



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 12:42 PM UTC

PDB ID : 4WF1 / pdb_00004wf1
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.; Juette, 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

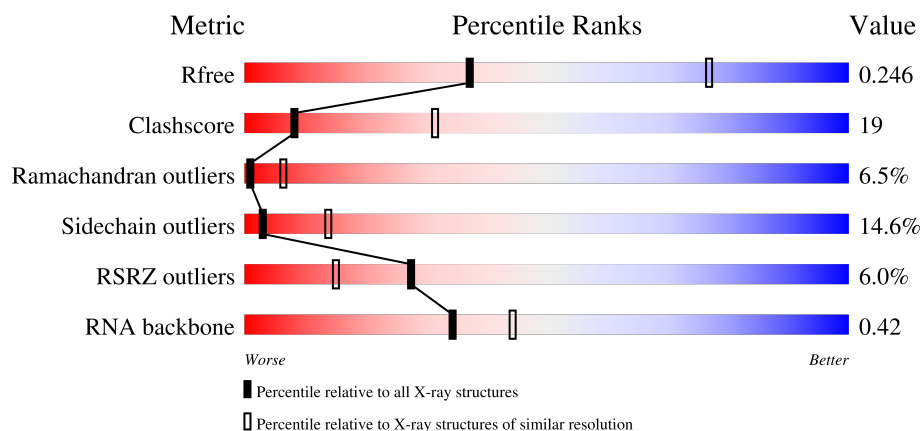
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	2% 36% 50% 14%
1	CA	1539	3% 36% 52% 12%
2	AB	218	6% 28% 50% 20%
2	CB	218	11% 35% 47% 16%

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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	

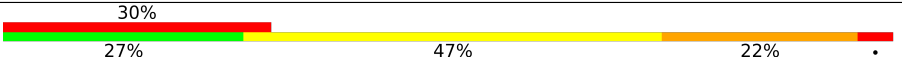
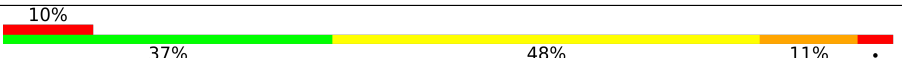
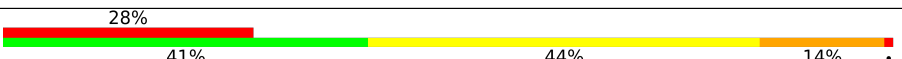
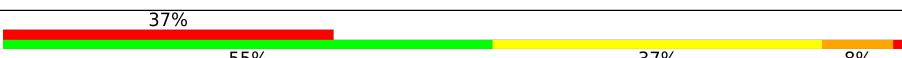
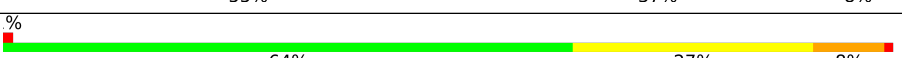
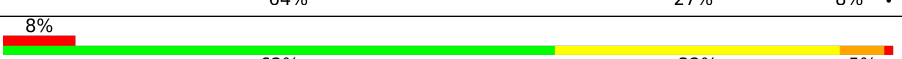
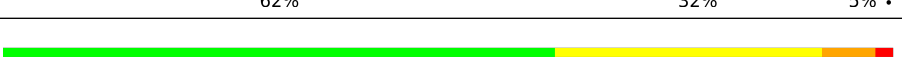
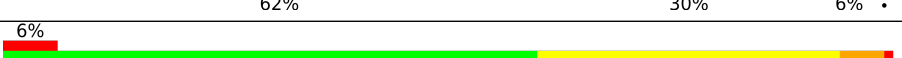
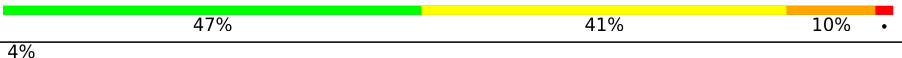
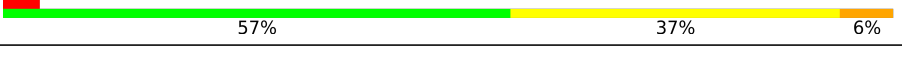
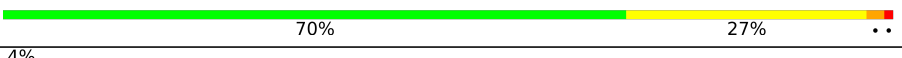
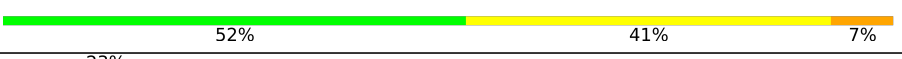
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Mol	Chain	Length	Quality of chain
15	CO	88	48% 42% 10%
16	AP	82	48% 32% 20%
16	CP	82	9% 43% 49% 9%
17	AQ	80	4% 42% 42% 10% 5%
17	CQ	80	2% 41% 40% 18%
18	AR	55	4% 64% 35%
18	CR	55	4% 44% 49% 5%
19	AS	79	9% 58% 32% 8%
19	CS	79	19% 56% 33% 10%
20	AT	85	5% 48% 35% 13%
20	CT	85	27% 49% 38% 12%
21	AU	51	12% 24% 47% 22% 8%
21	CU	51	18% 24% 49% 22% 6%
22	BA	2903	3% 51% 39% 10%
22	DA	2903	3% 34% 53% 13%
23	BB	119	59% 38%
23	DB	119	48% 46% 5%
24	BC	271	5% 54% 39% 7%
24	DC	271	13% 38% 49% 13%
25	BD	209	65% 30% 5%
25	DD	209	9% 59% 34% 7%
26	BE	201	60% 34% 5%
26	DE	201	15% 52% 44%
27	BF	177	49% 41% 8%
27	DF	177	11% 70% 27%

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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	BA	3179	-	-	-	X
54	MG	DA	3057	-	-	-	X
54	MG	DA	3061	-	-	-	X
54	MG	DA	3130	-	-	-	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			
			780	492	146	142	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

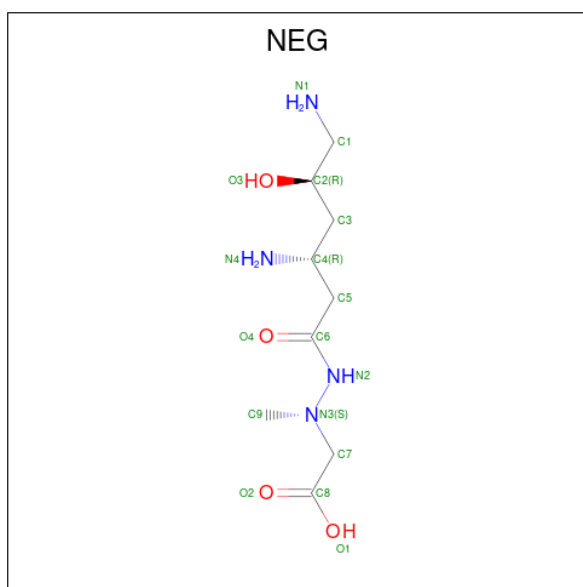
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 55 is ZINC ION (CCD ID: 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 (CCD ID: NEG) (formula: C₉H₂₀N₄O₄).



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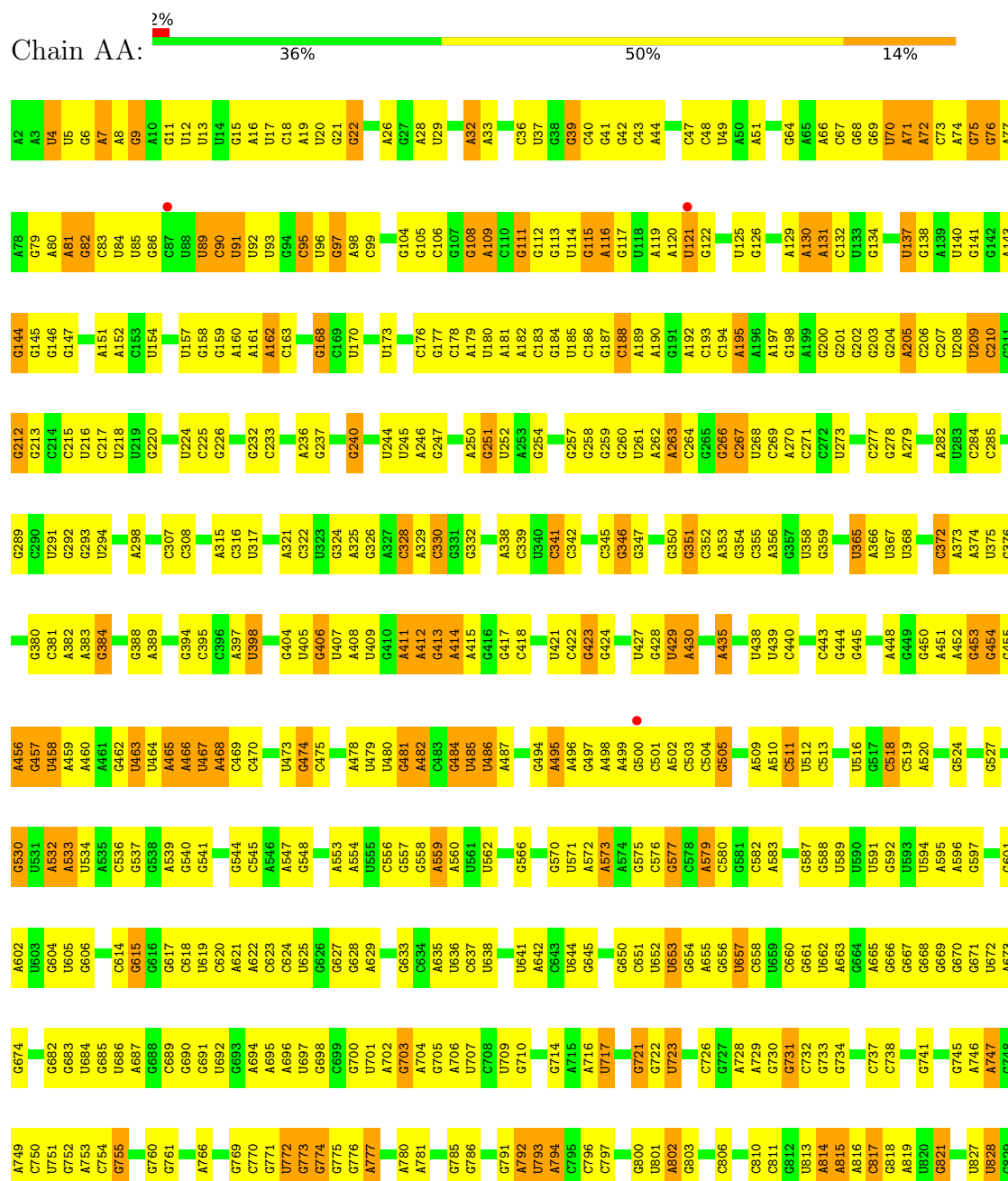
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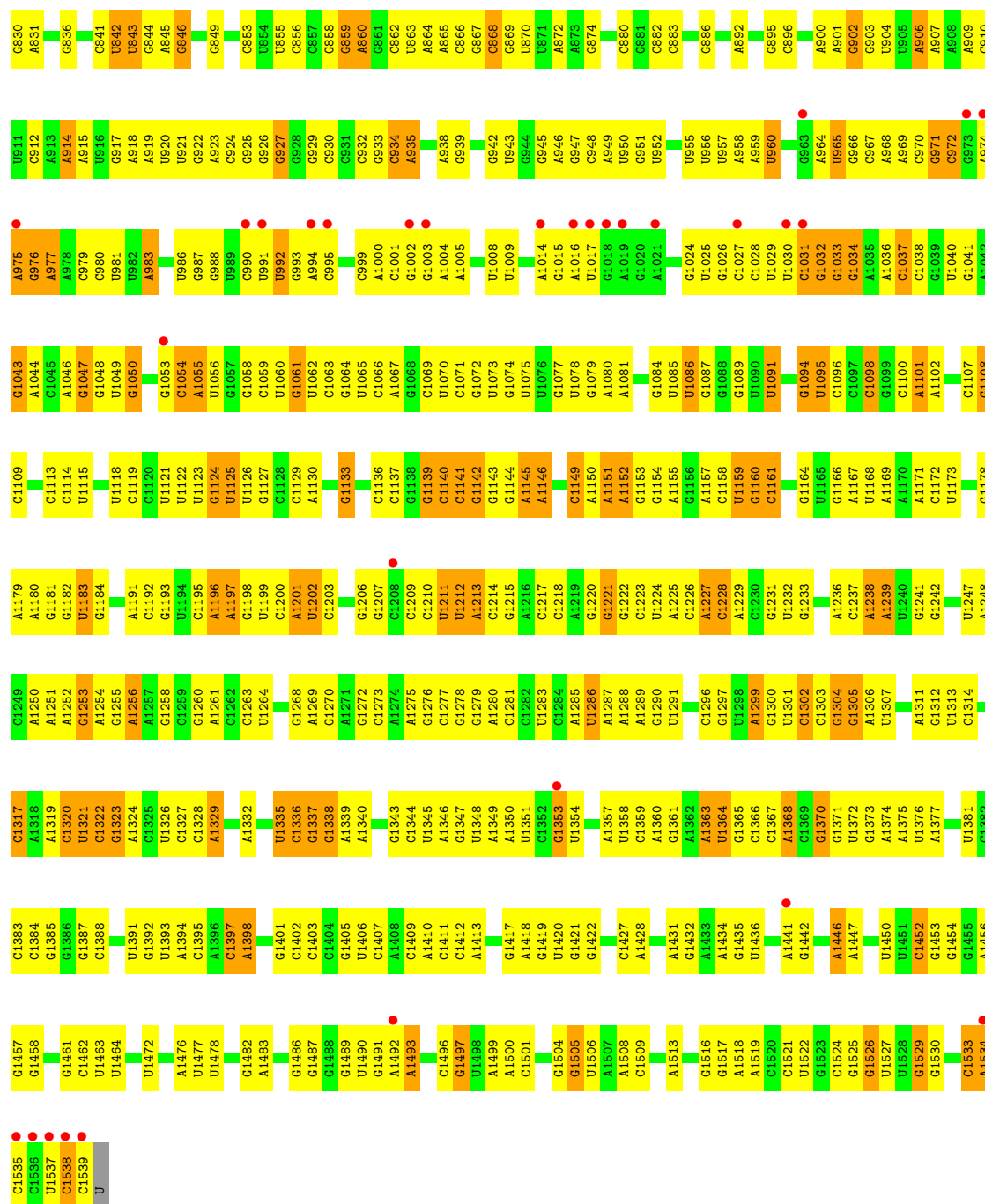
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DT	3	Total 3	O 3	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D3	2	Total 2	O 2	0	0
57	D4	1	Total 1	O 1	0	0

3 Residue-property plots

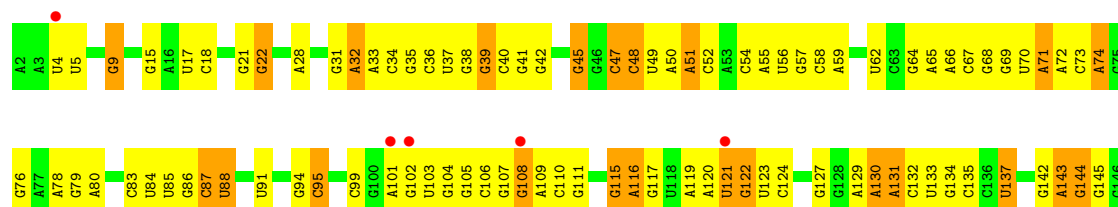
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

