



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 2, 2020 – 07:12 am BST

PDB ID : 4WF1  
Title : Crystal structure of the E. coli ribosome bound to negamycin.  
Authors : Olivier, N.B.; Altman, R.B.; Noeske, J.; Basarab, G.S.; Code, E.; Ferguson, A.D.; Gao, N.; Huang, J.; Juetten, M.F.; Livchak, S.; Miller, M.D.; Prince, D.B.; Cate, J.H.D.; Buurman, E.T.; Blanchard, S.C.  
Deposited on : 2014-09-11  
Resolution : 3.09 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

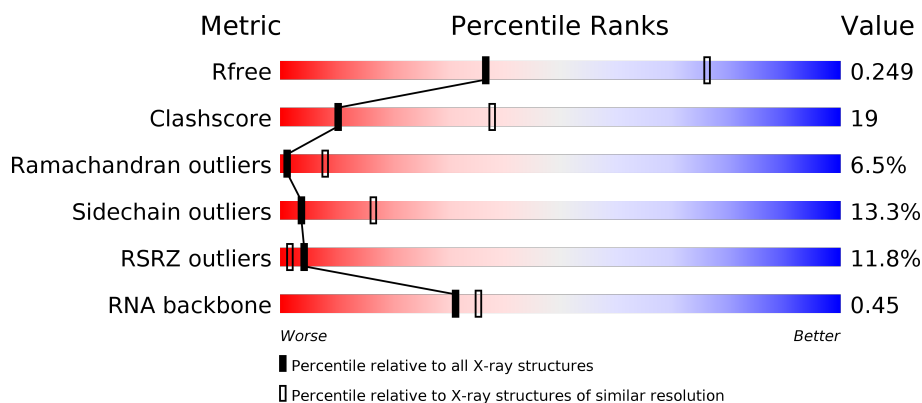
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.09 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1539	<div> <div>4%</div> <div>35% 49% 15%</div> </div>
1	CA	1539	<div> <div>9%</div> <div>35% 51% 13%</div> </div>
2	AB	218	<div> <div>6%</div> <div>31% 51% 16%</div> </div>
2	CB	218	<div> <div>11%</div> <div>36% 45% 16%</div> </div>

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




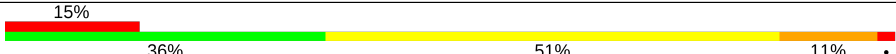
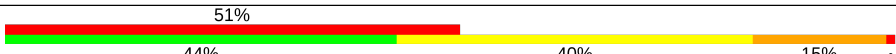

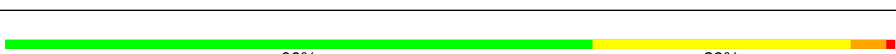
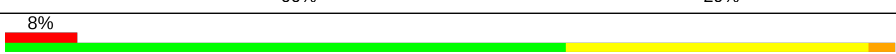

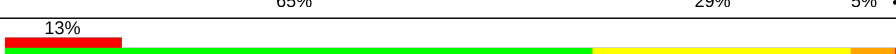

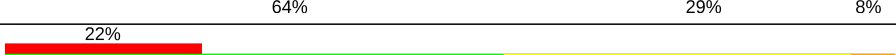
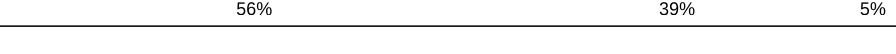
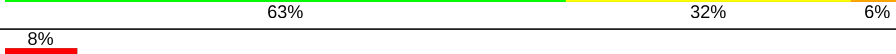











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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD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

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

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

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Mol	Chain	Length	Quality of chain
53	B5	207	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	1614	-	-	-	X
54	MG	AA	1617	-	-	-	X
54	MG	AA	1644	-	-	-	X
54	MG	AA	1646	-	-	-	X
54	MG	AA	1649	-	-	-	X
54	MG	AA	1657	-	-	-	X
54	MG	AA	1658	-	-	-	X
54	MG	AA	1659	-	-	-	X
54	MG	AA	1662	-	-	-	X
54	MG	AA	1669	-	-	-	X
54	MG	AA	1670	-	-	-	X
54	MG	AA	1671	-	-	-	X
54	MG	AM	201	-	-	-	X
54	MG	BA	3040	-	-	-	X
54	MG	BA	3060	-	-	-	X
54	MG	BA	3133	-	-	-	X
54	MG	BA	3161	-	-	-	X
54	MG	BA	3167	-	-	-	X
54	MG	BA	3168	-	-	-	X
54	MG	BA	3176	-	-	-	X
54	MG	BA	3179	-	-	-	X
54	MG	CA	1626	-	-	-	X
54	MG	CA	1629	-	-	-	X
54	MG	CA	1634	-	-	-	X
54	MG	CA	1644	-	-	-	X
54	MG	CA	1648	-	-	-	X
54	MG	CA	1650	-	-	-	X
54	MG	CA	1651	-	-	-	X
54	MG	CA	1654	-	-	-	X
54	MG	DA	3004	-	-	-	X
54	MG	DA	3025	-	-	-	X
54	MG	DA	3040	-	-	-	X
54	MG	DA	3055	-	-	-	X
54	MG	DA	3056	-	-	-	X
54	MG	DA	3057	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3060	-	-	-	X
54	MG	DA	3061	-	-	-	X
54	MG	DA	3076	-	-	-	X
54	MG	DA	3084	-	-	-	X
54	MG	DA	3091	-	-	-	X
54	MG	DA	3092	-	-	-	X
54	MG	DA	3114	-	-	-	X
54	MG	DA	3118	-	-	-	X
54	MG	DA	3130	-	-	-	X
54	MG	DA	3132	-	-	-	X
54	MG	DA	3135	-	-	-	X
54	MG	DA	3136	-	-	-	X
54	MG	DA	3140	-	-	-	X
54	MG	DA	3145	-	-	-	X
54	MG	DA	3153	-	-	-	X
54	MG	DA	3155	-	-	-	X
54	MG	DA	3159	-	-	-	X
54	MG	DA	3162	-	-	-	X
54	MG	DA	3164	-	-	-	X
54	MG	DL	201	-	-	-	X



## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288204 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

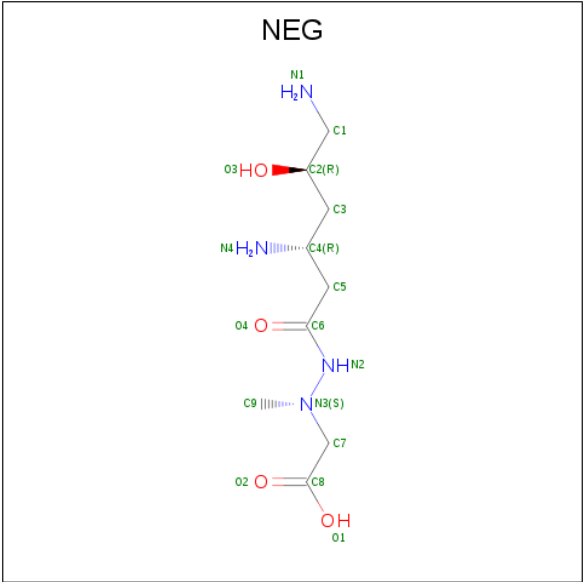
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	4	Total	Mg	0	0
			4	4		
54	DQ	1	Total	Mg	0	0
			1	1		
54	BA	194	Total	Mg	0	0
			194	194		
54	CA	56	Total	Mg	0	0
			56	56		
54	CT	1	Total	Mg	0	0
			1	1		
54	DL	2	Total	Mg	0	0
			2	2		
54	D2	1	Total	Mg	0	0
			1	1		
54	AA	71	Total	Mg	0	0
			71	71		
54	BQ	1	Total	Mg	0	0
			1	1		
54	DA	164	Total	Mg	0	0
			164	164		
54	DB	3	Total	Mg	0	0
			3	3		
54	AM	1	Total	Mg	0	0
			1	1		

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 56 is NEGAMYCIN (three-letter code: NEG) (formula: C<sub>9</sub>H<sub>20</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	CA	1	Total	C	N	O	0	0
			17	9	4	4		

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	196	Total	O	0	0
			196	196		
57	AE	1	Total	O	0	0
			1	1		
57	AL	1	Total	O	0	0
			1	1		
57	AN	3	Total	O	0	0
			3	3		
57	AT	1	Total	O	0	0
			1	1		
57	AU	1	Total	O	0	0
			1	1		
57	BA	620	Total	O	0	0
			620	620		
57	BB	14	Total	O	0	0
			14	14		
57	BC	10	Total	O	0	0
			10	10		
57	BD	4	Total	O	0	0
			4	4		
57	BF	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BG	1	Total 1	O 1	0	0
57	BL	6	Total 6	O 6	0	0
57	BN	3	Total 3	O 3	0	0
57	BS	1	Total 1	O 1	0	0
57	B2	1	Total 1	O 1	0	0
57	B3	3	Total 3	O 3	0	0
57	B4	2	Total 2	O 2	0	0
57	CA	186	Total 186	O 186	0	0
57	CL	1	Total 1	O 1	0	0
57	CN	3	Total 3	O 3	0	0
57	CT	3	Total 3	O 3	0	0
57	CU	1	Total 1	O 1	0	0
57	DA	611	Total 611	O 611	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	8	Total 8	O 8	0	0
57	DD	3	Total 3	O 3	0	0
57	DE	5	Total 5	O 5	0	0
57	DJ	1	Total 1	O 1	0	0
57	DL	4	Total 4	O 4	0	0
57	DN	1	Total 1	O 1	0	0
57	DS	1	Total 1	O 1	0	0

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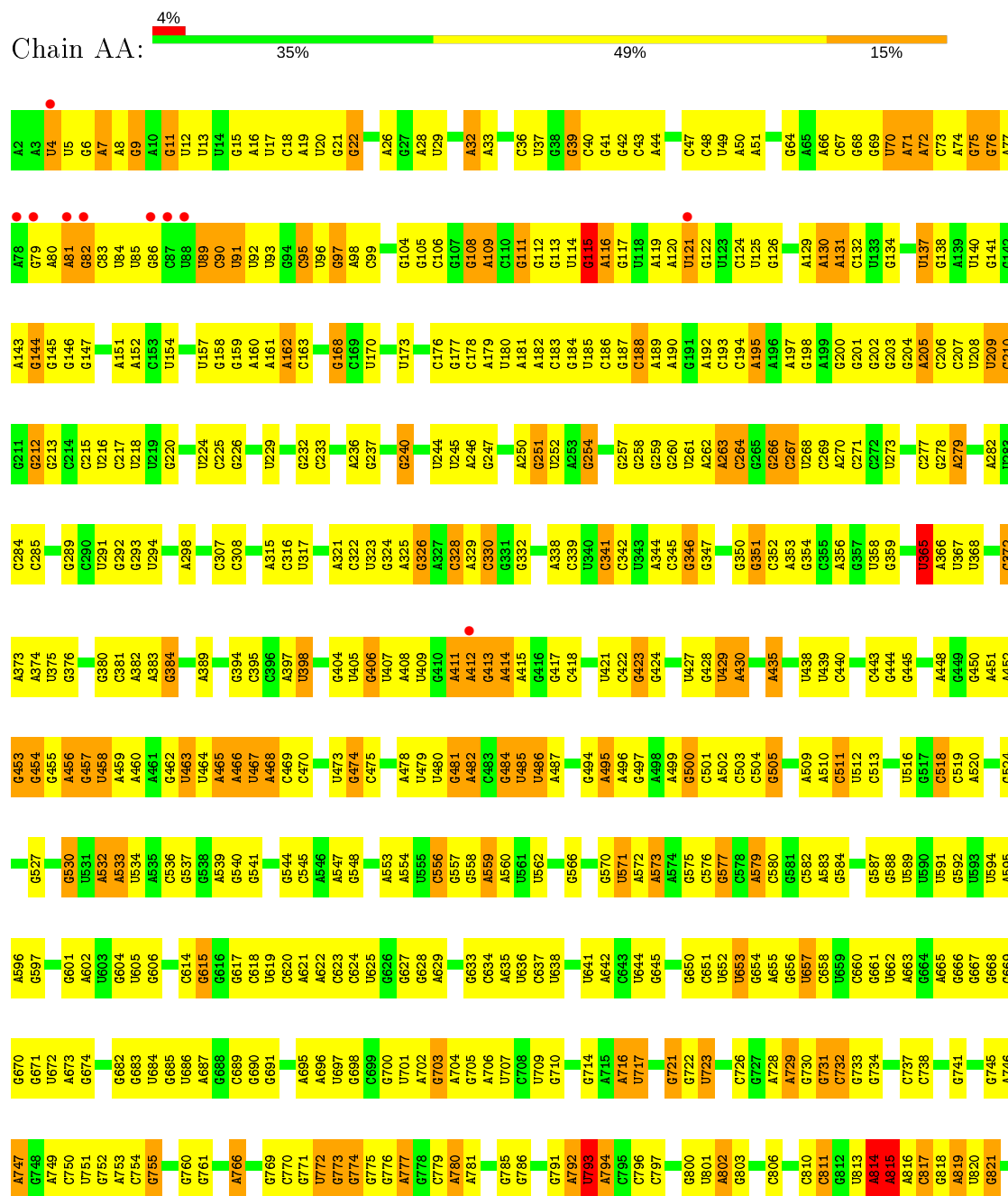
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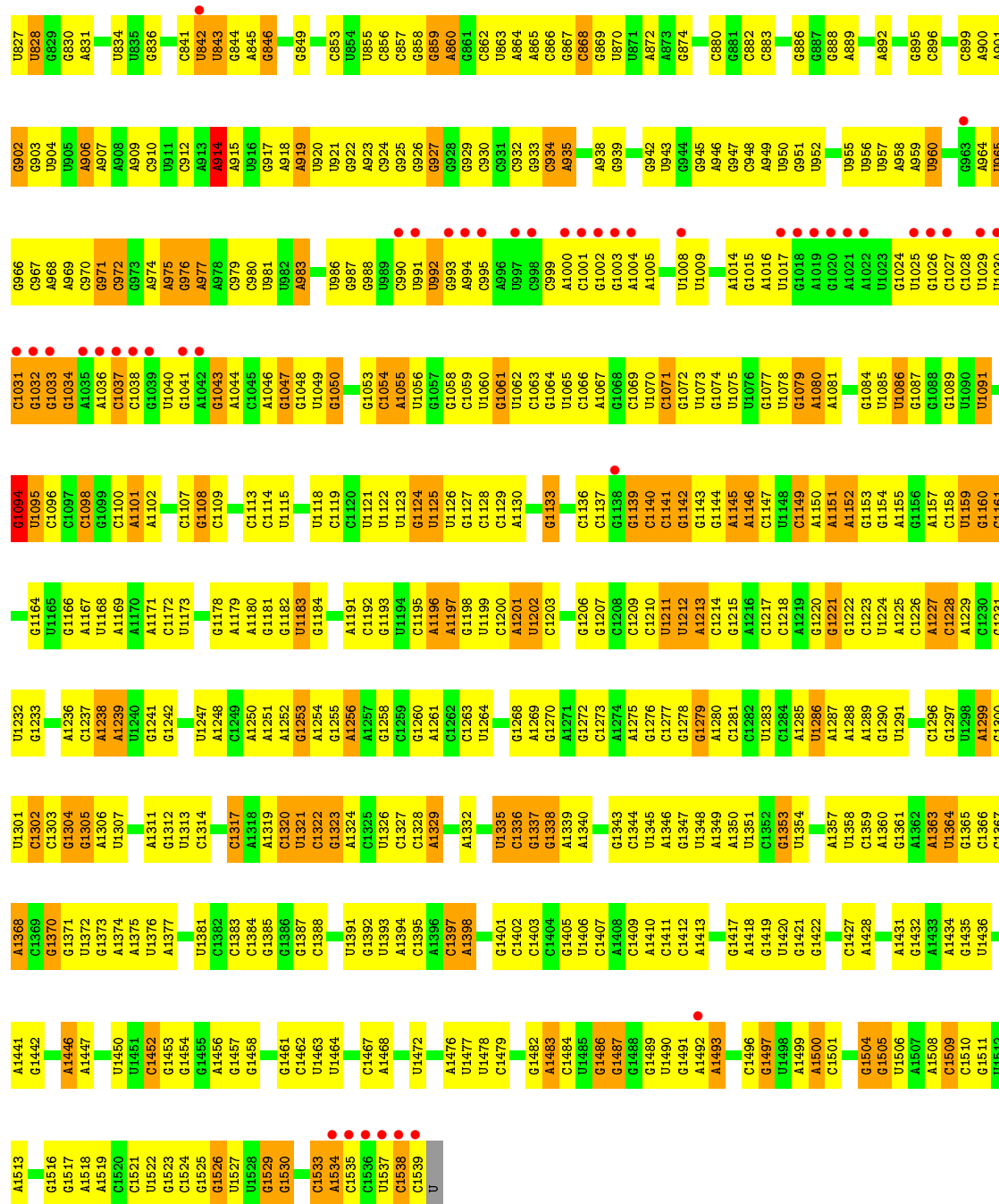
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DT	3	Total 3	O 3	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D3	2	Total 2	O 2	0	0
57	D4	1	Total 1	O 1	0	0

### 3 Residue-property plots [i](#)

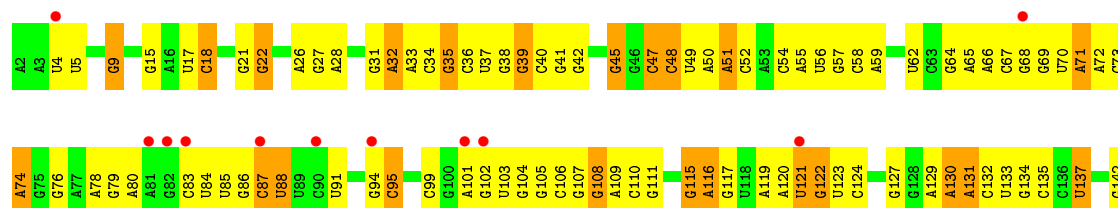
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 16S rRNA



