



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:02 am GMT

PDB ID : 4V57
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with spectinomycin and neomycin.
Authors : Borovinskaya, M.A.; Shoji, S.; Holton, J.M.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2007-07-21
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

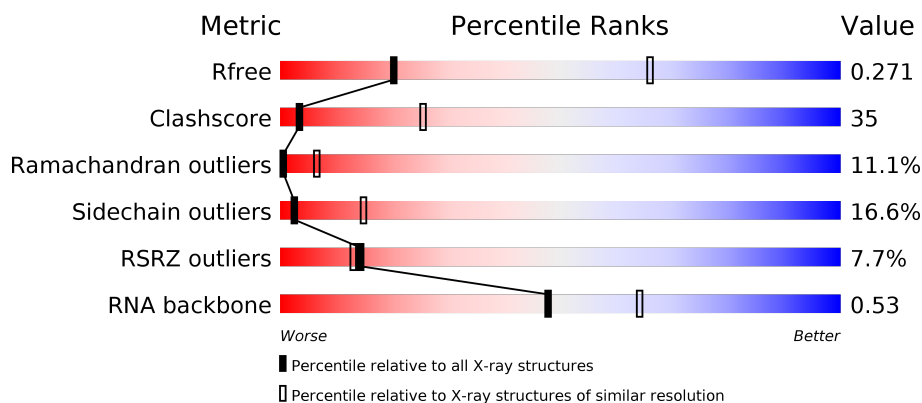
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)
RNA backbone	2435	1024 (4.10-2.86)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	<div> <div>23%</div> <div>62%</div> <div>14%</div> <div>..</div> </div>
1	CA	1542	<div> <div>24%</div> <div>62%</div> <div>13%</div> <div>.</div> </div>
2	AC	232	<div> <div>9%</div> <div>20%</div> <div>48%</div> <div>18%</div> <div>.</div> <div>11%</div> </div>
2	CC	232	<div> <div>6%</div> <div>28%</div> <div>46%</div> <div>14%</div> <div>.</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AP	82	
13	CP	82	
14	AQ	83	
14	CQ	83	
15	AR	74	

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Mol	Chain	Length	Quality of chain
15	CR	74	
16	AS	91	
16	CS	91	
17	AT	86	
17	CT	86	
18	AB	240	
18	CB	240	
19	AU	70	
19	CU	70	
20	AO	89	
20	CO	89	
21	AN	100	
21	CN	100	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
38	DM	136	
39	BX	63	
39	DX	63	
40	BH	149	

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Mol	Chain	Length	Quality of chain
40	DH	149	
41	BJ	142	
41	DJ	142	
42	BN	127	
42	DN	127	
43	BO	117	
43	DO	117	
44	BQ	117	
44	DQ	117	
45	BS	110	
45	DS	110	
46	BU	103	
46	DU	103	
47	BF	178	
47	DF	178	
48	BG	176	
48	DG	176	
49	BR	103	
49	DR	103	
50	BT	100	
50	DT	100	
51	BZ	78	
51	DZ	78	
52	BW	84	
52	DW	84	

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
53	NMY	AA	1601	-	-	-	X
53	NMY	BB	3001	-	-	-	X
53	NMY	CA	1601	-	-	-	X
53	NMY	DB	3001	-	-	-	X
54	MG	AA	1658	-	-	-	X
54	MG	BB	3088	-	-	-	X
54	MG	DB	3090	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 284201 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	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
2	CC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
4	CE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
5	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
9	CJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
12	CM	113	Total	C	N	O	S	0	0	0
			876	541	177	155	3			

- Molecule 13 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
13	CP	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

- Molecule 14 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
14	CQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

- Molecule 15 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
15	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 16 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
16	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

- Molecule 17 is a protein called 30S ribosomal protein S20.

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

- Molecule 18 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
18	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 19 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
19	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S14.

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

- Molecule 22 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	120	U	-	INSERTION	GB 85674274
DA	120	U	-	INSERTION	GB 85674274

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	2903	U	-	INSERTION	GB 85674274
BB	2904	U	-	INSERTION	GB 85674274
DB	2903	U	-	INSERTION	GB 85674274
DB	2904	U	-	INSERTION	GB 85674274

- Molecule 24 is a protein called 50S ribosomal protein L11.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
25	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

- Molecule 27 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
27	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
30	DY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
33	D1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
39	DX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 40 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
40	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
42	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BU	102	Total	C	N	O	0	0	0
			779	492	146	141			
46	DU	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 47 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
47	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 48 is a protein called 50S ribosomal protein L6.

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

- Molecule 49 is a protein called 50S ribosomal protein L21.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
50	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

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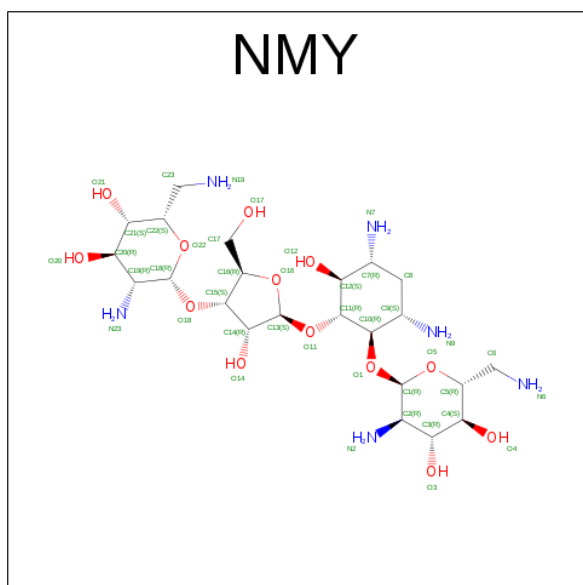
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 52 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
52	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 53 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).

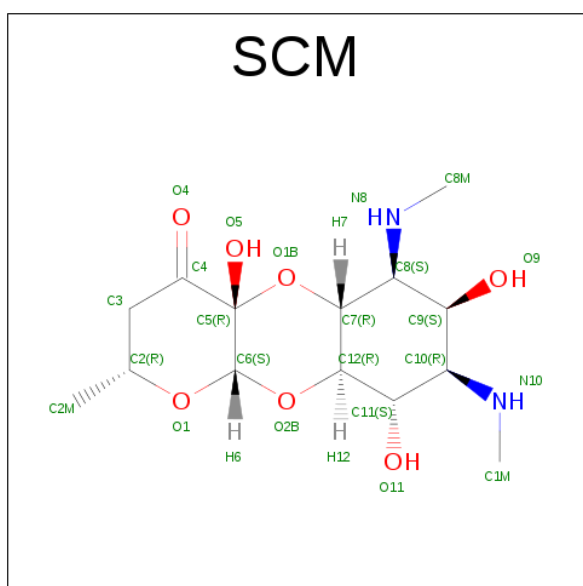


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
53	AA	1	Total	C	N	O	0	0
			42	23	6	13		
53	BB	1	Total	C	N	O	0	0
			42	23	6	13		
53	CA	1	Total	C	N	O	0	0
			42	23	6	13		
53	DB	1	Total	C	N	O	0	0
			42	23	6	13		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	BB	110	Total Mg 110 110	0	0
54	AA	60	Total Mg 60 60	0	0
54	CA	59	Total Mg 59 59	0	0
54	DB	111	Total Mg 111 111	0	0

- Molecule 55 is SPECTINOMYCIN (three-letter code: SCM) (formula: $C_{14}H_{24}N_2O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AA	1	Total C N O 23 14 2 7	0	0
55	CA	1	Total C N O 23 14 2 7	0	0

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	290	Total O 290 290	0	0
57	AE	1	Total O 1 1	0	0
57	AK	1	Total O 1 1	0	0
57	AL	4	Total O 4 4	0	0
57	AP	1	Total O 1 1	0	0
57	AT	2	Total O 2 2	0	0
57	AN	1	Total O 1 1	0	0
57	BB	492	Total O 492 492	0	0
57	BC	7	Total O 7 7	0	0
57	BD	1	Total O 1 1	0	0
57	BE	4	Total O 4 4	0	0
57	BL	2	Total O 2 2	0	0
57	BH	1	Total O 1 1	0	0
57	CA	282	Total O 282 282	0	0
57	CE	2	Total O 2 2	0	0
57	CL	4	Total O 4 4	0	0
57	CP	1	Total O 1 1	0	0
57	CT	1	Total O 1 1	0	0
57	CI	1	Total O 1 1	0	0
57	CN	3	Total O 3 3	0	0
57	DB	501	Total O 501 501	0	0
57	DC	4	Total O 4 4	0	0

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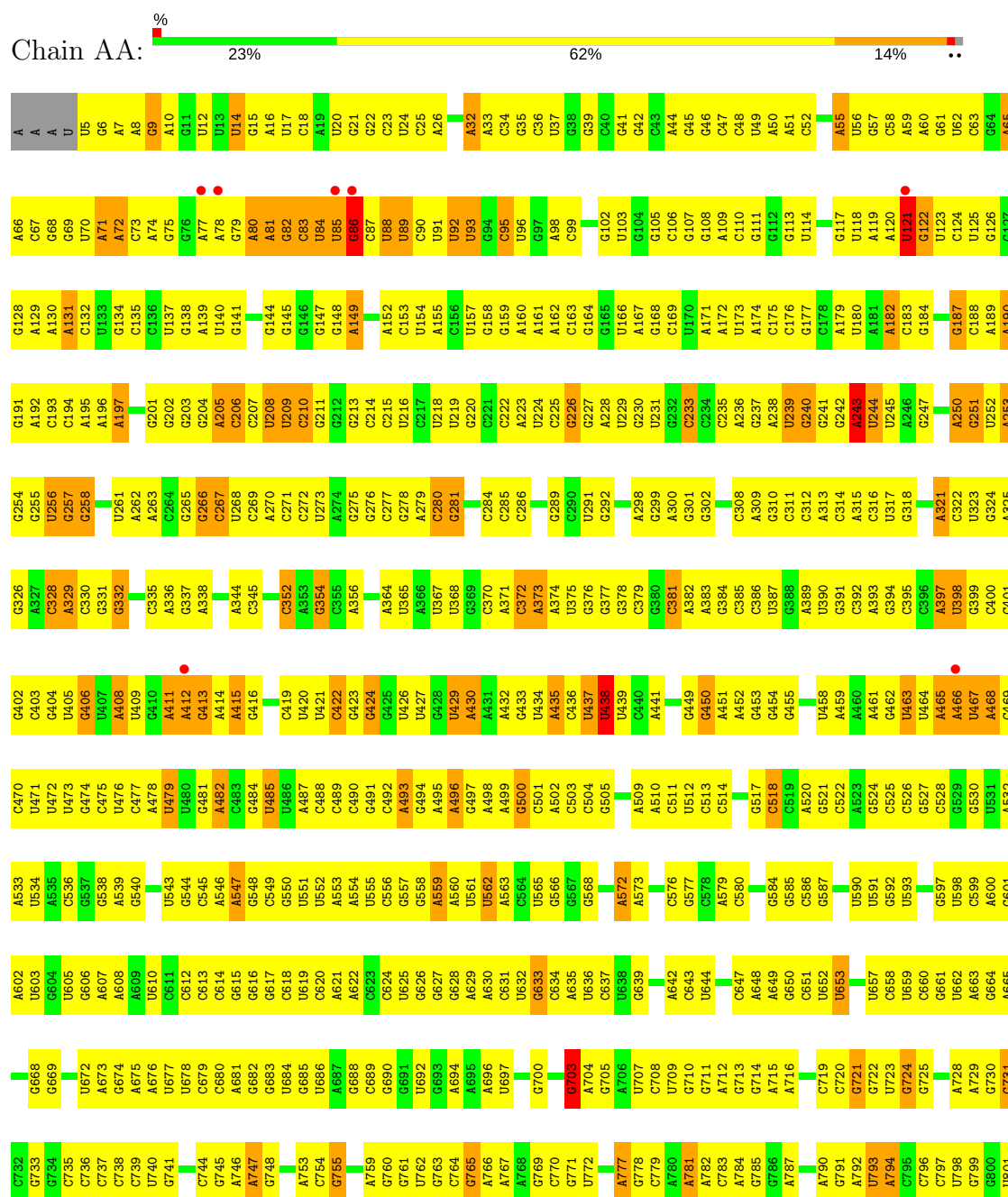
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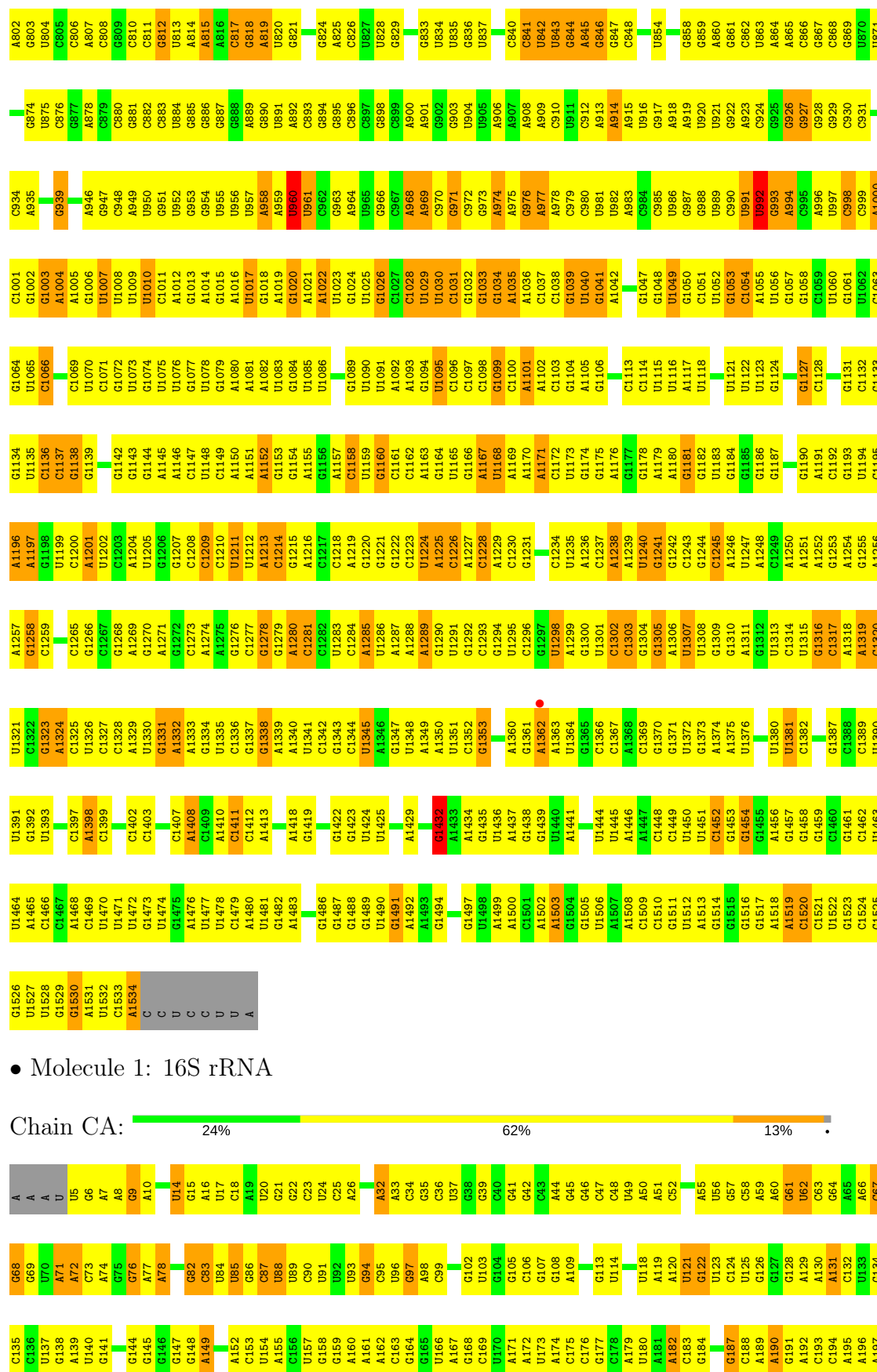
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DD	1	Total 1	O 1	0	0
57	DE	2	Total 2	O 2	0	0
57	DL	1	Total 1	O 1	0	0
57	DN	2	Total 2	O 2	0	0
57	DR	1	Total 1	O 1	0	0

3 Residue-property plots

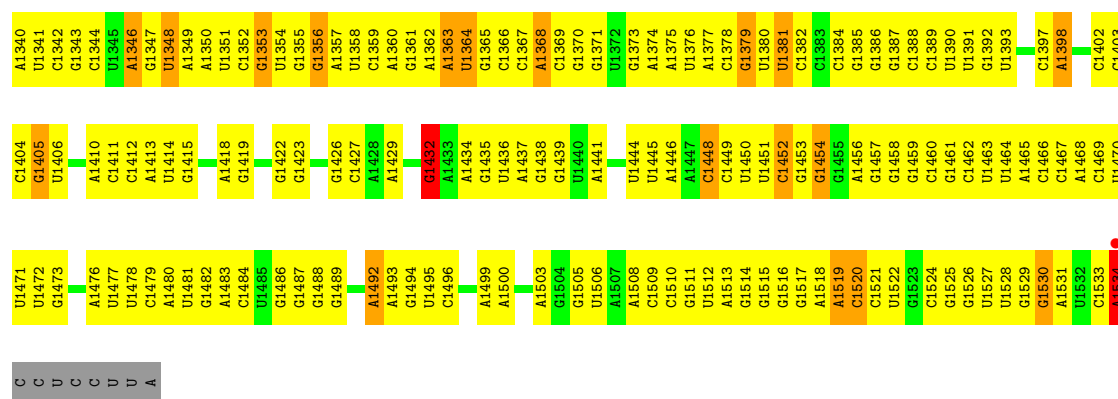
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA

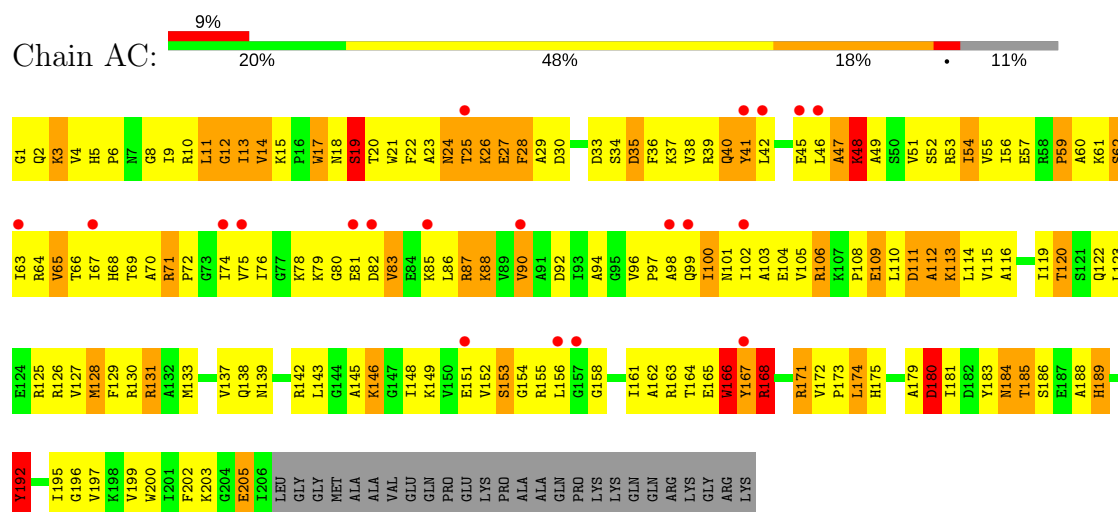




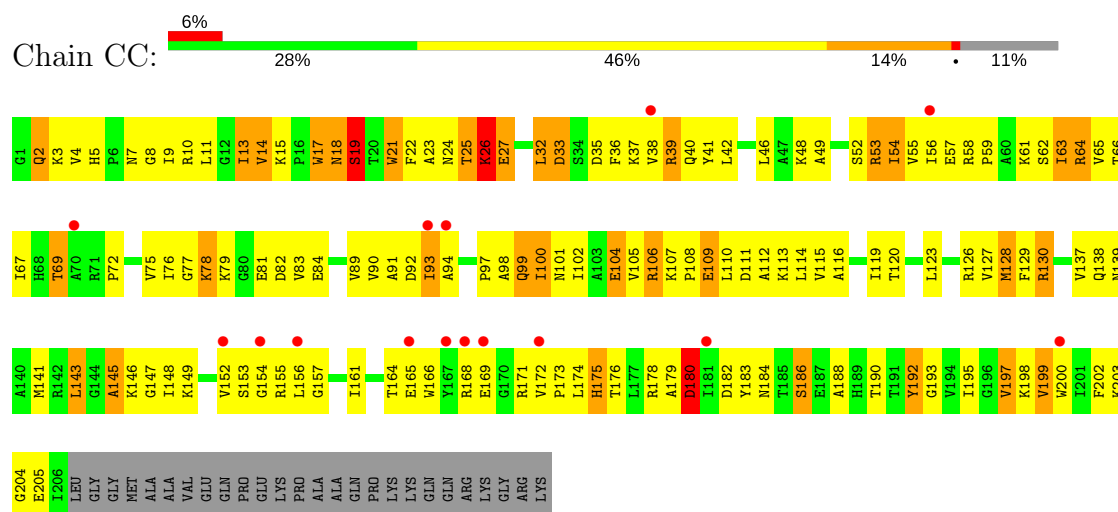
G1279	A1216	C1149	U1086	A1022	A959	A889	A816	A746	U678	U610	G544	U479	G410	C335	A262	G200
A1280	C1217	A1150	U1090	A1023	U960	G890	C817	A747	C679	C611	C545	U480	A411	C336	A263	G201
C1281	A1218	A1151	U1091	U1024	U961	U891	A818	G748	A680	C613	A547	A482	A412	G337	C264	G202
U1282	C1219	A1152	A1092	G1025	A964	A892	A819	A749	G682	C614	G548	C483	A413	G338	G265	G203
U1283	G1221	G1153	A1093	U1026	A965	G894	G821	C750	G683	G615	C549	G484	A414	C339	G266	G204
A1285	G1222	A1157	G1094	C1027	G966	G895	G824	G755	U684	G616	G550	U485	A415	C340	U268	A205
U1286	C1223	C1158	U1095	C1028	C967	C896	A825	G756	G685	G617	U551	U486	G416	A344	C269	A206
U1287	U1224	U1159	C1096	U1029	A968	C897	A826	A757	U686	G618	U552	A487	U420	C345	C207	C206
A1288	C1225	C1160	U1097	U1030	A969	A900	C826	A759	A687	U619	A553	A488	U421	C352	C271	U208
A1289	G1226	C1161	C1098	C1031	C970	A901	U827	G760	G688	U620	A554	C489	C422	C353	C272	U209
G1290	A1227	A1162	G1099	G1032	G971	A902	U828	G761	G689	A621	U555	C490	G423	A354	U273	G210
U1291	C1228	C1163	C1100	G1033	C972	G903	G833	G762	G690	A622	C556	G491	G424	G355	G211	G211
G1292	A1229	G1164	A1101	G1036	G973	G904	U834	G763	G691	C623	G557	C492	G425	C356	G212	G213
C1293	C1230	U1165	A1102	A1037	A974	U904	U835	G764	G692	U625	A558	G494	U426	A356	C214	C215
U1295	G1231	G1166	C1103	C1038	G975	U905	U836	G765	G693	G626	A559	G495	U427	C357	G276	G216
U1296	U1232	A1167	G1104	U1039	G976	A906	U837	A766	A694	U627	A560	A496	U428	C358	C280	U216
G1297	G1233	U1168	U1040	U1040	A977	A907	U838	G767	G700	G628	U562	G497	A430	A366	G281	C217
G1298	C1234	A1169	G1107	G1041	A978	A908	C840	G768	U701	U629	A563	A498	A431	U367	U218	U219
U1299	U1235	A1170	C1108	A1042	C979	A909	C841	C770	A702	A630	A564	A499	A432	U368	C284	C222
A1299	A1236	A1171	C1109	G1043	C980	C910	U842	G771	G703	C631	C565	C501	G433	C285	C285	A223
G1300	C1237	U1172	A1110	U1047	U981	C912	U843	U772	A704	U632	U566	C502	U434	C286	G287	A224
U1301	A1238	U1173	A1111	G1048	A983	A913	G844	A777	U707	C634	G567	A503	C436	C372	U288	U224
C1302	U1239	G1174	C1112	U1049	C984	A914	A845	G778	C708	A635	G568	C504	U437	A373	G289	C225
C1303	G1240	G1175	C1113	G1050	C985	C914	G846	C779	C709	U636	A572	C505	U438	A374	C290	G226
G1304	G1241	A1176	C1114	C1051	C986	G917	C847	G780	U709	U637	A573	C506	U439	C378	U291	G227
G1305	G1242	G1177	U1115	U1052	U987	A918	C848	A781	G710	C638	C576	A510	A440	C379	G292	A228
A1306	C1243	U1116	U1116	G1053	G988	A919	U849	A782	G711	U639	G577	C511	A441	G380	U299	U231
U1307	G1244	A1117	A1117	U1054	U989	A920	G850	A783	G712	C643	A578	C512	G449	C381	A300	G232
U1308	C1245	A1118	U1118	C1054	C990	U921	U851	C784	G713	U644	C580	C513	G450	A382	G301	C233
G1309	A1246	G1181	C1119	U1055	U991	G922	G858	G785	G714	A642	G584	C514	G451	C383	G302	G234
G1310	U1247	G1182	C1120	U1056	U992	A923	G859	G786	A715	C647	G585	C515	G452	C384	C235	C235
A1311	A1248	U1183	U1121	G1057	G993	C924	G860	A787	G716	C648	C586	C516	G453	C385	A236	G237
C1249	C1250	G1184	U1122	C1058	A994	G925	G861	C788	A717	U655	G587	C517	G454	C386	A309	G238
U1313	G1251	G1185	C1123	G1059	C995	G926	C862	A790	C719	C649	G588	C518	U458	G388	G310	A238
C1314	A1252	G1186	U1124	U1060	C996	G927	U863	G791	C720	A648	G589	C519	A459	A389	C311	U239
U1315	C1253	A1187	U1125	G1061	A997	G928	A864	A792	G721	A649	C590	C520	A460	U390	C312	G240
G1316	G1254	U1188	U1126	U1062	C998	G933	A865	U793	G722	G650	C591	C521	A461	G391	A313	G241
C1317	G1255	U1189	C1127	C1063	C999	C934	C866	A794	U723	C651	U590	C522	A462	G392	C314	G242
A1318	A1256	G1190	U1128	G1064	A1000	A935	G867	C795	G724	U652	U591	C523	A463	C393	A315	G243
C1319	C1257	A1191	C1129	U1065	C1001	A936	C868	C796	G725	U653	G592	C524	G464	G394	U244	U244
U1321	G1258	A1192	G1130	C1066	G1002	A938	G869	C797	G726	U656	U593	C525	U465	C395	U245	U245
C1322	C1259	U1193	C1131	G1067	G1003	G939	U870	U798	A728	G657	U594	C526	A466	C396	A246	G247
G1323	U1260	U1194	G1132	C1068	A1004	C940	U871	U801	C735	U658	A595	C527	U467	A397	A321	A250
A1324	C1262	C1200	G1133	C1069	G1005	G941	U872	A802	G736	C659	A596	C528	A468	U398	C322	G251
C1325	G1263	A1201	U1134	U1070	A1006	A946	U873	G803	G737	U660	A597	C529	C470	U399	U323	G252
U1326	U1264	U1202	C1135	C1071	G1007	A947	C876	G804	G738	C661	U598	C530	U471	C400	A324	A253
C1327	C1265	C1203	U1136	G1072	U1008	G947	G877	U804	C739	U662	U599	C531	U472	C401	A325	G254
G1328	G1266	U1204	G1137	U1073	C948	C948	A878	C805	G734	U663	C600	C532	U473	C402	G326	G255
U1267	G1267	G1206	U1138	G1074	U1009	A949	U879	C806	C735	A664	A600	A533	U474	C403	A327	G256
G1268	G1268	G1207	C1139	U1075	U1010	U950	C880	C807	G736	G665	G601	C534	U475	C404	G328	G257
A1269	C1269	U1208	U1140	G1076	A1011	U951	C881	A808	C737	A665	A602	U535	U476	C405	A329	G258
A1332	G1270	C1209	G1141	U1077	A1012	G951	C882	G809	C738	U672	G603	A536	U477	C406	C330	G331
A1333	U1271	U1209	C1142	G1078	G1013	U952	C883	G809	C739	U673	G604	C537	U478	C407	G332	G332
G1334	C1272	C1210	G1143	U1079	G1014	G953	C884	C810	G740	U674	U605	C538	U479	C408	A408	A409
U1335	U1273	U1211	G1144	A1081	A1015	G954	U884	C811	U740	G675	G606	A539	C475	G409	G409	G409
C1336	G1274	U1212	A1145	A1082	A1016	U955	C885	G812	G741	A676	A607	C540	U476	G410	G410	G410
G1337	A1274	A1213	A1146	U1083	U1017	U956	G886	U813	G742	A677	A608	C541	U477	G411	G411	G411
U1338	C1275	C1214	C1147	G1084	G887	U957	G887	U814	C744	A678	A609	C542	U478	G412	G412	G412
A1339	G1278	G1215	U1148	U1085	A1019	A958	G888	A815	G745	U679	A610	C543	U479	G413	G413	G413