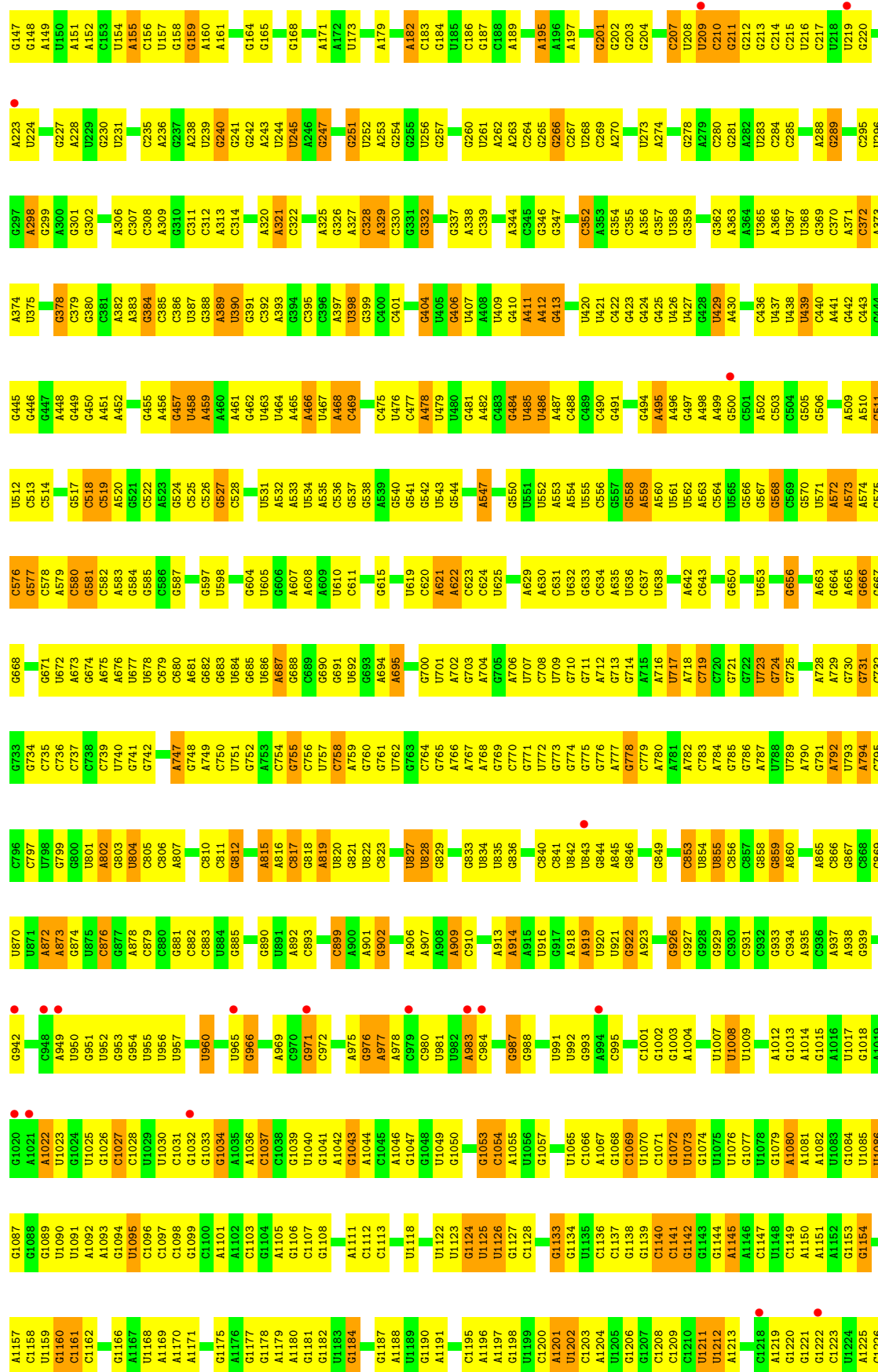
• Molecule 1: 16S rRNA

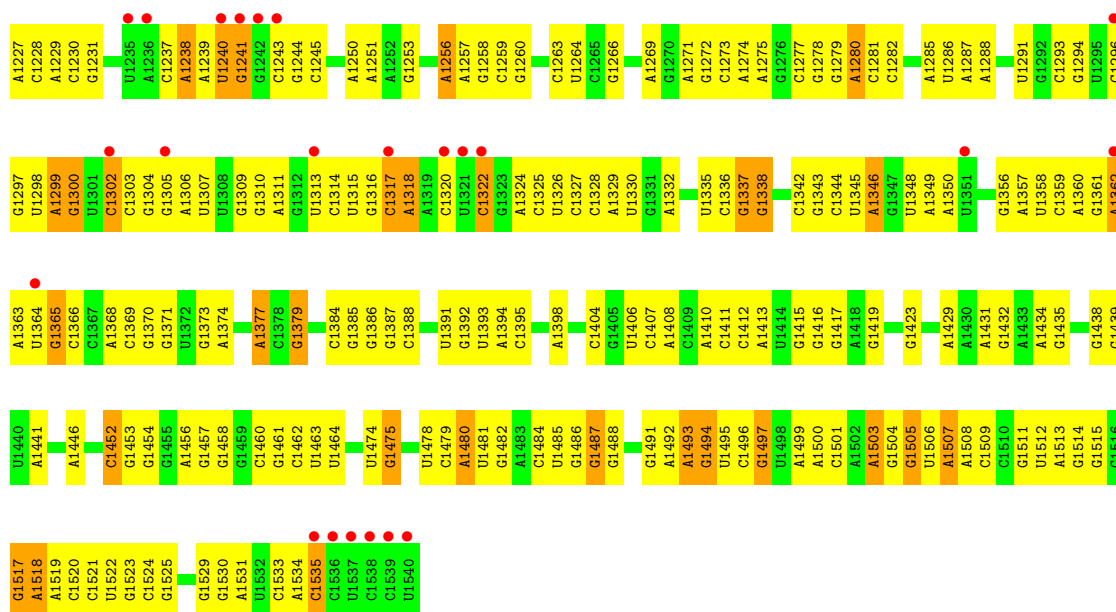




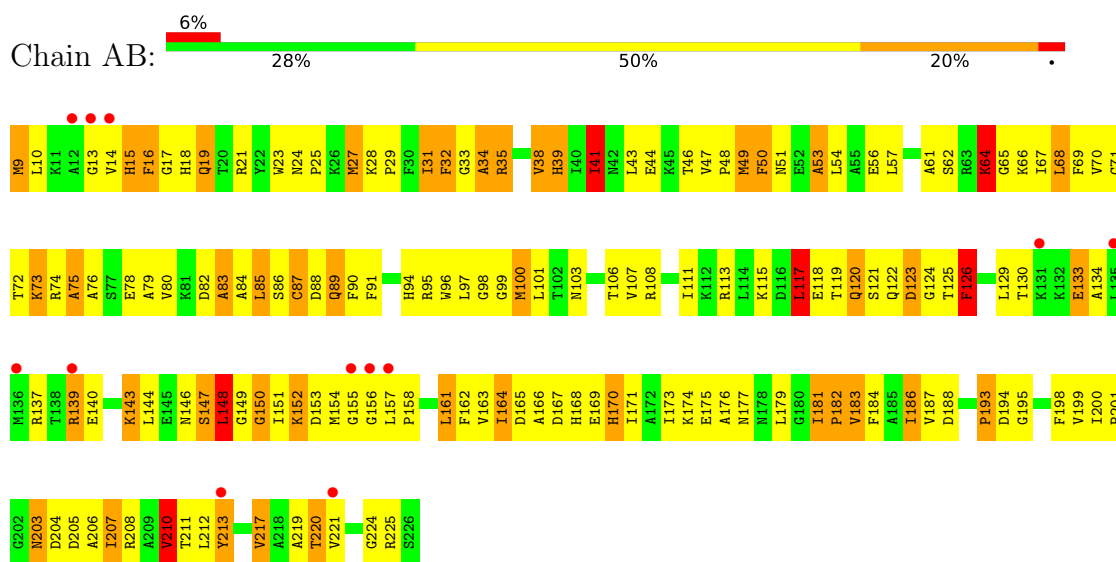
• Molecule 1: 16S rRNA



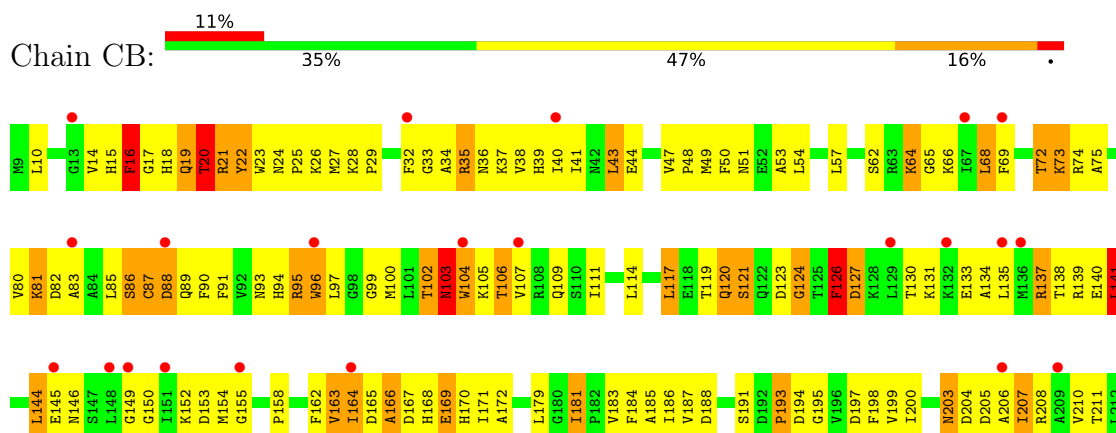


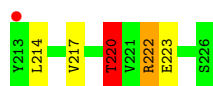


• Molecule 2: 30S ribosomal protein S2



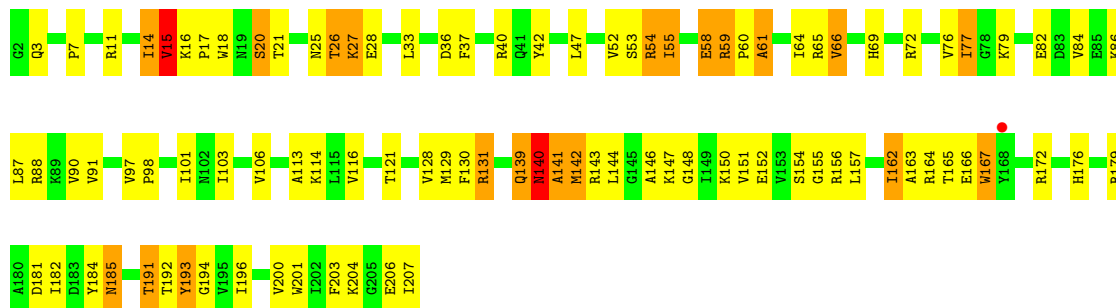
• Molecule 2: 30S ribosomal protein S2





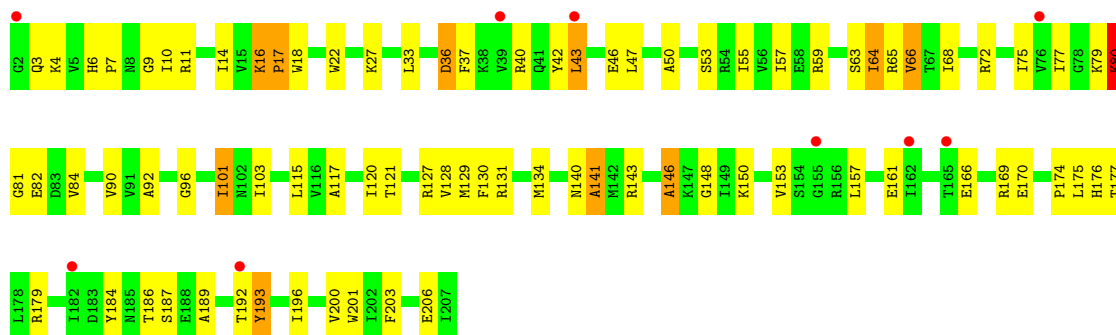
• Molecule 3: 30S ribosomal protein S3

Chain AC: 53% 36% 10%



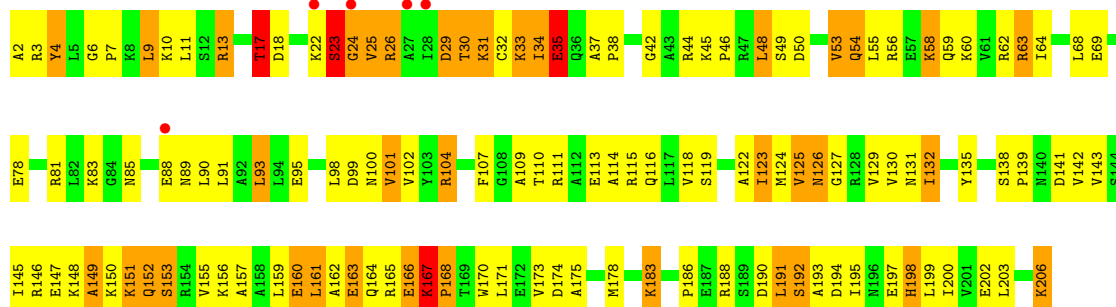
• Molecule 3: 30S ribosomal protein S3

Chain CC: 4% 60% 34% 5%



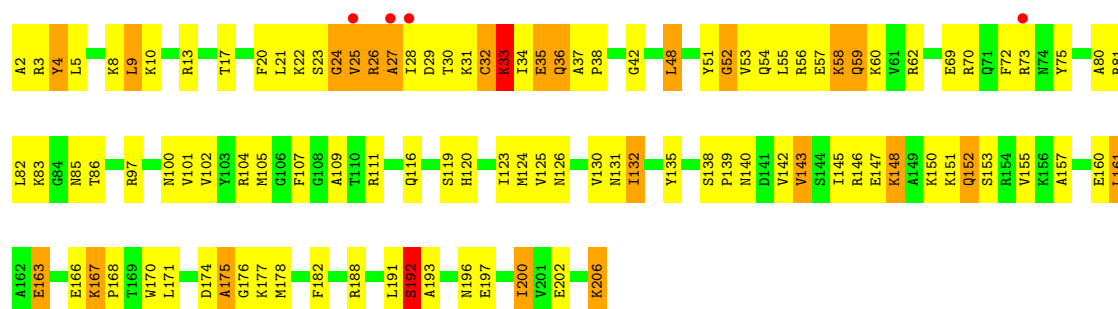
• Molecule 4: 30S ribosomal protein S4

Chain AD: 2% 37% 43% 18%

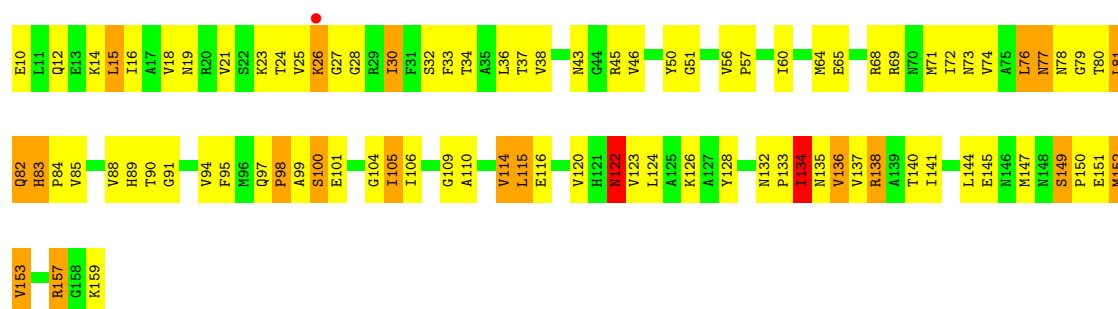


• Molecule 4: 30S ribosomal protein S4

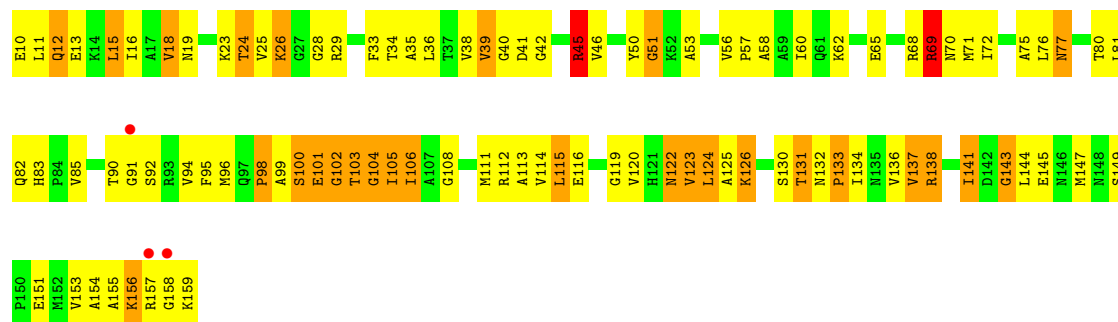
Chain CD: 2% 46% 41% 11%



• Molecule 5: 30S ribosomal protein S5



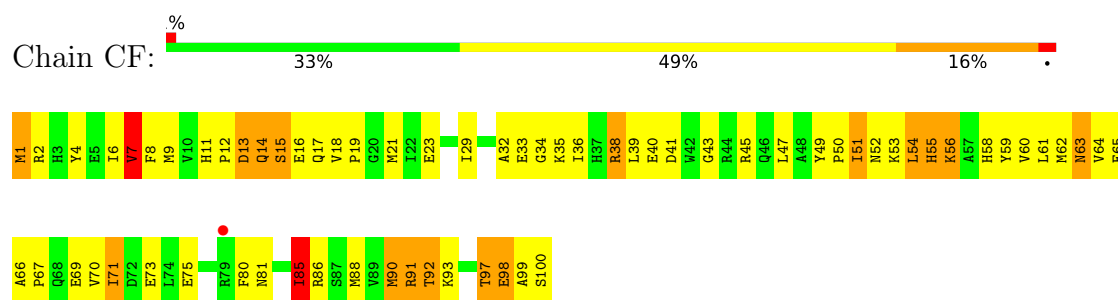
• Molecule 5: 30S ribosomal protein S5



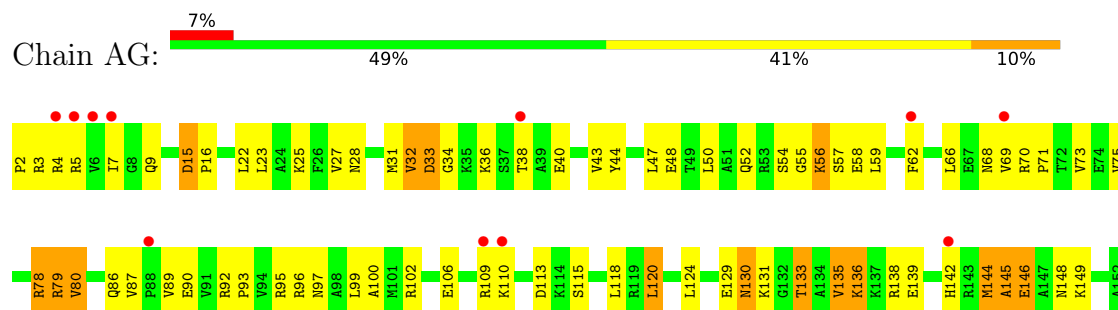
• Molecule 6: 30S ribosomal protein S6



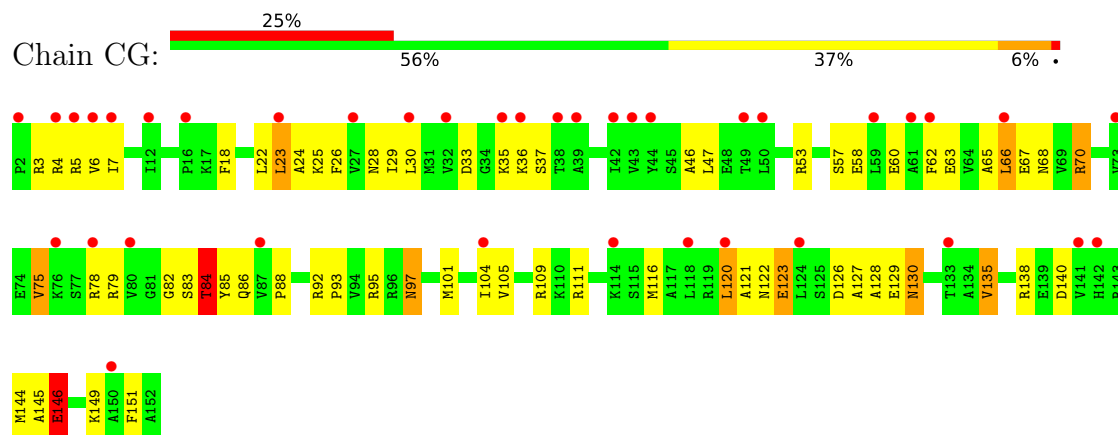
• Molecule 6: 30S ribosomal protein S6



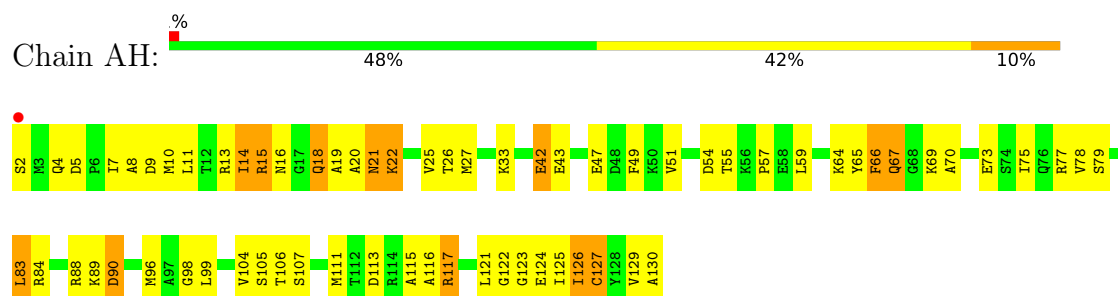
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7

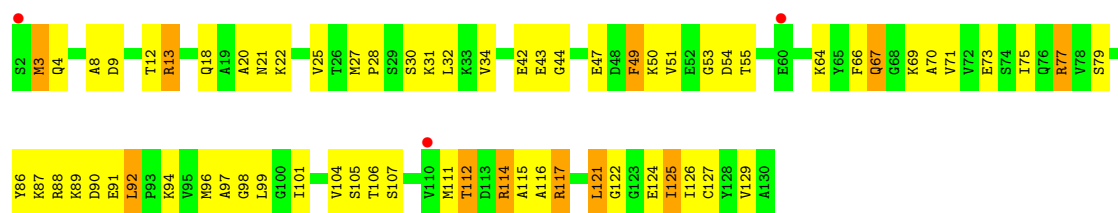


• Molecule 8: 30S ribosomal protein S8

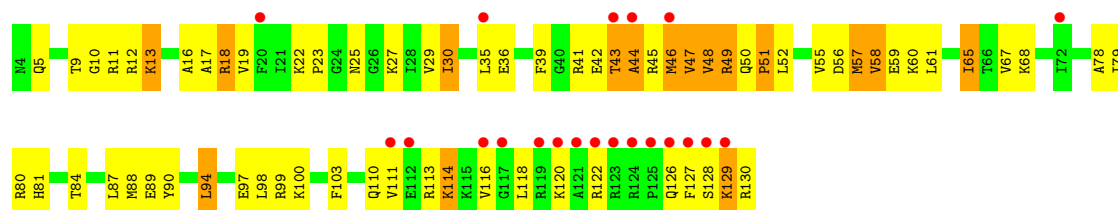


• Molecule 8: 30S ribosomal protein S8

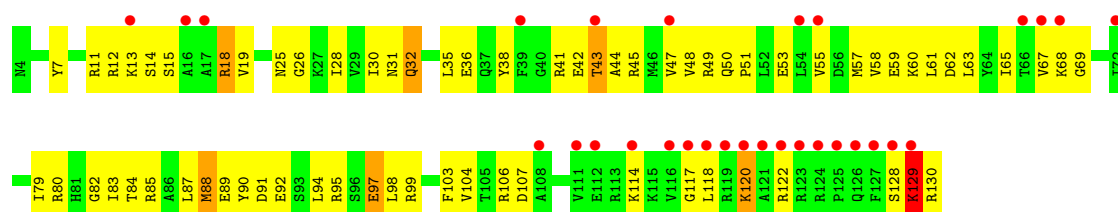




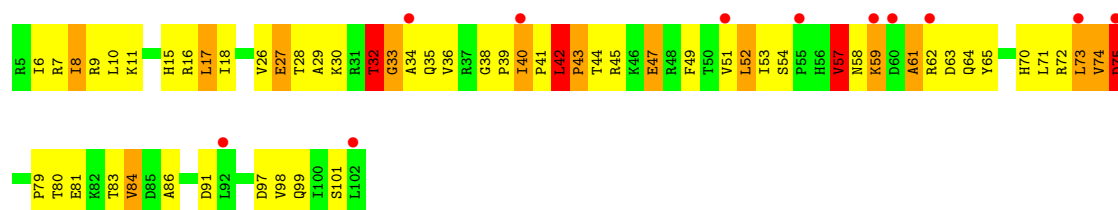
• Molecule 9: 30S ribosomal protein S9



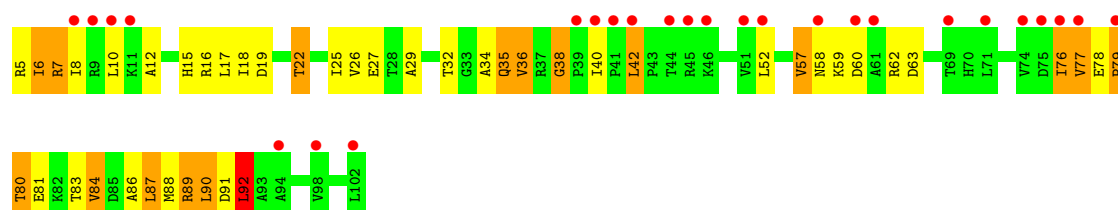
• Molecule 9: 30S ribosomal protein S9



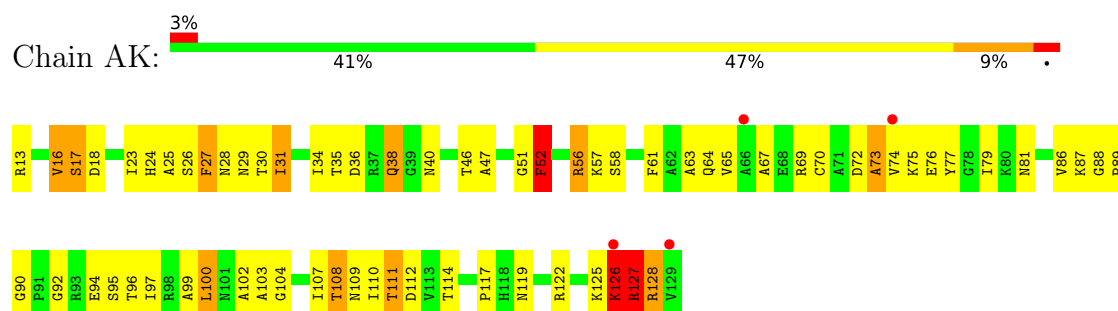
• Molecule 10: 30S ribosomal protein S10



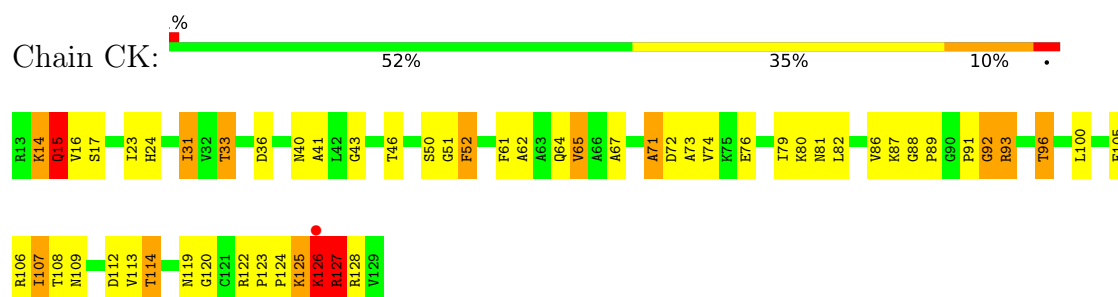
• Molecule 10: 30S ribosomal protein S10



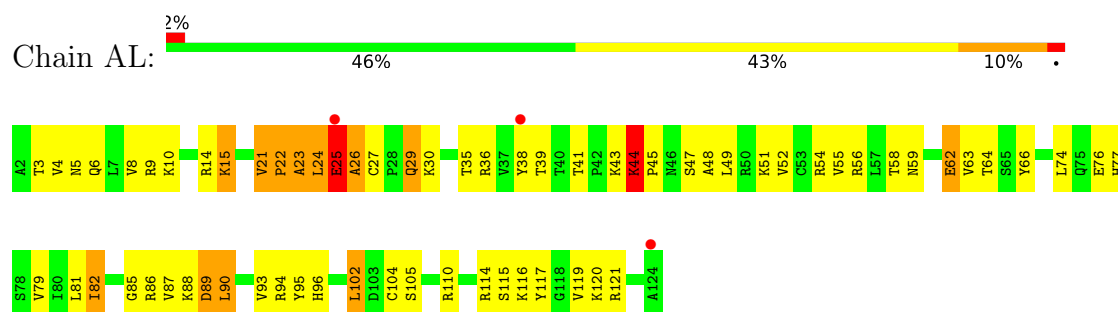
- Molecule 11: 30S ribosomal protein S11