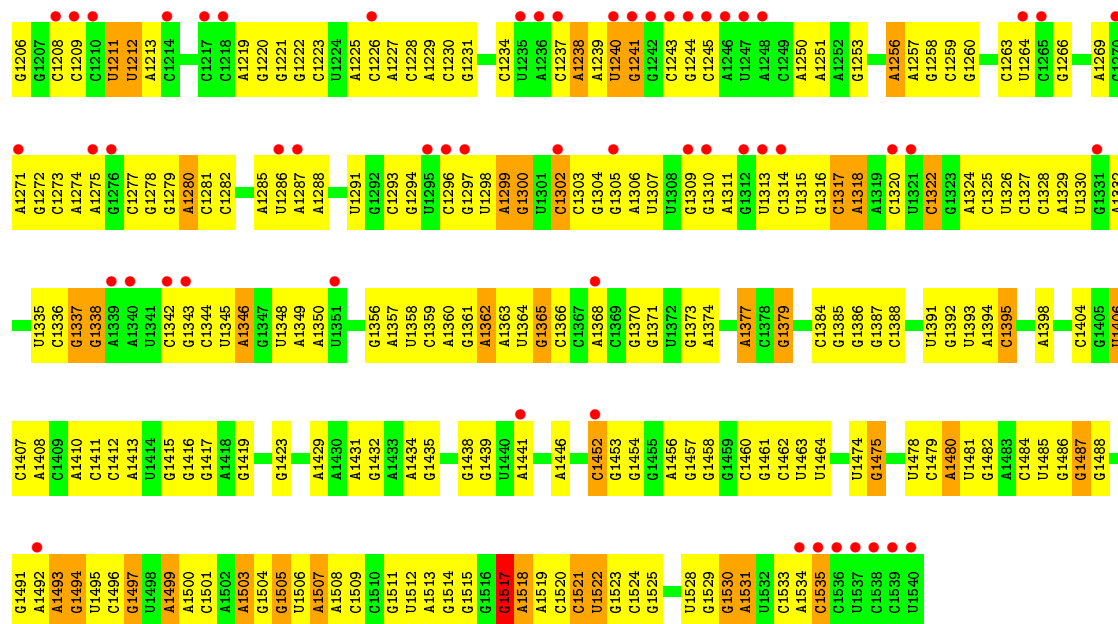


• Molecule 1: 16S rRNA

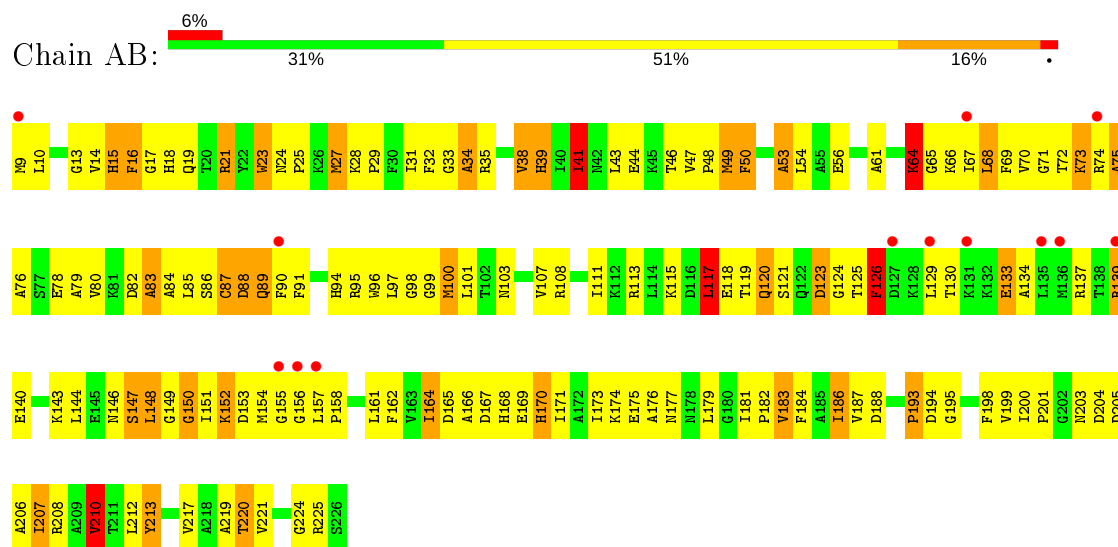




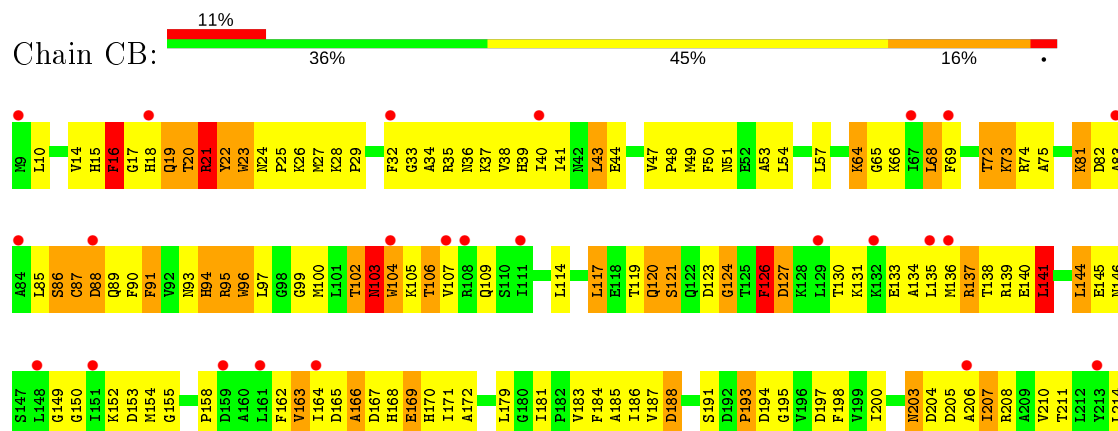
G1138	U1070	A865	G791	A728	A663	G570	G505	C217	A143
G1139	C1071	C866	A792	A729	A663	U571	G506	U218	G144
C1140	G1072	G867	A793	A730	G664	A572	G507	U219	G145
C1141	A1005	C868	A794	G731	A665	A573	A509	G220	G146
G1142	G1073	G869	A795	G732	G666	A574	A510	C295	G147
G1143	U1007	G870	A796	G733	G667	A575	C511	A223	G148
G1144	U1008	U871	A797	G734	G668	C576	U512	U224	A149
A1145	U1009	A872	A798	C735	G669	C577	C513	U296	U150
A1146	U1078	A873	A799	C736	G670	C578	C514	A298	A151
C1147	G1079	G874	A800	C737	G671	A579	A517	G227	A152
U1148	A1080	U875	U801	G738	A672	C580	G517	A228	C153
C1149	A1081	G876	A802	G739	G673	G581	C518	U229	G154
A1150	A1082	C877	A803	U740	G674	G582	C519	G230	U155
A1151	U1083	G878	U804	G741	A675	C583	C520	G302	A156
A1152	G1084	A879	C805	G742	A676	A583	A520	A306	C156
G1153	U1085	C880	C806	G743	U677	C584	G521	C307	U157
G1154	U1086	G881	A807	A747	U678	A585	C522	A436	G158
C1155	G1087	C882	C807	G748	C679	G586	A523	G237	C159
A1156	U1088	U883	C810	A749	G680	U587	C524	U239	A160
C1157	G1089	G884	C811	U750	G681	C588	C525	G240	A161
U1158	U1090	U885	G812	C751	G682	G597	C526	A388	G164
C1159	A1091	G886	A813	U752	U683	U598	C527	A389	G165
G1160	A1092	G887	A814	A753	U684	G604	C528	U390	C166
A1161	A1093	G888	A815	G754	G685	C587	C529	G391	G168
C1162	G1094	G889	A816	C755	U686	G605	U531	A320	C169
A1163	U1095	U891	C817	G756	G687	U606	A532	U444	U171
U1164	C1096	C892	C818	C757	G688	A607	A533	A321	A172
C1165	G1097	G893	A819	U758	C689	A608	U534	C322	U173
A1166	U1098	C894	U820	C759	G690	A609	A535	A325	A174
U1167	A1099	G895	G821	A759	C691	U610	C536	G326	G175
C1168	G1100	C896	U822	G760	G692	C611	C537	A327	A176
A1169	A1101	A800	C823	U761	G693	G612	C538	U328	A177
G1170	U1102	U801	A824	G762	A694	G613	A539	A329	C182
C1171	C1103	G802	U825	G763	A695	G614	A540	C330	C183
A1172	A1104	A906	G826	C764	G700	U615	G541	G331	G184
U1173	U1105	A907	U827	G765	U701	C621	U542	U405	C186
C1174	G1106	G908	G828	A766	A702	A622	U543	G406	G187
A1175	A1107	A909	U834	A767	A703	C623	G544	U407	C188
G1176	G1108	C910	U835	A768	G704	C624	A545	A408	A189
U1177	U1109	A913	G836	G769	A705	U625	A546	U409	C190
C1178	A1110	A914	U837	C770	U706	G626	A547	A410	A195
A1179	C1112	A915	C840	G771	U707	A629	G550	G411	A196
G1180	C1113	A916	U841	U772	C708	A630	U551	G412	A197
C1181	U1118	U917	U842	G773	U709	G631	U552	A413	C191
G1182	G1119	G918	U843	G774	G710	U632	A553	G414	C192
U1183	U1120	A919	U844	G775	G711	U633	U554	C415	C201
A1184	U1121	C920	G845	G776	A712	C634	U555	U421	G202
C1185	G1122	G921	U846	A777	G713	C635	C556	C422	G203
U1186	U1123	U922	U847	G778	G714	A636	G557	G423	G204
C1187	G1124	G923	U848	C779	A715	U637	A558	G424	A205
A1188	U1125	A924	C849	U780	U716	C638	A559	G425	C206
U1189	C1126	G925	C850	A781	U717	U639	A560	U426	C207
G1190	G1127	G926	U851	A782	A718	A642	A561	U427	U208
A1191	C1128	G927	U852	C783	C719	C643	U562	U428	U209
C1192	U1132	G928	C853	G784	U720	G644	A563	U429	C210
U1193	G1133	G929	U854	G785	C721	A635	C564	A430	G211
A1194	C1134	C930	U855	G786	G722	U636	U565	A431	C212
G1195	U1135	G931	C856	U787	U723	C637	A566	A363	G213
C1196	C1136	C932	U857	A788	G724	U638	A567	A364	C214
U1197	U1137	G933	U858	U789	G725	U639	A568	A365	C215
A1198	G1138	C934	U859	A790	G726	G650	C569	U367	U216
C1199	C1139	G935	A860			U653			
U1200	G1140	C936	G933			G656			
A1201	C1141	A937							
U1202	G1142	A938							
C1203	G1143	G939							
A1204	U1008	G942							
U1205	A1012	C945							
	G1013	A949							
	A1014	U950							
	G1015	G951							
	A1016	U952							
	U1017	G953							
	G1018	C954							
	U1019	U955							
	A1020	U956							
	G1021	U957							
	U1022	A958							
	A1023	U959							
	G1024	U960							
	U1025	C961							
	G1026	C962							
	A1027	U965							
	C1028	G966							
	U1029	C967							
	G1030	A968							
	A1031	U969							
	G1032	C970							
	U1033	G971							
	G1034	C972							
	A1035	A975							
	C1036	U976							
	G1037	A977							
	A1038	U978							
	G1039	C979							
	U1040	G980							
	G1041	U981							
	A1042	A983							
	G1043	C984							
	U1044	U985							
	C1045	G986							
	G1046	U987							
	A1047	C988							
	U1048	U989							
	G1049	C990							
	U1050	A991							
	A1051	U992							
	C1052	G993							
	G1053	U994							
	U1054	C995							
	A1055	G996							
	U1056	U997							
	G1057	C998							
	A1058	G999							
	U1059	U1000							
	C1060	C1001							
	G1061								
	A1062								
	U1063								
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	C1122								
	A1123								
	G1124								
	U1125								
	C1126								
	A1127								
	G1128								
	U1129								
	C1130								
	A1131								
	G1132								
	U1133								
	C1134								
	A1135								
	G1136								
	U1137								



• Molecule 2: 30S ribosomal protein S2



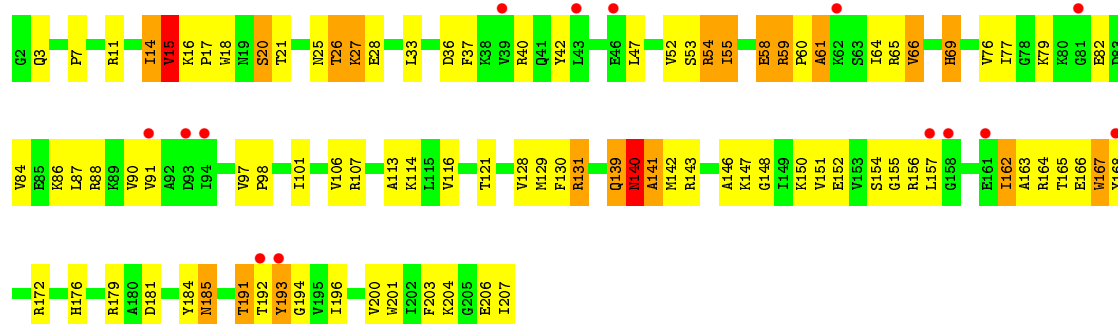
• Molecule 2: 30S ribosomal protein S2





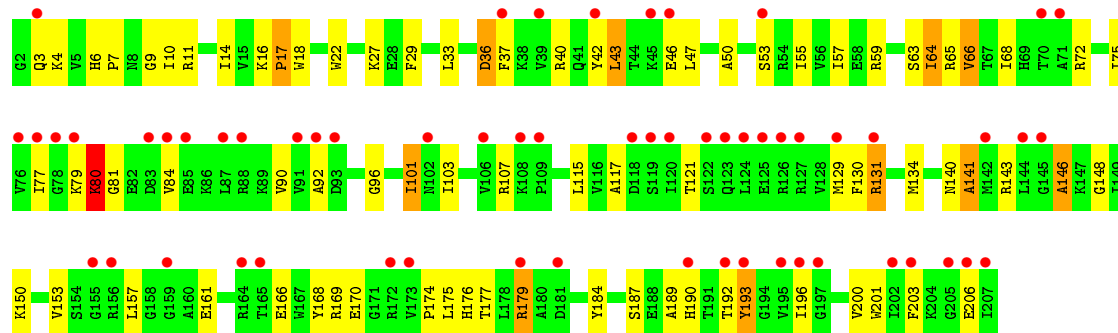
• Molecule 3: 30S ribosomal protein S3

Chain AC: 7% 54% 35% 9%



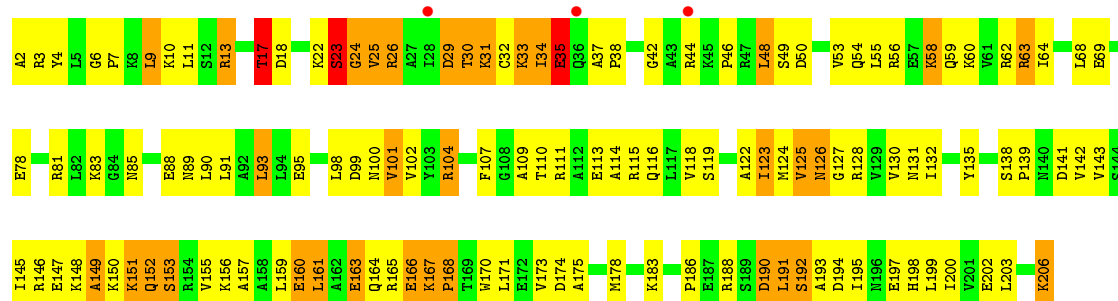
• Molecule 3: 30S ribosomal protein S3

Chain CC: 29% 61% 33% 5%



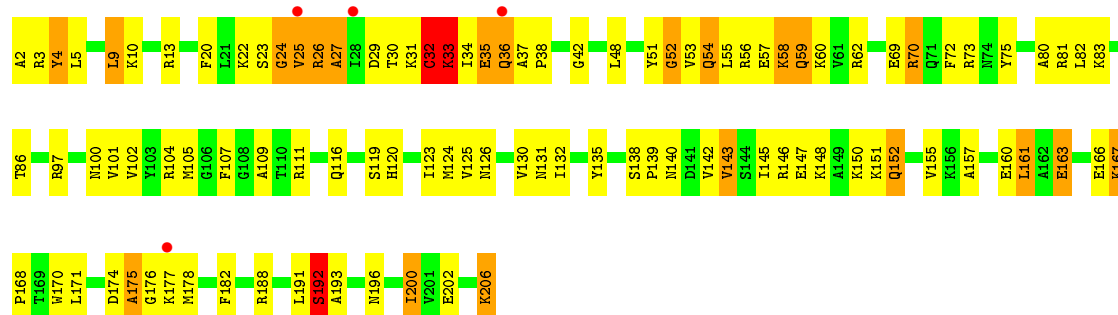
• Molecule 4: 30S ribosomal protein S4

Chain AD: 38% 45% 16%

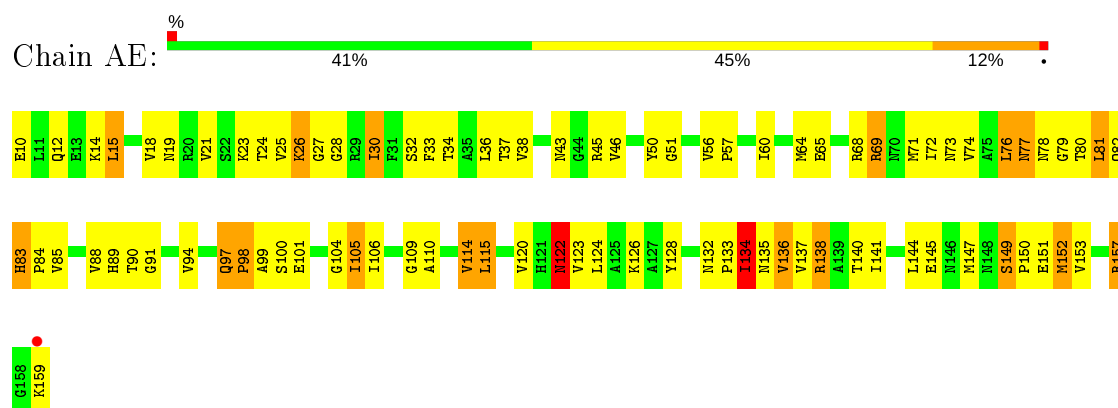


• Molecule 4: 30S ribosomal protein S4

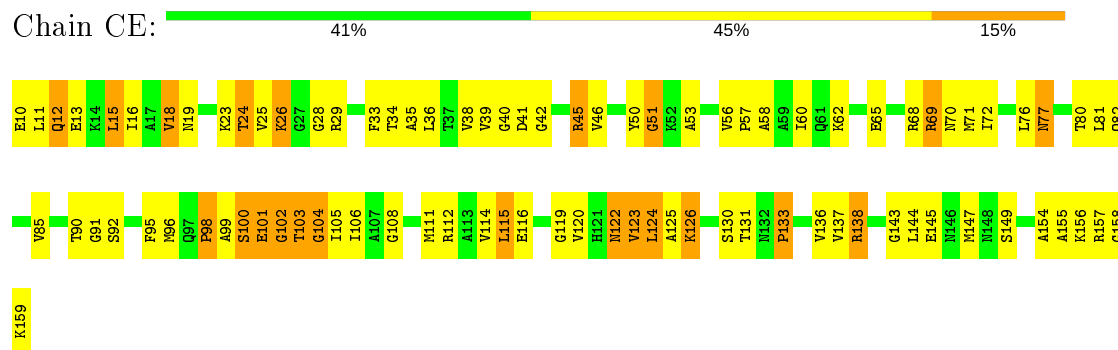
Chain CD: 2% 50% 39% 10%



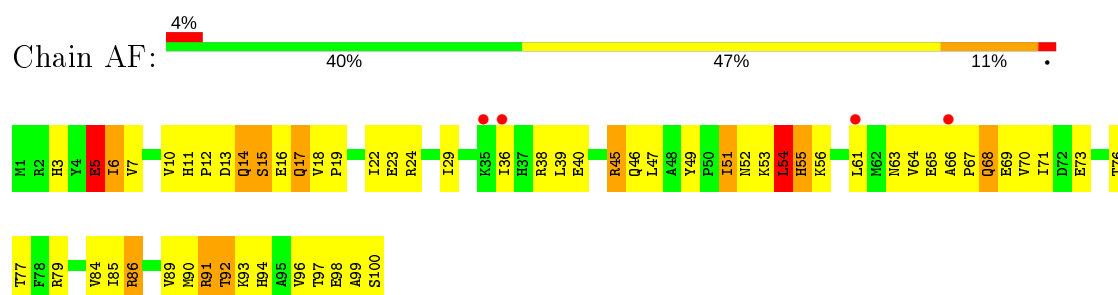
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

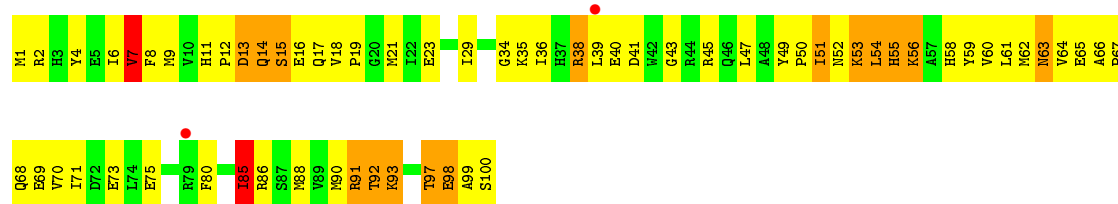


• Molecule 6: 30S ribosomal protein S6

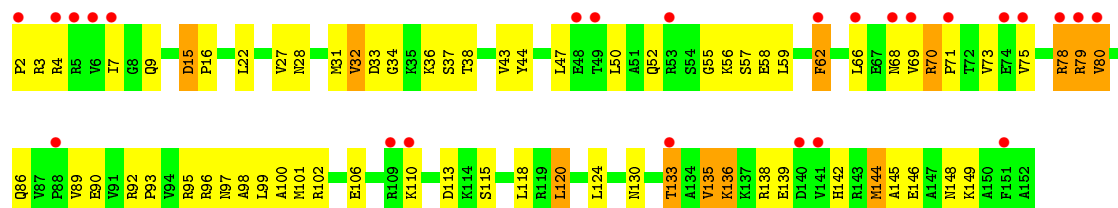


• Molecule 6: 30S ribosomal protein S6

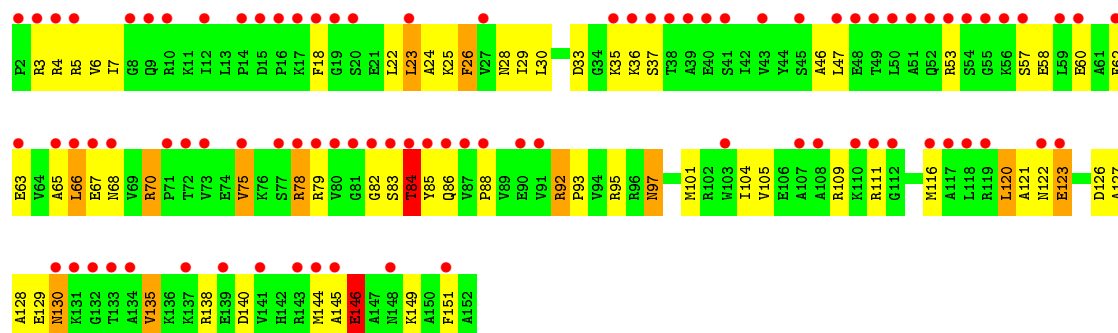




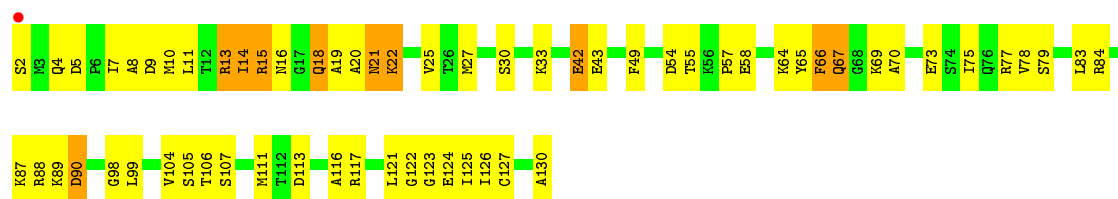
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

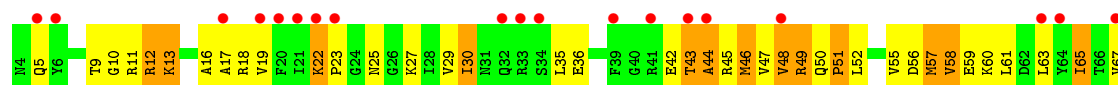


• Molecule 8: 30S ribosomal protein S8

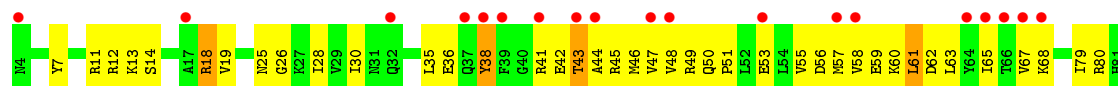
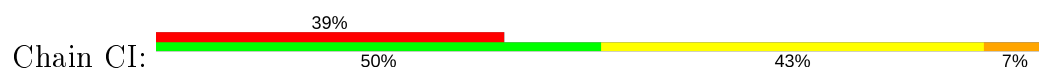




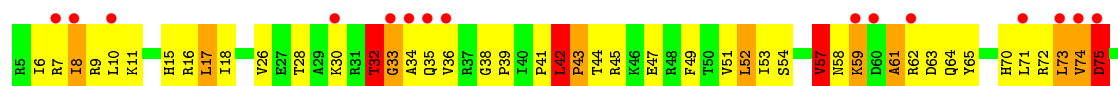
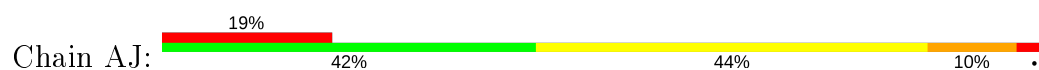
• Molecule 9: 30S ribosomal protein S9



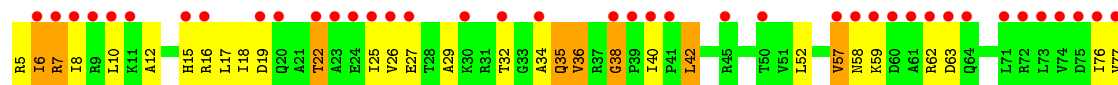
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

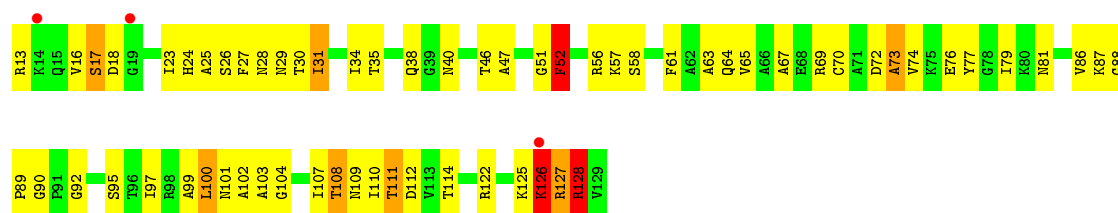


• Molecule 10: 30S ribosomal protein S10

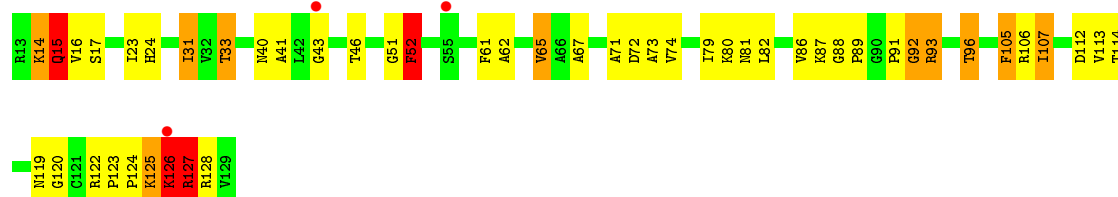


• Molecule 11: 30S ribosomal protein S11

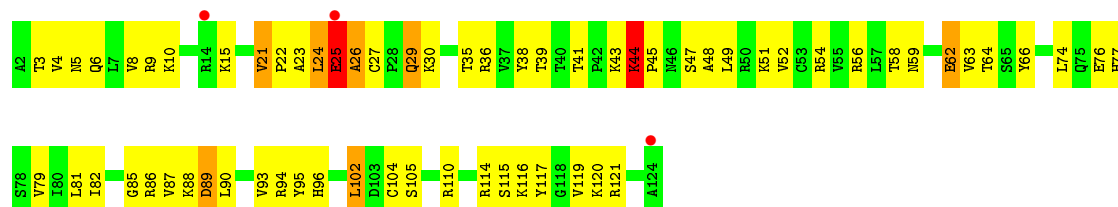




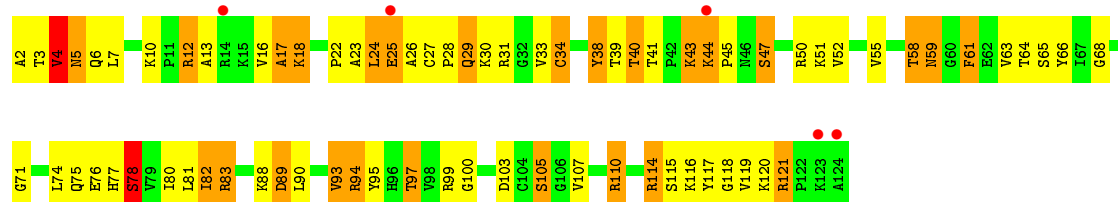
• Molecule 11: 30S ribosomal protein S11



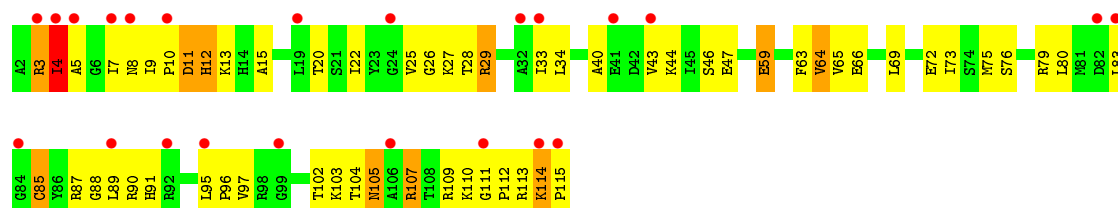
• Molecule 12: 30S ribosomal protein S12



