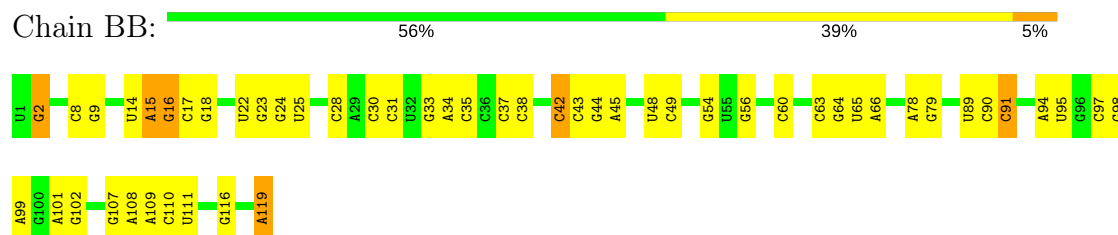




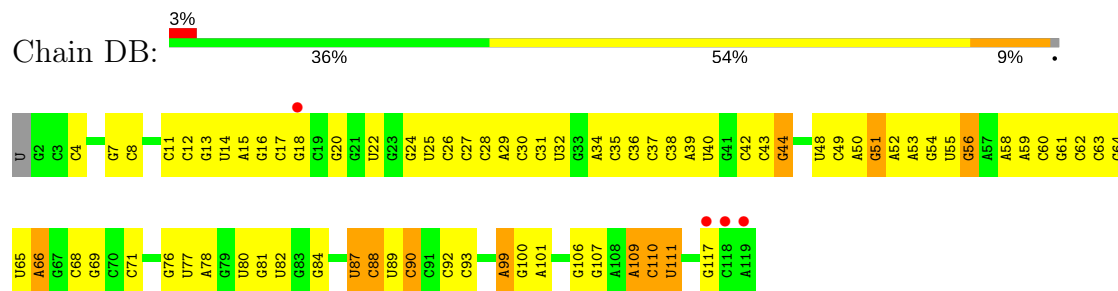
U2393	G2331	A2267	A2062	A1998	U1931	G1793	G1645	C1574	A1509	A1434
C2394	C2332	A2268	C2063	C1999	G1935	A1794	C1646	C1575	G1510	G1435
C2395	A2333	G2271	C2064	C2000	A1936	A1795	U1647	U1576	G1511	G1436
G2396	U2334	U2272	C2065	C2001	A1937	U1796	U1648	C1577	C1512	C1437
G2397	A2335	U2273	C2066	G2004	A1938	U1797	G1649	U1578	U1513	U1438
U2402	A2336	A2274	U2067	G2005	U1939	U1798	A1650	G1581	G1514	A1439
G2405	C2337	C2275	U2068	C2006	U1940	G1799	G1651	U1582	U1441	U1440
A2406	C2338	G2276	A2070	U2007	G1946	A1800	A1652	C1583	U1442	U1441
A2407	A2340	G2279	A2071	C2008	A2071	A1801	G1653	U1584	U1443	U1443
A2408	U2341	G2280	C2072	A2009	U1947	A1802	A1654	C1585	G1520	G1444
G2409	C2342	A2281	C2073	G2010	U1948	A1803	C1658	U1586	A1522	G1445
G2410	U2343	A2282	U2074	U2011	G1949	A1804	G1659	G1587	U1523	U1446
A2411	U2344	U2213	U2075	G2012	G1950	A1805	G1660	U1590	G1524	C1447
A2412	G2345	C2214	U2079	A2013	U1951	G1807	G1661	A1591	A1525	G1448
G2413	A2346	C2215	A2080	A2014	A1952	A1808	U1662	U1591	C1526	U1449
G2414	C2347	G2216	G2083	U2016	A1953	A1809	G1663	C1592	A1527	G1452
G2415	U2348	G2217	C2084	U2017	G1954	A1810	A1664	U1595	U1528	A1453
G2416	A2349	G2218	G2087	A2018	U1955	A1811	A1665	A1596	G1529	C1454
C2417	C2350	G2221	G2088	G2019	U1956	A1812	G1666	A1597	G1530	C1455
C2418	G2351	G2222	U2091	A2020	U1957	A1813	G1667	A1598	C1532	G1456
U2419	A2352	G2223	C2092	C2021	C1958	A1814	A1668	U1599	C1533	U1457
U2419	G2353	G2224	U2092	C2022	C1959	A1815	A1669	U1600	U1534	U1458
C2420	C2354	A2225	C2093	U2022	A1960	A1816	C1670	G1601	A1535	G1459
U2423	G2355	C2226	G2094	G2024	G1964	A1817	U1671	U1602	C1536	U1460
C2424	A2357	A2227	C2103	C2025	C1965	U1818	G1674	A1603	C1461	C1462
A2425	C2358	G2230	C2104	U2026	C1966	A1819	C1675	A1604	C1462	C1461
A2426	U2359	U2231	U2105	A2030	C1967	A1820	A1676	G1541	G1540	G1463
C2427	C2360	C2232	U2106	A2031	U1978	G1826	A1677	C1606	G1541	G1464
G2428	G2361	U2233	U2107	C2032	A1968	A1827	A1678	U1542	U1465	G1465
U2429	C2362	G2234	G2107	G2033	U1969	G1828	A1679	A1608	U1466	U1466
A2430	G2363	U2235	U2108	A2034	C1970	A1829	A1680	A1609	U1467	U1467
U2431	A2366	G2236	U2109	G2035	U1972	C1830	U1682	C1610	U1468	U1468
A2432	C2367	U2237	C2110	C2036	U1973	A1831	C1611	C1611	A1469	U1469
U2435	G2370	G2238	U2111	A2037	C1974	C1832	U1683	G1612	A1470	A1470
G2436	C2371	G2239	U2112	G2038	G1975	G1833	U1688	A1613	G1471	G1471
G2437	U2372	U2240	U2113	U2039	U1976	U1834	U1692	A1614	G1551	G1475
A2439	C2373	G2242	G2115	G2040	A1977	G1835	U1693	C1615	A1552	U1476
C2440	U2374	U2243	U2116	U2041	U1978	G1836	C1694	A1616	A1553	A1477
U2441	G2375	U2244	U2117	C2042	U1979	C1837	G1695	U1554	U1554	C1480
C2442	A2376	U2245	U2118	C2043	A1980	G1838	A1698	G1619	G1555	U1481
C2443	U2377	G2246	U2119	C2044	U1981	A1839	A1701	G1620	C1556	U1481
G2444	A2378	G2250	G2120	G2045	U1982	C1843	C1701	U1621	C1557	G1482
G2445	C2379	G2251	G2121	G2048	G1983	C1844	A1701	G1622	C1558	G1483
G2446	C2380	U2252	U2122	C2049	U1984	G1845	G1707	U1623	U1559	U1484
G2447	U2381	G2253	U2123	G2050	C1985	G1846	G1708	U1624	G1560	U1484
U2448	C2382	C2254	G2124	A2051	U1986	A1847	U1709	C1625	C1561	C1493
A2449	U2383	G2255	U2125	A2052	G1987	A1848	G1710	A1626	U1562	C1493
U2450	A2384	C2256	A2126	G2053	U1988	G1849	G1711	G1627	U1563	U1497
A2451	C2385	G2258	G2127	A2054	G1989	U1850	G1715	G1628	C1564	U1497
C2452	U2386	U2192	G2128	C2055	U1990	U1851	U1716	A1634	C1565	G1500
A2453	A2387	G2193	G2129	C2056	U1991	U1852	A1717	A1634	A1566	G1501
G2454	C2388	U2194	C2129	G2057	G1992	A1853	G1718	C1638	G1567	A1502
U2457	U2389	C2196	U2130	A2058	U1993	U1854	A1722	G1639	A1503	A1504
G2458	C2390	U2197	U2131	C2059	C1994	U1855	G1723	A1641	A1504	A1505
A2459	A2391	G2198	G2132	A2060	U1995	U1856	A1791	A1641	A1505	A1508
	A2392	A2199	A2134	G2061	C1997	G1930	G1724		A1571	



