



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:54 PM GMT

PDB ID : 4V7U
Title : Crystal structure of the E. coli ribosome bound to erythromycin.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-15
Resolution : 3.10 Å(reported)

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

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

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

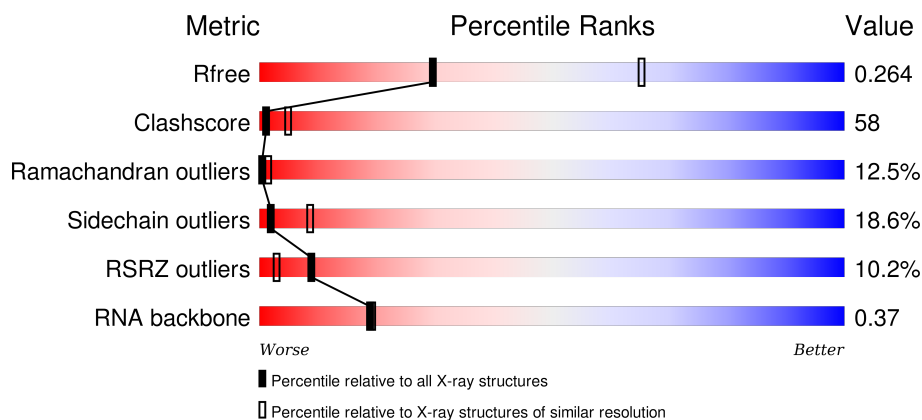
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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	1533	<div> <div>15%</div> <div>49%</div> <div>20%</div> <div>17%</div> </div>
1	CA	1533	<div> <div>3%</div> <div>12%</div> <div>48%</div> <div>25%</div> <div>14%</div> </div>
2	AB	218	<div> <div>33%</div> <div>21%</div> <div>54%</div> <div>23%</div> <div>.</div> </div>
2	CB	218	<div> <div>33%</div> <div>22%</div> <div>63%</div> <div>14%</div> <div>.</div> </div>

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

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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2904	
22	DA	2904	
23	BB	118	
23	DB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	178	
27	DF	178	

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

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	79	
44	DW	79	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	

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	MG	AA	1620	-	-	-	X
53	MG	BA	3027	-	-	-	X
53	MG	BA	3036	-	-	-	X
53	MG	BA	3040	-	-	-	X
53	MG	BA	3047	-	-	-	X
53	MG	BA	3057	-	-	-	X
53	MG	BA	3063	-	-	-	X
53	MG	BA	3070	-	-	-	X
53	MG	BA	3082	-	-	-	X
53	MG	BA	3100	-	-	-	X
53	MG	BA	3103	-	-	-	X
53	MG	BA	3104	-	-	-	X
53	MG	BA	3108	-	-	-	X
53	MG	BA	3123	-	-	-	X
53	MG	BA	3130	-	-	-	X
53	MG	BA	3135	-	-	-	X
53	MG	CA	1607	-	-	-	X
53	MG	CA	1618	-	-	-	X
53	MG	CA	1625	-	-	-	X
53	MG	CA	1628	-	-	-	X
53	MG	DA	3002	-	-	-	X
53	MG	DA	3013	-	-	-	X
53	MG	DA	3033	-	-	-	X
53	MG	DA	3043	-	-	-	X
53	MG	DA	3075	-	-	-	X
53	MG	DA	3076	-	-	-	X
53	MG	DA	3079	-	-	-	X
53	MG	DA	3082	-	-	-	X
53	MG	DA	3108	-	-	-	X
53	MG	DA	3129	-	-	-	X
53	MG	DA	3133	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284525 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	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
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 S2.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	CG	150	Total	C	N	O	S	0	0	0
			1175	730	226	215	4			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	CM	114	Total	C	N	O	S	0	0	1
			877	541	178	155	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	CN	95	Total	C	N	O	S	0	0	0
			769	480	159	127	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	CP	81	Total	C	N	O	S	0	0	1
			639	400	127	111	1			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
22	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
23	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	178	Total	C	N	O	S	0	0	1
			1411	899	250	256	6			
27	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

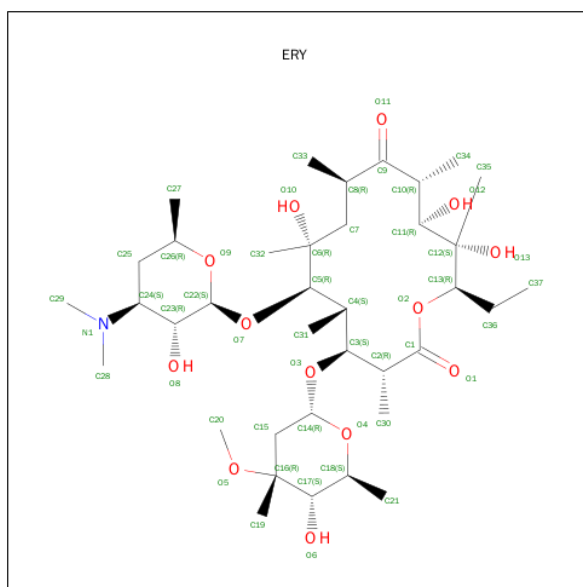
- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	BB	4	Total Mg 4 4	0	0
53	BA	135	Total Mg 135 135	0	0
53	CA	42	Total Mg 42 42	0	0
53	DJ	1	Total Mg 1 1	0	0
53	AA	41	Total Mg 41 41	0	0
53	AN	2	Total Mg 2 2	0	0
53	DA	133	Total Mg 133 133	0	0
53	DC	2	Total Mg 2 2	0	0
53	DB	1	Total Mg 1 1	0	0

- Molecule 54 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	BA	1	Total C N O 51 37 1 13	0	0

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

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	197	Total O 197 197	0	0
56	AE	1	Total O 1 1	0	0
56	AL	1	Total O 1 1	0	0
56	AN	7	Total O 7 7	0	0
56	AT	1	Total O 1 1	0	0
56	AU	1	Total O 1 1	0	0
56	BA	605	Total O 605 605	0	0
56	BB	19	Total O 19 19	0	0
56	BC	7	Total O 7 7	0	0
56	BD	3	Total O 3 3	0	0
56	BE	1	Total O 1 1	0	0
56	BL	4	Total O 4 4	0	0
56	BN	2	Total O 2 2	0	0
56	BR	1	Total O 1 1	0	0
56	BT	2	Total O 2 2	0	0
56	BV	1	Total O 1 1	0	0
56	B3	3	Total O 3 3	0	0
56	B4	2	Total O 2 2	0	0

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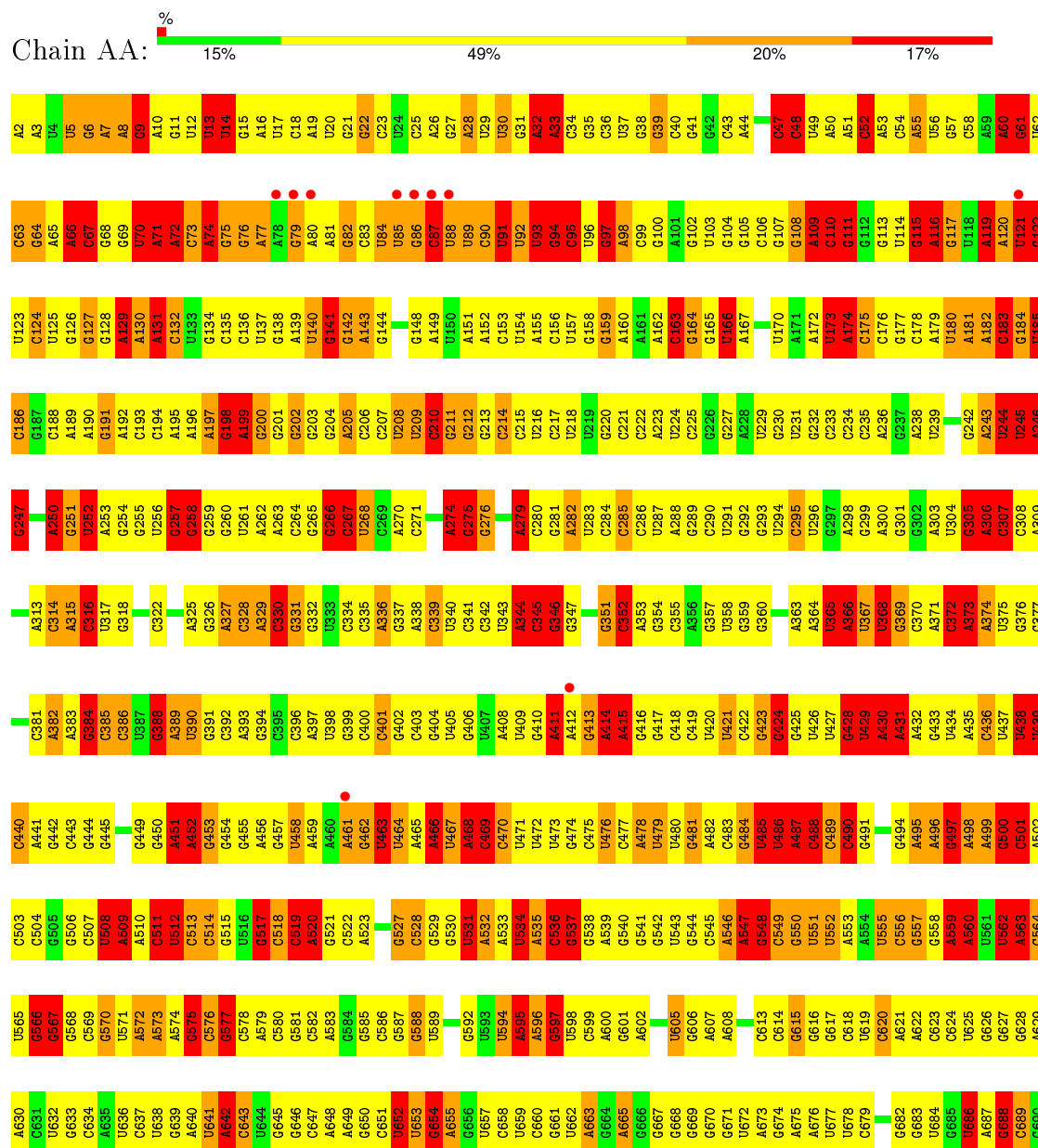
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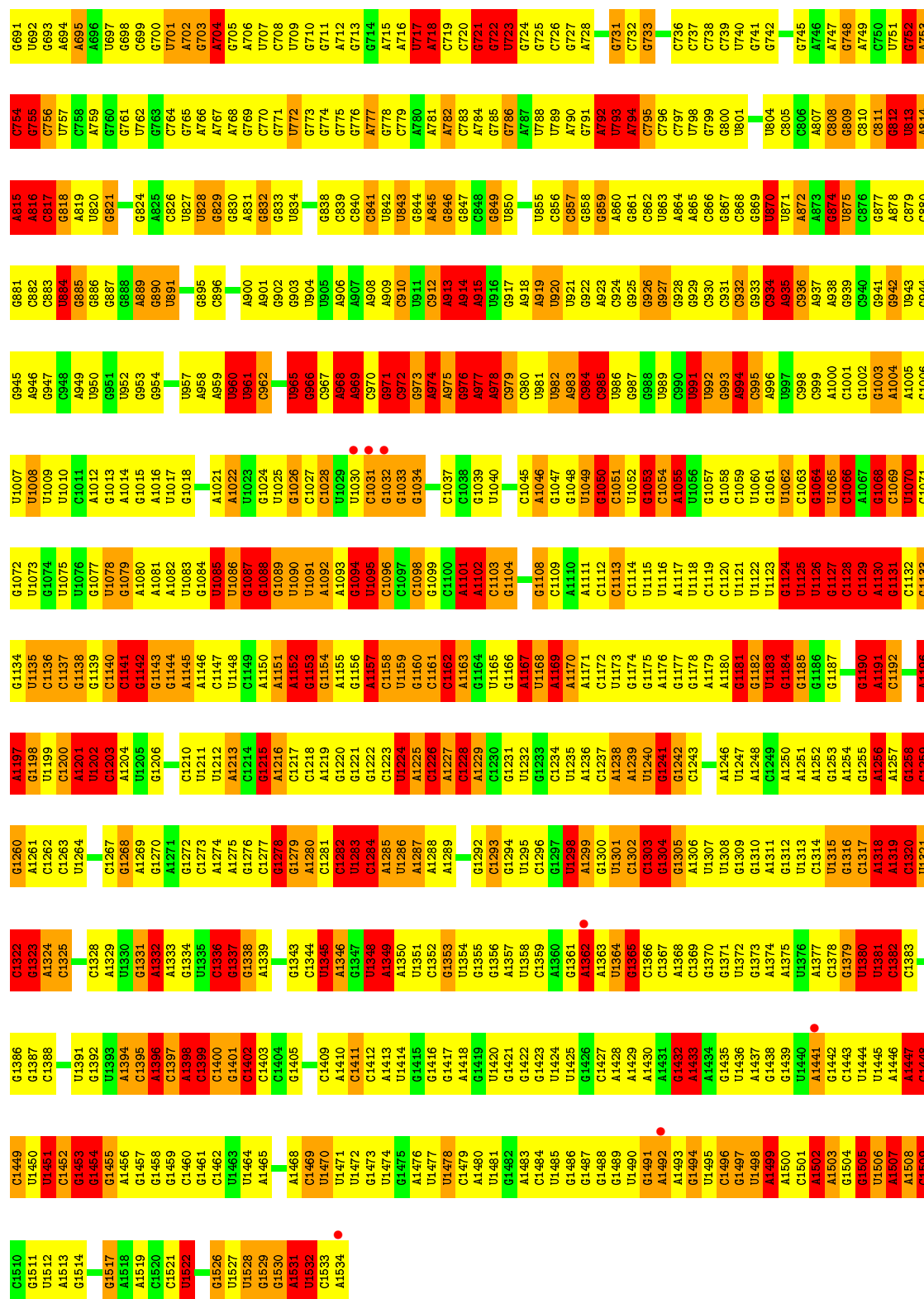
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CA	195	Total 195	O 195	0	0
56	CE	3	Total 3	O 3	0	0
56	CL	1	Total 1	O 1	0	0
56	CN	3	Total 3	O 3	0	0
56	CT	4	Total 4	O 4	0	0
56	CU	1	Total 1	O 1	0	0
56	DA	600	Total 600	O 600	0	0
56	DB	3	Total 3	O 3	0	0
56	DC	13	Total 13	O 13	0	0
56	DD	2	Total 2	O 2	0	0
56	DE	4	Total 4	O 4	0	0
56	DJ	3	Total 3	O 3	0	0
56	DL	4	Total 4	O 4	0	0
56	DN	2	Total 2	O 2	0	0
56	DT	2	Total 2	O 2	0	0
56	DU	2	Total 2	O 2	0	0
56	DV	2	Total 2	O 2	0	0
56	D2	1	Total 1	O 1	0	0
56	D3	1	Total 1	O 1	0	0
56	D4	4	Total 4	O 4	0	0

3 Residue-property plots

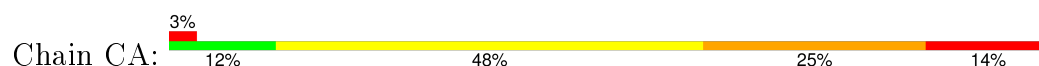
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA