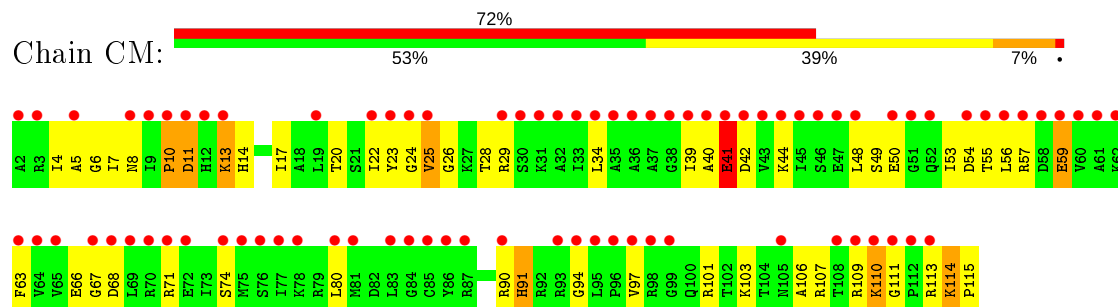
• Molecule 12: 30S ribosomal protein S12



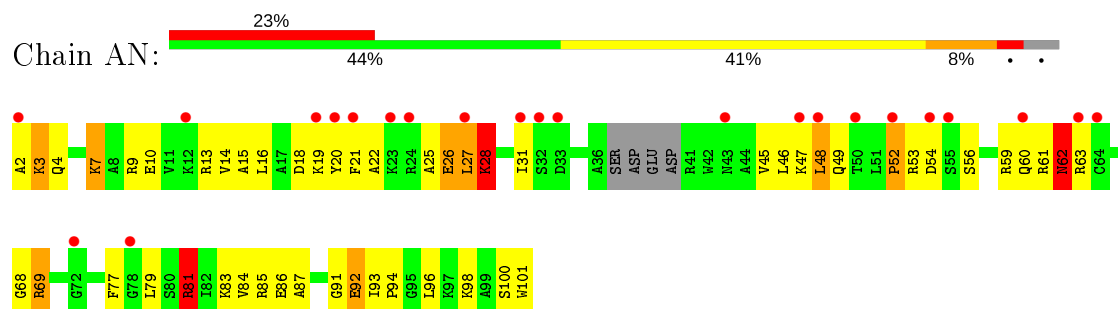
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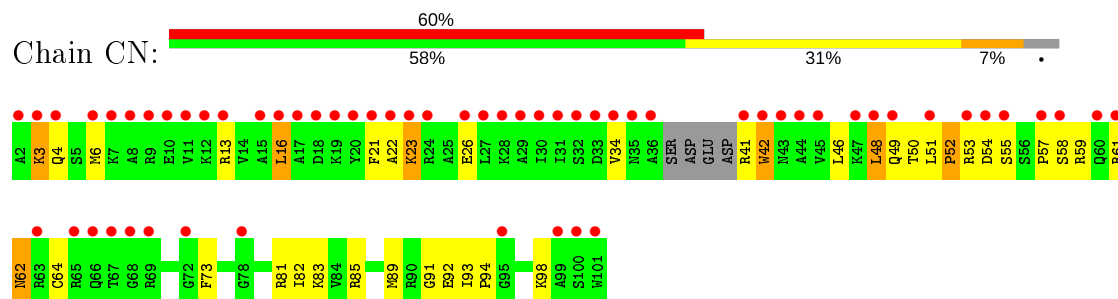
- Molecule 13: 30S ribosomal protein S13



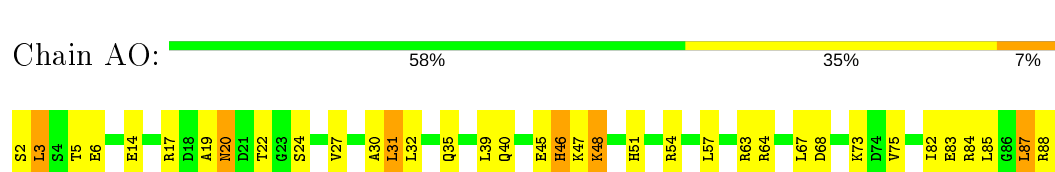
- Molecule 14: 30S ribosomal protein S14



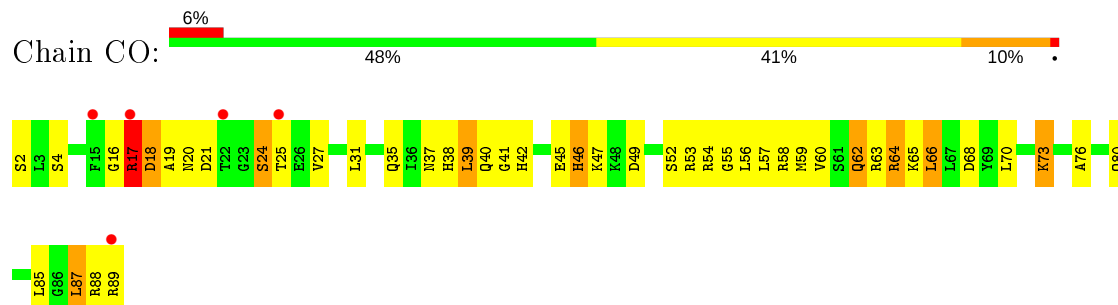
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

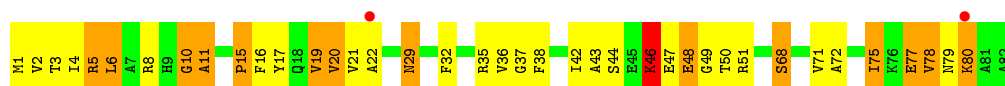


- Molecule 15: 30S ribosomal protein S15

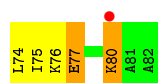
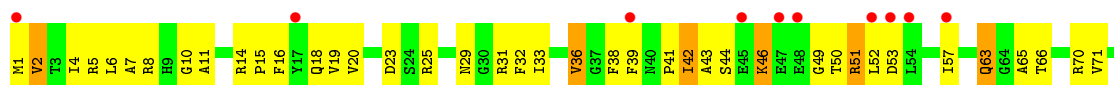




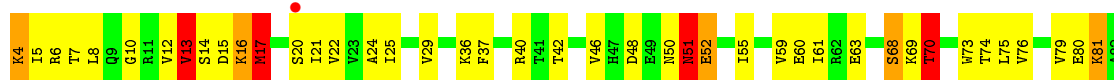
- Molecule 16: 30S ribosomal protein S16



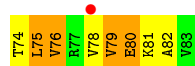
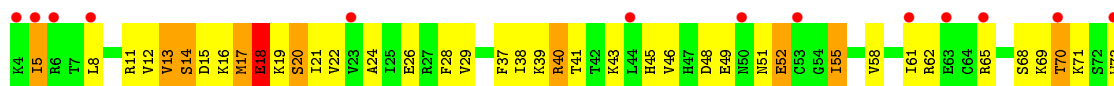
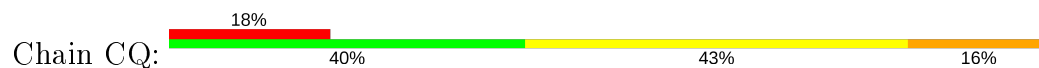
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



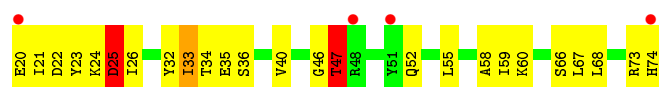
- Molecule 17: 30S ribosomal protein S17



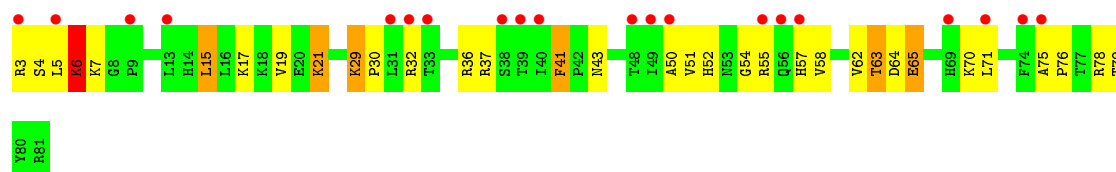
- Molecule 18: 30S ribosomal protein S18



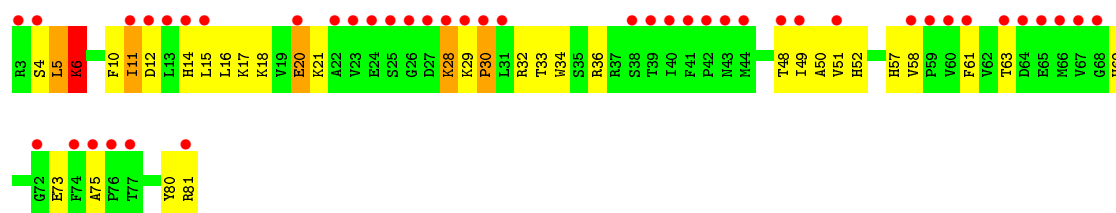
- Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19



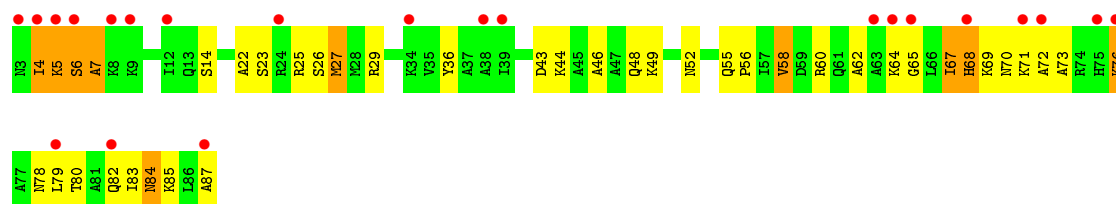
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20



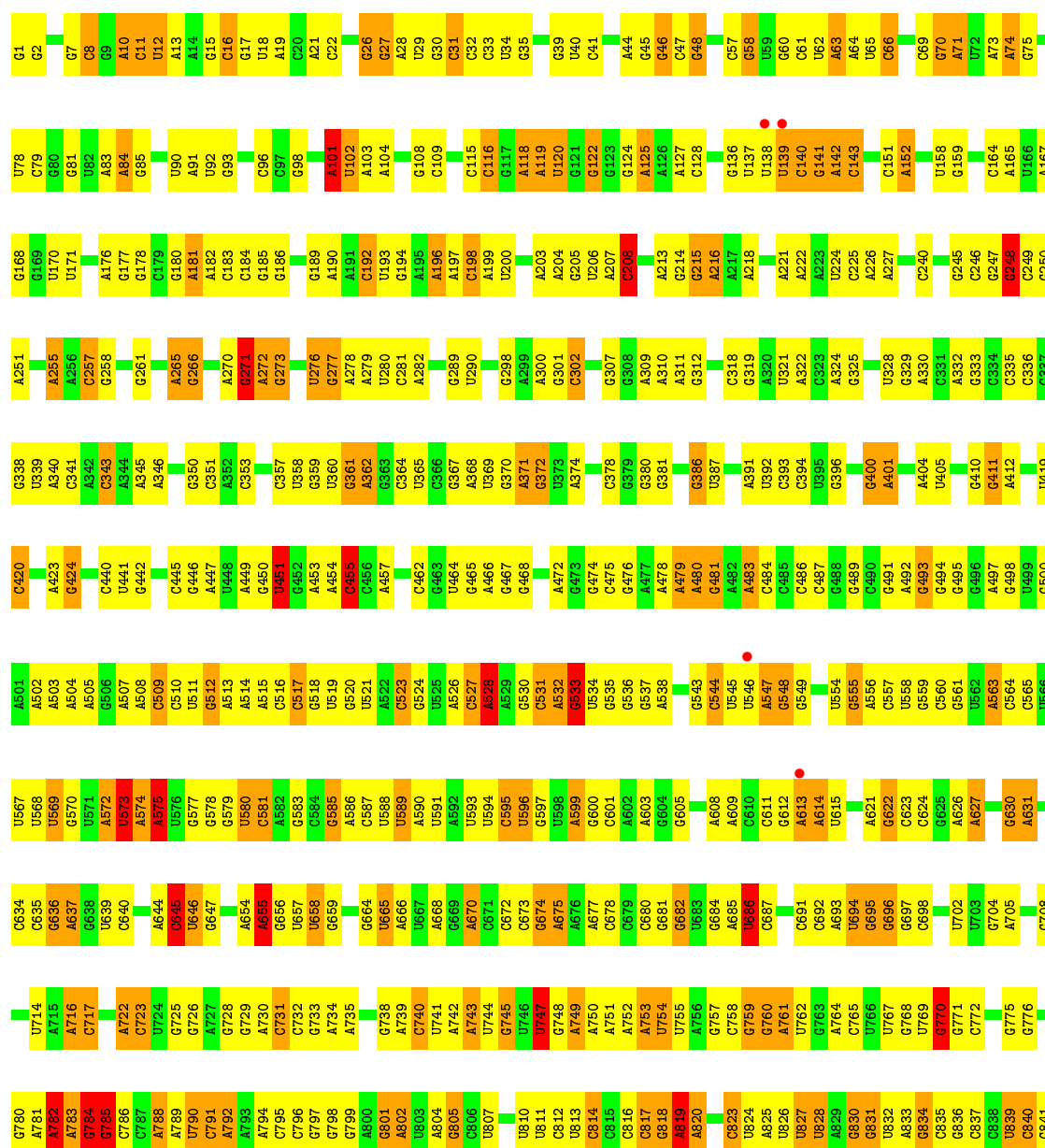
• Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

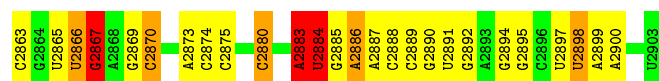


- Molecule 22: 23S rRNA

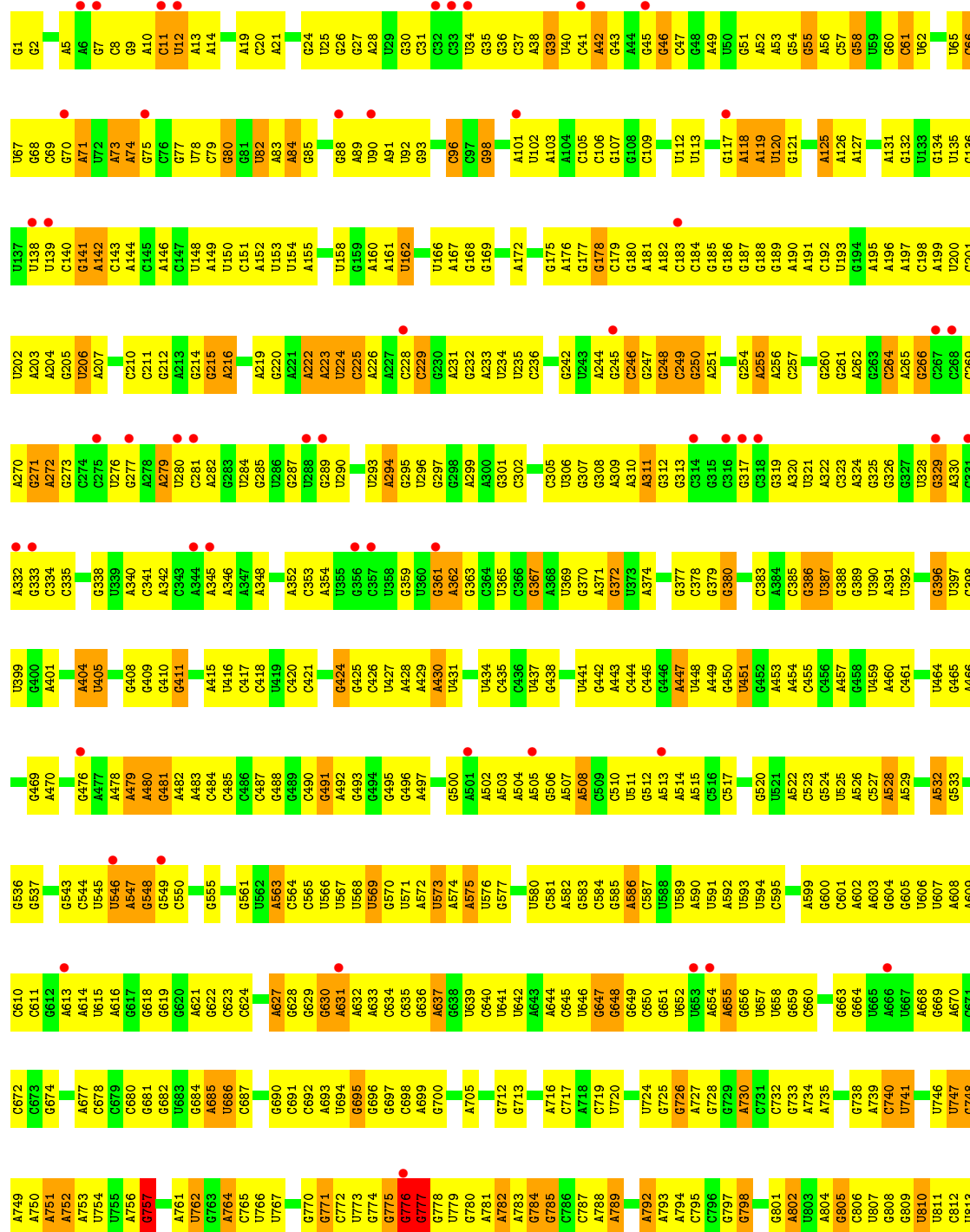








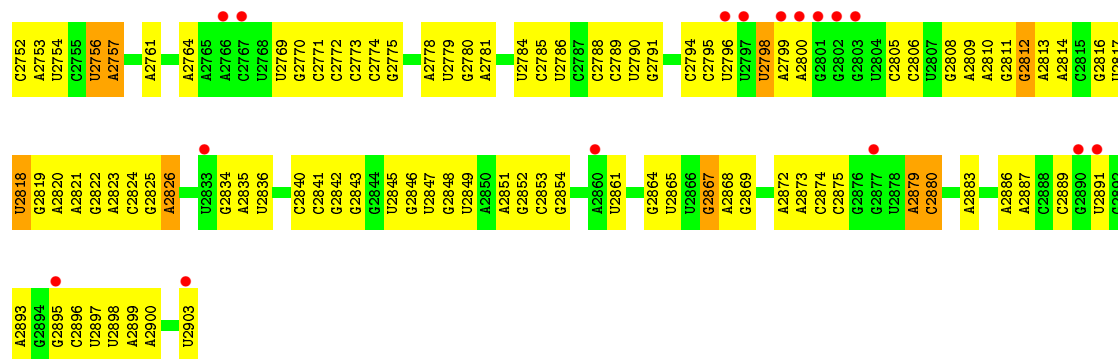
● Molecule 22: 23S rRNA



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A1677	U1680	G1681	U1682	G1683	C1686	U1687	U1688	U1692	U1693	C1694	G1695	A1698	U1699	A1705	C1708	U1709	A1784	G1710	G1710	G1710	A1713	U1714	G1715	U1716	A1717	G1718	U1722	C1723	C1724	U1725	U1726	U1727	U1728	U1729	G1730	G1731	C1732	G1733	U1736	G1737	G1738	A1739	U1742	G1743	A1744	A1745	A1746	U1747	U1748	A1749	G1750	U1751	U1752	A1753	A1754	A1755	G1756	A1757	U1758																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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G1531	A1532	C1533	U1534	A1535	C1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	A1544	A1545	A1546	C1547	A1548	A1549	C1550	A1551	A1552	G1555	C1556	U1559	C1560	U1561	U1562	C1563	C1564	C1565	G1566	G1567	G1568	A1569	A1570	A1571	A1572	C1577	U1578	C1579	A1580	C1581	C1582	U1583	U1584	C1585	A1586	U1594	C1595	A1596	A1597	A1598	U1599	C1600	G1601																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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A1677	U1680	G1681	U1682	G1683	C1686	U1687	U1688	U1692	U1693	C1694	G1695	A1698	U1699	A1705	C1708	U1709	A1784	G1710	G1710	G1710	A1713	U1714	G1715	U1716	A1717	G1718	U1722	C1723	C1724	U1725	U1726	U1727	U1728	U1729	G1730	G1731	C1732	G1733	U1736	G1737	G1738	A1739	U1742	G1743	A1744	A1745	A1746	U1747	U1748	A1749	G1750	U1751	U1752	A1753	A1754	A1755	G1756	A1757	U1758																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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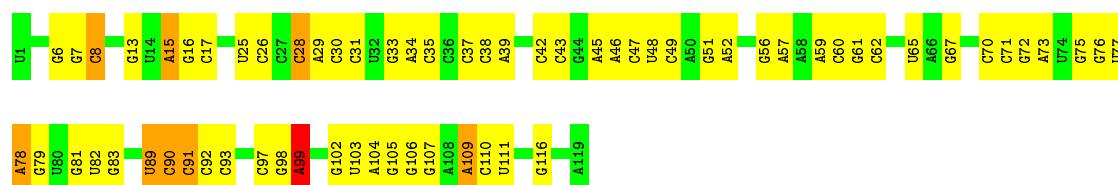