• Molecule 2: 30S ribosomal protein S3

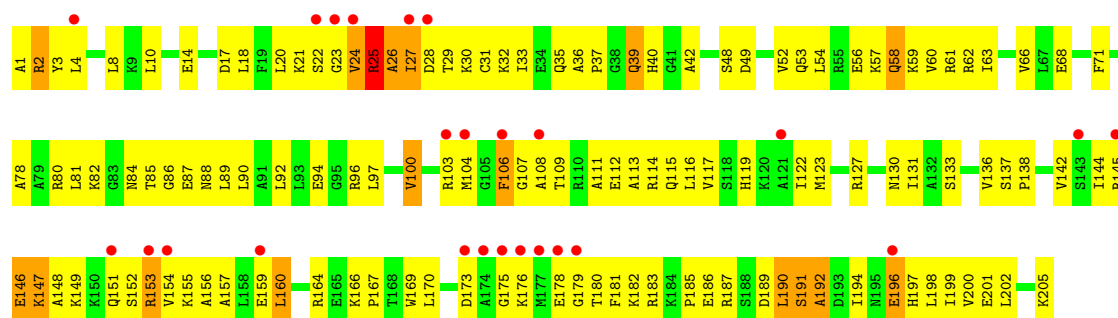


• Molecule 2: 30S ribosomal protein S3

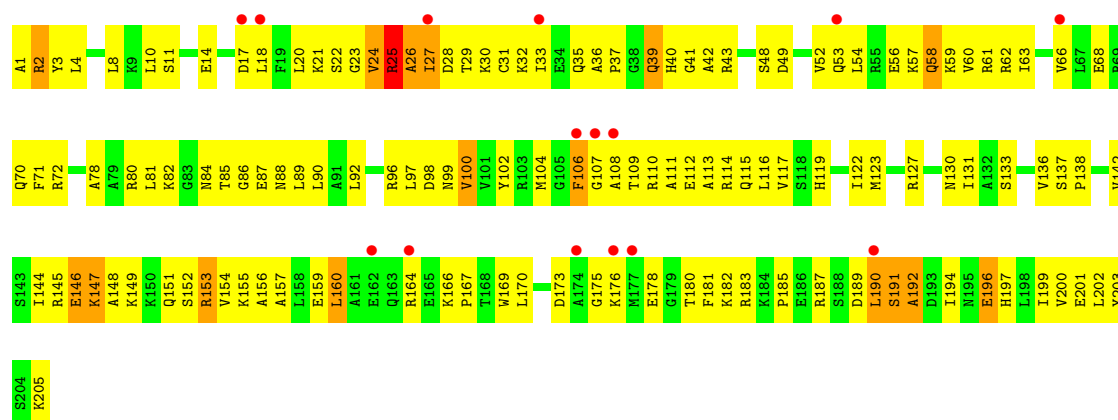


• Molecule 3: 30S ribosomal protein S4

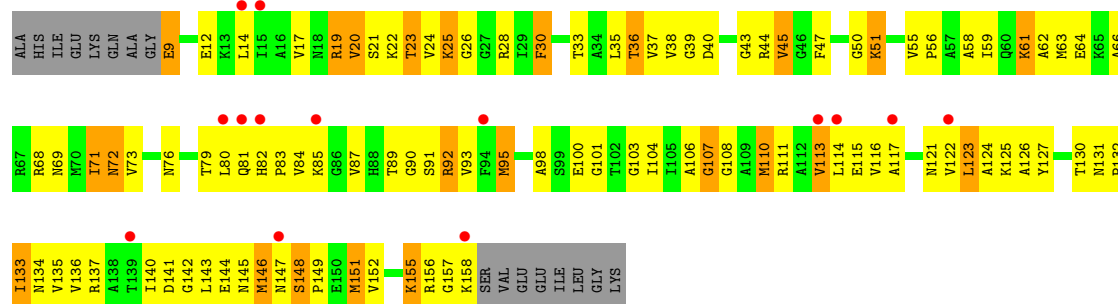




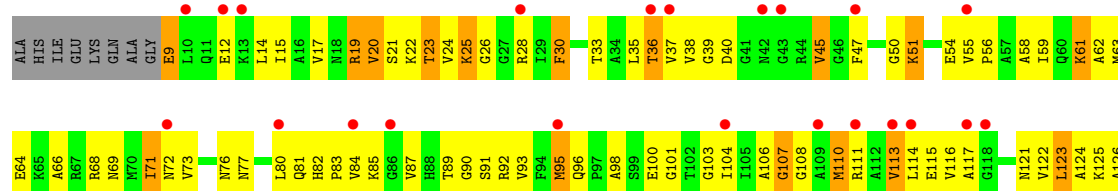
• Molecule 3: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S5

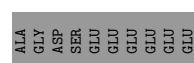
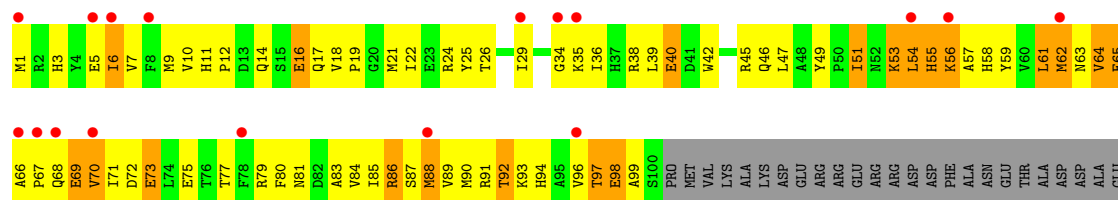
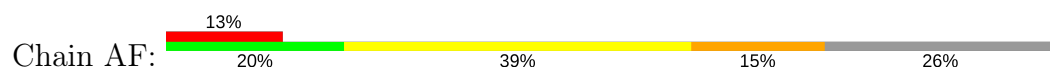


• Molecule 4: 30S ribosomal protein S5

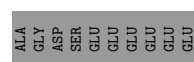
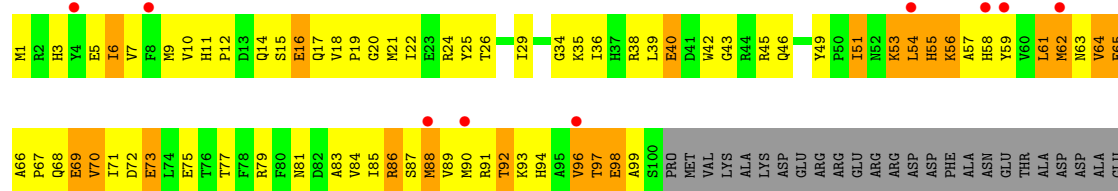
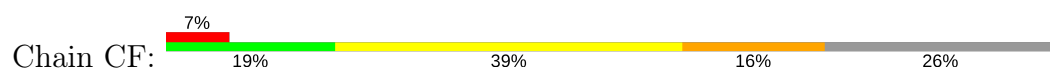




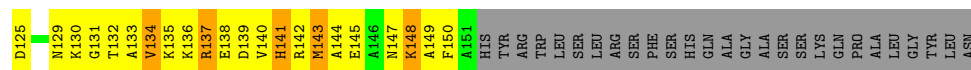
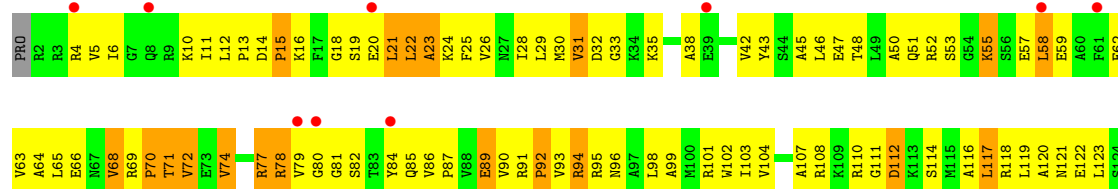
• Molecule 5: 30S ribosomal protein S6



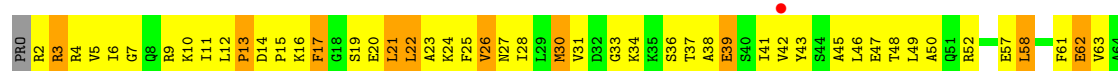
• Molecule 5: 30S ribosomal protein S6

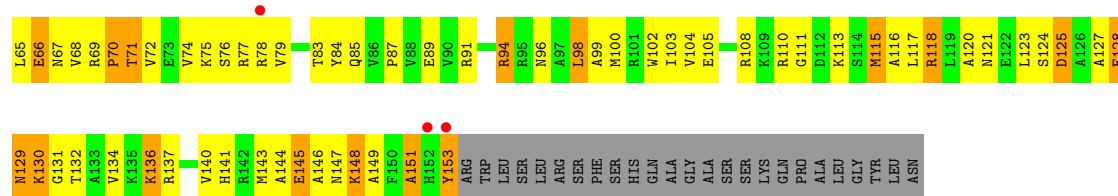


• Molecule 6: 30S ribosomal protein S7

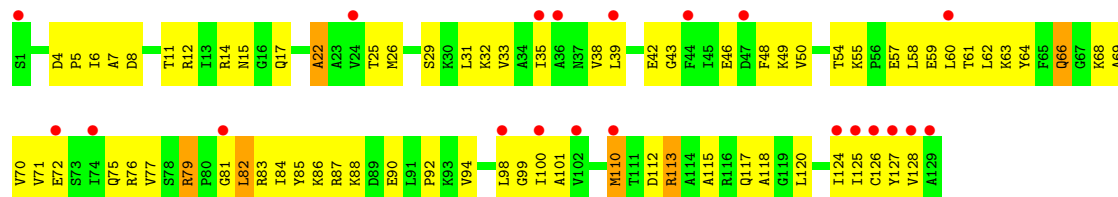
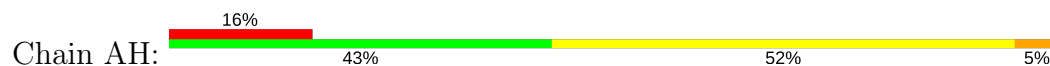


• Molecule 6: 30S ribosomal protein S7

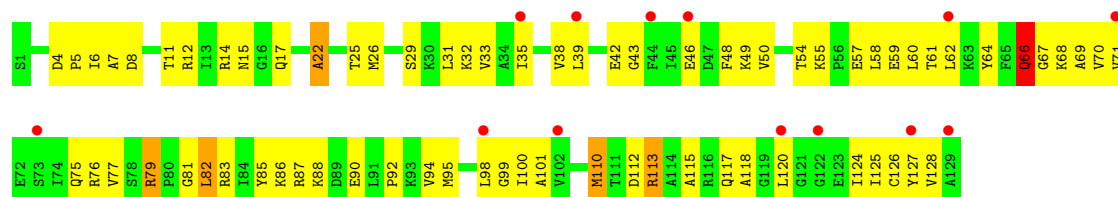




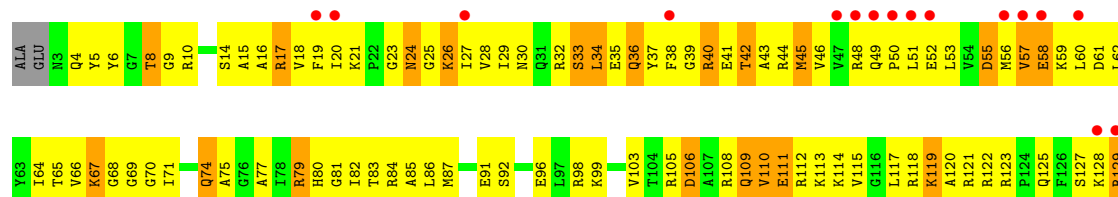
• Molecule 7: 30S ribosomal protein S8



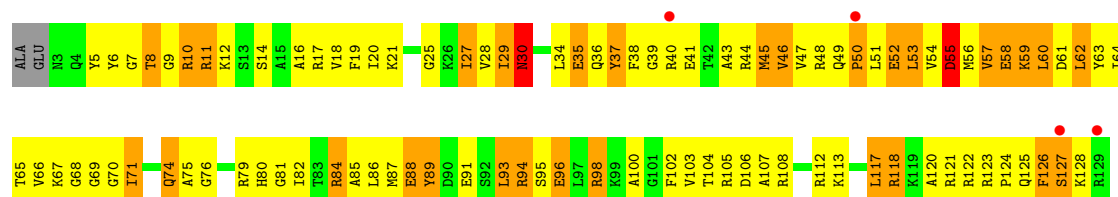
• Molecule 7: 30S ribosomal protein S8



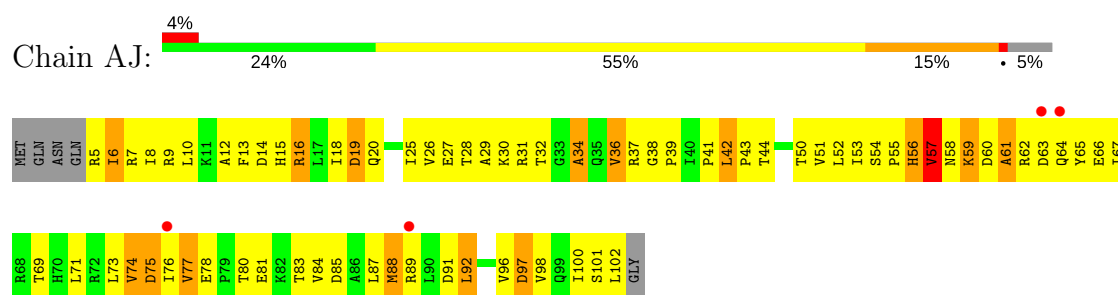
• Molecule 8: 30S ribosomal protein S9



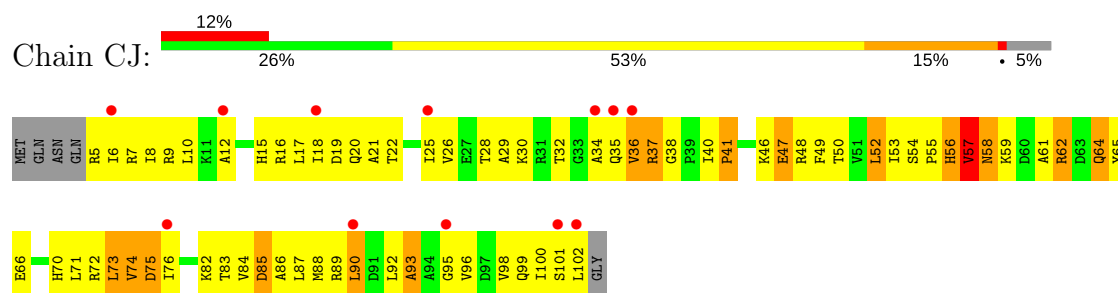
• Molecule 8: 30S ribosomal protein S9



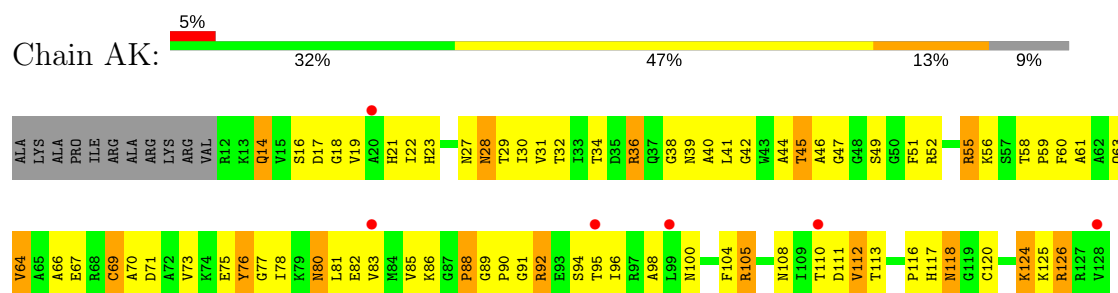
• Molecule 9: 30S ribosomal protein S10



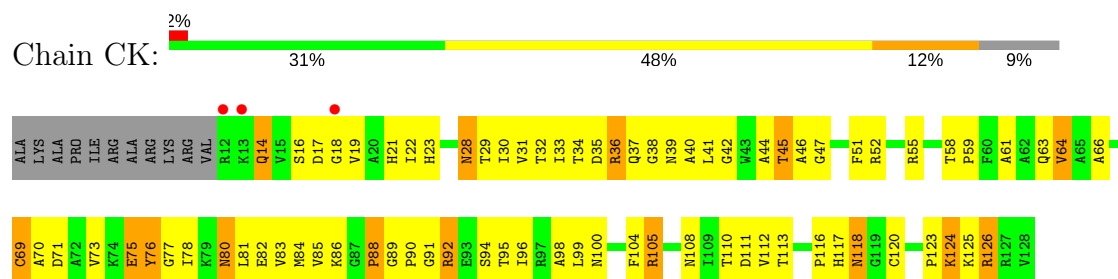
• Molecule 9: 30S ribosomal protein S10



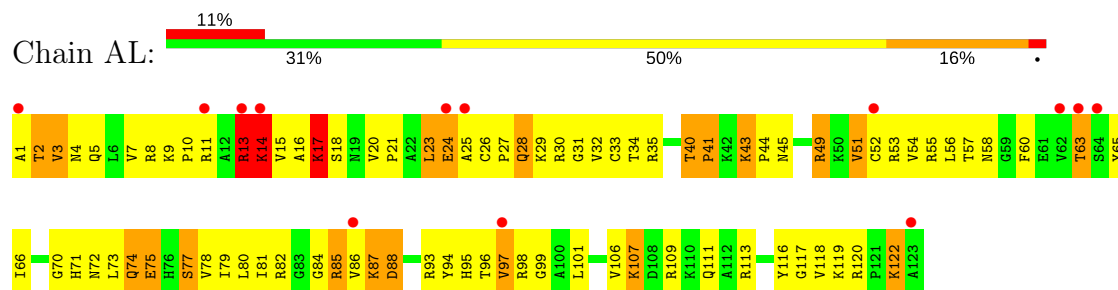
• Molecule 10: 30S ribosomal protein S11



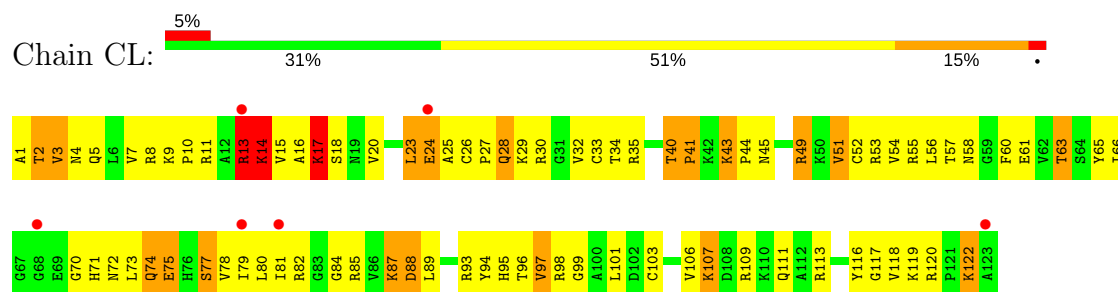
• Molecule 10: 30S ribosomal protein S11



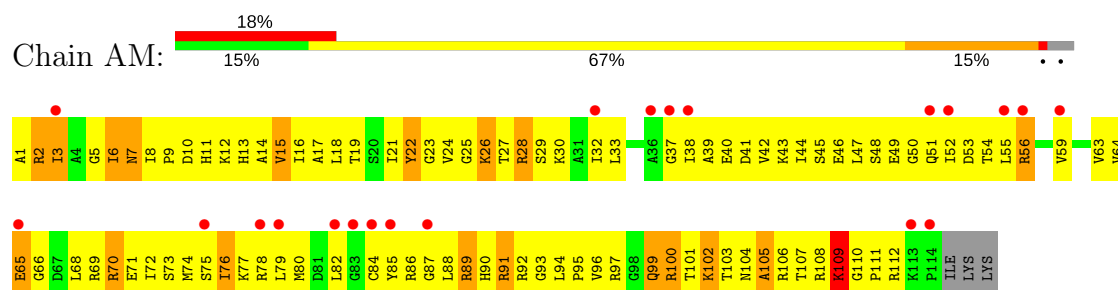
• Molecule 11: 30S ribosomal protein S12



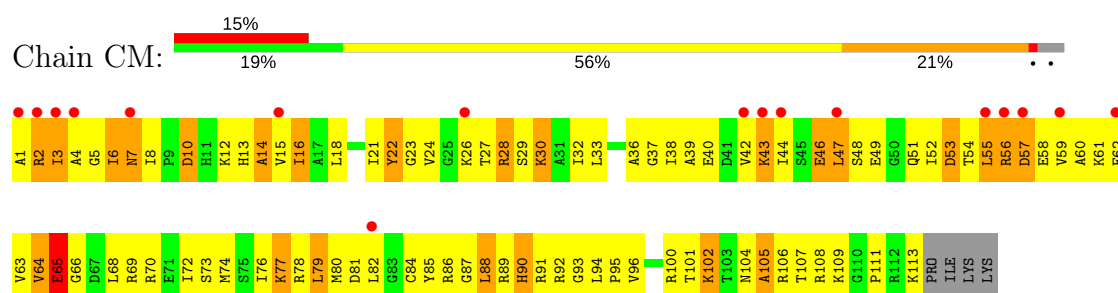
- Molecule 11: 30S ribosomal protein S12