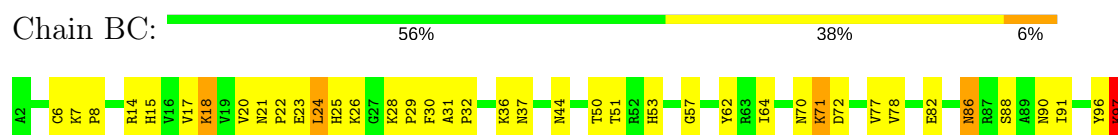
• Molecule 23: 5S rRNA

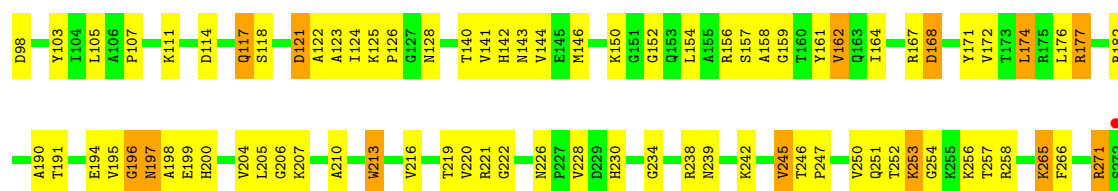


• Molecule 23: 5S rRNA

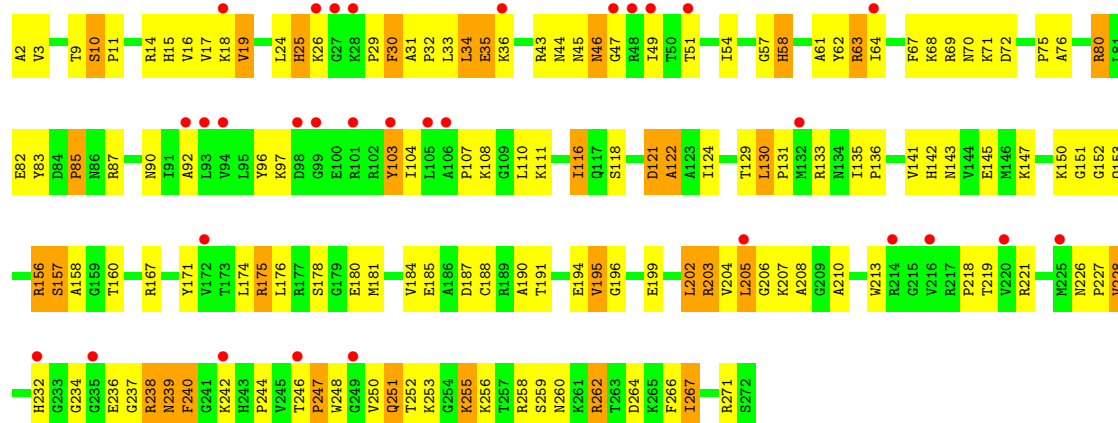


• Molecule 24: 50S ribosomal protein L2





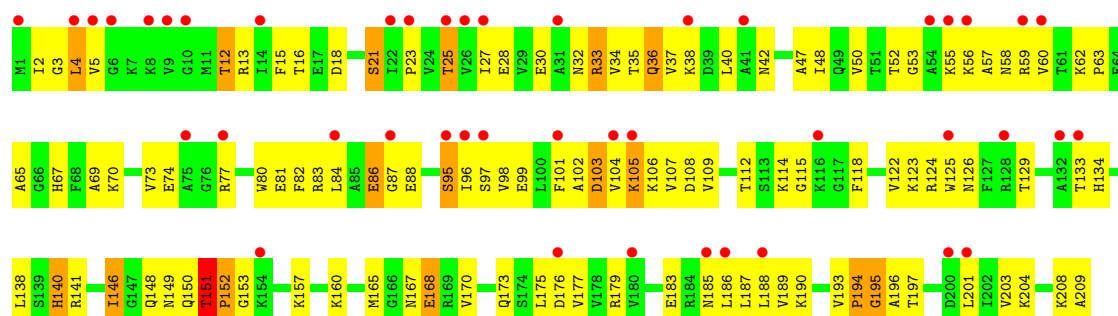
• Molecule 24: 50S ribosomal protein L2



• Molecule 25: 50S ribosomal protein L3

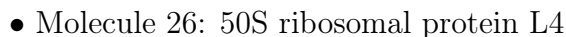


• Molecule 25: 50S ribosomal protein L3

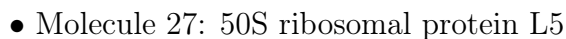


• Molecule 26: 50S ribosomal protein L4

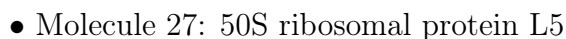
Response	Percentage
Yes, the U.S. is a democracy	59%
No, the U.S. is not a democracy	34%
Don't know	7%



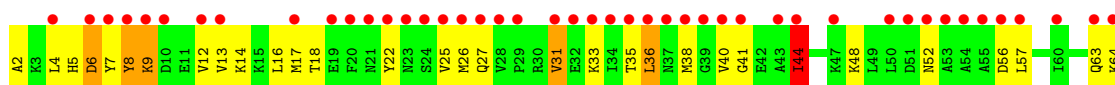
Group	Percentage
Red	40%
Green	49%
Yellow	38%
Orange	12%

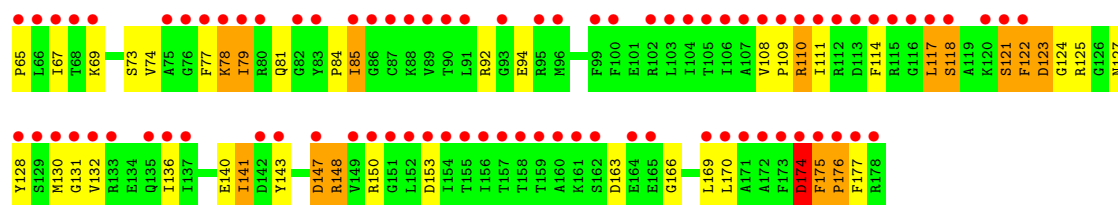


Frequency	Percentage
Very often	2%
Often	47%
Sometimes	37%
Never	14%

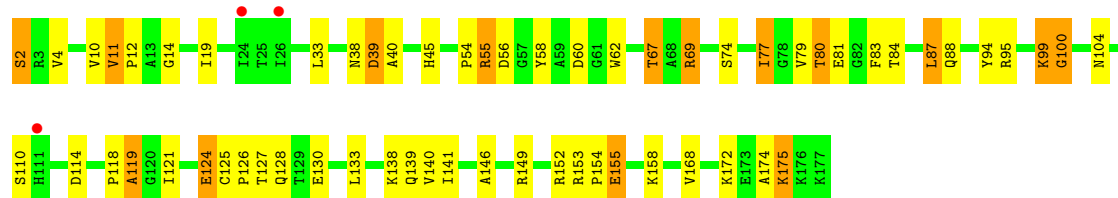


Response	Percentage
Yes, the current government is responsible	72%
No, the current government is not responsible	28%