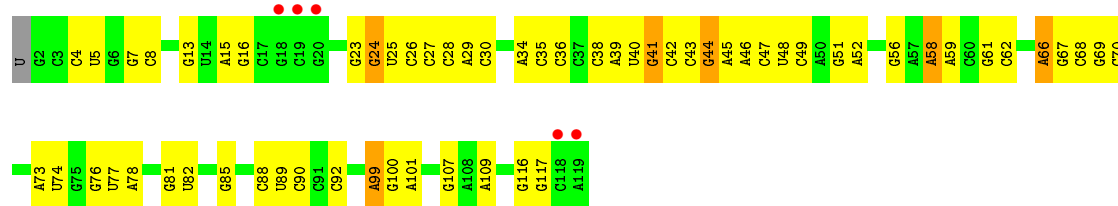
- Molecule 23: 5S rRNA

Chain BB: 45% 48% 7%



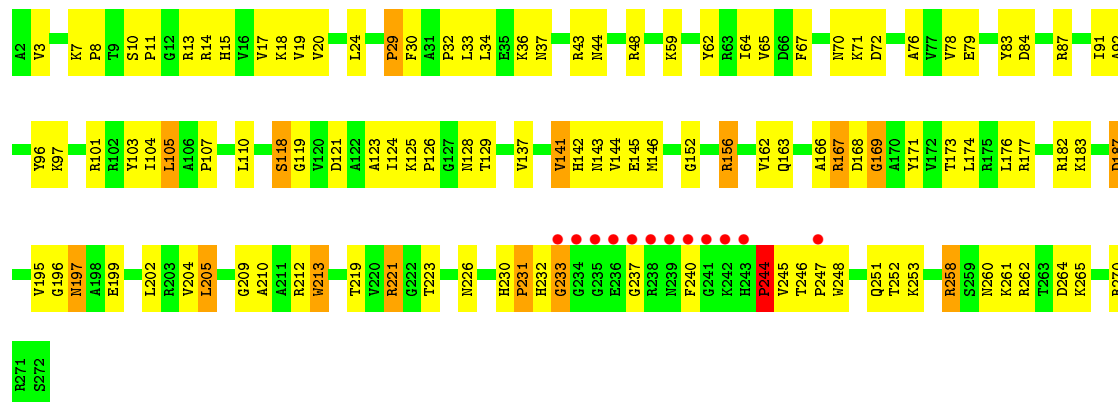
- Molecule 23: 5S rRNA

Chain DB: 4% 48% 46% 5%

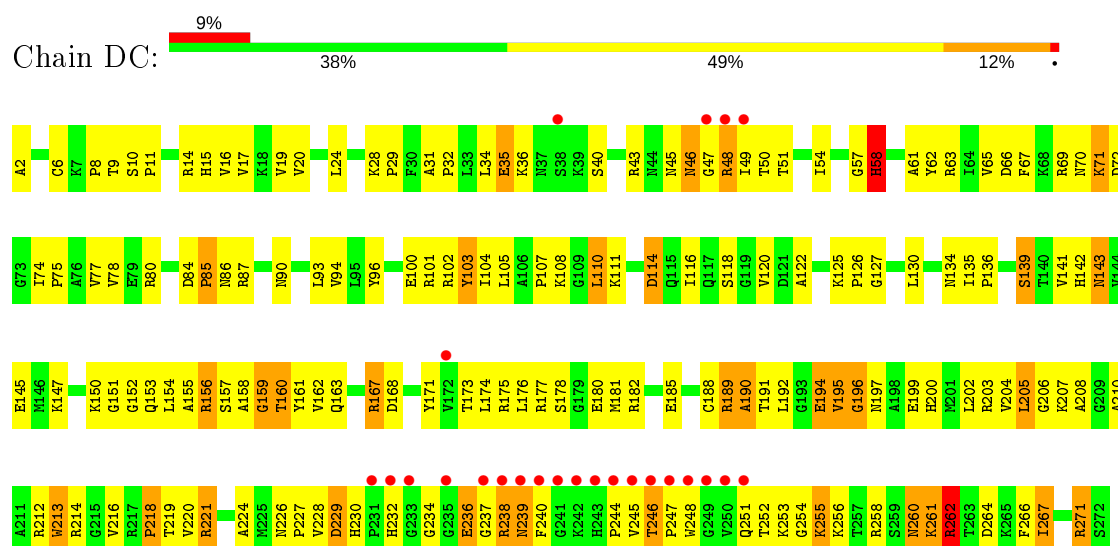


- Molecule 24: 50S ribosomal protein L2

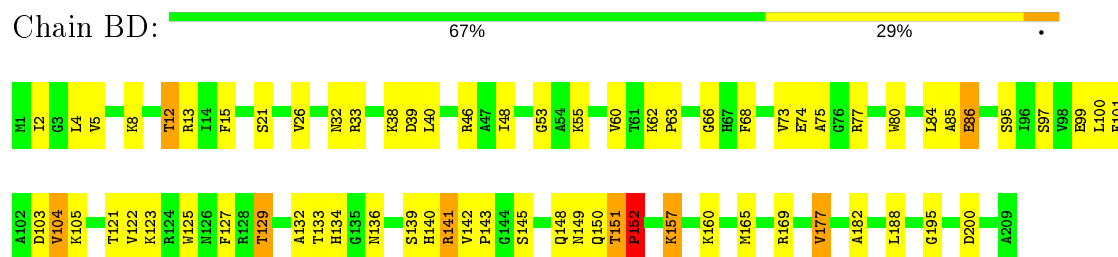
Chain BC: 4% 58% 37% 6%



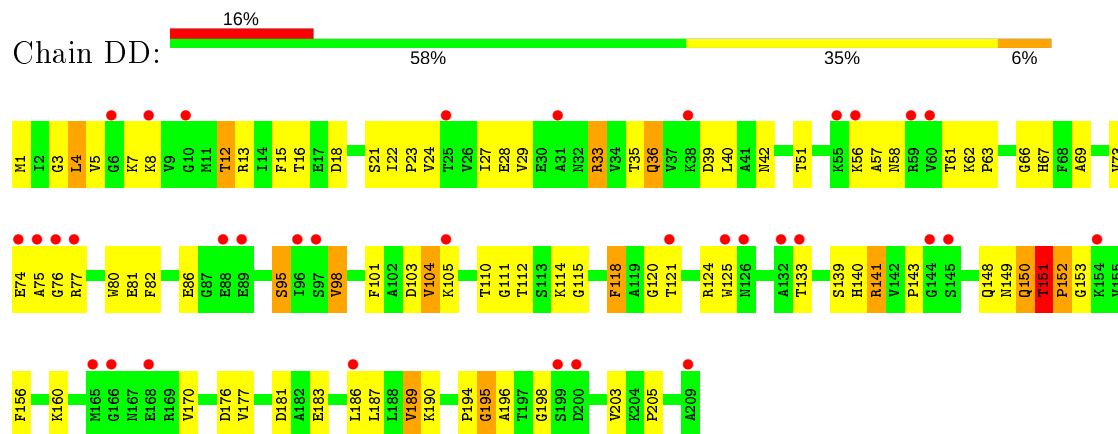
- Molecule 24: 50S ribosomal protein L2



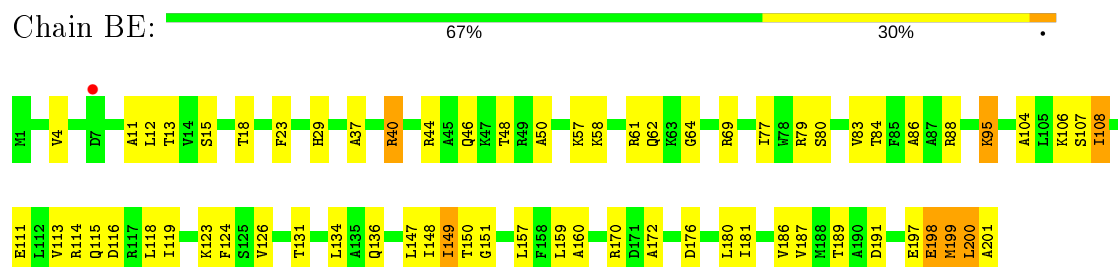
• Molecule 25: 50S ribosomal protein L3



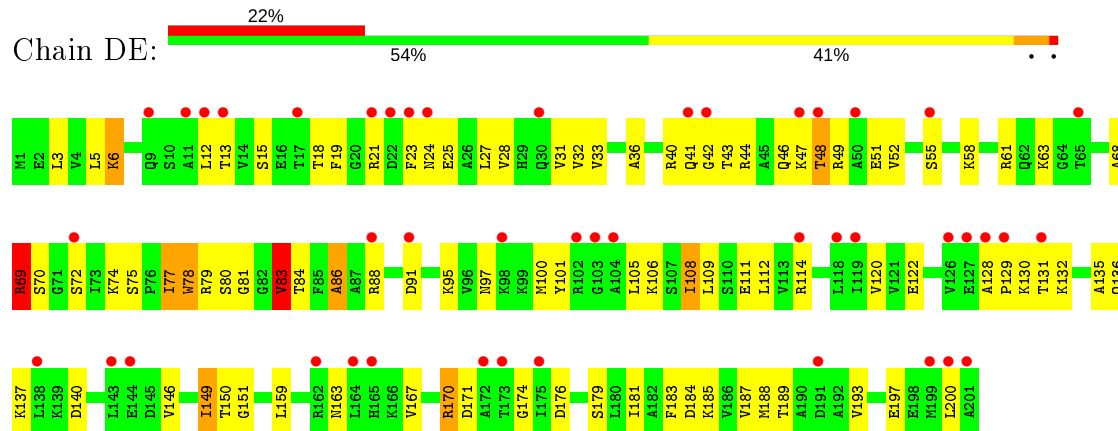
• Molecule 25: 50S ribosomal protein L3



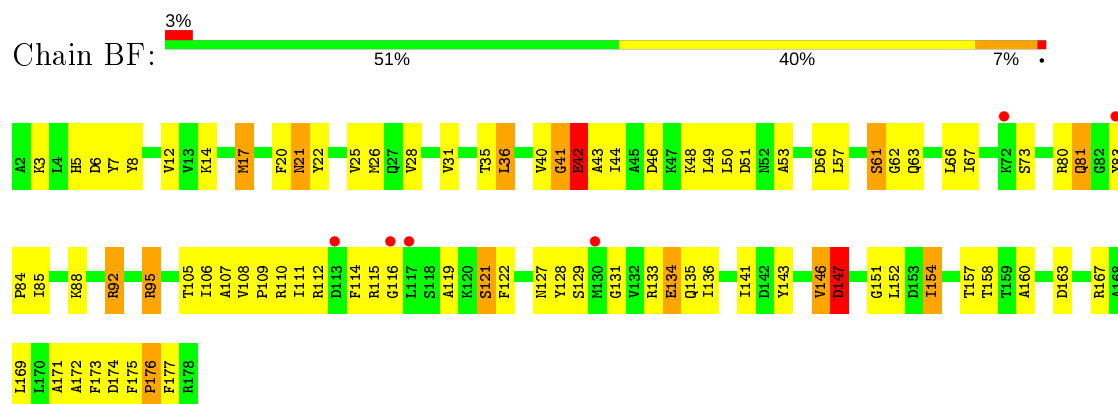
• Molecule 26: 50S ribosomal protein L4



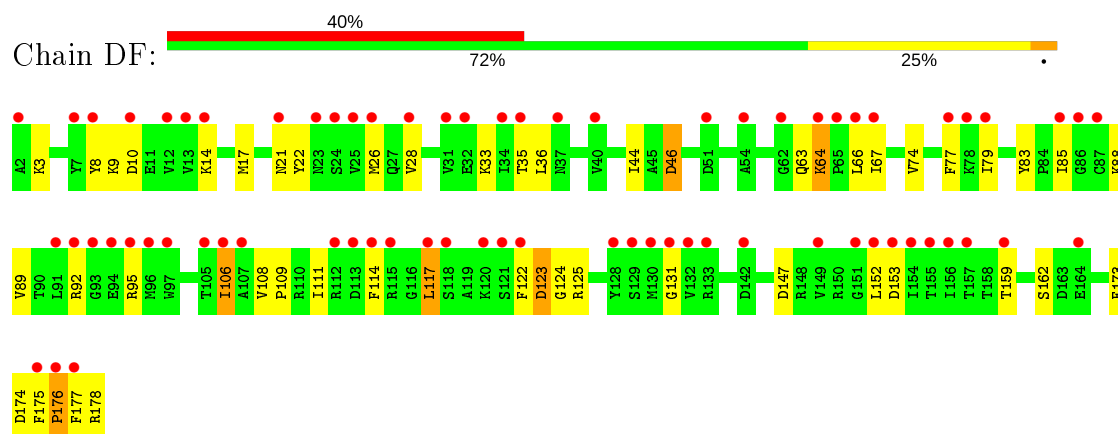
- Molecule 26: 50S ribosomal protein L4



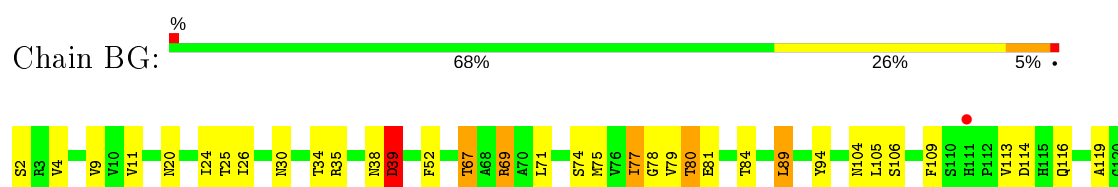
- Molecule 27: 50S ribosomal protein L5

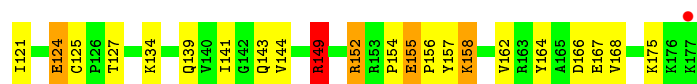


- Molecule 27: 50S ribosomal protein L5

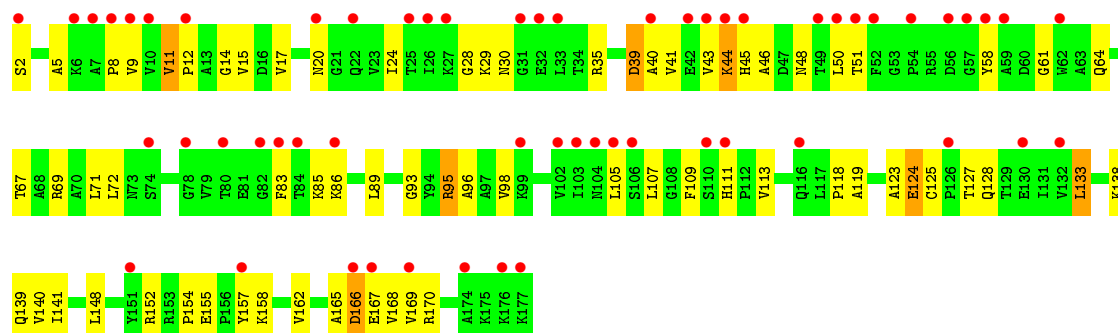


- Molecule 28: 50S ribosomal protein L6

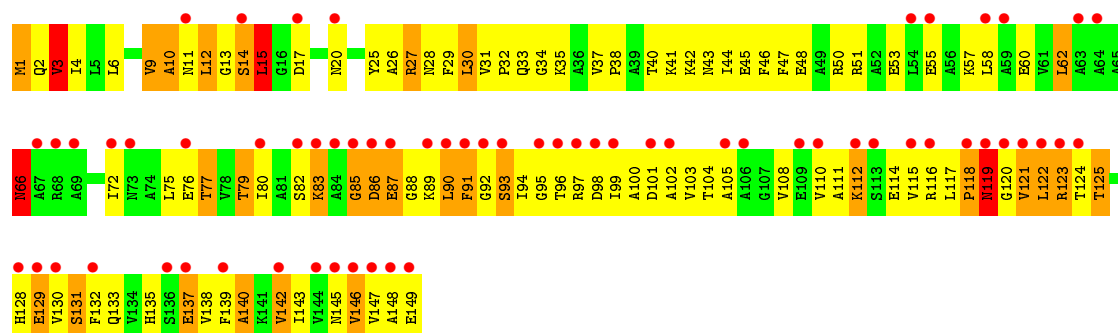




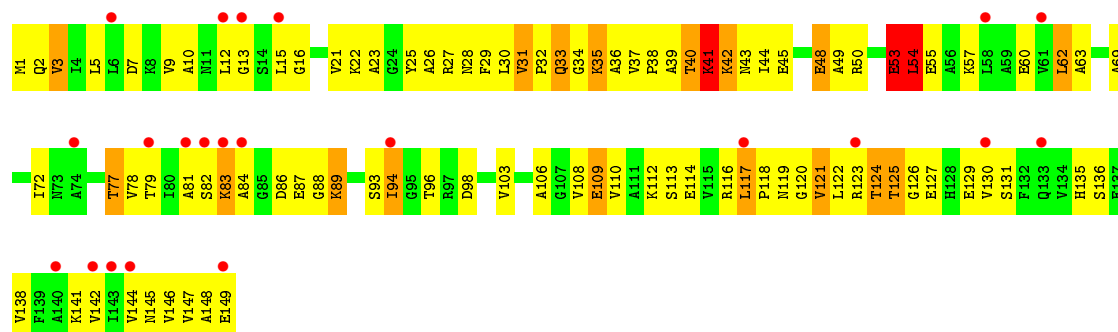
- Molecule 28: 50S ribosomal protein L6



- Molecule 29: 50S ribosomal protein L9

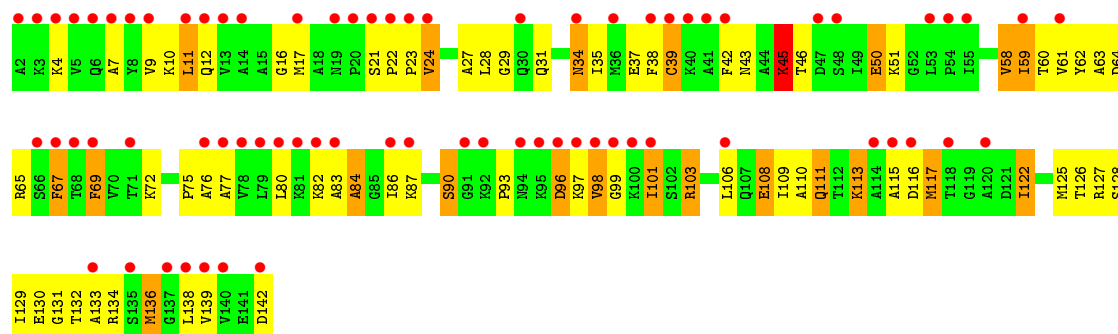


- Molecule 29: 50S ribosomal protein L9

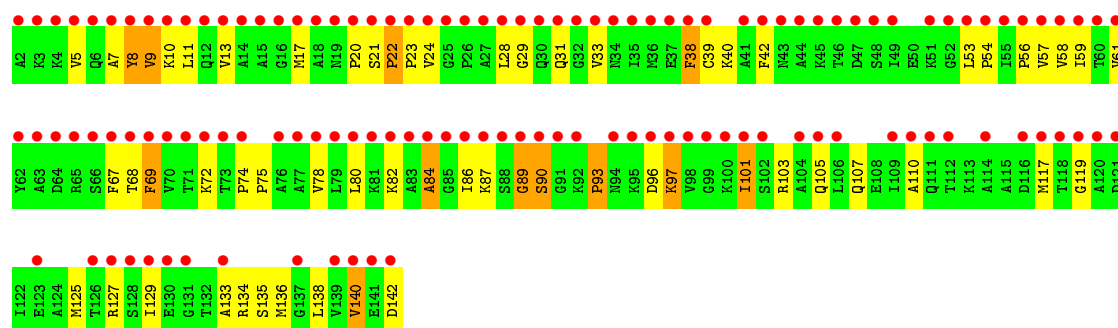
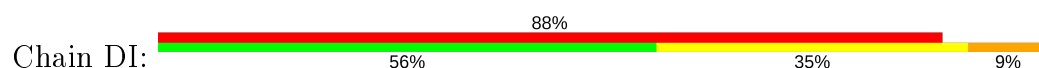


- Molecule 30: 50S ribosomal protein L11

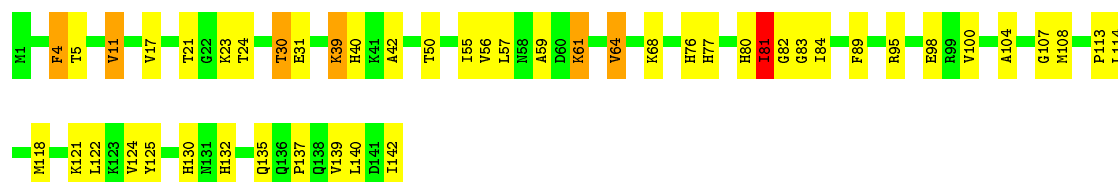




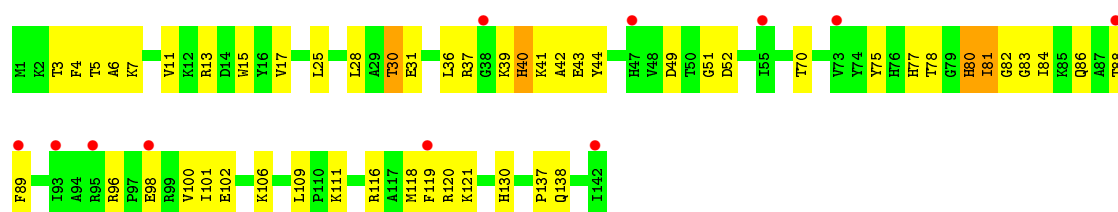
• Molecule 30: 50S ribosomal protein L11



• Molecule 31: 50S ribosomal protein L13

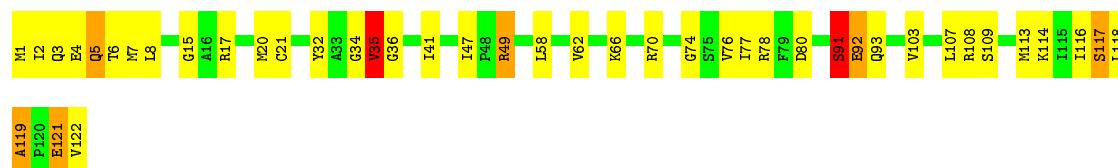


• Molecule 31: 50S ribosomal protein L13

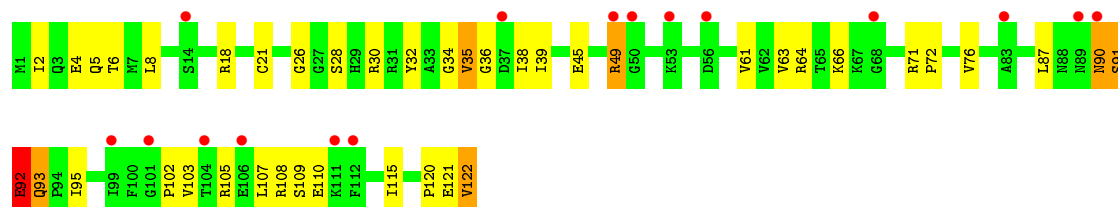


• Molecule 32: 50S ribosomal protein L14

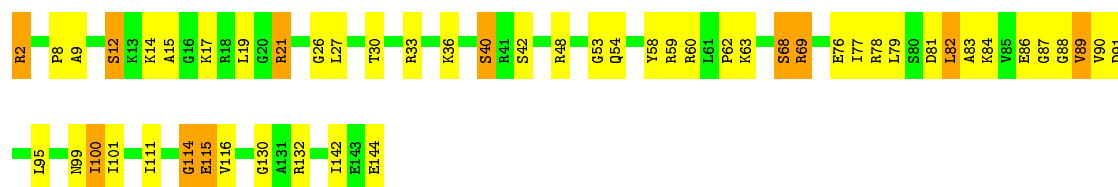




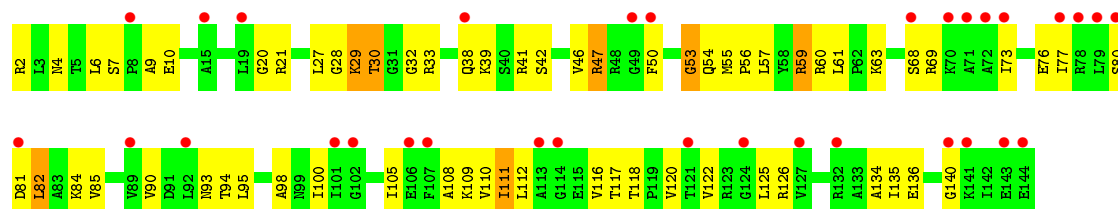
- Molecule 32: 50S ribosomal protein L14



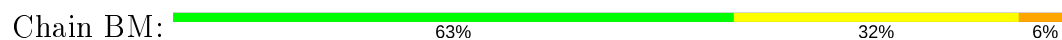
- Molecule 33: 50S ribosomal protein L15



- Molecule 33: 50S ribosomal protein L15



- Molecule 34: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L16

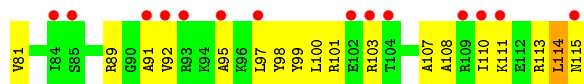
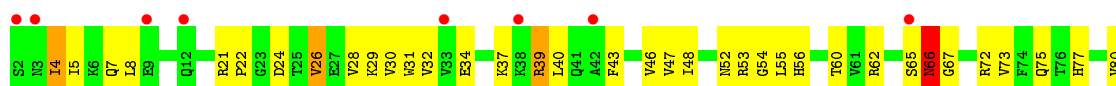




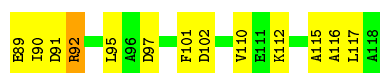
- Molecule 37: 50S ribosomal protein L19



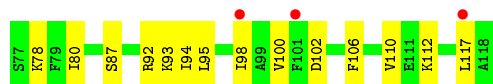
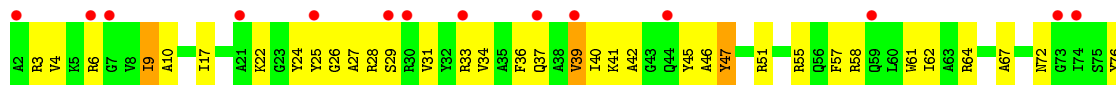
- Molecule 37: 50S ribosomal protein L19



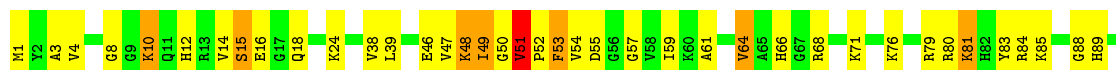
- Molecule 38: 50S ribosomal protein L20



- Molecule 38: 50S ribosomal protein L20



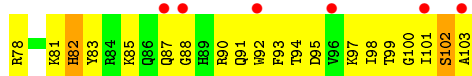
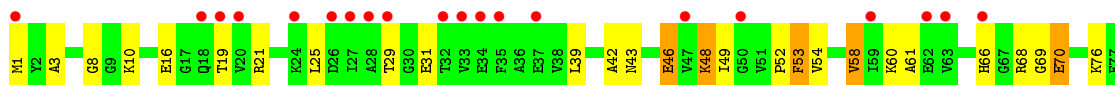
- Molecule 39: 50S ribosomal protein L21