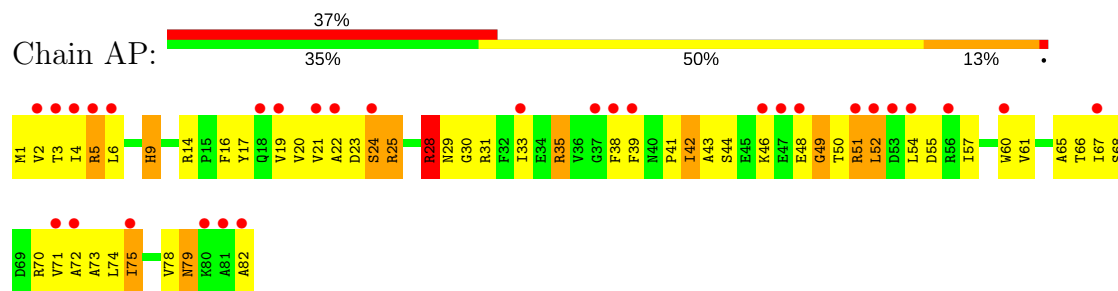
- Molecule 12: 30S ribosomal protein S13



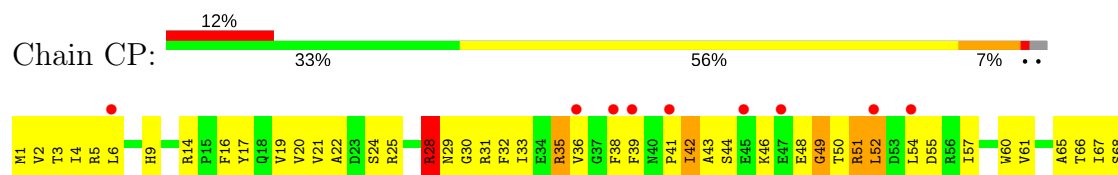
- Molecule 12: 30S ribosomal protein S13

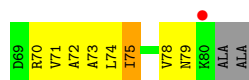


- Molecule 13: 30S ribosomal protein S16

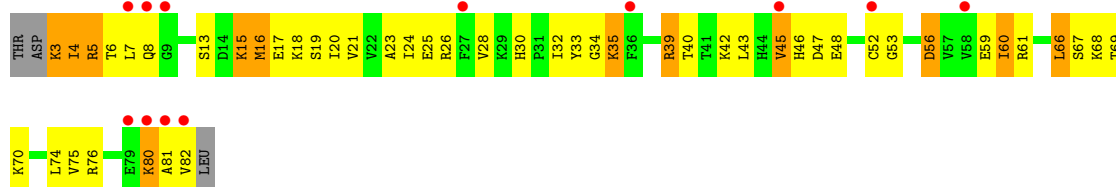


- Molecule 13: 30S ribosomal protein S16

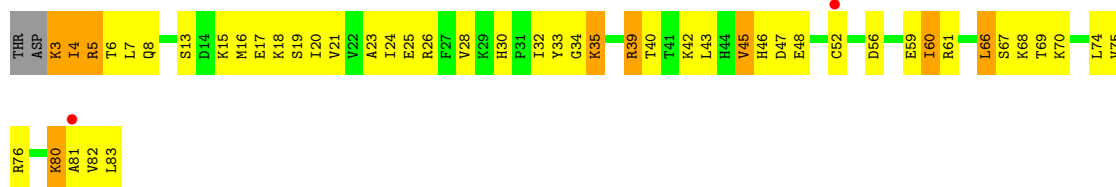
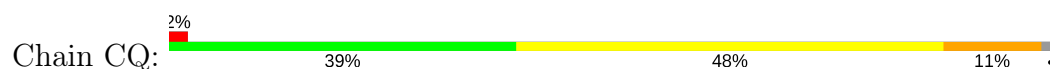




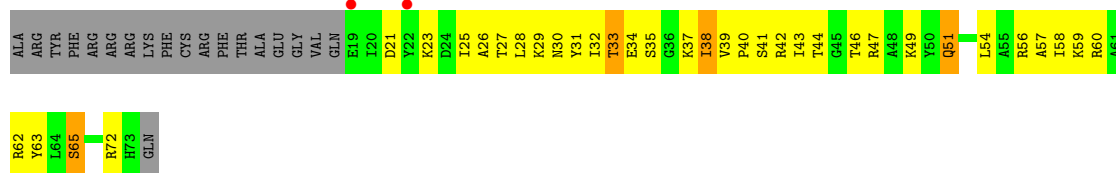
- Molecule 14: 30S ribosomal protein S17



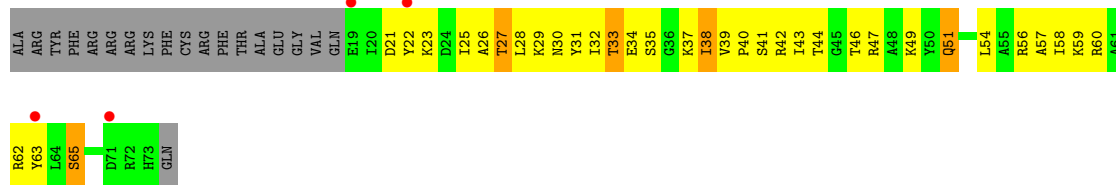
- Molecule 14: 30S ribosomal protein S17



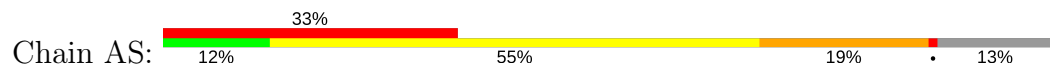
- Molecule 15: 30S ribosomal protein S18

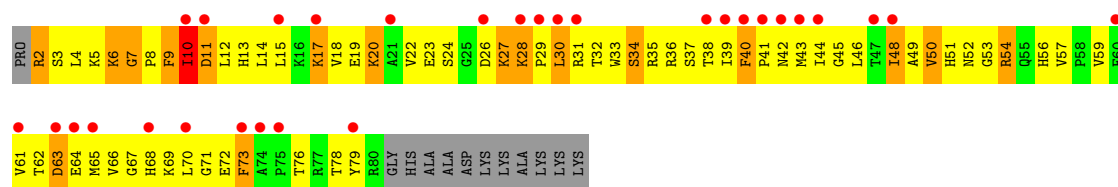


- Molecule 15: 30S ribosomal protein S18

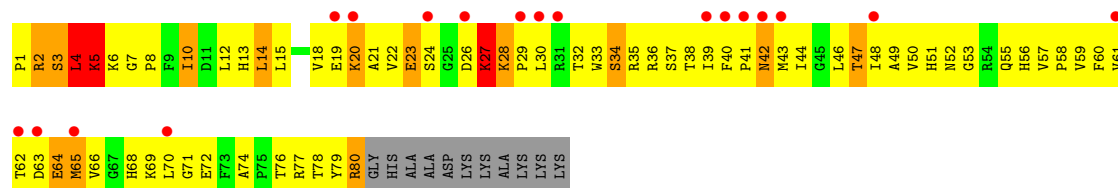
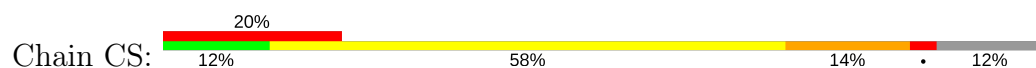


- Molecule 16: 30S ribosomal protein S19

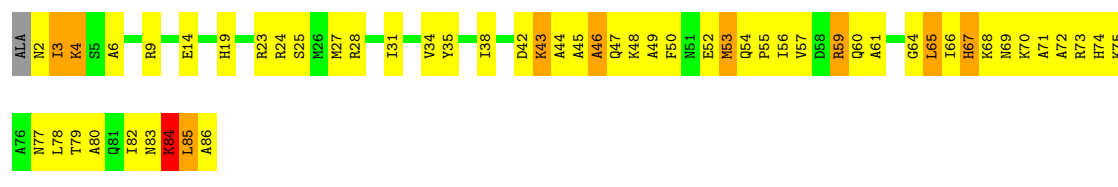




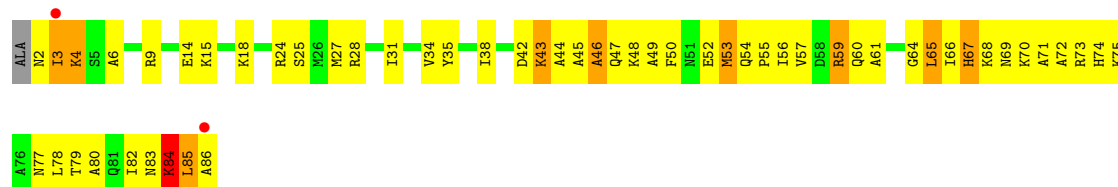
• Molecule 16: 30S ribosomal protein S19



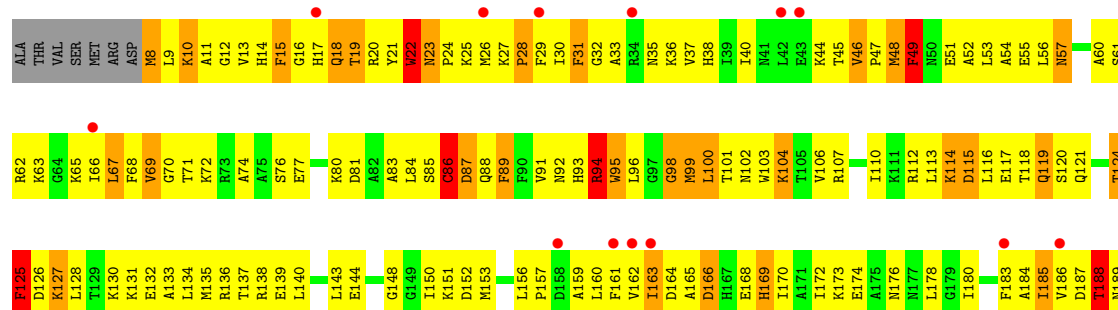
• Molecule 17: 30S ribosomal protein S20

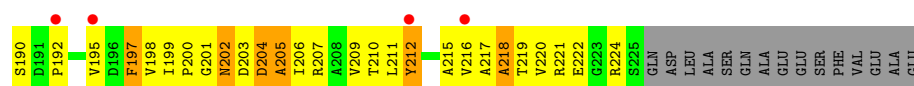


• Molecule 17: 30S ribosomal protein S20

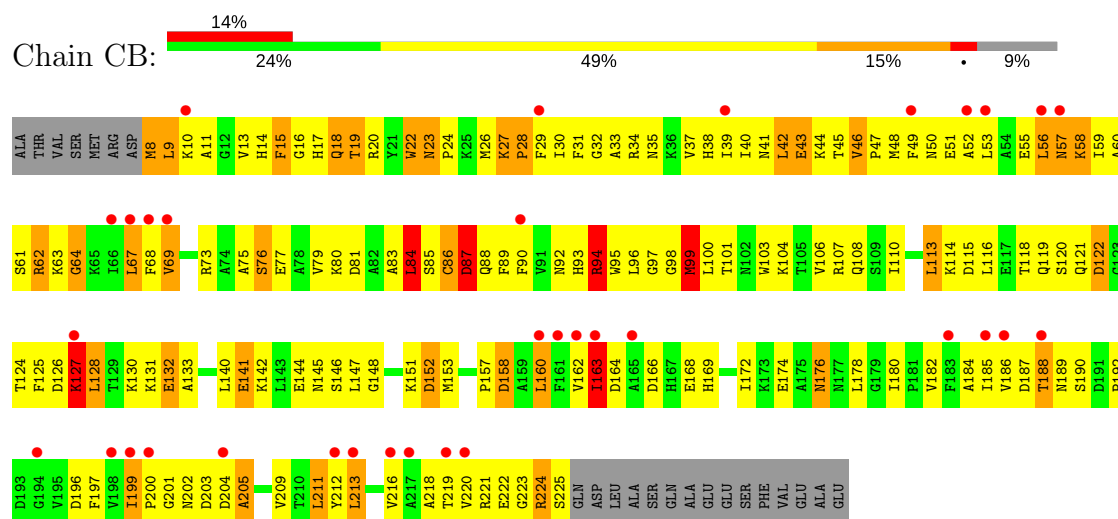


• Molecule 18: 30S ribosomal protein S2

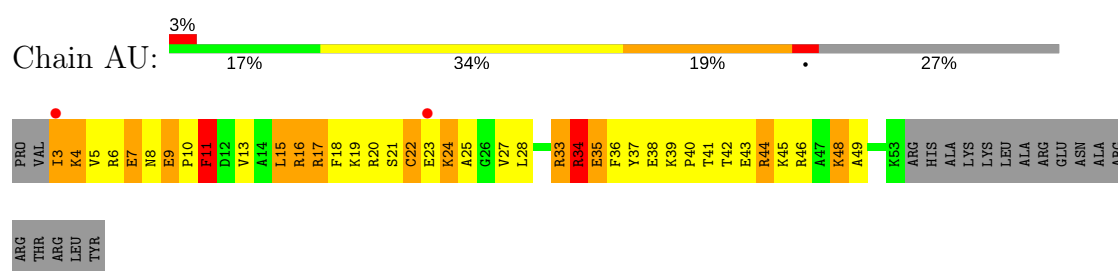




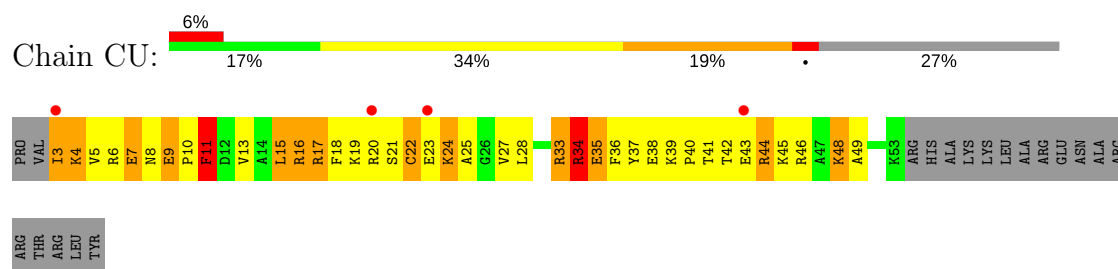
• Molecule 18: 30S ribosomal protein S2



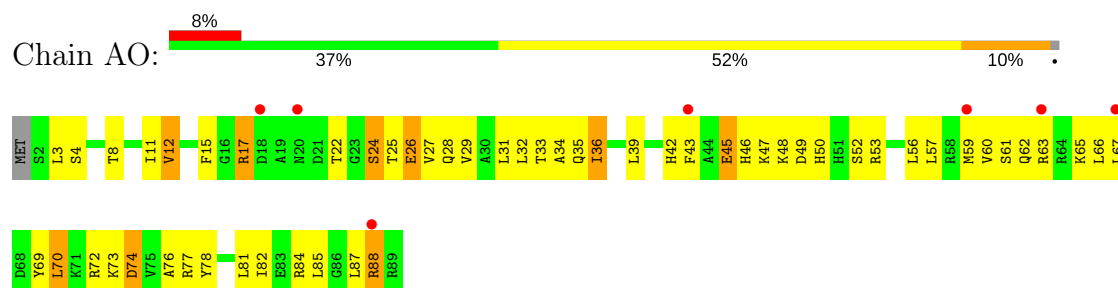
• Molecule 19: 30S ribosomal protein S21



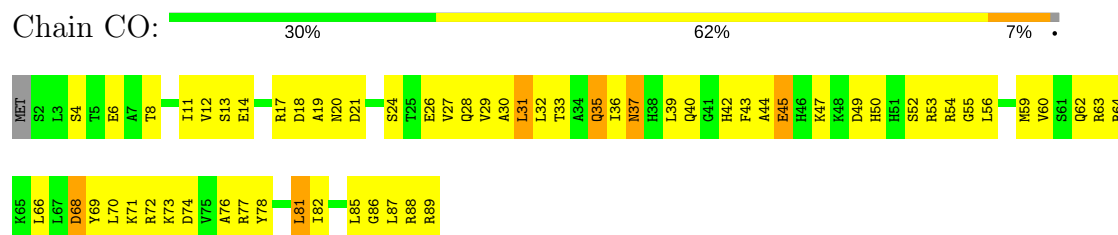
• Molecule 19: 30S ribosomal protein S21



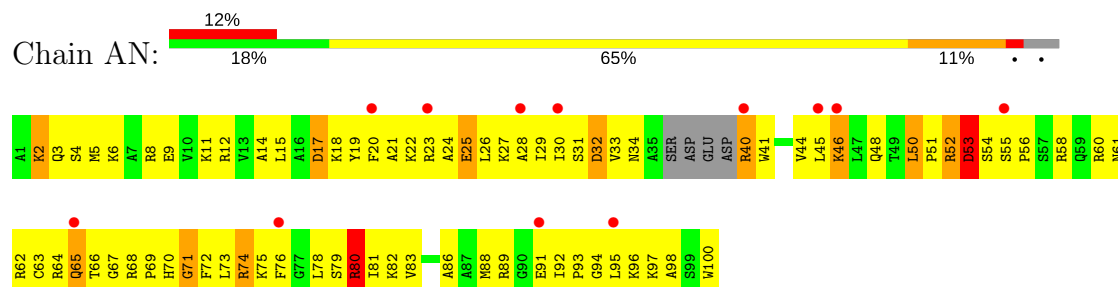
• Molecule 20: 30S ribosomal protein S15



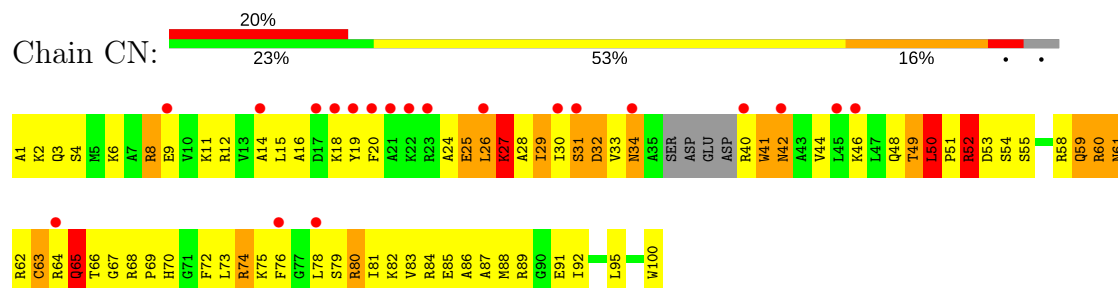
- Molecule 20: 30S ribosomal protein S15



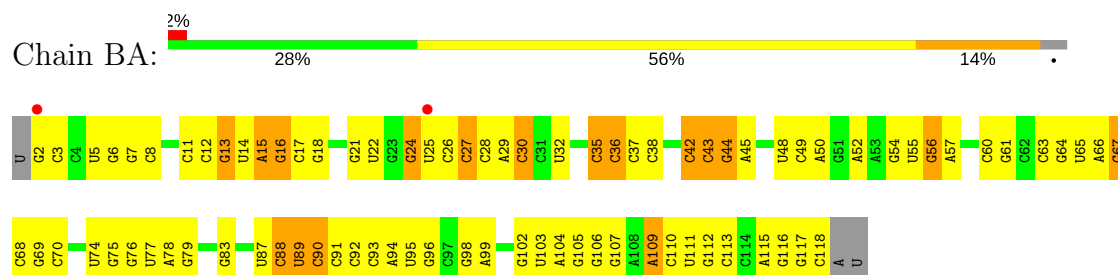
- Molecule 21: 30S ribosomal protein S14