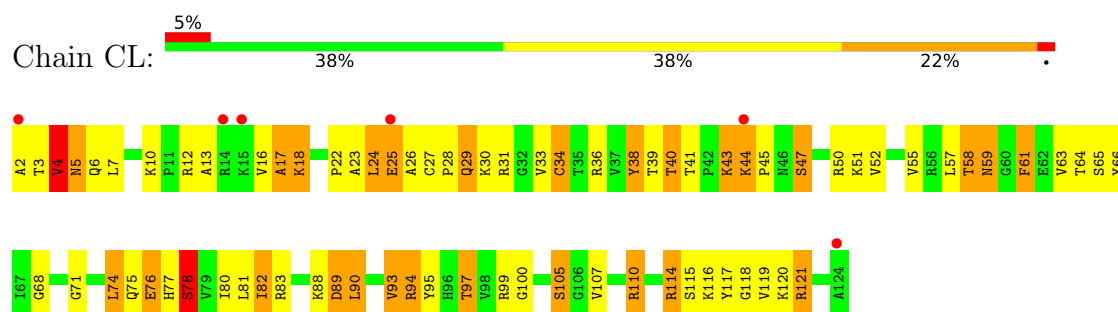
- Molecule 11: 30S ribosomal protein S11



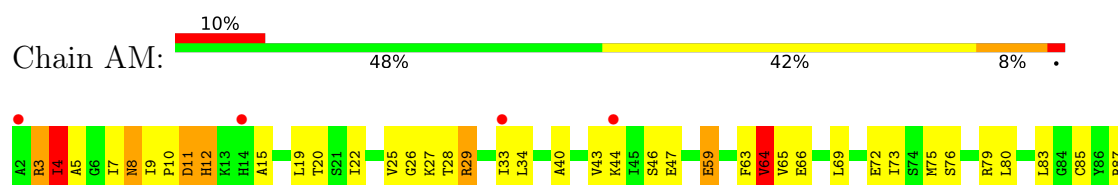
- Molecule 12: 30S ribosomal protein S12

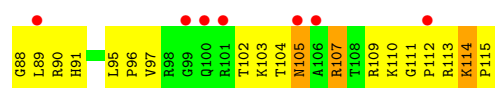


- Molecule 12: 30S ribosomal protein S12

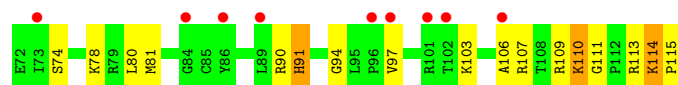
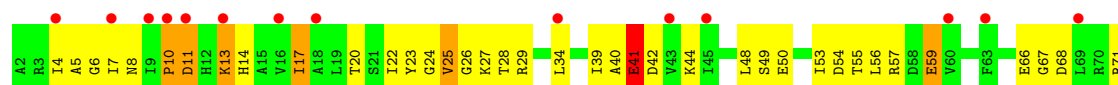


- Molecule 13: 30S ribosomal protein S13

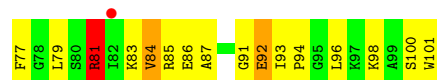
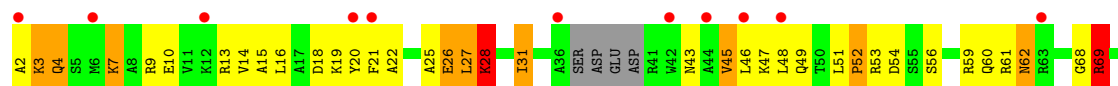
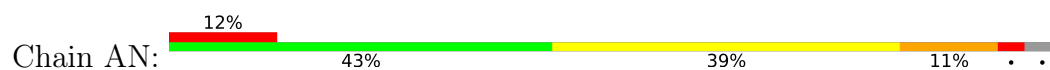




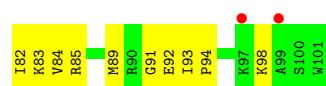
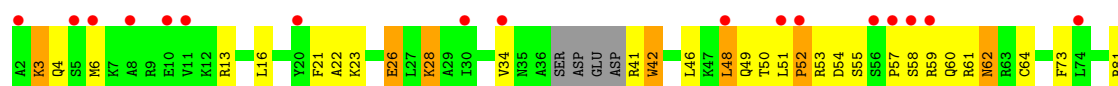
• Molecule 13: 30S ribosomal protein S13



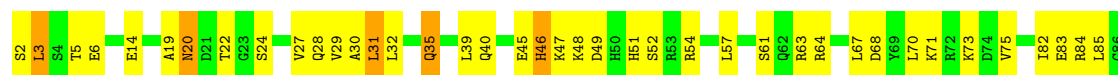
• Molecule 14: 30S ribosomal protein S14



• Molecule 14: 30S ribosomal protein S14

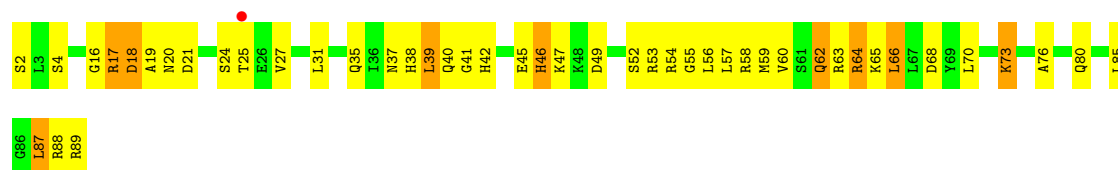


• Molecule 15: 30S ribosomal protein S15



• Molecule 15: 30S ribosomal protein S15

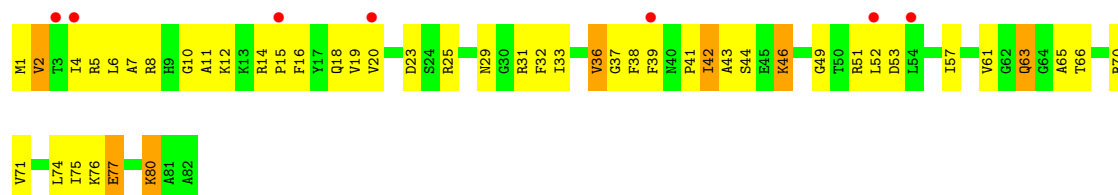
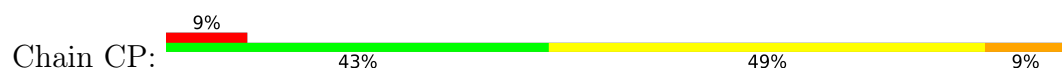




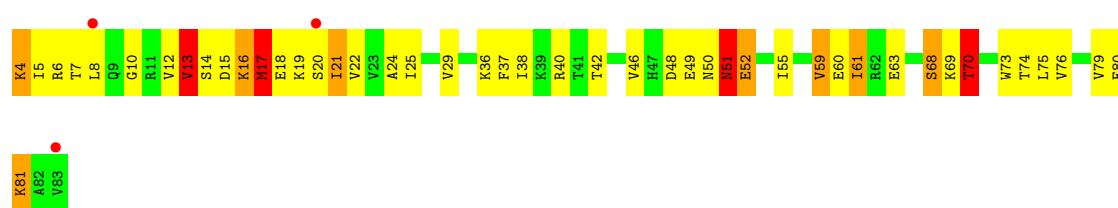
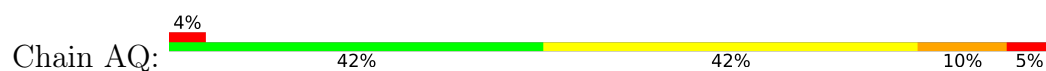
- Molecule 16: 30S ribosomal protein S16



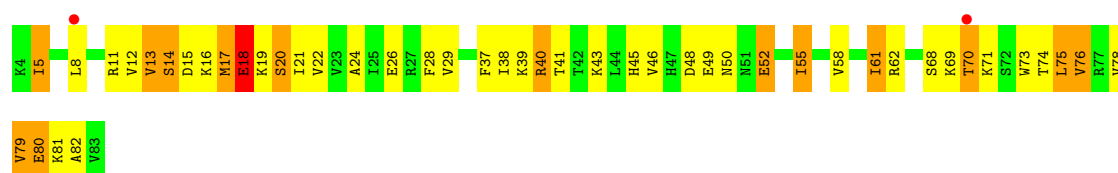
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

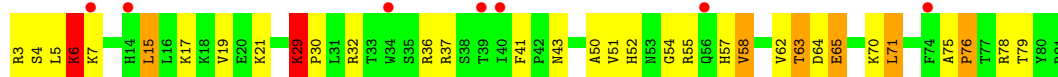




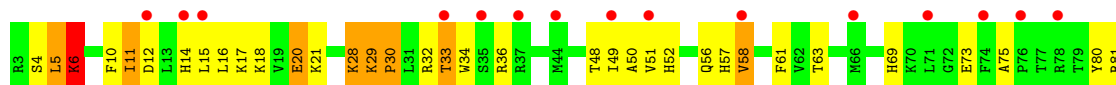
- Molecule 18: 30S ribosomal protein S18



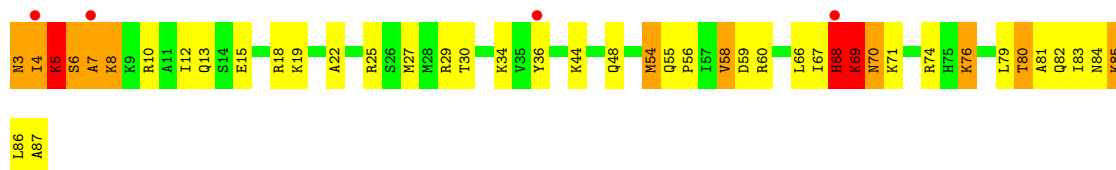
- Molecule 19: 30S ribosomal protein S19



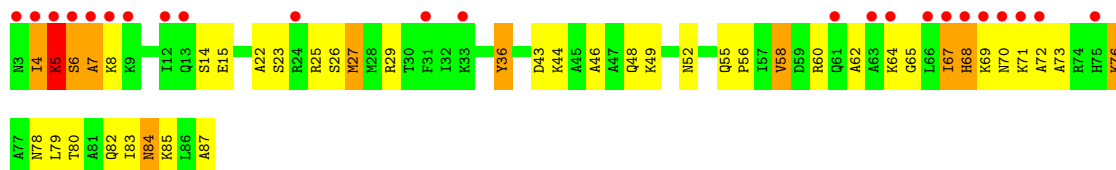
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

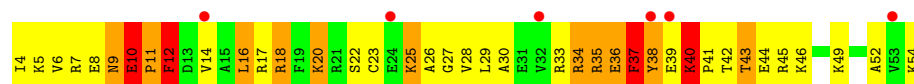


- Molecule 20: 30S ribosomal protein S20

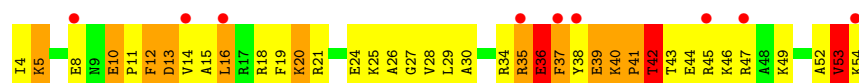


- Molecule 21: 30S ribosomal protein S21

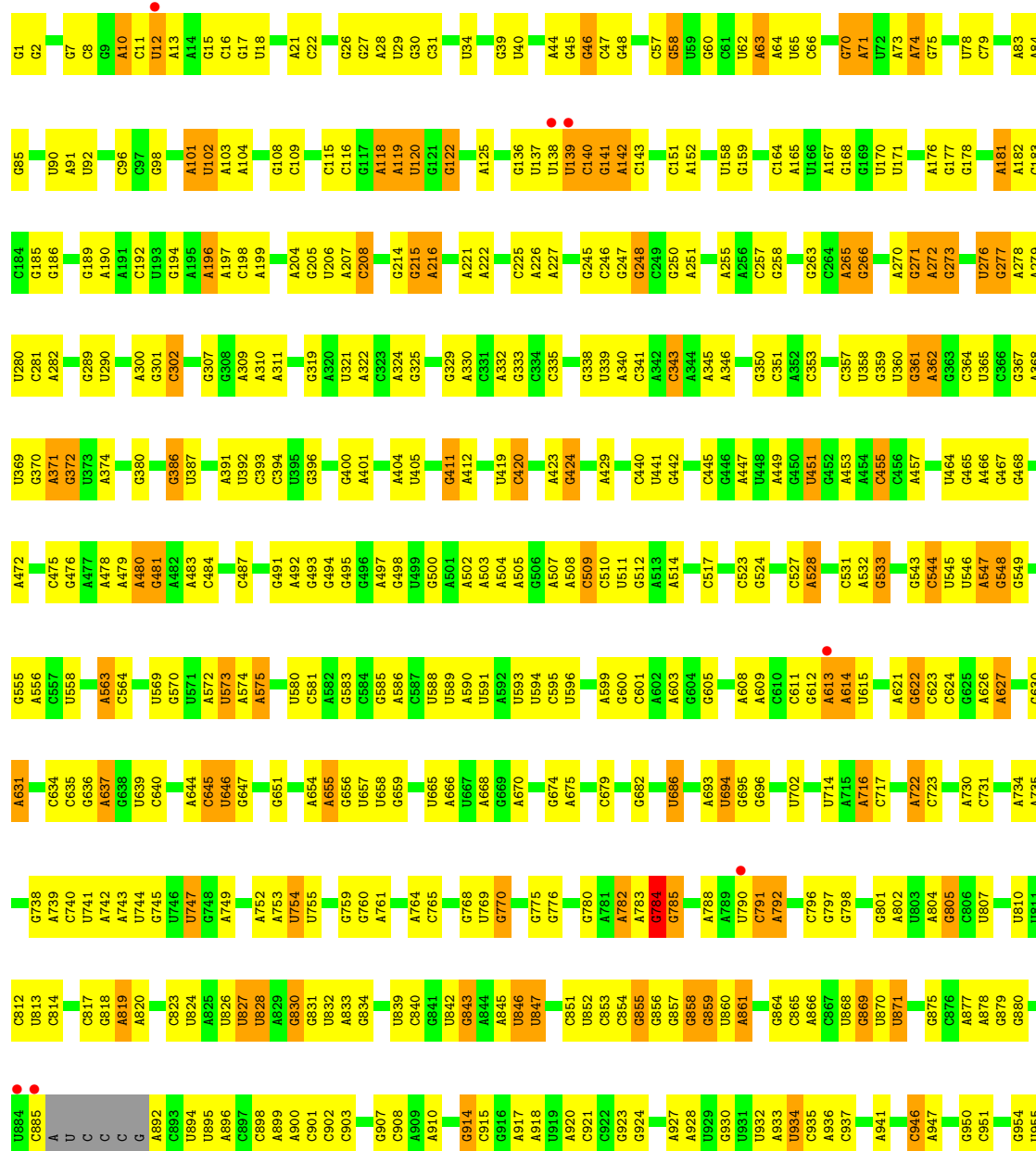




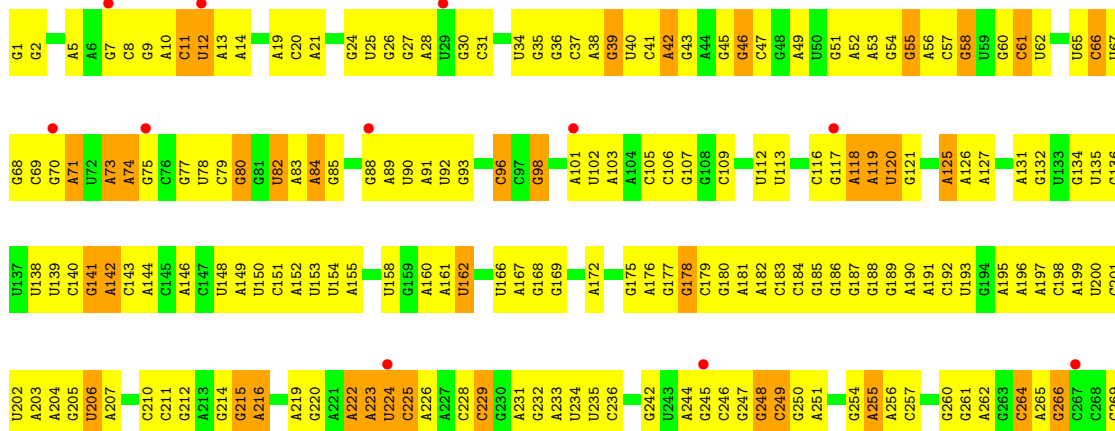
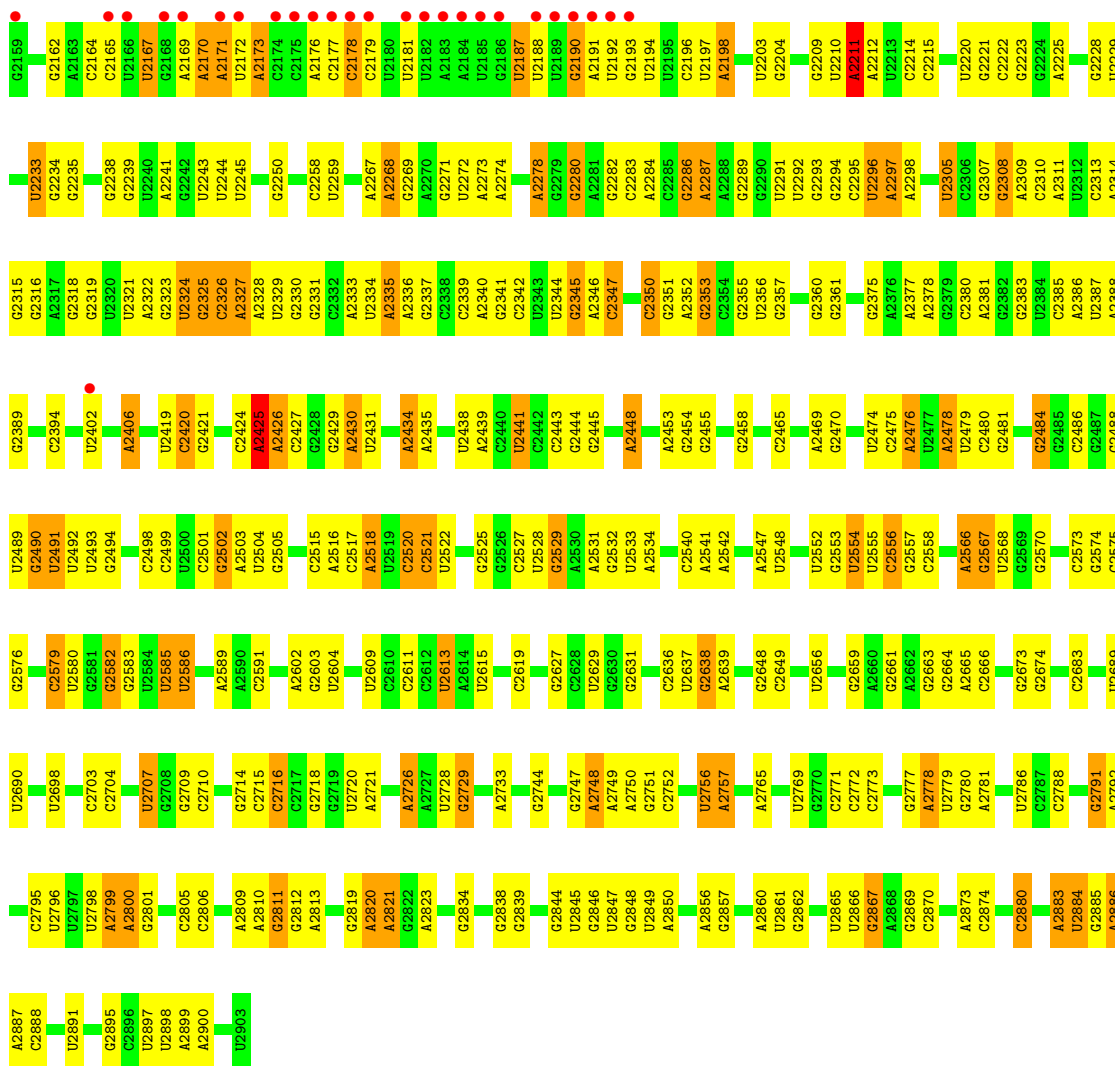
- Molecule 21: 30S ribosomal protein S21