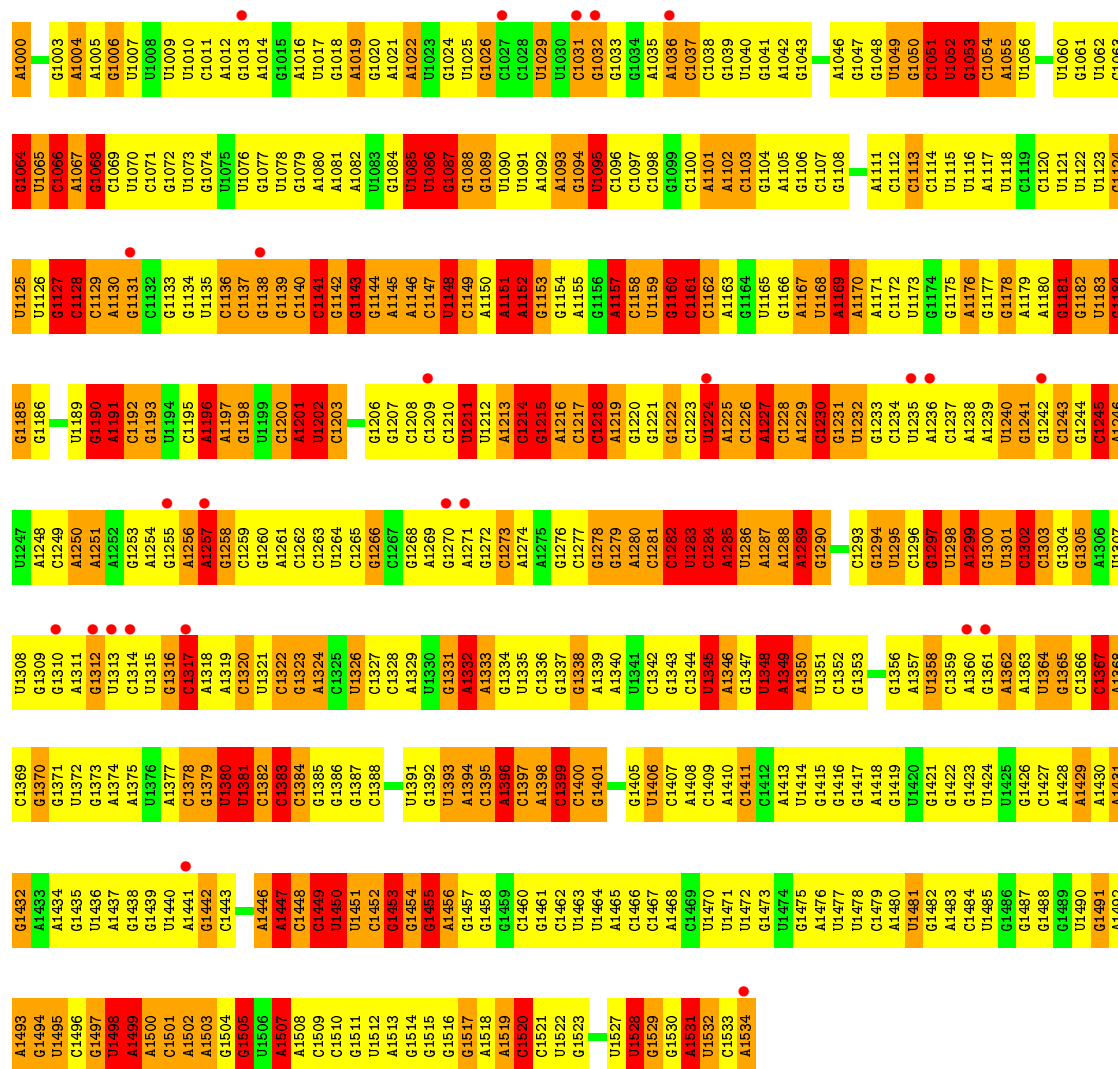




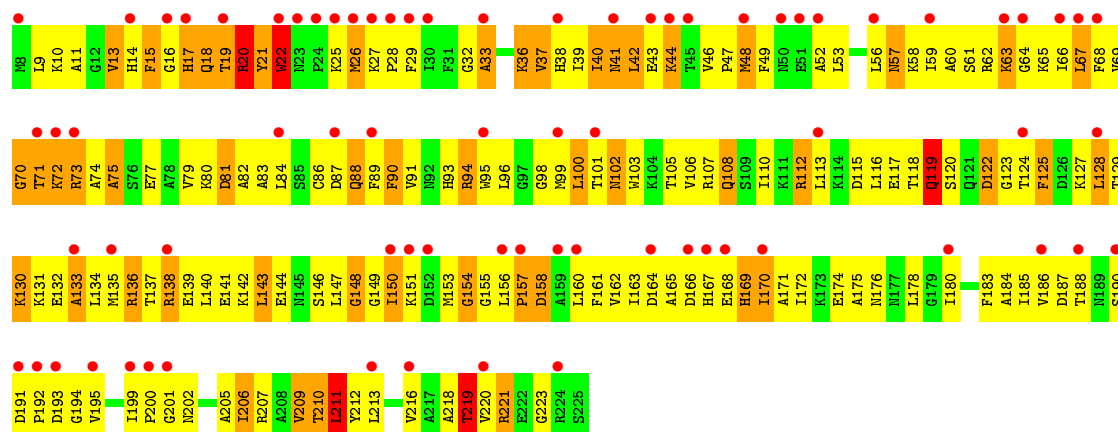
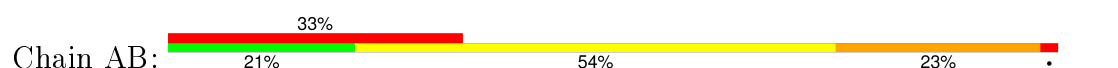
• Molecule 1: 16S rRNA



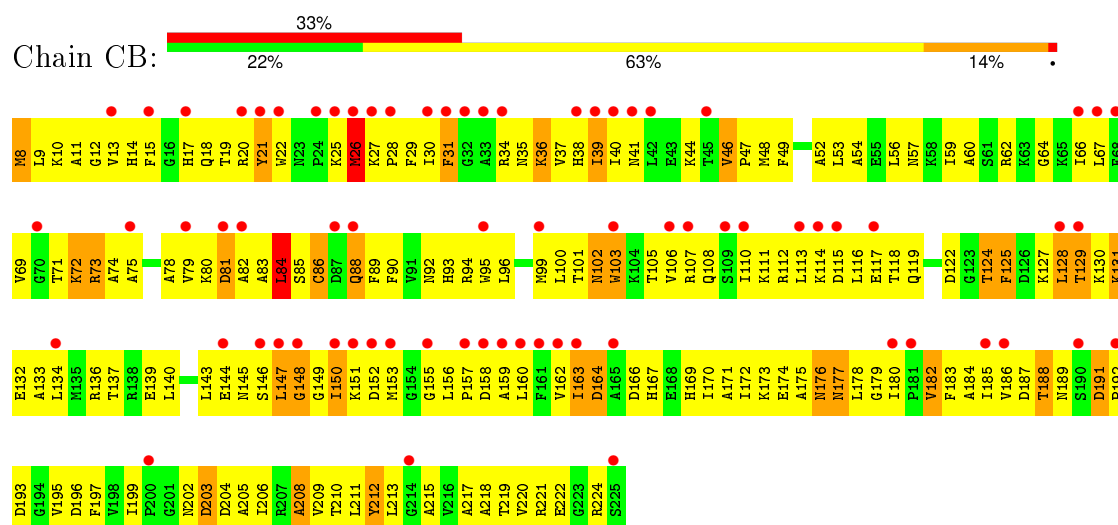




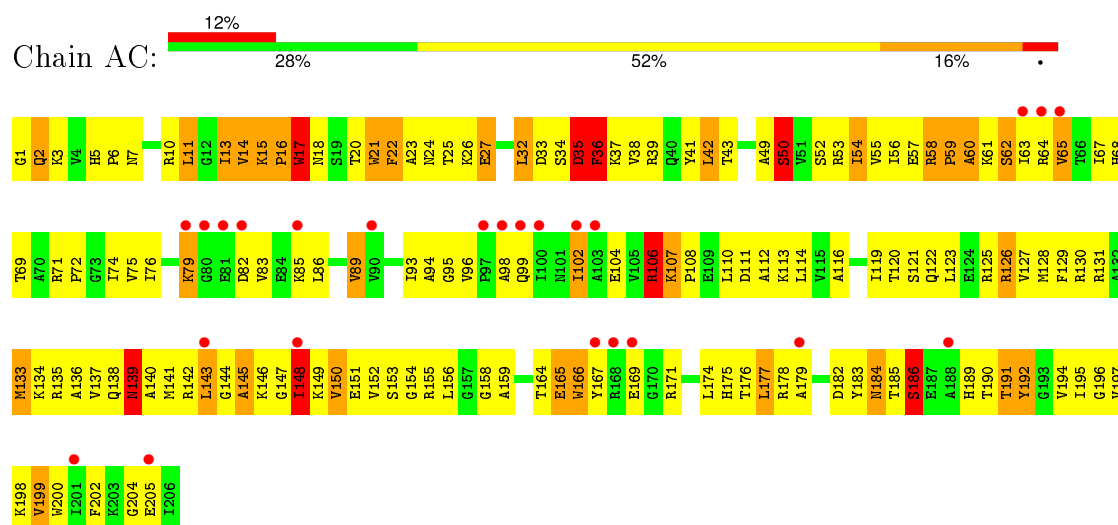
• Molecule 2: 30S ribosomal protein S2



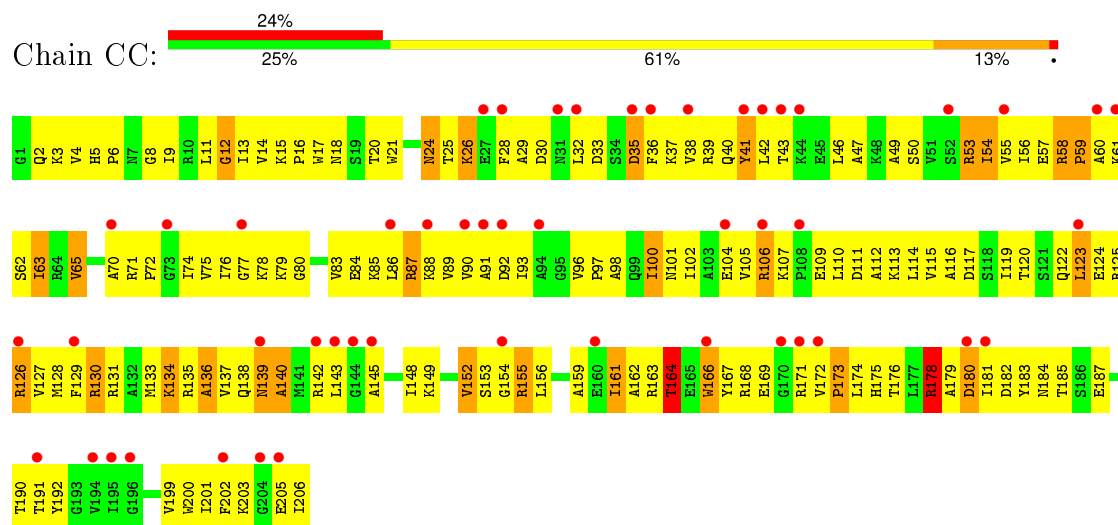
• Molecule 2: 30S ribosomal protein S2



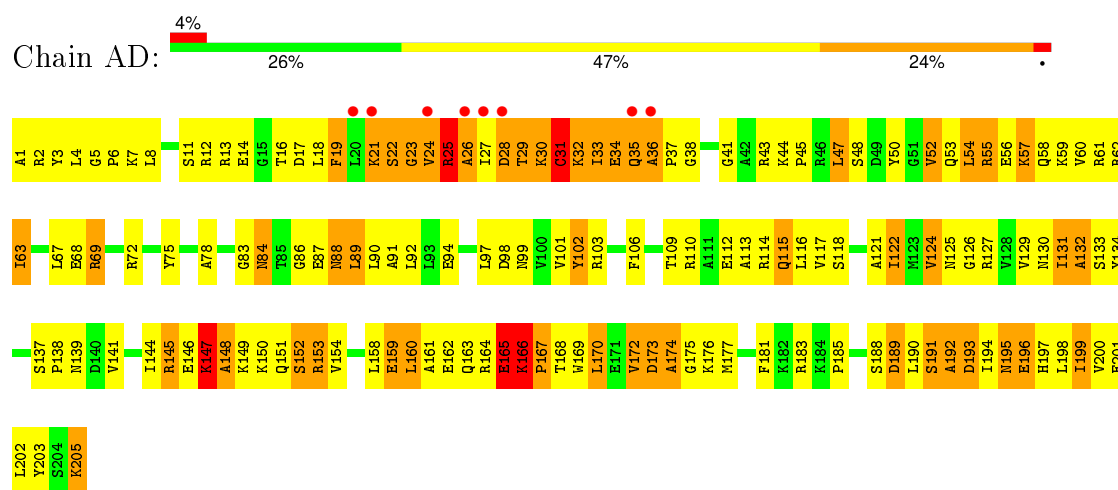
• Molecule 3: 30S ribosomal protein S3



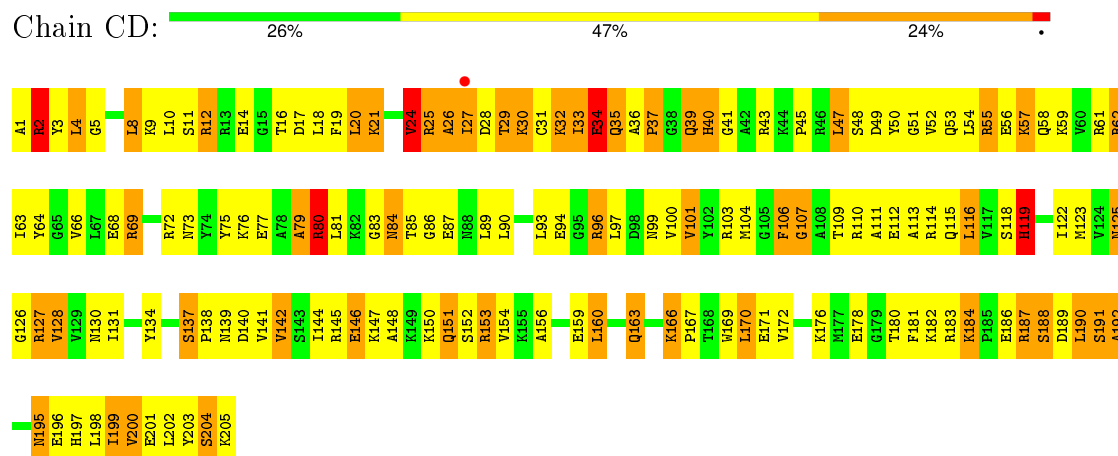
• Molecule 3: 30S ribosomal protein S3



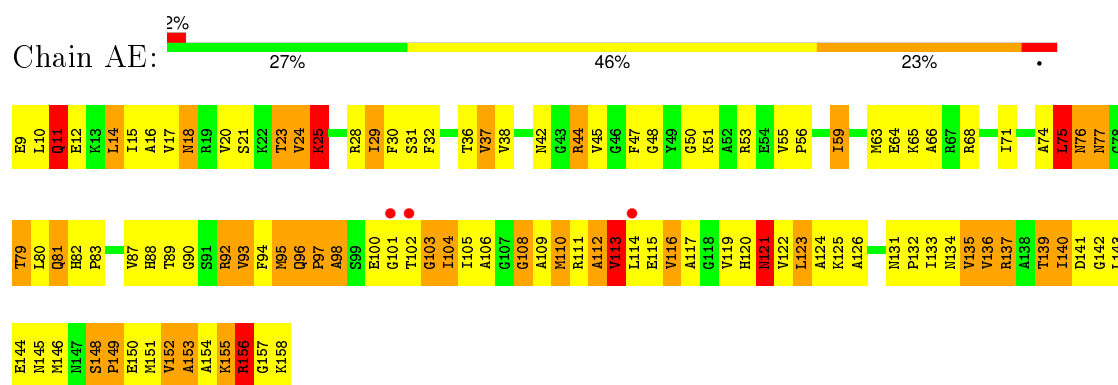
• Molecule 4: 30S ribosomal protein S4



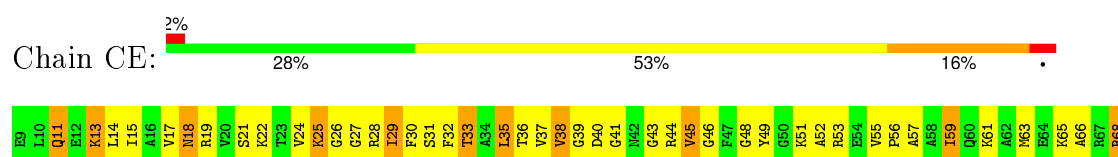
• Molecule 4: 30S ribosomal protein S4

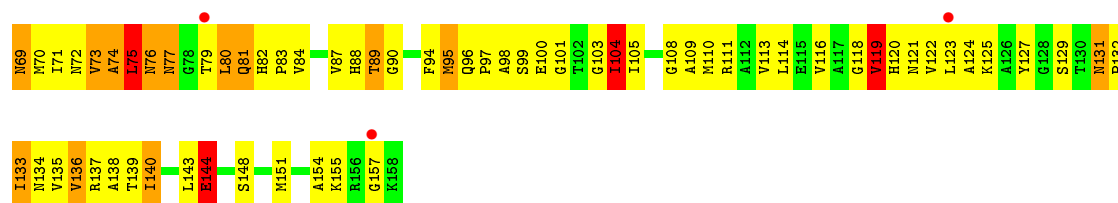


• Molecule 5: 30S ribosomal protein S5



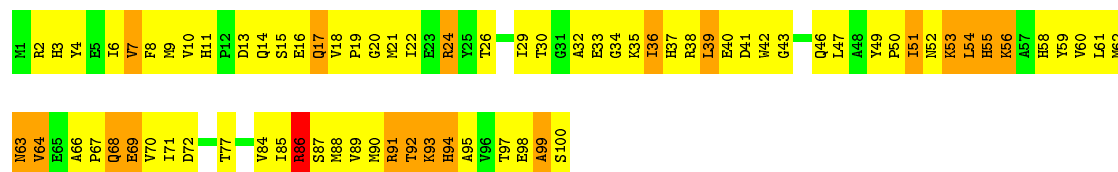
• Molecule 5: 30S ribosomal protein S5





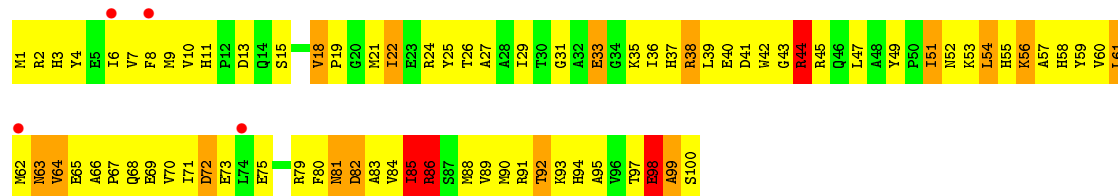
• Molecule 6: 30S ribosomal protein S6

Chain AF: 24% 56% 19%



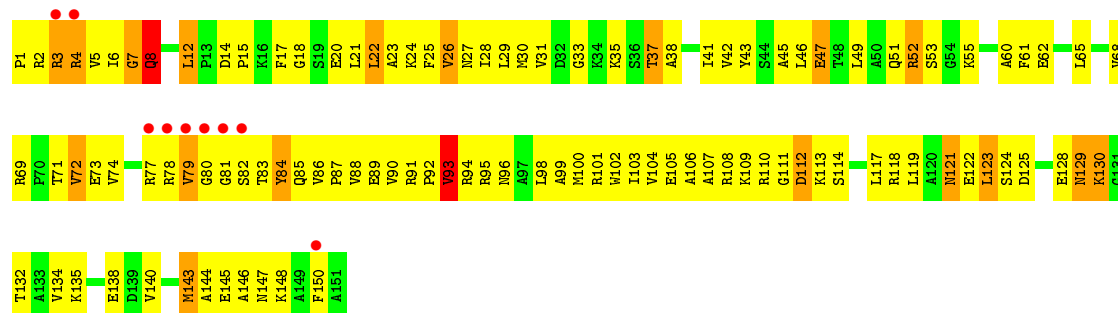
• Molecule 6: 30S ribosomal protein S6

Chain CF: 4% 20% 61% 15%



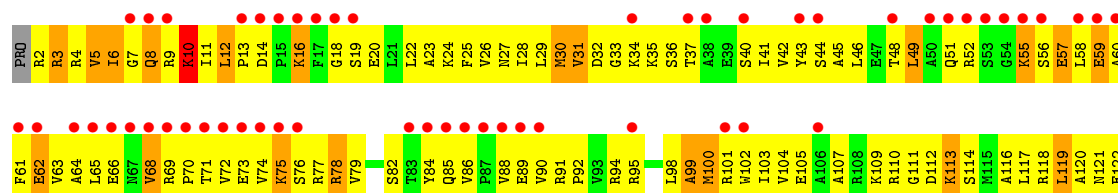
• Molecule 7: 30S ribosomal protein S7

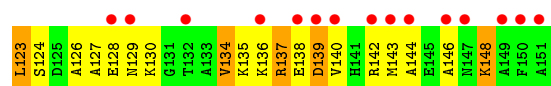
Chain AG: 6% 27% 60% 12%



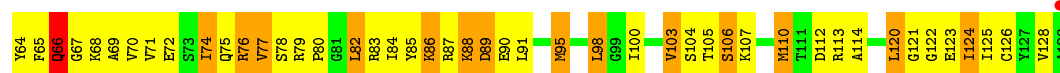
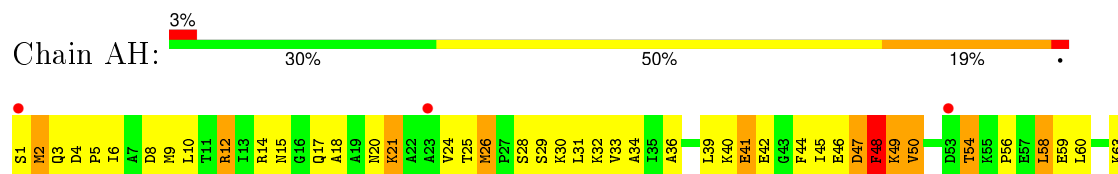
• Molecule 7: 30S ribosomal protein S7