- Molecule 21: 30S ribosomal protein S14



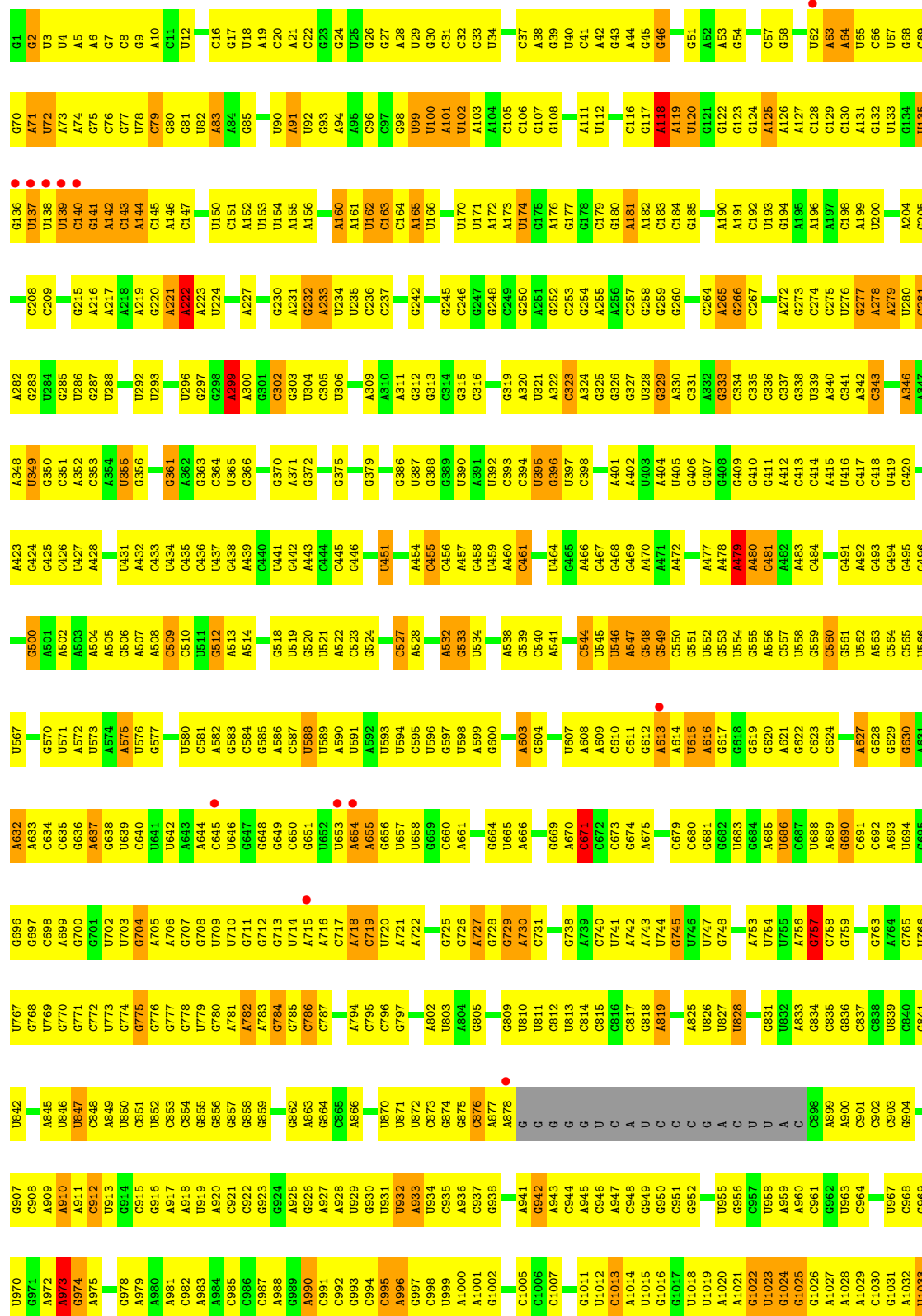
- Molecule 22: 5S rRNA



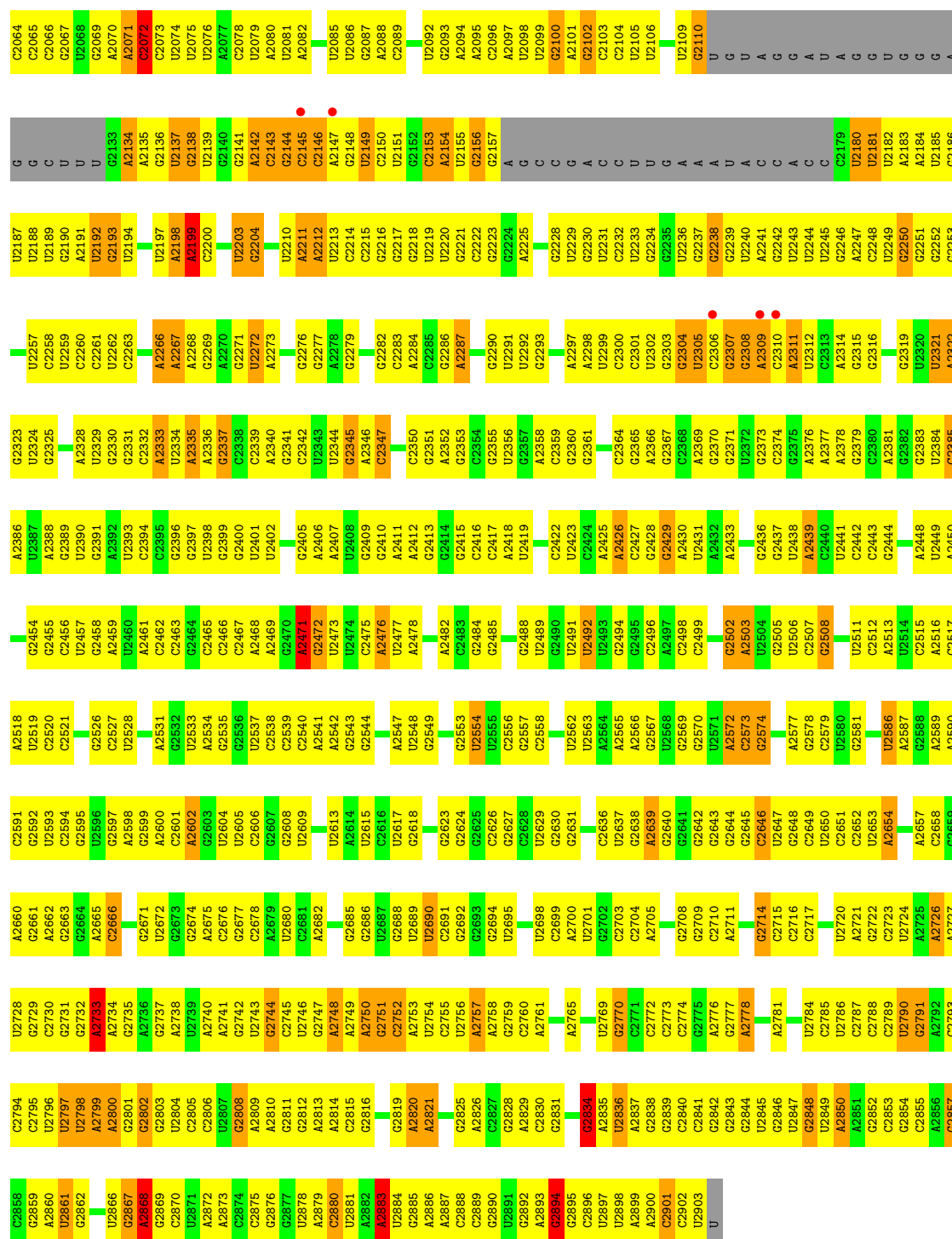
- Molecule 22: 5S rRNA



● Molecule 23: 23S rRNA

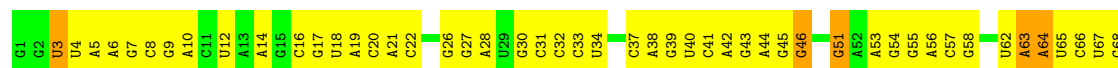






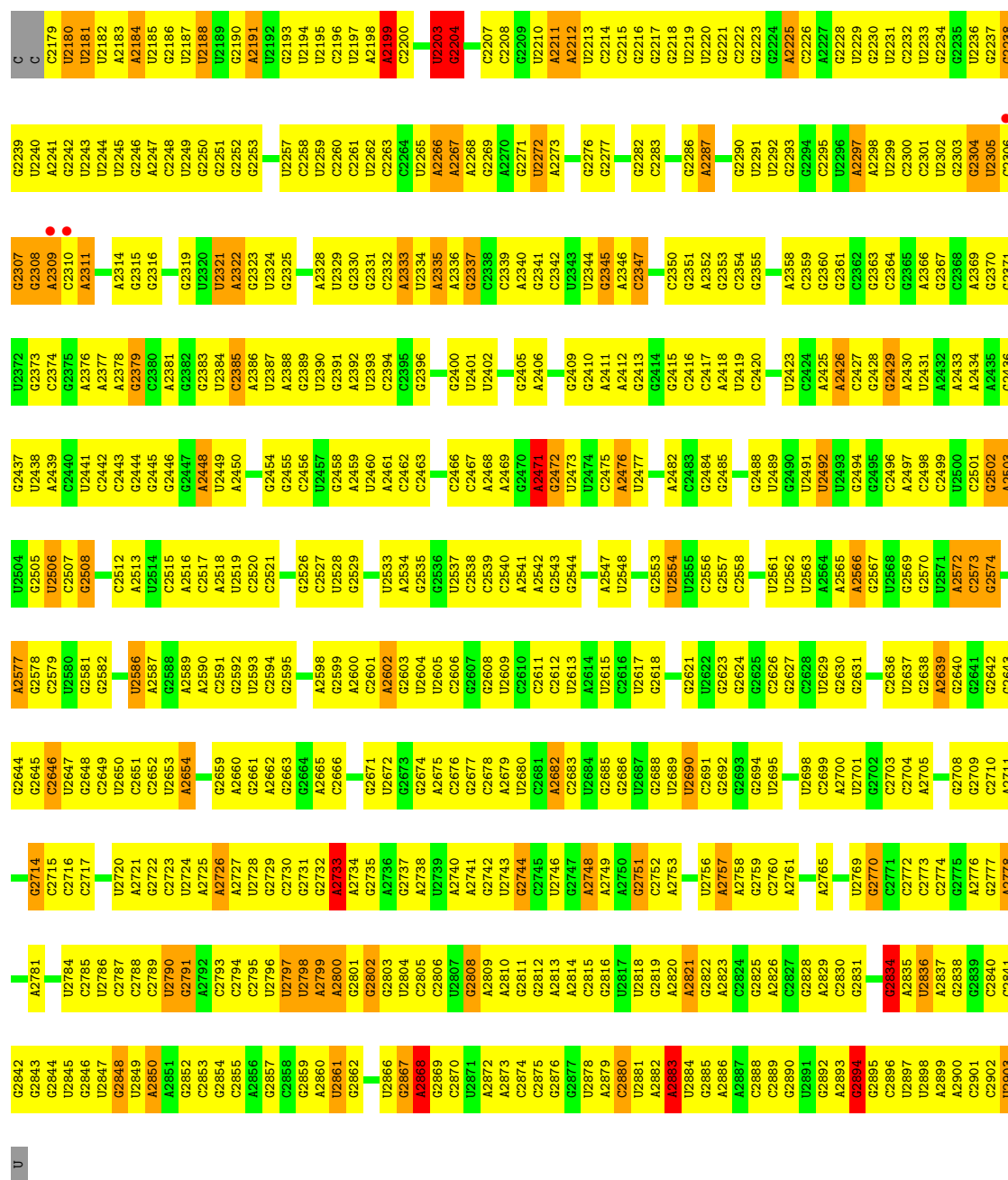
• Molecule 23: 23S rRNA

Chain DB: 26% 61% 10% ..

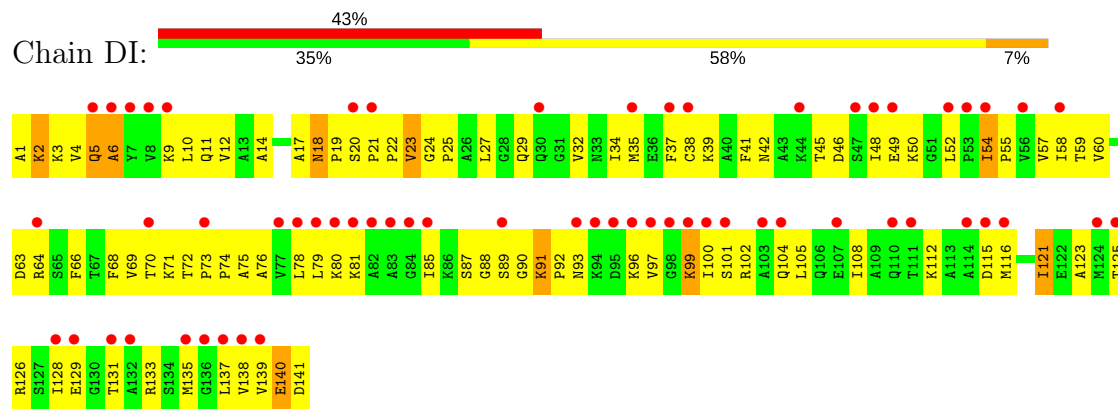


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C1100	U1026	U963	A899	U755	U686		G555	G491	C417	A348	U286		C143	U72
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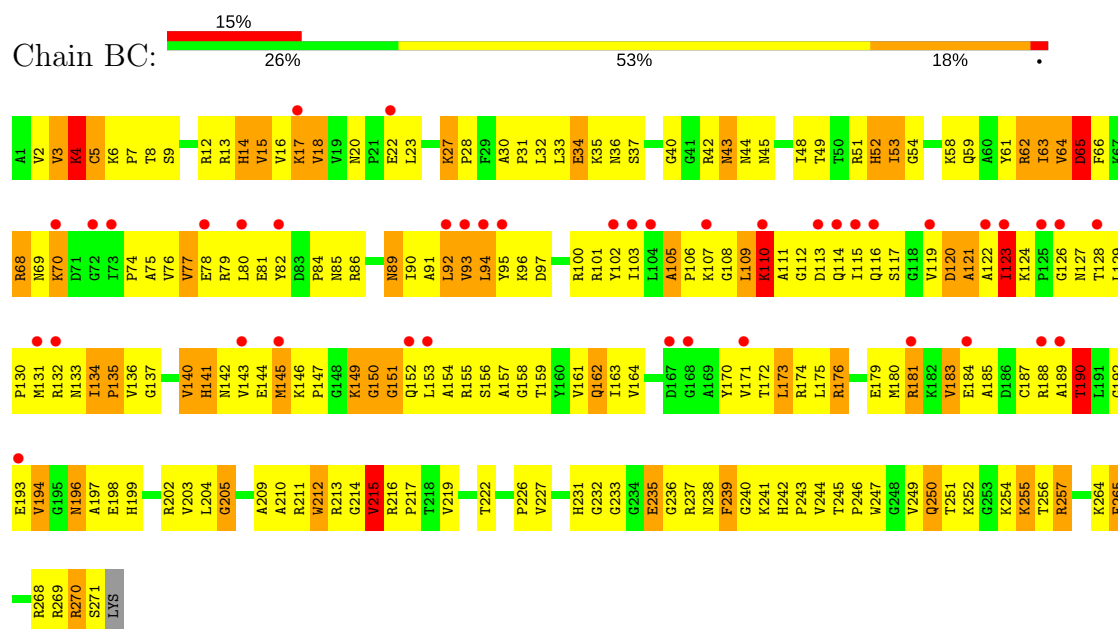
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U	U2044	U1971	U1824	C1761	C1704	A1636	U1563	A1495	G1432		C1306	
U	U2045	C1907	C1830	G1767	A1705	U1636	C1564	A1496	G1433		A1307	G1236
G	A2108	C1908	G1831	C1768	A1706	U1637	C1565		A1434		G1308	G1237
A	U2109	C1909	C1832		G1707	C1638		C1499			A1309	G1238
A	G2110	U1911		C1771	C1708	G1639	G1568		A1372	A1373		
U	C2047			A1772								
G	G2048											
U	G2049											
C	C2050											
A	A2051											



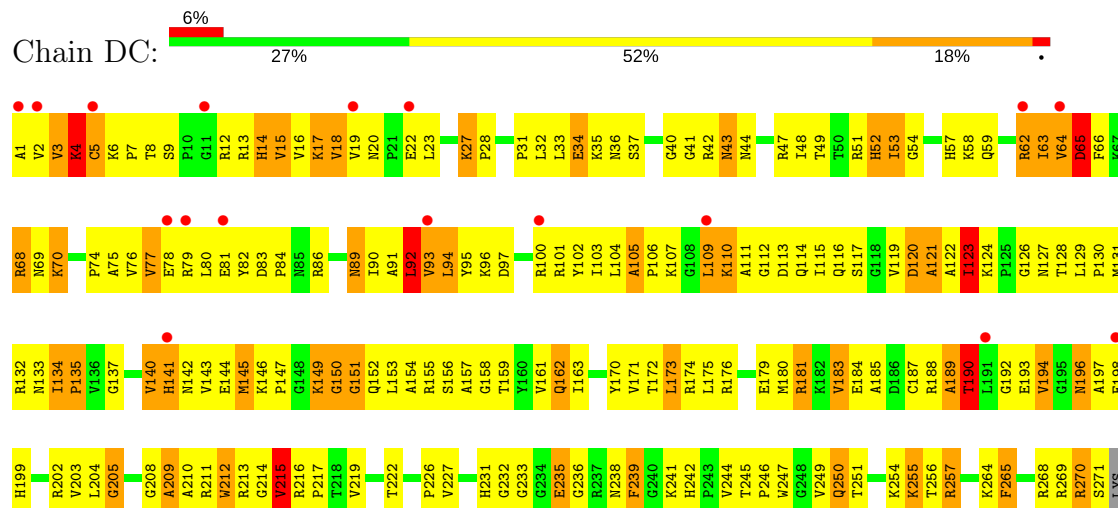
Chain DI:



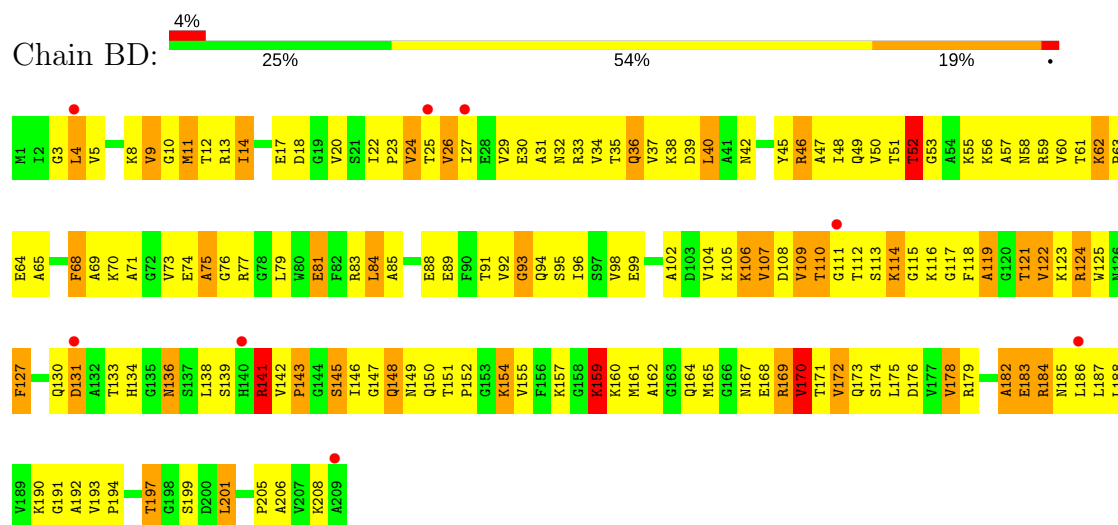
Chain BC:



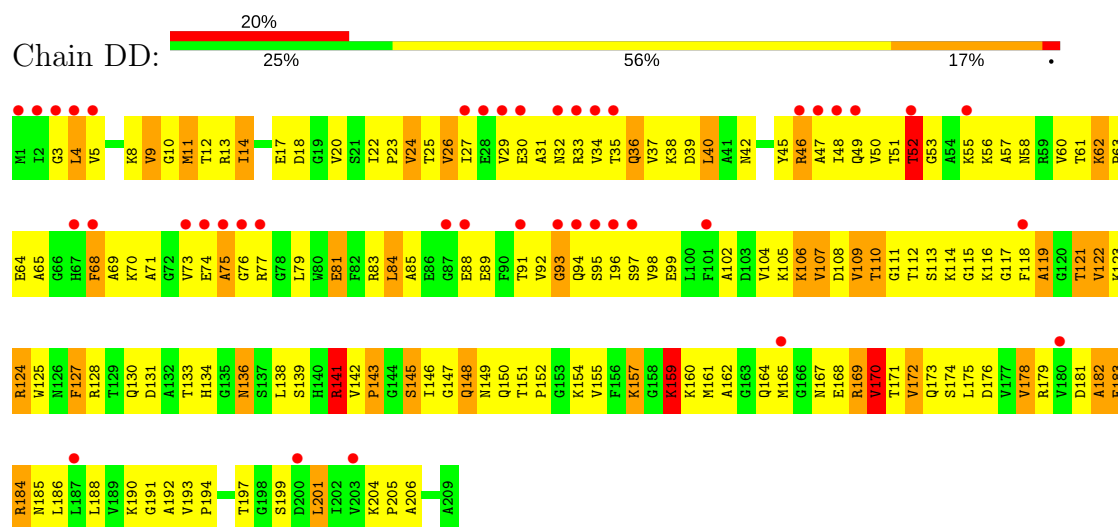
Chain DC:



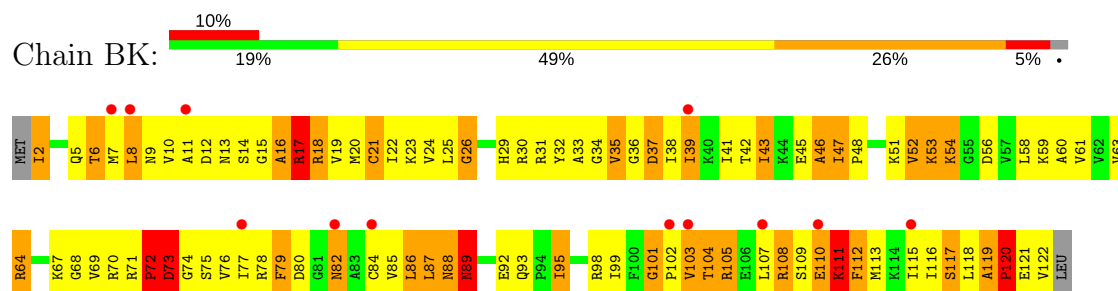
• Molecule 26: 50S ribosomal protein L3



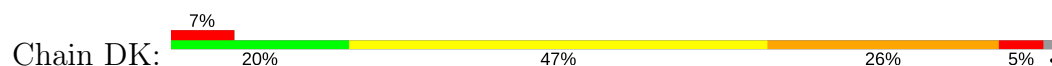
• Molecule 26: 50S ribosomal protein L3



• Molecule 27: 50S ribosomal protein L14

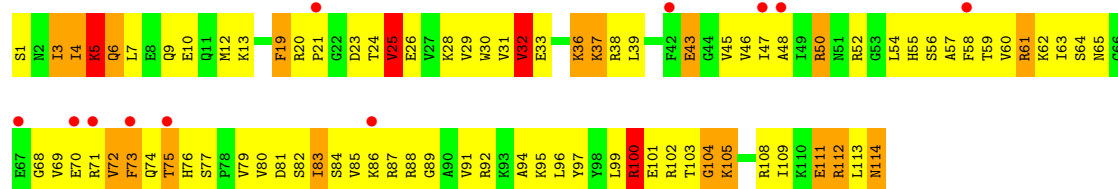


• Molecule 27: 50S ribosomal protein L14

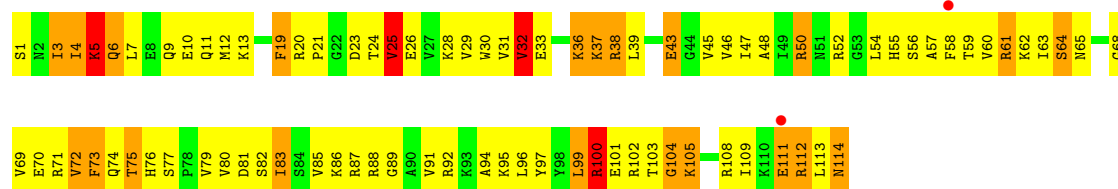




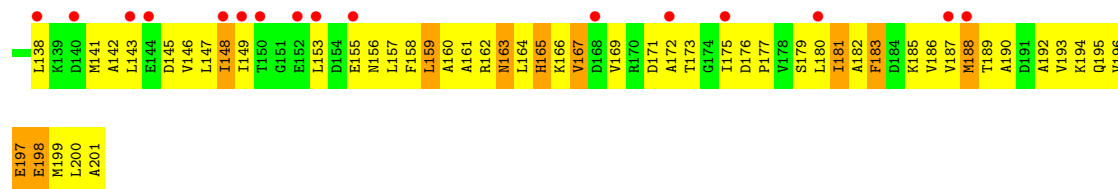
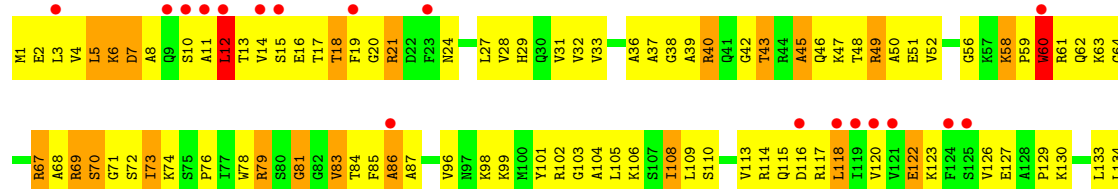
• Molecule 28: 50S ribosomal protein L19



• Molecule 28: 50S ribosomal protein L19

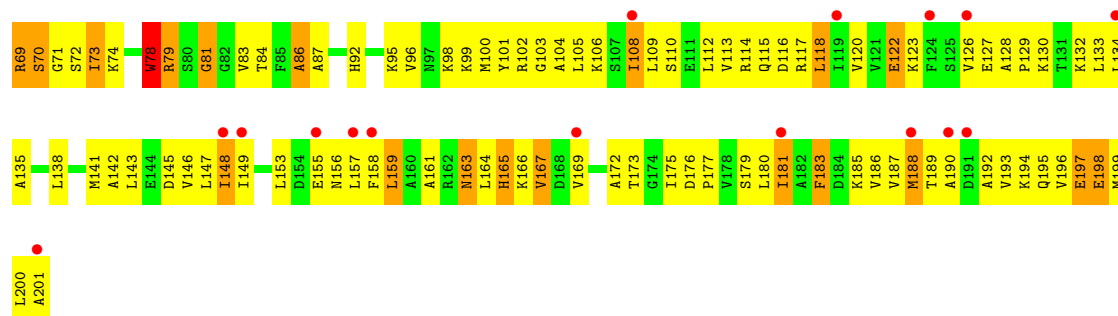


• Molecule 29: 50S ribosomal protein L4

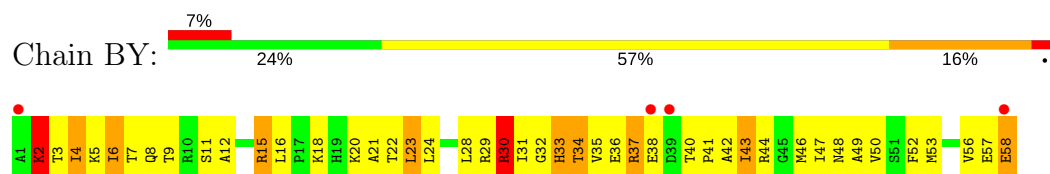


• Molecule 29: 50S ribosomal protein L4

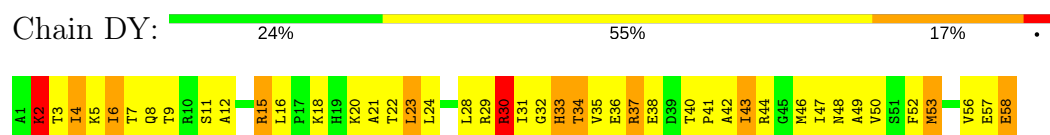




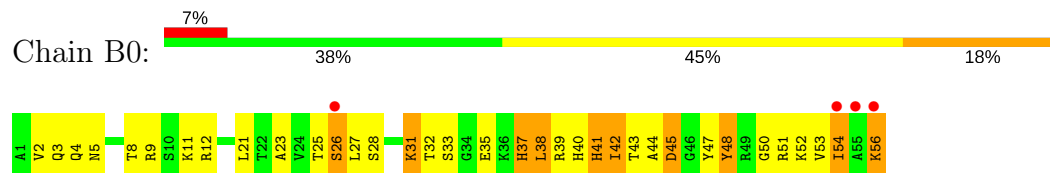
- Molecule 30: 50S ribosomal protein L30



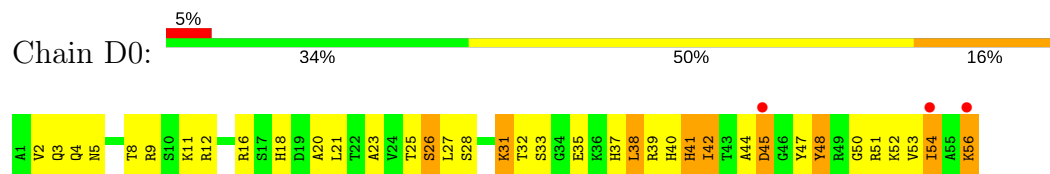
- Molecule 30: 50S ribosomal protein L30



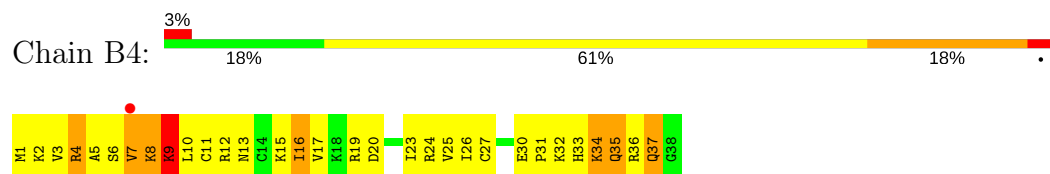
- Molecule 31: 50S ribosomal protein L32



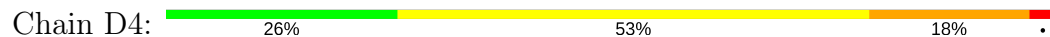
- Molecule 31: 50S ribosomal protein L32