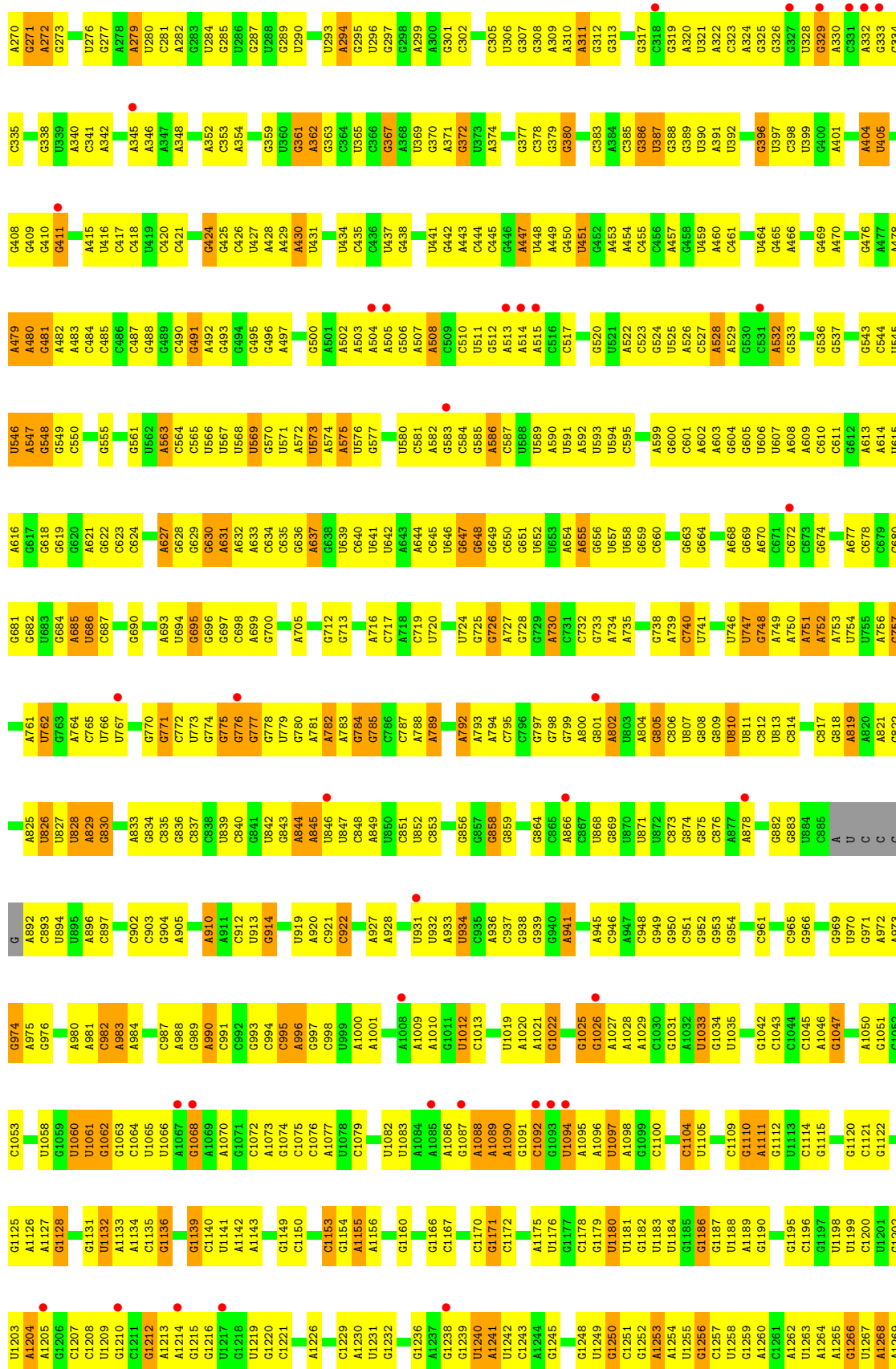


- Molecule 22: 23S rRNA



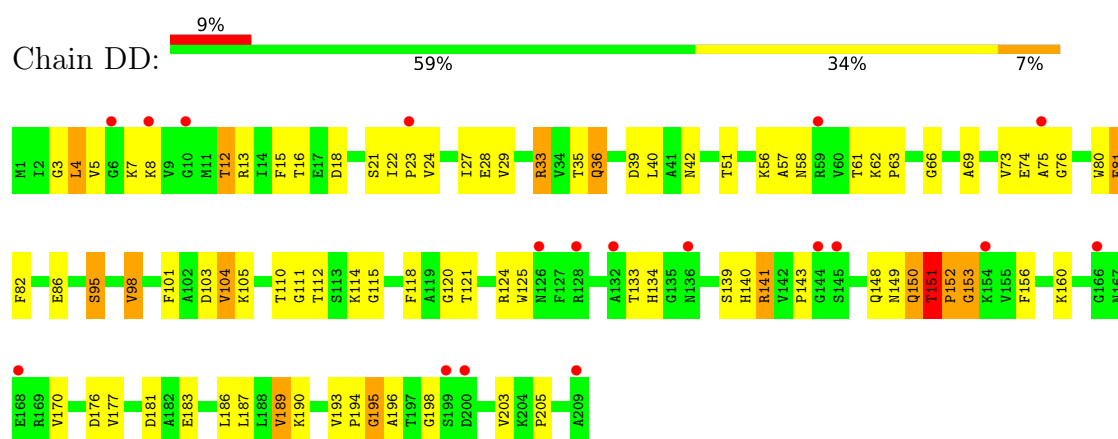
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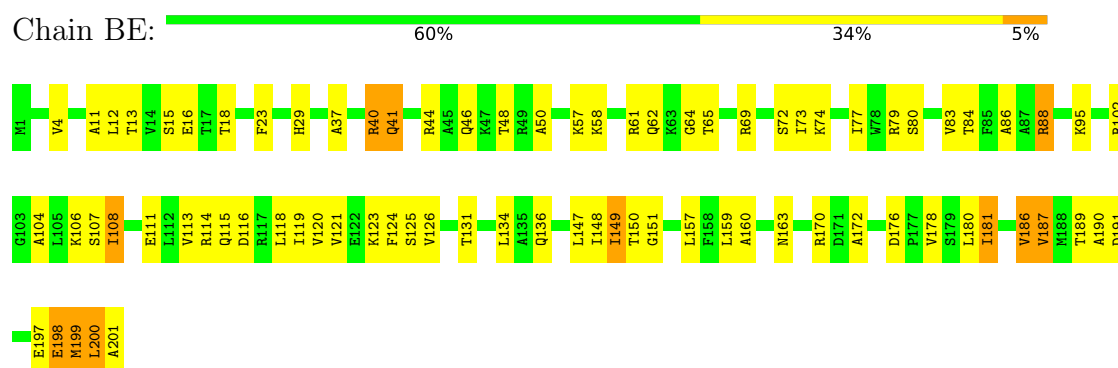


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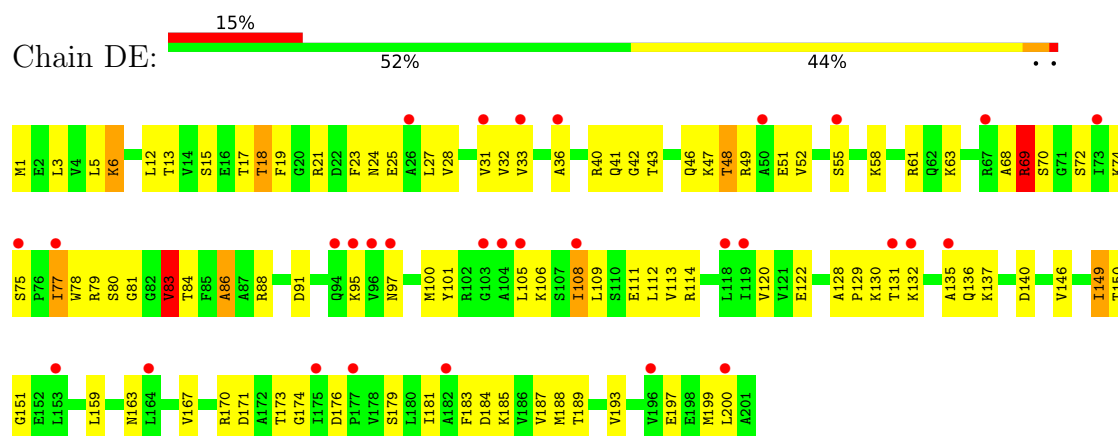




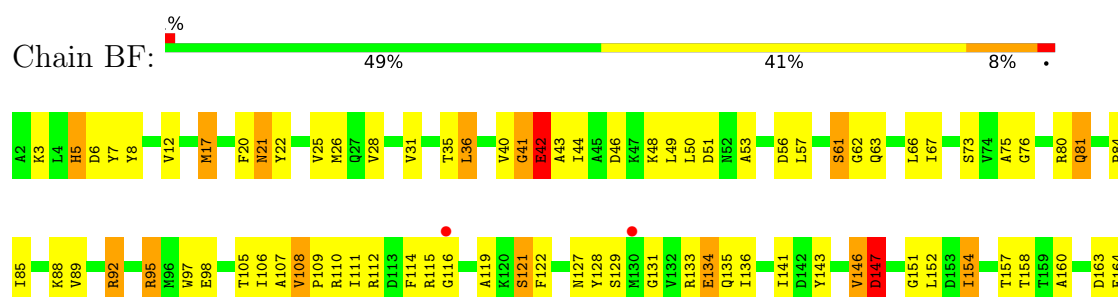
- Molecule 26: 50S ribosomal protein L4



- Molecule 26: 50S ribosomal protein L4

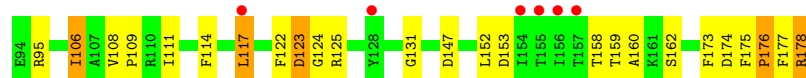
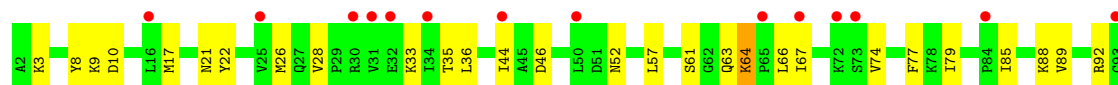
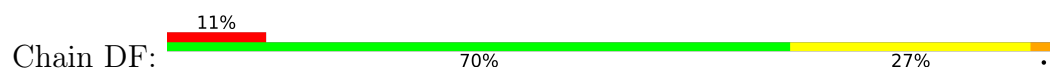


- Molecule 27: 50S ribosomal protein L5

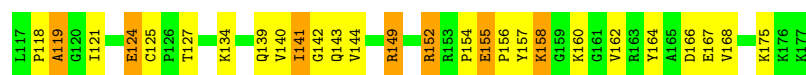
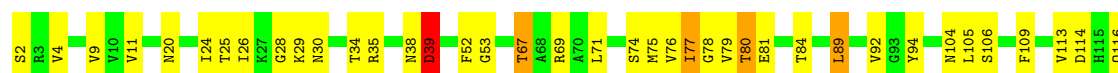




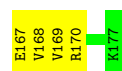
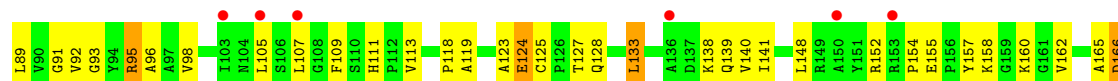
- Molecule 27: 50S ribosomal protein L5



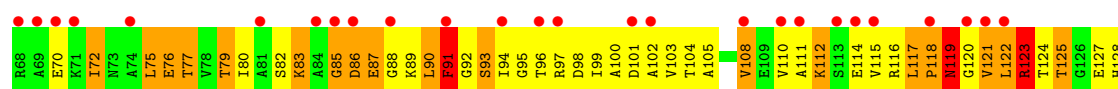
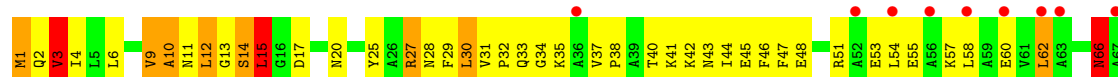
- Molecule 28: 50S ribosomal protein L6

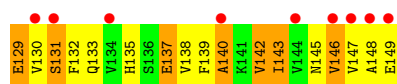


- Molecule 28: 50S ribosomal protein L6

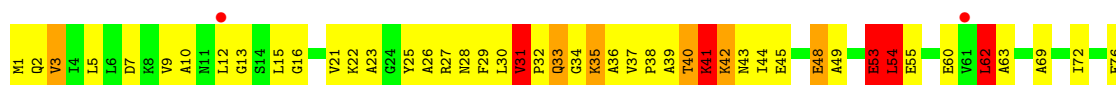


- Molecule 29: 50S ribosomal protein L9

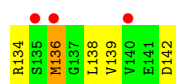
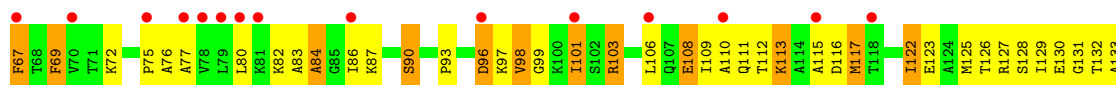
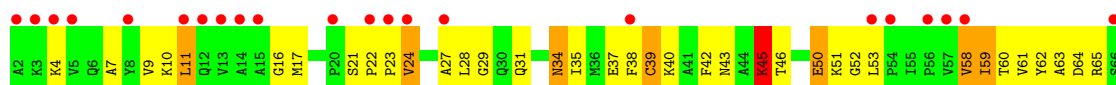




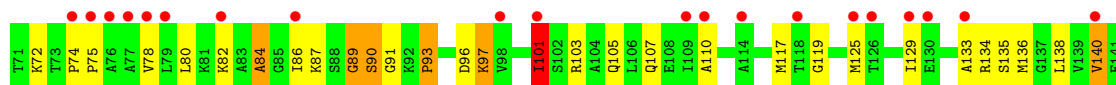
• Molecule 29: 50S ribosomal protein L9



• Molecule 30: 50S ribosomal protein L11

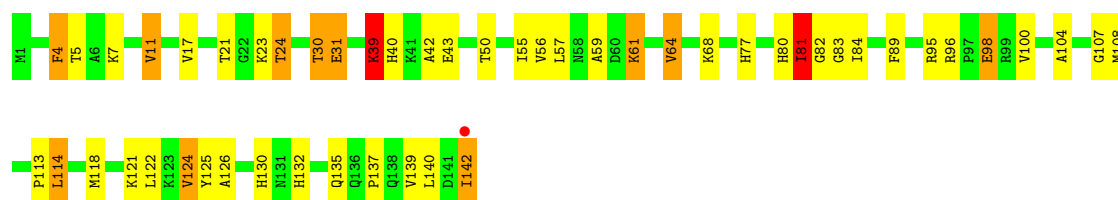


• Molecule 30: 50S ribosomal protein L11

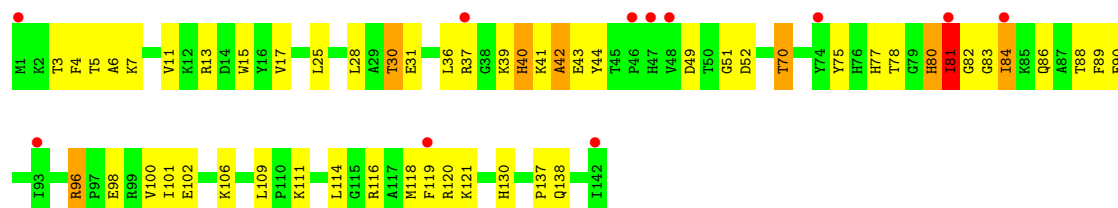


• Molecule 31: 50S ribosomal protein L13

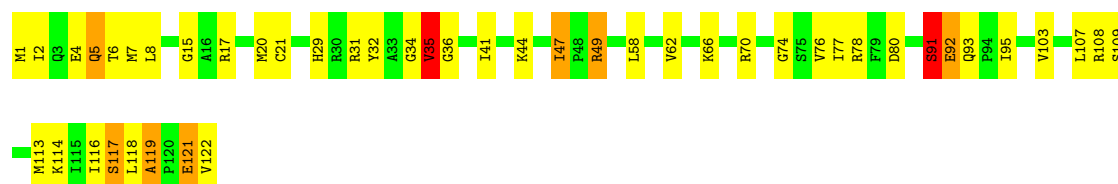




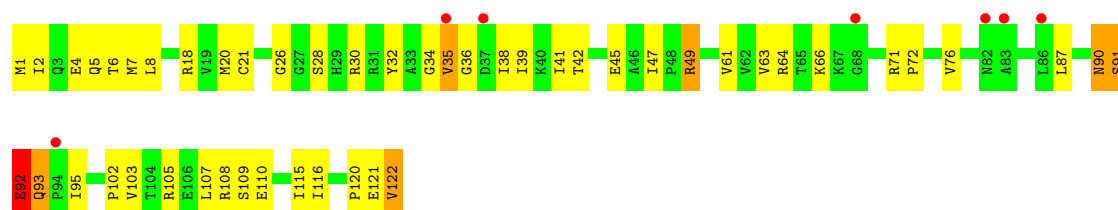
• Molecule 31: 50S ribosomal protein L13



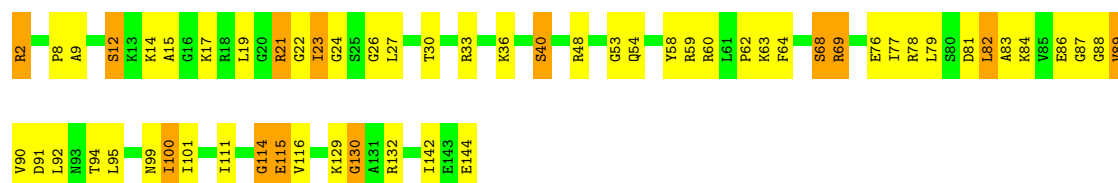
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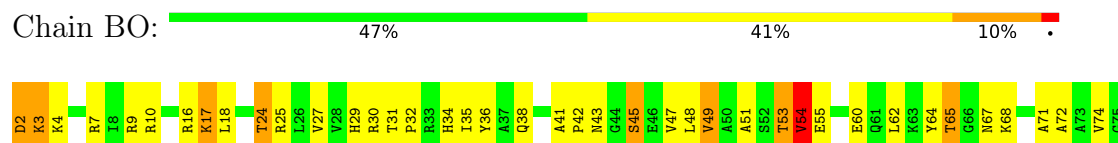
• Molecule 32: 50S ribosomal protein L14



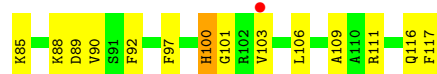
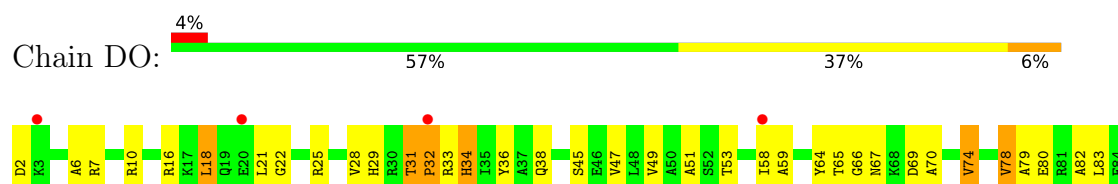
• Molecule 33: 50S ribosomal protein L15



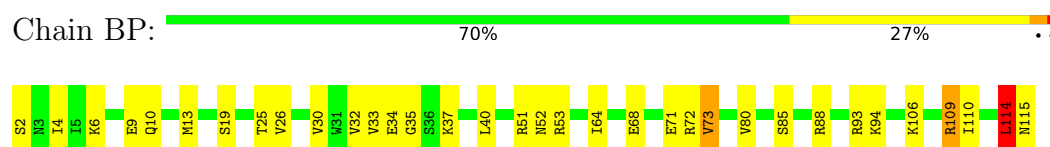
• Molecule 33: 50S ribosomal protein L15



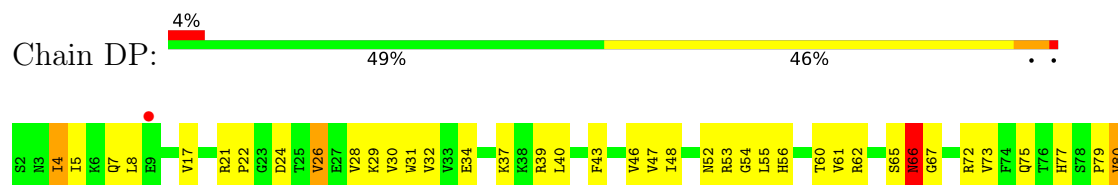
• Molecule 36: 50S ribosomal protein L18



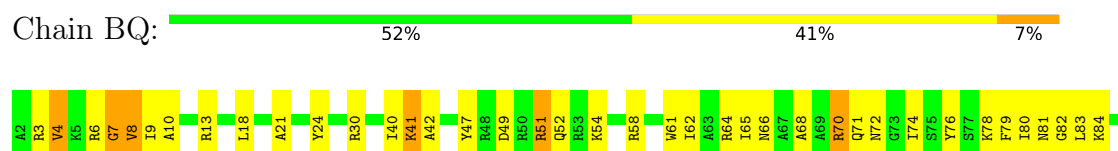
• Molecule 37: 50S ribosomal protein L19



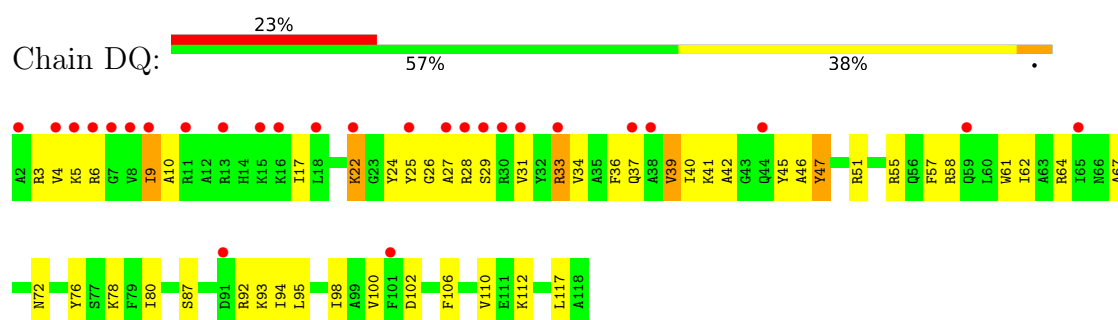
• Molecule 37: 50S ribosomal protein L19



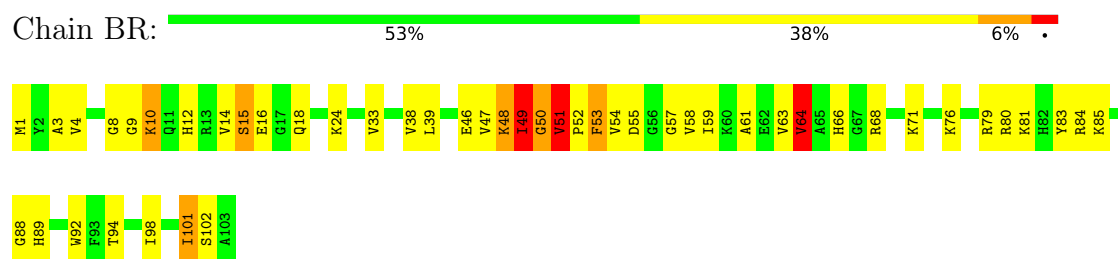
• Molecule 38: 50S ribosomal protein L20



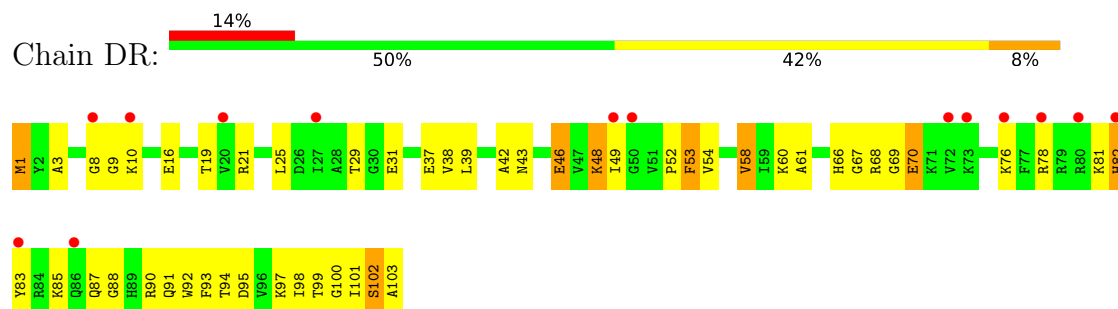
• Molecule 38: 50S ribosomal protein L20