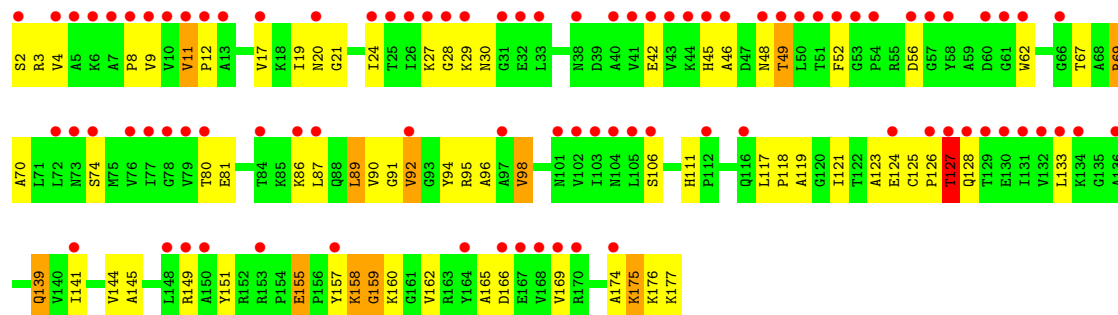




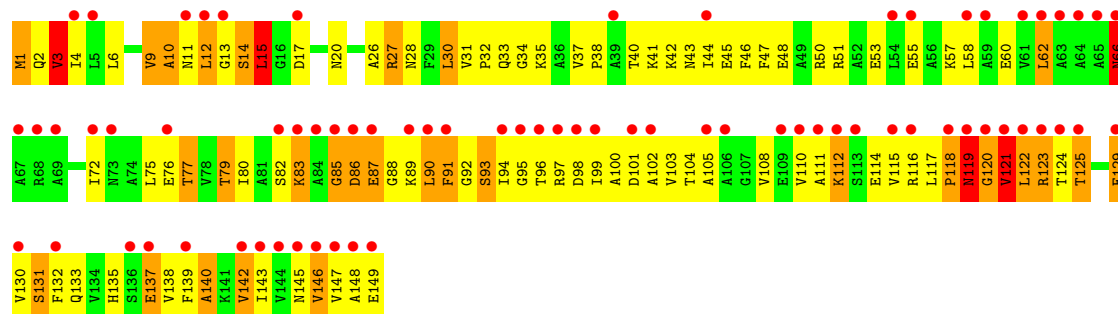
• Molecule 28: 50S ribosomal protein L6



• Molecule 28: 50S ribosomal protein L6

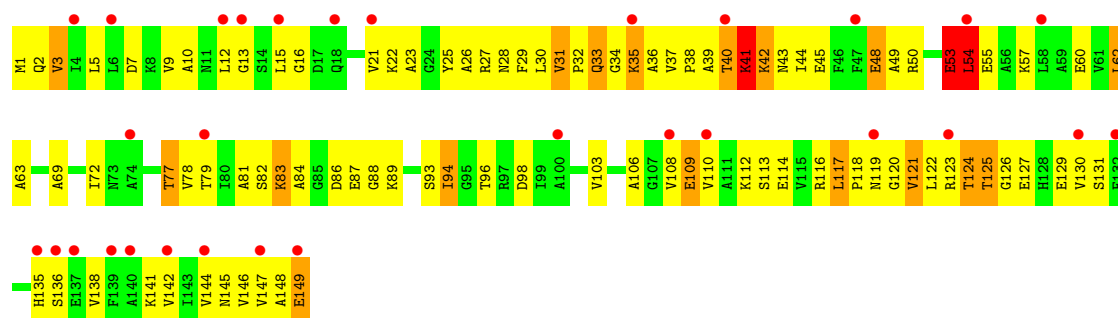


• Molecule 29: 50S ribosomal protein L9

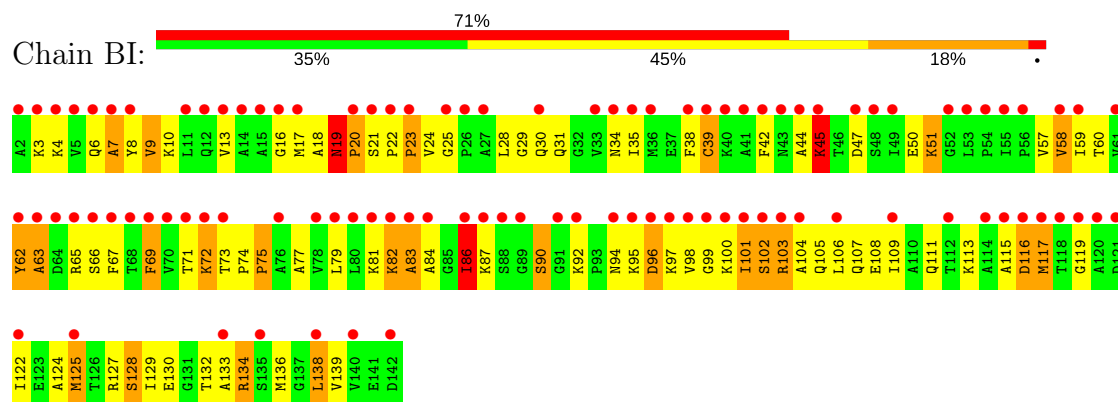


• Molecule 29: 50S ribosomal protein L9

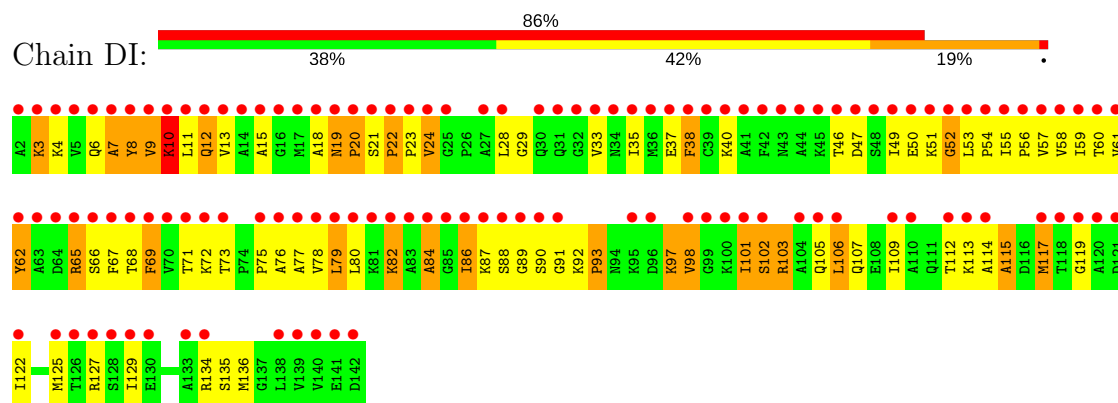




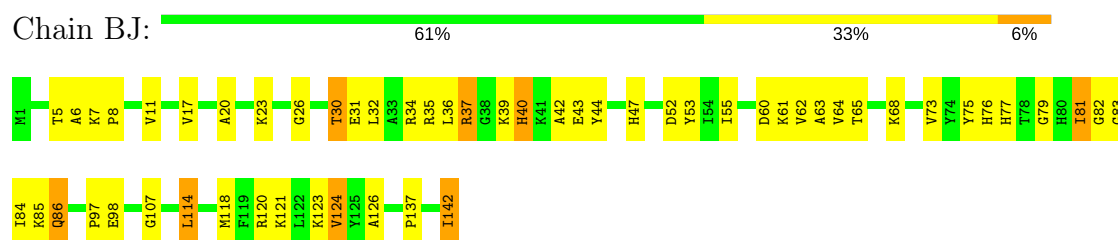
- Molecule 30: 50S ribosomal protein L11



- Molecule 30: 50S ribosomal protein L11

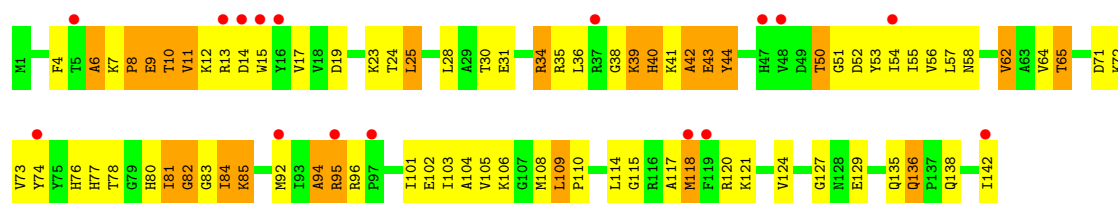


- Molecule 31: 50S ribosomal protein L13



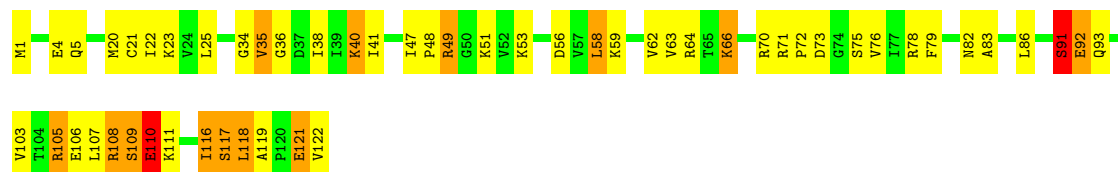
- Molecule 31: 50S ribosomal protein L13





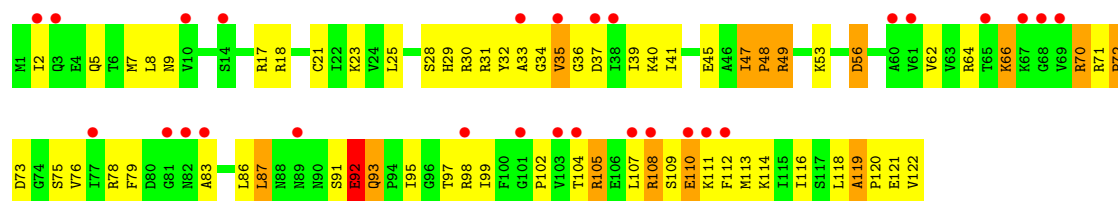
• Molecule 32: 50S ribosomal protein L14

Chain BK: 56% 32% 11% .



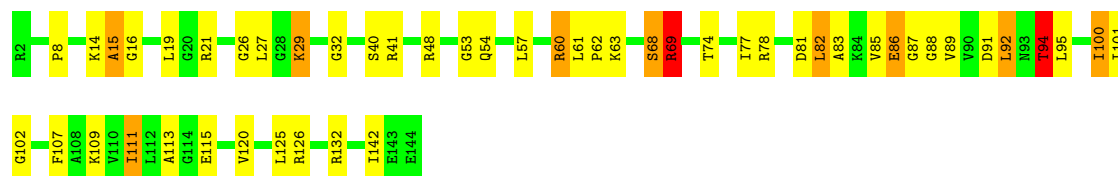
• Molecule 32: 50S ribosomal protein L14

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



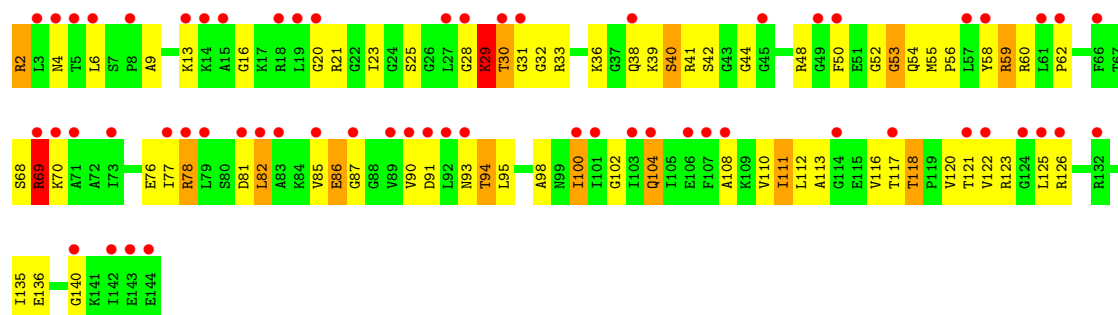
• Molecule 33: 50S ribosomal protein L15

Chain BL: 65% 27% 6% .