- Molecule 32: 50S ribosomal protein L36

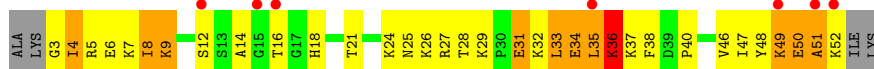


- Molecule 32: 50S ribosomal protein L36

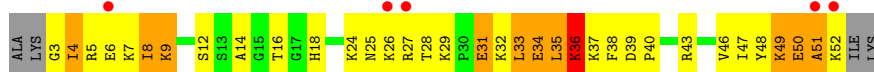




- Molecule 33: 50S ribosomal protein L33



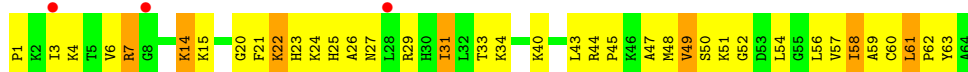
- Molecule 33: 50S ribosomal protein L33



- Molecule 34: 50S ribosomal protein L35



- Molecule 34: 50S ribosomal protein L35

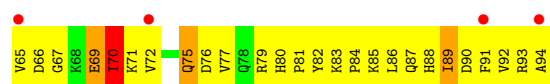


- Molecule 35: 50S ribosomal protein L25



- Molecule 35: 50S ribosomal protein L25

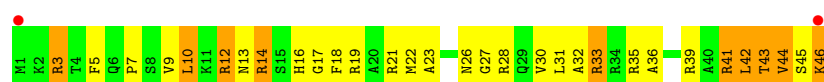




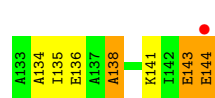
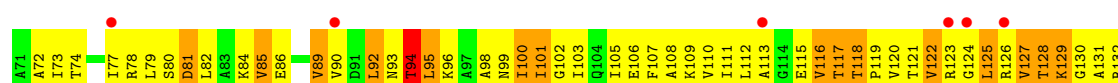
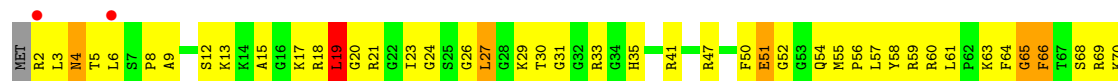
- Molecule 36: 50S ribosomal protein L34



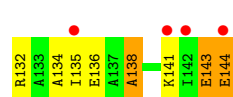
- Molecule 36: 50S ribosomal protein L34



- Molecule 37: 50S ribosomal protein L15

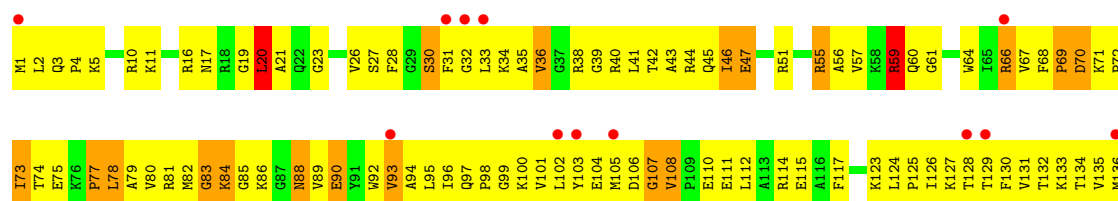


- Molecule 37: 50S ribosomal protein L15

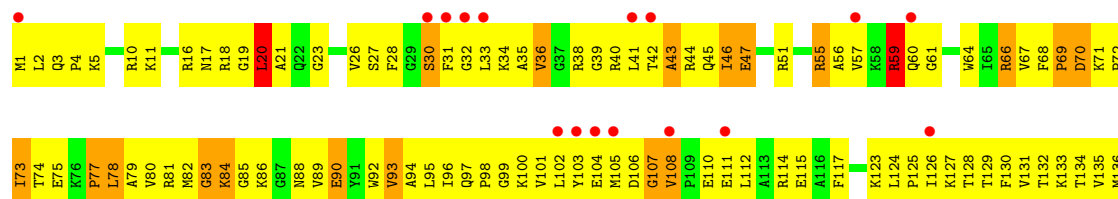


- Molecule 38: 50S ribosomal protein L16

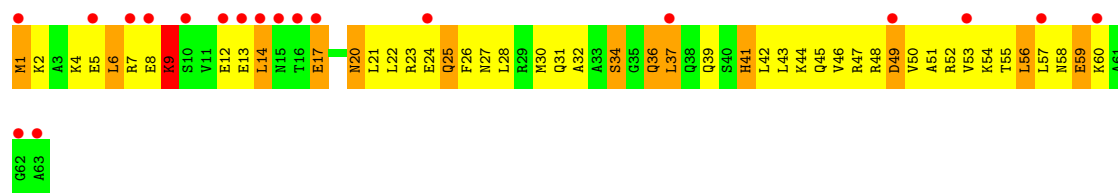




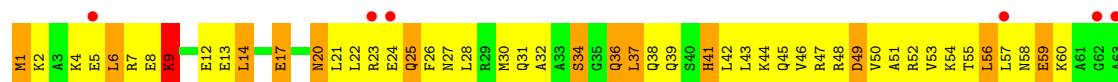
• Molecule 38: 50S ribosomal protein L16



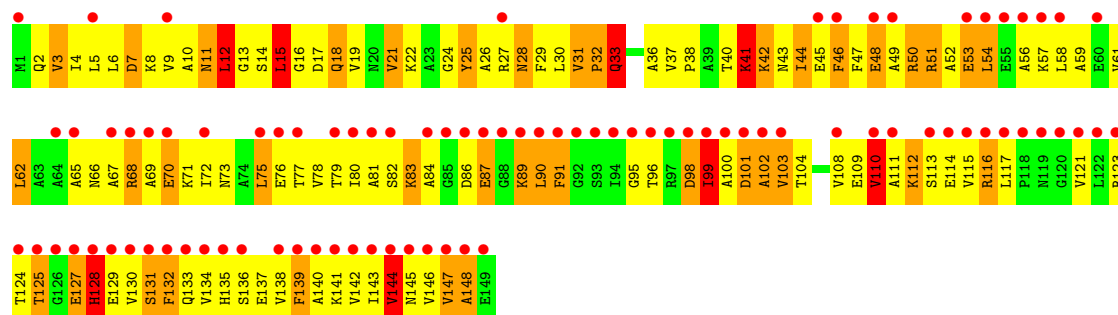
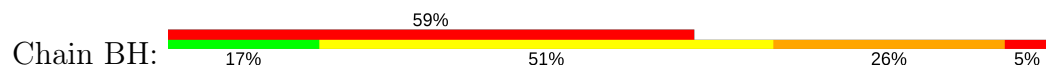
• Molecule 39: 50S ribosomal protein L29



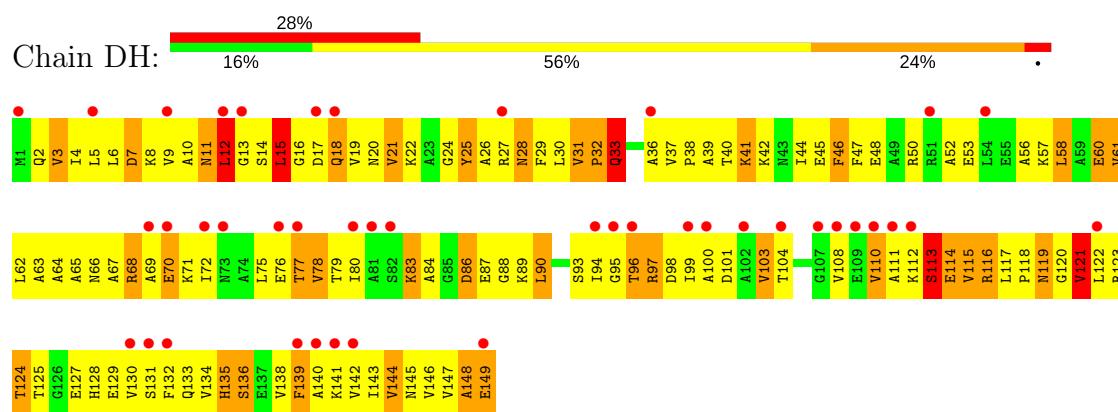
• Molecule 39: 50S ribosomal protein L29



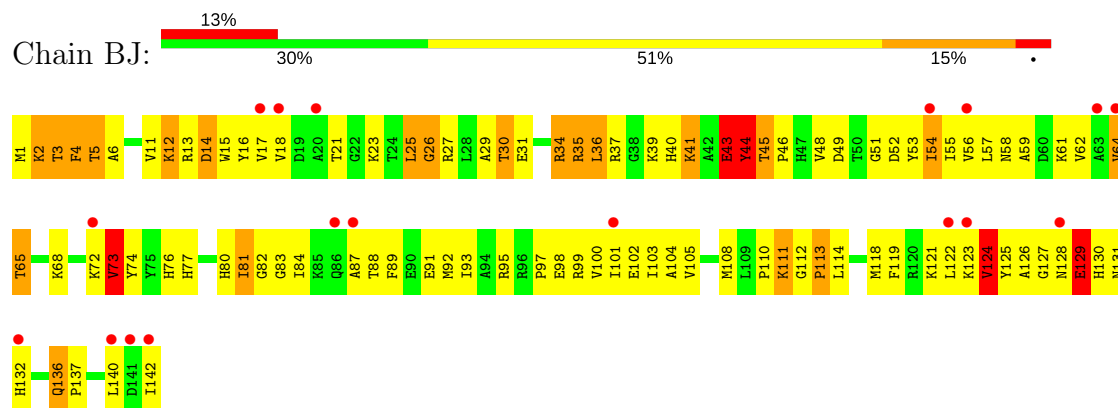
• Molecule 40: 50S ribosomal protein L9



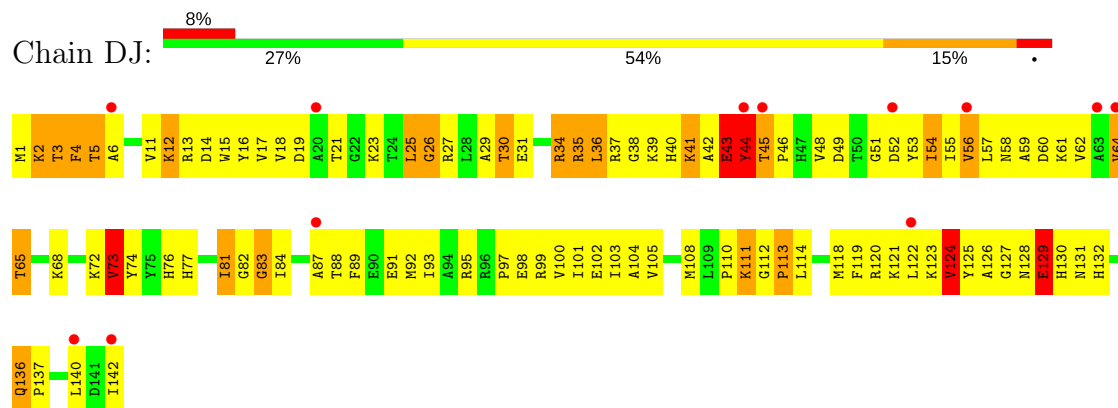
• Molecule 40: 50S ribosomal protein L9



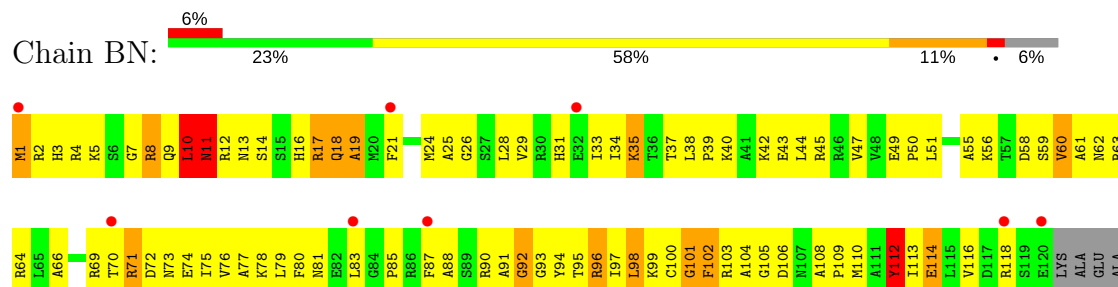
• Molecule 41: 50S ribosomal protein L13



• Molecule 41: 50S ribosomal protein L13



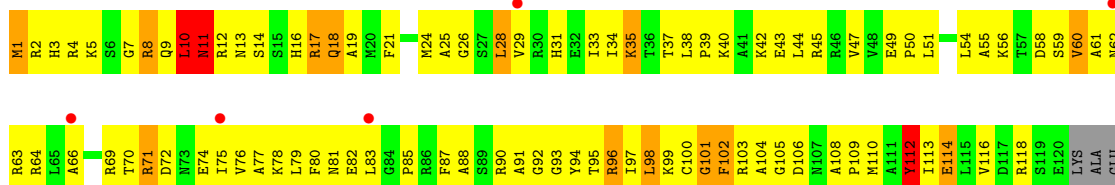
• Molecule 42: 50S ribosomal protein L17



ALA
ALA
GLU

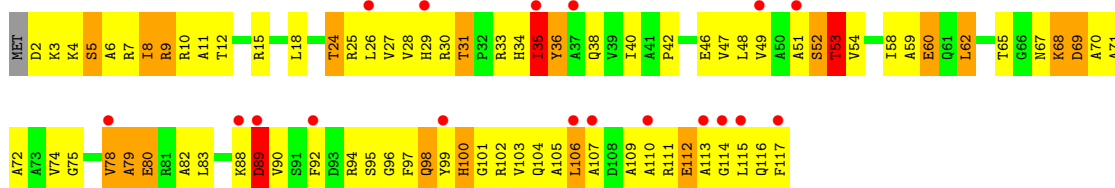
- Molecule 42: 50S ribosomal protein L17

Chain DN: 

ALA
ALA
GLU

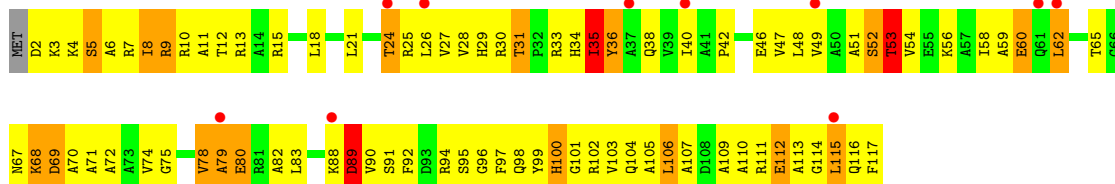
- Molecule 43: 50S ribosomal protein L18

Chain BO: 



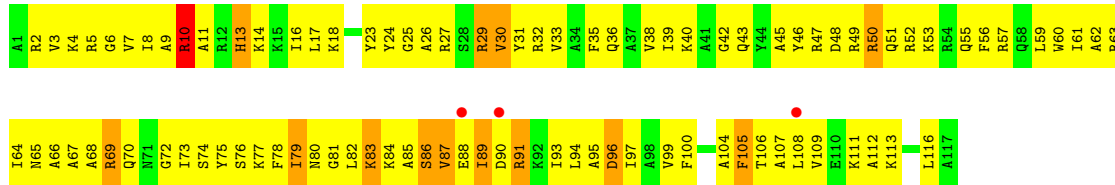
- Molecule 43: 50S ribosomal protein L18

Chain DO: 



- Molecule 44: 50S ribosomal protein L20

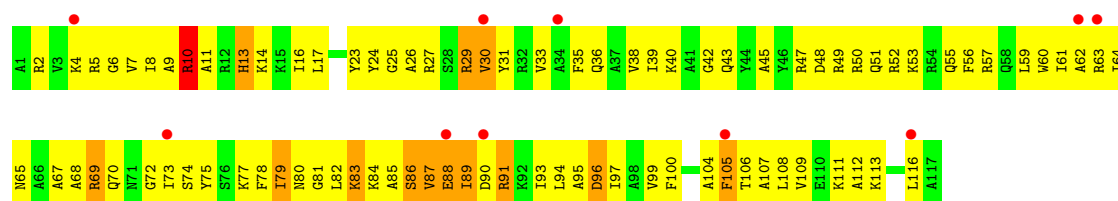
Chain BQ: 



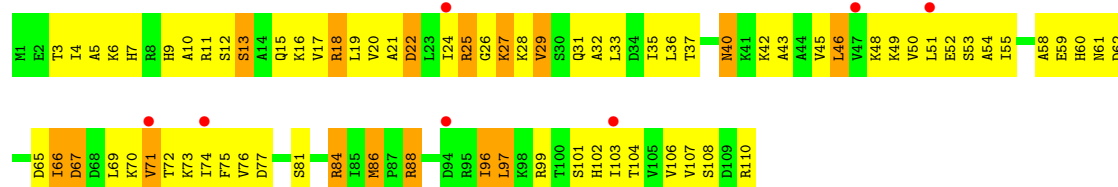
- Molecule 44: 50S ribosomal protein L20

Chain DQ: 

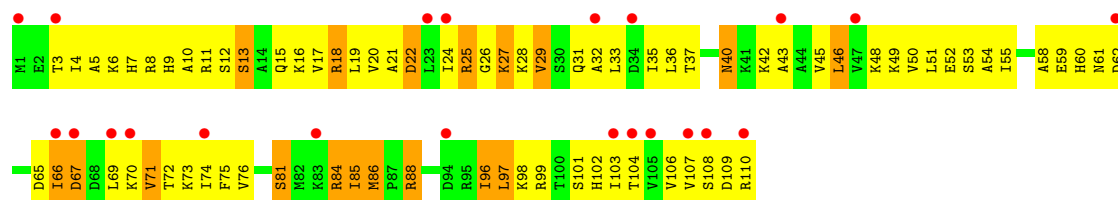




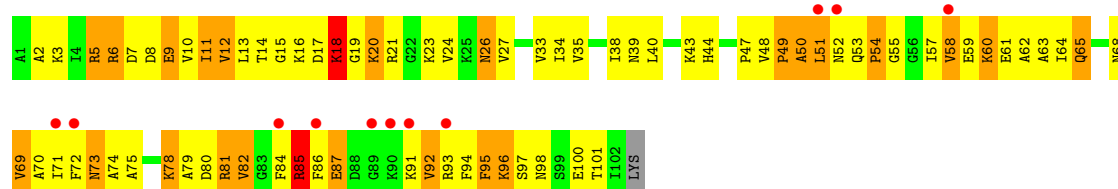
• Molecule 45: 50S ribosomal protein L22



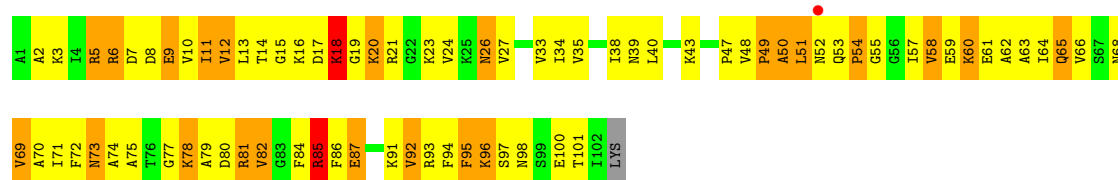
• Molecule 45: 50S ribosomal protein L22



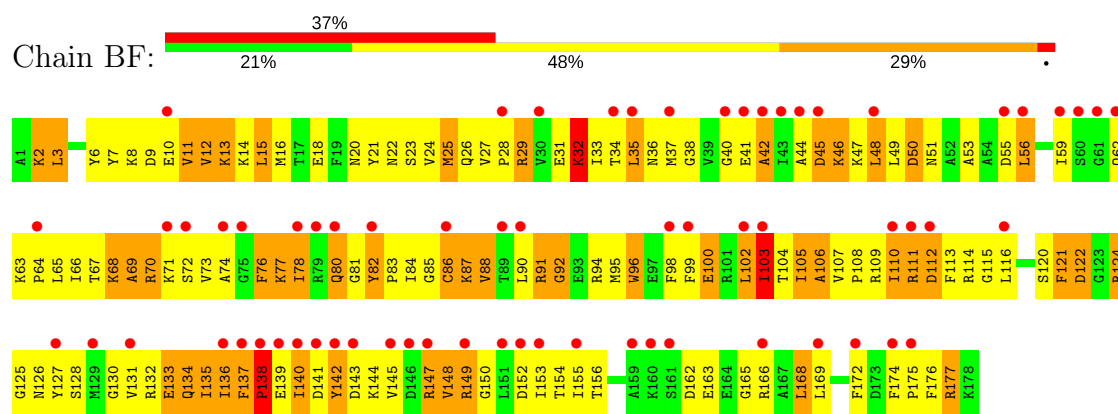
• Molecule 46: 50S ribosomal protein L24



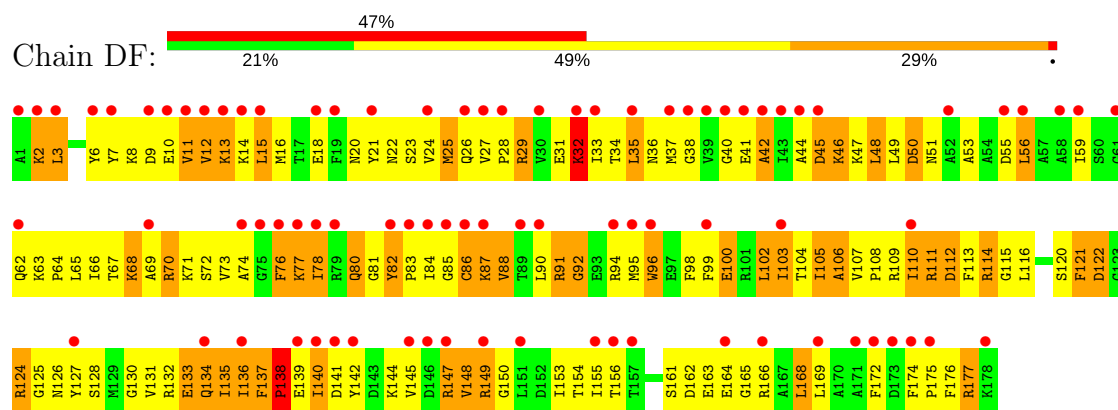
• Molecule 46: 50S ribosomal protein L24



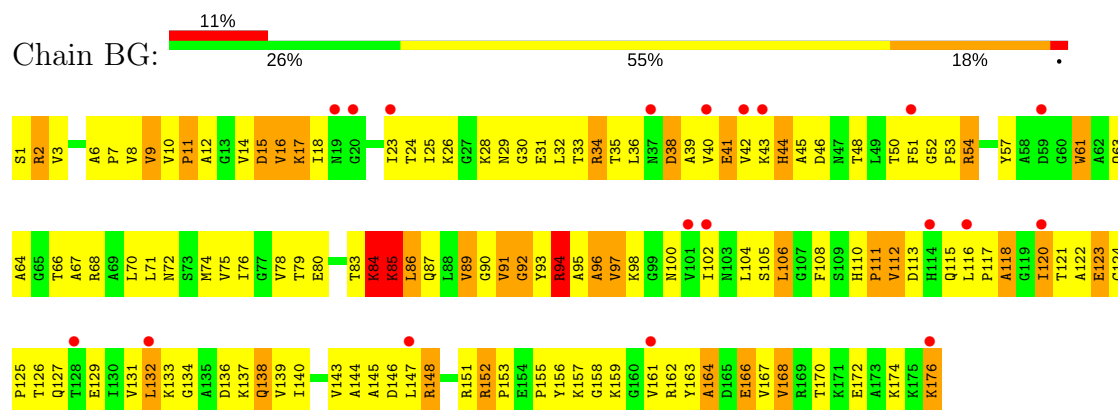
• Molecule 47: 50S ribosomal protein L5



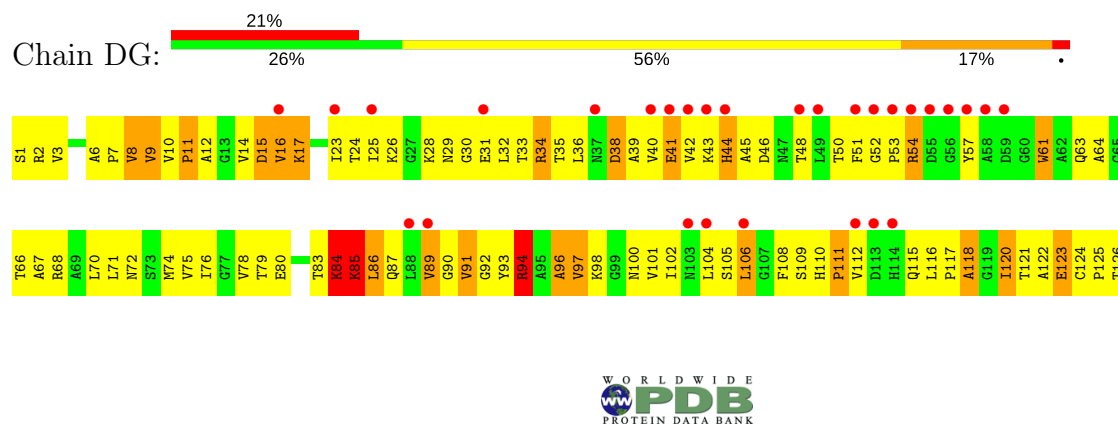
• Molecule 47: 50S ribosomal protein L5

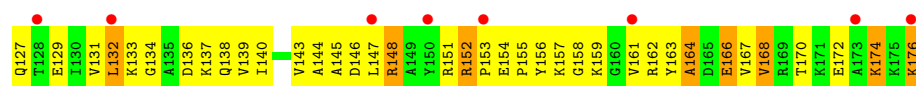


• Molecule 48: 50S ribosomal protein L6



• Molecule 48: 50S ribosomal protein L6

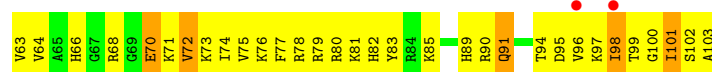
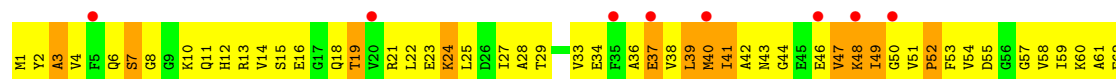