Chain CG: 46% 20% 62% 17%

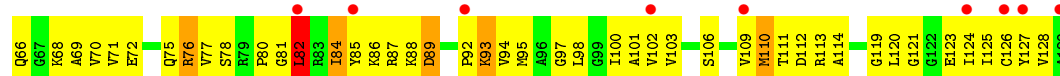
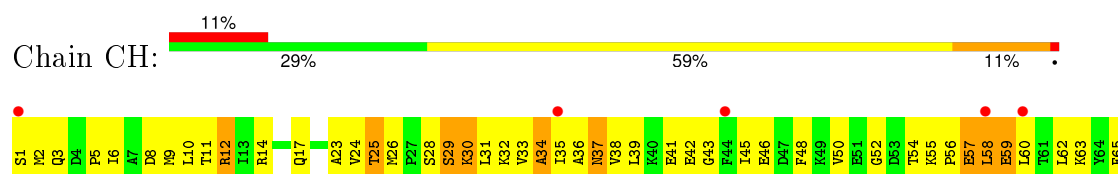




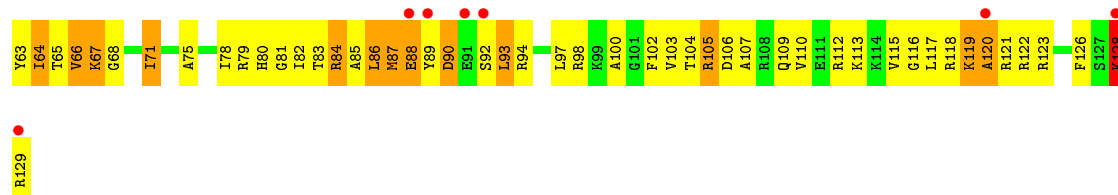
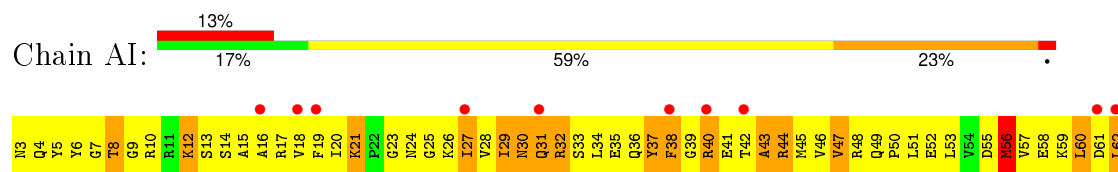
• Molecule 8: 30S ribosomal protein S8



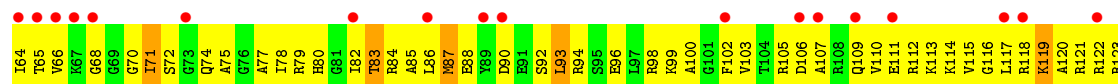
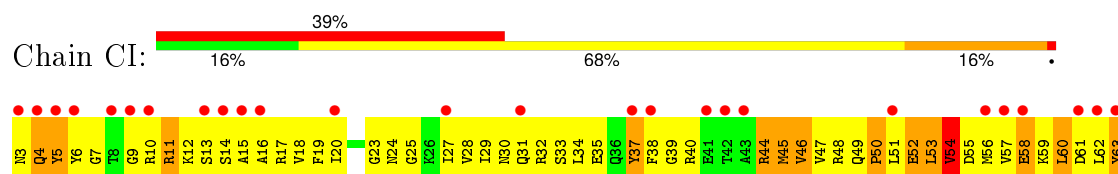
• Molecule 8: 30S ribosomal protein S8



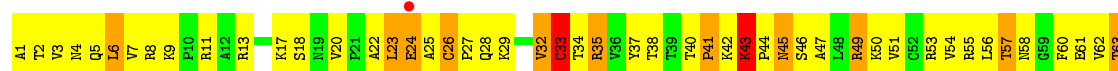
• Molecule 9: 30S ribosomal protein S9



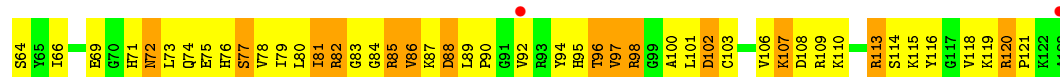
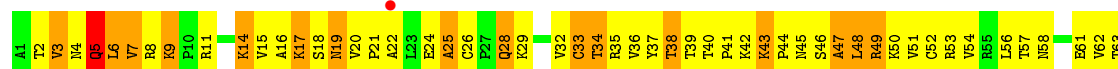
• Molecule 9: 30S ribosomal protein S9



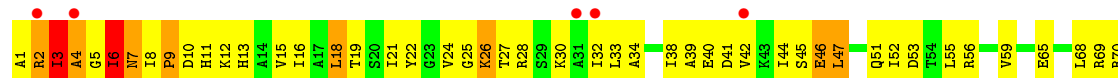




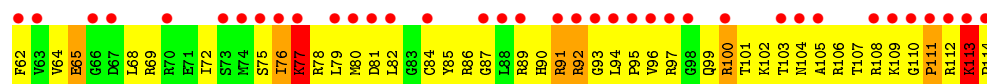
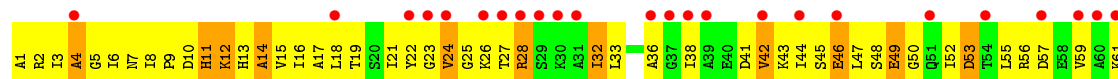
• Molecule 12: 30S ribosomal protein S12



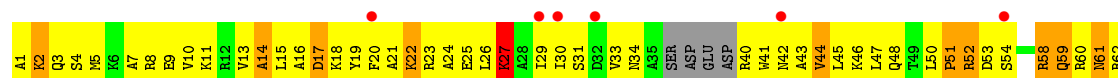
• Molecule 13: 30S ribosomal protein S13



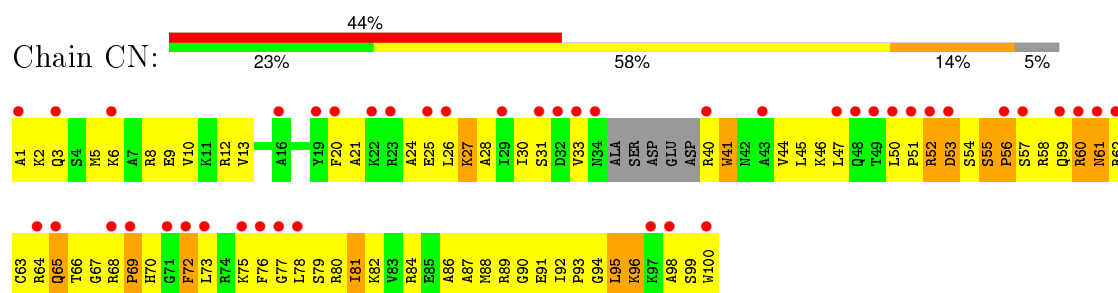
• Molecule 13: 30S ribosomal protein S13



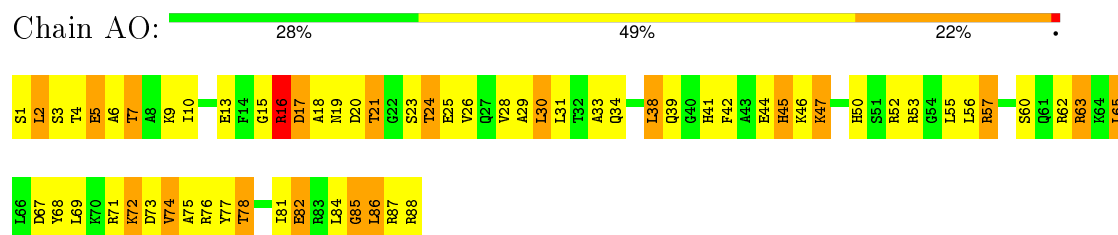
• Molecule 14: 30S ribosomal protein S14



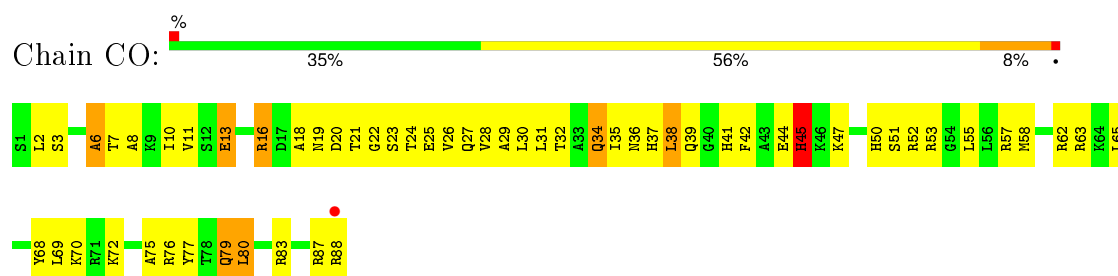
• Molecule 14: 30S ribosomal protein S14



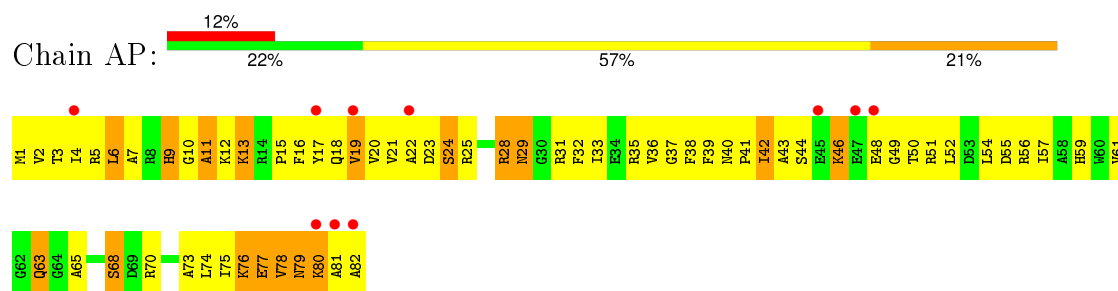
- Molecule 15: 30S ribosomal protein S15



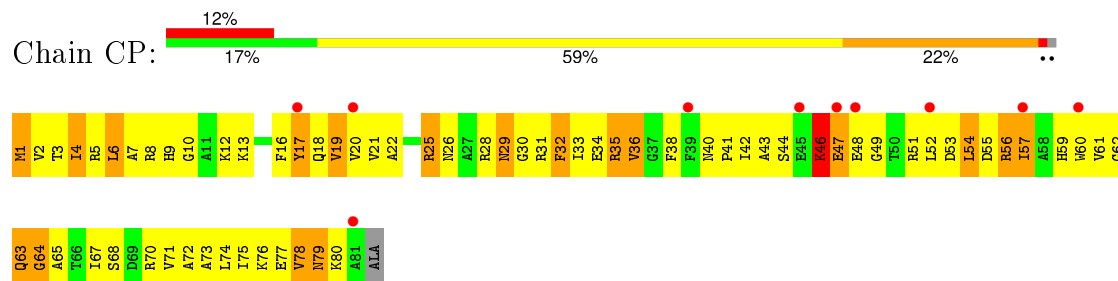
- Molecule 15: 30S ribosomal protein S15



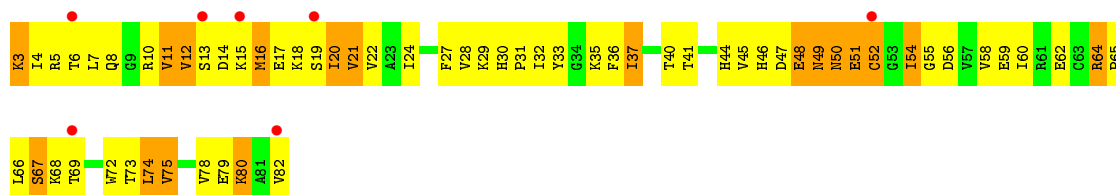
- Molecule 16: 30S ribosomal protein S16



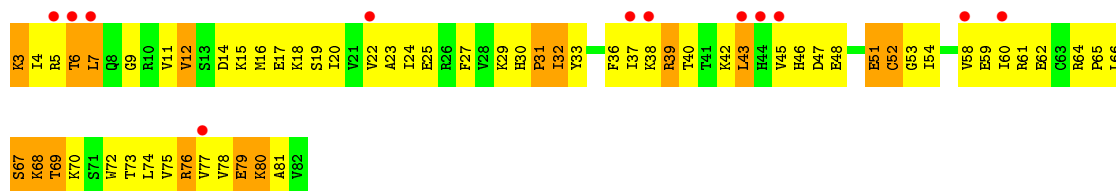
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



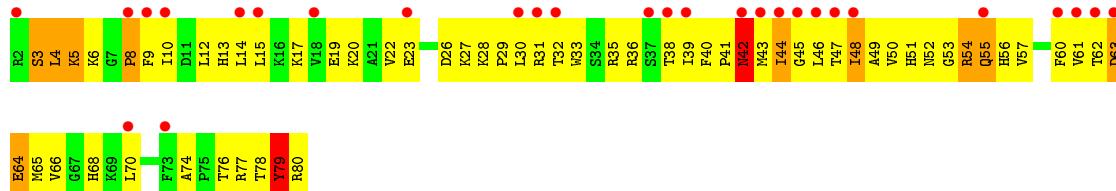
- Molecule 18: 30S ribosomal protein S18



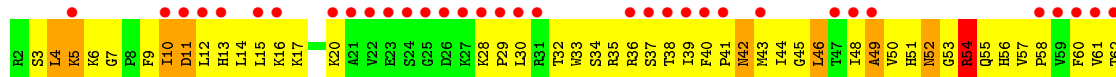
- Molecule 18: 30S ribosomal protein S18

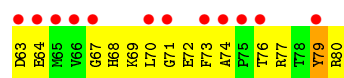


- Molecule 19: 30S ribosomal protein S19



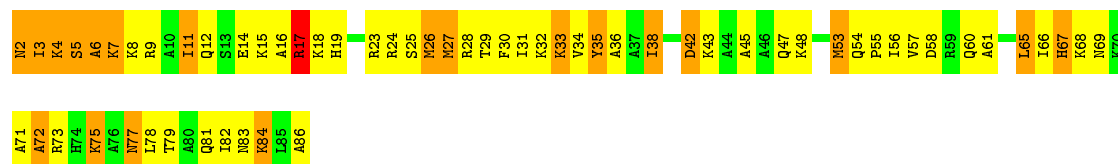
- Molecule 19: 30S ribosomal protein S19





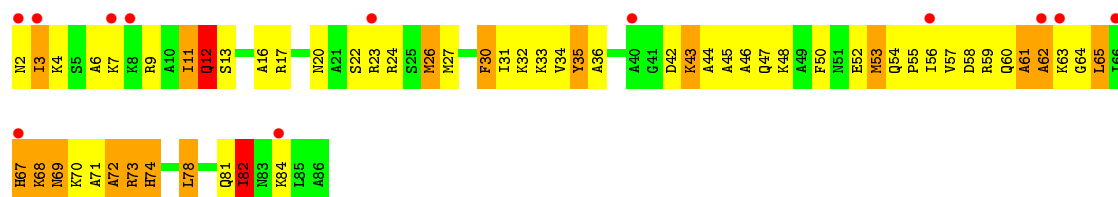
• Molecule 20: 30S ribosomal protein S20