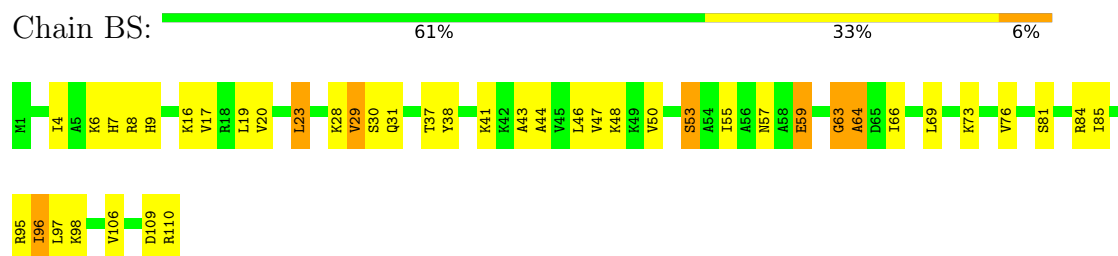
• Molecule 39: 50S ribosomal protein L21



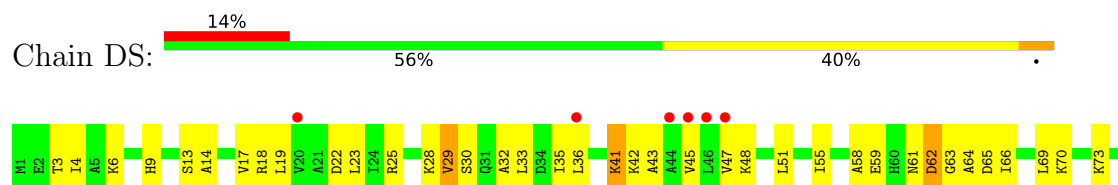
• Molecule 39: 50S ribosomal protein L21



• Molecule 40: 50S ribosomal protein L22

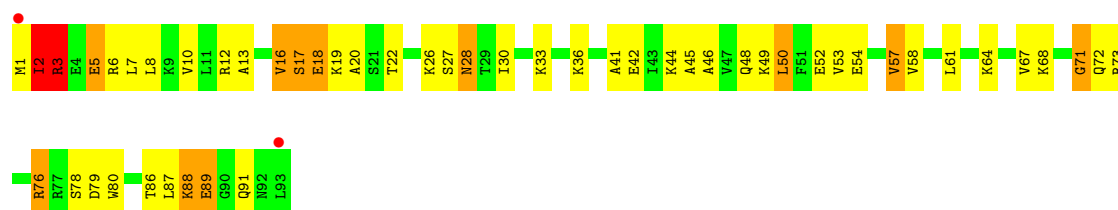


• Molecule 40: 50S ribosomal protein L22

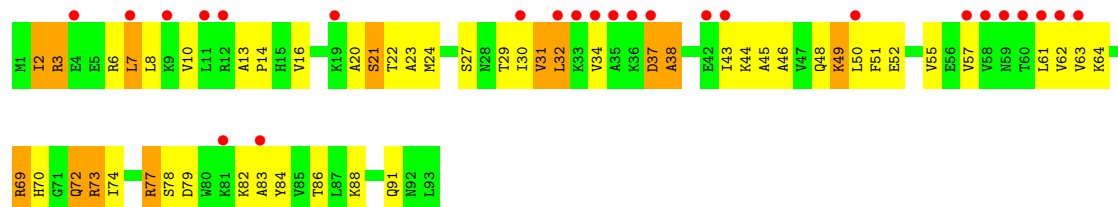




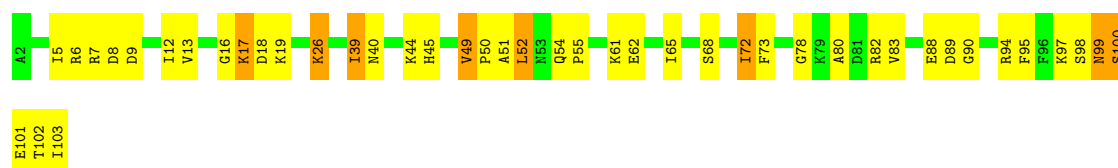
- Molecule 41: 50S ribosomal protein L23



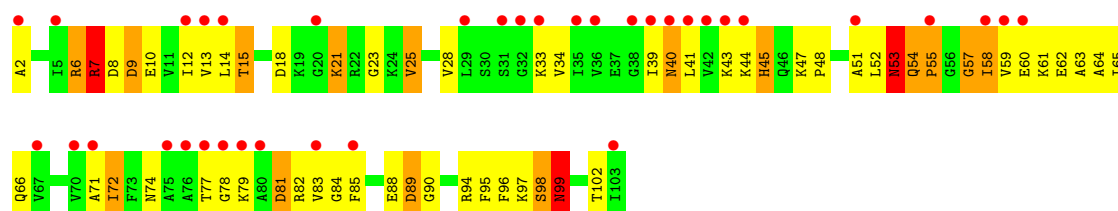
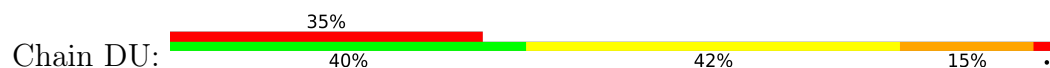
- Molecule 41: 50S ribosomal protein L23



- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24

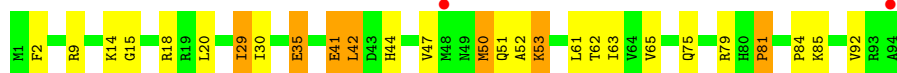
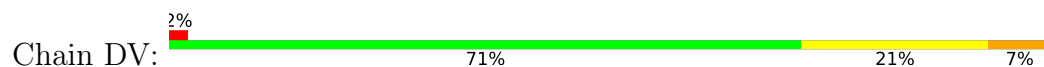


- Molecule 43: 50S ribosomal protein L25

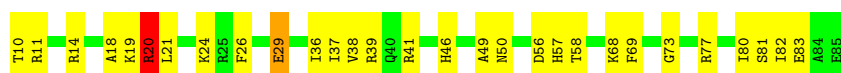




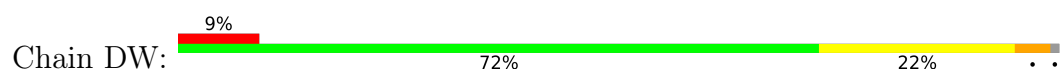
- Molecule 43: 50S ribosomal protein L25



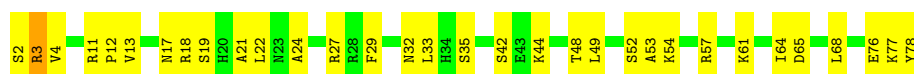
- Molecule 44: 50S ribosomal protein L27



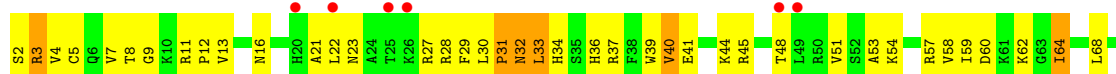
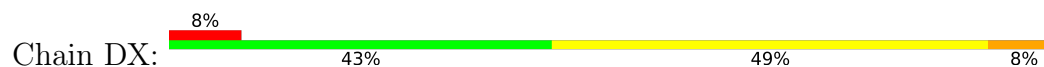
- Molecule 44: 50S ribosomal protein L27



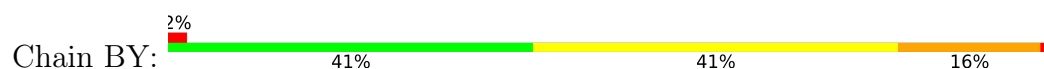
- Molecule 45: 50S ribosomal protein L28



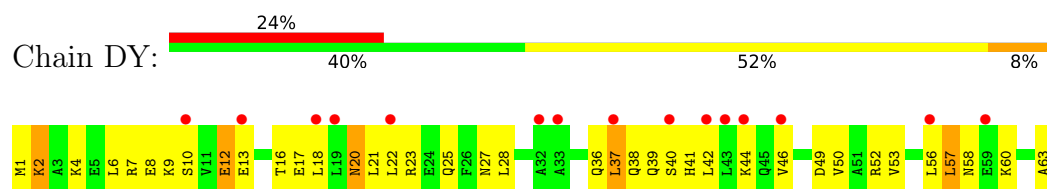
- Molecule 45: 50S ribosomal protein L28



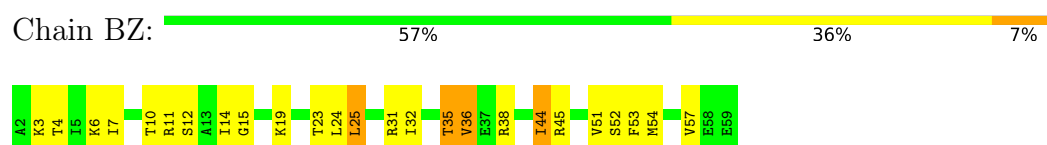
- Molecule 46: 50S ribosomal protein L29



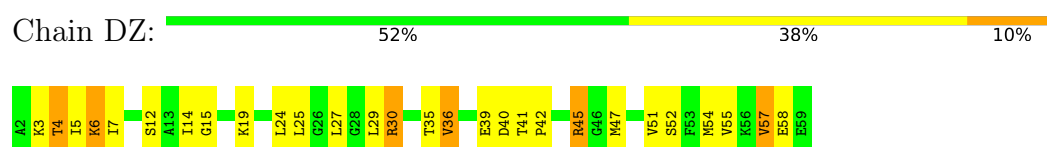
- Molecule 46: 50S ribosomal protein L29



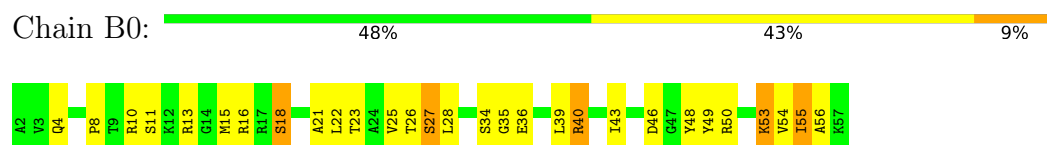
- Molecule 47: 50S ribosomal protein L30



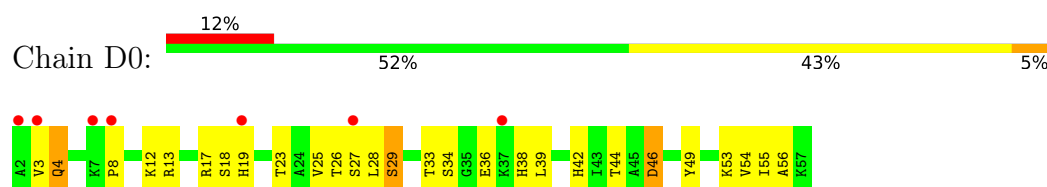
- Molecule 47: 50S ribosomal protein L30



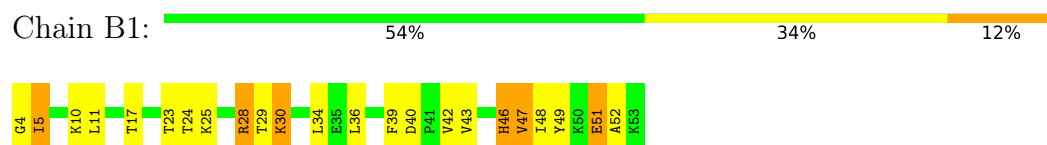
- Molecule 48: 50S ribosomal protein L32



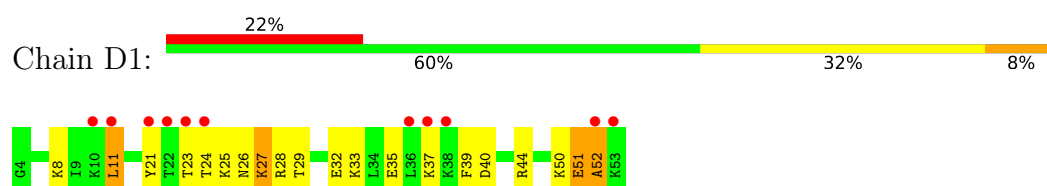
- Molecule 48: 50S ribosomal protein L32



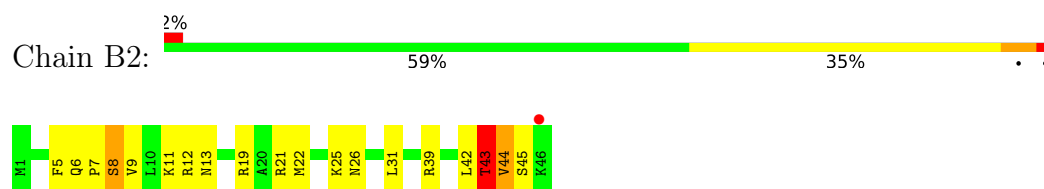
- Molecule 49: 50S ribosomal protein L33



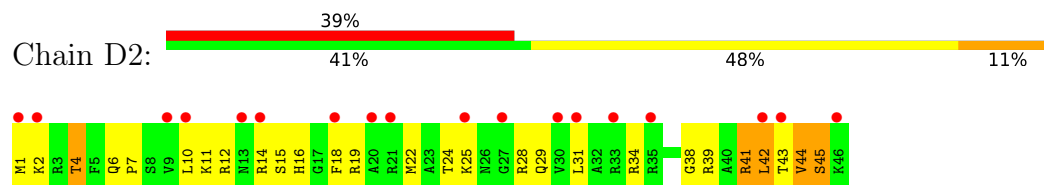
- Molecule 49: 50S ribosomal protein L33



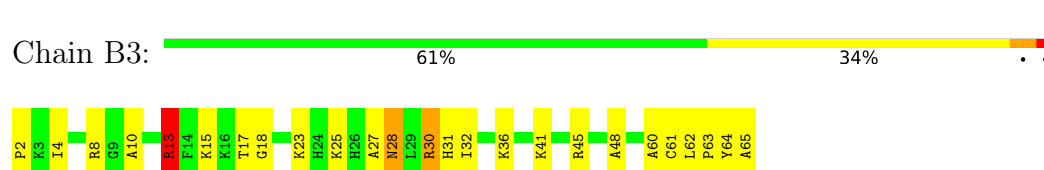
- Molecule 50: 50S ribosomal protein L34



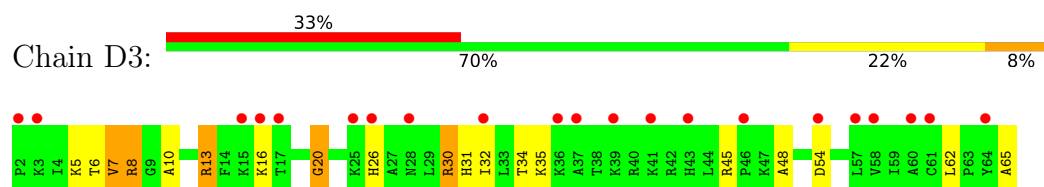
- Molecule 50: 50S ribosomal protein L34



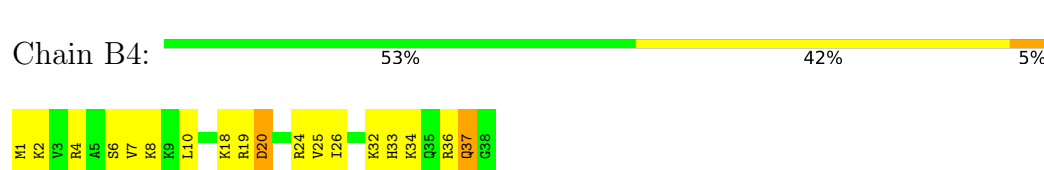
- Molecule 51: 50S ribosomal protein L35



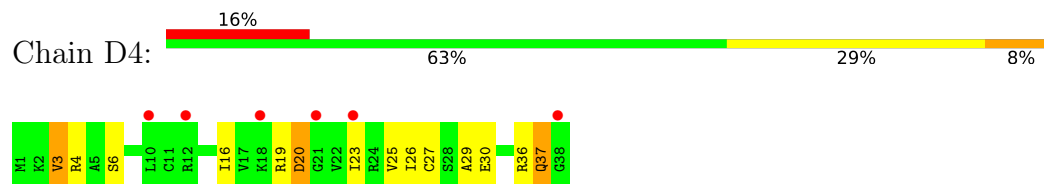
- Molecule 51: 50S ribosomal protein L35



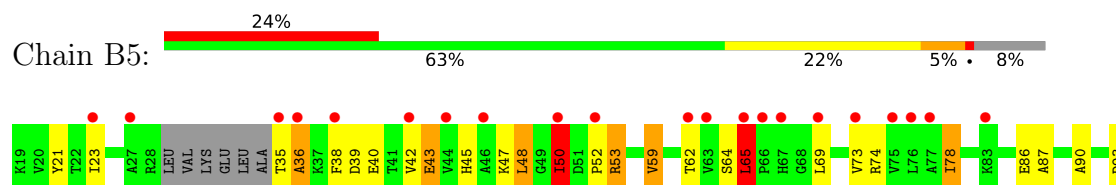
- Molecule 52: 50S ribosomal protein L36

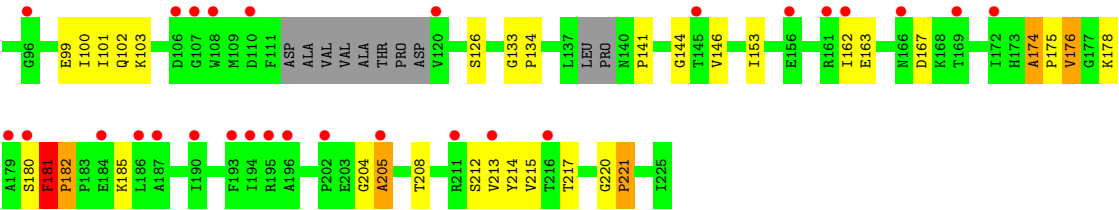


- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.202 , 0.244 0.204 , 0.246	Depositor DCC
R_{free} test set	4190 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NEG, 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	0.32	0/36944	0.52	0/57632
1	CA	0.28	0/36966	0.47	0/57666
2	AB	0.52	0/1736	0.92	4/2338 (0.2%)
2	CB	0.47	1/1736 (0.1%)	0.82	0/2338
3	AC	0.47	0/1652	0.82	2/2225 (0.1%)
3	CC	0.49	0/1652	0.77	0/2225
4	AD	0.49	0/1665	0.85	3/2227 (0.1%)
4	CD	0.61	0/1665	0.92	1/2227 (0.0%)
5	AE	0.57	0/1119	0.96	1/1504 (0.1%)
5	CE	0.58	0/1119	0.96	2/1504 (0.1%)
6	AF	0.57	0/836	0.85	1/1128 (0.1%)
6	CF	0.51	0/836	0.84	1/1128 (0.1%)
7	AG	0.47	0/1196	0.82	2/1602 (0.1%)
7	CG	0.51	0/1196	0.79	0/1602
8	AH	0.51	0/989	0.93	2/1326 (0.2%)
8	CH	0.44	0/989	0.83	0/1326
9	AI	0.46	0/1034	0.78	1/1375 (0.1%)
9	CI	0.45	0/1034	0.74	0/1375
10	AJ	0.48	0/797	0.80	2/1077 (0.2%)
10	CJ	0.52	0/797	0.78	1/1077 (0.1%)
11	AK	0.50	0/893	0.85	1/1205 (0.1%)
11	CK	0.47	0/893	0.90	2/1205 (0.2%)
12	AL	0.64	2/969 (0.2%)	1.02	1/1300 (0.1%)
12	CL	0.54	0/969	1.00	1/1300 (0.1%)
13	AM	0.50	0/893	0.86	0/1193
13	CM	0.53	0/893	0.81	1/1193 (0.1%)
14	AN	0.44	0/785	0.86	3/1043 (0.3%)
14	CN	0.44	0/785	0.75	0/1043
15	AO	0.49	0/722	0.83	0/964
15	CO	0.41	0/722	0.81	0/964
16	AP	0.55	0/659	0.82	0/884
16	CP	0.53	0/659	0.87	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.59	0/658	0.90	0/881
17	CQ	0.51	0/658	0.78	0/881
18	AR	0.53	0/463	0.82	0/621
18	CR	0.49	0/463	0.83	1/621 (0.2%)
19	AS	0.51	0/653	0.84	2/877 (0.2%)
19	CS	0.50	0/653	0.80	2/877 (0.2%)
20	AT	0.55	0/671	0.93	2/888 (0.2%)
20	CT	0.48	0/671	0.86	1/888 (0.1%)
21	AU	0.72	0/431	1.05	4/570 (0.7%)
21	CU	0.61	0/431	0.88	2/570 (0.4%)
22	BA	0.57	0/69659	0.72	10/108672 (0.0%)
22	DA	0.27	0/69659	0.44	0/108672
23	BB	0.48	0/2850	0.68	1/4444 (0.0%)
23	DB	0.21	0/2828	0.34	0/4410
24	BC	0.82	0/2122	1.11	13/2852 (0.5%)
24	DC	0.50	0/2122	0.90	2/2852 (0.1%)
25	BD	1.03	2/1586 (0.1%)	1.73	6/2134 (0.3%)
25	DD	0.49	0/1586	0.86	3/2134 (0.1%)
26	BE	0.79	0/1571	1.00	4/2113 (0.2%)
26	DE	0.52	0/1571	0.81	0/2113
27	BF	0.56	0/1435	0.91	3/1926 (0.2%)
27	DF	0.43	0/1435	0.74	0/1926
28	BG	0.65	0/1343	1.02	3/1816 (0.2%)
28	DG	0.43	0/1343	0.76	2/1816 (0.1%)
29	BH	0.46	0/1121	0.94	4/1515 (0.3%)
29	DH	0.47	0/1121	0.91	5/1515 (0.3%)
30	BI	0.59	0/1046	0.84	0/1410
30	DI	0.59	0/1046	0.86	1/1410 (0.1%)
31	BJ	0.96	0/1152	1.13	4/1551 (0.3%)
31	DJ	0.45	0/1152	0.86	2/1551 (0.1%)
32	BK	0.89	0/948	1.23	4/1268 (0.3%)
32	DK	0.50	0/948	0.83	2/1268 (0.2%)
33	BL	0.81	0/1054	1.12	2/1403 (0.1%)
33	DL	0.50	0/1054	0.90	1/1403 (0.1%)
34	BM	0.90	1/1093 (0.1%)	1.08	6/1460 (0.4%)
34	DM	0.42	0/1093	0.81	2/1460 (0.1%)
35	BN	0.95	1/974 (0.1%)	1.23	6/1301 (0.5%)
35	DN	0.50	0/974	0.81	0/1301
36	BO	0.67	0/902	0.98	2/1209 (0.2%)
36	DO	0.41	0/902	0.75	0/1209
37	BP	0.80	0/929	0.99	1/1242 (0.1%)
37	DP	0.48	0/929	0.83	3/1242 (0.2%)
38	BQ	1.04	2/960 (0.2%)	1.28	5/1278 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.44	0/960	0.80	0/1278
39	BR	0.97	0/829	1.34	6/1107 (0.5%)
39	DR	0.47	0/829	0.80	0/1107
40	BS	1.09	0/864	1.13	2/1156 (0.2%)
40	DS	0.50	0/864	0.83	0/1156
41	BT	0.86	1/745 (0.1%)	1.05	1/994 (0.1%)
41	DT	0.48	0/745	0.80	0/994
42	BU	0.69	0/788	0.98	0/1051
42	DU	0.58	0/788	0.88	2/1051 (0.2%)
43	BV	0.81	0/766	1.02	0/1025
43	DV	0.39	0/766	0.73	0/1025
44	BW	0.85	0/587	1.12	2/776 (0.3%)
44	DW	0.39	0/576	0.73	0/762
45	BX	0.74	0/635	0.97	0/848
45	DX	0.51	0/635	0.86	0/848
46	BY	0.70	0/510	1.01	3/677 (0.4%)
46	DY	0.44	0/510	0.85	0/677
47	BZ	0.99	0/453	1.11	1/605 (0.2%)
47	DZ	0.46	0/453	0.87	1/605 (0.2%)
48	B0	1.00	1/450 (0.2%)	1.07	1/599 (0.2%)
48	D0	0.48	0/450	0.75	0/599
49	B1	0.61	0/417	0.97	2/554 (0.4%)
49	D1	0.49	0/417	0.70	0/554
50	B2	0.99	0/380	1.28	2/498 (0.4%)
50	D2	0.49	0/380	0.86	0/498
51	B3	0.80	0/513	1.13	3/676 (0.4%)
51	D3	0.46	0/513	0.78	0/676
52	B4	0.91	0/303	1.11	0/397
52	D4	0.44	0/303	0.81	0/397
53	B5	0.54	0/1145	0.99	8/1556 (0.5%)
All	All	0.47	11/310634 (0.0%)	0.68	177/464376 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BD	151	THR	C-O	13.08	1.40	1.24
34	BM	36	VAL	CA-CB	-6.74	1.46	1.54
25	BD	152	PRO	N-CA	-5.97	1.39	1.47
38	BQ	42	ALA	CA-CB	-5.68	1.44	1.53
48	B0	21	ALA	CA-CB	-5.52	1.44	1.53