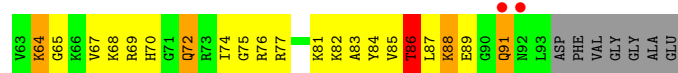
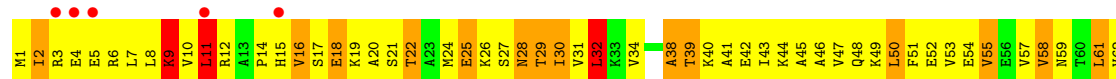
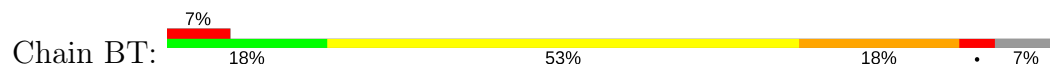
• Molecule 49: 50S ribosomal protein L21



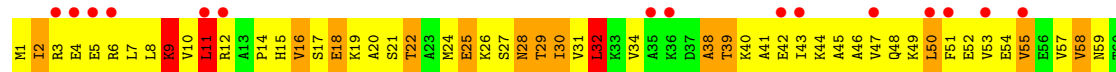
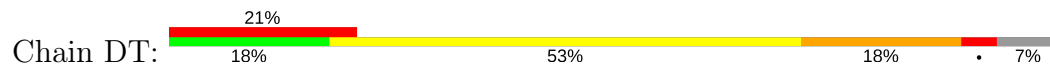
• Molecule 49: 50S ribosomal protein L21



• Molecule 50: 50S ribosomal protein L23

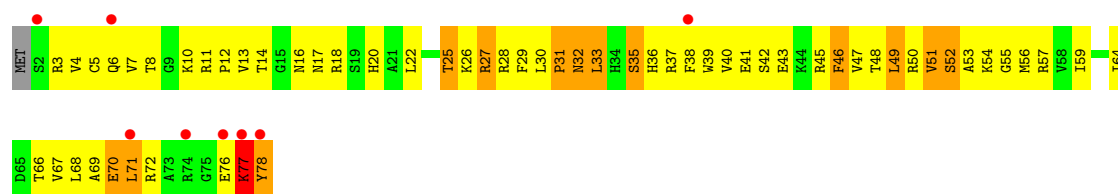


• Molecule 50: 50S ribosomal protein L23

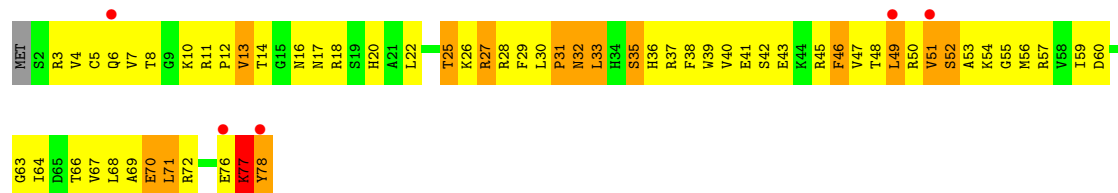


• Molecule 51: 50S ribosomal protein L28

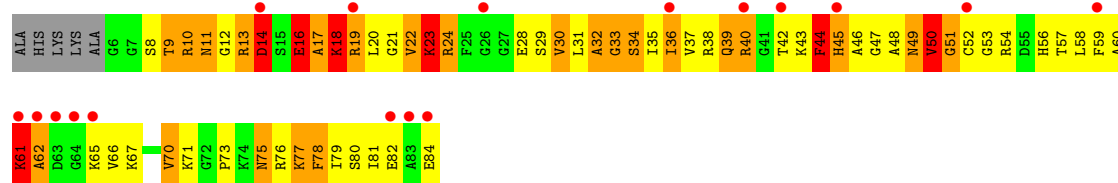
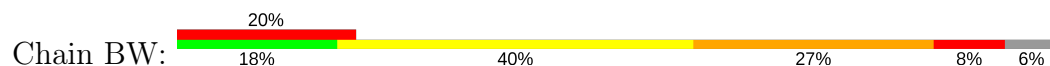




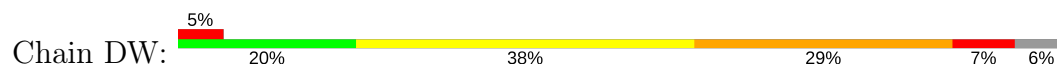
• Molecule 51: 50S ribosomal protein L28



• Molecule 52: 50S ribosomal protein L27



• Molecule 52: 50S ribosomal protein L27



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.50 182.94 – 3.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.50) 73.0 (182.94-3.53)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.306 0.232 , 0.271	Depositor DCC
R_{free} test set	25277 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	132.6	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 79.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284201	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% 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: SCM, ZN, MG, NMY

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	0.26	1/36762 (0.0%)	0.75	9/57350 (0.0%)
1	CA	0.32	2/36762 (0.0%)	0.77	8/57350 (0.0%)
2	AC	0.23	0/1651	0.45	0/2225
2	CC	0.23	0/1651	0.46	0/2225
3	AD	0.23	0/1665	0.43	0/2227
3	CD	0.23	0/1665	0.43	0/2227
4	AE	0.23	0/1118	0.46	0/1504
4	CE	0.23	0/1118	0.46	0/1504
5	AF	0.24	0/835	0.44	0/1128
5	CF	0.24	0/835	0.44	0/1128
6	AG	0.23	0/1187	0.44	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.45	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.44	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.23	0/796	0.47	0/1077
10	AK	0.24	0/893	0.45	0/1205
10	CK	0.24	0/893	0.45	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AP	0.25	0/659	0.46	0/884
13	CP	0.25	0/648	0.46	0/870
14	AQ	0.24	0/657	0.46	0/881
14	CQ	0.24	0/666	0.46	0/892
15	AR	0.23	0/462	0.44	0/621
15	CR	0.23	0/462	0.45	0/621
16	AS	0.25	0/652	0.45	0/877
16	CS	0.25	0/660	0.49	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.24	0/671	0.40	0/888
17	CT	0.23	0/671	0.40	0/888
18	AB	0.25	0/1735	0.44	0/2338
18	CB	0.25	0/1735	0.45	0/2338
19	AU	0.26	0/430	0.46	0/570
19	CU	0.26	0/430	0.46	0/570
20	AO	0.23	0/722	0.44	0/964
20	CO	0.23	0/722	0.43	0/964
21	AN	0.24	0/785	0.43	0/1043
21	CN	0.24	0/785	0.45	0/1043
22	BA	0.25	0/2803	0.75	0/4371
22	DA	0.25	0/2803	0.74	0/4371
23	BB	0.28	6/68314 (0.0%)	0.77	42/106569 (0.0%)
23	DB	0.28	6/68314 (0.0%)	0.77	41/106569 (0.0%)
24	BI	0.24	0/1046	0.46	0/1410
24	DI	0.25	0/1046	0.47	0/1410
25	BC	0.22	0/2121	0.47	0/2852
25	DC	0.22	0/2121	0.47	0/2852
26	BD	0.24	0/1586	0.47	0/2134
26	DD	0.24	0/1586	0.47	0/2134
27	BK	0.23	0/939	0.52	0/1258
27	DK	0.23	0/939	0.52	0/1258
28	BP	0.24	0/929	0.49	0/1242
28	DP	0.24	0/929	0.49	0/1242
29	BE	0.24	0/1571	0.49	0/2113
29	DE	0.24	0/1571	0.49	0/2113
30	BY	0.24	0/453	0.48	0/605
30	DY	0.24	0/453	0.48	0/605
31	B0	0.22	0/450	0.51	0/599
31	D0	0.22	0/450	0.51	0/599
32	B4	0.23	0/303	0.44	0/397
32	D4	0.23	0/303	0.44	0/397
33	B1	0.27	0/416	0.47	0/554
33	D1	0.27	0/416	0.47	0/554
34	B3	0.24	0/513	0.47	0/676
34	D3	0.24	0/513	0.47	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.26	0/380	0.47	0/498
36	D2	0.26	0/380	0.47	0/498
37	BL	0.23	0/1054	0.47	0/1403
37	DL	0.23	0/1054	0.47	0/1403
38	BM	0.25	0/1093	0.47	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.47	0/1460
39	BX	0.24	0/510	0.52	0/677
39	DX	0.24	0/510	0.52	0/677
40	BH	0.25	0/1122	0.45	0/1515
40	DH	0.25	0/1122	0.46	0/1515
41	BJ	0.23	0/1152	0.47	0/1551
41	DJ	0.23	0/1152	0.47	0/1551
42	BN	0.24	0/973	0.49	0/1301
42	DN	0.24	0/973	0.49	0/1301
43	BO	0.23	0/902	0.47	0/1209
43	DO	0.23	0/902	0.47	0/1209
44	BQ	0.25	0/960	0.46	0/1278
44	DQ	0.25	0/960	0.46	0/1278
45	BS	0.21	0/864	0.50	0/1156
45	DS	0.21	0/864	0.50	0/1156
46	BU	0.25	0/787	0.45	0/1051
46	DU	0.25	0/787	0.45	0/1051
47	BF	0.25	0/1444	0.50	0/1937
47	DF	0.25	0/1444	0.50	0/1937
48	BG	0.23	0/1343	0.46	0/1816
48	DG	0.23	0/1343	0.46	0/1816
49	BR	0.25	0/829	0.46	0/1107
49	DR	0.25	0/829	0.46	0/1107
50	BT	0.22	0/744	0.51	0/994
50	DT	0.22	0/744	0.51	0/994
51	BZ	0.25	0/635	0.48	0/848
51	DZ	0.25	0/635	0.48	0/848
52	BW	0.28	0/603	0.48	0/797
52	DW	0.27	0/603	0.48	0/797
All	All	0.27	15/306360 (0.0%)	0.70	100/457969 (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
1	AA	0	13
1	CA	0	20
23	BB	0	44
23	DB	0	43
All	All	0	120

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-15.92	1.26	1.41
23	DB	1086	A	C5-C6	-15.80	1.26	1.41
23	BB	1088	A	C6-N1	-10.61	1.28	1.35
23	DB	1088	A	C6-N1	-10.48	1.28	1.35
23	DB	1060	U	C2-N3	7.81	1.43	1.37

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-29.68	75.09	110.70
23	BB	2204	G	O5'-P-OP2	-28.72	76.23	110.70
23	DB	2791	G	O5'-P-OP2	-27.53	77.67	110.70
23	BB	2791	G	O5'-P-OP1	-27.53	77.67	110.70
23	DB	2791	G	O5'-P-OP1	17.94	132.23	110.70

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	437	U	Sidechain
1	AA	438	U	Sidechain
1	AA	86	G	Sidechain

5.2 Too-close contacts [i](#)

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	32831	0	16521	1291	0
1	CA	32831	0	16521	1302	0
2	AC	1624	0	1699	189	0
2	CC	1624	0	1699	189	0
3	AD	1643	0	1710	127	0
3	CD	1643	0	1710	128	0
4	AE	1105	0	1148	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CE	1105	0	1148	93	0
5	AF	817	0	808	95	0
5	CF	817	0	808	91	0
6	AG	1174	0	1230	150	0
6	CG	1196	0	1246	114	0
7	AH	979	0	1034	68	0
7	CH	979	0	1034	70	0
8	AI	1022	0	1070	146	0
8	CI	1022	0	1070	136	0
9	AJ	786	0	828	100	0
9	CJ	786	0	828	98	0
10	AK	877	0	887	108	0
10	CK	877	0	887	97	0
11	AL	955	0	1019	96	0
11	CL	955	0	1019	97	0
12	AM	883	0	944	160	0
12	CM	876	0	937	116	0
13	AP	649	0	666	58	0
13	CP	638	0	656	50	0
14	AQ	648	0	691	63	0
14	CQ	657	0	702	59	0
15	AR	455	0	478	40	0
15	CR	455	0	478	43	0
16	AS	637	0	665	107	0
16	CS	644	0	675	106	0
17	AT	665	0	714	60	0
17	CT	665	0	714	64	0
18	AB	1704	0	1732	193	0
18	CB	1704	0	1732	210	0
19	AU	425	0	449	74	0
19	CU	425	0	449	67	0
20	AO	714	0	734	65	0
20	CO	714	0	734	50	0
21	AN	774	0	827	109	0
21	CN	774	0	827	113	0
22	BA	2507	0	1270	104	0
22	DA	2507	0	1270	107	0
23	BB	60995	0	30679	2216	0
23	DB	60995	0	30678	2313	0
24	BI	1032	0	1088	112	0
24	DI	1032	0	1088	176	0
25	BC	2082	0	2157	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DC	2082	0	2157	218	0
26	BD	1565	0	1616	206	0
26	DD	1565	0	1616	207	0
27	BK	930	0	1000	130	0
27	DK	930	0	1000	138	0
28	BP	917	0	965	115	0
28	DP	917	0	965	118	0
29	BE	1552	0	1619	199	0
29	DE	1552	0	1619	183	0
30	BY	449	0	491	58	0
30	DY	449	0	491	57	0
31	B0	444	0	461	35	0
31	D0	444	0	461	40	0
32	B4	302	0	340	42	0
32	D4	302	0	340	39	0
33	B1	409	0	440	34	0
33	D1	409	0	440	38	0
34	B3	504	0	574	50	0
34	D3	504	0	574	44	0
35	BV	753	0	780	102	0
35	DV	753	0	780	100	0
36	B2	377	0	418	48	0
36	D2	377	0	418	45	0
37	BL	1045	0	1117	139	0
37	DL	1045	0	1117	153	0
38	BM	1074	0	1157	116	0
38	DM	1074	0	1157	115	0
39	BX	509	0	543	63	0
39	DX	509	0	543	67	0
40	BH	1111	0	1148	193	0
40	DH	1111	0	1148	179	0
41	BJ	1129	0	1162	130	0
41	DJ	1129	0	1162	127	0
42	BN	960	0	1000	115	0
42	DN	960	0	1000	114	0
43	BO	892	0	923	93	0
43	DO	892	0	923	102	0
44	BQ	947	0	1022	143	0
44	DQ	947	0	1022	143	0
45	BS	857	0	922	86	0
45	DS	857	0	922	92	0
46	BU	779	0	834	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DU	779	0	834	111	0
47	BF	1420	0	1460	223	0
47	DF	1420	0	1460	216	0
48	BG	1323	0	1374	188	0
48	DG	1323	0	1374	178	0
49	BR	816	0	839	110	0
49	DR	816	0	839	105	0
50	BT	738	0	807	107	0
50	DT	738	0	807	116	0
51	BZ	625	0	652	68	0
51	DZ	625	0	652	67	0
52	BW	596	0	610	134	0
52	DW	596	0	610	127	0
53	AA	42	0	46	0	0
53	BB	42	0	46	0	0
53	CA	42	0	46	0	0
53	DB	42	0	46	1	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	59	0	0	0	0
54	DB	111	0	0	0	0
55	AA	23	0	24	5	0
55	CA	23	0	24	1	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	290	0	0	2	0
57	AE	1	0	0	0	0
57	AK	1	0	0	0	0
57	AL	4	0	0	0	0
57	AN	1	0	0	0	0
57	AP	1	0	0	0	0
57	AT	2	0	0	0	0
57	BB	492	0	0	4	0
57	BC	7	0	0	0	0
57	BD	1	0	0	0	0
57	BE	4	0	0	0	0
57	BH	1	0	0	0	0
57	BL	2	0	0	0	0
57	CA	282	0	0	2	0
57	CE	2	0	0	0	0
57	CI	1	0	0	0	0
57	CL	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CN	3	0	0	0	0
57	CP	1	0	0	0	0
57	CT	1	0	0	0	0
57	DB	501	0	0	14	0
57	DC	4	0	0	0	0
57	DD	1	0	0	0	0
57	DE	2	0	0	0	0
57	DL	1	0	0	0	0
57	DN	2	0	0	0	0
57	DR	1	0	0	0	0
All	All	284201	0	190895	16740	0

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 35.

The worst 5 of 16740 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)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.32	1.27
23:BB:2305:U:H1'	47:BF:132:ARG:HA	1.33	1.10
40:BH:125:THR:HA	40:BH:146:VAL:HB	1.28	1.10
18:CB:69:VAL:HG23	18:CB:162:VAL:HB	1.34	1.09
23:DB:1098:A:H3'	24:DI:3:LYS:HA	1.32	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AC	204/232 (88%)	130 (64%)	44 (22%)	30 (15%)	0 3
2	CC	204/232 (88%)	137 (67%)	49 (24%)	18 (9%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	153 (75%)	40 (20%)	10 (5%)	2	24
3	CD	203/205 (99%)	153 (75%)	40 (20%)	10 (5%)	2	24
4	AE	148/166 (89%)	116 (78%)	24 (16%)	8 (5%)	2	22
4	CE	148/166 (89%)	114 (77%)	25 (17%)	9 (6%)	2	19
5	AF	98/135 (73%)	63 (64%)	25 (26%)	10 (10%)	1	8
5	CF	98/135 (73%)	64 (65%)	24 (24%)	10 (10%)	1	8
6	AG	148/178 (83%)	110 (74%)	30 (20%)	8 (5%)	2	22
6	CG	150/178 (84%)	111 (74%)	28 (19%)	11 (7%)	1	14
7	AH	127/129 (98%)	92 (72%)	31 (24%)	4 (3%)	5	37
7	CH	127/129 (98%)	92 (72%)	31 (24%)	4 (3%)	5	37
8	AI	125/129 (97%)	80 (64%)	35 (28%)	10 (8%)	1	12
8	CI	125/129 (97%)	80 (64%)	34 (27%)	11 (9%)	1	10
9	AJ	96/103 (93%)	59 (62%)	25 (26%)	12 (12%)	0	5
9	CJ	96/103 (93%)	64 (67%)	22 (23%)	10 (10%)	0	7
10	AK	115/128 (90%)	87 (76%)	23 (20%)	5 (4%)	3	28
10	CK	115/128 (90%)	86 (75%)	24 (21%)	5 (4%)	3	28
11	AL	121/123 (98%)	69 (57%)	37 (31%)	15 (12%)	0	5
11	CL	121/123 (98%)	72 (60%)	34 (28%)	15 (12%)	0	5
12	AM	112/117 (96%)	74 (66%)	25 (22%)	13 (12%)	0	6
12	CM	111/117 (95%)	78 (70%)	21 (19%)	12 (11%)	0	7
13	AP	80/82 (98%)	53 (66%)	20 (25%)	7 (9%)	1	10
13	CP	78/82 (95%)	52 (67%)	19 (24%)	7 (9%)	1	10
14	AQ	78/83 (94%)	59 (76%)	15 (19%)	4 (5%)	2	23
14	CQ	79/83 (95%)	57 (72%)	18 (23%)	4 (5%)	2	23
15	AR	53/74 (72%)	40 (76%)	13 (24%)	0	100	100
15	CR	53/74 (72%)	41 (77%)	11 (21%)	1 (2%)	9	47
16	AS	77/91 (85%)	49 (64%)	24 (31%)	4 (5%)	2	23
16	CS	78/91 (86%)	57 (73%)	16 (20%)	5 (6%)	1	18
17	AT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	2	19
17	CT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	2	19
18	AB	216/240 (90%)	135 (62%)	56 (26%)	25 (12%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CB	216/240 (90%)	145 (67%)	52 (24%)	19 (9%)	1	10
19	AU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	0	5
19	CU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	0	5
20	AO	86/89 (97%)	62 (72%)	18 (21%)	6 (7%)	1	15
20	CO	86/89 (97%)	60 (70%)	25 (29%)	1 (1%)	15	57
21	AN	92/100 (92%)	53 (58%)	30 (33%)	9 (10%)	1	9
21	CN	92/100 (92%)	49 (53%)	31 (34%)	12 (13%)	0	5
24	BI	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	5	38
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	4	33
25	BC	269/272 (99%)	163 (61%)	63 (23%)	43 (16%)	0	3
25	DC	269/272 (99%)	162 (60%)	61 (23%)	46 (17%)	0	2
26	BD	207/209 (99%)	118 (57%)	57 (28%)	32 (16%)	0	3
26	DD	207/209 (99%)	118 (57%)	58 (28%)	31 (15%)	0	3
27	BK	119/123 (97%)	70 (59%)	27 (23%)	22 (18%)	0	2
27	DK	119/123 (97%)	69 (58%)	29 (24%)	21 (18%)	0	2
28	BP	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	3
28	DP	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	3
29	BE	199/201 (99%)	124 (62%)	51 (26%)	24 (12%)	0	5
29	DE	199/201 (99%)	124 (62%)	48 (24%)	27 (14%)	0	4
30	BY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	10
30	DY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	10
31	B0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	0	6
31	D0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	0	6
32	B4	36/38 (95%)	20 (56%)	9 (25%)	7 (19%)	0	1
32	D4	36/38 (95%)	21 (58%)	8 (22%)	7 (19%)	0	1
33	B1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	11
33	D1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	11
34	B3	62/64 (97%)	39 (63%)	17 (27%)	6 (10%)	1	9
34	D3	62/64 (97%)	39 (63%)	18 (29%)	5 (8%)	1	12
35	BV	92/94 (98%)	60 (65%)	22 (24%)	10 (11%)	0	7
35	DV	92/94 (98%)	59 (64%)	23 (25%)	10 (11%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	B2	44/46 (96%)	25 (57%)	16 (36%)	3 (7%)	1	17
36	D2	44/46 (96%)	24 (54%)	16 (36%)	4 (9%)	1	9
37	BL	141/144 (98%)	78 (55%)	44 (31%)	19 (14%)	0	4
37	DL	141/144 (98%)	78 (55%)	42 (30%)	21 (15%)	0	3
38	BM	134/136 (98%)	90 (67%)	28 (21%)	16 (12%)	0	6
38	DM	134/136 (98%)	91 (68%)	26 (19%)	17 (13%)	0	5
39	BX	61/63 (97%)	35 (57%)	22 (36%)	4 (7%)	1	17
39	DX	61/63 (97%)	35 (57%)	22 (36%)	4 (7%)	1	17
40	BH	147/149 (99%)	74 (50%)	42 (29%)	31 (21%)	0	1
40	DH	147/149 (99%)	86 (58%)	38 (26%)	23 (16%)	0	3
41	BJ	140/142 (99%)	88 (63%)	33 (24%)	19 (14%)	0	4
41	DJ	140/142 (99%)	88 (63%)	32 (23%)	20 (14%)	0	3
42	BN	118/127 (93%)	74 (63%)	31 (26%)	13 (11%)	0	7
42	DN	118/127 (93%)	74 (63%)	32 (27%)	12 (10%)	1	8
43	BO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	12
43	DO	114/117 (97%)	79 (69%)	25 (22%)	10 (9%)	1	10
44	BQ	115/117 (98%)	76 (66%)	32 (28%)	7 (6%)	2	19
44	DQ	115/117 (98%)	75 (65%)	33 (29%)	7 (6%)	2	19
45	BS	108/110 (98%)	67 (62%)	28 (26%)	13 (12%)	0	6
45	DS	108/110 (98%)	67 (62%)	28 (26%)	13 (12%)	0	6
46	BU	100/103 (97%)	50 (50%)	35 (35%)	15 (15%)	0	3
46	DU	100/103 (97%)	54 (54%)	31 (31%)	15 (15%)	0	3
47	BF	176/178 (99%)	102 (58%)	48 (27%)	26 (15%)	0	3
47	DF	176/178 (99%)	102 (58%)	48 (27%)	26 (15%)	0	3
48	BG	174/176 (99%)	111 (64%)	40 (23%)	23 (13%)	0	4
48	DG	174/176 (99%)	110 (63%)	40 (23%)	24 (14%)	0	4
49	BR	101/103 (98%)	59 (58%)	31 (31%)	11 (11%)	0	7
49	DR	101/103 (98%)	59 (58%)	31 (31%)	11 (11%)	0	7
50	BT	91/100 (91%)	49 (54%)	25 (28%)	17 (19%)	0	2
50	DT	91/100 (91%)	47 (52%)	27 (30%)	17 (19%)	0	2
51	BZ	75/78 (96%)	50 (67%)	17 (23%)	8 (11%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DZ	75/78 (96%)	48 (64%)	19 (25%)	8 (11%)	0	7
52	BW	77/84 (92%)	26 (34%)	26 (34%)	25 (32%)	0	0
52	DW	77/84 (92%)	26 (34%)	25 (32%)	26 (34%)	0	0
All	All	11241/11914 (94%)	7227 (64%)	2767 (25%)	1247 (11%)	0	6

5 of 1247 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	11	LEU
2	AC	14	VAL
2	AC	25	THR
2	AC	54	ILE
2	AC	83	VAL