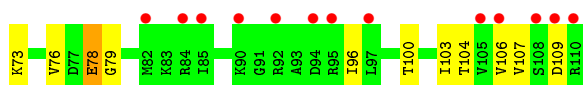
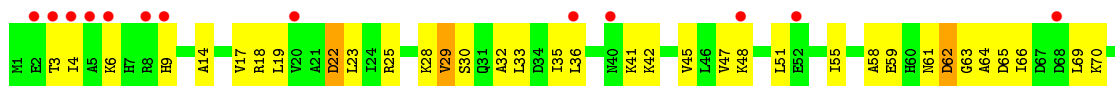
- Molecule 39: 50S ribosomal protein L21



- Molecule 40: 50S ribosomal protein L22



- Molecule 40: 50S ribosomal protein L22

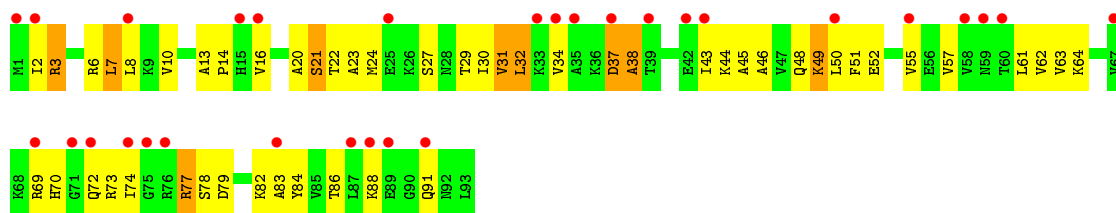


- Molecule 41: 50S ribosomal protein L23

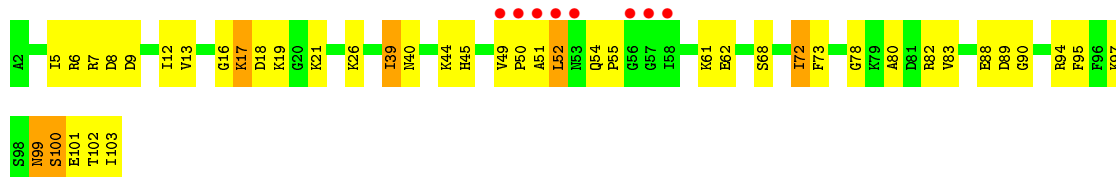


- Molecule 41: 50S ribosomal protein L23

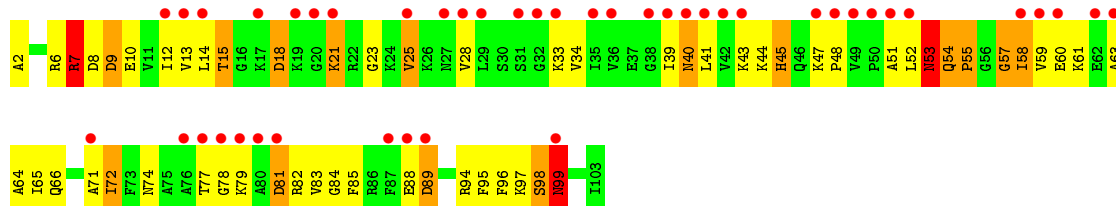
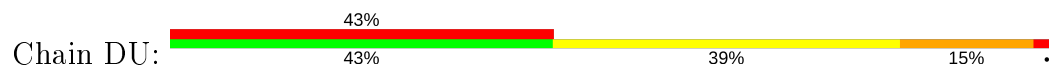




- Molecule 42: 50S ribosomal protein L24



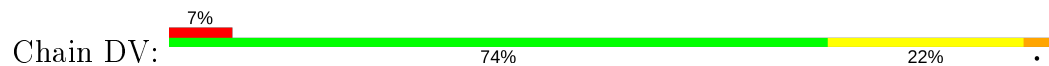
- Molecule 42: 50S ribosomal protein L24



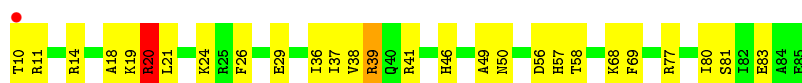
- Molecule 43: 50S ribosomal protein L25



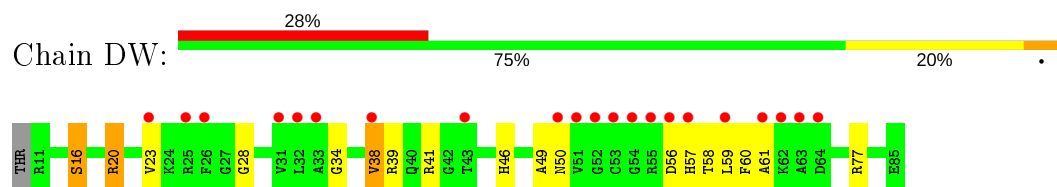
- Molecule 43: 50S ribosomal protein L25



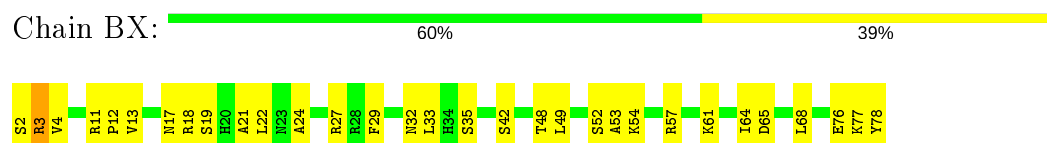
- Molecule 44: 50S ribosomal protein L27



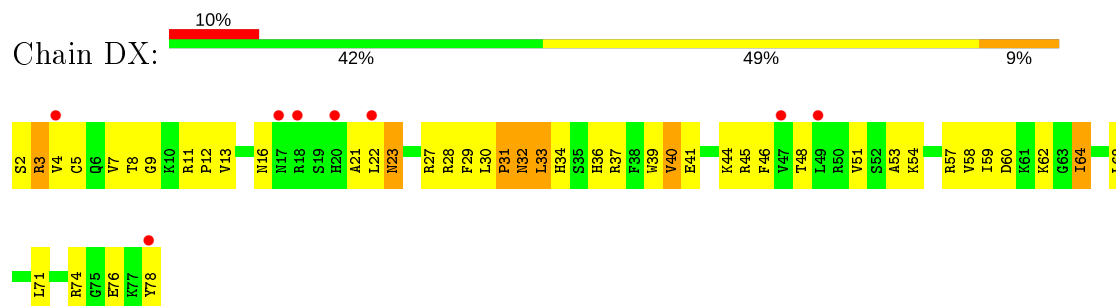
- Molecule 44: 50S ribosomal protein L27



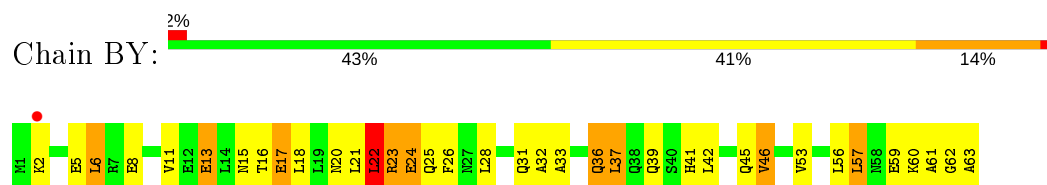
- Molecule 45: 50S ribosomal protein L28



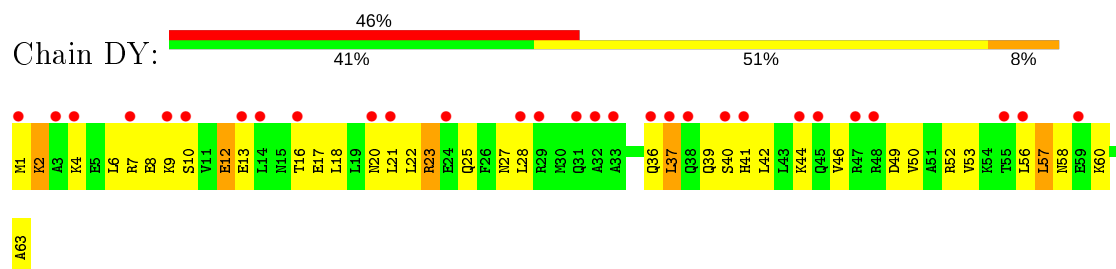
- Molecule 45: 50S ribosomal protein L28



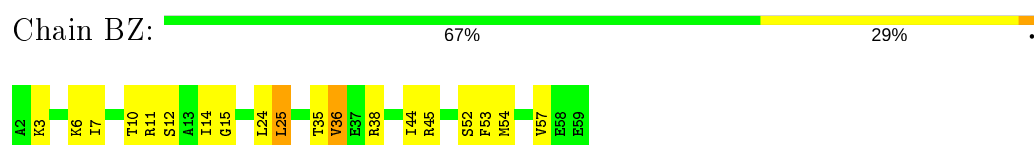
- Molecule 46: 50S ribosomal protein L29



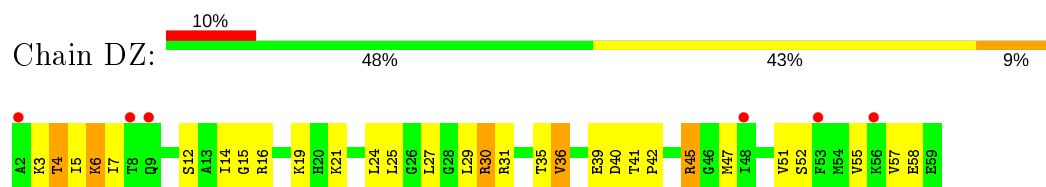
- Molecule 46: 50S ribosomal protein L29



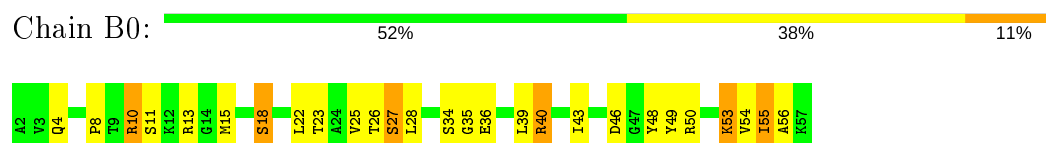
- Molecule 47: 50S ribosomal protein L30



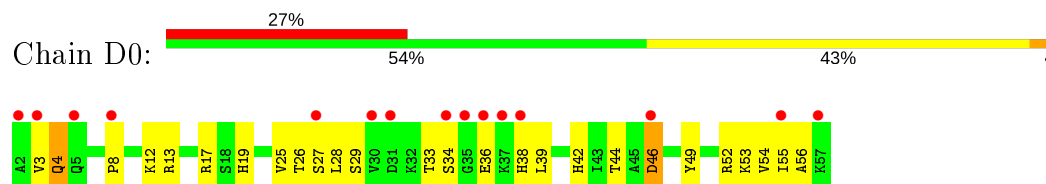
## • Molecule 47: 50S ribosomal protein L30



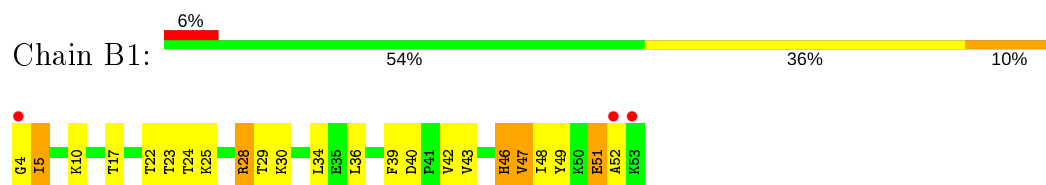
## • Molecule 48: 50S ribosomal protein L32



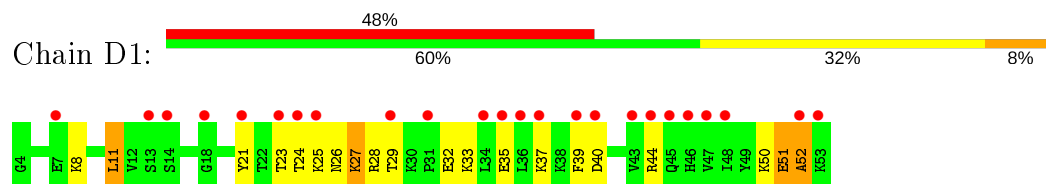
## • Molecule 48: 50S ribosomal protein L32



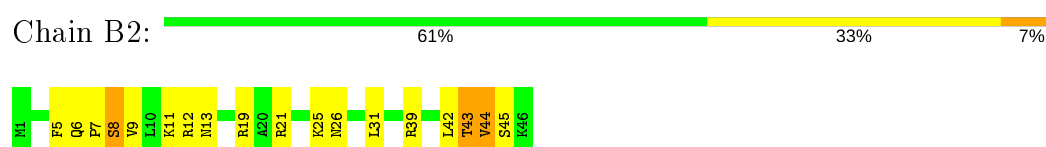
## • Molecule 49: 50S ribosomal protein L33



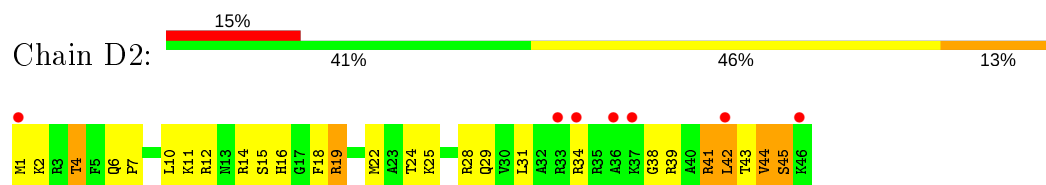
## • Molecule 49: 50S ribosomal protein L33



## • Molecule 50: 50S ribosomal protein L34

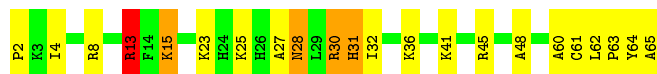


## • Molecule 50: 50S ribosomal protein L34



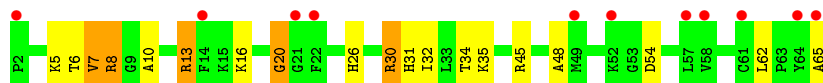
- Molecule 51: 50S ribosomal protein L35

Chain B3:  66% 27% 6%



- Molecule 51: 50S ribosomal protein L35

Chain D3:  17% 70% 22% 8%



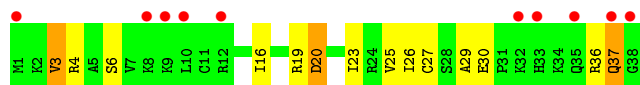
- Molecule 52: 50S ribosomal protein L36

Chain B4:  63% 34%




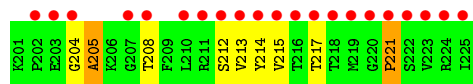
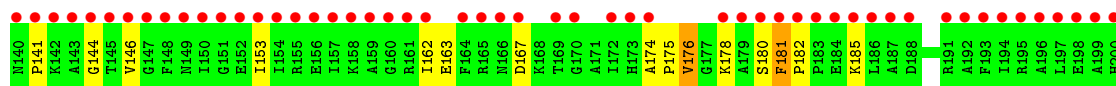
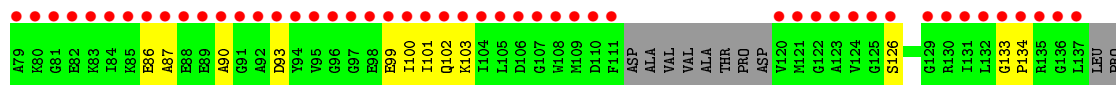
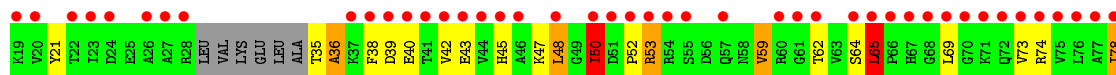
- Molecule 52: 50S ribosomal protein L36

Chain D4:  26% 63% 29% 8%



- Molecule 53: 50S ribosomal protein L1

Chain B5:  81% 64% 23% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.91Å 434.31Å 624.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.14 – 3.09 41.14 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.14-3.09) 99.9 (41.14-3.09)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.202 , 0.244 0.206 , 0.249	Depositor DCC
$R_{free}$ test set	4190 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	288204	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	0.58	3/36944 (0.0%)	1.07	91/57632 (0.2%)
1	CA	0.51	3/36966 (0.0%)	1.00	57/57666 (0.1%)
2	AB	0.42	0/1736	0.60	0/2338
2	CB	0.35	0/1736	0.55	0/2338
3	AC	0.36	0/1652	0.52	0/2225
3	CC	0.36	0/1652	0.48	0/2225
4	AD	0.40	0/1665	0.60	0/2227
4	CD	0.50	0/1665	0.66	0/2227
5	AE	0.46	0/1119	0.71	0/1504
5	CE	0.44	0/1119	0.68	0/1504
6	AF	0.46	0/836	0.63	0/1128
6	CF	0.39	0/836	0.54	0/1128
7	AG	0.37	0/1196	0.53	0/1602
7	CG	0.37	0/1196	0.48	0/1602
8	AH	0.41	0/989	0.59	0/1326
8	CH	0.34	0/989	0.55	0/1326
9	AI	0.35	0/1034	0.54	0/1375
9	CI	0.35	0/1034	0.50	0/1375
10	AJ	0.35	0/797	0.54	0/1077
10	CJ	0.34	0/797	0.51	0/1077
11	AK	0.38	0/893	0.59	0/1205
11	CK	0.35	0/893	0.59	0/1205
12	AL	0.49	0/969	0.73	0/1300
12	CL	0.41	0/969	0.71	0/1300
13	AM	0.36	0/893	0.57	0/1193
13	CM	0.36	0/893	0.54	0/1193
14	AN	0.36	0/785	0.52	0/1043
14	CN	0.34	0/785	0.48	0/1043
15	AO	0.38	0/722	0.60	0/964
15	CO	0.34	0/722	0.54	0/964
16	AP	0.42	0/659	0.59	0/884
16	CP	0.40	0/659	0.62	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.47	0/658	0.62	0/881
17	CQ	0.37	0/658	0.56	0/881
18	AR	0.39	0/463	0.59	0/621
18	CR	0.37	0/463	0.57	0/621
19	AS	0.37	0/653	0.53	0/877
19	CS	0.35	0/653	0.48	0/877
20	AT	0.44	0/671	0.62	0/888
20	CT	0.37	0/671	0.54	0/888
21	AU	0.58	0/431	0.70	0/570
21	CU	0.57	0/431	0.67	0/570
22	BA	1.11	160/69659 (0.2%)	1.57	1390/108672 (1.3%)
22	DA	0.49	0/69659	0.96	49/108672 (0.0%)
23	BB	0.92	4/2850 (0.1%)	1.50	47/4444 (1.1%)
23	DB	0.39	0/2828	0.83	0/4410
24	BC	0.68	1/2122 (0.0%)	0.79	0/2852
24	DC	0.39	0/2122	0.60	0/2852
25	BD	0.80	1/1586 (0.1%)	0.98	4/2134 (0.2%)
25	DD	0.37	0/1586	0.56	0/2134
26	BE	0.60	0/1571	0.72	0/2113
26	DE	0.37	0/1571	0.53	0/2113
27	BF	0.43	0/1435	0.61	0/1926
27	DF	0.32	0/1435	0.46	0/1926
28	BG	0.50	0/1343	0.70	1/1816 (0.1%)
28	DG	0.32	0/1343	0.46	0/1816
29	BH	0.32	0/1121	0.63	0/1515
29	DH	0.34	0/1121	0.56	0/1515
30	BI	0.39	0/1046	0.51	0/1410
30	DI	0.38	0/1046	0.51	0/1410
31	BJ	0.77	0/1152	0.76	0/1551
31	DJ	0.36	0/1152	0.56	0/1551
32	BK	0.70	0/948	0.86	0/1268
32	DK	0.39	0/948	0.55	0/1268
33	BL	0.66	0/1054	0.80	0/1403
33	DL	0.36	0/1054	0.57	0/1403
34	BM	0.71	0/1093	0.86	1/1460 (0.1%)
34	DM	0.34	0/1093	0.53	0/1460
35	BN	0.71	0/974	0.89	0/1301
35	DN	0.36	0/974	0.53	0/1301
36	BO	0.50	0/902	0.67	0/1209
36	DO	0.32	0/902	0.46	0/1209
37	BP	0.64	0/929	0.74	0/1242
37	DP	0.39	0/929	0.55	0/1242
38	BQ	0.86	0/960	0.92	1/1278 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DQ	0.37	0/960	0.52	0/1278
39	BR	0.82	0/829	0.91	1/1107 (0.1%)
39	DR	0.35	0/829	0.55	0/1107
40	BS	0.85	0/864	0.91	1/1156 (0.1%)
40	DS	0.35	0/864	0.55	0/1156
41	BT	0.67	1/745 (0.1%)	0.77	1/994 (0.1%)
41	DT	0.38	0/745	0.57	0/994
42	BU	0.54	0/788	0.71	0/1051
42	DU	0.41	0/788	0.57	0/1051
43	BV	0.63	0/766	0.70	0/1025
43	DV	0.31	0/766	0.45	0/1025
44	BW	0.70	0/587	0.80	1/776 (0.1%)
44	DW	0.33	0/576	0.48	0/762
45	BX	0.52	0/635	0.71	0/848
45	DX	0.40	0/635	0.60	0/848
46	BY	0.55	0/510	0.74	0/677
46	DY	0.37	0/510	0.54	0/677
47	BZ	0.77	0/453	0.86	0/605
47	DZ	0.34	0/453	0.50	0/605
48	B0	0.77	0/450	0.81	0/599
48	D0	0.36	0/450	0.57	0/599
49	B1	0.50	0/417	0.60	0/554
49	D1	0.36	0/417	0.49	0/554
50	B2	0.77	0/380	0.95	0/498
50	D2	0.39	0/380	0.62	0/498
51	B3	0.63	0/513	0.86	1/676 (0.1%)
51	D3	0.33	0/513	0.53	0/676
52	B4	0.71	0/303	0.87	0/397
52	D4	0.32	0/303	0.51	0/397
53	B5	0.34	0/1145	0.47	0/1556
All	All	0.69	173/310634 (0.1%)	1.09	1646/464376 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	2
11	AK	0	1
11	CK	0	1
12	CL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	BD	0	1
25	DD	0	1
41	BT	0	1
47	BZ	0	1
All	All	0	9

The worst 5 of 173 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2777	G	N7-C5	15.93	1.48	1.39
22	BA	984	A	N9-C4	-14.44	1.29	1.37
22	BA	2777	G	N9-C8	13.80	1.47	1.37
22	BA	1142	A	N9-C4	-12.51	1.30	1.37
1	CA	500	G	N9-C8	10.22	1.45	1.37