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BD	151	THR	CA-C-N	41.74	172.01	119.84
25	BD	151	THR	C-N-CA	41.74	172.01	119.84
25	BD	151	THR	C-N-CD	-12.44	73.98	125.00
39	BR	51	VAL	CA-C-N	-12.19	108.51	120.21
39	BR	51	VAL	C-N-CA	-12.19	108.51	120.21

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	896	5
1	CA	33015	0	16617	1016	0
2	AB	1705	0	1732	122	0
2	CB	1705	0	1732	115	0
3	AC	1625	0	1696	61	0
3	CC	1625	0	1696	50	0
4	AD	1643	0	1707	128	0
4	CD	1643	0	1707	104	0
5	AE	1106	0	1148	84	0
5	CE	1106	0	1148	100	0
6	AF	818	0	808	50	0
6	CF	818	0	808	55	0
7	AG	1182	0	1238	53	0
7	CG	1182	0	1238	46	0
8	AH	979	0	1031	48	0
8	CH	979	0	1031	43	0
9	AI	1022	0	1070	59	0
9	CI	1022	0	1070	42	0
10	AJ	787	0	828	43	0
10	CJ	787	0	828	34	0
11	AK	877	0	887	62	0
11	CK	877	0	887	55	0
12	AL	955	0	1016	63	0
12	CL	955	0	1016	75	0
13	AM	884	0	941	52	0
13	CM	884	0	941	37	0
14	AN	774	0	824	47	0
14	CN	774	0	824	28	0
15	AO	714	0	734	31	0
15	CO	714	0	734	38	0
16	AP	649	0	666	30	0
16	CP	649	0	666	46	0
17	AQ	649	0	691	48	0
17	CQ	649	0	691	41	0
18	AR	456	0	478	11	0
18	CR	456	0	478	28	0
19	AS	638	0	665	33	0
19	CS	638	0	665	22	0
20	AT	665	0	714	42	0
20	CT	665	0	714	35	0
21	AU	426	0	449	60	0
21	CU	426	0	449	47	0
22	BA	62195	0	31278	1189	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	62195	0	31280	2066	0
23	BB	2549	0	1291	36	0
23	DB	2529	0	1281	42	0
24	BC	2083	0	2154	85	0
24	DC	2083	0	2154	168	0
25	BD	1565	0	1616	62	0
25	DD	1565	0	1616	71	0
26	BE	1552	0	1619	62	0
26	DE	1552	0	1619	84	0
27	BF	1411	0	1444	71	0
27	DF	1411	0	1444	29	0
28	BG	1323	0	1371	49	0
28	DG	1323	0	1371	44	0
29	BH	1110	0	1148	172	0
29	DH	1110	0	1148	91	5
30	BI	1032	0	1085	58	0
30	DI	1032	0	1085	40	0
31	BJ	1129	0	1162	43	0
31	DJ	1129	0	1162	48	0
32	BK	939	0	1012	32	0
32	DK	939	0	1012	36	0
33	BL	1045	0	1117	57	0
33	DL	1045	0	1117	64	0
34	BM	1074	0	1157	45	0
34	DM	1074	0	1157	26	0
35	BN	961	0	1000	49	0
35	DN	961	0	1000	49	0
36	BO	892	0	923	52	0
36	DO	892	0	923	36	0
37	BP	917	0	962	23	0
37	DP	917	0	962	41	0
38	BQ	947	0	1019	52	0
38	DQ	947	0	1019	48	0
39	BR	816	0	839	60	0
39	DR	816	0	839	47	0
40	BS	857	0	922	30	0
40	DS	857	0	922	32	0
41	BT	739	0	807	52	0
41	DT	739	0	807	28	0
42	BU	780	0	831	34	0
42	DU	780	0	831	64	0
43	BV	753	0	780	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DV	753	0	780	17	0
44	BW	580	0	594	22	0
44	DW	569	0	581	12	0
45	BX	625	0	652	21	0
45	DX	625	0	652	55	0
46	BY	509	0	543	31	0
46	DY	509	0	543	24	0
47	BZ	449	0	488	13	0
47	DZ	449	0	488	15	0
48	B0	444	0	458	26	0
48	D0	444	0	458	19	0
49	B1	410	0	440	15	0
49	D1	410	0	440	12	0
50	B2	377	0	418	16	0
50	D2	377	0	418	41	0
51	B3	504	0	572	24	0
51	D3	504	0	572	22	0
52	B4	302	0	340	12	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	9120	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 9120 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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	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%)	1	9
3	CC	204/206 (99%)	165 (81%)	29 (14%)	10 (5%)	1	11
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	5
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	7
6	CF	98/100 (98%)	72 (74%)	17 (17%)	9 (9%)	0	3

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	99 (92%)	7 (6%)	2 (2%)	6	27
40	DS	108/110 (98%)	91 (84%)	13 (12%)	4 (4%)	2	15
41	BT	91/93 (98%)	73 (80%)	9 (10%)	9 (10%)	0	3
41	DT	91/93 (98%)	65 (71%)	18 (20%)	8 (9%)	0	3
42	BU	100/102 (98%)	79 (79%)	15 (15%)	6 (6%)	1	7
42	DU	100/102 (98%)	74 (74%)	13 (13%)	13 (13%)	0	1
43	BV	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	11	39
43	DV	92/94 (98%)	83 (90%)	7 (8%)	2 (2%)	5	24
44	BW	74/76 (97%)	66 (89%)	7 (10%)	1 (1%)	9	34
44	DW	73/76 (96%)	61 (84%)	11 (15%)	1 (1%)	9	34
45	BX	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	9	35
45	DX	75/77 (97%)	54 (72%)	17 (23%)	4 (5%)	1	10
46	BY	61/63 (97%)	47 (77%)	5 (8%)	9 (15%)	0	0
46	DY	61/63 (97%)	50 (82%)	8 (13%)	3 (5%)	1	11
47	BZ	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
47	DZ	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	2	16
48	B0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	2	15
48	D0	54/56 (96%)	37 (68%)	14 (26%)	3 (6%)	1	8
49	B1	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	2	13
49	D1	48/50 (96%)	35 (73%)	9 (19%)	4 (8%)	0	4
50	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	2	12
50	D2	44/46 (96%)	38 (86%)	3 (7%)	3 (7%)	1	5
51	B3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	7	30
51	D3	62/64 (97%)	54 (87%)	6 (10%)	2 (3%)	3	18
52	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
52	D4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	1	8
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	6

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%)	133 (74%)	47 (26%)	0	2
2	CB	180/180 (100%)	142 (79%)	38 (21%)	1	5
3	AC	170/170 (100%)	138 (81%)	32 (19%)	1	7
3	CC	170/170 (100%)	151 (89%)	19 (11%)	6	24
4	AD	172/172 (100%)	144 (84%)	28 (16%)	2	11
4	CD	172/172 (100%)	147 (86%)	25 (14%)	3	14
5	AE	113/113 (100%)	88 (78%)	25 (22%)	1	4
5	CE	113/113 (100%)	86 (76%)	27 (24%)	1	3
6	AF	87/87 (100%)	71 (82%)	16 (18%)	1	8
6	CF	87/87 (100%)	68 (78%)	19 (22%)	1	5
7	AG	124/124 (100%)	101 (82%)	23 (18%)	1	8
7	CG	124/124 (100%)	105 (85%)	19 (15%)	3	12
8	AH	104/104 (100%)	91 (88%)	13 (12%)	4	19
8	CH	104/104 (100%)	82 (79%)	22 (21%)	1	5
9	AI	105/105 (100%)	83 (79%)	22 (21%)	1	5
9	CI	105/105 (100%)	87 (83%)	18 (17%)	2	10
10	AJ	86/86 (100%)	69 (80%)	17 (20%)	1	6
10	CJ	86/86 (100%)	72 (84%)	14 (16%)	2	11
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	4
11	CK	90/90 (100%)	74 (82%)	16 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	87 (84%)	16 (16%)	2	12
12	CL	103/103 (100%)	81 (79%)	22 (21%)	1	5
13	AM	92/92 (100%)	81 (88%)	11 (12%)	5	21
13	CM	92/92 (100%)	83 (90%)	9 (10%)	7	29
14	AN	79/83 (95%)	71 (90%)	8 (10%)	7	28
14	CN	79/83 (95%)	73 (92%)	6 (8%)	12	39
15	AO	76/76 (100%)	67 (88%)	9 (12%)	5	21
15	CO	76/76 (100%)	63 (83%)	13 (17%)	2	10
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	4
16	CP	65/65 (100%)	56 (86%)	9 (14%)	3	15
17	AQ	74/74 (100%)	54 (73%)	20 (27%)	0	2
17	CQ	74/74 (100%)	60 (81%)	14 (19%)	1	7
18	AR	48/48 (100%)	44 (92%)	4 (8%)	10	35
18	CR	48/48 (100%)	42 (88%)	6 (12%)	4	19
19	AS	70/70 (100%)	63 (90%)	7 (10%)	7	29
19	CS	70/70 (100%)	60 (86%)	10 (14%)	3	14
20	AT	65/65 (100%)	48 (74%)	17 (26%)	0	2
20	CT	65/65 (100%)	53 (82%)	12 (18%)	1	8
21	AU	44/44 (100%)	30 (68%)	14 (32%)	0	0
21	CU	44/44 (100%)	34 (77%)	10 (23%)	1	4
24	BC	216/216 (100%)	189 (88%)	27 (12%)	4	19
24	DC	216/216 (100%)	189 (88%)	27 (12%)	4	19
25	BD	164/164 (100%)	151 (92%)	13 (8%)	11	37
25	DD	164/164 (100%)	149 (91%)	15 (9%)	9	32
26	BE	165/165 (100%)	143 (87%)	22 (13%)	4	17
26	DE	165/165 (100%)	154 (93%)	11 (7%)	15	43
27	BF	148/148 (100%)	126 (85%)	22 (15%)	3	13
27	DF	148/148 (100%)	133 (90%)	15 (10%)	7	28
28	BG	137/137 (100%)	121 (88%)	16 (12%)	5	22
28	DG	137/137 (100%)	125 (91%)	12 (9%)	9	33
29	BH	114/114 (100%)	83 (73%)	31 (27%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	90 (79%)	24 (21%)	1	5
30	BI	109/109 (100%)	86 (79%)	23 (21%)	1	5
30	DI	109/109 (100%)	90 (83%)	19 (17%)	2	9
31	BJ	116/116 (100%)	100 (86%)	16 (14%)	3	15
31	DJ	116/116 (100%)	108 (93%)	8 (7%)	14	41
32	BK	103/103 (100%)	93 (90%)	10 (10%)	8	30
32	DK	103/103 (100%)	94 (91%)	9 (9%)	9	34
33	BL	102/102 (100%)	87 (85%)	15 (15%)	3	14
33	DL	102/102 (100%)	94 (92%)	8 (8%)	11	38
34	BM	109/109 (100%)	95 (87%)	14 (13%)	4	18
34	DM	109/109 (100%)	104 (95%)	5 (5%)	24	55
35	BN	100/100 (100%)	87 (87%)	13 (13%)	4	18
35	DN	100/100 (100%)	89 (89%)	11 (11%)	6	24
36	BO	86/86 (100%)	69 (80%)	17 (20%)	1	6
36	DO	86/86 (100%)	75 (87%)	11 (13%)	4	18
37	BP	99/99 (100%)	88 (89%)	11 (11%)	6	24
37	DP	99/99 (100%)	89 (90%)	10 (10%)	7	28
38	BQ	89/89 (100%)	79 (89%)	10 (11%)	6	24
38	DQ	89/89 (100%)	81 (91%)	8 (9%)	9	33
39	BR	84/84 (100%)	69 (82%)	15 (18%)	2	9
39	DR	84/84 (100%)	76 (90%)	8 (10%)	8	30
40	BS	93/93 (100%)	79 (85%)	14 (15%)	3	13
40	DS	93/93 (100%)	86 (92%)	7 (8%)	12	39
41	BT	80/80 (100%)	66 (82%)	14 (18%)	2	9
41	DT	80/80 (100%)	66 (82%)	14 (18%)	2	9
42	BU	83/83 (100%)	72 (87%)	11 (13%)	4	17
42	DU	83/83 (100%)	73 (88%)	10 (12%)	5	21
43	BV	78/78 (100%)	66 (85%)	12 (15%)	2	12
43	DV	78/78 (100%)	68 (87%)	10 (13%)	4	18
44	BW	57/58 (98%)	53 (93%)	4 (7%)	14	41
44	DW	56/58 (97%)	52 (93%)	4 (7%)	13	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	63 (94%)	4 (6%)	17	47
45	DX	67/67 (100%)	63 (94%)	4 (6%)	17	47
46	BY	55/55 (100%)	49 (89%)	6 (11%)	6	24
46	DY	55/55 (100%)	45 (82%)	10 (18%)	2	8
47	BZ	48/48 (100%)	36 (75%)	12 (25%)	0	2
47	DZ	48/48 (100%)	41 (85%)	7 (15%)	3	14
48	B0	47/47 (100%)	41 (87%)	6 (13%)	4	18
48	D0	47/47 (100%)	41 (87%)	6 (13%)	4	18
49	B1	45/45 (100%)	39 (87%)	6 (13%)	4	17
49	D1	45/45 (100%)	43 (96%)	2 (4%)	25	56
50	B2	38/38 (100%)	34 (90%)	4 (10%)	6	26
50	D2	38/38 (100%)	33 (87%)	5 (13%)	4	17
51	B3	51/51 (100%)	48 (94%)	3 (6%)	18	48
51	D3	51/51 (100%)	48 (94%)	3 (6%)	18	48
52	B4	34/34 (100%)	28 (82%)	6 (18%)	2	9
52	D4	34/34 (100%)	31 (91%)	3 (9%)	9	33
53	B5	61/161 (38%)	48 (79%)	13 (21%)	1	5
All	All	9388/9499 (99%)	8020 (85%)	1368 (15%)	3	14

5 of 1368 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	CI	36	GLU
27	DF	147	ASP
10	CJ	89	ARG
9	CI	32	GLN
17	CQ	75	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
13	CM	8	ASN
29	DH	28	ASN
16	CP	26	ASN
25	DD	140	HIS

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Mol	Chain	Res	Type
36	DO	100	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%)	304 (19%)	7 (0%)
22	BA	2895/2903 (99%)	519 (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%)	1697 (18%)	77 (0%)

5 of 1697 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	DA	404	A
22	DA	2225	A
22	DA	982	C
22	DA	1900	A
22	DA	2425	A

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 oligosaccharides 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	14,16,16	0.66	0	12,20,20	0.64	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	-	10/18/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	CA	1657	NEG	N3-C7-C8-O1
56	CA	1657	NEG	N3-C7-C8-O2
56	CA	1657	NEG	C8-C7-N3-N2
56	CA	1657	NEG	C6-N2-N3-C9
56	CA	1657	NEG	N4-C4-C5-C6