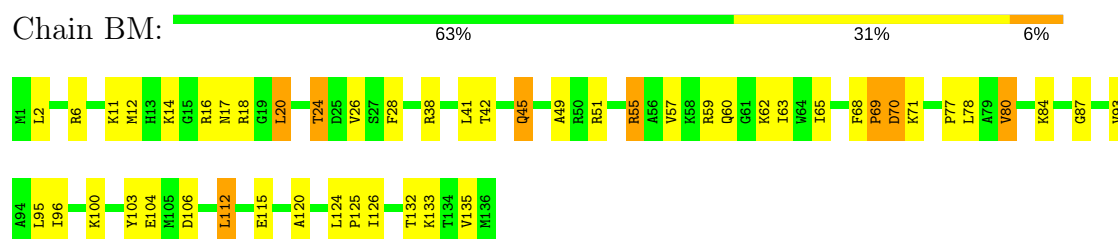


• Molecule 33: 50S ribosomal protein L15

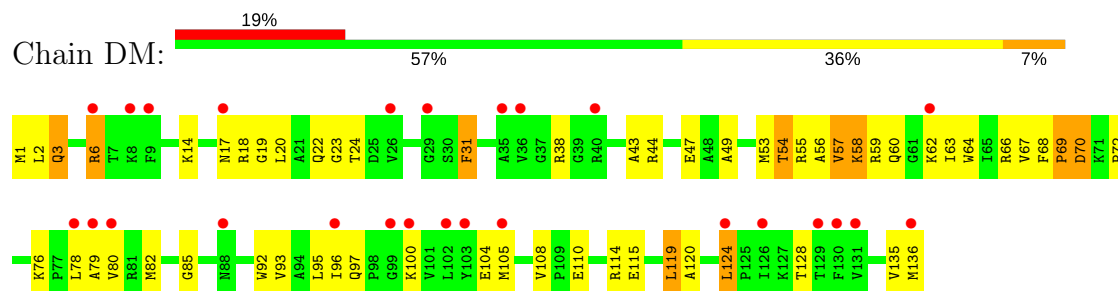
Chain DL: 42% 50% 39% 9% .



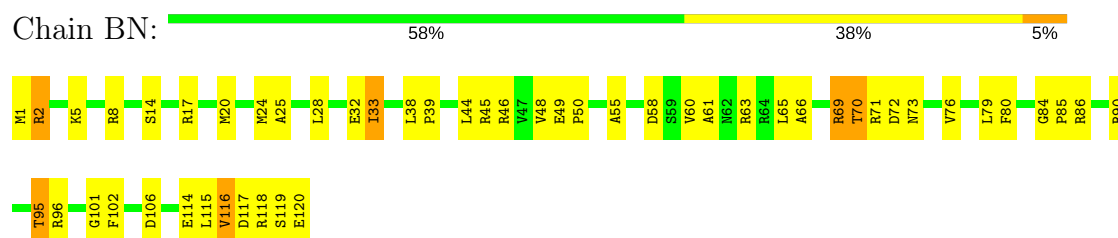
- Molecule 34: 50S ribosomal protein L16



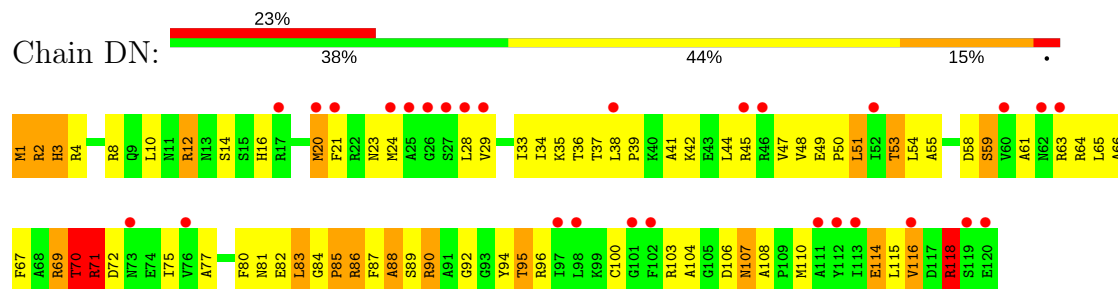
- Molecule 34: 50S ribosomal protein L16



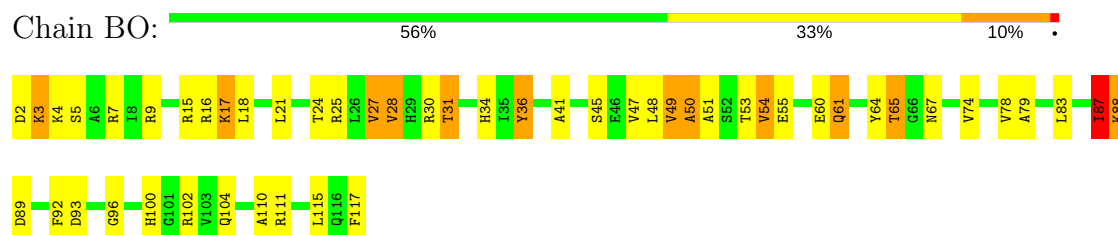
- Molecule 35: 50S ribosomal protein L17



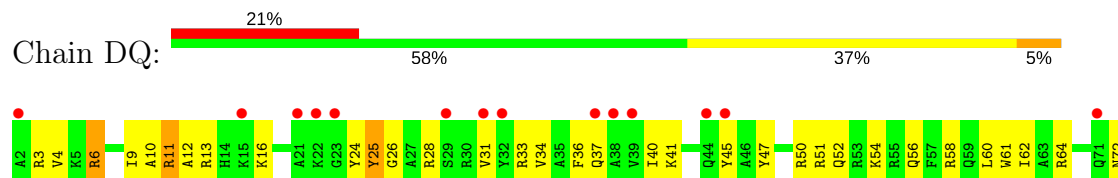
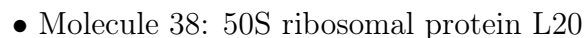
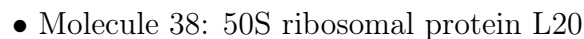
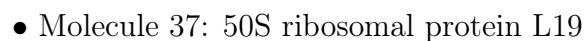
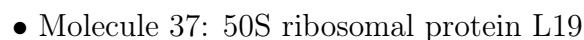
- Molecule 35: 50S ribosomal protein L17

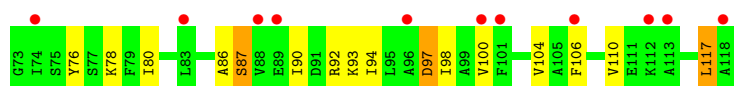


- Molecule 36: 50S ribosomal protein L18



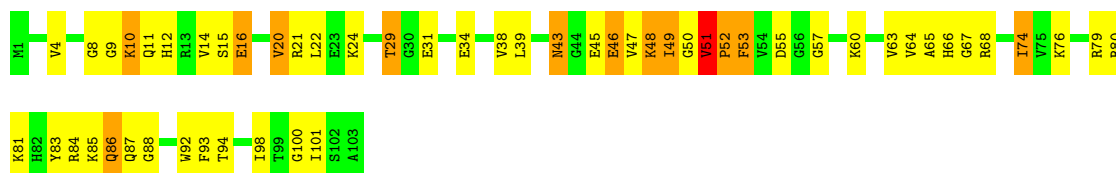
- Chain DO:





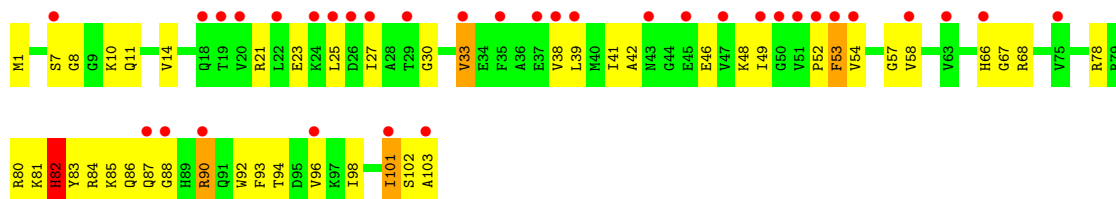
• Molecule 39: 50S ribosomal protein L21

Chain BR: 48% 40% 12%



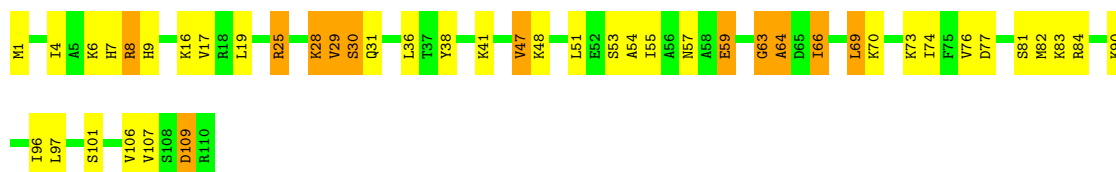
• Molecule 39: 50S ribosomal protein L21