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	AC	170/189 (90%)	137 (81%)	33 (19%)	1	8
2	CC	170/189 (90%)	139 (82%)	31 (18%)	2	11
3	AD	172/172 (100%)	153 (89%)	19 (11%)	7	33
3	CD	172/172 (100%)	154 (90%)	18 (10%)	8	35
4	AE	113/125 (90%)	90 (80%)	23 (20%)	1	7
4	CE	113/125 (90%)	91 (80%)	22 (20%)	1	8
5	AF	87/116 (75%)	75 (86%)	12 (14%)	4	23
5	CF	87/116 (75%)	74 (85%)	13 (15%)	3	20
6	AG	123/146 (84%)	104 (85%)	19 (15%)	3	18
6	CG	125/146 (86%)	102 (82%)	23 (18%)	2	10
7	AH	104/104 (100%)	96 (92%)	8 (8%)	15	50
7	CH	104/104 (100%)	97 (93%)	7 (7%)	19	57
8	AI	105/106 (99%)	88 (84%)	17 (16%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	77 (73%)	28 (27%)	0	3
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	4	22
9	CJ	86/90 (96%)	75 (87%)	11 (13%)	5	25
10	AK	90/98 (92%)	77 (86%)	13 (14%)	4	21
10	CK	90/98 (92%)	76 (84%)	14 (16%)	3	18
11	AL	103/103 (100%)	84 (82%)	19 (18%)	2	10
11	CL	103/103 (100%)	84 (82%)	19 (18%)	2	10
12	AM	92/95 (97%)	79 (86%)	13 (14%)	4	22
12	CM	91/95 (96%)	70 (77%)	21 (23%)	1	5
13	AP	65/65 (100%)	56 (86%)	9 (14%)	4	23
13	CP	65/65 (100%)	56 (86%)	9 (14%)	4	23
14	AQ	74/77 (96%)	65 (88%)	9 (12%)	6	27
14	CQ	75/77 (97%)	66 (88%)	9 (12%)	6	28
15	AR	48/64 (75%)	42 (88%)	6 (12%)	5	26
15	CR	48/64 (75%)	42 (88%)	6 (12%)	5	26
16	AS	70/78 (90%)	48 (69%)	22 (31%)	0	2
16	CS	71/78 (91%)	53 (75%)	18 (25%)	0	4
17	AT	65/65 (100%)	56 (86%)	9 (14%)	4	23
17	CT	65/65 (100%)	56 (86%)	9 (14%)	4	23
18	AB	180/198 (91%)	149 (83%)	31 (17%)	2	13
18	CB	180/198 (91%)	141 (78%)	39 (22%)	1	6
19	AU	44/60 (73%)	33 (75%)	11 (25%)	1	4
19	CU	44/60 (73%)	33 (75%)	11 (25%)	1	4
20	AO	76/77 (99%)	69 (91%)	7 (9%)	11	41
20	CO	76/77 (99%)	64 (84%)	12 (16%)	3	17
21	AN	79/83 (95%)	69 (87%)	10 (13%)	5	25
21	CN	79/83 (95%)	64 (81%)	15 (19%)	2	9
24	BI	109/109 (100%)	108 (99%)	1 (1%)	82	93
24	DI	109/109 (100%)	103 (94%)	6 (6%)	25	62
25	BC	216/217 (100%)	184 (85%)	32 (15%)	3	20
25	DC	216/217 (100%)	184 (85%)	32 (15%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	136 (83%)	28 (17%)	2	14
26	DD	164/164 (100%)	136 (83%)	28 (17%)	2	14
27	BK	102/104 (98%)	74 (72%)	28 (28%)	0	3
27	DK	102/104 (98%)	73 (72%)	29 (28%)	0	3
28	BP	99/99 (100%)	83 (84%)	16 (16%)	3	16
28	DP	99/99 (100%)	83 (84%)	16 (16%)	3	16
29	BE	165/165 (100%)	146 (88%)	19 (12%)	6	30
29	DE	165/165 (100%)	145 (88%)	20 (12%)	6	27
30	BY	48/48 (100%)	38 (79%)	10 (21%)	1	7
30	DY	48/48 (100%)	37 (77%)	11 (23%)	1	5
31	B0	47/47 (100%)	38 (81%)	9 (19%)	2	9
31	D0	47/47 (100%)	38 (81%)	9 (19%)	2	9
32	B4	34/34 (100%)	31 (91%)	3 (9%)	12	43
32	D4	34/34 (100%)	31 (91%)	3 (9%)	12	43
33	B1	45/48 (94%)	35 (78%)	10 (22%)	1	6
33	D1	45/48 (94%)	35 (78%)	10 (22%)	1	6
34	B3	51/51 (100%)	48 (94%)	3 (6%)	23	61
34	D3	51/51 (100%)	48 (94%)	3 (6%)	23	61
35	BV	78/78 (100%)	65 (83%)	13 (17%)	2	14
35	DV	78/78 (100%)	65 (83%)	13 (17%)	2	14
36	B2	38/38 (100%)	28 (74%)	10 (26%)	0	3
36	D2	38/38 (100%)	28 (74%)	10 (26%)	0	3
37	BL	102/103 (99%)	85 (83%)	17 (17%)	2	14
37	DL	102/103 (99%)	85 (83%)	17 (17%)	2	14
38	BM	109/109 (100%)	93 (85%)	16 (15%)	3	20
38	DM	109/109 (100%)	93 (85%)	16 (15%)	3	20
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	6
39	DX	55/55 (100%)	43 (78%)	12 (22%)	1	6
40	BH	114/114 (100%)	83 (73%)	31 (27%)	0	3
40	DH	114/114 (100%)	87 (76%)	27 (24%)	1	4
41	BJ	116/116 (100%)	100 (86%)	16 (14%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DJ	116/116 (100%)	100 (86%)	16 (14%)	4	23
42	BN	100/103 (97%)	86 (86%)	14 (14%)	4	22
42	DN	100/103 (97%)	85 (85%)	15 (15%)	3	19
43	BO	86/87 (99%)	68 (79%)	18 (21%)	1	7
43	DO	86/87 (99%)	67 (78%)	19 (22%)	1	6
44	BQ	89/89 (100%)	77 (86%)	12 (14%)	4	24
44	DQ	89/89 (100%)	77 (86%)	12 (14%)	4	24
45	BS	93/93 (100%)	85 (91%)	8 (9%)	12	45
45	DS	93/93 (100%)	83 (89%)	10 (11%)	7	34
46	BU	83/84 (99%)	68 (82%)	15 (18%)	2	11
46	DU	83/84 (99%)	68 (82%)	15 (18%)	2	11
47	BF	149/149 (100%)	111 (74%)	38 (26%)	0	4
47	DF	149/149 (100%)	112 (75%)	37 (25%)	1	4
48	BG	137/137 (100%)	114 (83%)	23 (17%)	2	14
48	DG	137/137 (100%)	113 (82%)	24 (18%)	2	13
49	BR	84/84 (100%)	71 (84%)	13 (16%)	3	18
49	DR	84/84 (100%)	72 (86%)	12 (14%)	4	22
50	BT	80/84 (95%)	66 (82%)	14 (18%)	2	13
50	DT	80/84 (95%)	66 (82%)	14 (18%)	2	13
51	BZ	67/68 (98%)	57 (85%)	10 (15%)	3	20
51	DZ	67/68 (98%)	56 (84%)	11 (16%)	2	15
52	BW	59/62 (95%)	44 (75%)	15 (25%)	0	4
52	DW	59/62 (95%)	44 (75%)	15 (25%)	0	4
All	All	9333/9700 (96%)	7780 (83%)	1553 (17%)	2	15

5 of 1553 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BG	174	LYS
15	CR	38	ILE
46	DU	78	LYS
50	BT	25	GLU
4	CE	115	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 349 such sidechains are listed below:

Mol	Chain	Res	Type
48	BG	127	GLN
10	CK	21	HIS
46	DU	26	ASN
49	BR	86	GLN
3	CD	70	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	285 (18%)	0
1	CA	1529/1542 (99%)	255 (16%)	0
22	BA	116/120 (96%)	21 (18%)	0
22	DA	116/120 (96%)	20 (17%)	0
23	BB	2837/2904 (97%)	444 (15%)	0
23	DB	2837/2904 (97%)	437 (15%)	0
All	All	8964/9132 (98%)	1462 (16%)	0

5 of 1462 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	15	G
1	AA	32	A
1	AA	39	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 348 ligands modelled in this entry, 342 are monoatomic - leaving 6 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$
53	NMY	AA	1601	-	45,45,45	1.96	13 (28%)	59,67,67	1.18	6 (10%)
55	SCM	AA	1662	-	22,25,25	1.67	7 (31%)	25,39,39	0.91	2 (8%)
53	NMY	BB	3001	-	45,45,45	1.89	13 (28%)	59,67,67	1.24	7 (11%)
53	NMY	CA	1601	-	45,45,45	1.88	13 (28%)	59,67,67	1.21	6 (10%)
55	SCM	CA	1661	-	22,25,25	1.69	8 (36%)	25,39,39	0.92	2 (8%)
53	NMY	DB	3001	-	45,45,45	1.92	13 (28%)	59,67,67	1.26	6 (10%)

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
53	NMY	AA	1601	-	-	0/18/94/94	0/4/4/4
55	SCM	AA	1662	-	-	0/4/57/57	0/3/3/3
53	NMY	BB	3001	-	-	0/18/94/94	0/4/4/4
53	NMY	CA	1601	-	-	0/18/94/94	0/4/4/4
55	SCM	CA	1661	-	-	0/4/57/57	0/3/3/3
53	NMY	DB	3001	-	-	0/18/94/94	0/4/4/4

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	CA	1661	SCM	C10-N10	-2.00	1.44	1.47
53	DB	3001	NMY	C6-C5	2.01	1.57	1.51
53	CA	1601	NMY	C6-C5	2.03	1.57	1.51
53	AA	1601	NMY	C6-C5	2.05	1.57	1.51
53	BB	3001	NMY	O18-C15	2.07	1.48	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	CA	1661	SCM	C2M-C2-C3	-2.62	108.15	113.27
55	AA	1662	SCM	C2M-C2-C3	-2.55	108.28	113.27
55	AA	1662	SCM	C6-O1-C2	-2.07	105.54	112.06
55	CA	1661	SCM	C6-O1-C2	-2.03	105.64	112.06
53	CA	1601	NMY	O11-C13-C14	2.05	112.21	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	AA	1662	SCM	5	0
55	CA	1661	SCM	1	0
53	DB	3001	NMY	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	1530/1542 (99%)	-0.79	8 (0%)	90 86	16, 81, 159, 180	0
1	CA	1530/1542 (99%)	-0.72	1 (0%)	95 94	9, 57, 133, 180	0
2	AC	206/232 (88%)	0.45	20 (9%)	8 9	9, 76, 136, 180	0
2	CC	206/232 (88%)	0.28	15 (7%)	16 14	7, 75, 127, 180	0
3	AD	205/205 (100%)	0.60	25 (12%)	5 6	24, 92, 157, 180	0
3	CD	205/205 (100%)	0.50	15 (7%)	16 14	10, 64, 139, 180	0
4	AE	150/166 (90%)	0.50	14 (9%)	9 10	11, 74, 139, 176	0
4	CE	150/166 (90%)	0.80	25 (16%)	2 2	5, 61, 132, 180	0
5	AF	100/135 (74%)	1.04	17 (17%)	2 2	11, 86, 144, 172	0
5	CF	100/135 (74%)	0.56	9 (9%)	10 10	7, 83, 173, 180	0
6	AG	150/178 (84%)	0.23	9 (6%)	23 19	23, 104, 153, 180	0
6	CG	152/178 (85%)	-0.04	4 (2%)	56 47	27, 90, 147, 180	0
7	AH	129/129 (100%)	0.91	21 (16%)	2 2	13, 88, 155, 180	0
7	CH	129/129 (100%)	0.57	13 (10%)	8 8	5, 61, 127, 180	0
8	AI	127/129 (98%)	0.45	16 (12%)	4 5	36, 91, 150, 180	0
8	CI	127/129 (98%)	0.07	4 (3%)	49 41	20, 92, 148, 180	0
9	AJ	98/103 (95%)	0.40	4 (4%)	38 31	22, 94, 151, 180	0
9	CJ	98/103 (95%)	0.75	12 (12%)	5 6	17, 89, 156, 180	0
10	AK	117/128 (91%)	0.05	6 (5%)	29 23	14, 67, 125, 180	0
10	CK	117/128 (91%)	0.07	3 (2%)	56 47	5, 56, 125, 178	0
11	AL	123/123 (100%)	0.48	13 (10%)	7 8	19, 80, 133, 180	0
11	CL	123/123 (100%)	0.18	6 (4%)	30 24	7, 51, 135, 180	0
12	AM	114/117 (97%)	0.71	21 (18%)	1 2	56, 120, 166, 180	0
12	CM	113/117 (96%)	0.59	17 (15%)	3 3	38, 109, 165, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	82/82 (100%)	2.16	30 (36%) 0 0	38, 91, 152, 180	0
13	CP	80/82 (97%)	0.50	10 (12%) 4 5	6, 63, 141, 180	0
14	AQ	80/83 (96%)	0.85	12 (15%) 3 3	37, 99, 151, 180	0
14	CQ	81/83 (97%)	0.54	2 (2%) 58 48	17, 71, 129, 180	0
15	AR	55/74 (74%)	0.54	2 (3%) 43 37	16, 76, 149, 180	0
15	CR	55/74 (74%)	0.41	4 (7%) 16 14	21, 66, 126, 180	0
16	AS	79/91 (86%)	1.60	30 (37%) 0 0	55, 121, 180, 180	0
16	CS	80/91 (87%)	1.05	18 (22%) 1 1	70, 109, 174, 180	0
17	AT	85/86 (98%)	-0.22	0 100 100	49, 106, 179, 180	0
17	CT	85/86 (98%)	-0.07	2 (2%) 59 50	19, 65, 143, 159	0
18	AB	218/240 (90%)	0.23	17 (7%) 14 13	22, 94, 153, 180	0
18	CB	218/240 (90%)	0.75	34 (15%) 2 3	19, 102, 160, 180	0
19	AU	51/70 (72%)	0.25	2 (3%) 40 33	29, 101, 151, 180	0
19	CU	51/70 (72%)	0.42	4 (7%) 14 13	24, 113, 155, 180	0
20	AO	88/89 (98%)	0.52	7 (7%) 13 12	18, 83, 137, 179	0
20	CO	88/89 (98%)	-0.11	0 100 100	7, 60, 118, 161	0
21	AN	96/100 (96%)	0.72	12 (12%) 4 5	13, 98, 151, 180	0
21	CN	96/100 (96%)	0.87	20 (20%) 1 1	12, 81, 150, 180	0
22	BA	117/120 (97%)	-0.26	2 (1%) 70 62	35, 74, 117, 167	0
22	DA	117/120 (97%)	-0.56	1 (0%) 84 77	36, 86, 127, 180	0
23	BB	2841/2904 (97%)	-0.48	28 (0%) 82 75	6, 54, 148, 180	0
23	DB	2841/2904 (97%)	-0.49	15 (0%) 90 86	5, 48, 146, 180	0
24	BI	141/141 (100%)	2.71	78 (55%) 0 0	95, 172, 180, 180	0
24	DI	141/141 (100%)	2.06	61 (43%) 0 0	91, 179, 180, 180	0
25	BC	271/272 (99%)	0.80	41 (15%) 3 3	5, 50, 103, 180	0
25	DC	271/272 (99%)	0.44	17 (6%) 21 17	5, 40, 100, 146	0
26	BD	209/209 (100%)	0.08	8 (3%) 41 35	7, 68, 146, 180	0
26	DD	209/209 (100%)	0.85	41 (19%) 1 1	5, 49, 129, 180	0
27	BK	121/123 (98%)	0.68	12 (9%) 8 8	7, 69, 139, 180	0
27	DK	121/123 (98%)	0.74	9 (7%) 15 14	5, 41, 118, 180	0
28	BP	114/114 (100%)	0.51	11 (9%) 9 9	26, 85, 142, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.32	2 (1%) 69 60	5, 49, 103, 145	0
29	BE	201/201 (100%)	0.86	34 (16%) 2 2	5, 63, 143, 180	0
29	DE	201/201 (100%)	0.42	17 (8%) 11 12	5, 70, 144, 180	0
30	BY	58/58 (100%)	0.40	4 (6%) 18 15	20, 62, 140, 180	0
30	DY	58/58 (100%)	-0.17	0 100 100	5, 66, 116, 142	0
31	B0	56/56 (100%)	0.16	4 (7%) 17 15	20, 80, 163, 180	0
31	D0	56/56 (100%)	0.21	3 (5%) 26 22	12, 58, 116, 165	0
32	B4	38/38 (100%)	0.16	1 (2%) 56 47	5, 75, 120, 137	0
32	D4	38/38 (100%)	-0.35	0 100 100	7, 60, 114, 135	0
33	B1	50/54 (92%)	1.27	7 (14%) 3 4	15, 70, 135, 180	0
33	D1	50/54 (92%)	0.66	5 (10%) 8 8	20, 69, 142, 157	0
34	B3	64/64 (100%)	0.48	5 (7%) 14 13	13, 50, 102, 148	0
34	D3	64/64 (100%)	0.33	3 (4%) 32 26	5, 42, 88, 133	0
35	BV	94/94 (100%)	0.54	9 (9%) 9 9	21, 89, 143, 180	0
35	DV	94/94 (100%)	0.29	13 (13%) 3 4	9, 96, 151, 169	0
36	B2	46/46 (100%)	0.49	3 (6%) 20 16	5, 43, 120, 143	0
36	D2	46/46 (100%)	0.14	2 (4%) 36 29	11, 43, 103, 159	0
37	BL	143/144 (99%)	0.29	9 (6%) 21 17	8, 67, 133, 172	0
37	DL	143/144 (99%)	0.59	20 (13%) 3 4	5, 56, 119, 164	0
38	BM	136/136 (100%)	0.56	12 (8%) 11 11	9, 59, 117, 170	0
38	DM	136/136 (100%)	0.61	16 (11%) 5 6	7, 60, 116, 137	0
39	BX	63/63 (100%)	1.33	19 (30%) 1 1	6, 86, 135, 180	0
39	DX	63/63 (100%)	0.64	6 (9%) 9 9	38, 106, 178, 180	0
40	BH	149/149 (100%)	2.92	88 (59%) 0 0	26, 134, 177, 180	0
40	DH	149/149 (100%)	1.36	42 (28%) 1 1	11, 112, 162, 180	0
41	BJ	142/142 (100%)	0.53	18 (12%) 4 5	5, 74, 127, 180	0
41	DJ	142/142 (100%)	0.62	12 (8%) 11 12	5, 59, 125, 180	0
42	BN	120/127 (94%)	0.39	8 (6%) 19 16	20, 65, 126, 180	0
42	DN	120/127 (94%)	0.18	5 (4%) 37 30	5, 43, 103, 180	0
43	BO	116/117 (99%)	0.63	18 (15%) 2 3	12, 77, 140, 180	0
43	DO	116/117 (99%)	0.41	10 (8%) 11 11	32, 85, 152, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	-0.27	3 (2%) 56 47	6, 57, 133, 175	0
44	DQ	117/117 (100%)	0.35	10 (8%) 11 12	5, 52, 112, 161	0
45	BS	110/110 (100%)	0.48	7 (6%) 20 17	5, 50, 125, 180	0
45	DS	110/110 (100%)	0.98	22 (20%) 1 1	5, 52, 131, 180	0
46	BU	102/103 (99%)	0.82	11 (10%) 6 7	5, 70, 146, 180	0
46	DU	102/103 (99%)	0.02	1 (0%) 82 75	22, 97, 158, 180	0
47	BF	178/178 (100%)	1.52	66 (37%) 0 0	52, 123, 180, 180	0
47	DF	178/178 (100%)	2.24	84 (47%) 0 0	33, 110, 176, 180	0
48	BG	176/176 (100%)	0.61	19 (10%) 6 7	26, 104, 165, 180	0
48	DG	176/176 (100%)	0.88	37 (21%) 1 1	26, 98, 169, 180	0
49	BR	103/103 (100%)	0.35	8 (7%) 14 13	11, 76, 142, 180	0
49	DR	103/103 (100%)	0.52	10 (9%) 8 9	13, 79, 144, 180	0
50	BT	93/100 (93%)	0.60	7 (7%) 15 14	16, 75, 150, 180	0
50	DT	93/100 (93%)	1.00	21 (22%) 1 1	13, 79, 154, 180	0
51	BZ	77/78 (98%)	0.65	8 (10%) 7 8	5, 53, 122, 137	0
51	DZ	77/78 (98%)	0.20	5 (6%) 20 16	5, 47, 124, 144	0
52	BW	79/84 (94%)	1.15	17 (21%) 1 1	8, 74, 121, 180	0
52	DW	79/84 (94%)	0.10	4 (5%) 29 23	9, 77, 144, 164	0
All	All	20417/21046 (97%)	0.11	1563 (7%) 14 13	5, 69, 155, 180	0