Chain AT: 28% 47% 24%



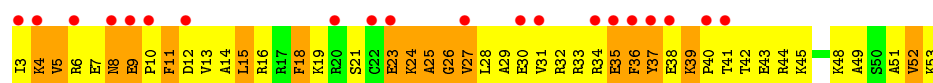
• Molecule 20: 30S ribosomal protein S20

Chain CT: 14% 32% 46% 20%



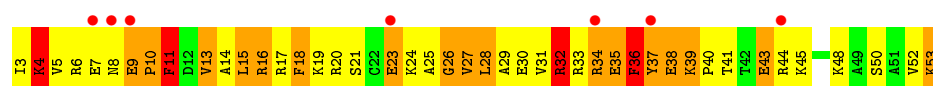
• Molecule 21: 30S ribosomal protein S21

Chain AU: 12% 39% 55% 33%



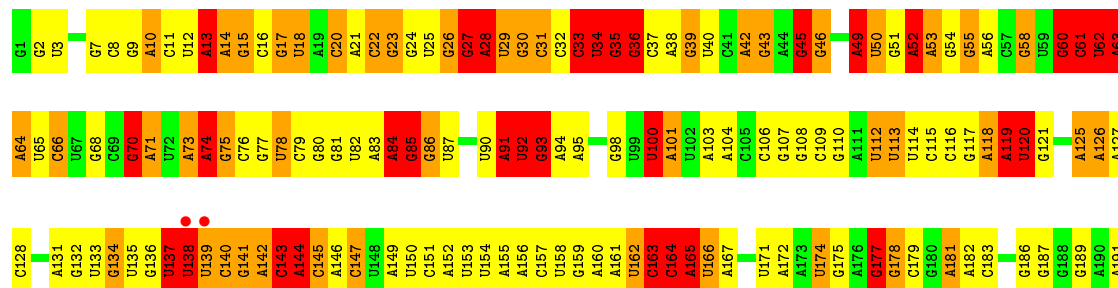
• Molecule 21: 30S ribosomal protein S21

Chain CU: 14% 14% 45% 33% 8%



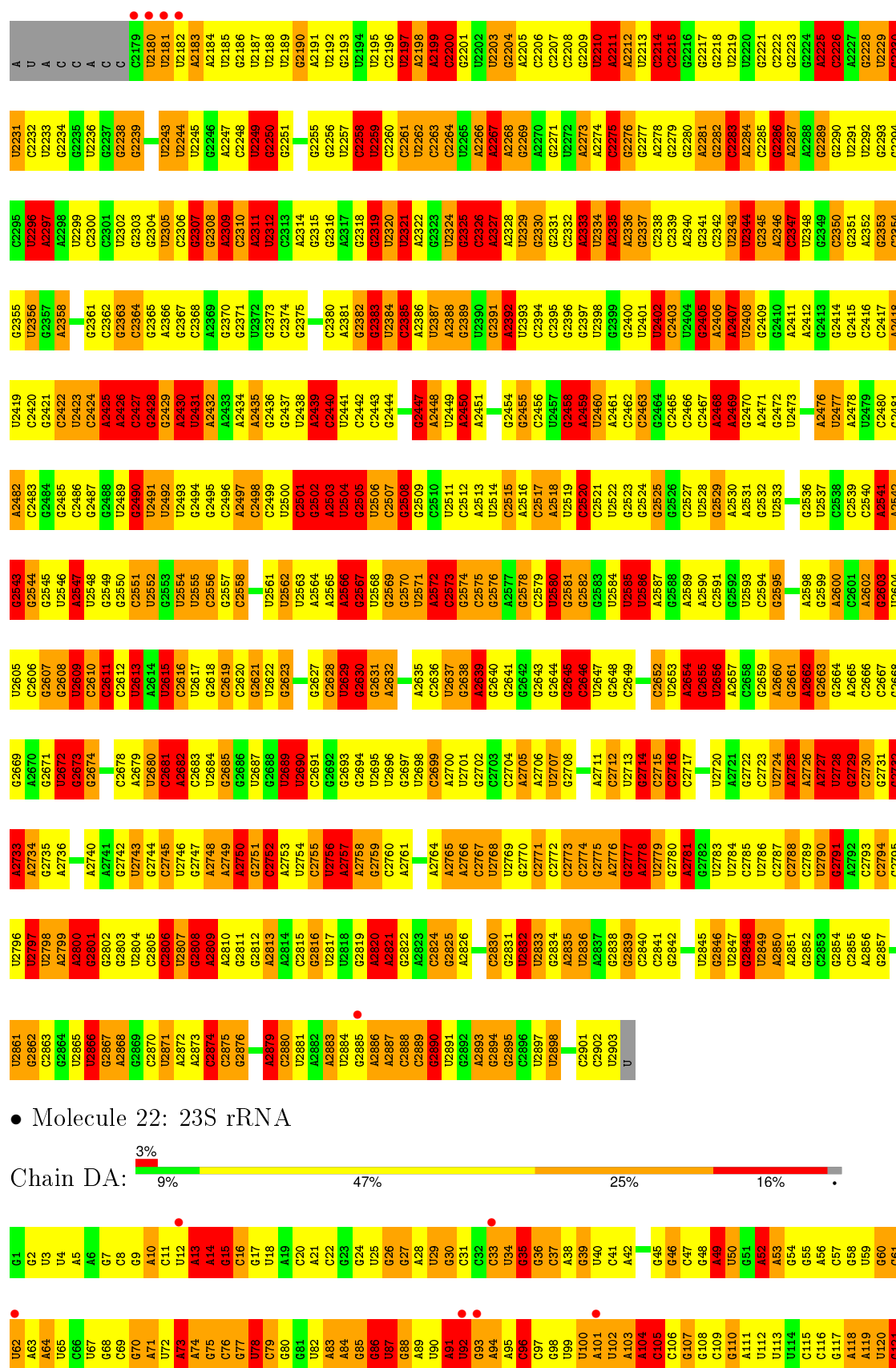
• Molecule 22: 23S rRNA

Chain BA: 17% 40% 24% 17%



G1139	C1079	C1013	C951	C	A825	G763	A699	G638	G577	C510	U448	A382	C318	C257	G192
C1140	A1080	A1014	G951	C	U826	A764	U702	U639	G578	U511	A449	C383	G319	G258	A196
U1141	U1081	U1015	G954	G	U827	C765	U703	C640	G579	U512	G450	A384	A320	G259	A197
A1142	G1016	G1016	U955	A892	U828	U766	G702	U641	U580	A513	U451	C385	U321	G260	C198
A1143	G1017	G1017	U955	C893	A829	U767	G704	U642	A582	A514	G452	G386	A322	G261	C199
A1144	U1018	U1018	G956	U894	G830	G768	A705	C845	C581	A453	G453	U387	C323	A262	A199
C1145	U1085	U1019	C957	U895	G831	U769	A706	C845	C583	G520	A454	C388	C324	G263	U200
A1146	A1086	A1020	U958	A896	U832	U770	G707	U646	C584	U521	C455	C389	G325	C264	C201
A1147	G1087	A1021	A959	C897	A833	C772	G708	U647	C585	A522	C456	U390	G326	A265	
G1148	A1088	G1022	A960	A898	G834	U773	U709	G648	C587	C523	A457	A391	G329	G266	A204
G1149	C1089	U1023	C961	A899	C835	U774	U710	G649	C588		G458		G330	G267	G205
A1150	A1090	G1024	G962	A900	G836	G775	G711	C650	U583	A526	U459	U395	A330	C268	U206
A1151	C1091	G1025	U963	C901	C837	G776	G712	C651	U589	A527	A460	C386	A331	C269	A207
C1152	C1092	G1026	C964	C902	C838	G777	G713	U852	A590	A528	C461	U397	A332	A270	C208
C1153	G1093	A1027	C965	G903	U839	U778	U715	U853	U591	A529	C462	U398	G333	G271	C209
G1154	U1094	C840	G966	G904	U841	U779	A715	A854	A592	G530	G463	U399	C334	A272	C210
A1155	A1095	U841	U967	A905	G842	G780	G716	A855	U593	C531	U464	G400	C335	G273	C211
A1156	C968	U842	C968	U906	U842	A781	C717	G656	U594	A532	G465		C336	G274	G212
G1157	G969	G907	G969	G907	U842	A782	A718	U657	C595	G533	A466	U403	C337	G275	A213
A1158	A1098	G1033	A972	C908	A845	A783	G719	U658	U596	U534	G467	A404	U338	G276	G214
U1159	C1099	U1033	A973	A909	U846	G784	U720	U658	C597	G535	G468	U405	U339	G277	G215
G1160	U1100	A1040	A974	A910	U847	G785	A721	C660		G536	G469	G406	U340	A278	A216
C1161	C1101	G1041	G974	A911	C848	G786	A722	A661	G600	U537	A470	G407	C341	A279	A217
G1162	A1102	G1042	A975	C912		C787	G723	G662	C601	A538	A471	G408	A342	U280	
	C1103	G1043	G976	U913	C851	A788	U724	G663	A602	G539	A472	G409	C343	C281	A221
A1165	C1104	C1044	G977	C914	U852	A789	G725	G664	A603	U540	G473	G410	A344	A282	A222
G1166	U1105	C1045	G978	C915	C853	U790	G726	U665	G604	A541	G474	G411	A345	G283	A223
	G1106	A1046	A979	G916	C854	G791	A727	U666	G605	C542	C475	A412	A346	U284	U224
C1170	G1107	G1047	A980	A917	G855	A792	G728	U667	U606	G543	G476	C413	A347	G285	C225
G1171	A1108	A1048	A981	A918	G856	A793	G729	U668	U607	C544	A477	C414	A348	U286	A226
C1172	C1109	U1049	C982	U919	G857	A794	A730	G669	A608	U545	A478	A415	U349	G287	A227
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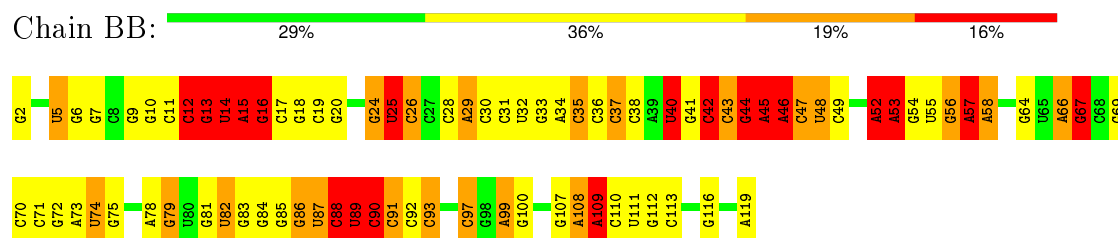


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G985	G924	G924	A861	A800	G738	A675	U615	G554	C491	A431	A371	A311	A251	A191	G132
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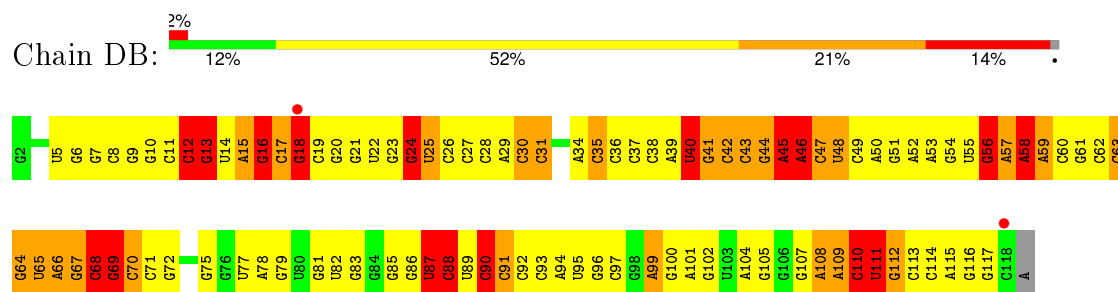
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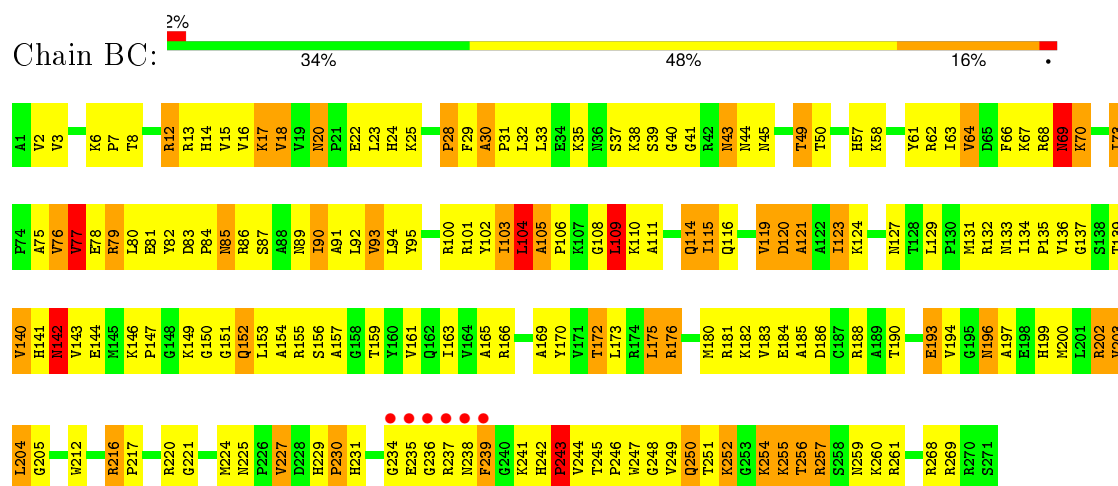
- Molecule 23: 5S rRNA