Chain DR: 33% 55% 40%



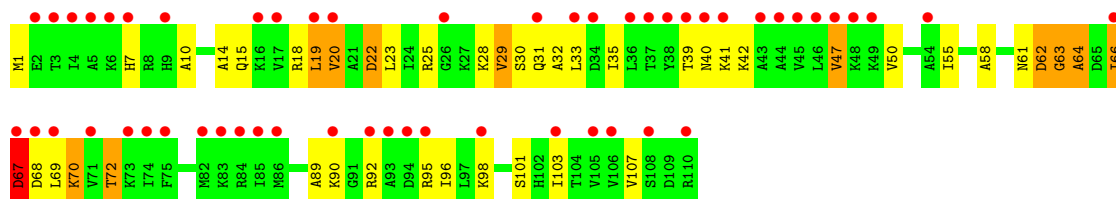
• Molecule 40: 50S ribosomal protein L22

Chain BS: 59% 30% 11%



• Molecule 40: 50S ribosomal protein L22

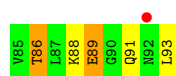
Chain DS: 48% 59% 30% 10%



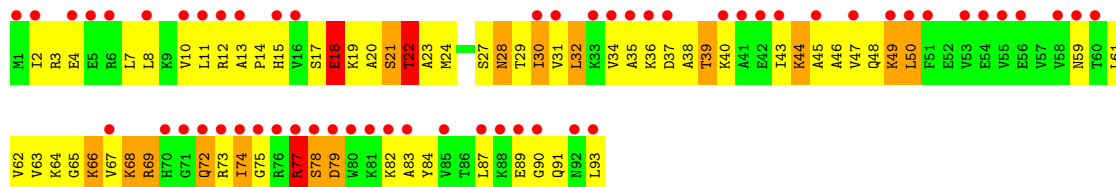
• Molecule 41: 50S ribosomal protein L23

Chain BT: 3% 49% 39% 11%

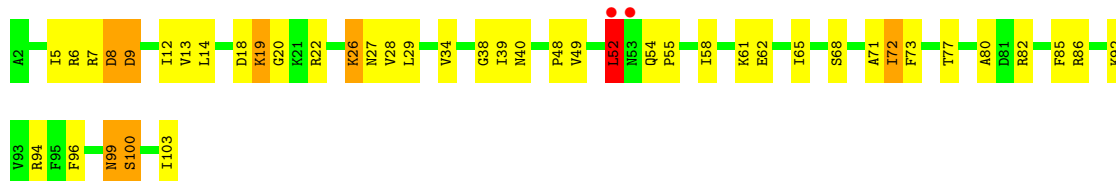




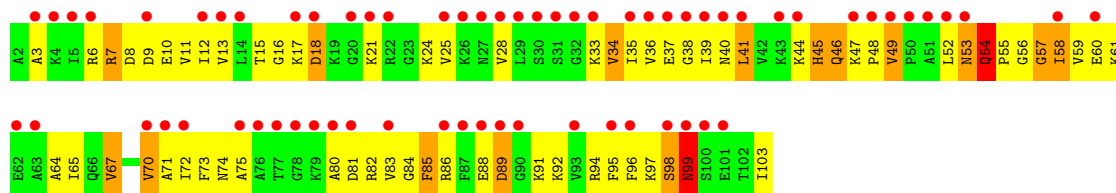
• Molecule 41: 50S ribosomal protein L23



• Molecule 42: 50S ribosomal protein L24



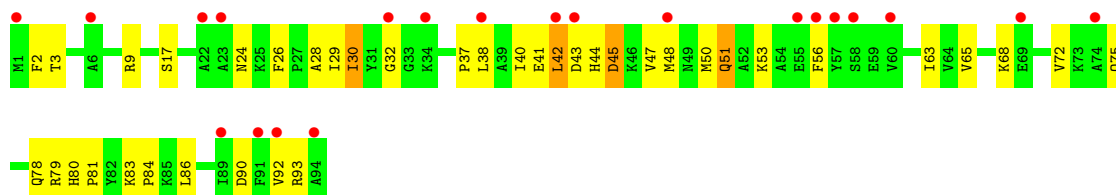
• Molecule 42: 50S ribosomal protein L24



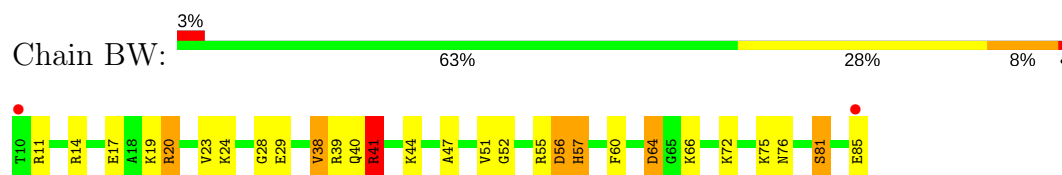
• Molecule 43: 50S ribosomal protein L25



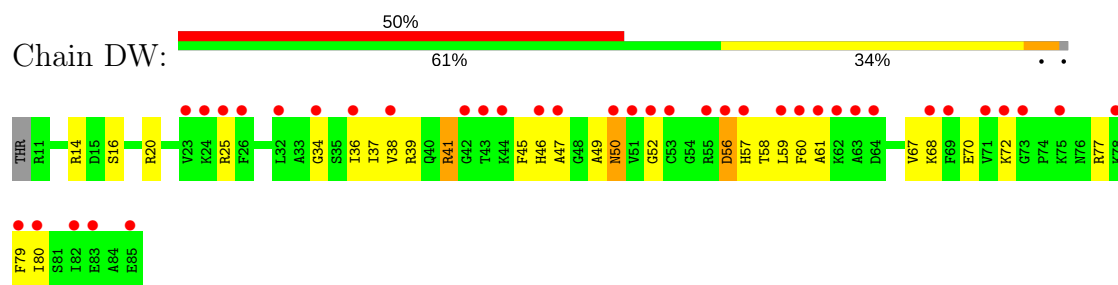
• Molecule 43: 50S ribosomal protein L25



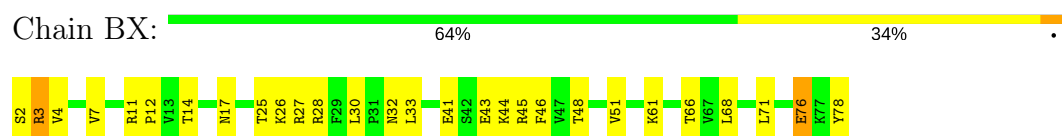
- Molecule 44: 50S ribosomal protein L27



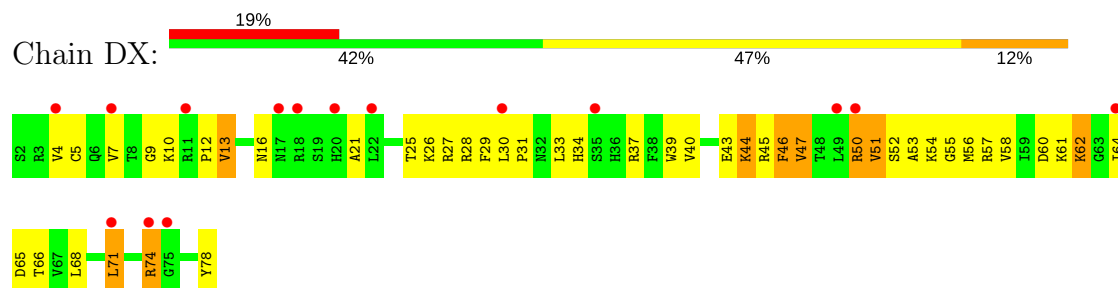
- Molecule 44: 50S ribosomal protein L27



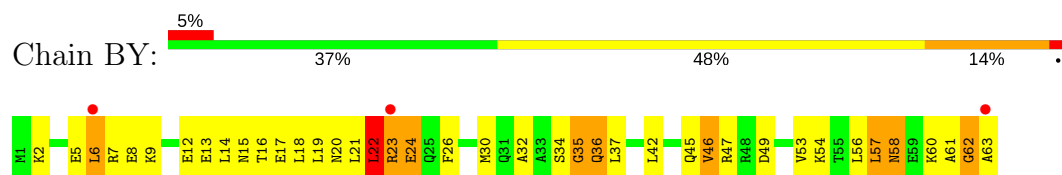
- Molecule 45: 50S ribosomal protein L28



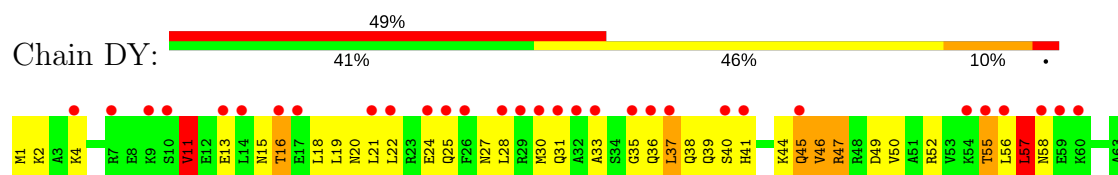
- Molecule 45: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29



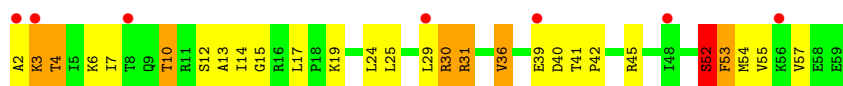
- Molecule 47: 50S ribosomal protein L30

Chain BZ:  69% 29% .