The worst 5 of 1563 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AP	82	ALA	19.5
24	BI	49	GLU	12.0
13	AP	81	ALA	11.9
47	DF	75	GLY	11.0
40	BH	142	VAL	10.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
53	NMY	BB	3001	42/42	0.58	0.68	17.78	89,89,89,89	42
53	NMY	DB	3001	42/42	0.70	0.51	13.07	68,68,68,68	42
54	MG	AA	1658	1/1	0.83	0.26	7.04	120,120,120,120	0
54	MG	DB	3090	1/1	0.99	0.25	7.04	99,99,99,99	0
54	MG	BB	3088	1/1	0.95	0.25	5.98	87,87,87,87	0
53	NMY	CA	1601	42/42	0.90	0.22	2.78	47,47,47,47	0
53	NMY	AA	1601	42/42	0.86	0.23	2.55	75,75,75,75	0
54	MG	BB	3087	1/1	0.99	0.20	1.80	23,23,23,23	0
54	MG	CA	1613	1/1	0.88	0.18	1.41	108,108,108,108	0
54	MG	AA	1636	1/1	0.09	0.15	1.13	121,121,121,121	0
55	SCM	CA	1661	23/23	0.94	0.16	0.99	37,37,37,37	0
54	MG	BB	3041	1/1	0.97	0.17	0.53	34,34,34,34	0
54	MG	BB	3111	1/1	0.97	0.12	0.51	90,90,90,90	0
55	SCM	AA	1662	23/23	0.96	0.15	0.37	23,23,23,23	0
54	MG	DB	3013	1/1	0.99	0.17	0.29	12,12,12,12	0
54	MG	BB	3012	1/1	0.97	0.17	0.19	33,33,33,33	0
54	MG	CA	1634	1/1	0.95	0.12	-0.31	75,75,75,75	0
54	MG	BB	3086	1/1	0.84	0.16	-0.32	18,18,18,18	0
54	MG	BB	3084	1/1	0.95	0.16	-0.34	61,61,61,61	0
54	MG	BB	3076	1/1	0.98	0.16	-0.51	33,33,33,33	0
54	MG	AA	1616	1/1	0.92	0.14	-0.63	113,113,113,113	0
54	MG	AA	1634	1/1	0.85	0.10	-0.65	88,88,88,88	0
54	MG	AA	1653	1/1	0.78	0.11	-0.79	110,110,110,110	0
54	MG	DB	3111	1/1	0.98	0.09	-0.82	36,36,36,36	0
54	MG	DB	3091	1/1	0.86	0.06	-0.83	55,55,55,55	0
54	MG	DB	3015	1/1	0.97	0.07	-0.99	37,37,37,37	0
54	MG	DB	3031	1/1	0.86	0.16	-1.01	21,21,21,21	0
54	MG	DB	3100	1/1	0.96	0.15	-1.06	6,6,6,6	0
54	MG	CA	1654	1/1	0.80	0.09	-1.10	82,82,82,82	0
54	MG	DB	3088	1/1	0.97	0.16	-1.16	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3097	1/1	0.95	0.15	-1.18	12,12,12,12	0
54	MG	DB	3093	1/1	0.90	0.12	-1.18	98,98,98,98	0
54	MG	DB	3079	1/1	0.95	0.12	-1.22	80,80,80,80	0
54	MG	DB	3026	1/1	0.97	0.08	-1.27	16,16,16,16	0
54	MG	AA	1654	1/1	0.93	0.09	-1.31	49,49,49,49	0
54	MG	CA	1648	1/1	0.83	0.05	-1.38	69,69,69,69	0
54	MG	AA	1614	1/1	0.93	0.05	-1.41	66,66,66,66	0
56	ZN	B4	101	1/1	0.96	0.08	-1.46	49,49,49,49	0
54	MG	BB	3013	1/1	0.98	0.11	-1.51	81,81,81,81	0
54	MG	DB	3095	1/1	0.96	0.05	-1.58	39,39,39,39	0
56	ZN	D4	101	1/1	0.95	0.08	-1.59	40,40,40,40	0
54	MG	DB	3008	1/1	0.97	0.15	-1.65	41,41,41,41	0
54	MG	BB	3024	1/1	0.92	0.15	-1.68	12,12,12,12	0
54	MG	AA	1644	1/1	0.98	0.09	-1.71	42,42,42,42	0
54	MG	CA	1611	1/1	0.99	0.10	-1.71	5,5,5,5	0
54	MG	BB	3006	1/1	0.97	0.09	-1.72	9,9,9,9	0
54	MG	BB	3093	1/1	0.87	0.07	-1.79	32,32,32,32	0
54	MG	BB	3002	1/1	0.95	0.08	-1.80	19,19,19,19	0
54	MG	AA	1604	1/1	0.95	0.13	-1.82	43,43,43,43	0
54	MG	BB	3099	1/1	0.94	0.12	-1.86	23,23,23,23	0
54	MG	DB	3048	1/1	0.98	0.16	-1.92	14,14,14,14	0
54	MG	CA	1656	1/1	0.87	0.09	-1.92	135,135,135,135	0
54	MG	DB	3007	1/1	0.93	0.14	-1.98	9,9,9,9	0
54	MG	DB	3110	1/1	0.96	0.09	-2.02	17,17,17,17	0
54	MG	AA	1608	1/1	0.96	0.07	-2.05	53,53,53,53	0
54	MG	CA	1646	1/1	0.90	0.03	-2.08	52,52,52,52	0
54	MG	DB	3010	1/1	0.98	0.12	-2.08	8,8,8,8	0
54	MG	AA	1610	1/1	0.98	0.10	-2.15	5,5,5,5	0
54	MG	DB	3021	1/1	0.99	0.13	-2.36	5,5,5,5	0
54	MG	AA	1611	1/1	0.98	0.04	-2.39	73,73,73,73	0
54	MG	CA	1622	1/1	0.96	0.11	-2.53	44,44,44,44	0
54	MG	BB	3083	1/1	0.94	0.13	-2.55	5,5,5,5	0
54	MG	DB	3036	1/1	0.90	0.10	-2.61	85,85,85,85	0
54	MG	DB	3004	1/1	0.95	0.12	-2.65	41,41,41,41	0
54	MG	BB	3050	1/1	0.91	0.07	-2.68	16,16,16,16	0
54	MG	BB	3104	1/1	0.98	0.12	-2.68	6,6,6,6	0
54	MG	BB	3003	1/1	0.97	0.10	-2.75	17,17,17,17	0
54	MG	DB	3070	1/1	0.98	0.15	-2.77	38,38,38,38	0
54	MG	DB	3104	1/1	0.97	0.11	-2.88	31,31,31,31	0
54	MG	AA	1652	1/1	0.88	0.04	-2.91	101,101,101,101	0
54	MG	DB	3023	1/1	0.88	0.07	-2.93	7,7,7,7	0
54	MG	AA	1645	1/1	0.86	0.08	-2.94	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3086	1/1	0.98	0.11	-2.95	41,41,41,41	0
54	MG	DB	3056	1/1	0.93	0.11	-2.97	34,34,34,34	0
54	MG	BB	3066	1/1	0.94	0.06	-2.98	10,10,10,10	0
54	MG	DB	3011	1/1	0.97	0.09	-3.08	9,9,9,9	0
54	MG	DB	3073	1/1	0.91	0.07	-3.08	62,62,62,62	0
54	MG	DB	3071	1/1	0.93	0.14	-3.10	93,93,93,93	0
54	MG	DB	3089	1/1	0.98	0.10	-3.28	13,13,13,13	0
54	MG	BB	3030	1/1	0.95	0.08	-3.32	16,16,16,16	0
54	MG	DB	3069	1/1	0.97	0.08	-3.40	8,8,8,8	0
54	MG	CA	1628	1/1	0.93	0.09	-3.48	41,41,41,41	0
54	MG	CA	1612	1/1	0.98	0.07	-3.49	25,25,25,25	0
54	MG	DB	3052	1/1	0.96	0.12	-3.56	40,40,40,40	0
54	MG	CA	1621	1/1	0.97	0.10	-3.59	34,34,34,34	0
54	MG	AA	1642	1/1	0.98	0.04	-3.61	51,51,51,51	0
54	MG	CA	1635	1/1	0.91	0.07	-3.62	64,64,64,64	0
54	MG	BB	3022	1/1	0.96	0.09	-3.63	35,35,35,35	0
54	MG	AA	1631	1/1	0.96	0.04	-3.64	84,84,84,84	0
54	MG	BB	3082	1/1	0.92	0.11	-3.67	34,34,34,34	0
54	MG	AA	1639	1/1	0.96	0.05	-3.83	65,65,65,65	0
54	MG	BB	3089	1/1	0.95	0.07	-3.83	7,7,7,7	0
54	MG	BB	3091	1/1	0.95	0.05	-3.91	105,105,105,105	0
54	MG	DB	3057	1/1	0.97	0.09	-4.00	11,11,11,11	0
54	MG	AA	1637	1/1	0.95	0.03	-4.09	62,62,62,62	0
54	MG	CA	1637	1/1	0.99	0.08	-4.18	26,26,26,26	0
54	MG	BB	3095	1/1	0.90	0.08	-4.20	36,36,36,36	0
54	MG	DB	3002	1/1	0.98	0.13	-4.25	5,5,5,5	0
54	MG	BB	3075	1/1	0.95	0.08	-4.57	6,6,6,6	0
54	MG	DB	3085	1/1	0.96	0.13	-4.57	12,12,12,12	0
54	MG	DB	3109	1/1	0.98	0.08	-4.64	33,33,33,33	0
54	MG	CA	1625	1/1	0.99	0.06	-4.65	36,36,36,36	0
54	MG	CA	1636	1/1	0.99	0.07	-4.81	37,37,37,37	0
54	MG	AA	1655	1/1	0.92	0.06	-4.85	73,73,73,73	0
54	MG	AA	1602	1/1	0.96	0.06	-4.91	28,28,28,28	0
54	MG	BB	3063	1/1	0.99	0.10	-4.99	7,7,7,7	0
54	MG	BB	3014	1/1	0.92	0.06	-5.20	11,11,11,11	0
54	MG	BB	3080	1/1	0.93	0.10	-5.24	44,44,44,44	0
54	MG	DB	3003	1/1	0.99	0.07	-5.98	21,21,21,21	0
54	MG	BB	3070	1/1	0.97	0.08	-6.05	9,9,9,9	0
54	MG	BB	3033	1/1	0.99	0.05	-6.17	25,25,25,25	0
54	MG	CA	1602	1/1	0.99	0.04	-6.36	7,7,7,7	0
54	MG	CA	1606	1/1	0.95	0.06	-6.38	7,7,7,7	0
54	MG	BB	3057	1/1	0.97	0.05	-6.62	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3109	1/1	0.97	0.07	-6.66	19,19,19,19	0
54	MG	DB	3045	1/1	0.85	0.05	-6.69	32,32,32,32	0
54	MG	DB	3076	1/1	0.99	0.05	-6.86	22,22,22,22	0
54	MG	BB	3020	1/1	0.97	0.08	-8.07	28,28,28,28	0
54	MG	DB	3035	1/1	0.86	0.09	-9.10	80,80,80,80	0
54	MG	BB	3060	1/1	0.97	0.06	-9.57	5,5,5,5	0
54	MG	BB	3036	1/1	0.91	0.05	-11.17	26,26,26,26	0
54	MG	BB	3053	1/1	0.95	0.07	-14.14	30,30,30,30	0
54	MG	DB	3081	1/1	0.98	0.08	-15.48	35,35,35,35	0
54	MG	CA	1605	1/1	0.98	0.06	-17.16	12,12,12,12	0
54	MG	BB	3049	1/1	0.96	0.05	-27.29	24,24,24,24	0
54	MG	DB	3046	1/1	0.88	0.08	-	104,104,104,104	0
54	MG	BB	3034	1/1	0.82	0.40	-	130,130,130,130	0
54	MG	BB	3061	1/1	0.99	0.11	-	5,5,5,5	0
54	MG	DB	3055	1/1	0.98	0.09	-	22,22,22,22	0
54	MG	DB	3032	1/1	0.96	0.14	-	5,5,5,5	0
54	MG	CA	1640	1/1	0.97	0.13	-	43,43,43,43	0
54	MG	DB	3051	1/1	0.90	0.11	-	67,67,67,67	0
54	MG	BB	3032	1/1	0.95	0.12	-	38,38,38,38	0
54	MG	BB	3077	1/1	0.99	0.09	-	5,5,5,5	0
54	MG	BB	3039	1/1	0.89	0.09	-	107,107,107,107	0
54	MG	DB	3072	1/1	0.99	0.08	-	36,36,36,36	0
54	MG	BB	3069	1/1	0.87	0.07	-	41,41,41,41	0
54	MG	BB	3044	1/1	0.88	0.15	-	118,118,118,118	0
54	MG	BB	3027	1/1	0.89	0.14	-	42,42,42,42	0
54	MG	BB	3102	1/1	0.98	0.09	-	10,10,10,10	0
54	MG	DB	3024	1/1	0.93	0.07	-	32,32,32,32	0
54	MG	DB	3068	1/1	0.95	0.11	-	36,36,36,36	0
54	MG	DB	3060	1/1	0.49	0.08	-	96,96,96,96	0
54	MG	BB	3081	1/1	0.83	0.09	-	77,77,77,77	0
54	MG	AA	1620	1/1	0.73	0.12	-	132,132,132,132	0
54	MG	CA	1657	1/1	0.97	0.06	-	14,14,14,14	0
54	MG	BB	3015	1/1	0.96	0.03	-	32,32,32,32	0
54	MG	AA	1630	1/1	0.97	0.08	-	36,36,36,36	0
54	MG	DB	3019	1/1	0.99	0.08	-	25,25,25,25	0
54	MG	CA	1653	1/1	0.71	0.10	-	96,96,96,96	0
54	MG	BB	3046	1/1	0.98	0.10	-	50,50,50,50	0
54	MG	BB	3055	1/1	0.98	0.06	-	46,46,46,46	0
54	MG	BB	3097	1/1	0.99	0.07	-	5,5,5,5	0
54	MG	CA	1638	1/1	0.95	0.10	-	123,123,123,123	0
54	MG	BB	3010	1/1	0.98	0.06	-	123,123,123,123	0
54	MG	BB	3064	1/1	0.99	0.07	-	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1638	1/1	0.53	0.31	-	126,126,126,126	0
54	MG	DB	3099	1/1	0.99	0.13	-	9,9,9,9	0
54	MG	AA	1649	1/1	0.97	0.10	-	31,31,31,31	0
54	MG	CA	1627	1/1	0.96	0.07	-	40,40,40,40	0
54	MG	AA	1609	1/1	0.86	0.11	-	107,107,107,107	0
54	MG	CA	1660	1/1	0.98	0.07	-	77,77,77,77	0
54	MG	BB	3096	1/1	0.94	0.08	-	5,5,5,5	0
54	MG	CA	1658	1/1	0.97	0.14	-	50,50,50,50	0
54	MG	BB	3042	1/1	1.00	0.10	-	10,10,10,10	0
54	MG	DB	3105	1/1	0.97	0.10	-	41,41,41,41	0
54	MG	AA	1621	1/1	0.73	0.05	-	82,82,82,82	0
54	MG	AA	1647	1/1	0.82	0.12	-	133,133,133,133	0
54	MG	DB	3018	1/1	0.96	0.15	-	5,5,5,5	0
54	MG	DB	3047	1/1	0.98	0.08	-	27,27,27,27	0
54	MG	AA	1656	1/1	0.97	0.14	-	95,95,95,95	0
54	MG	AA	1626	1/1	0.53	0.24	-	87,87,87,87	1
54	MG	DB	3059	1/1	0.63	0.80	-	180,180,180,180	0
54	MG	AA	1643	1/1	0.94	0.13	-	43,43,43,43	0
54	MG	CA	1647	1/1	0.61	0.08	-	153,153,153,153	0
54	MG	CA	1633	1/1	0.69	0.07	-	48,48,48,48	0
54	MG	DB	3038	1/1	0.95	0.20	-	10,10,10,10	0
54	MG	BB	3079	1/1	0.85	0.08	-	68,68,68,68	0
54	MG	BB	3071	1/1	0.97	0.08	-	33,33,33,33	0
54	MG	DB	3050	1/1	0.97	0.12	-	6,6,6,6	0
54	MG	BB	3065	1/1	0.98	0.09	-	24,24,24,24	0
54	MG	AA	1635	1/1	0.98	0.06	-	86,86,86,86	0
54	MG	DB	3108	1/1	0.99	0.06	-	27,27,27,27	0
54	MG	CA	1644	1/1	0.93	0.08	-	49,49,49,49	0
54	MG	DB	3042	1/1	0.99	0.09	-	17,17,17,17	0
54	MG	DB	3016	1/1	0.89	0.10	-	53,53,53,53	0
54	MG	CA	1610	1/1	0.95	0.09	-	103,103,103,103	0
54	MG	BB	3085	1/1	0.96	0.15	-	43,43,43,43	0
54	MG	BB	3100	1/1	0.96	0.11	-	34,34,34,34	0
54	MG	DB	3077	1/1	0.98	0.12	-	28,28,28,28	0
54	MG	BB	3052	1/1	0.93	0.12	-	67,67,67,67	0
54	MG	BB	3098	1/1	0.95	0.09	-	85,85,85,85	0
54	MG	CA	1619	1/1	0.92	0.08	-	53,53,53,53	0
54	MG	CA	1609	1/1	0.79	0.07	-	110,110,110,110	0
54	MG	BB	3101	1/1	0.84	0.23	-	157,157,157,157	0
54	MG	BB	3068	1/1	0.96	0.11	-	65,65,65,65	0
54	MG	DB	3033	1/1	0.95	0.07	-	82,82,82,82	0
54	MG	CA	1632	1/1	0.98	0.05	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1648	1/1	0.86	0.40	-	110,110,110,110	0
54	MG	CA	1614	1/1	0.82	0.34	-	139,139,139,139	0
54	MG	BB	3056	1/1	0.94	0.14	-	23,23,23,23	0
54	MG	DB	3067	1/1	0.49	0.09	-	137,137,137,137	0
54	MG	DB	3043	1/1	0.97	0.09	-	32,32,32,32	0
54	MG	CA	1642	1/1	0.99	0.12	-	49,49,49,49	0
54	MG	DB	3030	1/1	0.82	0.15	-	81,81,81,81	0
54	MG	BB	3040	1/1	0.96	0.18	-	44,44,44,44	0
54	MG	DB	3084	1/1	0.86	0.16	-	109,109,109,109	0
54	MG	CA	1652	1/1	0.29	0.12	-	128,128,128,128	0
54	MG	DB	3005	1/1	0.96	0.14	-	23,23,23,23	0
54	MG	DB	3098	1/1	0.97	0.17	-	41,41,41,41	0
54	MG	AA	1659	1/1	0.87	0.05	-	111,111,111,111	0
54	MG	DB	3101	1/1	0.94	0.12	-	20,20,20,20	0
54	MG	DB	3040	1/1	0.97	0.08	-	78,78,78,78	0
54	MG	AA	1651	1/1	0.88	0.07	-	97,97,97,97	0
54	MG	BB	3025	1/1	0.94	0.11	-	32,32,32,32	0
54	MG	CA	1649	1/1	0.85	0.08	-	92,92,92,92	0
54	MG	BB	3009	1/1	0.95	0.08	-	80,80,80,80	0
54	MG	DB	3066	1/1	0.95	0.06	-	32,32,32,32	0
54	MG	CA	1623	1/1	0.96	0.12	-	21,21,21,21	0
54	MG	DB	3082	1/1	0.98	0.07	-	9,9,9,9	0
54	MG	AA	1660	1/1	0.38	0.40	-	148,148,148,148	0
54	MG	BB	3045	1/1	0.91	0.13	-	42,42,42,42	0
54	MG	BB	3110	1/1	0.98	0.15	-	61,61,61,61	0
54	MG	CA	1641	1/1	0.95	0.14	-	61,61,61,61	0
54	MG	BB	3090	1/1	0.97	0.10	-	54,54,54,54	0
54	MG	CA	1608	1/1	0.94	0.04	-	31,31,31,31	0
54	MG	BB	3028	1/1	0.98	0.05	-	24,24,24,24	0
54	MG	DB	3103	1/1	0.98	0.13	-	14,14,14,14	0
54	MG	DB	3106	1/1	0.97	0.16	-	53,53,53,53	0
54	MG	AA	1627	1/1	0.97	0.11	-	5,5,5,5	1
54	MG	DB	3006	1/1	0.97	0.14	-	13,13,13,13	0
54	MG	BB	3062	1/1	0.93	0.08	-	38,38,38,38	0
54	MG	DB	3061	1/1	0.28	0.17	-	117,117,117,117	0
54	MG	BB	3008	1/1	0.98	0.18	-	81,81,81,81	0
54	MG	CA	1618	1/1	0.87	0.15	-	104,104,104,104	0
54	MG	AA	1661	1/1	0.94	0.11	-	62,62,62,62	0
54	MG	AA	1633	1/1	0.93	0.14	-	65,65,65,65	0
54	MG	CA	1659	1/1	0.95	0.06	-	45,45,45,45	0
54	MG	CA	1639	1/1	0.96	0.06	-	108,108,108,108	0
54	MG	BB	3073	1/1	0.97	0.06	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3092	1/1	0.97	0.16	-	12,12,12,12	0
54	MG	DB	3078	1/1	0.98	0.11	-	24,24,24,24	0
54	MG	AA	1650	1/1	0.91	0.06	-	105,105,105,105	0
54	MG	BB	3048	1/1	0.90	0.09	-	145,145,145,145	0
54	MG	CA	1630	1/1	0.88	0.10	-	81,81,81,81	0
54	MG	DB	3094	1/1	0.91	0.15	-	5,5,5,5	0
54	MG	AA	1612	1/1	0.99	0.06	-	70,70,70,70	0
54	MG	BB	3017	1/1	0.96	0.08	-	43,43,43,43	0
54	MG	BB	3092	1/1	0.98	0.11	-	5,5,5,5	0
54	MG	DB	3029	1/1	0.95	0.04	-	30,30,30,30	0
54	MG	BB	3004	1/1	0.96	0.06	-	31,31,31,31	0
54	MG	CA	1616	1/1	0.96	0.07	-	15,15,15,15	0
54	MG	CA	1655	1/1	0.97	0.06	-	52,52,52,52	0
54	MG	CA	1643	1/1	0.82	0.11	-	75,75,75,75	0
54	MG	DB	3012	1/1	0.96	0.14	-	32,32,32,32	0
54	MG	CA	1603	1/1	0.99	0.15	-	25,25,25,25	0
54	MG	CA	1650	1/1	0.39	0.50	-	180,180,180,180	0
54	MG	DB	3075	1/1	0.94	0.17	-	58,58,58,58	0
54	MG	BB	3106	1/1	0.97	0.20	-	11,11,11,11	0
54	MG	CA	1620	1/1	0.98	0.09	-	62,62,62,62	0
54	MG	CA	1615	1/1	0.98	0.07	-	29,29,29,29	0
54	MG	BB	3103	1/1	0.97	0.13	-	25,25,25,25	0
54	MG	AA	1625	1/1	0.84	0.20	-	102,102,102,102	0
54	MG	AA	1618	1/1	0.69	0.20	-	160,160,160,160	0
54	MG	DB	3027	1/1	0.87	0.11	-	72,72,72,72	0
54	MG	AA	1629	1/1	0.96	0.09	-	55,55,55,55	0
54	MG	BB	3051	1/1	0.98	0.05	-	34,34,34,34	0
54	MG	BB	3018	1/1	0.95	0.15	-	31,31,31,31	0
54	MG	BB	3026	1/1	0.98	0.17	-	68,68,68,68	0
54	MG	DB	3020	1/1	0.98	0.10	-	6,6,6,6	0
54	MG	AA	1622	1/1	0.92	0.06	-	24,24,24,24	0
54	MG	AA	1613	1/1	0.95	0.08	-	80,80,80,80	0
54	MG	BB	3021	1/1	0.97	0.15	-	30,30,30,30	0
54	MG	BB	3054	1/1	0.93	0.07	-	46,46,46,46	0
54	MG	BB	3031	1/1	0.95	0.06	-	53,53,53,53	0
54	MG	DB	3107	1/1	1.00	0.07	-	20,20,20,20	0
54	MG	BB	3011	1/1	0.92	0.10	-	62,62,62,62	0
54	MG	BB	3058	1/1	0.91	0.17	-	63,63,63,63	0
54	MG	DB	3034	1/1	0.99	0.11	-	5,5,5,5	0
54	MG	DB	3014	1/1	0.77	0.15	-	80,80,80,80	0
54	MG	CA	1629	1/1	0.94	0.10	-	57,57,57,57	0
54	MG	CA	1624	1/1	0.97	0.07	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3065	1/1	0.98	0.07	-	20,20,20,20	0
54	MG	BB	3059	1/1	0.99	0.05	-	13,13,13,13	0
54	MG	BB	3043	1/1	0.29	0.23	-	145,145,145,145	0
54	MG	DB	3009	1/1	0.97	0.09	-	49,49,49,49	0
54	MG	DB	3074	1/1	0.86	0.12	-	29,29,29,29	0
54	MG	BB	3038	1/1	0.92	0.13	-	46,46,46,46	0
54	MG	DB	3049	1/1	0.95	0.06	-	66,66,66,66	0
54	MG	DB	3087	1/1	0.97	0.10	-	11,11,11,11	0
54	MG	AA	1624	1/1	0.95	0.32	-	13,13,13,13	1
54	MG	BB	3016	1/1	0.99	0.09	-	31,31,31,31	0
54	MG	DB	3028	1/1	0.95	0.10	-	17,17,17,17	0
54	MG	AA	1607	1/1	0.66	0.12	-	93,93,93,93	0
54	MG	BB	3108	1/1	0.96	0.14	-	36,36,36,36	0
54	MG	DB	3054	1/1	0.84	0.10	-	80,80,80,80	0
54	MG	AA	1606	1/1	0.95	0.19	-	56,56,56,56	0
54	MG	BB	3007	1/1	0.93	0.06	-	37,37,37,37	0
54	MG	BB	3067	1/1	0.95	0.09	-	26,26,26,26	0
54	MG	AA	1615	1/1	0.89	0.10	-	123,123,123,123	0
54	MG	BB	3029	1/1	0.91	0.22	-	21,21,21,21	0
54	MG	AA	1646	1/1	0.86	0.08	-	89,89,89,89	0
54	MG	BB	3037	1/1	0.98	0.20	-	35,35,35,35	0
54	MG	DB	3112	1/1	0.93	0.23	-	87,87,87,87	0
54	MG	CA	1631	1/1	0.99	0.15	-	43,43,43,43	0
54	MG	DB	3083	1/1	0.98	0.06	-	37,37,37,37	0
54	MG	BB	3072	1/1	0.94	0.08	-	54,54,54,54	0
54	MG	CA	1617	1/1	0.81	0.07	-	83,83,83,83	0
54	MG	CA	1604	1/1	0.95	0.07	-	66,66,66,66	0
54	MG	BB	3094	1/1	0.75	0.08	-	75,75,75,75	0
54	MG	DB	3064	1/1	0.99	0.04	-	34,34,34,34	0
54	MG	BB	3105	1/1	0.96	0.17	-	18,18,18,18	0
54	MG	AA	1605	1/1	0.95	0.09	-	46,46,46,46	0
54	MG	DB	3096	1/1	0.91	0.07	-	115,115,115,115	0
54	MG	AA	1657	1/1	0.81	0.23	-	95,95,95,95	0
54	MG	DB	3058	1/1	0.95	0.08	-	39,39,39,39	0
54	MG	CA	1651	1/1	0.84	0.46	-	161,161,161,161	0
54	MG	BB	3019	1/1	0.99	0.11	-	44,44,44,44	0
54	MG	CA	1607	1/1	0.92	0.16	-	129,129,129,129	0
54	MG	BB	3023	1/1	0.99	0.21	-	12,12,12,12	0
54	MG	DB	3017	1/1	0.97	0.11	-	29,29,29,29	0
54	MG	AA	1640	1/1	0.81	0.15	-	110,110,110,110	0
54	MG	AA	1628	1/1	0.96	0.07	-	53,53,53,53	0
54	MG	AA	1619	1/1	0.98	0.06	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3022	1/1	0.97	0.09	-	5,5,5,5	0
54	MG	AA	1603	1/1	0.87	0.07	-	100,100,100,100	0
54	MG	DB	3063	1/1	0.98	0.04	-	50,50,50,50	0
54	MG	DB	3037	1/1	0.94	0.09	-	23,23,23,23	0
54	MG	CA	1645	1/1	0.90	0.08	-	70,70,70,70	0
54	MG	BB	3074	1/1	0.99	0.09	-	28,28,28,28	0
54	MG	BB	3107	1/1	0.97	0.07	-	30,30,30,30	0
54	MG	AA	1641	1/1	0.96	0.15	-	88,88,88,88	0
54	MG	DB	3102	1/1	0.96	0.17	-	6,6,6,6	0
54	MG	AA	1617	1/1	0.96	0.11	-	47,47,47,47	0
54	MG	DB	3062	1/1	0.96	0.06	-	75,75,75,75	0
54	MG	BB	3047	1/1	0.96	0.11	-	66,66,66,66	0
54	MG	DB	3025	1/1	0.98	0.11	-	47,47,47,47	0
54	MG	DB	3044	1/1	0.98	0.07	-	11,11,11,11	0
54	MG	CA	1626	1/1	0.88	0.08	-	117,117,117,117	0
54	MG	AA	1623	1/1	0.68	0.19	-	157,157,157,157	0
54	MG	BB	3005	1/1	0.91	0.07	-	29,29,29,29	0
54	MG	BB	3035	1/1	0.94	0.06	-	41,41,41,41	0
54	MG	DB	3080	1/1	0.98	0.09	-	46,46,46,46	0
54	MG	BB	3078	1/1	0.96	0.15	-	47,47,47,47	0
54	MG	AA	1632	1/1	0.97	0.11	-	29,29,29,29	0
54	MG	DB	3039	1/1	0.97	0.11	-	19,19,19,19	0
54	MG	DB	3053	1/1	0.91	0.07	-	90,90,90,90	0
54	MG	DB	3041	1/1	0.98	0.09	-	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.