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.39	33 (2%) 63 42	12, 56, 146, 187	0
1	CA	1539/1539 (100%)	0.07	47 (3%) 51 30	24, 78, 151, 182	0
2	AB	218/218 (100%)	0.34	12 (5%) 30 16	38, 79, 106, 130	0
2	CB	218/218 (100%)	0.74	23 (10%) 11 6	62, 97, 114, 127	0
3	AC	206/206 (100%)	0.06	1 (0%) 87 73	57, 83, 97, 110	0
3	CC	206/206 (100%)	0.62	9 (4%) 39 21	83, 101, 112, 120	0
4	AD	205/205 (100%)	0.02	5 (2%) 59 38	39, 64, 88, 106	0
4	CD	205/205 (100%)	-0.21	4 (1%) 65 44	21, 41, 70, 92	0
5	AE	150/150 (100%)	-0.09	1 (0%) 84 68	31, 50, 83, 105	0
5	CE	150/150 (100%)	0.06	3 (2%) 65 44	28, 58, 89, 109	0
6	AF	100/100 (100%)	-0.03	3 (3%) 52 31	36, 60, 80, 92	0
6	CF	100/100 (100%)	0.08	1 (1%) 79 61	48, 81, 103, 108	0
7	AG	151/151 (100%)	0.54	11 (7%) 21 11	68, 93, 106, 116	0
7	CG	151/151 (100%)	1.50	38 (25%) 1 1	95, 117, 127, 130	0
8	AH	129/129 (100%)	-0.25	1 (0%) 82 65	31, 52, 72, 90	0
8	CH	129/129 (100%)	0.08	3 (2%) 61 39	55, 75, 93, 105	0
9	AI	127/127 (100%)	0.94	21 (16%) 4 2	70, 95, 110, 122	0
9	CI	127/127 (100%)	1.32	30 (23%) 2 1	100, 112, 123, 131	0
10	AJ	98/98 (100%)	0.73	11 (11%) 10 5	76, 90, 107, 127	0
10	CJ	98/98 (100%)	1.52	26 (26%) 1 1	97, 114, 122, 133	0
11	AK	117/117 (100%)	0.20	4 (3%) 48 28	26, 70, 98, 117	0
11	CK	117/117 (100%)	0.01	1 (0%) 81 63	36, 75, 94, 98	0
12	AL	123/123 (100%)	-0.17	3 (2%) 59 38	23, 39, 70, 100	0
12	CL	123/123 (100%)	0.34	6 (4%) 35 18	34, 56, 84, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.75	11 (9%) 13 7	70, 87, 104, 111	0
13	CM	114/114 (100%)	1.49	23 (20%) 3 1	105, 122, 130, 134	0
14	AN	96/100 (96%)	1.04	12 (12%) 8 5	79, 91, 108, 117	0
14	CN	96/100 (96%)	1.29	19 (19%) 3 1	98, 112, 125, 129	0
15	AO	88/88 (100%)	-0.22	0 100 100	30, 51, 72, 92	0
15	CO	88/88 (100%)	0.19	1 (1%) 78 59	45, 71, 89, 106	0
16	AP	82/82 (100%)	0.11	0 100 100	34, 51, 92, 108	0
16	CP	82/82 (100%)	0.83	7 (8%) 16 9	52, 73, 105, 117	0
17	AQ	80/80 (100%)	0.26	3 (3%) 44 25	30, 53, 77, 120	0
17	CQ	80/80 (100%)	0.46	2 (2%) 58 37	48, 88, 102, 109	0
18	AR	55/55 (100%)	0.14	2 (3%) 46 26	44, 56, 87, 108	0
18	CR	55/55 (100%)	0.05	2 (3%) 46 26	41, 58, 85, 109	0
19	AS	79/79 (100%)	0.74	7 (8%) 15 8	78, 95, 107, 113	0
19	CS	79/79 (100%)	1.38	15 (18%) 3 1	105, 123, 130, 133	0
20	AT	85/85 (100%)	0.24	4 (4%) 36 19	35, 52, 79, 98	0
20	CT	85/85 (100%)	1.35	23 (27%) 1 1	61, 86, 102, 106	0
21	AU	51/51 (100%)	0.85	6 (11%) 9 5	39, 73, 105, 115	0
21	CU	51/51 (100%)	0.98	9 (17%) 4 2	46, 73, 101, 107	0
22	BA	2897/2903 (99%)	-0.85	98 (3%) 48 28	1, 14, 135, 195	0
22	DA	2897/2903 (99%)	0.45	82 (2%) 55 34	38, 91, 152, 183	0
23	BB	119/119 (100%)	-1.07	0 100 100	2, 25, 59, 89	0
23	DB	118/119 (99%)	0.16	0 100 100	80, 119, 136, 145	0
24	BC	271/271 (100%)	-0.26	14 (5%) 33 17	2, 21, 52, 65	0
24	DC	271/271 (100%)	0.73	34 (12%) 8 5	45, 70, 90, 96	0
25	BD	209/209 (100%)	-0.64	0 100 100	1, 12, 38, 77	0
25	DD	209/209 (100%)	0.70	18 (8%) 16 9	56, 82, 97, 107	0
26	BE	201/201 (100%)	-0.47	0 100 100	1, 27, 64, 92	0
26	DE	201/201 (100%)	0.94	30 (14%) 5 3	63, 98, 114, 122	0
27	BF	177/177 (100%)	-0.15	2 (1%) 78 59	20, 51, 84, 100	0
27	DF	177/177 (100%)	0.97	20 (11%) 10 5	100, 119, 131, 137	0
28	BG	176/176 (100%)	-0.48	0 100 100	12, 38, 66, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	0.68	6 (3%) 48 28	87, 105, 116, 126	0
29	BH	149/149 (100%)	1.39	44 (29%) 1 1	25, 102, 121, 129	0
29	DH	149/149 (100%)	0.87	15 (10%) 12 6	25, 92, 107, 115	0
30	BI	141/141 (100%)	1.56	40 (28%) 1 1	103, 122, 132, 139	0
30	DI	141/141 (100%)	1.66	52 (36%) 1 0	109, 130, 140, 149	0
31	BJ	142/142 (100%)	-0.63	1 (0%) 84 68	1, 8, 28, 41	0
31	DJ	142/142 (100%)	0.60	11 (7%) 19 10	57, 79, 92, 103	0
32	BK	122/122 (100%)	-0.60	0 100 100	4, 13, 35, 66	0
32	DK	122/122 (100%)	0.51	7 (5%) 29 16	56, 75, 94, 106	0
33	BL	143/143 (100%)	-0.45	0 100 100	1, 22, 52, 87	0
33	DL	143/143 (100%)	1.31	34 (23%) 2 1	58, 92, 106, 127	0
34	BM	136/136 (100%)	-0.67	0 100 100	1, 11, 34, 82	0
34	DM	136/136 (100%)	0.29	3 (2%) 62 41	50, 79, 94, 113	0
35	BN	120/120 (100%)	-0.67	0 100 100	2, 10, 21, 70	0
35	DN	120/120 (100%)	0.98	15 (12%) 8 5	65, 88, 100, 123	0
36	BO	116/116 (100%)	-0.53	0 100 100	12, 30, 47, 57	0
36	DO	116/116 (100%)	0.76	5 (4%) 40 22	91, 106, 114, 121	0
37	BP	114/114 (100%)	-0.60	0 100 100	5, 18, 46, 67	0
37	DP	114/114 (100%)	0.72	5 (4%) 39 21	65, 81, 94, 103	0
38	BQ	117/117 (100%)	-0.63	0 100 100	1, 4, 15, 52	0
38	DQ	117/117 (100%)	1.14	27 (23%) 2 1	62, 79, 89, 94	0
39	BR	103/103 (100%)	-0.60	0 100 100	1, 13, 35, 67	0
39	DR	103/103 (100%)	0.92	14 (13%) 7 4	67, 91, 101, 103	0
40	BS	110/110 (100%)	-0.72	0 100 100	1, 5, 27, 79	0
40	DS	110/110 (100%)	0.92	15 (13%) 7 4	68, 88, 105, 112	0
41	BT	93/93 (100%)	-0.27	2 (2%) 62 41	8, 27, 77, 106	0
41	DT	93/93 (100%)	1.45	25 (26%) 1 1	80, 98, 117, 125	0
42	BU	102/102 (100%)	-0.39	0 100 100	13, 32, 67, 96	0
42	DU	102/102 (100%)	1.70	36 (35%) 1 0	88, 106, 122, 129	0
43	BV	94/94 (100%)	-0.61	0 100 100	7, 23, 51, 63	0
43	DV	94/94 (100%)	0.35	2 (2%) 63 42	74, 95, 107, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.58	0 100 100	3, 13, 32, 61	0
44	DW	75/76 (98%)	0.78	7 (9%) 14 8	60, 90, 99, 114	0
45	BX	77/77 (100%)	-0.48	0 100 100	5, 26, 54, 77	0
45	DX	77/77 (100%)	0.76	6 (7%) 19 10	57, 80, 94, 101	0
46	BY	63/63 (100%)	-0.01	1 (1%) 70 49	17, 40, 74, 92	0
46	DY	63/63 (100%)	1.24	15 (23%) 2 1	89, 105, 112, 115	0
47	BZ	58/58 (100%)	-0.52	0 100 100	2, 8, 35, 48	0
47	DZ	58/58 (100%)	0.50	0 100 100	64, 81, 96, 102	0
48	B0	56/56 (100%)	-0.73	0 100 100	1, 11, 44, 65	0
48	D0	56/56 (100%)	1.20	7 (12%) 8 5	58, 89, 102, 109	0
49	B1	50/50 (100%)	-0.39	0 100 100	25, 38, 63, 84	0
49	D1	50/50 (100%)	1.15	11 (22%) 2 1	79, 99, 108, 112	0
50	B2	46/46 (100%)	-0.43	1 (2%) 62 41	3, 8, 17, 80	0
50	D2	46/46 (100%)	1.85	18 (39%) 1 0	58, 80, 89, 105	0
51	B3	64/64 (100%)	-0.54	0 100 100	5, 11, 20, 33	0
51	D3	64/64 (100%)	1.57	21 (32%) 1 0	66, 82, 93, 98	0
52	B4	38/38 (100%)	-0.47	0 100 100	4, 13, 33, 51	0
52	D4	38/38 (100%)	1.24	6 (15%) 5 2	65, 84, 98, 109	0
53	B5	191/207 (92%)	1.41	49 (25%) 1 1	108, 127, 138, 143	0
All	All	20734/20773 (99%)	0.13	1242 (5%) 27 15	1, 73, 130, 195	0

The worst 5 of 1242 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	CT	4	ILE	9.6
22	BA	2184	A	8.5
50	D2	46	LYS	8.2
24	DC	242	LYS	8.1
24	DC	241	GLY	7.8