- Molecule 47: 50S ribosomal protein L30

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



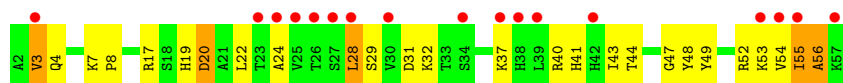
- Molecule 48: 50S ribosomal protein L32

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% .

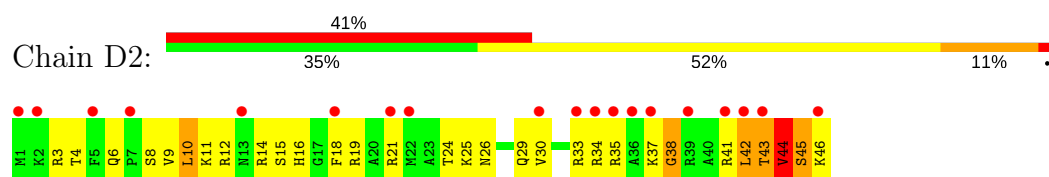


- Molecule 50: 50S ribosomal protein L34

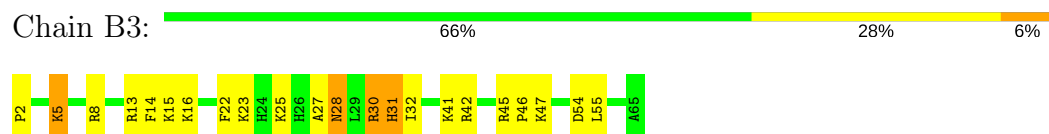
Chain B2:  2% 70% 26% .



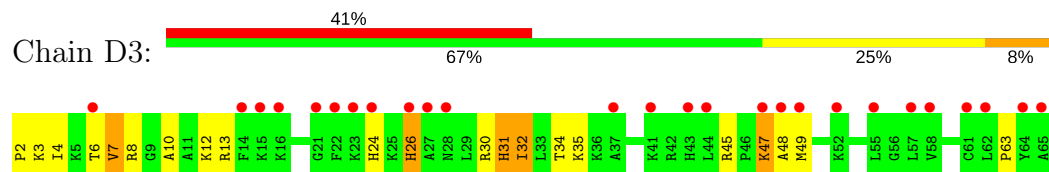
- Molecule 50: 50S ribosomal protein L34



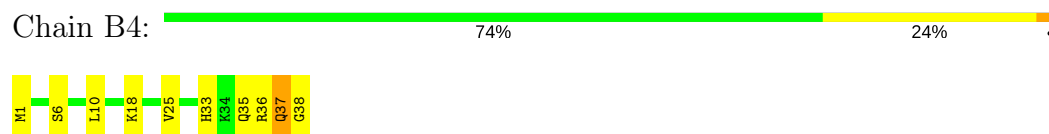
- Molecule 51: 50S ribosomal protein L35



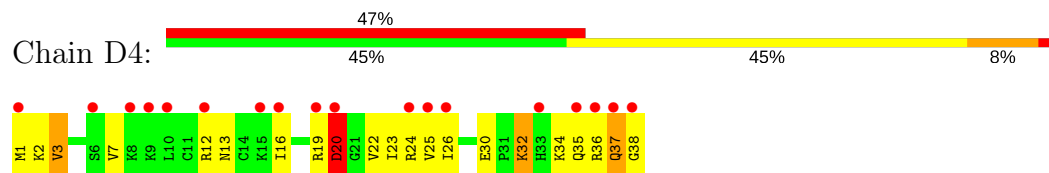
- Molecule 51: 50S ribosomal protein L35



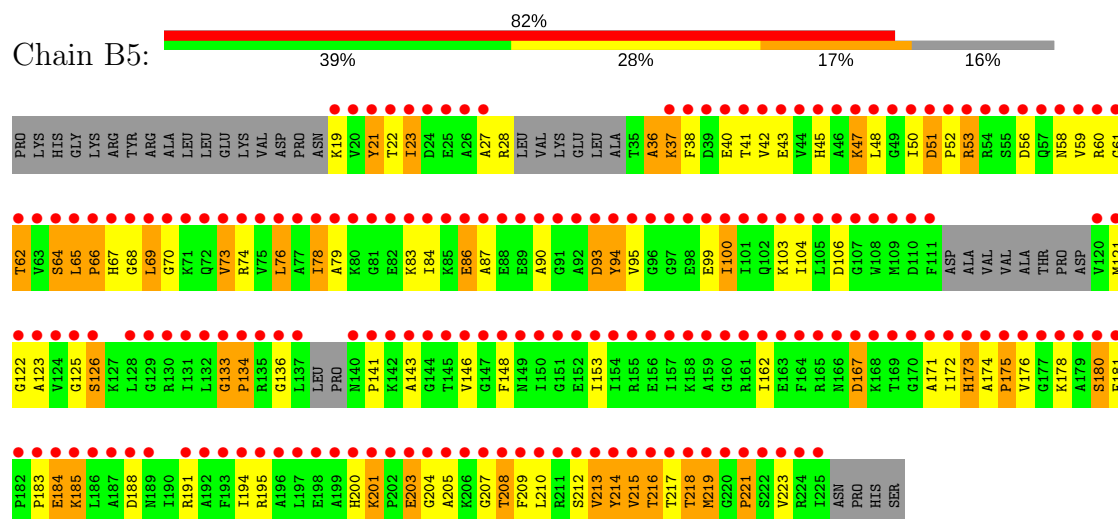
- Molecule 52: 50S ribosomal protein L36



- 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
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288423	wwPDB-VP
Average B, all atoms (Å 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	126 (58%)	45 (21%)	45 (21%)	0	0
2	CB	216/218 (99%)	140 (65%)	51 (24%)	25 (12%)	0	1
3	AC	204/206 (99%)	148 (72%)	35 (17%)	21 (10%)	0	1
3	CC	204/206 (99%)	154 (76%)	39 (19%)	11 (5%)	2	6
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	6
8	AH	127/129 (98%)	90 (71%)	28 (22%)	9 (7%)	1	3

Continued on next page...

Continued from previous page...

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	1
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	1
17	CQ	78/80 (98%)	56 (72%)	15 (19%)	7 (9%)	1	1
18	AR	53/55 (96%)	42 (79%)	11 (21%)	0	100	100
18	CR	53/55 (96%)	37 (70%)	12 (23%)	4 (8%)	1	2
19	AS	77/79 (98%)	57 (74%)	11 (14%)	9 (12%)	0	1
19	CS	77/79 (98%)	55 (71%)	11 (14%)	11 (14%)	0	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	9
24	DC	269/271 (99%)	196 (73%)	48 (18%)	25 (9%)	1	1
25	BD	207/209 (99%)	180 (87%)	21 (10%)	6 (3%)	5	18
25	DD	207/209 (99%)	153 (74%)	43 (21%)	11 (5%)	2	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BE	199/201 (99%)	165 (83%)	30 (15%)	4 (2%)	9	28
26	DE	199/201 (99%)	154 (77%)	27 (14%)	18 (9%)	1	1
27	BF	175/177 (99%)	142 (81%)	24 (14%)	9 (5%)	2	7
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	5
28	DG	174/176 (99%)	127 (73%)	36 (21%)	11 (6%)	1	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%)	25	59
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	2
32	DK	120/122 (98%)	95 (79%)	15 (12%)	10 (8%)	1	2
33	BL	141/143 (99%)	112 (79%)	21 (15%)	8 (6%)	2	5
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	26
34	DM	134/136 (98%)	112 (84%)	17 (13%)	5 (4%)	4	13
35	BN	118/120 (98%)	95 (80%)	21 (18%)	2 (2%)	11	34
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	14
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	9
37	DP	112/114 (98%)	88 (79%)	18 (16%)	6 (5%)	2	6
38	BQ	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	20	52
38	DQ	115/117 (98%)	92 (80%)	22 (19%)	1 (1%)	20	52
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	13
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	DT	91/93 (98%)	53 (58%)	28 (31%)	10 (11%)	0	1
42	BU	100/102 (98%)	77 (77%)	19 (19%)	4 (4%)	3	11
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	47
43	DV	92/94 (98%)	76 (83%)	14 (15%)	2 (2%)	8	26
44	BW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	6	20
44	DW	73/76 (96%)	61 (84%)	12 (16%)	0	100	100
45	BX	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	14	41
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	9
50	D2	44/46 (96%)	34 (77%)	6 (14%)	4 (9%)	1	1
51	B3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	11	36
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	19
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

Continued on next page...

Continued from previous page...