The worst 5 of 1646 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BD	151	THR	C-N-CD	-21.19	73.98	120.60
22	BA	2777	G	C5-N7-C8	-19.20	94.70	104.30
22	BA	984	A	C2-N3-C4	-18.54	101.33	110.60
22	BA	2777	G	C4-C5-C6	-17.34	108.40	118.80
22	BA	528	A	N1-C6-N6	16.96	128.78	118.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
25	BD	132	ALA	Peptide
41	BT	2	ILE	Peptide
47	BZ	15	GLY	Peptide
5	CE	102	GLY	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	893	5
1	CA	33015	0	16617	1011	0
2	AB	1705	0	1732	112	0
2	CB	1705	0	1732	107	0
3	AC	1625	0	1696	57	0
3	CC	1625	0	1696	49	0
4	AD	1643	0	1707	117	0
4	CD	1643	0	1707	96	0
5	AE	1106	0	1148	81	0
5	CE	1106	0	1148	88	0
6	AF	818	0	808	47	0
6	CF	818	0	808	47	0
7	AG	1182	0	1238	47	0
7	CG	1182	0	1238	46	0
8	AH	979	0	1031	41	0
8	CH	979	0	1031	36	0
9	AI	1022	0	1070	55	0
9	CI	1022	0	1070	36	0
10	AJ	787	0	828	42	0
10	CJ	787	0	828	32	0
11	AK	877	0	887	59	0
11	CK	877	0	887	52	0
12	AL	955	0	1016	61	0
12	CL	955	0	1016	73	0
13	AM	884	0	941	51	0
13	CM	884	0	941	35	0
14	AN	774	0	824	44	0
14	CN	774	0	824	26	0
15	AO	714	0	734	28	0
15	CO	714	0	734	36	0
16	AP	649	0	666	27	0
16	CP	649	0	666	43	0
17	AQ	649	0	691	46	0
17	CQ	649	0	691	38	0
18	AR	456	0	478	9	0
18	CR	456	0	478	22	0
19	AS	638	0	665	33	0
19	CS	638	0	665	22	0
20	AT	665	0	714	41	0
20	CT	665	0	714	34	0
21	AU	426	0	449	59	0
21	CU	426	0	449	44	0
22	BA	62195	0	31278	1182	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	62195	0	31280	2055	0
23	BB	2549	0	1291	36	0
23	DB	2529	0	1281	42	0
24	BC	2083	0	2154	81	0
24	DC	2083	0	2154	161	0
25	BD	1565	0	1616	59	0
25	DD	1565	0	1616	69	0
26	BE	1552	0	1619	57	0
26	DE	1552	0	1619	80	0
27	BF	1411	0	1444	66	0
27	DF	1411	0	1444	26	0
28	BG	1323	0	1371	44	0
28	DG	1323	0	1371	41	0
29	BH	1110	0	1148	166	0
29	DH	1110	0	1148	86	5
30	BI	1032	0	1085	54	0
30	DI	1032	0	1085	38	0
31	BJ	1129	0	1162	41	0
31	DJ	1129	0	1162	43	0
32	BK	939	0	1012	29	0
32	DK	939	0	1012	33	0
33	BL	1045	0	1117	54	0
33	DL	1045	0	1117	59	0
34	BM	1074	0	1157	40	0
34	DM	1074	0	1157	23	0
35	BN	961	0	1000	46	0
35	DN	961	0	1000	47	0
36	BO	892	0	923	48	0
36	DO	892	0	923	36	0
37	BP	917	0	962	24	0
37	DP	917	0	962	40	0
38	BQ	947	0	1019	49	0
38	DQ	947	0	1019	47	0
39	BR	816	0	839	59	0
39	DR	816	0	839	45	0
40	BS	857	0	922	29	0
40	DS	857	0	922	29	0
41	BT	739	0	807	49	0
41	DT	739	0	807	27	0
42	BU	780	0	831	33	0
42	DU	780	0	831	61	0
43	BV	753	0	780	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DV	753	0	780	14	0
44	BW	580	0	594	22	0
44	DW	569	0	581	11	0
45	BX	625	0	652	21	0
45	DX	625	0	652	54	0
46	BY	509	0	543	30	0
46	DY	509	0	543	24	0
47	BZ	449	0	488	12	0
47	DZ	449	0	488	15	0
48	B0	444	0	458	24	0
48	D0	444	0	458	18	0
49	B1	410	0	440	15	0
49	D1	410	0	440	12	0
50	B2	377	0	418	14	0
50	D2	377	0	418	41	0
51	B3	504	0	572	23	0
51	D3	504	0	572	22	0
52	B4	302	0	340	9	0
52	D4	302	0	342	10	0
53	B5	1142	0	865	26	0
54	AA	71	0	0	0	0
54	AM	1	0	0	0	0
54	BA	194	0	0	0	0
54	BB	4	0	0	0	0
54	BQ	1	0	0	0	0
54	CA	56	0	0	0	0
54	CT	1	0	0	0	0
54	D2	1	0	0	0	0
54	DA	164	0	0	0	0
54	DB	3	0	0	0	0
54	DL	2	0	0	0	0
54	DQ	1	0	0	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	CA	17	0	19	1	0
57	AA	196	0	0	18	0
57	AE	1	0	0	0	0
57	AL	1	0	0	0	0
57	AN	3	0	0	1	0
57	AT	1	0	0	0	0
57	AU	1	0	0	0	0
57	B2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B3	3	0	0	0	0
57	B4	2	0	0	0	0
57	BA	620	0	0	82	0
57	BB	14	0	0	0	0
57	BC	10	0	0	1	0
57	BD	4	0	0	2	0
57	BF	1	0	0	0	0
57	BG	1	0	0	0	0
57	BL	6	0	0	2	0
57	BN	3	0	0	0	0
57	BS	1	0	0	0	0
57	CA	186	0	0	16	0
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	3	0	0	1	0
57	CU	1	0	0	0	0
57	D2	1	0	0	1	0
57	D3	2	0	0	0	0
57	D4	1	0	0	1	0
57	DA	611	0	0	87	0
57	DB	13	0	0	1	0
57	DC	8	0	0	0	0
57	DD	3	0	0	1	0
57	DE	5	0	0	0	0
57	DJ	1	0	0	0	0
57	DL	4	0	0	0	0
57	DN	1	0	0	0	0
57	DS	1	0	0	0	0
57	DT	3	0	0	0	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
All	All	288204	0	192819	8827	5

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 19.

The worst 5 of 8827 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:94:ILE:H	29:BH:122:LEU:CB	1.08	1.58
29:BH:94:ILE:O	29:BH:122:LEU:CD1	1.69	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:94:ILE:N	29:BH:122:LEU:CB	1.88	1.34
29:BH:94:ILE:N	29:BH:122:LEU:HB3	1.41	1.28
29:BH:122:LEU:HD21	1:CA:368:U:OP2	1.09	1.25

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:368:U:OP2	29:DH:123:ARG:NH2[4_455]	2.03	0.17
1:AA:368:U:OP2	29:DH:123:ARG:NE[4_455]	2.07	0.13
1:AA:368:U:OP1	29:DH:93:SER:OG[4_455]	2.08	0.12
1:AA:368:U:OP2	29:DH:123:ARG:CZ[4_455]	2.18	0.02
1:AA:359:G:OP1	29:DH:89:LYS:NZ[4_455]	2.19	0.01

## 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%)	140 (65%)	41 (19%)	35 (16%)	0	0
2	CB	216/218 (99%)	144 (67%)	44 (20%)	28 (13%)	0	1
3	AC	204/206 (99%)	161 (79%)	32 (16%)	11 (5%)	2	12
3	CC	204/206 (99%)	165 (81%)	29 (14%)	10 (5%)	2	14
4	AD	203/205 (99%)	149 (73%)	29 (14%)	25 (12%)	0	1
4	CD	203/205 (99%)	155 (76%)	34 (17%)	14 (7%)	1	7
5	AE	148/150 (99%)	109 (74%)	24 (16%)	15 (10%)	0	3
5	CE	148/150 (99%)	104 (70%)	29 (20%)	15 (10%)	0	3
6	AF	98/100 (98%)	75 (76%)	17 (17%)	6 (6%)	1	9
6	CF	98/100 (98%)	72 (74%)	17 (17%)	9 (9%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	111 (74%)	31 (21%)	7 (5%)	2	14
7	CG	149/151 (99%)	127 (85%)	18 (12%)	4 (3%)	5	25
8	AH	127/129 (98%)	97 (76%)	20 (16%)	10 (8%)	1	5
8	CH	127/129 (98%)	100 (79%)	24 (19%)	3 (2%)	6	27
9	AI	125/127 (98%)	93 (74%)	28 (22%)	4 (3%)	4	22
9	CI	125/127 (98%)	95 (76%)	23 (18%)	7 (6%)	2	11
10	AJ	96/98 (98%)	67 (70%)	13 (14%)	16 (17%)	0	0
10	CJ	96/98 (98%)	69 (72%)	15 (16%)	12 (12%)	0	1
11	AK	115/117 (98%)	91 (79%)	15 (13%)	9 (8%)	1	5
11	CK	115/117 (98%)	87 (76%)	23 (20%)	5 (4%)	2	16
12	AL	121/123 (98%)	84 (69%)	31 (26%)	6 (5%)	2	13
12	CL	121/123 (98%)	90 (74%)	16 (13%)	15 (12%)	0	1
13	AM	112/114 (98%)	84 (75%)	20 (18%)	8 (7%)	1	6
13	CM	112/114 (98%)	83 (74%)	16 (14%)	13 (12%)	0	2
14	AN	92/100 (92%)	65 (71%)	17 (18%)	10 (11%)	0	2
14	CN	92/100 (92%)	71 (77%)	13 (14%)	8 (9%)	1	4
15	AO	86/88 (98%)	72 (84%)	10 (12%)	4 (5%)	2	14
15	CO	86/88 (98%)	69 (80%)	14 (16%)	3 (4%)	3	20
16	AP	80/82 (98%)	49 (61%)	18 (22%)	13 (16%)	0	0
16	CP	80/82 (98%)	61 (76%)	14 (18%)	5 (6%)	1	8
17	AQ	78/80 (98%)	53 (68%)	20 (26%)	5 (6%)	1	8
17	CQ	78/80 (98%)	59 (76%)	12 (15%)	7 (9%)	1	4
18	AR	53/55 (96%)	44 (83%)	8 (15%)	1 (2%)	8	33
18	CR	53/55 (96%)	41 (77%)	8 (15%)	4 (8%)	1	6
19	AS	77/79 (98%)	61 (79%)	13 (17%)	3 (4%)	3	18
19	CS	77/79 (98%)	66 (86%)	6 (8%)	5 (6%)	1	8
20	AT	83/85 (98%)	68 (82%)	8 (10%)	7 (8%)	1	5
20	CT	83/85 (98%)	67 (81%)	10 (12%)	6 (7%)	1	6
21	AU	49/51 (96%)	29 (59%)	11 (22%)	9 (18%)	0	0
21	CU	49/51 (96%)	24 (49%)	11 (22%)	14 (29%)	0	0
24	BC	269/271 (99%)	219 (81%)	38 (14%)	12 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	200 (74%)	43 (16%)	26 (10%)	0	3
25	BD	207/209 (99%)	186 (90%)	18 (9%)	3 (1%)	11	40
25	DD	207/209 (99%)	165 (80%)	32 (16%)	10 (5%)	2	14
26	BE	199/201 (99%)	174 (87%)	22 (11%)	3 (2%)	10	39
26	DE	199/201 (99%)	167 (84%)	24 (12%)	8 (4%)	3	17
27	BF	175/177 (99%)	144 (82%)	19 (11%)	12 (7%)	1	7
27	DF	175/177 (99%)	143 (82%)	24 (14%)	8 (5%)	2	15
28	BG	174/176 (99%)	150 (86%)	18 (10%)	6 (3%)	3	21
28	DG	174/176 (99%)	145 (83%)	21 (12%)	8 (5%)	2	15
29	BH	147/149 (99%)	91 (62%)	35 (24%)	21 (14%)	0	1
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	0	3
30	BI	139/141 (99%)	85 (61%)	37 (27%)	17 (12%)	0	1
30	DI	139/141 (99%)	89 (64%)	39 (28%)	11 (8%)	1	5
31	BJ	140/142 (99%)	127 (91%)	9 (6%)	4 (3%)	4	24
31	DJ	140/142 (99%)	116 (83%)	22 (16%)	2 (1%)	11	40
32	BK	120/122 (98%)	98 (82%)	16 (13%)	6 (5%)	2	13
32	DK	120/122 (98%)	100 (83%)	14 (12%)	6 (5%)	2	13
33	BL	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	2	16
33	DL	141/143 (99%)	106 (75%)	28 (20%)	7 (5%)	2	13
34	BM	134/136 (98%)	118 (88%)	13 (10%)	3 (2%)	6	29
34	DM	134/136 (98%)	111 (83%)	18 (13%)	5 (4%)	3	19
35	BN	118/120 (98%)	98 (83%)	18 (15%)	2 (2%)	9	36
35	DN	118/120 (98%)	93 (79%)	18 (15%)	7 (6%)	1	10
36	BO	114/116 (98%)	94 (82%)	18 (16%)	2 (2%)	8	34
36	DO	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	3	20
37	BP	112/114 (98%)	104 (93%)	5 (4%)	3 (3%)	5	25
37	DP	112/114 (98%)	89 (80%)	18 (16%)	5 (4%)	2	15
38	BQ	115/117 (98%)	107 (93%)	5 (4%)	3 (3%)	5	26
38	DQ	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	5	26
39	BR	101/103 (98%)	90 (89%)	5 (5%)	6 (6%)	1	10
39	DR	101/103 (98%)	79 (78%)	17 (17%)	5 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	99 (92%)	7 (6%)	2 (2%)	8	33
40	DS	108/110 (98%)	91 (84%)	13 (12%)	4 (4%)	3	19
41	BT	91/93 (98%)	73 (80%)	9 (10%)	9 (10%)	0	3
41	DT	91/93 (98%)	65 (71%)	18 (20%)	8 (9%)	1	4
42	BU	100/102 (98%)	79 (79%)	15 (15%)	6 (6%)	1	9
42	DU	100/102 (98%)	74 (74%)	13 (13%)	13 (13%)	0	1
43	BV	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	14	46
43	DV	92/94 (98%)	83 (90%)	7 (8%)	2 (2%)	6	29
44	BW	74/76 (97%)	66 (89%)	7 (10%)	1 (1%)	11	40
44	DW	73/76 (96%)	61 (84%)	11 (15%)	1 (1%)	11	40
45	BX	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	12	42
45	DX	75/77 (97%)	54 (72%)	17 (23%)	4 (5%)	2	12
46	BY	61/63 (97%)	47 (77%)	5 (8%)	9 (15%)	0	0
46	DY	61/63 (97%)	50 (82%)	8 (13%)	3 (5%)	2	14
47	BZ	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
47	DZ	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	3	20
48	B0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	3	19
48	D0	54/56 (96%)	37 (68%)	14 (26%)	3 (6%)	2	11
49	B1	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	3	16
49	D1	48/50 (96%)	35 (73%)	9 (19%)	4 (8%)	1	5
50	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	2	15
50	D2	44/46 (96%)	38 (86%)	3 (7%)	3 (7%)	1	7
51	B3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	37
51	D3	62/64 (97%)	54 (87%)	6 (10%)	2 (3%)	4	22
52	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
52	D4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	2	11
53	B5	183/207 (88%)	100 (55%)	58 (32%)	25 (14%)	0	1
All	All	11418/11651 (98%)	8949 (78%)	1727 (15%)	742 (6%)	1	8

5 of 742 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE

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Mol	Chain	Res	Type
2	AB	34	ALA
2	AB	73	LYS
2	AB	74	ARG
2	AB	120	GLN

### 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%)	142 (79%)	38 (21%)	1	5
2	CB	180/180 (100%)	141 (78%)	39 (22%)	1	4
3	AC	170/170 (100%)	138 (81%)	32 (19%)	1	6
3	CC	170/170 (100%)	150 (88%)	20 (12%)	5	21
4	AD	172/172 (100%)	148 (86%)	24 (14%)	3	15
4	CD	172/172 (100%)	149 (87%)	23 (13%)	4	16
5	AE	113/113 (100%)	89 (79%)	24 (21%)	1	5
5	CE	113/113 (100%)	94 (83%)	19 (17%)	2	9
6	AF	87/87 (100%)	71 (82%)	16 (18%)	1	7
6	CF	87/87 (100%)	67 (77%)	20 (23%)	1	3
7	AG	124/124 (100%)	103 (83%)	21 (17%)	2	9
7	CG	124/124 (100%)	102 (82%)	22 (18%)	2	8
8	AH	104/104 (100%)	92 (88%)	12 (12%)	5	22
8	CH	104/104 (100%)	88 (85%)	16 (15%)	2	11
9	AI	105/105 (100%)	82 (78%)	23 (22%)	1	4
9	CI	105/105 (100%)	84 (80%)	21 (20%)	1	5
10	AJ	86/86 (100%)	71 (83%)	15 (17%)	2	9
10	CJ	86/86 (100%)	75 (87%)	11 (13%)	4	18
11	AK	90/90 (100%)	73 (81%)	17 (19%)	1	6
11	CK	90/90 (100%)	75 (83%)	15 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	90 (87%)	13 (13%)	4	18
12	CL	103/103 (100%)	81 (79%)	22 (21%)	1	4
13	AM	92/92 (100%)	82 (89%)	10 (11%)	6	25
13	CM	92/92 (100%)	82 (89%)	10 (11%)	6	25
14	AN	79/83 (95%)	71 (90%)	8 (10%)	7	28
14	CN	79/83 (95%)	74 (94%)	5 (6%)	18	48
15	AO	76/76 (100%)	66 (87%)	10 (13%)	4	17
15	CO	76/76 (100%)	61 (80%)	15 (20%)	1	6
16	AP	65/65 (100%)	54 (83%)	11 (17%)	2	9
16	CP	65/65 (100%)	55 (85%)	10 (15%)	2	11
17	AQ	74/74 (100%)	58 (78%)	16 (22%)	1	4
17	CQ	74/74 (100%)	59 (80%)	15 (20%)	1	5
18	AR	48/48 (100%)	44 (92%)	4 (8%)	11	38
18	CR	48/48 (100%)	43 (90%)	5 (10%)	7	27
19	AS	70/70 (100%)	63 (90%)	7 (10%)	7	28
19	CS	70/70 (100%)	63 (90%)	7 (10%)	7	28
20	AT	65/65 (100%)	55 (85%)	10 (15%)	2	11
20	CT	65/65 (100%)	55 (85%)	10 (15%)	2	11
21	AU	44/44 (100%)	29 (66%)	15 (34%)	0	0
21	CU	44/44 (100%)	31 (70%)	13 (30%)	0	1
24	BC	216/216 (100%)	195 (90%)	21 (10%)	8	30
24	DC	216/216 (100%)	191 (88%)	25 (12%)	5	22
25	BD	164/164 (100%)	154 (94%)	10 (6%)	18	49
25	DD	164/164 (100%)	147 (90%)	17 (10%)	7	27
26	BE	165/165 (100%)	152 (92%)	13 (8%)	12	40
26	DE	165/165 (100%)	152 (92%)	13 (8%)	12	40
27	BF	148/148 (100%)	127 (86%)	21 (14%)	3	14
27	DF	148/148 (100%)	131 (88%)	17 (12%)	5	22
28	BG	137/137 (100%)	122 (89%)	15 (11%)	6	25
28	DG	137/137 (100%)	124 (90%)	13 (10%)	8	31
29	BH	114/114 (100%)	89 (78%)	25 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	89 (78%)	25 (22%)	1	4
30	BI	109/109 (100%)	86 (79%)	23 (21%)	1	5
30	DI	109/109 (100%)	91 (84%)	18 (16%)	2	10
31	BJ	116/116 (100%)	106 (91%)	10 (9%)	10	37
31	DJ	116/116 (100%)	110 (95%)	6 (5%)	23	55
32	BK	103/103 (100%)	93 (90%)	10 (10%)	8	30
32	DK	103/103 (100%)	96 (93%)	7 (7%)	16	45
33	BL	102/102 (100%)	88 (86%)	14 (14%)	3	16
33	DL	102/102 (100%)	94 (92%)	8 (8%)	12	40
34	BM	109/109 (100%)	98 (90%)	11 (10%)	7	28
34	DM	109/109 (100%)	104 (95%)	5 (5%)	27	59
35	BN	100/100 (100%)	87 (87%)	13 (13%)	4	18
35	DN	100/100 (100%)	89 (89%)	11 (11%)	6	25
36	BO	86/86 (100%)	72 (84%)	14 (16%)	2	10
36	DO	86/86 (100%)	78 (91%)	8 (9%)	9	32
37	BP	99/99 (100%)	89 (90%)	10 (10%)	7	28
37	DP	99/99 (100%)	89 (90%)	10 (10%)	7	28
38	BQ	89/89 (100%)	81 (91%)	8 (9%)	9	34
38	DQ	89/89 (100%)	84 (94%)	5 (6%)	21	52
39	BR	84/84 (100%)	71 (84%)	13 (16%)	2	11
39	DR	84/84 (100%)	79 (94%)	5 (6%)	19	49
40	BS	93/93 (100%)	80 (86%)	13 (14%)	3	15
40	DS	93/93 (100%)	86 (92%)	7 (8%)	13	42
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	12
41	DT	80/80 (100%)	68 (85%)	12 (15%)	3	12
42	BU	83/83 (100%)	74 (89%)	9 (11%)	6	25
42	DU	83/83 (100%)	73 (88%)	10 (12%)	5	20
43	BV	78/78 (100%)	68 (87%)	10 (13%)	4	18
43	DV	78/78 (100%)	71 (91%)	7 (9%)	9	34
44	BW	57/58 (98%)	55 (96%)	2 (4%)	36	68
44	DW	56/58 (97%)	52 (93%)	4 (7%)	14	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	64 (96%)	3 (4%)	27	60
45	DX	67/67 (100%)	61 (91%)	6 (9%)	9	34
46	BY	55/55 (100%)	47 (86%)	8 (14%)	3	13
46	DY	55/55 (100%)	46 (84%)	9 (16%)	2	10
47	BZ	48/48 (100%)	41 (85%)	7 (15%)	3	13
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	2	9
48	B0	47/47 (100%)	40 (85%)	7 (15%)	3	13
48	D0	47/47 (100%)	42 (89%)	5 (11%)	6	26
49	B1	45/45 (100%)	39 (87%)	6 (13%)	4	16
49	D1	45/45 (100%)	43 (96%)	2 (4%)	28	61
50	B2	38/38 (100%)	34 (90%)	4 (10%)	7	26
50	D2	38/38 (100%)	32 (84%)	6 (16%)	2	11
51	B3	51/51 (100%)	47 (92%)	4 (8%)	12	40
51	D3	51/51 (100%)	48 (94%)	3 (6%)	19	50
52	B4	34/34 (100%)	29 (85%)	5 (15%)	3	13
52	D4	34/34 (100%)	31 (91%)	3 (9%)	10	36
53	B5	61/161 (38%)	50 (82%)	11 (18%)	1	7
All	All	9388/9499 (99%)	8137 (87%)	1251 (13%)	4	16

5 of 1251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	BS	59	GLU
3	CC	27	LYS
37	DP	80	VAL
42	BU	9	ASP
50	B2	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
27	BF	21	ASN
6	CF	37	HIS
40	DS	7	HIS
36	BO	29	HIS

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Mol	Chain	Res	Type
15	CO	46	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	304 (19%)	13 (0%)
1	CA	1538/1539 (99%)	303 (19%)	7 (0%)
22	BA	2895/2903 (99%)	518 (17%)	34 (1%)
22	DA	2895/2903 (99%)	536 (18%)	22 (0%)
23	BB	118/119 (99%)	16 (13%)	1 (0%)
23	DB	117/119 (98%)	18 (15%)	0
All	All	9100/9122 (99%)	1695 (18%)	77 (0%)

5 of 1695 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	7	A
1	AA	9	G
1	AA	13	U

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	1610	A
22	BA	2425	A
22	DA	2225	A
22	BA	1738	G
22	BA	2286	G