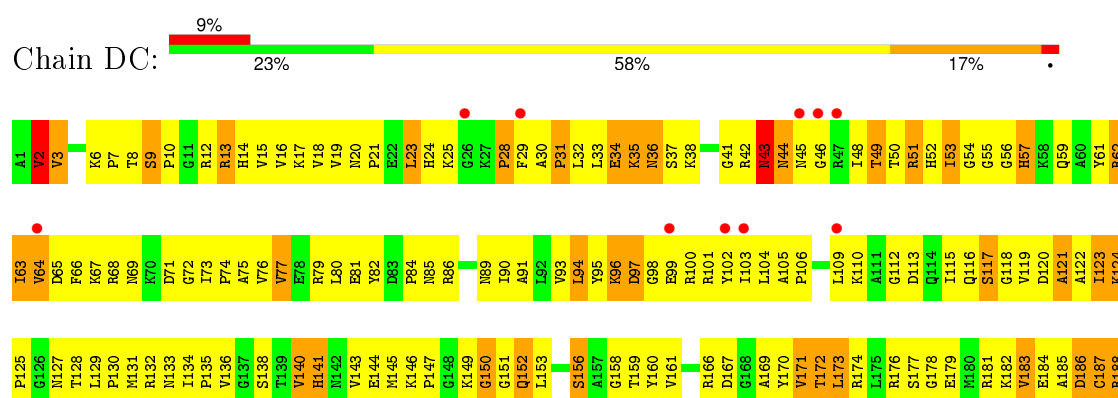
- Molecule 23: 5S rRNA

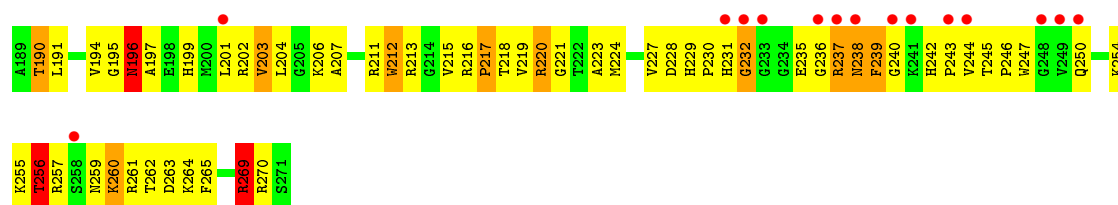


- Molecule 24: 50S ribosomal protein L2



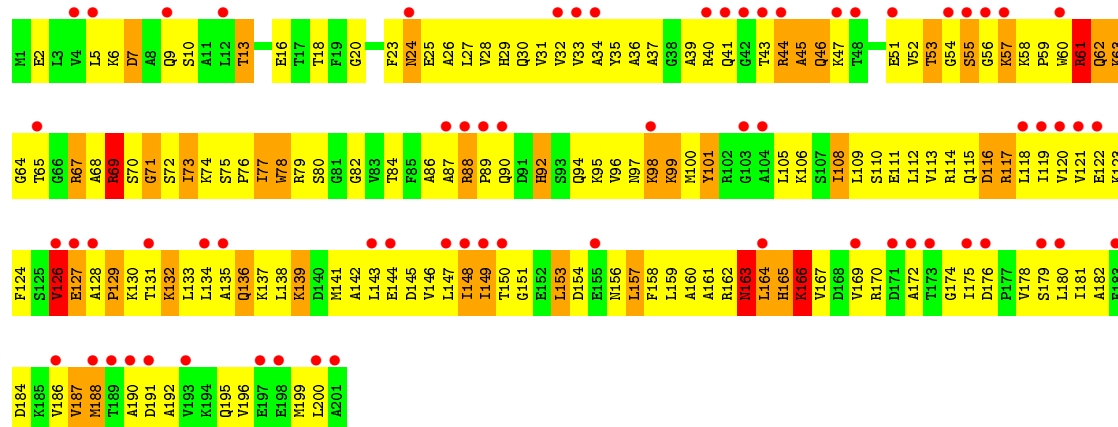
- Molecule 24: 50S ribosomal protein L2



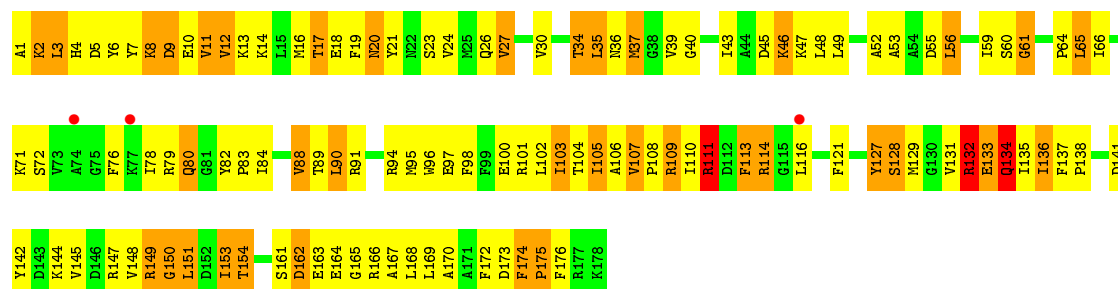




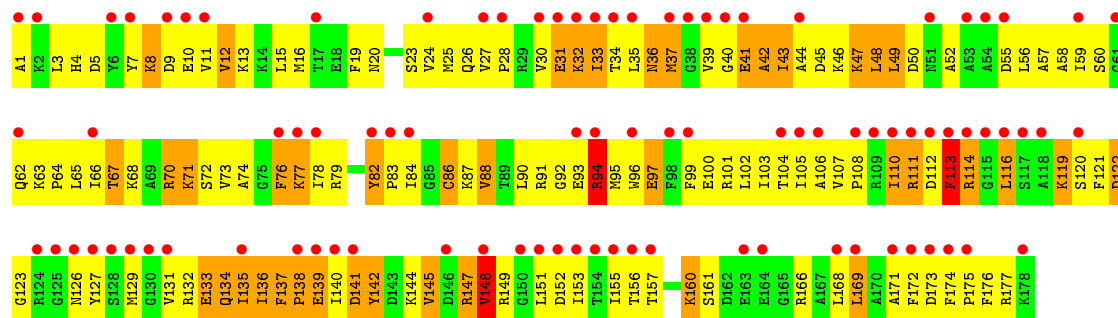
• Molecule 26: 50S ribosomal protein L4



• Molecule 27: 50S ribosomal protein L5

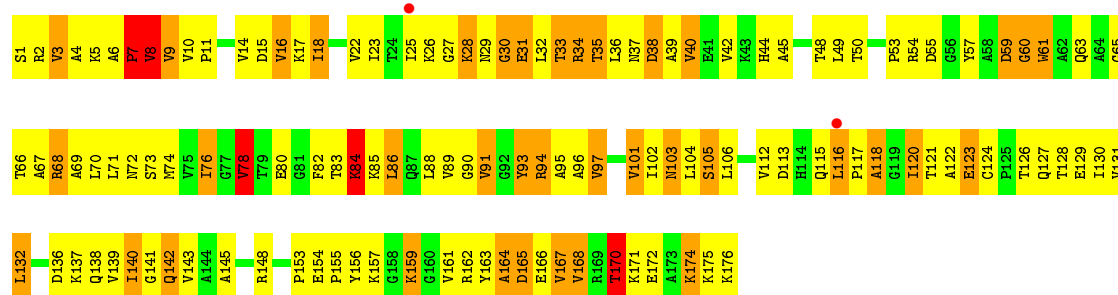


• Molecule 27: 50S ribosomal protein L5

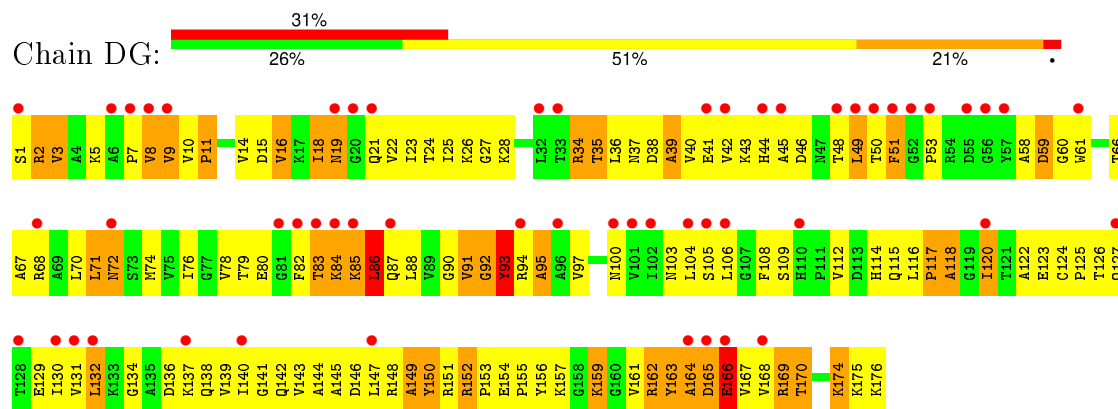


• Molecule 28: 50S ribosomal protein L6

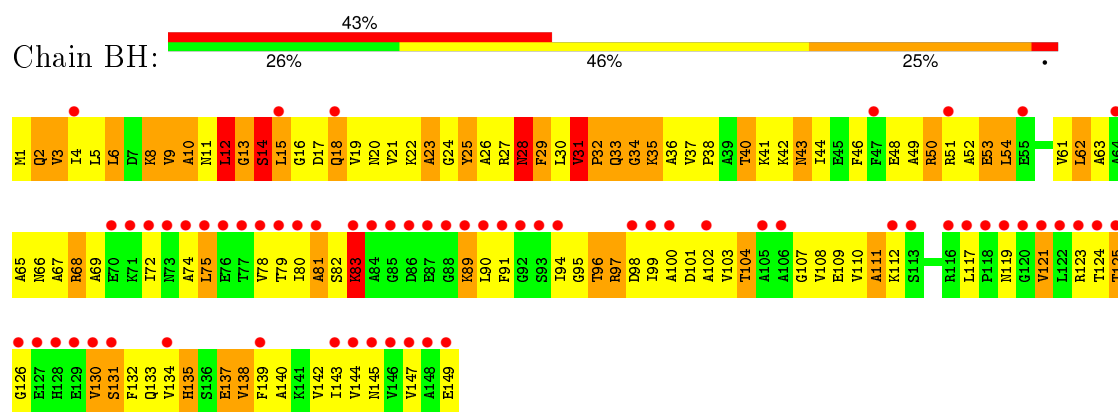




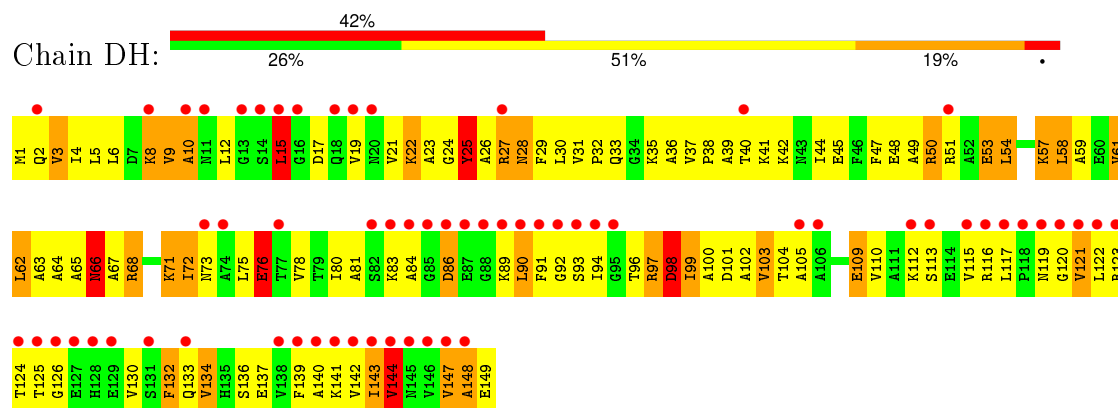
• Molecule 28: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L9



• Molecule 29: 50S ribosomal protein L9



Chain BI:

45%

29%

55%

15%

Chain DI:

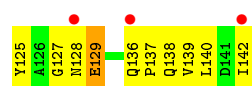
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V8	69%
K9	69%
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V23	69%
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Chain BJ:

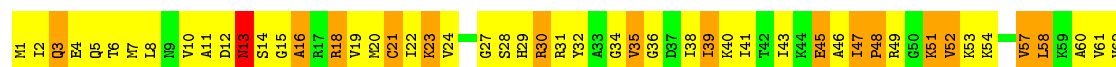
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Chain DJ:

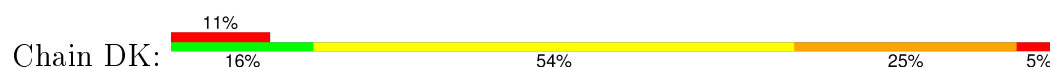
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Green	20%
Yellow	63%
Red (End)	15%



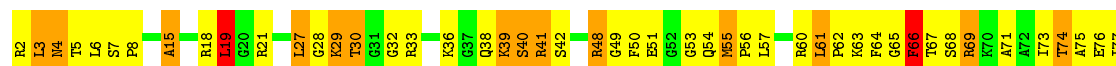
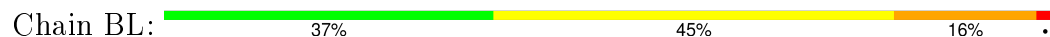
- Molecule 32: 50S ribosomal protein L14



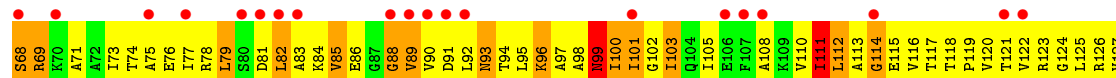
- Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15

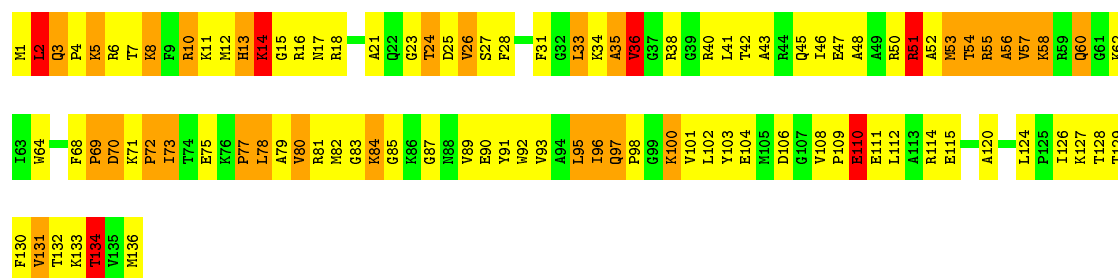


- Molecule 33: 50S ribosomal protein L15

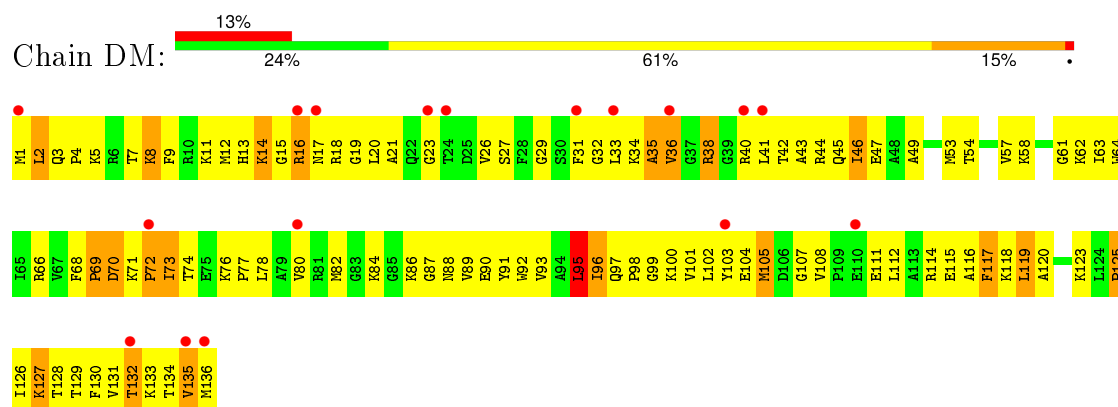


- Molecule 34: 50S ribosomal protein L16

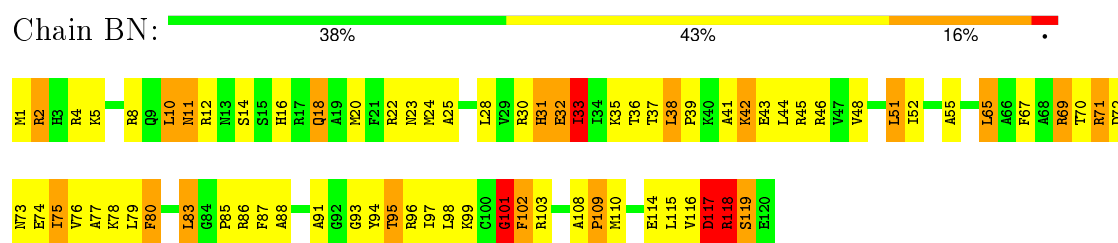




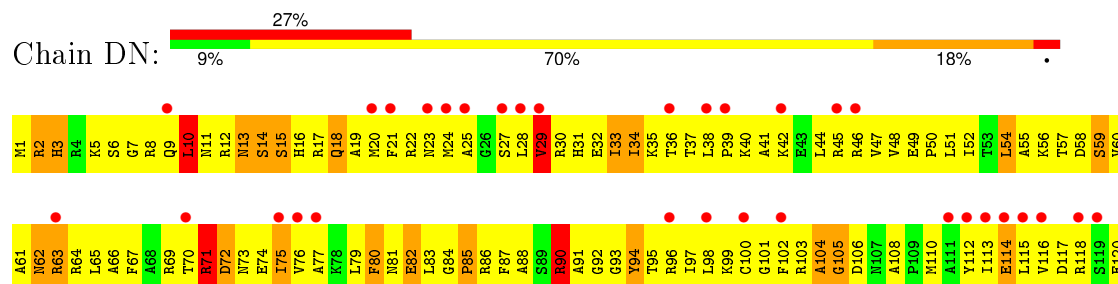
• Molecule 34: 50S ribosomal protein L16



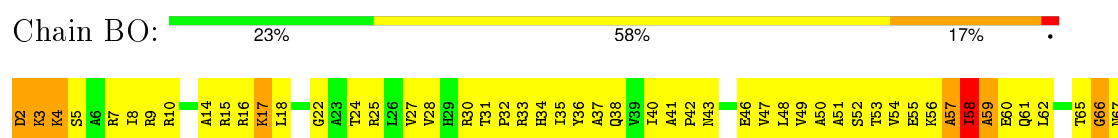
• Molecule 35: 50S ribosomal protein L17



• Molecule 35: 50S ribosomal protein L17

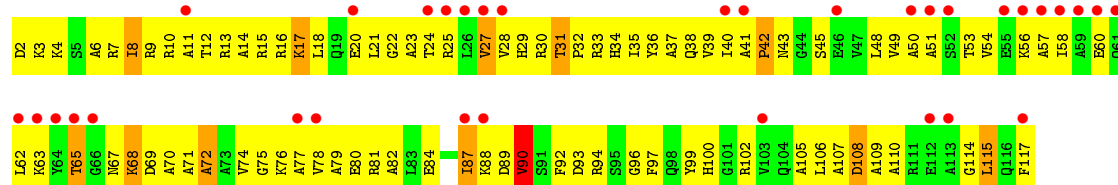


• Molecule 36: 50S ribosomal protein L18

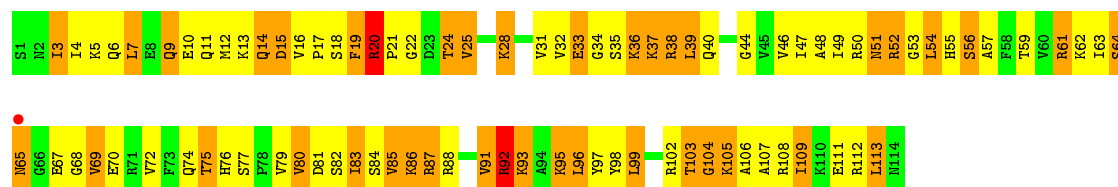
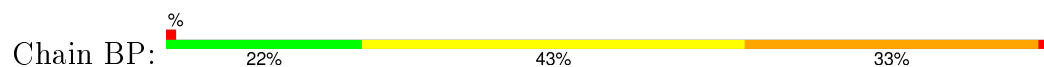




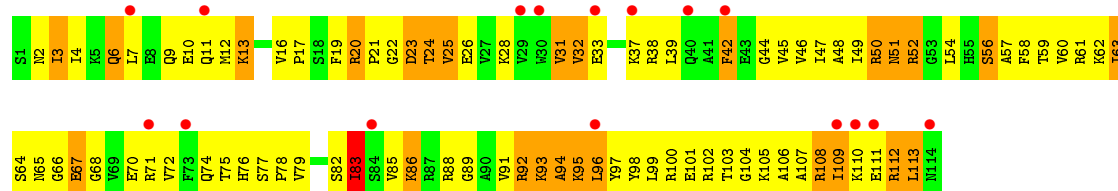
• Molecule 36: 50S ribosomal protein L18



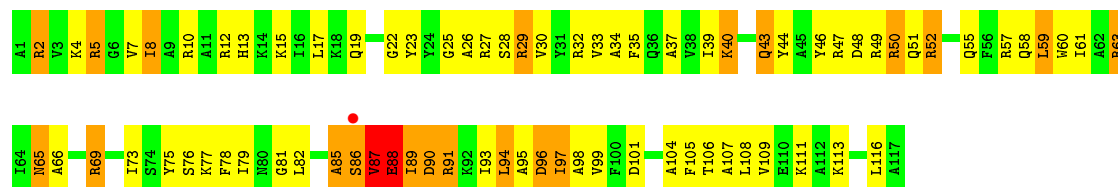
• Molecule 37: 50S ribosomal protein L19