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	9
4	AD	172/172 (100%)	139 (81%)	33 (19%)	1	5
4	CD	172/172 (100%)	143 (83%)	29 (17%)	2	7
5	AE	113/113 (100%)	84 (74%)	29 (26%)	0	1
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	5
7	CG	124/124 (100%)	99 (80%)	25 (20%)	1	4
8	AH	104/104 (100%)	84 (81%)	20 (19%)	1	5
8	CH	104/104 (100%)	82 (79%)	22 (21%)	1	3
9	AI	105/105 (100%)	77 (73%)	28 (27%)	0	1
9	CI	105/105 (100%)	88 (84%)	17 (16%)	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	3
12	AL	103/103 (100%)	89 (86%)	14 (14%)	4	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	103/103 (100%)	82 (80%)	21 (20%)	1	4
13	AM	92/92 (100%)	74 (80%)	18 (20%)	1	4
13	CM	92/92 (100%)	75 (82%)	17 (18%)	2	5
14	AN	79/83 (95%)	64 (81%)	15 (19%)	2	5
14	CN	79/83 (95%)	70 (89%)	9 (11%)	7	20
15	AO	75/76 (99%)	63 (84%)	12 (16%)	3	8
15	CO	75/76 (99%)	65 (87%)	10 (13%)	4	13
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	2
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%)	5	17
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%)	5	16
24	DC	216/216 (100%)	197 (91%)	19 (9%)	12	33
25	BD	164/164 (100%)	148 (90%)	16 (10%)	9	27
25	DD	164/164 (100%)	145 (88%)	19 (12%)	6	19
26	BE	165/165 (100%)	136 (82%)	29 (18%)	2	6
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	4
28	BG	137/137 (100%)	118 (86%)	19 (14%)	4	12
28	DG	137/137 (100%)	114 (83%)	23 (17%)	2	7
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	3
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	3

Continued on next page...

Continued from previous page...

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%)	10	28
31	DJ	116/116 (100%)	94 (81%)	22 (19%)	2	5
32	BK	103/103 (100%)	89 (86%)	14 (14%)	4	13
32	DK	103/103 (100%)	90 (87%)	13 (13%)	5	16
33	BL	102/102 (100%)	91 (89%)	11 (11%)	7	22
33	DL	102/102 (100%)	86 (84%)	16 (16%)	3	9
34	BM	109/109 (100%)	99 (91%)	10 (9%)	11	30
34	DM	109/109 (100%)	95 (87%)	14 (13%)	5	15
35	BN	100/100 (100%)	94 (94%)	6 (6%)	22	54
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	5
37	BP	99/99 (100%)	81 (82%)	18 (18%)	2	6
37	DP	99/99 (100%)	90 (91%)	9 (9%)	11	31
38	BQ	89/89 (100%)	78 (88%)	11 (12%)	5	16
38	DQ	89/89 (100%)	78 (88%)	11 (12%)	5	16
39	BR	84/84 (100%)	74 (88%)	10 (12%)	6	18
39	DR	84/84 (100%)	76 (90%)	8 (10%)	10	28
40	BS	93/93 (100%)	76 (82%)	17 (18%)	2	6
40	DS	93/93 (100%)	83 (89%)	10 (11%)	7	22
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	10
41	DT	80/80 (100%)	66 (82%)	14 (18%)	2	6
42	BU	83/83 (100%)	72 (87%)	11 (13%)	4	13
42	DU	83/83 (100%)	68 (82%)	15 (18%)	2	6
43	BV	78/78 (100%)	63 (81%)	15 (19%)	1	5
43	DV	78/78 (100%)	65 (83%)	13 (17%)	2	7
44	BW	57/58 (98%)	47 (82%)	10 (18%)	2	6
44	DW	56/58 (97%)	50 (89%)	6 (11%)	8	22
45	BX	67/67 (100%)	61 (91%)	6 (9%)	11	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DX	67/67 (100%)	58 (87%)	9 (13%)	4	13
46	BY	55/55 (100%)	50 (91%)	5 (9%)	11	31
46	DY	55/55 (100%)	43 (78%)	12 (22%)	1	3
47	BZ	48/48 (100%)	41 (85%)	7 (15%)	3	11
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	4
48	B0	47/47 (100%)	42 (89%)	5 (11%)	8	23
48	D0	47/47 (100%)	43 (92%)	4 (8%)	12	35
49	B1	45/45 (100%)	42 (93%)	3 (7%)	19	48
49	D1	45/45 (100%)	39 (87%)	6 (13%)	4	13
50	B2	38/38 (100%)	34 (90%)	4 (10%)	8	23
50	D2	38/38 (100%)	31 (82%)	7 (18%)	2	5
51	B3	51/51 (100%)	45 (88%)	6 (12%)	6	18
51	D3	51/51 (100%)	46 (90%)	5 (10%)	9	27
52	B4	34/34 (100%)	32 (94%)	2 (6%)	23	54
52	D4	34/34 (100%)	26 (76%)	8 (24%)	1	2
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1	3
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7747 (82%)	1643 (18%)	2	6

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

Mol	Chain	Res	Type
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

Continued on next page...

Continued from previous page...

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%)	0
1	CA	1538/1539 (99%)	342 (22%)	0
22	BA	2895/2903 (99%)	579 (20%)	0
22	DA	2895/2903 (99%)	704 (24%)	0
23	BB	118/119 (99%)	16 (13%)	0
23	DB	117/119 (98%)	20 (17%)	0
All	All	9100/9122 (99%)	1985 (21%)	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

There are no RNA pucker outliers to report.

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	1.52	1 (11%)	9,11,13	2.92	4 (44%)
54	DBB	B6	3	54	5,5,6	1.17	0	3,5,7	1.98	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	MHU	B6	5	54	15,15,16	1.82	4 (26%)	18,19,21	1.17	2 (11%)
54	MHV	B6	6	54	9,9,10	1.54	1 (11%)	9,11,13	3.23	4 (44%)
54	004	B6	7	54	8,10,11	1.53	1 (12%)	11,12,14	2.44	5 (45%)
54	MHW	D6	1	54	9,9,10	1.77	1 (11%)	9,11,13	3.17	3 (33%)
54	DBB	D6	3	54	5,5,6	1.05	0	3,5,7	1.78	1 (33%)
54	MHU	D6	5	54	15,15,16	1.65	4 (26%)	18,19,21	1.34	3 (16%)
54	MHV	D6	6	54	9,9,10	1.12	0	9,11,13	3.04	4 (44%)
54	004	D6	7	54	8,10,11	0.79	0	11,12,14	1.28	1 (9%)

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 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-4.05	1.48	1.52
54	B6	6	MHV	CB-CG	-2.84	1.45	1.50
54	B6	5	MHU	CA-C	-2.33	1.47	1.50
54	D6	5	MHU	CA-C	-2.03	1.47	1.50
54	D6	5	MHU	CD2-CE2	2.04	1.42	1.38

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	MHV	CD2-CE-N	-5.21	98.62	109.91
54	D6	1	MHW	CG2-CD-CE	-4.87	111.66	118.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B6	6	MHV	CD2-CE-N	-4.78	99.55	109.91
54	D6	1	MHW	O-C-CA	-4.62	120.32	124.32
54	B6	1	MHW	O-C-CA	-4.51	120.42	124.32

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	3.35	14 (32%)	54,70,70	3.15	16 (29%)
56	DOL	DA	3001	-	43,50,50	3.32	13 (30%)	54,70,70	3.11	12 (22%)

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 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BA	3001	DOL	C1-C2	-8.95	1.43	1.55
56	DA	3001	DOL	C1-C2	-7.77	1.45	1.55
56	BA	3001	DOL	O36-C32	-3.53	1.39	1.44
56	BA	3001	DOL	C16-C17	-3.39	1.49	1.54
56	DA	3001	DOL	C16-C17	-3.32	1.49	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DA	3001	DOL	O40-S39-O41	-18.89	100.57	117.94
56	BA	3001	DOL	O40-S39-O41	-17.92	101.47	117.94
56	BA	3001	DOL	C29-C28-C26	-5.73	107.93	122.90
56	DA	3001	DOL	C4-N5-C1	-5.53	106.22	112.33
56	BA	3001	DOL	C23-C22-C20	-4.62	118.91	125.89