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 502 ligands modelled in this entry, 501 are monoatomic - leaving 1 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	NEG	CA	1657	54	9,16,16	0.74	0	10,20,20	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	NEG	CA	1657	54	-	8/15/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	CA	1657	NEG	C8-C7-N3-N2
56	CA	1657	NEG	C6-N2-N3-C9
56	CA	1657	NEG	N4-C4-C5-C6
56	CA	1657	NEG	C3-C4-C5-C6
56	CA	1657	NEG	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	1657	NEG	1	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1538/1539 (99%)	-0.07	54 (3%) 44 23	12, 56, 146, 187	0
1	CA	1539/1539 (100%)	0.38	132 (8%) 10 4	24, 78, 151, 182	0
2	AB	218/218 (100%)	0.25	13 (5%) 21 10	38, 79, 106, 130	0
2	CB	218/218 (100%)	0.49	24 (11%) 5 2	62, 97, 114, 127	0
3	AC	206/206 (100%)	0.37	14 (6%) 17 7	57, 83, 97, 110	0
3	CC	206/206 (100%)	1.39	59 (28%) 0 0	83, 101, 112, 120	0
4	AD	205/205 (100%)	-0.10	3 (1%) 73 54	39, 64, 88, 106	0
4	CD	205/205 (100%)	-0.20	4 (1%) 65 44	21, 41, 70, 92	0
5	AE	150/150 (100%)	-0.08	1 (0%) 87 75	31, 50, 83, 105	0
5	CE	150/150 (100%)	-0.06	0 100 100	28, 58, 89, 109	0
6	AF	100/100 (100%)	0.17	4 (4%) 38 19	36, 60, 80, 92	0
6	CF	100/100 (100%)	0.12	2 (2%) 65 44	48, 81, 103, 108	0
7	AG	151/151 (100%)	0.75	25 (16%) 1 1	68, 93, 106, 116	0
7	CG	151/151 (100%)	2.68	88 (58%) 0 0	95, 117, 127, 130	0
8	AH	129/129 (100%)	-0.18	1 (0%) 86 72	31, 52, 72, 90	0
8	CH	129/129 (100%)	0.09	7 (5%) 25 12	55, 75, 93, 105	0
9	AI	127/127 (100%)	1.45	42 (33%) 0 0	70, 95, 110, 122	0
9	CI	127/127 (100%)	2.03	50 (39%) 0 0	100, 112, 123, 131	0
10	AJ	98/98 (100%)	0.89	19 (19%) 1 0	76, 90, 107, 127	0
10	CJ	98/98 (100%)	3.19	55 (56%) 0 0	97, 114, 122, 133	0
11	AK	117/117 (100%)	0.08	3 (2%) 56 33	26, 70, 98, 117	0
11	CK	117/117 (100%)	0.06	3 (2%) 56 33	36, 75, 94, 98	0
12	AL	123/123 (100%)	-0.13	3 (2%) 59 37	23, 39, 70, 100	0
12	CL	123/123 (100%)	0.19	5 (4%) 37 18	34, 56, 84, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/114 (100%)	0.92	23 (20%) 1 0	70, 87, 104, 111	0
13	CM	114/114 (100%)	3.30	82 (71%) 0 0	105, 122, 130, 134	0
14	AN	96/100 (96%)	1.05	23 (23%) 0 0	79, 91, 108, 117	0
14	CN	96/100 (96%)	2.56	60 (62%) 0 0	98, 112, 125, 129	0
15	AO	88/88 (100%)	-0.15	0 100 100	30, 51, 72, 92	0
15	CO	88/88 (100%)	0.25	5 (5%) 23 11	45, 71, 89, 106	0
16	AP	82/82 (100%)	0.10	2 (2%) 59 37	34, 51, 92, 108	0
16	CP	82/82 (100%)	0.73	11 (13%) 3 1	52, 73, 105, 117	0
17	AQ	80/80 (100%)	0.26	2 (2%) 57 34	30, 53, 77, 120	0
17	CQ	80/80 (100%)	0.88	14 (17%) 1 0	48, 88, 102, 109	0
18	AR	55/55 (100%)	0.20	3 (5%) 25 11	44, 57, 87, 108	0
18	CR	55/55 (100%)	0.22	4 (7%) 15 6	41, 58, 85, 109	0
19	AS	79/79 (100%)	1.40	20 (25%) 0 0	78, 95, 107, 113	0
19	CS	79/79 (100%)	2.43	44 (55%) 0 0	105, 123, 130, 133	0
20	AT	85/85 (100%)	0.21	3 (3%) 44 23	35, 52, 79, 98	0
20	CT	85/85 (100%)	1.41	22 (25%) 0 0	61, 86, 102, 106	0
21	AU	51/51 (100%)	0.28	3 (5%) 22 10	39, 73, 105, 115	0
21	CU	51/51 (100%)	0.27	3 (5%) 22 10	46, 73, 101, 107	0
22	BA	2897/2903 (99%)	0.08	130 (4%) 33 16	1, 14, 135, 195	0
22	DA	2897/2903 (99%)	0.53	214 (7%) 14 5	38, 91, 152, 183	0
23	BB	119/119 (100%)	-0.39	0 100 100	2, 25, 59, 89	0
23	DB	118/119 (99%)	0.42	5 (4%) 36 18	80, 119, 136, 145	0
24	BC	271/271 (100%)	-0.15	12 (4%) 34 17	2, 21, 52, 65	0
24	DC	271/271 (100%)	0.47	24 (8%) 9 3	45, 70, 90, 96	0
25	BD	209/209 (100%)	-0.34	0 100 100	1, 12, 38, 77	0
25	DD	209/209 (100%)	0.78	34 (16%) 1 1	56, 82, 97, 107	0
26	BE	201/201 (100%)	-0.34	1 (0%) 91 81	1, 27, 64, 92	0
26	DE	201/201 (100%)	1.13	45 (22%) 0 0	63, 98, 114, 122	0
27	BF	177/177 (100%)	-0.12	6 (3%) 45 24	20, 51, 84, 100	0
27	DF	177/177 (100%)	2.08	71 (40%) 0 0	100, 119, 131, 137	0
28	BG	176/176 (100%)	-0.29	2 (1%) 80 64	12, 38, 66, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DG	176/176 (100%)	1.66	57 (32%) 0 0	87, 105, 116, 126	0
29	BH	149/149 (100%)	2.45	64 (42%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	0.93	22 (14%) 2 1	25, 92, 107, 115	0
30	BI	141/141 (100%)	2.93	72 (51%) 0 0	103, 122, 132, 139	0
30	DI	141/141 (100%)	4.25	124 (87%) 0 0	109, 130, 140, 149	0
31	BJ	142/142 (100%)	-0.33	0 100 100	1, 8, 28, 41	0
31	DJ	142/142 (100%)	0.45	11 (7%) 13 5	57, 79, 92, 103	0
32	BK	122/122 (100%)	-0.37	0 100 100	4, 13, 35, 66	0
32	DK	122/122 (100%)	0.56	16 (13%) 3 1	56, 75, 94, 106	0
33	BL	143/143 (100%)	-0.33	0 100 100	1, 22, 52, 87	0
33	DL	143/143 (100%)	1.26	32 (22%) 0 0	58, 92, 106, 127	0
34	BM	136/136 (100%)	-0.41	0 100 100	1, 11, 34, 82	0
34	DM	136/136 (100%)	0.36	11 (8%) 12 5	50, 79, 94, 113	0
35	BN	120/120 (100%)	-0.39	0 100 100	2, 10, 21, 70	0
35	DN	120/120 (100%)	0.83	18 (15%) 2 1	65, 88, 100, 123	0
36	BO	116/116 (100%)	-0.32	0 100 100	12, 30, 47, 57	0
36	DO	116/116 (100%)	1.77	50 (43%) 0 0	91, 106, 114, 121	0
37	BP	114/114 (100%)	-0.35	0 100 100	5, 18, 46, 67	0
37	DP	114/114 (100%)	0.83	22 (19%) 1 0	65, 81, 94, 103	0
38	BQ	117/117 (100%)	-0.27	0 100 100	1, 4, 15, 52	0
38	DQ	117/117 (100%)	0.86	17 (14%) 2 1	62, 79, 89, 94	0
39	BR	103/103 (100%)	-0.42	0 100 100	1, 13, 35, 67	0
39	DR	103/103 (100%)	1.29	26 (25%) 0 0	67, 91, 101, 103	0
40	BS	110/110 (100%)	-0.40	0 100 100	1, 5, 27, 79	0
40	DS	110/110 (100%)	1.27	26 (23%) 0 0	68, 88, 105, 112	0
41	BT	93/93 (100%)	-0.04	2 (2%) 62 41	8, 27, 77, 106	0
41	DT	93/93 (100%)	1.64	30 (32%) 0 0	80, 98, 117, 125	0
42	BU	102/102 (100%)	0.10	8 (7%) 13 5	13, 32, 67, 96	0
42	DU	102/102 (100%)	2.28	44 (43%) 0 0	88, 106, 122, 129	0
43	BV	94/94 (100%)	-0.36	0 100 100	7, 23, 51, 63	0
43	DV	94/94 (100%)	0.50	7 (7%) 14 5	74, 95, 107, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BW	76/76 (100%)	-0.27	1 (1%) 77 59	3, 13, 32, 61	0
44	DW	75/76 (98%)	1.57	21 (28%) 0 0	60, 90, 99, 114	0
45	BX	77/77 (100%)	-0.33	0 100 100	5, 26, 54, 77	0
45	DX	77/77 (100%)	0.74	8 (10%) 6 2	57, 80, 94, 101	0
46	BY	63/63 (100%)	0.04	1 (1%) 72 51	17, 40, 74, 92	0
46	DY	63/63 (100%)	1.78	29 (46%) 0 0	89, 105, 112, 115	0
47	BZ	58/58 (100%)	-0.28	0 100 100	2, 8, 35, 48	0
47	DZ	58/58 (100%)	0.63	6 (10%) 6 2	64, 81, 96, 102	0
48	B0	56/56 (100%)	-0.47	0 100 100	1, 11, 44, 65	0
48	D0	56/56 (100%)	1.12	15 (26%) 0 0	58, 89, 102, 109	0
49	B1	50/50 (100%)	0.33	3 (6%) 21 10	25, 38, 63, 84	0
49	D1	50/50 (100%)	2.29	24 (48%) 0 0	79, 99, 108, 112	0
50	B2	46/46 (100%)	-0.21	0 100 100	3, 8, 17, 80	0
50	D2	46/46 (100%)	0.92	7 (15%) 2 1	58, 80, 89, 105	0
51	B3	64/64 (100%)	-0.28	0 100 100	5, 11, 20, 33	0
51	D3	64/64 (100%)	0.92	11 (17%) 1 0	66, 82, 93, 98	0
52	B4	38/38 (100%)	-0.17	0 100 100	4, 13, 33, 51	0
52	D4	38/38 (100%)	1.48	10 (26%) 0 0	65, 84, 99, 109	0
53	B5	191/207 (92%)	4.94	167 (87%) 0 0	108, 127, 138, 143	0
All	All	20734/20773 (99%)	0.51	2441 (11%) 4 2	1, 73, 130, 195	0