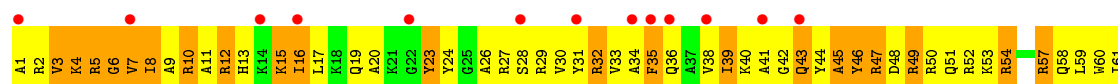
• Molecule 37: 50S ribosomal protein L19

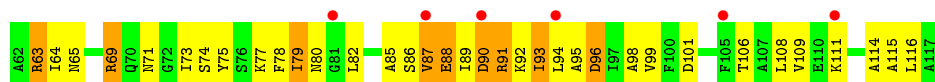


• Molecule 38: 50S ribosomal protein L20

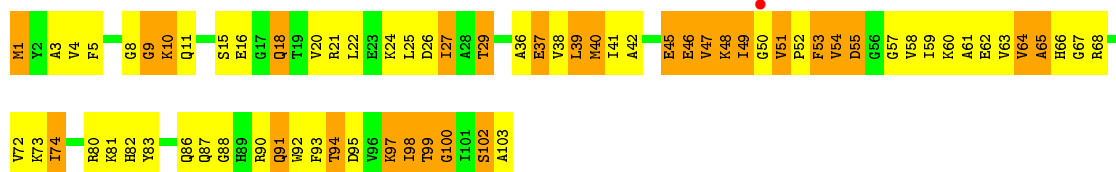


• Molecule 38: 50S ribosomal protein L20

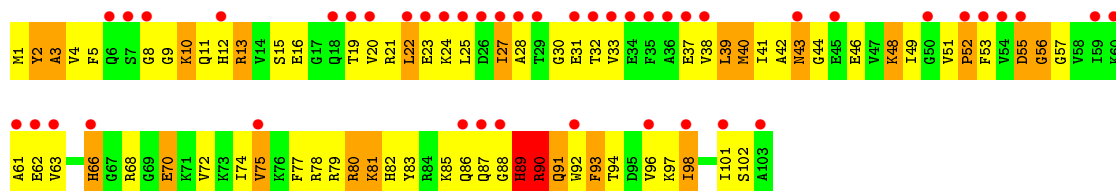




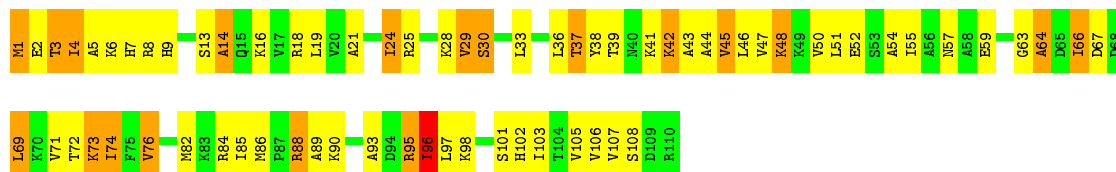
- Molecule 39: 50S ribosomal protein L21



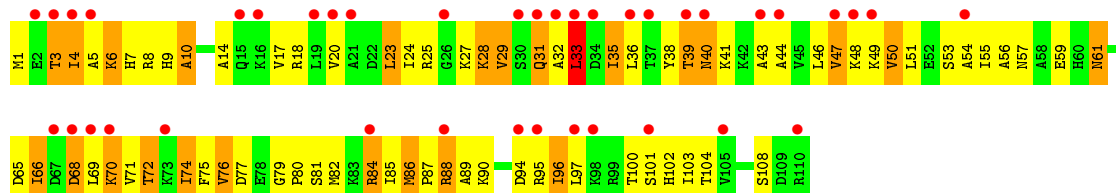
- Molecule 39: 50S ribosomal protein L21



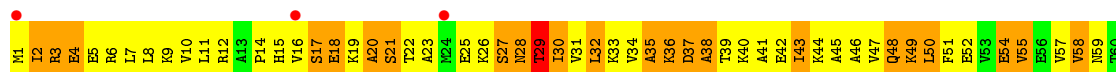
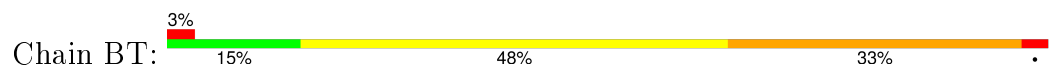
- Molecule 40: 50S ribosomal protein L22



- Molecule 40: 50S ribosomal protein L22

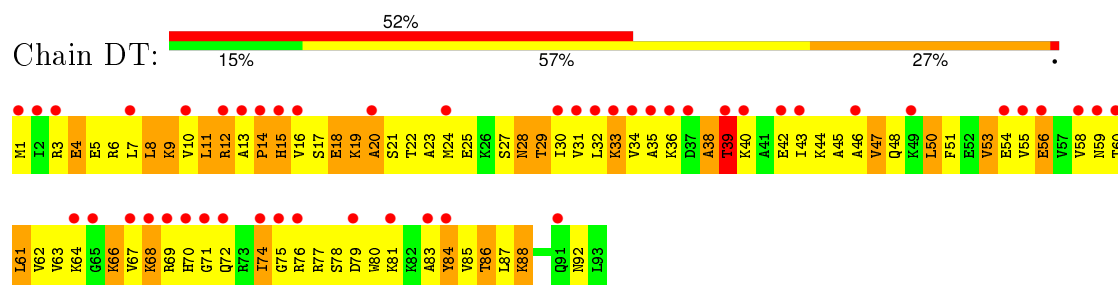


- Molecule 41: 50S ribosomal protein L23

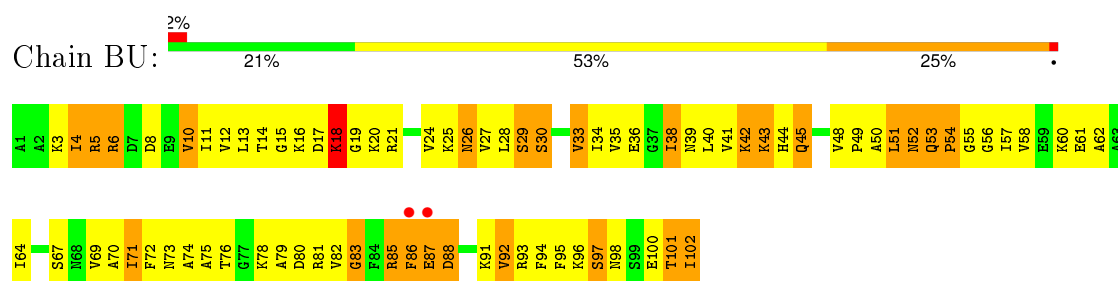




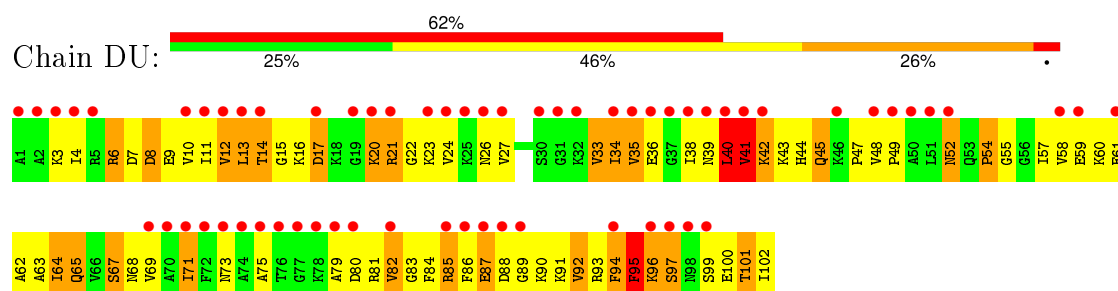
• Molecule 41: 50S ribosomal protein L23



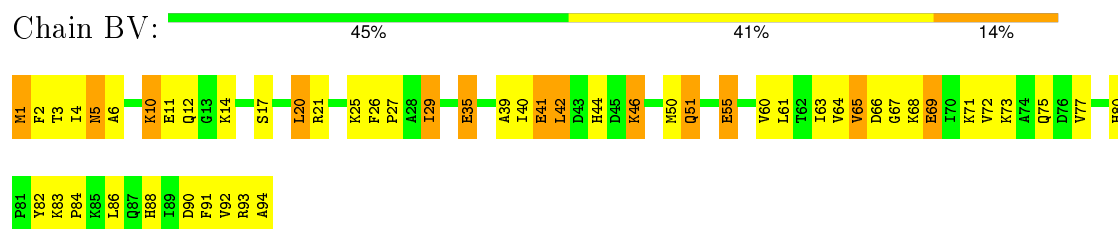
• Molecule 42: 50S ribosomal protein L24



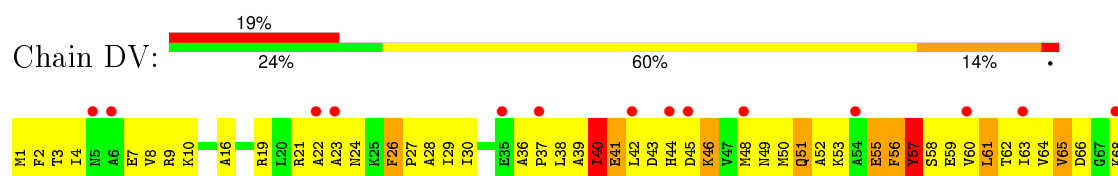
• Molecule 42: 50S ribosomal protein L24

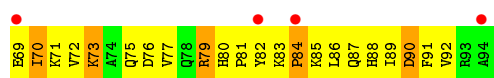


• Molecule 43: 50S ribosomal protein L25

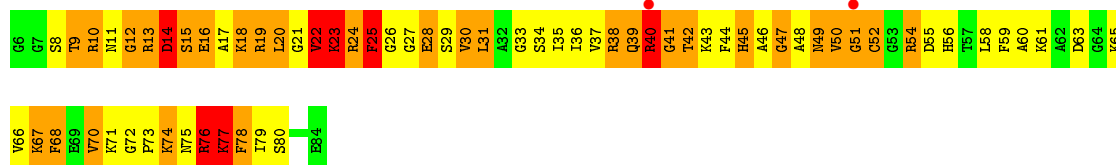
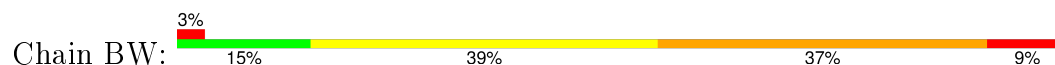


• Molecule 43: 50S ribosomal protein L25

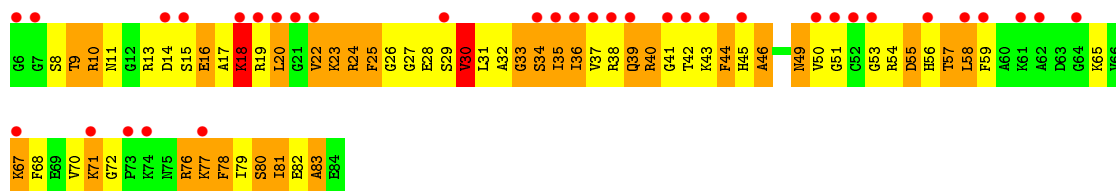
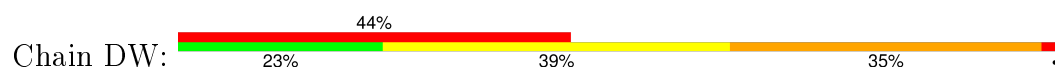




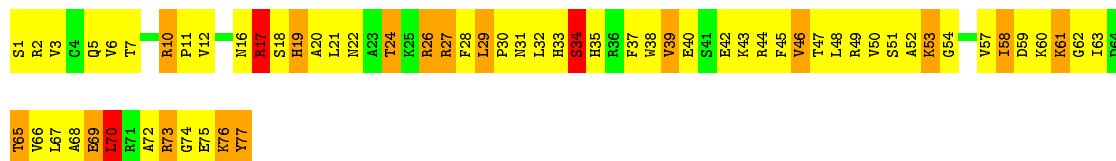
- Molecule 44: 50S ribosomal protein L27



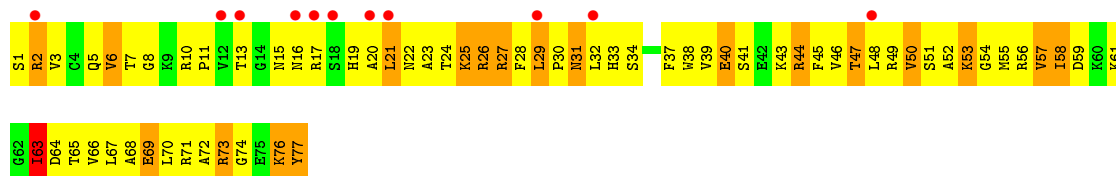
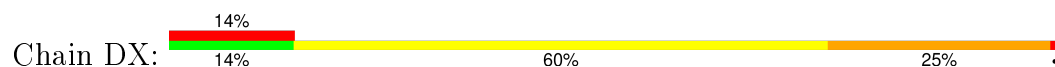
- Molecule 44: 50S ribosomal protein L27



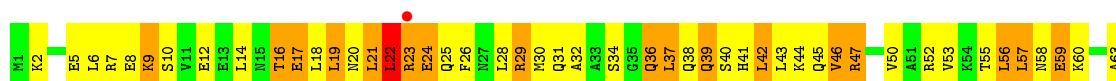
- Molecule 45: 50S ribosomal protein L28



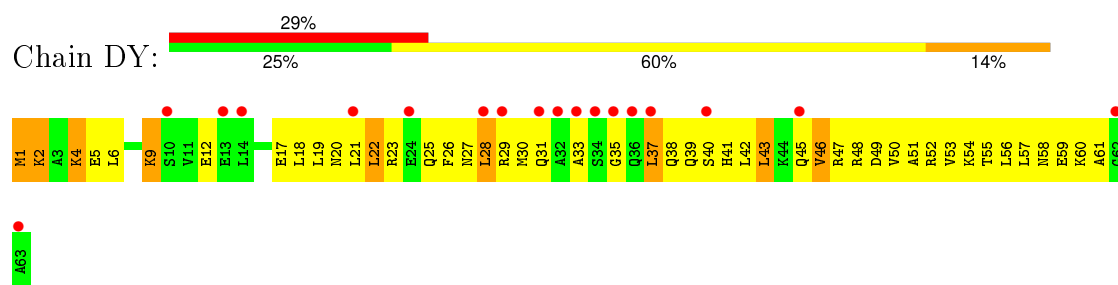
- Molecule 45: 50S ribosomal protein L28



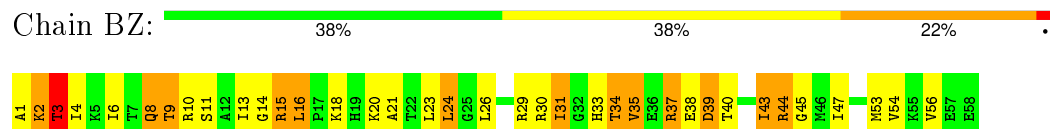
- Molecule 46: 50S ribosomal protein L29



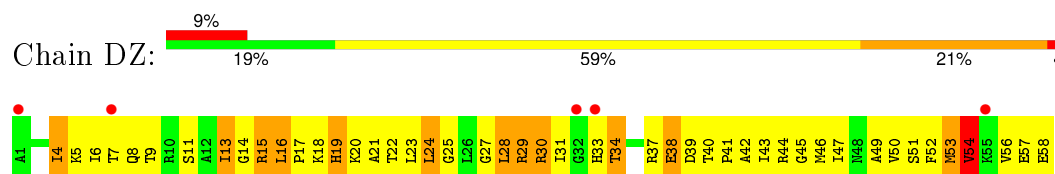
- Molecule 46: 50S ribosomal protein L29



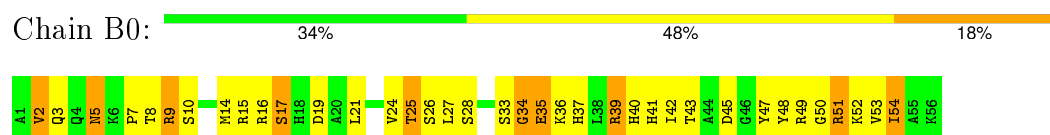
- Molecule 47: 50S ribosomal protein L30



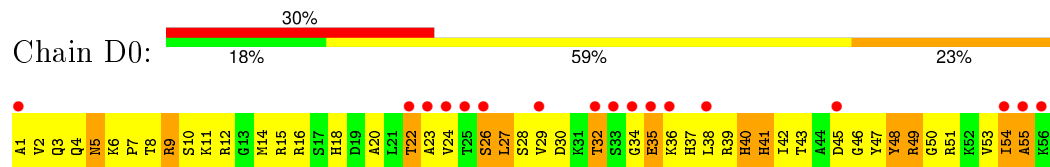
- Molecule 47: 50S ribosomal protein L30



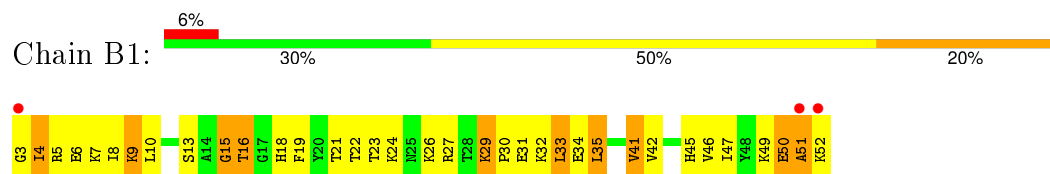
- Molecule 48: 50S ribosomal protein L32