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%)	-0.15	23 (1%) 74 67	10, 49, 132, 182	0
1	CA	1539/1539 (100%)	0.16	56 (3%) 43 32	22, 70, 146, 178	0
2	AB	218/218 (100%)	0.80	29 (13%) 4 2	36, 73, 100, 117	0
2	CB	218/218 (100%)	1.04	45 (20%) 1 1	57, 86, 108, 121	0
3	AC	206/206 (100%)	0.15	9 (4%) 35 25	33, 57, 78, 95	0
3	CC	206/206 (100%)	1.18	50 (24%) 1 1	55, 80, 96, 107	0
4	AD	205/205 (100%)	0.36	8 (3%) 40 29	31, 56, 79, 99	0
4	CD	205/205 (100%)	-0.03	5 (2%) 59 49	13, 35, 60, 82	0
5	AE	150/150 (100%)	0.10	2 (1%) 77 71	26, 47, 78, 93	0
5	CE	150/150 (100%)	0.18	1 (0%) 87 83	25, 52, 84, 104	0
6	AF	100/100 (100%)	-0.17	1 (1%) 82 77	32, 54, 73, 77	0
6	CF	100/100 (100%)	0.53	10 (10%) 8 4	41, 74, 92, 103	0
7	AG	151/151 (100%)	0.25	3 (1%) 65 56	51, 75, 92, 100	0
7	CG	151/151 (100%)	2.55	83 (54%) 0 0	82, 106, 114, 118	0
8	AH	129/129 (100%)	0.18	2 (1%) 72 65	29, 46, 67, 79	0
8	CH	129/129 (100%)	0.45	10 (7%) 14 7	46, 64, 80, 94	0
9	AI	127/127 (100%)	0.93	22 (17%) 2 1	40, 74, 98, 107	0
9	CI	127/127 (100%)	1.84	45 (35%) 0 0	79, 96, 112, 121	0
10	AJ	98/98 (100%)	0.63	8 (8%) 12 6	38, 66, 86, 116	0
10	CJ	98/98 (100%)	2.70	59 (60%) 0 0	72, 97, 115, 123	0
11	AK	117/117 (100%)	0.48	10 (8%) 11 6	25, 61, 89, 119	0
11	CK	117/117 (100%)	0.23	2 (1%) 70 63	35, 68, 79, 90	0
12	AL	123/123 (100%)	0.15	6 (4%) 30 20	20, 34, 65, 97	0
12	CL	123/123 (100%)	0.32	3 (2%) 59 49	30, 50, 74, 95	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.41	10 (8%) 11 5	47, 69, 91, 103	0
13	CM	114/114 (100%)	3.13	76 (66%) 0 0	93, 113, 122, 125	0
14	AN	96/100 (96%)	0.67	11 (11%) 5 3	36, 60, 96, 105	0
14	CN	96/100 (96%)	2.15	43 (44%) 0 0	70, 96, 115, 122	0
15	AO	88/88 (100%)	0.35	3 (3%) 46 34	29, 47, 64, 91	0
15	CO	88/88 (100%)	0.33	3 (3%) 46 34	36, 64, 80, 102	0
16	AP	82/82 (100%)	0.69	6 (7%) 16 8	34, 47, 83, 109	0
16	CP	82/82 (100%)	0.97	11 (13%) 4 2	45, 62, 91, 112	0
17	AQ	80/80 (100%)	0.26	3 (3%) 41 30	27, 48, 75, 111	0
17	CQ	80/80 (100%)	1.15	19 (23%) 1 1	42, 77, 97, 99	0
18	AR	55/55 (100%)	0.21	3 (5%) 26 17	40, 52, 77, 102	0
18	CR	55/55 (100%)	0.28	4 (7%) 16 8	36, 54, 78, 108	0
19	AS	79/79 (100%)	0.70	13 (16%) 2 1	54, 70, 88, 97	0
19	CS	79/79 (100%)	3.94	58 (73%) 0 0	95, 114, 122, 128	0
20	AT	85/85 (100%)	0.42	4 (4%) 32 22	35, 48, 68, 96	0
20	CT	85/85 (100%)	1.81	33 (38%) 0 0	53, 78, 96, 101	0
21	AU	51/51 (100%)	1.26	12 (23%) 1 1	41, 74, 95, 105	0
21	CU	51/51 (100%)	0.68	6 (11%) 5 3	42, 69, 98, 102	0
22	BA	2897/2903 (99%)	0.14	107 (3%) 42 31	0, 14, 129, 195	0
22	DA	2897/2903 (99%)	0.40	130 (4%) 34 24	41, 85, 148, 181	0
23	BB	119/119 (100%)	-0.36	0 100 100	2, 23, 46, 81	0
23	DB	118/119 (99%)	0.19	4 (3%) 46 34	69, 115, 134, 142	0
24	BC	271/271 (100%)	-0.18	1 (0%) 92 90	2, 18, 35, 55	0
24	DC	271/271 (100%)	0.73	31 (11%) 6 3	46, 64, 77, 95	0
25	BD	209/209 (100%)	-0.25	0 100 100	0, 9, 34, 65	0
25	DD	209/209 (100%)	1.17	44 (21%) 1 1	53, 72, 87, 97	0
26	BE	201/201 (100%)	-0.30	0 100 100	1, 23, 54, 88	0
26	DE	201/201 (100%)	1.86	80 (39%) 0 0	52, 89, 105, 113	0
27	BF	177/177 (100%)	0.18	4 (2%) 61 51	21, 40, 74, 88	0
27	DF	177/177 (100%)	3.26	128 (72%) 0 0	94, 113, 124, 131	0
28	BG	176/176 (100%)	0.04	3 (1%) 70 63	15, 35, 58, 72	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	2.22	89 (50%) 0 0	78, 96, 110, 121	0
29	BH	149/149 (100%)	3.02	72 (48%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.18	30 (20%) 1 1	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.57	100 (70%) 0 0	89, 116, 126, 134	0
30	DI	141/141 (100%)	4.83	121 (85%) 0 0	105, 124, 135, 142	0
31	BJ	142/142 (100%)	-0.27	0 100 100	1, 6, 26, 35	0
31	DJ	142/142 (100%)	0.83	16 (11%) 6 3	49, 69, 83, 91	0
32	BK	122/122 (100%)	-0.34	0 100 100	3, 11, 28, 60	0
32	DK	122/122 (100%)	1.12	28 (22%) 1 1	48, 66, 84, 95	0
33	BL	143/143 (100%)	-0.13	0 100 100	1, 18, 42, 65	0
33	DL	143/143 (100%)	1.94	60 (41%) 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%)	1.01	26 (19%) 1 1	44, 70, 85, 99	0
35	BN	120/120 (100%)	-0.24	0 100 100	2, 7, 17, 65	0
35	DN	120/120 (100%)	1.29	28 (23%) 1 1	58, 78, 92, 112	0
36	BO	116/116 (100%)	-0.21	0 100 100	14, 24, 42, 54	0
36	DO	116/116 (100%)	2.77	75 (64%) 0 0	85, 99, 110, 117	0
37	BP	114/114 (100%)	-0.22	1 (0%) 84 79	6, 16, 41, 71	0
37	DP	114/114 (100%)	1.07	26 (22%) 1 1	61, 74, 86, 94	0
38	BQ	117/117 (100%)	-0.31	0 100 100	0, 3, 12, 30	0
38	DQ	117/117 (100%)	1.14	25 (21%) 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%)	1.67	34 (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%)	2.11	53 (48%) 0 0	60, 79, 94, 105	0
41	BT	93/93 (100%)	0.19	3 (3%) 48 37	10, 24, 68, 99	0
41	DT	93/93 (100%)	2.70	57 (61%) 0 0	73, 91, 106, 115	0
42	BU	102/102 (100%)	-0.22	2 (1%) 65 56	10, 25, 58, 77	0
42	DU	102/102 (100%)	3.21	65 (63%) 0 0	77, 95, 109, 120	0
43	BV	94/94 (100%)	-0.27	0 100 100	4, 18, 39, 52	0
43	DV	94/94 (100%)	1.13	21 (22%) 1 1	72, 86, 98, 105	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.15	2 (2%) 56 45	4, 11, 27, 57	0
44	DW	75/76 (98%)	2.03	38 (50%) 0 0	58, 83, 93, 104	0
45	BX	77/77 (100%)	-0.24	0 100 100	8, 22, 48, 68	0
45	DX	77/77 (100%)	1.11	15 (19%) 1 1	47, 72, 87, 91	0
46	BY	63/63 (100%)	0.23	3 (4%) 31 21	18, 38, 71, 94	0
46	DY	63/63 (100%)	1.95	31 (49%) 0 0	81, 99, 106, 109	0
47	BZ	58/58 (100%)	-0.22	0 100 100	2, 6, 25, 34	0
47	DZ	58/58 (100%)	0.83	7 (12%) 5 2	60, 73, 85, 103	0
48	B0	56/56 (100%)	-0.30	0 100 100	0, 7, 33, 60	0
48	D0	56/56 (100%)	1.48	17 (30%) 0 0	51, 82, 95, 103	0
49	B1	50/50 (100%)	-0.23	1 (2%) 65 56	13, 25, 49, 57	0
49	D1	50/50 (100%)	1.74	16 (32%) 0 0	73, 89, 94, 106	0
50	B2	46/46 (100%)	-0.14	1 (2%) 62 52	4, 8, 15, 79	0
50	D2	46/46 (100%)	1.93	19 (41%) 0 0	58, 72, 86, 101	0
51	B3	64/64 (100%)	-0.18	0 100 100	4, 9, 17, 29	0
51	D3	64/64 (100%)	1.70	26 (40%) 0 0	60, 75, 84, 94	0
52	B4	38/38 (100%)	-0.13	0 100 100	5, 15, 29, 52	0
52	D4	38/38 (100%)	2.24	18 (47%) 0 0	62, 77, 88, 98	0
53	B5	191/228 (83%)	6.24	186 (97%) 0 0	100, 121, 133, 141	0
54	B6	2/8 (25%)	0.46	0 100 100	1, 1, 1, 1	0
54	D6	2/8 (25%)	-0.03	0 100 100	46, 46, 46, 51	0
All	All	20738/20810 (99%)	0.62	2654 (12%) 4 2	0, 63, 124, 195	0

The worst 5 of 2654 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	25.2
53	B5	55	SER	19.9
22	BA	2184	A	17.4
22	BA	2101	A	17.3
22	BA	2185	U	16.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	DA	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.