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	DA	3040	1/1	-0.06	0.28	94,94,94,94	0
54	MG	DA	3132	1/1	-0.00	0.33	123,123,123,123	0
54	MG	DA	3144	1/1	0.06	0.24	96,96,96,96	0
54	MG	DA	3025	1/1	0.23	0.38	120,120,120,120	0
54	MG	DA	3130	1/1	0.23	0.44	108,108,108,108	0
54	MG	AA	1617	1/1	0.34	0.25	124,124,124,124	0
54	MG	CA	1634	1/1	0.44	0.13	143,143,143,143	0
54	MG	CA	1651	1/1	0.46	0.26	70,70,70,70	0
54	MG	BA	3102	1/1	0.48	0.21	68,68,68,68	0
54	MG	CA	1644	1/1	0.52	0.32	86,86,86,86	0
54	MG	DA	3091	1/1	0.54	0.23	128,128,128,128	0
54	MG	DA	3055	1/1	0.55	0.23	109,109,109,109	0
54	MG	CA	1626	1/1	0.57	0.24	125,125,125,125	0
54	MG	DA	3146	1/1	0.57	0.26	68,68,68,68	0
54	MG	DA	3092	1/1	0.58	0.15	123,123,123,123	0
54	MG	DA	3061	1/1	0.61	0.42	91,91,91,91	0
54	MG	AA	1658	1/1	0.62	0.09	71,71,71,71	0
54	MG	DA	3127	1/1	0.63	0.27	91,91,91,91	0
54	MG	CA	1633	1/1	0.67	0.11	134,134,134,134	0
54	MG	DA	3056	1/1	0.67	0.17	103,103,103,103	0
54	MG	DA	3060	1/1	0.69	0.25	92,92,92,92	0
54	MG	DA	3135	1/1	0.70	0.19	112,112,112,112	0
54	MG	DA	3114	1/1	0.70	0.16	126,126,126,126	0
54	MG	DA	3145	1/1	0.70	0.28	60,60,60,60	0
54	MG	DA	3093	1/1	0.70	0.12	119,119,119,119	0
54	MG	DA	3158	1/1	0.70	0.20	52,52,52,52	0
54	MG	DA	3041	1/1	0.71	0.09	96,96,96,96	0
54	MG	DA	3150	1/1	0.71	0.18	86,86,86,86	0
54	MG	DA	3136	1/1	0.71	0.31	46,46,46,46	0
54	MG	CA	1627	1/1	0.72	0.09	116,116,116,116	0
54	MG	DA	3031	1/1	0.73	0.35	95,95,95,95	0
54	MG	DA	3047	1/1	0.73	0.08	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DL	201	1/1	0.73	0.39	95,95,95,95	0
54	MG	AA	1660	1/1	0.74	0.27	72,72,72,72	0
54	MG	DA	3071	1/1	0.74	0.20	99,99,99,99	0
54	MG	DA	3089	1/1	0.74	0.12	106,106,106,106	0
54	MG	AA	1665	1/1	0.74	0.14	61,61,61,61	0
54	MG	DA	3004	1/1	0.74	0.22	112,112,112,112	0
54	MG	BA	3057	1/1	0.74	0.32	40,40,40,40	0
54	MG	DA	3027	1/1	0.74	0.20	106,106,106,106	0
54	MG	DA	3059	1/1	0.74	0.16	87,87,87,87	0
54	MG	AA	1659	1/1	0.74	0.21	68,68,68,68	0
54	MG	DA	3057	1/1	0.75	0.47	99,99,99,99	0
54	MG	DA	3155	1/1	0.76	0.19	51,51,51,51	0
54	MG	DA	3118	1/1	0.76	0.20	113,113,113,113	0
54	MG	DA	3162	1/1	0.76	0.24	66,66,66,66	0
54	MG	CA	1628	1/1	0.76	0.10	137,137,137,137	0
54	MG	DA	3104	1/1	0.77	0.16	97,97,97,97	0
54	MG	CA	1650	1/1	0.77	0.09	85,85,85,85	0
54	MG	DA	3159	1/1	0.77	0.15	71,71,71,71	0
54	MG	DA	3147	1/1	0.77	0.33	49,49,49,49	0
54	MG	BA	3179	1/1	0.77	0.47	29,29,29,29	0
54	MG	CA	1654	1/1	0.78	0.10	70,70,70,70	0
54	MG	DA	3074	1/1	0.78	0.10	96,96,96,96	0
54	MG	AA	1667	1/1	0.78	0.07	54,54,54,54	0
54	MG	CA	1647	1/1	0.79	0.31	72,72,72,72	0
54	MG	CA	1629	1/1	0.79	0.22	123,123,123,123	0
54	MG	DA	3149	1/1	0.79	0.35	77,77,77,77	0
54	MG	BA	3176	1/1	0.79	0.21	37,37,37,37	0
54	MG	DA	3154	1/1	0.79	0.17	63,63,63,63	0
54	MG	AA	1652	1/1	0.80	0.21	63,63,63,63	0
54	MG	DA	3083	1/1	0.80	0.08	116,116,116,116	0
54	MG	DA	3139	1/1	0.80	0.24	49,49,49,49	0
54	MG	AA	1670	1/1	0.80	0.30	49,49,49,49	0
54	MG	AA	1671	1/1	0.80	0.38	52,52,52,52	0
54	MG	AM	201	1/1	0.80	0.13	63,63,63,63	0
54	MG	BA	3055	1/1	0.80	0.36	89,89,89,89	0
54	MG	AA	1657	1/1	0.80	0.20	42,42,42,42	0
54	MG	DA	3006	1/1	0.80	0.09	127,127,127,127	0
54	MG	DA	3116	1/1	0.80	0.12	106,106,106,106	0
54	MG	DA	3008	1/1	0.80	0.13	96,96,96,96	0
54	MG	DA	3156	1/1	0.80	0.15	72,72,72,72	0
54	MG	DA	3016	1/1	0.80	0.11	103,103,103,103	0
54	MG	BA	3059	1/1	0.80	0.25	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1614	1/1	0.80	0.23	97,97,97,97	0
54	MG	DA	3134	1/1	0.80	0.11	112,112,112,112	0
54	MG	DA	3105	1/1	0.81	0.10	77,77,77,77	0
54	MG	DA	3094	1/1	0.81	0.12	99,99,99,99	0
54	MG	CA	1641	1/1	0.81	0.35	49,49,49,49	0
54	MG	DA	3024	1/1	0.82	0.11	77,77,77,77	0
54	MG	DA	3084	1/1	0.82	0.13	104,104,104,104	0
54	MG	CA	1642	1/1	0.82	0.23	53,53,53,53	0
54	MG	DA	3070	1/1	0.82	0.12	105,105,105,105	0
54	MG	DA	3043	1/1	0.82	0.11	104,104,104,104	0
54	MG	DA	3142	1/1	0.82	0.32	53,53,53,53	0
54	MG	DA	3143	1/1	0.82	0.11	63,63,63,63	0
54	MG	DA	3125	1/1	0.82	0.16	83,83,83,83	0
54	MG	DA	3036	1/1	0.82	0.08	114,114,114,114	0
54	MG	DA	3076	1/1	0.82	0.14	114,114,114,114	0
54	MG	DA	3039	1/1	0.83	0.10	96,96,96,96	0
54	MG	CA	1655	1/1	0.83	0.17	85,85,85,85	0
54	MG	AA	1662	1/1	0.83	0.29	76,76,76,76	0
54	MG	BA	3040	1/1	0.83	0.32	1,1,1,1	0
54	MG	DA	3137	1/1	0.83	0.29	38,38,38,38	0
54	MG	CA	1614	1/1	0.83	0.18	60,60,60,60	0
54	MG	BA	3146	1/1	0.83	0.33	32,32,32,32	0
56	NEG	CA	1657	17/17	0.83	0.09	62,88,103,104	0
54	MG	AA	1666	1/1	0.84	0.24	55,55,55,55	0
54	MG	AA	1651	1/1	0.84	0.37	52,52,52,52	0
54	MG	DA	3164	1/1	0.84	0.08	60,60,60,60	0
54	MG	CA	1640	1/1	0.84	0.19	29,29,29,29	0
54	MG	AA	1644	1/1	0.84	0.10	60,60,60,60	0
54	MG	BA	3133	1/1	0.85	0.28	63,63,63,63	0
54	MG	BA	3034	1/1	0.85	0.38	39,39,39,39	0
54	MG	BA	3173	1/1	0.85	0.14	40,40,40,40	0
54	MG	DA	3015	1/1	0.85	0.14	90,90,90,90	0
54	MG	BA	3060	1/1	0.85	0.31	72,72,72,72	0
54	MG	AA	1669	1/1	0.85	1.16	83,83,83,83	0
54	MG	BQ	201	1/1	0.85	0.10	17,17,17,17	0
54	MG	CA	1635	1/1	0.85	0.29	99,99,99,99	0
54	MG	BA	3112	1/1	0.85	0.08	25,25,25,25	0
54	MG	AA	1649	1/1	0.86	0.12	52,52,52,52	0
54	MG	DA	3072	1/1	0.86	0.13	78,78,78,78	0
54	MG	AA	1648	1/1	0.86	0.22	34,34,34,34	0
54	MG	DA	3048	1/1	0.86	0.10	109,109,109,109	0
54	MG	CA	1649	1/1	0.86	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3098	1/1	0.86	0.17	89,89,89,89	0
54	MG	DA	3140	1/1	0.86	0.20	51,51,51,51	0
54	MG	DL	202	1/1	0.86	0.12	116,116,116,116	0
54	MG	D2	101	1/1	0.86	0.09	111,111,111,111	0
54	MG	BA	3105	1/1	0.86	0.11	10,10,10,10	0
54	MG	BA	3061	1/1	0.87	0.25	56,56,56,56	0
54	MG	BA	3145	1/1	0.87	0.22	35,35,35,35	0
54	MG	DA	3107	1/1	0.87	0.10	70,70,70,70	0
54	MG	DA	3161	1/1	0.87	0.11	65,65,65,65	0
54	MG	DA	3111	1/1	0.87	0.09	71,71,71,71	0
54	MG	BA	3131	1/1	0.87	0.23	49,49,49,49	0
54	MG	BA	3147	1/1	0.87	0.13	13,13,13,13	0
54	MG	BA	3163	1/1	0.87	0.42	36,36,36,36	0
54	MG	CA	1622	1/1	0.87	0.15	84,84,84,84	0
54	MG	DA	3026	1/1	0.87	0.08	93,93,93,93	0
54	MG	BA	3076	1/1	0.88	0.16	60,60,60,60	0
54	MG	AA	1646	1/1	0.88	0.06	49,49,49,49	0
54	MG	DA	3119	1/1	0.88	0.09	83,83,83,83	0
54	MG	AA	1628	1/1	0.88	0.08	84,84,84,84	0
54	MG	CA	1631	1/1	0.88	0.15	85,85,85,85	0
54	MG	BA	3183	1/1	0.88	0.20	35,35,35,35	0
54	MG	AA	1630	1/1	0.88	0.15	78,78,78,78	0
54	MG	CA	1653	1/1	0.88	0.29	54,54,54,54	0
54	MG	BA	3148	1/1	0.88	0.28	44,44,44,44	0
54	MG	AA	1618	1/1	0.88	0.07	89,89,89,89	0
54	MG	BA	3167	1/1	0.88	0.09	25,25,25,25	0
54	MG	AA	1663	1/1	0.89	0.09	36,36,36,36	0
54	MG	BA	3132	1/1	0.89	0.24	45,45,45,45	0
54	MG	DA	3123	1/1	0.89	0.18	88,88,88,88	0
54	MG	AA	1635	1/1	0.89	0.17	73,73,73,73	0
54	MG	BA	3084	1/1	0.89	0.17	33,33,33,33	0
54	MG	DA	3152	1/1	0.89	0.10	59,59,59,59	0
54	MG	CA	1643	1/1	0.89	0.18	43,43,43,43	0
54	MG	BA	3166	1/1	0.89	0.18	36,36,36,36	0
54	MG	CA	1645	1/1	0.89	0.18	52,52,52,52	0
54	MG	DA	3124	1/1	0.90	0.15	55,55,55,55	0
54	MG	CA	1605	1/1	0.90	0.08	110,110,110,110	0
54	MG	BA	3110	1/1	0.90	0.12	61,61,61,61	0
54	MG	BA	3185	1/1	0.90	0.22	17,17,17,17	0
54	MG	DA	3005	1/1	0.90	0.06	113,113,113,113	0
54	MG	CA	1636	1/1	0.90	0.08	93,93,93,93	0
54	MG	BA	3150	1/1	0.90	0.20	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3014	1/1	0.90	0.16	86,86,86,86	0
54	MG	DA	3002	1/1	0.91	0.17	94,94,94,94	0
54	MG	AA	1661	1/1	0.91	0.06	40,40,40,40	0
54	MG	BA	3073	1/1	0.91	0.08	16,16,16,16	0
54	MG	DA	3151	1/1	0.91	0.22	42,42,42,42	0
54	MG	CA	1652	1/1	0.91	0.06	73,73,73,73	0
54	MG	BA	3001	1/1	0.91	0.07	39,39,39,39	0
54	MG	DA	3028	1/1	0.91	0.08	83,83,83,83	0
54	MG	DA	3078	1/1	0.91	0.08	103,103,103,103	0
54	MG	DA	3109	1/1	0.91	0.22	64,64,64,64	0
54	MG	DA	3080	1/1	0.91	0.10	74,74,74,74	0
54	MG	DA	3160	1/1	0.91	0.14	86,86,86,86	0
54	MG	DA	3112	1/1	0.91	0.06	78,78,78,78	0
54	MG	DA	3011	1/1	0.91	0.11	98,98,98,98	0
54	MG	DA	3033	1/1	0.91	0.14	77,77,77,77	0
54	MG	DA	3087	1/1	0.91	0.07	84,84,84,84	0
54	MG	BA	3169	1/1	0.91	0.07	33,33,33,33	0
54	MG	DQ	201	1/1	0.91	0.20	51,51,51,51	0
54	MG	DA	3120	1/1	0.91	0.10	82,82,82,82	0
54	MG	BA	3004	1/1	0.91	0.11	55,55,55,55	0
54	MG	DA	3110	1/1	0.92	0.11	89,89,89,89	0
54	MG	DA	3153	1/1	0.92	0.11	58,58,58,58	0
54	MG	DA	3086	1/1	0.92	0.08	81,81,81,81	0
54	MG	BA	3164	1/1	0.92	0.06	13,13,13,13	0
54	MG	DA	3069	1/1	0.92	0.08	121,121,121,121	0
54	MG	DA	3157	1/1	0.92	0.17	61,61,61,61	0
54	MG	AA	1623	1/1	0.92	0.10	60,60,60,60	0
54	MG	BA	3111	1/1	0.92	0.08	40,40,40,40	0
54	MG	DA	3007	1/1	0.92	0.09	114,114,114,114	0
54	MG	BA	3015	1/1	0.92	0.20	62,62,62,62	0
54	MG	CA	1632	1/1	0.92	0.07	85,85,85,85	0
54	MG	DA	3103	1/1	0.92	0.09	85,85,85,85	0
54	MG	AA	1620	1/1	0.92	0.06	100,100,100,100	0
54	MG	DA	3034	1/1	0.92	0.11	90,90,90,90	0
54	MG	BA	3036	1/1	0.92	0.32	20,20,20,20	0
54	MG	DA	3131	1/1	0.92	0.13	79,79,79,79	0
54	MG	AA	1638	1/1	0.92	0.08	88,88,88,88	0
54	MG	BA	3158	1/1	0.93	0.12	15,15,15,15	0
54	MG	BA	3174	1/1	0.93	0.10	25,25,25,25	0
54	MG	DA	3148	1/1	0.93	0.07	53,53,53,53	0
54	MG	BA	3175	1/1	0.93	0.11	38,38,38,38	0
54	MG	BA	3144	1/1	0.93	0.23	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3178	1/1	0.93	0.29	41,41,41,41	0
54	MG	BA	3115	1/1	0.93	0.11	58,58,58,58	0
54	MG	BA	3137	1/1	0.93	0.23	11,11,11,11	0
54	MG	BA	3151	1/1	0.93	0.06	7,7,7,7	0
54	MG	BA	3194	1/1	0.93	0.10	42,42,42,42	0
54	MG	DA	3013	1/1	0.93	0.11	72,72,72,72	0
54	MG	DA	3106	1/1	0.93	0.05	60,60,60,60	0
54	MG	BA	3168	1/1	0.93	0.12	43,43,43,43	0
54	MG	BA	3152	1/1	0.93	0.24	1,1,1,1	0
54	MG	DA	3079	1/1	0.93	0.08	91,91,91,91	0
54	MG	DA	3138	1/1	0.93	0.17	41,41,41,41	0
54	MG	CA	1608	1/1	0.93	0.08	86,86,86,86	0
54	MG	DA	3018	1/1	0.93	0.07	88,88,88,88	0
54	MG	DA	3141	1/1	0.93	0.28	45,45,45,45	0
54	MG	DA	3020	1/1	0.93	0.24	76,76,76,76	0
54	MG	DA	3115	1/1	0.93	0.10	79,79,79,79	0
54	MG	DA	3023	1/1	0.93	0.12	57,57,57,57	0
54	MG	DA	3117	1/1	0.93	0.12	79,79,79,79	0
54	MG	BA	3170	1/1	0.94	0.07	44,44,44,44	0
54	MG	BA	3171	1/1	0.94	0.14	29,29,29,29	0
54	MG	AA	1653	1/1	0.94	0.19	27,27,27,27	0
54	MG	BA	3079	1/1	0.94	0.09	29,29,29,29	0
54	MG	CA	1656	1/1	0.94	0.10	88,88,88,88	0
54	MG	BA	3080	1/1	0.94	0.06	24,24,24,24	0
54	MG	BA	3056	1/1	0.94	0.20	27,27,27,27	0
54	MG	BA	3135	1/1	0.94	0.10	23,23,23,23	0
54	MG	BA	3159	1/1	0.94	0.23	18,18,18,18	0
54	MG	BA	3181	1/1	0.94	0.23	33,33,33,33	0
54	MG	DA	3088	1/1	0.94	0.09	81,81,81,81	0
54	MG	BA	3160	1/1	0.94	0.05	7,7,7,7	0
54	MG	DA	3090	1/1	0.94	0.06	85,85,85,85	0
54	MG	DA	3046	1/1	0.94	0.07	80,80,80,80	0
54	MG	DA	3009	1/1	0.94	0.05	91,91,91,91	0
54	MG	BA	3161	1/1	0.94	0.18	30,30,30,30	0
54	MG	DA	3133	1/1	0.94	0.09	78,78,78,78	0
54	MG	BA	3186	1/1	0.94	0.10	29,29,29,29	0
54	MG	BA	3191	1/1	0.94	0.13	17,17,17,17	0
54	MG	BA	3136	1/1	0.94	0.22	50,50,50,50	0
54	MG	AA	1654	1/1	0.94	0.24	46,46,46,46	0
54	MG	AA	1645	1/1	0.94	0.16	52,52,52,52	0
54	MG	AA	1643	1/1	0.94	0.33	7,7,7,7	0
54	MG	AA	1668	1/1	0.94	0.13	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	CA	1620	1/1	0.94	0.07	81,81,81,81	0
54	MG	BA	3047	1/1	0.94	0.07	43,43,43,43	0
54	MG	DA	3077	1/1	0.95	0.08	114,114,114,114	0
54	MG	BA	3180	1/1	0.95	0.14	45,45,45,45	0
54	MG	AA	1627	1/1	0.95	0.17	68,68,68,68	0
54	MG	CA	1646	1/1	0.95	0.36	21,21,21,21	0
54	MG	AA	1615	1/1	0.95	0.15	52,52,52,52	0
54	MG	CA	1648	1/1	0.95	0.24	47,47,47,47	0
54	MG	BA	3021	1/1	0.95	0.05	1,1,1,1	0
54	MG	BA	3143	1/1	0.95	0.19	18,18,18,18	0
54	MG	DA	3121	1/1	0.95	0.09	62,62,62,62	0
54	MG	BA	3187	1/1	0.95	0.10	41,41,41,41	0
54	MG	DA	3051	1/1	0.95	0.09	51,51,51,51	0
54	MG	BA	3188	1/1	0.95	0.09	5,5,5,5	0
54	MG	BA	3120	1/1	0.95	0.09	10,10,10,10	0
54	MG	BA	3121	1/1	0.95	0.16	50,50,50,50	0
54	MG	BA	3124	1/1	0.95	0.23	44,44,44,44	0
54	MG	CA	1604	1/1	0.95	0.06	102,102,102,102	0
54	MG	BA	3070	1/1	0.95	0.07	6,6,6,6	0
54	MG	DA	3099	1/1	0.95	0.07	69,69,69,69	0
54	MG	CA	1607	1/1	0.95	0.07	96,96,96,96	0
54	MG	DA	3029	1/1	0.95	0.10	83,83,83,83	0
54	MG	DA	3030	1/1	0.95	0.07	71,71,71,71	0
54	MG	DB	202	1/1	0.95	0.07	89,89,89,89	0
54	MG	DB	203	1/1	0.95	0.06	106,106,106,106	0
54	MG	AA	1664	1/1	0.95	0.12	58,58,58,58	0
54	MG	DA	3073	1/1	0.95	0.10	69,69,69,69	0
54	MG	AA	1629	1/1	0.95	0.07	73,73,73,73	0
54	MG	DA	3075	1/1	0.95	0.13	78,78,78,78	0
54	MG	CA	1619	1/1	0.95	0.09	85,85,85,85	0
54	MG	DA	3067	1/1	0.96	0.09	70,70,70,70	0
54	MG	DA	3068	1/1	0.96	0.07	81,81,81,81	0
54	MG	DA	3101	1/1	0.96	0.07	85,85,85,85	0
54	MG	BA	3014	1/1	0.96	0.13	8,8,8,8	0
54	MG	DA	3001	1/1	0.96	0.05	93,93,93,93	0
54	MG	BA	3193	1/1	0.96	0.21	46,46,46,46	0
54	MG	BA	3098	1/1	0.96	0.19	41,41,41,41	0
54	MG	BA	3172	1/1	0.96	0.15	29,29,29,29	0
54	MG	CA	1602	1/1	0.96	0.11	93,93,93,93	0
54	MG	BA	3156	1/1	0.96	0.35	40,40,40,40	0
54	MG	AA	1632	1/1	0.96	0.07	60,60,60,60	0
54	MG	AA	1655	1/1	0.96	0.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1656	1/1	0.96	0.09	46,46,46,46	0
54	MG	BA	3069	1/1	0.96	0.06	72,72,72,72	0
54	MG	BA	3162	1/1	0.96	0.18	30,30,30,30	0
54	MG	DA	3081	1/1	0.96	0.05	75,75,75,75	0
54	MG	DA	3082	1/1	0.96	0.04	80,80,80,80	0
54	MG	AA	1650	1/1	0.96	0.36	49,49,49,49	0
54	MG	AA	1601	1/1	0.96	0.06	59,59,59,59	0
54	MG	DA	3085	1/1	0.96	0.08	71,71,71,71	0
54	MG	BA	3165	1/1	0.96	0.24	29,29,29,29	0
54	MG	DA	3053	1/1	0.96	0.11	49,49,49,49	0
54	MG	DA	3054	1/1	0.96	0.06	64,64,64,64	0
54	MG	AA	1604	1/1	0.96	0.05	81,81,81,81	0
54	MG	DA	3128	1/1	0.96	0.08	60,60,60,60	0
54	MG	DA	3163	1/1	0.96	0.21	45,45,45,45	0
54	MG	BA	3003	1/1	0.96	0.06	29,29,29,29	0
54	MG	AA	1619	1/1	0.96	0.15	57,57,57,57	0
54	MG	CA	1630	1/1	0.96	0.04	79,79,79,79	0
54	MG	BA	3083	1/1	0.96	0.17	44,44,44,44	0
54	MG	BA	3189	1/1	0.96	0.15	43,43,43,43	0
54	MG	DA	3095	1/1	0.96	0.05	77,77,77,77	0
54	MG	DA	3096	1/1	0.96	0.12	81,81,81,81	0
54	MG	DA	3097	1/1	0.96	0.06	67,67,67,67	0
54	MG	BA	3119	1/1	0.97	0.16	40,40,40,40	0
54	MG	BA	3157	1/1	0.97	0.20	26,26,26,26	0
54	MG	DA	3062	1/1	0.97	0.04	67,67,67,67	0
54	MG	CA	1606	1/1	0.97	0.09	61,61,61,61	0
54	MG	BA	3138	1/1	0.97	0.21	1,1,1,1	0
54	MG	DA	3102	1/1	0.97	0.10	77,77,77,77	0
54	MG	BA	3177	1/1	0.97	0.11	24,24,24,24	0
54	MG	CA	1613	1/1	0.97	0.06	51,51,51,51	0
54	MG	BA	3139	1/1	0.97	0.24	1,1,1,1	0
54	MG	CA	1616	1/1	0.97	0.12	43,43,43,43	0
54	MG	BA	3141	1/1	0.97	0.33	2,2,2,2	0
54	MG	DA	3108	1/1	0.97	0.15	22,22,22,22	0
54	MG	BA	3142	1/1	0.97	0.38	17,17,17,17	0
54	MG	BA	3093	1/1	0.97	0.05	11,11,11,11	0
54	MG	AA	1624	1/1	0.97	0.07	36,36,36,36	0
54	MG	BA	3184	1/1	0.97	0.05	24,24,24,24	0
54	MG	DA	3113	1/1	0.97	0.07	54,54,54,54	0
54	MG	BA	3025	1/1	0.97	0.18	38,38,38,38	0
54	MG	CT	101	1/1	0.97	0.10	91,91,91,91	0
54	MG	BA	3128	1/1	0.97	0.30	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	BA	3029	1/1	0.97	0.06	20,20,20,20	0
54	MG	DA	3003	1/1	0.97	0.06	83,83,83,83	0
54	MG	AA	1625	1/1	0.97	0.07	47,47,47,47	0
54	MG	DA	3045	1/1	0.97	0.06	74,74,74,74	0
54	MG	BA	3149	1/1	0.97	0.26	48,48,48,48	0
54	MG	DA	3122	1/1	0.97	0.07	51,51,51,51	0
54	MG	BA	3190	1/1	0.97	0.08	46,46,46,46	0
54	MG	AA	1616	1/1	0.97	0.05	94,94,94,94	0
54	MG	AA	1634	1/1	0.97	0.05	58,58,58,58	0
54	MG	AA	1608	1/1	0.97	0.07	26,26,26,26	0
54	MG	DB	201	1/1	0.97	0.09	118,118,118,118	0
54	MG	DA	3010	1/1	0.97	0.09	60,60,60,60	0
54	MG	DA	3129	1/1	0.97	0.04	93,93,93,93	0
54	MG	CA	1639	1/1	0.97	0.16	59,59,59,59	0
54	MG	BA	3153	1/1	0.97	0.11	33,33,33,33	0
54	MG	CA	1601	1/1	0.97	0.07	45,45,45,45	0
54	MG	DA	3058	1/1	0.97	0.05	64,64,64,64	0
54	MG	BA	3155	1/1	0.97	0.22	21,21,21,21	0
54	MG	BA	3048	1/1	0.98	0.15	10,10,10,10	0
54	MG	BA	3099	1/1	0.98	0.06	1,1,1,1	0
54	MG	BA	3027	1/1	0.98	0.12	10,10,10,10	0
54	MG	BA	3182	1/1	0.98	0.17	25,25,25,25	0
54	MG	DA	3032	1/1	0.98	0.06	67,67,67,67	0
54	MG	CA	1637	1/1	0.98	0.07	35,35,35,35	0
54	MG	AA	1636	1/1	0.98	0.09	46,46,46,46	0
54	MG	AA	1639	1/1	0.98	0.08	60,60,60,60	0
54	MG	BA	3016	1/1	0.98	0.11	13,13,13,13	0
54	MG	BA	3005	1/1	0.98	0.04	44,44,44,44	0
54	MG	CA	1615	1/1	0.98	0.06	39,39,39,39	0
54	MG	DA	3042	1/1	0.98	0.09	67,67,67,67	0
54	MG	BA	3154	1/1	0.98	0.10	18,18,18,18	0
54	MG	CA	1617	1/1	0.98	0.04	38,38,38,38	0
54	MG	BA	3114	1/1	0.98	0.04	14,14,14,14	0
54	MG	BA	3046	1/1	0.98	0.09	5,5,5,5	0
54	MG	CA	1621	1/1	0.98	0.07	75,75,75,75	0
54	MG	DA	3049	1/1	0.98	0.04	61,61,61,61	0
54	MG	DA	3050	1/1	0.98	0.04	41,41,41,41	0
54	MG	BA	3118	1/1	0.98	0.08	14,14,14,14	0
54	MG	DA	3052	1/1	0.98	0.05	50,50,50,50	0
54	MG	DA	3017	1/1	0.98	0.06	71,71,71,71	0
54	MG	BA	3085	1/1	0.98	0.06	9,9,9,9	0
54	MG	DA	3019	1/1	0.98	0.20	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3192	1/1	0.98	0.12	30,30,30,30	0
54	MG	DA	3021	1/1	0.98	0.08	69,69,69,69	0
54	MG	BA	3089	1/1	0.98	0.04	8,8,8,8	0
54	MG	BA	3091	1/1	0.98	0.08	53,53,53,53	0
54	MG	BB	204	1/1	0.98	0.28	6,6,6,6	0
54	MG	BA	3123	1/1	0.98	0.08	6,6,6,6	0
54	MG	BA	3010	1/1	0.98	0.03	1,1,1,1	0
54	MG	DA	3064	1/1	0.98	0.04	61,61,61,61	0
54	MG	DA	3065	1/1	0.98	0.05	44,44,44,44	0
54	MG	DA	3100	1/1	0.98	0.05	74,74,74,74	0
55	ZN	D4	101	1/1	0.98	0.03	95,95,95,95	0
54	MG	DA	3066	1/1	0.98	0.08	58,58,58,58	0
54	MG	DA	3037	1/1	0.99	0.09	66,66,66,66	0
54	MG	DA	3038	1/1	0.99	0.05	68,68,68,68	0
54	MG	BA	3108	1/1	0.99	0.09	1,1,1,1	0
54	MG	BA	3109	1/1	0.99	0.11	1,1,1,1	0
54	MG	AA	1611	1/1	0.99	0.04	32,32,32,32	0
54	MG	AA	1647	1/1	0.99	0.10	51,51,51,51	0
54	MG	AA	1631	1/1	0.99	0.02	32,32,32,32	0
54	MG	DA	3044	1/1	0.99	0.19	51,51,51,51	0
54	MG	BA	3113	1/1	0.99	0.04	4,4,4,4	0
54	MG	BA	3006	1/1	0.99	0.05	29,29,29,29	0
54	MG	BA	3007	1/1	0.99	0.03	29,29,29,29	0
54	MG	BA	3116	1/1	0.99	0.05	1,1,1,1	0
54	MG	BA	3009	1/1	0.99	0.06	1,1,1,1	0
54	MG	AA	1612	1/1	0.99	0.06	42,42,42,42	0
54	MG	BA	3011	1/1	0.99	0.12	16,16,16,16	0
54	MG	BA	3062	1/1	0.99	0.03	4,4,4,4	0
54	MG	BA	3063	1/1	0.99	0.03	6,6,6,6	0
54	MG	BA	3064	1/1	0.99	0.05	5,5,5,5	0
54	MG	BA	3126	1/1	0.99	0.09	3,3,3,3	0
54	MG	BA	3127	1/1	0.99	0.03	3,3,3,3	0
54	MG	BA	3067	1/1	0.99	0.06	2,2,2,2	0
54	MG	DA	3126	1/1	0.99	0.04	58,58,58,58	0
54	MG	BA	3129	1/1	0.99	0.04	1,1,1,1	0
54	MG	BA	3012	1/1	0.99	0.08	1,1,1,1	0
54	MG	AA	1633	1/1	0.99	0.04	25,25,25,25	0
54	MG	BA	3071	1/1	0.99	0.09	13,13,13,13	0
54	MG	BA	3134	1/1	0.99	0.06	3,3,3,3	0
54	MG	DA	3063	1/1	0.99	0.07	64,64,64,64	0
54	MG	AA	1621	1/1	0.99	0.04	32,32,32,32	0
54	MG	BA	3074	1/1	0.99	0.05	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1622	1/1	0.99	0.13	21,21,21,21	0
54	MG	BA	3077	1/1	0.99	0.03	16,16,16,16	0
54	MG	BA	3078	1/1	0.99	0.03	48,48,48,48	0
54	MG	BA	3140	1/1	0.99	0.18	34,34,34,34	0
54	MG	AA	1613	1/1	0.99	0.03	13,13,13,13	0
54	MG	BA	3023	1/1	0.99	0.04	1,1,1,1	0
54	MG	BB	201	1/1	0.99	0.06	32,32,32,32	0
54	MG	BA	3081	1/1	0.99	0.03	1,1,1,1	0
54	MG	BA	3082	1/1	0.99	0.10	8,8,8,8	0
54	MG	AA	1606	1/1	0.99	0.02	42,42,42,42	0
54	MG	AA	1607	1/1	0.99	0.04	48,48,48,48	0
54	MG	CA	1603	1/1	0.99	0.03	40,40,40,40	0
54	MG	AA	1640	1/1	0.99	0.05	39,39,39,39	0
54	MG	BA	3087	1/1	0.99	0.04	18,18,18,18	0
54	MG	DA	3012	1/1	0.99	0.07	46,46,46,46	0
54	MG	BA	3088	1/1	0.99	0.12	25,25,25,25	0
54	MG	BA	3031	1/1	0.99	0.09	11,11,11,11	0
54	MG	BA	3090	1/1	0.99	0.09	13,13,13,13	0
54	MG	CA	1609	1/1	0.99	0.05	56,56,56,56	0
54	MG	CA	1610	1/1	0.99	0.03	57,57,57,57	0
54	MG	CA	1611	1/1	0.99	0.04	42,42,42,42	0
54	MG	CA	1612	1/1	0.99	0.07	20,20,20,20	0
54	MG	AA	1605	1/1	0.99	0.07	35,35,35,35	0
54	MG	BA	3092	1/1	0.99	0.09	33,33,33,33	0
54	MG	DA	3022	1/1	0.99	0.09	74,74,74,74	0
54	MG	AA	1609	1/1	0.99	0.04	23,23,23,23	0
54	MG	BA	3094	1/1	0.99	0.06	19,19,19,19	0
54	MG	BA	3095	1/1	0.99	0.04	6,6,6,6	0
54	MG	CA	1618	1/1	0.99	0.06	35,35,35,35	0
54	MG	BA	3039	1/1	0.99	0.04	1,1,1,1	0
54	MG	AA	1610	1/1	0.99	0.04	64,64,64,64	0
54	MG	BA	3101	1/1	0.99	0.03	14,14,14,14	0
54	MG	BA	3045	1/1	0.99	0.10	5,5,5,5	0
54	MG	CA	1623	1/1	0.99	0.03	48,48,48,48	0
54	MG	CA	1625	1/1	0.99	0.02	44,44,44,44	0
54	MG	BA	3104	1/1	0.99	0.08	1,1,1,1	0
54	MG	BA	3002	1/1	0.99	0.05	11,11,11,11	0
54	MG	DA	3035	1/1	0.99	0.07	54,54,54,54	0
54	MG	BA	3107	1/1	0.99	0.03	3,3,3,3	0
54	MG	BA	3018	1/1	1.00	0.03	14,14,14,14	0
54	MG	CA	1624	1/1	1.00	0.19	4,4,4,4	0
54	MG	BA	3125	1/1	1.00	0.06	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3041	1/1	1.00	0.08	3,3,3,3	0
54	MG	BA	3042	1/1	1.00	0.04	1,1,1,1	0
54	MG	BA	3043	1/1	1.00	0.02	11,11,11,11	0
54	MG	BA	3044	1/1	1.00	0.25	1,1,1,1	0
54	MG	BA	3130	1/1	1.00	0.08	7,7,7,7	0
54	MG	BA	3019	1/1	1.00	0.26	1,1,1,1	0
54	MG	BA	3020	1/1	1.00	0.04	1,1,1,1	0
54	MG	AA	1603	1/1	1.00	0.02	30,30,30,30	0
54	MG	BA	3086	1/1	1.00	0.04	2,2,2,2	0
54	MG	BA	3022	1/1	1.00	0.04	1,1,1,1	0
54	MG	BA	3049	1/1	1.00	0.04	3,3,3,3	0
54	MG	BA	3050	1/1	1.00	0.04	7,7,7,7	0
54	MG	CA	1638	1/1	1.00	0.09	28,28,28,28	0
54	MG	BA	3051	1/1	1.00	0.04	2,2,2,2	0
54	MG	BA	3052	1/1	1.00	0.02	1,1,1,1	0
54	MG	BA	3053	1/1	1.00	0.08	1,1,1,1	0
54	MG	BA	3054	1/1	1.00	0.02	4,4,4,4	0
54	MG	AA	1626	1/1	1.00	0.19	1,1,1,1	0
54	MG	BA	3024	1/1	1.00	0.02	13,13,13,13	0
54	MG	BA	3096	1/1	1.00	0.02	2,2,2,2	0
54	MG	BA	3097	1/1	1.00	0.09	1,1,1,1	0
54	MG	AA	1602	1/1	1.00	0.06	37,37,37,37	0
54	MG	BA	3058	1/1	1.00	0.02	14,14,14,14	0
54	MG	BB	202	1/1	1.00	0.02	10,10,10,10	0
54	MG	BB	203	1/1	1.00	0.05	12,12,12,12	0
54	MG	BA	3100	1/1	1.00	0.02	4,4,4,4	0
54	MG	BA	3026	1/1	1.00	0.01	2,2,2,2	0
54	MG	AA	1641	1/1	1.00	0.07	12,12,12,12	0
54	MG	BA	3103	1/1	1.00	0.02	2,2,2,2	0
54	MG	BA	3028	1/1	1.00	0.03	1,1,1,1	0
54	MG	BA	3013	1/1	1.00	0.08	1,1,1,1	0
54	MG	BA	3106	1/1	1.00	0.06	1,1,1,1	0
54	MG	BA	3030	1/1	1.00	0.05	4,4,4,4	0
54	MG	AA	1642	1/1	1.00	0.04	23,23,23,23	0
54	MG	BA	3065	1/1	1.00	0.06	1,1,1,1	0
54	MG	BA	3066	1/1	1.00	0.02	3,3,3,3	0
54	MG	BA	3032	1/1	1.00	0.05	4,4,4,4	0
54	MG	BA	3068	1/1	1.00	0.01	1,1,1,1	0
54	MG	BA	3033	1/1	1.00	0.10	1,1,1,1	0
54	MG	AA	1637	1/1	1.00	0.04	13,13,13,13	0
54	MG	BA	3035	1/1	1.00	0.05	1,1,1,1	0
54	MG	BA	3072	1/1	1.00	0.04	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	BA	3117	1/1	1.00	0.05	1,1,1,1	0
54	MG	BA	3008	1/1	1.00	0.07	3,3,3,3	0
54	MG	BA	3037	1/1	1.00	0.10	1,1,1,1	0
54	MG	BA	3075	1/1	1.00	0.05	3,3,3,3	0
54	MG	BA	3038	1/1	1.00	0.04	1,1,1,1	0
55	ZN	B4	101	1/1	1.00	0.04	28,28,28,28	0
54	MG	BA	3122	1/1	1.00	0.10	1,1,1,1	0
54	MG	BA	3017	1/1	1.00	0.06	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.