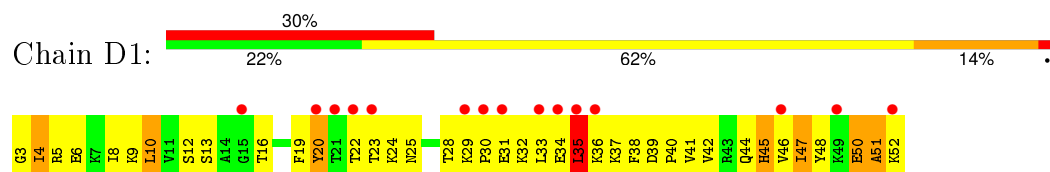
- Molecule 48: 50S ribosomal protein L32



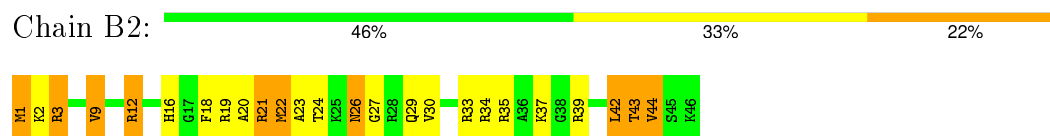
- Molecule 49: 50S ribosomal protein L33



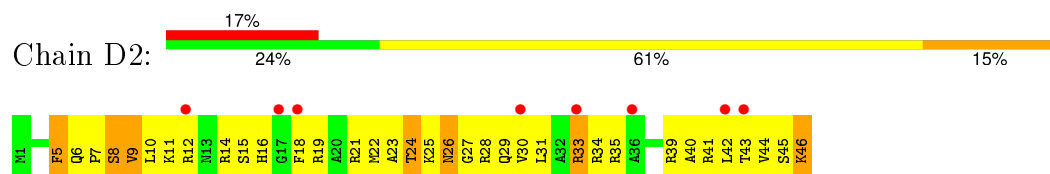
- Molecule 49: 50S ribosomal protein L33



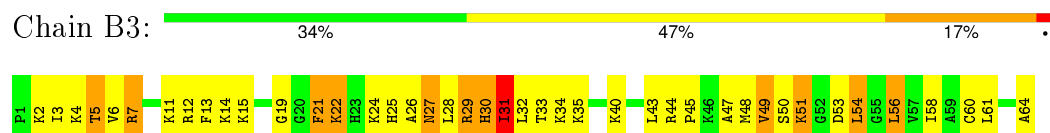
- Molecule 50: 50S ribosomal protein L34



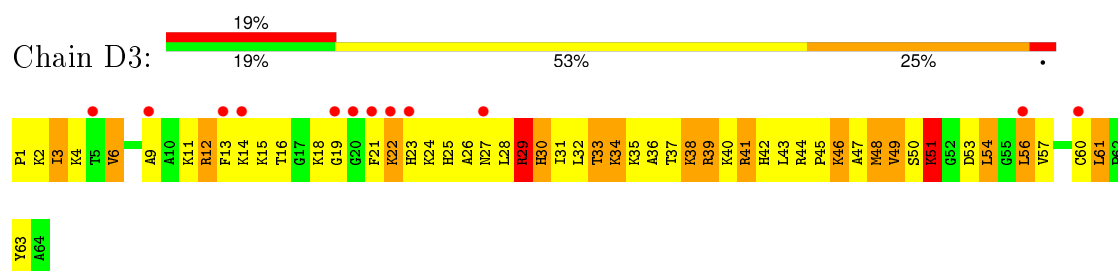
- Molecule 50: 50S ribosomal protein L34



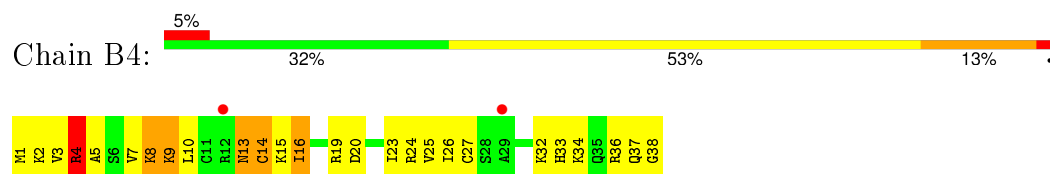
- Molecule 51: 50S ribosomal protein L35



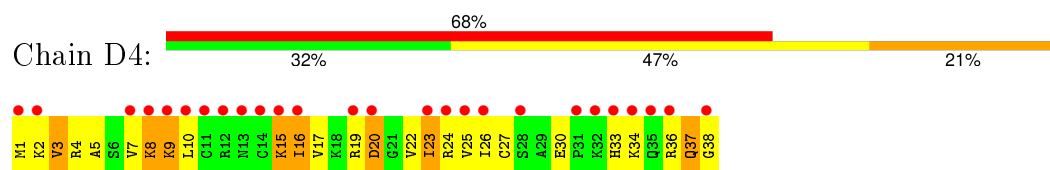
- Molecule 51: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.96Å 434.53Å 623.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.40 – 3.10 82.42 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (82.40-3.10) 83.9 (82.42-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.205 , 0.254 0.217 , 0.264	Depositor DCC
R_{free} test set	18658 reflections (2.21%)	DCC
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 79.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 925668 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	284525	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.53	0/36834	1.32	524/57462 (0.9%)
1	CA	0.46	0/36762	1.21	433/57350 (0.8%)
2	AB	0.24	0/1736	0.47	0/2338
2	CB	0.22	0/1736	0.44	0/2338
3	AC	0.27	0/1652	0.50	0/2225
3	CC	0.24	0/1652	0.44	0/2225
4	AD	0.30	0/1665	0.52	0/2227
4	CD	0.37	0/1665	0.61	0/2227
5	AE	0.34	0/1119	0.61	0/1504
5	CE	0.31	0/1119	0.55	0/1504
6	AF	0.29	0/836	0.47	0/1128
6	CF	0.28	0/836	0.51	0/1128
7	AG	0.22	0/1196	0.44	0/1602
7	CG	0.22	0/1188	0.44	0/1591
8	AH	0.32	0/989	0.56	0/1326
8	CH	0.27	0/989	0.49	0/1326
9	AI	0.23	0/1034	0.45	0/1375
9	CI	0.22	0/1034	0.41	0/1375
10	AJ	0.24	0/797	0.47	0/1077
10	CJ	0.21	0/797	0.47	0/1077
11	AK	0.27	0/893	0.53	0/1205
11	CK	0.26	0/893	0.50	0/1205
12	AL	0.38	0/969	0.69	0/1300
12	CL	0.32	0/969	0.56	0/1300
13	AM	0.23	0/893	0.49	0/1193
13	CM	0.27	1/885 (0.1%)	0.39	0/1183
14	AN	0.25	0/785	0.48	0/1043
14	CN	0.21	0/780	0.38	0/1036
15	AO	0.30	0/722	0.49	0/964
15	CO	0.25	0/722	0.44	0/964
16	AP	0.31	0/659	0.51	0/884
16	CP	0.33	0/649	0.53	0/872

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/658	0.59	0/881
17	CQ	0.26	0/658	0.50	0/881
18	AR	0.29	0/463	0.49	0/621
18	CR	0.28	0/463	0.46	0/621
19	AS	0.23	0/653	0.46	0/877
19	CS	0.21	0/653	0.41	0/877
20	AT	0.34	0/671	0.57	0/888
20	CT	0.26	0/671	0.51	0/888
21	AU	0.25	0/431	0.46	0/570
21	CU	0.31	0/431	0.58	0/570
22	BA	0.85	15/68626 (0.0%)	1.69	1674/107056 (1.6%)
22	DA	0.46	0/68314	1.26	901/106569 (0.8%)
23	BB	0.74	0/2828	1.56	46/4410 (1.0%)
23	DB	0.40	0/2803	1.09	27/4371 (0.6%)
24	BC	0.48	0/2122	0.74	1/2852 (0.0%)
24	DC	0.29	0/2122	0.54	0/2852
25	BD	0.61	0/1586	0.80	2/2134 (0.1%)
25	DD	0.28	0/1586	0.55	0/2134
26	BE	0.51	0/1571	0.73	0/2113
26	DE	0.25	0/1571	0.48	0/2113
27	BF	0.35	0/1435	0.55	0/1928
27	DF	0.21	0/1444	0.44	0/1937
28	BG	0.38	0/1343	0.61	0/1816
28	DG	0.21	0/1343	0.44	0/1816
29	BH	0.28	0/1122	0.51	0/1515
29	DH	0.26	0/1122	0.48	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.20	0/1046	0.42	0/1410
31	BJ	0.60	0/1152	0.84	1/1551 (0.1%)
31	DJ	0.27	0/1152	0.55	1/1551 (0.1%)
32	BK	0.61	1/948 (0.1%)	0.83	0/1268
32	DK	0.30	0/948	0.56	0/1268
33	BL	0.50	0/1054	0.80	2/1403 (0.1%)
33	DL	0.25	0/1054	0.51	0/1403
34	BM	0.55	0/1093	0.78	0/1460
34	DM	0.27	0/1093	0.49	0/1460
35	BN	0.55	0/974	0.82	2/1301 (0.2%)
35	DN	0.27	0/974	0.50	0/1301
36	BO	0.42	0/902	0.66	0/1209
36	DO	0.22	0/902	0.41	0/1209
37	BP	0.52	0/929	0.72	0/1242
37	DP	0.28	0/929	0.49	0/1242
38	BQ	0.72	0/960	0.89	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.27	0/960	0.46	0/1278
39	BR	0.67	2/829 (0.2%)	0.85	1/1107 (0.1%)
39	DR	0.27	0/829	0.48	0/1107
40	BS	0.63	0/864	0.84	0/1156
40	DS	0.26	0/864	0.51	0/1156
41	BT	0.51	0/745	0.80	0/994
41	DT	0.22	0/745	0.46	0/994
42	BU	0.44	0/788	0.75	0/1051
42	DU	0.23	0/788	0.45	0/1051
43	BV	0.47	0/766	0.65	0/1025
43	DV	0.23	0/766	0.43	0/1025
44	BW	0.67	0/603	0.93	1/797 (0.1%)
44	DW	0.24	0/603	0.48	0/797
45	BX	0.43	0/635	0.75	1/848 (0.1%)
45	DX	0.28	0/635	0.54	0/848
46	BY	0.39	0/510	0.63	0/677
46	DY	0.21	0/510	0.41	0/677
47	BZ	0.58	0/453	0.93	2/605 (0.3%)
47	DZ	0.25	0/453	0.49	0/605
48	B0	0.52	0/450	0.79	0/599
48	D0	0.27	0/450	0.49	0/599
49	B1	0.38	0/417	0.64	0/554
49	D1	0.23	0/417	0.46	0/554
50	B2	0.52	0/380	0.71	0/498
50	D2	0.27	0/380	0.52	0/498
51	B3	0.50	0/513	0.70	1/676 (0.1%)
51	D3	0.26	0/513	0.54	0/676
52	B4	0.41	0/303	0.64	0/397
52	D4	0.24	0/303	0.43	0/397
All	All	0.56	19/306773 (0.0%)	1.25	3621/458571 (0.8%)

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
12	AL	0	1
20	AT	0	1
25	BD	0	1
31	BJ	0	1
35	BN	0	1
All	All	0	5

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-8.33	1.32	1.37
22	BA	984	A	C5-C6	-7.40	1.34	1.41
39	BR	86	GLN	CB-CG	7.19	1.72	1.52
22	BA	1783	A	N7-C5	-6.87	1.35	1.39
22	BA	984	A	N9-C4	-5.90	1.34	1.37

The worst 5 of 3621 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	571	U	O4'-C1'-N1	17.46	122.17	108.20
22	BA	2848	G	P-O3'-C3'	17.00	140.09	119.70
22	BA	627	A	P-O3'-C3'	16.24	139.19	119.70
22	BA	984	A	N1-C6-N6	16.11	128.26	118.60
22	BA	1603	A	P-O3'-C3'	-15.84	100.69	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	AL	22	ALA	Peptide
20	AT	6	ALA	Peptide
25	BD	191	GLY	Peptide
31	BJ	110	PRO	Peptide
35	BN	101	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32895	0	16553	2319	0
1	CA	32831	0	16521	2706	0
2	AB	1705	0	1732	283	0
2	CB	1705	0	1732	260	0
3	AC	1625	0	1699	194	0
3	CC	1625	0	1699	238	0
4	AD	1643	0	1710	284	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CD	1643	0	1710	269	0
5	AE	1106	0	1148	203	0
5	CE	1106	0	1148	183	0
6	AF	818	0	808	113	0
6	CF	818	0	808	134	0
7	AG	1182	0	1240	150	0
7	CG	1175	0	1230	209	0
8	AH	979	0	1034	162	0
8	CH	979	0	1034	140	0
9	AI	1022	0	1070	165	0
9	CI	1022	0	1070	178	0
10	AJ	787	0	828	169	0
10	CJ	787	0	828	142	0
11	AK	877	0	887	165	0
11	CK	877	0	887	138	0
12	AL	955	0	1019	132	0
12	CL	955	0	1019	173	0
13	AM	884	0	944	120	0
13	CM	877	0	937	176	0
14	AN	774	0	827	131	0
14	CN	769	0	822	149	0
15	AO	714	0	737	93	0
15	CO	714	0	737	71	0
16	AP	649	0	666	105	0
16	CP	639	0	656	135	0
17	AQ	649	0	691	141	0
17	CQ	649	0	691	98	0
18	AR	456	0	478	51	0
18	CR	456	0	478	95	0
19	AS	638	0	665	97	0
19	CS	638	0	665	118	0
20	AT	665	0	714	117	0
20	CT	665	0	714	99	0
21	AU	426	0	449	131	0
21	CU	426	0	449	126	0
22	BA	61274	0	30819	3116	1
22	DA	60995	0	30679	5725	1
23	BB	2529	0	1281	109	0
23	DB	2507	0	1270	238	0
24	BC	2083	0	2157	313	0
24	DC	2083	0	2157	347	0
25	BD	1565	0	1616	274	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DD	1565	0	1616	319	0
26	BE	1552	0	1619	199	0
26	DE	1552	0	1619	321	0
27	BF	1411	0	1447	210	0
27	DF	1420	0	1460	289	0
28	BG	1323	0	1374	225	0
28	DG	1323	0	1374	229	0
29	BH	1111	0	1148	184	0
29	DH	1111	0	1148	208	0
30	BI	1032	0	1088	135	0
30	DI	1032	0	1088	149	0
31	BJ	1129	0	1162	214	0
31	DJ	1129	0	1162	205	0
32	BK	939	0	1012	150	0
32	DK	939	0	1012	188	0
33	BL	1045	0	1117	169	0
33	DL	1045	0	1117	224	0
34	BM	1074	0	1157	148	0
34	DM	1074	0	1157	156	0
35	BN	961	0	1000	131	0
35	DN	961	0	1000	228	0
36	BO	892	0	923	120	0
36	DO	892	0	923	118	0
37	BP	917	0	965	189	0
37	DP	917	0	965	184	0
38	BQ	947	0	1022	192	0
38	DQ	947	0	1022	203	0
39	BR	816	0	839	145	0
39	DR	816	0	839	147	0
40	BS	857	0	922	93	0
40	DS	857	0	922	125	0
41	BT	739	0	807	155	0
41	DT	739	0	807	174	0
42	BU	780	0	834	103	0
42	DU	780	0	834	147	0
43	BV	753	0	780	63	0
43	DV	753	0	780	118	0
44	BW	596	0	610	286	0
44	DW	596	0	610	180	0
45	BX	625	0	655	113	0
45	DX	625	0	655	128	0
46	BY	509	0	543	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DY	509	0	543	114	0
47	BZ	449	0	491	44	0
47	DZ	449	0	491	69	0
48	B0	444	0	461	52	0
48	D0	444	0	461	92	0
49	B1	410	0	440	66	0
49	D1	410	0	440	55	0
50	B2	377	0	418	29	0
50	D2	377	0	418	65	0
51	B3	504	0	574	71	0
51	D3	504	0	574	105	0
52	B4	302	0	340	48	0
52	D4	302	0	343	48	0
53	AA	41	0	0	0	0
53	AN	2	0	0	0	0
53	BA	135	0	0	0	0
53	BB	4	0	0	0	0
53	CA	42	0	0	0	0
53	DA	133	0	0	0	0
53	DB	1	0	0	0	0
53	DC	2	0	0	0	0
53	DJ	1	0	0	0	0
54	BA	51	0	67	4	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	197	0	0	12	0
56	AE	1	0	0	0	0
56	AL	1	0	0	0	0
56	AN	7	0	0	0	0
56	AT	1	0	0	0	0
56	AU	1	0	0	0	0
56	B3	3	0	0	0	0
56	B4	2	0	0	0	0
56	BA	605	0	0	46	0
56	BB	19	0	0	0	0
56	BC	7	0	0	0	0
56	BD	3	0	0	2	0
56	BE	1	0	0	1	0
56	BL	4	0	0	1	0
56	BN	2	0	0	0	0
56	BR	1	0	0	0	0
56	BT	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BV	1	0	0	1	0
56	CA	195	0	0	3	0
56	CE	3	0	0	1	0
56	CL	1	0	0	0	0
56	CN	3	0	0	0	0
56	CT	4	0	0	0	0
56	CU	1	0	0	0	0
56	D2	1	0	0	1	0
56	D3	1	0	0	0	0
56	D4	4	0	0	0	0
56	DA	600	0	0	30	0
56	DB	3	0	0	0	0
56	DC	13	0	0	2	0
56	DD	2	0	0	0	0
56	DE	4	0	0	0	0
56	DJ	3	0	0	0	0
56	DL	4	0	0	1	0
56	DN	2	0	0	0	0
56	DT	2	0	0	0	0
56	DU	2	0	0	0	0
56	DV	2	0	0	0	0
All	All	284525	0	190908	27236	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 58.