The worst 5 of 2441 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	BA	2184	A	19.4
30	BI	3	LYS	16.7
22	BA	2101	A	16.1
30	BI	2	ALA	15.3
30	BI	4	LYS	15.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	DA	3092	1/1	-0.22	0.48	123,123,123,123	0
54	MG	CA	1644	1/1	-0.04	1.57	86,86,86,86	0
54	MG	DA	3040	1/1	0.07	0.64	94,94,94,94	0
54	MG	DA	3144	1/1	0.08	0.34	96,96,96,96	0
54	MG	CA	1651	1/1	0.15	0.46	70,70,70,70	0
54	MG	DA	3146	1/1	0.23	0.19	68,68,68,68	0
54	MG	DA	3132	1/1	0.26	1.09	123,123,123,123	0
54	MG	AA	1617	1/1	0.27	0.84	124,124,124,124	0
54	MG	BA	3102	1/1	0.29	0.36	68,68,68,68	0
54	MG	DA	3026	1/1	0.33	0.14	93,93,93,93	0
54	MG	BA	3179	1/1	0.33	1.42	29,29,29,29	0
54	MG	DL	201	1/1	0.38	0.48	95,95,95,95	0
54	MG	CA	1628	1/1	0.40	0.14	137,137,137,137	0
54	MG	DA	3055	1/1	0.42	0.60	109,109,109,109	0
54	MG	DA	3114	1/1	0.42	0.42	126,126,126,126	0
54	MG	DA	3006	1/1	0.43	0.13	127,127,127,127	0
54	MG	DA	3024	1/1	0.46	0.25	77,77,77,77	0
54	MG	DA	3004	1/1	0.47	0.53	112,112,112,112	0
54	MG	DA	3091	1/1	0.50	0.71	128,128,128,128	0
54	MG	DA	3047	1/1	0.51	0.16	132,132,132,132	0
54	MG	AM	201	1/1	0.52	1.28	63,63,63,63	0
54	MG	DA	3071	1/1	0.52	0.33	99,99,99,99	0
54	MG	AA	1658	1/1	0.52	0.51	71,71,71,71	0
54	MG	DA	3164	1/1	0.53	0.55	60,60,60,60	0
54	MG	CA	1626	1/1	0.54	0.93	125,125,125,125	0
54	MG	DA	3059	1/1	0.56	0.34	87,87,87,87	0
54	MG	DA	3083	1/1	0.57	0.28	116,116,116,116	0
54	MG	DA	3159	1/1	0.58	0.45	71,71,71,71	0
54	MG	DA	3056	1/1	0.58	0.64	103,103,103,103	0
54	MG	DA	3060	1/1	0.60	0.66	92,92,92,92	0
54	MG	AA	1671	1/1	0.60	0.54	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1633	1/1	0.61	0.29	134,134,134,134	0
54	MG	DA	3089	1/1	0.61	0.15	106,106,106,106	0
54	MG	AA	1644	1/1	0.62	0.61	60,60,60,60	0
54	MG	BA	3060	1/1	0.63	0.70	72,72,72,72	0
54	MG	CA	1619	1/1	0.64	0.10	85,85,85,85	0
54	MG	AA	1662	1/1	0.64	0.75	76,76,76,76	0
54	MG	DA	3043	1/1	0.64	0.31	104,104,104,104	0
54	MG	DA	3130	1/1	0.65	1.53	108,108,108,108	0
54	MG	CA	1634	1/1	0.65	0.59	143,143,143,143	0
54	MG	DA	3013	1/1	0.65	0.22	72,72,72,72	0
54	MG	BA	3015	1/1	0.65	0.32	62,62,62,62	0
54	MG	DA	3036	1/1	0.66	0.14	114,114,114,114	0
54	MG	DA	3162	1/1	0.67	0.49	66,66,66,66	0
54	MG	DA	3025	1/1	0.67	1.86	120,120,120,120	0
54	MG	DA	3070	1/1	0.68	0.20	105,105,105,105	0
54	MG	DA	3118	1/1	0.68	0.61	113,113,113,113	0
54	MG	CA	1627	1/1	0.68	0.07	116,116,116,116	0
54	MG	DA	3076	1/1	0.68	0.52	114,114,114,114	0
54	MG	CA	1654	1/1	0.69	0.68	70,70,70,70	0
54	MG	BA	3168	1/1	0.69	0.74	43,43,43,43	0
54	MG	AA	1666	1/1	0.69	0.36	55,55,55,55	0
54	MG	DA	3081	1/1	0.69	0.12	75,75,75,75	0
54	MG	AA	1628	1/1	0.69	0.12	84,84,84,84	0
54	MG	BA	3131	1/1	0.70	0.29	49,49,49,49	0
54	MG	DA	3098	1/1	0.70	0.20	89,89,89,89	0
54	MG	DA	3057	1/1	0.70	0.85	99,99,99,99	0
54	MG	CA	1653	1/1	0.70	0.39	54,54,54,54	0
54	MG	BA	3176	1/1	0.70	0.45	37,37,37,37	0
54	MG	AA	1649	1/1	0.70	0.65	52,52,52,52	0
54	MG	DA	3145	1/1	0.70	1.24	60,60,60,60	0
54	MG	CA	1629	1/1	0.70	0.51	123,123,123,123	0
54	MG	AA	1646	1/1	0.71	0.60	49,49,49,49	0
54	MG	DA	3134	1/1	0.71	0.30	112,112,112,112	0
54	MG	DA	3155	1/1	0.71	0.74	51,51,51,51	0
54	MG	DA	3136	1/1	0.72	0.54	46,46,46,46	0
54	MG	AA	1614	1/1	0.72	0.64	97,97,97,97	0
54	MG	DA	3120	1/1	0.72	0.27	82,82,82,82	0
54	MG	DA	3088	1/1	0.72	0.22	81,81,81,81	0
54	MG	DA	3074	1/1	0.72	0.18	96,96,96,96	0
54	MG	BA	3115	1/1	0.72	0.16	58,58,58,58	0
54	MG	AA	1657	1/1	0.73	0.45	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1605	1/1	0.73	0.20	110,110,110,110	0
54	MG	AA	1659	1/1	0.73	0.45	68,68,68,68	0
54	MG	BA	3167	1/1	0.73	0.41	25,25,25,25	0
54	MG	DB	201	1/1	0.73	0.09	118,118,118,118	0
54	MG	DA	3163	1/1	0.74	0.25	45,45,45,45	0
54	MG	AA	1624	1/1	0.74	0.12	36,36,36,36	0
54	MG	DA	3028	1/1	0.74	0.14	83,83,83,83	0
54	MG	DA	3041	1/1	0.74	0.15	96,96,96,96	0
54	MG	DA	3105	1/1	0.75	0.17	77,77,77,77	0
54	MG	AA	1670	1/1	0.75	0.43	49,49,49,49	0
54	MG	DA	3087	1/1	0.76	0.10	84,84,84,84	0
54	MG	CA	1650	1/1	0.76	0.41	85,85,85,85	0
54	MG	DA	3016	1/1	0.76	0.18	103,103,103,103	0
54	MG	DA	3008	1/1	0.76	0.27	96,96,96,96	0
54	MG	AA	1669	1/1	0.76	0.72	83,83,83,83	0
54	MG	DA	3093	1/1	0.76	0.23	119,119,119,119	0
54	MG	DA	3061	1/1	0.76	1.24	91,91,91,91	0
54	MG	DA	3094	1/1	0.76	0.38	99,99,99,99	0
54	MG	DA	3084	1/1	0.76	0.42	104,104,104,104	0
54	MG	CA	1648	1/1	0.76	0.43	47,47,47,47	0
54	MG	DA	3100	1/1	0.76	0.17	74,74,74,74	0
54	MG	BA	3061	1/1	0.77	0.33	56,56,56,56	0
54	MG	BA	3133	1/1	0.77	0.56	63,63,63,63	0
54	MG	DA	3072	1/1	0.77	0.27	78,78,78,78	0
54	MG	CA	1636	1/1	0.77	0.18	93,93,93,93	0
54	MG	DA	3152	1/1	0.77	0.29	59,59,59,59	0
54	MG	DA	3158	1/1	0.77	0.33	52,52,52,52	0
54	MG	DA	3069	1/1	0.78	0.06	121,121,121,121	0
54	MG	DA	3116	1/1	0.78	0.20	106,106,106,106	0
54	MG	DA	3018	1/1	0.78	0.11	88,88,88,88	0
54	MG	DA	3099	1/1	0.78	0.13	69,69,69,69	0
54	MG	DA	3140	1/1	0.78	0.48	51,51,51,51	0
54	MG	BA	3161	1/1	0.78	0.40	30,30,30,30	0
54	MG	DA	3135	1/1	0.78	0.62	112,112,112,112	0
54	MG	AA	1620	1/1	0.79	0.12	100,100,100,100	0
54	MG	DA	3005	1/1	0.79	0.19	113,113,113,113	0
54	MG	AA	1652	1/1	0.79	0.21	63,63,63,63	0
54	MG	CA	1620	1/1	0.79	0.10	81,81,81,81	0
54	MG	DA	3153	1/1	0.80	0.42	58,58,58,58	0
54	MG	DA	3078	1/1	0.80	0.09	103,103,103,103	0
54	MG	DA	3001	1/1	0.80	0.13	93,93,93,93	0
54	MG	CA	1614	1/1	0.80	0.27	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1630	1/1	0.80	0.06	79,79,79,79	0
54	MG	BA	3040	1/1	0.80	0.47	1,1,1,1	0
54	MG	BA	3149	1/1	0.80	0.23	48,48,48,48	0
54	MG	DA	3029	1/1	0.80	0.18	83,83,83,83	0
54	MG	BA	3160	1/1	0.81	0.35	7,7,7,7	0
54	MG	DA	3103	1/1	0.81	0.10	85,85,85,85	0
54	MG	DA	3147	1/1	0.81	0.41	49,49,49,49	0
54	MG	D2	101	1/1	0.81	0.18	111,111,111,111	0
54	MG	CA	1632	1/1	0.81	0.16	85,85,85,85	0
54	MG	AA	1650	1/1	0.81	0.80	49,49,49,49	0
54	MG	CA	1608	1/1	0.81	0.17	86,86,86,86	0
54	MG	AA	1638	1/1	0.82	0.15	88,88,88,88	0
54	MG	DA	3149	1/1	0.82	0.38	77,77,77,77	0
54	MG	BA	3191	1/1	0.82	0.30	17,17,17,17	0
54	MG	BA	3073	1/1	0.82	0.12	16,16,16,16	0
54	MG	DA	3048	1/1	0.82	0.36	109,109,109,109	0
54	MG	BA	3150	1/1	0.83	0.34	23,23,23,23	0
54	MG	DA	3007	1/1	0.83	0.29	114,114,114,114	0
54	MG	BA	3189	1/1	0.83	0.17	43,43,43,43	0
54	MG	BA	3057	1/1	0.83	0.48	40,40,40,40	0
54	MG	DA	3154	1/1	0.83	0.36	63,63,63,63	0
54	MG	AA	1625	1/1	0.83	0.08	47,47,47,47	0
54	MG	CA	1642	1/1	0.83	0.28	53,53,53,53	0
54	MG	DA	3002	1/1	0.83	0.47	94,94,94,94	0
54	MG	DA	3143	1/1	0.84	0.45	63,63,63,63	0
54	MG	AA	1604	1/1	0.84	0.09	81,81,81,81	0
54	MG	DA	3067	1/1	0.84	0.17	70,70,70,70	0
54	MG	DA	3077	1/1	0.84	0.13	114,114,114,114	0
54	MG	AA	1663	1/1	0.84	0.66	36,36,36,36	0
54	MG	DA	3027	1/1	0.84	0.55	106,106,106,106	0
54	MG	DA	3009	1/1	0.84	0.07	91,91,91,91	0
54	MG	AA	1635	1/1	0.85	0.26	73,73,73,73	0
54	MG	BA	3055	1/1	0.85	0.64	89,89,89,89	0
54	MG	CA	1607	1/1	0.85	0.20	96,96,96,96	0
54	MG	BA	3148	1/1	0.85	0.62	44,44,44,44	0
54	MG	BA	3121	1/1	0.85	0.14	50,50,50,50	0
54	MG	CA	1613	1/1	0.85	0.10	51,51,51,51	0
54	MG	DA	3095	1/1	0.85	0.08	77,77,77,77	0
54	MG	DL	202	1/1	0.85	0.39	116,116,116,116	0
54	MG	DQ	201	1/1	0.85	0.76	51,51,51,51	0
54	MG	BA	3003	1/1	0.85	0.09	29,29,29,29	0
54	MG	AA	1601	1/1	0.85	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3053	1/1	0.85	0.19	49,49,49,49	0
54	MG	DA	3031	1/1	0.85	0.52	95,95,95,95	0
54	MG	CA	1645	1/1	0.86	0.38	52,52,52,52	0
54	MG	BA	3170	1/1	0.86	0.25	44,44,44,44	0
54	MG	BA	3114	1/1	0.86	0.14	14,14,14,14	0
54	MG	AA	1634	1/1	0.86	0.12	58,58,58,58	0
54	MG	DA	3104	1/1	0.86	0.46	97,97,97,97	0
54	MG	DA	3161	1/1	0.86	0.35	65,65,65,65	0
54	MG	BA	3185	1/1	0.86	0.28	17,17,17,17	0
54	MG	BA	3163	1/1	0.86	0.99	36,36,36,36	0
54	MG	DA	3037	1/1	0.86	0.25	66,66,66,66	0
54	MG	DA	3157	1/1	0.86	0.36	61,61,61,61	0
54	MG	CA	1604	1/1	0.87	0.07	102,102,102,102	0
54	MG	BA	3036	1/1	0.87	0.53	20,20,20,20	0
54	MG	DA	3090	1/1	0.87	0.09	85,85,85,85	0
56	NEG	CA	1657	17/17	0.87	0.13	62,88,103,104	0
54	MG	DA	3106	1/1	0.87	0.10	60,60,60,60	0
54	MG	CA	1649	1/1	0.87	0.63	50,50,50,50	0
54	MG	DA	3124	1/1	0.87	0.26	55,55,55,55	0
54	MG	CA	1616	1/1	0.87	0.11	43,43,43,43	0
54	MG	DA	3133	1/1	0.87	0.14	78,78,78,78	0
54	MG	BA	3174	1/1	0.87	0.82	25,25,25,25	0
54	MG	AA	1618	1/1	0.87	0.10	89,89,89,89	0
54	MG	CA	1641	1/1	0.87	0.56	49,49,49,49	0
54	MG	DA	3137	1/1	0.87	0.49	38,38,38,38	0
54	MG	BA	3105	1/1	0.87	0.22	10,10,10,10	0
54	MG	DA	3052	1/1	0.88	0.09	50,50,50,50	0
54	MG	AA	1619	1/1	0.88	0.24	57,57,57,57	0
54	MG	DA	3049	1/1	0.88	0.10	61,61,61,61	0
54	MG	DA	3115	1/1	0.88	0.29	79,79,79,79	0
54	MG	BA	3188	1/1	0.88	0.20	5,5,5,5	0
54	MG	CA	1652	1/1	0.88	0.45	73,73,73,73	0
54	MG	BA	3166	1/1	0.88	0.45	36,36,36,36	0
54	MG	DA	3015	1/1	0.88	0.32	90,90,90,90	0
54	MG	BQ	201	1/1	0.88	0.33	17,17,17,17	0
54	MG	AA	1648	1/1	0.88	0.32	34,34,34,34	0
54	MG	DA	3102	1/1	0.88	0.15	77,77,77,77	0
54	MG	CA	1639	1/1	0.88	0.15	59,59,59,59	0
54	MG	BA	3169	1/1	0.88	0.19	33,33,33,33	0
54	MG	AA	1667	1/1	0.88	0.49	54,54,54,54	0
54	MG	BA	3186	1/1	0.88	0.35	29,29,29,29	0
54	MG	BA	3034	1/1	0.88	0.50	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3110	1/1	0.88	0.23	61,61,61,61	0
54	MG	DA	3107	1/1	0.88	0.18	70,70,70,70	0
54	MG	DA	3030	1/1	0.88	0.18	71,71,71,71	0
54	MG	BA	3101	1/1	0.88	0.12	14,14,14,14	0
54	MG	CA	1640	1/1	0.88	0.35	29,29,29,29	0
54	MG	DA	3039	1/1	0.89	0.18	96,96,96,96	0
54	MG	DA	3111	1/1	0.89	0.12	71,71,71,71	0
54	MG	DA	3054	1/1	0.89	0.14	64,64,64,64	0
54	MG	BA	3011	1/1	0.89	0.07	16,16,16,16	0
54	MG	CA	1655	1/1	0.89	0.07	85,85,85,85	0
54	MG	BA	3155	1/1	0.89	0.26	21,21,21,21	0
54	MG	BA	3184	1/1	0.89	0.19	24,24,24,24	0
54	MG	DA	3068	1/1	0.89	0.08	81,81,81,81	0
54	MG	AA	1668	1/1	0.89	0.24	39,39,39,39	0
54	MG	BA	3173	1/1	0.89	0.24	40,40,40,40	0
54	MG	BA	3190	1/1	0.89	0.27	46,46,46,46	0
54	MG	BA	3165	1/1	0.89	0.30	29,29,29,29	0
54	MG	CA	1635	1/1	0.89	0.76	99,99,99,99	0
54	MG	BA	3153	1/1	0.89	0.58	33,33,33,33	0
54	MG	DA	3033	1/1	0.89	0.20	77,77,77,77	0
54	MG	DA	3128	1/1	0.89	0.14	60,60,60,60	0
54	MG	AA	1665	1/1	0.89	0.57	61,61,61,61	0
54	MG	DA	3097	1/1	0.90	0.09	67,67,67,67	0
54	MG	BA	3079	1/1	0.90	0.18	29,29,29,29	0
54	MG	CA	1631	1/1	0.90	0.19	85,85,85,85	0
54	MG	BA	3154	1/1	0.90	0.25	18,18,18,18	0
54	MG	DA	3113	1/1	0.90	0.13	54,54,54,54	0
54	MG	DA	3156	1/1	0.90	0.16	72,72,72,72	0
54	MG	BA	3193	1/1	0.90	0.29	46,46,46,46	0
54	MG	CA	1656	1/1	0.90	0.08	88,88,88,88	0
54	MG	DA	3148	1/1	0.90	0.25	53,53,53,53	0
54	MG	AA	1630	1/1	0.90	0.30	78,78,78,78	0
54	MG	AA	1651	1/1	0.90	0.80	52,52,52,52	0
54	MG	DA	3119	1/1	0.90	0.25	83,83,83,83	0
54	MG	DA	3139	1/1	0.90	0.58	49,49,49,49	0
54	MG	BA	3172	1/1	0.90	0.19	29,29,29,29	0
54	MG	AA	1661	1/1	0.90	0.55	40,40,40,40	0
54	MG	BA	3056	1/1	0.90	0.36	27,27,27,27	0
54	MG	DA	3096	1/1	0.90	0.26	81,81,81,81	0
54	MG	BA	3047	1/1	0.90	0.13	43,43,43,43	0
54	MG	DA	3020	1/1	0.90	0.74	76,76,76,76	0
54	MG	DA	3046	1/1	0.90	0.13	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3131	1/1	0.90	0.30	79,79,79,79	0
54	MG	DA	3014	1/1	0.90	0.30	86,86,86,86	0
54	MG	CA	1602	1/1	0.90	0.11	93,93,93,93	0
54	MG	DA	3064	1/1	0.90	0.12	61,61,61,61	0
54	MG	DB	202	1/1	0.90	0.08	89,89,89,89	0
54	MG	BA	3001	1/1	0.90	0.13	39,39,39,39	0
54	MG	CA	1621	1/1	0.90	0.17	75,75,75,75	0
54	MG	BA	3194	1/1	0.91	0.16	42,42,42,42	0
54	MG	BA	3112	1/1	0.91	0.10	25,25,25,25	0
54	MG	AA	1610	1/1	0.91	0.09	64,64,64,64	0
54	MG	BA	3082	1/1	0.91	0.07	8,8,8,8	0
54	MG	CA	1646	1/1	0.91	0.80	21,21,21,21	0
54	MG	DA	3086	1/1	0.91	0.20	81,81,81,81	0
54	MG	DA	3123	1/1	0.91	0.23	88,88,88,88	0
54	MG	BA	3139	1/1	0.91	0.50	1,1,1,1	0
54	MG	BA	3083	1/1	0.91	0.33	44,44,44,44	0
54	MG	BA	3059	1/1	0.91	0.41	27,27,27,27	0
54	MG	BA	3067	1/1	0.91	0.16	2,2,2,2	0
54	MG	BA	3164	1/1	0.92	0.15	13,13,13,13	0
54	MG	BA	3069	1/1	0.92	0.10	72,72,72,72	0
54	MG	DA	3112	1/1	0.92	0.28	78,78,78,78	0
54	MG	BA	3084	1/1	0.92	0.25	33,33,33,33	0
54	MG	AA	1621	1/1	0.92	0.08	32,32,32,32	0
54	MG	DA	3085	1/1	0.92	0.14	71,71,71,71	0
54	MG	DA	3010	1/1	0.92	0.16	60,60,60,60	0
54	MG	BA	3085	1/1	0.92	0.13	9,9,9,9	0
54	MG	DA	3023	1/1	0.92	0.22	57,57,57,57	0
54	MG	BA	3076	1/1	0.92	0.26	60,60,60,60	0
54	MG	CA	1643	1/1	0.92	0.22	43,43,43,43	0
54	MG	AA	1640	1/1	0.92	0.06	39,39,39,39	0
54	MG	BA	3151	1/1	0.92	0.24	7,7,7,7	0
54	MG	DA	3138	1/1	0.92	0.42	41,41,41,41	0
54	MG	BA	3025	1/1	0.92	0.34	38,38,38,38	0
54	MG	AA	1627	1/1	0.93	0.47	68,68,68,68	0
54	MG	DA	3117	1/1	0.93	0.21	79,79,79,79	0
54	MG	AA	1660	1/1	0.93	0.37	72,72,72,72	0
54	MG	DA	3073	1/1	0.93	0.15	69,69,69,69	0
54	MG	CA	1609	1/1	0.93	0.10	56,56,56,56	0
54	MG	DA	3127	1/1	0.93	0.38	91,91,91,91	0
54	MG	AA	1611	1/1	0.93	0.10	32,32,32,32	0
54	MG	DA	3050	1/1	0.93	0.09	41,41,41,41	0
54	MG	DA	3034	1/1	0.93	0.12	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DB	203	1/1	0.93	0.07	106,106,106,106	0
54	MG	CA	1603	1/1	0.93	0.06	40,40,40,40	0
54	MG	BA	3146	1/1	0.93	0.36	32,32,32,32	0
54	MG	BA	3108	1/1	0.93	0.21	1,1,1,1	0
54	MG	BA	3007	1/1	0.93	0.06	29,29,29,29	0
54	MG	BA	3180	1/1	0.93	0.28	45,45,45,45	0
54	MG	BA	3136	1/1	0.93	0.26	50,50,50,50	0
54	MG	BA	3175	1/1	0.93	0.23	38,38,38,38	0
54	MG	AA	1653	1/1	0.93	0.38	27,27,27,27	0
54	MG	BA	3140	1/1	0.93	0.29	34,34,34,34	0
54	MG	CA	1612	1/1	0.93	0.19	20,20,20,20	0
54	MG	DA	3065	1/1	0.93	0.16	44,44,44,44	0
54	MG	AA	1629	1/1	0.93	0.20	73,73,73,73	0
54	MG	DA	3110	1/1	0.93	0.24	89,89,89,89	0
54	MG	AA	1623	1/1	0.93	0.21	60,60,60,60	0
54	MG	BA	3045	1/1	0.93	0.25	5,5,5,5	0
54	MG	BA	3042	1/1	0.93	0.14	1,1,1,1	0
54	MG	DA	3066	1/1	0.94	0.15	58,58,58,58	0
54	MG	DA	3080	1/1	0.94	0.17	74,74,74,74	0
54	MG	CA	1617	1/1	0.94	0.15	38,38,38,38	0
54	MG	AA	1615	1/1	0.94	0.23	52,52,52,52	0
54	MG	BA	3145	1/1	0.94	0.57	35,35,35,35	0
54	MG	BA	3177	1/1	0.94	0.21	24,24,24,24	0
54	MG	BA	3118	1/1	0.94	0.07	14,14,14,14	0
54	MG	AA	1605	1/1	0.94	0.18	35,35,35,35	0
54	MG	DA	3017	1/1	0.94	0.23	71,71,71,71	0
54	MG	BA	3014	1/1	0.94	0.12	8,8,8,8	0
54	MG	CA	1601	1/1	0.94	0.12	45,45,45,45	0
54	MG	BA	3178	1/1	0.94	0.76	41,41,41,41	0
54	MG	CA	1622	1/1	0.94	0.60	84,84,84,84	0
54	MG	BA	3130	1/1	0.94	0.29	7,7,7,7	0
54	MG	BA	3077	1/1	0.94	0.12	16,16,16,16	0
54	MG	BA	3182	1/1	0.94	0.33	25,25,25,25	0
54	MG	DA	3129	1/1	0.94	0.17	93,93,93,93	0
54	MG	DA	3125	1/1	0.94	0.27	83,83,83,83	0
54	MG	BA	3162	1/1	0.94	0.39	30,30,30,30	0
54	MG	DA	3051	1/1	0.94	0.19	51,51,51,51	0
54	MG	BA	3120	1/1	0.94	0.14	10,10,10,10	0
54	MG	BA	3004	1/1	0.94	0.20	55,55,55,55	0
54	MG	BA	3099	1/1	0.94	0.18	1,1,1,1	0
54	MG	DA	3151	1/1	0.94	0.27	42,42,42,42	0
54	MG	BA	3021	1/1	0.94	0.13	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3021	1/1	0.94	0.09	69,69,69,69	0
54	MG	CT	101	1/1	0.94	0.19	91,91,91,91	0
54	MG	DA	3062	1/1	0.94	0.13	67,67,67,67	0
54	MG	DA	3042	1/1	0.94	0.11	67,67,67,67	0
54	MG	DA	3101	1/1	0.94	0.20	85,85,85,85	0
54	MG	DA	3121	1/1	0.94	0.19	62,62,62,62	0
54	MG	AA	1607	1/1	0.94	0.06	48,48,48,48	0
54	MG	BA	3143	1/1	0.95	0.48	18,18,18,18	0
54	MG	BA	3119	1/1	0.95	0.29	40,40,40,40	0
54	MG	DA	3035	1/1	0.95	0.27	54,54,54,54	0
54	MG	AA	1633	1/1	0.95	0.10	25,25,25,25	0
54	MG	DA	3122	1/1	0.95	0.10	51,51,51,51	0
54	MG	BA	3135	1/1	0.95	0.15	23,23,23,23	0
54	MG	AA	1654	1/1	0.95	0.41	46,46,46,46	0
54	MG	DA	3045	1/1	0.95	0.11	74,74,74,74	0
54	MG	BA	3032	1/1	0.95	0.18	4,4,4,4	0
54	MG	BA	3068	1/1	0.95	0.11	1,1,1,1	0
54	MG	BA	3008	1/1	0.95	0.16	3,3,3,3	0
54	MG	BA	3002	1/1	0.95	0.09	11,11,11,11	0
54	MG	BA	3012	1/1	0.95	0.24	1,1,1,1	0
54	MG	AA	1645	1/1	0.95	0.89	52,52,52,52	0
54	MG	BA	3009	1/1	0.95	0.14	1,1,1,1	0
54	MG	BA	3092	1/1	0.95	0.13	33,33,33,33	0
54	MG	BA	3063	1/1	0.95	0.11	6,6,6,6	0
54	MG	BB	201	1/1	0.95	0.15	32,32,32,32	0
54	MG	DA	3003	1/1	0.95	0.10	83,83,83,83	0
54	MG	AA	1631	1/1	0.95	0.08	32,32,32,32	0
54	MG	AA	1616	1/1	0.95	0.08	94,94,94,94	0
54	MG	BA	3029	1/1	0.95	0.08	20,20,20,20	0
54	MG	BA	3158	1/1	0.95	0.26	15,15,15,15	0
54	MG	BA	3187	1/1	0.95	0.22	41,41,41,41	0
54	MG	AA	1613	1/1	0.95	0.08	13,13,13,13	0
54	MG	DA	3058	1/1	0.95	0.10	64,64,64,64	0
54	MG	DA	3022	1/1	0.95	0.09	74,74,74,74	0
54	MG	BA	3171	1/1	0.95	0.23	29,29,29,29	0
54	MG	CA	1647	1/1	0.95	0.57	72,72,72,72	0
54	MG	DA	3079	1/1	0.95	0.11	91,91,91,91	0
54	MG	DA	3012	1/1	0.95	0.23	46,46,46,46	0
54	MG	BA	3027	1/1	0.95	0.14	10,10,10,10	0
54	MG	DA	3142	1/1	0.95	0.44	53,53,53,53	0
54	MG	BA	3019	1/1	0.95	0.41	1,1,1,1	0
54	MG	BA	3127	1/1	0.95	0.13	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3157	1/1	0.95	0.23	26,26,26,26	0
54	MG	BA	3088	1/1	0.95	0.12	25,25,25,25	0
54	MG	DA	3011	1/1	0.95	0.18	98,98,98,98	0
54	MG	BA	3134	1/1	0.95	0.18	3,3,3,3	0
54	MG	BA	3142	1/1	0.95	0.61	17,17,17,17	0
54	MG	DA	3108	1/1	0.96	0.25	22,22,22,22	0
54	MG	AA	1655	1/1	0.96	0.41	55,55,55,55	0
54	MG	DA	3082	1/1	0.96	0.09	80,80,80,80	0
54	MG	BA	3022	1/1	0.96	0.14	1,1,1,1	0
54	MG	CA	1638	1/1	0.96	0.17	28,28,28,28	0
54	MG	BA	3138	1/1	0.96	0.54	1,1,1,1	0
54	MG	BA	3078	1/1	0.96	0.07	48,48,48,48	0
54	MG	BA	3064	1/1	0.96	0.13	5,5,5,5	0
54	MG	BA	3124	1/1	0.96	0.33	44,44,44,44	0
54	MG	BA	3038	1/1	0.96	0.16	1,1,1,1	0
54	MG	CA	1625	1/1	0.96	0.04	44,44,44,44	0
54	MG	BA	3109	1/1	0.96	0.21	1,1,1,1	0
54	MG	AA	1602	1/1	0.96	0.10	37,37,37,37	0
54	MG	AA	1647	1/1	0.96	0.19	51,51,51,51	0
54	MG	BA	3116	1/1	0.96	0.19	1,1,1,1	0
54	MG	CA	1615	1/1	0.96	0.17	39,39,39,39	0
54	MG	BA	3156	1/1	0.96	0.88	40,40,40,40	0
54	MG	AA	1636	1/1	0.96	0.16	46,46,46,46	0
54	MG	DA	3019	1/1	0.96	0.32	38,38,38,38	0
54	MG	BA	3132	1/1	0.96	0.37	45,45,45,45	0
54	MG	BA	3152	1/1	0.96	0.45	1,1,1,1	0
54	MG	BA	3080	1/1	0.96	0.15	24,24,24,24	0
54	MG	BA	3192	1/1	0.96	0.18	30,30,30,30	0
54	MG	AA	1622	1/1	0.96	0.25	21,21,21,21	0
54	MG	BA	3147	1/1	0.96	0.39	13,13,13,13	0
54	MG	DA	3126	1/1	0.96	0.13	58,58,58,58	0
54	MG	CA	1637	1/1	0.96	0.12	35,35,35,35	0
54	MG	BA	3066	1/1	0.96	0.12	3,3,3,3	0
54	MG	AA	1643	1/1	0.96	0.71	7,7,7,7	0
54	MG	BA	3098	1/1	0.96	0.36	41,41,41,41	0
54	MG	BA	3111	1/1	0.96	0.10	40,40,40,40	0
54	MG	AA	1612	1/1	0.96	0.10	42,42,42,42	0
54	MG	BA	3016	1/1	0.96	0.12	13,13,13,13	0
54	MG	BA	3181	1/1	0.96	0.49	33,33,33,33	0
54	MG	BA	3159	1/1	0.96	0.33	18,18,18,18	0
54	MG	DA	3109	1/1	0.96	0.36	64,64,64,64	0
54	MG	BA	3070	1/1	0.96	0.10	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1610	1/1	0.96	0.04	57,57,57,57	0
54	MG	BA	3074	1/1	0.97	0.08	24,24,24,24	0
54	MG	BA	3033	1/1	0.97	0.23	1,1,1,1	0
54	MG	DA	3075	1/1	0.97	0.28	78,78,78,78	0
54	MG	BA	3100	1/1	0.97	0.17	4,4,4,4	0
54	MG	BA	3065	1/1	0.97	0.13	1,1,1,1	0
54	MG	BA	3048	1/1	0.97	0.15	10,10,10,10	0
54	MG	AA	1639	1/1	0.97	0.12	60,60,60,60	0
54	MG	AA	1632	1/1	0.97	0.09	60,60,60,60	0
54	MG	BA	3020	1/1	0.97	0.05	1,1,1,1	0
54	MG	BA	3052	1/1	0.97	0.08	1,1,1,1	0
54	MG	CA	1623	1/1	0.97	0.06	48,48,48,48	0
54	MG	DA	3063	1/1	0.97	0.14	64,64,64,64	0
54	MG	BA	3123	1/1	0.97	0.15	6,6,6,6	0
54	MG	BA	3046	1/1	0.97	0.20	5,5,5,5	0
55	ZN	D4	101	1/1	0.97	0.10	95,95,95,95	0
54	MG	BA	3035	1/1	0.97	0.21	1,1,1,1	0
54	MG	BA	3010	1/1	0.97	0.13	1,1,1,1	0
54	MG	DA	3038	1/1	0.97	0.15	68,68,68,68	0
54	MG	DA	3044	1/1	0.97	0.30	51,51,51,51	0
54	MG	BA	3013	1/1	0.97	0.22	1,1,1,1	0
54	MG	CA	1606	1/1	0.97	0.11	61,61,61,61	0
54	MG	AA	1606	1/1	0.97	0.08	42,42,42,42	0
54	MG	BA	3081	1/1	0.97	0.15	1,1,1,1	0
54	MG	BA	3054	1/1	0.97	0.14	4,4,4,4	0
54	MG	BB	204	1/1	0.97	0.69	6,6,6,6	0
54	MG	BA	3039	1/1	0.97	0.19	1,1,1,1	0
54	MG	BA	3005	1/1	0.97	0.06	44,44,44,44	0
54	MG	BA	3087	1/1	0.97	0.07	18,18,18,18	0
54	MG	BA	3137	1/1	0.97	0.59	11,11,11,11	0
54	MG	CA	1611	1/1	0.97	0.12	42,42,42,42	0
54	MG	AA	1609	1/1	0.97	0.05	23,23,23,23	0
54	MG	DA	3032	1/1	0.97	0.06	67,67,67,67	0
54	MG	BA	3086	1/1	0.97	0.17	2,2,2,2	0
54	MG	BA	3129	1/1	0.97	0.17	1,1,1,1	0
54	MG	BA	3089	1/1	0.97	0.07	8,8,8,8	0
54	MG	BA	3028	1/1	0.97	0.16	1,1,1,1	0
54	MG	BA	3125	1/1	0.97	0.20	4,4,4,4	0
54	MG	DA	3141	1/1	0.97	0.56	45,45,45,45	0
54	MG	BA	3072	1/1	0.97	0.13	1,1,1,1	0
54	MG	BA	3091	1/1	0.97	0.27	53,53,53,53	0
54	MG	AA	1608	1/1	0.97	0.17	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3094	1/1	0.97	0.07	19,19,19,19	0
54	MG	AA	1637	1/1	0.98	0.10	13,13,13,13	0
54	MG	BA	3093	1/1	0.98	0.12	11,11,11,11	0
54	MG	BA	3023	1/1	0.98	0.18	1,1,1,1	0
54	MG	BB	202	1/1	0.98	0.08	10,10,10,10	0
54	MG	BA	3051	1/1	0.98	0.15	2,2,2,2	0
54	MG	AA	1603	1/1	0.98	0.04	30,30,30,30	0
54	MG	DA	3160	1/1	0.98	0.30	86,86,86,86	0
54	MG	BB	203	1/1	0.98	0.08	12,12,12,12	0
54	MG	BA	3024	1/1	0.98	0.10	13,13,13,13	0
54	MG	BA	3141	1/1	0.98	0.65	2,2,2,2	0
54	MG	BA	3006	1/1	0.98	0.14	29,29,29,29	0
54	MG	BA	3126	1/1	0.98	0.15	3,3,3,3	0
54	MG	BA	3062	1/1	0.98	0.13	4,4,4,4	0
54	MG	DA	3150	1/1	0.98	0.16	86,86,86,86	0
54	MG	BA	3071	1/1	0.98	0.08	13,13,13,13	0
54	MG	CA	1618	1/1	0.98	0.10	35,35,35,35	0
54	MG	BA	3144	1/1	0.98	0.46	34,34,34,34	0
54	MG	AA	1664	1/1	0.98	0.29	58,58,58,58	0
54	MG	BA	3096	1/1	0.98	0.09	2,2,2,2	0
54	MG	BA	3017	1/1	0.98	0.20	1,1,1,1	0
54	MG	BA	3049	1/1	0.98	0.20	3,3,3,3	0
54	MG	AA	1626	1/1	0.98	0.25	1,1,1,1	0
54	MG	BA	3095	1/1	0.98	0.07	6,6,6,6	0
54	MG	BA	3018	1/1	0.98	0.10	14,14,14,14	0
54	MG	BA	3183	1/1	0.98	0.42	35,35,35,35	0
54	MG	BA	3031	1/1	0.98	0.04	11,11,11,11	0
54	MG	BA	3106	1/1	0.98	0.18	1,1,1,1	0
54	MG	BA	3058	1/1	0.98	0.09	14,14,14,14	0
54	MG	BA	3026	1/1	0.99	0.09	2,2,2,2	0
54	MG	BA	3043	1/1	0.99	0.08	11,11,11,11	0
54	MG	BA	3128	1/1	0.99	0.41	1,1,1,1	0
54	MG	BA	3107	1/1	0.99	0.16	3,3,3,3	0
54	MG	BA	3050	1/1	0.99	0.12	7,7,7,7	0
54	MG	BA	3117	1/1	0.99	0.21	1,1,1,1	0
54	MG	AA	1641	1/1	0.99	0.13	12,12,12,12	0
54	MG	BA	3122	1/1	0.99	0.24	1,1,1,1	0
54	MG	BA	3113	1/1	0.99	0.15	4,4,4,4	0
54	MG	BA	3103	1/1	0.99	0.13	2,2,2,2	0
54	MG	AA	1656	1/1	0.99	0.15	46,46,46,46	0
54	MG	CA	1624	1/1	0.99	0.28	4,4,4,4	0
54	MG	BA	3037	1/1	0.99	0.25	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1642	1/1	0.99	0.11	23,23,23,23	0
54	MG	BA	3053	1/1	0.99	0.23	1,1,1,1	0
54	MG	BA	3030	1/1	0.99	0.17	4,4,4,4	0
54	MG	BA	3104	1/1	0.99	0.29	1,1,1,1	0
54	MG	BA	3075	1/1	0.99	0.17	3,3,3,3	0
54	MG	BA	3044	1/1	0.99	0.34	1,1,1,1	0
54	MG	BA	3090	1/1	0.99	0.18	13,13,13,13	0
54	MG	BA	3041	1/1	0.99	0.16	3,3,3,3	0
54	MG	BA	3097	1/1	0.99	0.17	1,1,1,1	0
55	ZN	B4	101	1/1	1.00	0.17	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.