The worst 5 of 27236 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)
37:BP:50:ARG:CG	37:BP:57:ALA:H	1.24	1.44
37:BP:50:ARG:HD2	37:BP:51:ASN:N	1.27	1.42
37:BP:50:ARG:HG2	37:BP:57:ALA:N	1.13	1.41
1:CA:238:A:C2'	1:CA:239:U:H5''	1.57	1.34
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.37	1.34

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:138:U:O4	22:DA:305:C:OP1[3_545]	2.02	0.18

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	133 (62%)	51 (24%)	32 (15%)	0	1
2	CB	216/218 (99%)	158 (73%)	38 (18%)	20 (9%)	1	4
3	AC	204/206 (99%)	144 (71%)	36 (18%)	24 (12%)	0	2
3	CC	204/206 (99%)	138 (68%)	47 (23%)	19 (9%)	1	4
4	AD	203/205 (99%)	127 (63%)	43 (21%)	33 (16%)	0	0
4	CD	203/205 (99%)	138 (68%)	40 (20%)	25 (12%)	0	2
5	AE	148/150 (99%)	97 (66%)	28 (19%)	23 (16%)	0	0
5	CE	148/150 (99%)	111 (75%)	21 (14%)	16 (11%)	0	3
6	AF	98/100 (98%)	71 (72%)	15 (15%)	12 (12%)	0	2
6	CF	98/100 (98%)	66 (67%)	19 (19%)	13 (13%)	0	1
7	AG	149/151 (99%)	100 (67%)	37 (25%)	12 (8%)	1	6
7	CG	148/151 (98%)	96 (65%)	38 (26%)	14 (10%)	1	4
8	AH	127/129 (98%)	101 (80%)	15 (12%)	11 (9%)	1	5
8	CH	127/129 (98%)	96 (76%)	23 (18%)	8 (6%)	2	10
9	AI	125/127 (98%)	81 (65%)	28 (22%)	16 (13%)	0	1
9	CI	125/127 (98%)	84 (67%)	32 (26%)	9 (7%)	1	7
10	AJ	96/98 (98%)	69 (72%)	10 (10%)	17 (18%)	0	0
10	CJ	96/98 (98%)	61 (64%)	21 (22%)	14 (15%)	0	1
11	AK	115/117 (98%)	80 (70%)	20 (17%)	15 (13%)	0	1
11	CK	115/117 (98%)	87 (76%)	16 (14%)	12 (10%)	1	3
12	AL	121/123 (98%)	88 (73%)	21 (17%)	12 (10%)	1	4
12	CL	121/123 (98%)	84 (69%)	24 (20%)	13 (11%)	0	3
13	AM	112/114 (98%)	83 (74%)	19 (17%)	10 (9%)	1	5
13	CM	112/114 (98%)	62 (55%)	37 (33%)	13 (12%)	0	2
14	AN	92/100 (92%)	60 (65%)	18 (20%)	14 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	91/100 (91%)	57 (63%)	26 (29%)	8 (9%)	1	5
15	AO	86/88 (98%)	59 (69%)	19 (22%)	8 (9%)	1	4
15	CO	86/88 (98%)	53 (62%)	30 (35%)	3 (4%)	4	24
16	AP	80/82 (98%)	59 (74%)	12 (15%)	9 (11%)	0	2
16	CP	79/82 (96%)	48 (61%)	23 (29%)	8 (10%)	1	4
17	AQ	78/80 (98%)	48 (62%)	24 (31%)	6 (8%)	1	6
17	CQ	78/80 (98%)	59 (76%)	11 (14%)	8 (10%)	1	4
18	AR	53/55 (96%)	40 (76%)	10 (19%)	3 (6%)	2	12
18	CR	53/55 (96%)	33 (62%)	17 (32%)	3 (6%)	2	12
19	AS	77/79 (98%)	51 (66%)	15 (20%)	11 (14%)	0	1
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	5
20	AT	83/85 (98%)	57 (69%)	21 (25%)	5 (6%)	2	11
20	CT	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	0	2
21	AU	49/51 (96%)	25 (51%)	12 (24%)	12 (24%)	0	0
21	CU	49/51 (96%)	20 (41%)	13 (26%)	16 (33%)	0	0
24	BC	269/271 (99%)	197 (73%)	46 (17%)	26 (10%)	1	4
24	DC	269/271 (99%)	174 (65%)	64 (24%)	31 (12%)	0	2
25	BD	207/209 (99%)	141 (68%)	32 (16%)	34 (16%)	0	0
25	DD	207/209 (99%)	131 (63%)	41 (20%)	35 (17%)	0	0
26	BE	199/201 (99%)	144 (72%)	35 (18%)	20 (10%)	1	4
26	DE	199/201 (99%)	115 (58%)	54 (27%)	30 (15%)	0	0
27	BF	176/178 (99%)	124 (70%)	36 (20%)	16 (9%)	1	5
27	DF	176/178 (99%)	87 (49%)	58 (33%)	31 (18%)	0	0
28	BG	174/176 (99%)	111 (64%)	38 (22%)	25 (14%)	0	1
28	DG	174/176 (99%)	99 (57%)	40 (23%)	35 (20%)	0	0
29	BH	147/149 (99%)	62 (42%)	50 (34%)	35 (24%)	0	0
29	DH	147/149 (99%)	70 (48%)	54 (37%)	23 (16%)	0	0
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	1	4
30	DI	139/141 (99%)	75 (54%)	48 (34%)	16 (12%)	0	2
31	BJ	140/142 (99%)	104 (74%)	24 (17%)	12 (9%)	1	5
31	DJ	140/142 (99%)	92 (66%)	28 (20%)	20 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BK	120/122 (98%)	89 (74%)	17 (14%)	14 (12%)	0	2
32	DK	120/122 (98%)	76 (63%)	17 (14%)	27 (22%)	0	0
33	BL	141/143 (99%)	100 (71%)	30 (21%)	11 (8%)	1	6
33	DL	141/143 (99%)	77 (55%)	44 (31%)	20 (14%)	0	1
34	BM	134/136 (98%)	96 (72%)	18 (13%)	20 (15%)	0	1
34	DM	134/136 (98%)	90 (67%)	26 (19%)	18 (13%)	0	1
35	BN	118/120 (98%)	91 (77%)	16 (14%)	11 (9%)	1	4
35	DN	118/120 (98%)	74 (63%)	25 (21%)	19 (16%)	0	0
36	BO	114/116 (98%)	85 (75%)	18 (16%)	11 (10%)	1	4
36	DO	114/116 (98%)	74 (65%)	30 (26%)	10 (9%)	1	5
37	BP	112/114 (98%)	78 (70%)	20 (18%)	14 (12%)	0	1
37	DP	112/114 (98%)	60 (54%)	31 (28%)	21 (19%)	0	0
38	BQ	115/117 (98%)	100 (87%)	7 (6%)	8 (7%)	1	8
38	DQ	115/117 (98%)	75 (65%)	27 (24%)	13 (11%)	0	2
39	BR	101/103 (98%)	76 (75%)	14 (14%)	11 (11%)	0	3
39	DR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	1
40	BS	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	3	17
40	DS	108/110 (98%)	72 (67%)	25 (23%)	11 (10%)	1	4
41	BT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	0
41	DT	91/93 (98%)	41 (45%)	26 (29%)	24 (26%)	0	0
42	BU	100/102 (98%)	66 (66%)	16 (16%)	18 (18%)	0	0
42	DU	100/102 (98%)	52 (52%)	22 (22%)	26 (26%)	0	0
43	BV	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	8	36
43	DV	92/94 (98%)	60 (65%)	24 (26%)	8 (9%)	1	5
44	BW	77/79 (98%)	31 (40%)	22 (29%)	24 (31%)	0	0
44	DW	77/79 (98%)	30 (39%)	25 (32%)	22 (29%)	0	0
45	BX	75/77 (97%)	58 (77%)	10 (13%)	7 (9%)	1	4
45	DX	75/77 (97%)	44 (59%)	20 (27%)	11 (15%)	0	1
46	BY	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	1
46	DY	61/63 (97%)	40 (66%)	16 (26%)	5 (8%)	1	6
47	BZ	56/58 (97%)	47 (84%)	5 (9%)	4 (7%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DZ	56/58 (97%)	31 (55%)	20 (36%)	5 (9%)	1	5
48	B0	54/56 (96%)	41 (76%)	9 (17%)	4 (7%)	1	7
48	D0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	1	4
49	B1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	1	3
49	D1	48/50 (96%)	35 (73%)	8 (17%)	5 (10%)	1	3
50	B2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
50	D2	44/46 (96%)	29 (66%)	10 (23%)	5 (11%)	0	2
51	B3	62/64 (97%)	53 (86%)	5 (8%)	4 (6%)	1	9
51	D3	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0	1
52	B4	36/38 (95%)	24 (67%)	9 (25%)	3 (8%)	1	6
52	D4	36/38 (95%)	21 (58%)	9 (25%)	6 (17%)	0	0
All	All	11241/11452 (98%)	7412 (66%)	2420 (22%)	1409 (12%)	0	1

5 of 1409 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	21	TYR
2	AB	33	ALA
2	AB	37	VAL
2	AB	72	LYS
2	AB	75	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	142 (79%)	38 (21%)	1	6
2	CB	180/180 (100%)	154 (86%)	26 (14%)	4	17
3	AC	170/170 (100%)	136 (80%)	34 (20%)	1	7
3	CC	170/170 (100%)	153 (90%)	17 (10%)	9	34
4	AD	172/172 (100%)	138 (80%)	34 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/172 (100%)	131 (76%)	41 (24%)	1	3
5	AE	113/113 (100%)	77 (68%)	36 (32%)	0	0
5	CE	113/113 (100%)	89 (79%)	24 (21%)	1	6
6	AF	87/87 (100%)	71 (82%)	16 (18%)	2	9
6	CF	87/87 (100%)	73 (84%)	14 (16%)	3	13
7	AG	124/124 (100%)	111 (90%)	13 (10%)	8	31
7	CG	123/124 (99%)	101 (82%)	22 (18%)	2	10
8	AH	104/104 (100%)	83 (80%)	21 (20%)	1	7
8	CH	104/104 (100%)	91 (88%)	13 (12%)	6	22
9	AI	105/105 (100%)	82 (78%)	23 (22%)	1	5
9	CI	105/105 (100%)	89 (85%)	16 (15%)	3	14
10	AJ	86/86 (100%)	70 (81%)	16 (19%)	2	9
10	CJ	86/86 (100%)	73 (85%)	13 (15%)	3	15
11	AK	90/90 (100%)	73 (81%)	17 (19%)	2	8
11	CK	90/90 (100%)	79 (88%)	11 (12%)	6	24
12	AL	103/103 (100%)	76 (74%)	27 (26%)	0	2
12	CL	103/103 (100%)	78 (76%)	25 (24%)	1	3
13	AM	92/92 (100%)	84 (91%)	8 (9%)	13	44
13	CM	91/92 (99%)	81 (89%)	10 (11%)	8	30
14	AN	79/83 (95%)	71 (90%)	8 (10%)	9	33
14	CN	79/83 (95%)	69 (87%)	10 (13%)	5	22
15	AO	76/76 (100%)	59 (78%)	17 (22%)	1	4
15	CO	76/76 (100%)	69 (91%)	7 (9%)	11	40
16	AP	65/65 (100%)	54 (83%)	11 (17%)	2	11
16	CP	65/65 (100%)	50 (77%)	15 (23%)	1	4
17	AQ	74/74 (100%)	60 (81%)	14 (19%)	2	8
17	CQ	74/74 (100%)	62 (84%)	12 (16%)	3	12
18	AR	48/48 (100%)	44 (92%)	4 (8%)	14	46
18	CR	48/48 (100%)	40 (83%)	8 (17%)	3	11
19	AS	70/70 (100%)	63 (90%)	7 (10%)	9	34
19	CS	70/70 (100%)	64 (91%)	6 (9%)	13	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AT	65/65 (100%)	48 (74%)	17 (26%)	0	2
20	CT	65/65 (100%)	52 (80%)	13 (20%)	1	7
21	AU	44/44 (100%)	36 (82%)	8 (18%)	2	9
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0	0
24	BC	216/216 (100%)	170 (79%)	46 (21%)	1	6
24	DC	216/216 (100%)	178 (82%)	38 (18%)	2	10
25	BD	164/164 (100%)	133 (81%)	31 (19%)	2	8
25	DD	164/164 (100%)	131 (80%)	33 (20%)	1	7
26	BE	165/165 (100%)	111 (67%)	54 (33%)	0	0
26	DE	165/165 (100%)	143 (87%)	22 (13%)	5	20
27	BF	148/149 (99%)	116 (78%)	32 (22%)	1	5
27	DF	149/149 (100%)	124 (83%)	25 (17%)	2	11
28	BG	137/137 (100%)	106 (77%)	31 (23%)	1	4
28	DG	137/137 (100%)	117 (85%)	20 (15%)	4	16
29	BH	114/114 (100%)	96 (84%)	18 (16%)	3	13
29	DH	114/114 (100%)	90 (79%)	24 (21%)	1	6
30	BI	109/109 (100%)	91 (84%)	18 (16%)	3	12
30	DI	109/109 (100%)	103 (94%)	6 (6%)	27	63
31	BJ	116/116 (100%)	92 (79%)	24 (21%)	1	6
31	DJ	116/116 (100%)	101 (87%)	15 (13%)	5	21
32	BK	103/103 (100%)	77 (75%)	26 (25%)	1	2
32	DK	103/103 (100%)	84 (82%)	19 (18%)	2	9
33	BL	102/102 (100%)	82 (80%)	20 (20%)	1	7
33	DL	102/102 (100%)	89 (87%)	13 (13%)	5	22
34	BM	109/109 (100%)	81 (74%)	28 (26%)	0	2
34	DM	109/109 (100%)	98 (90%)	11 (10%)	9	33
35	BN	100/100 (100%)	82 (82%)	18 (18%)	2	10
35	DN	100/100 (100%)	85 (85%)	15 (15%)	3	15
36	BO	86/86 (100%)	67 (78%)	19 (22%)	1	5
36	DO	86/86 (100%)	79 (92%)	7 (8%)	15	47
37	BP	99/99 (100%)	66 (67%)	33 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DP	99/99 (100%)	88 (89%)	11 (11%)	8	29
38	BQ	89/89 (100%)	68 (76%)	21 (24%)	1	3
38	DQ	89/89 (100%)	69 (78%)	20 (22%)	1	4
39	BR	84/84 (100%)	66 (79%)	18 (21%)	1	5
39	DR	84/84 (100%)	69 (82%)	15 (18%)	2	10
40	BS	93/93 (100%)	72 (77%)	21 (23%)	1	4
40	DS	93/93 (100%)	72 (77%)	21 (23%)	1	4
41	BT	80/80 (100%)	53 (66%)	27 (34%)	0	0
41	DT	80/80 (100%)	75 (94%)	5 (6%)	22	58
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	6
42	DU	83/83 (100%)	72 (87%)	11 (13%)	5	20
43	BV	78/78 (100%)	62 (80%)	16 (20%)	1	6
43	DV	78/78 (100%)	66 (85%)	12 (15%)	3	14
44	BW	59/59 (100%)	38 (64%)	21 (36%)	0	0
44	DW	59/59 (100%)	45 (76%)	14 (24%)	1	3
45	BX	67/67 (100%)	51 (76%)	16 (24%)	1	3
45	DX	67/67 (100%)	55 (82%)	12 (18%)	2	10
46	BY	55/55 (100%)	42 (76%)	13 (24%)	1	3
46	DY	55/55 (100%)	51 (93%)	4 (7%)	17	52
47	BZ	48/48 (100%)	35 (73%)	13 (27%)	0	1
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	6
48	B0	47/47 (100%)	39 (83%)	8 (17%)	2	11
48	D0	47/47 (100%)	38 (81%)	9 (19%)	2	8
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	10
49	D1	45/45 (100%)	38 (84%)	7 (16%)	3	14
50	B2	38/38 (100%)	27 (71%)	11 (29%)	0	1
50	D2	38/38 (100%)	33 (87%)	5 (13%)	5	20
51	B3	51/51 (100%)	42 (82%)	9 (18%)	2	10
51	D3	51/51 (100%)	37 (72%)	14 (28%)	0	1
52	B4	34/34 (100%)	28 (82%)	6 (18%)	2	10
52	D4	34/34 (100%)	30 (88%)	4 (12%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9331/9342 (100%)	7599 (81%)	1732 (19%)	2 9

5 of 1732 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	BQ	89	ILE
50	B2	12	ARG
39	DR	86	GLN
40	BS	1	MET
43	BV	41	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 360 such sidechains are listed below:

Mol	Chain	Res	Type
41	BT	48	GLN
3	CC	139	ASN
42	DU	39	ASN
42	BU	73	ASN
48	B0	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	518 (33%)	236 (15%)
1	CA	1529/1533 (99%)	572 (37%)	242 (15%)
22	BA	2850/2904 (98%)	913 (32%)	429 (15%)
22	DA	2839/2904 (97%)	1105 (38%)	498 (17%)
23	BB	117/118 (99%)	34 (29%)	17 (14%)
23	DB	116/118 (98%)	44 (37%)	16 (13%)
All	All	8983/9110 (98%)	3186 (35%)	1438 (16%)

5 of 3186 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G

5 of 1438 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2781	A
1	CA	701	U
22	DA	2300	C
23	BB	25	U
1	CA	279	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 364 ligands modelled in this entry, 363 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	ERY	BA	3136	-	53,53,53	0.74	0	82,82,82	1.65	16 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	ERY	BA	3136	-	-	0/72/107/107	0/3/3/3

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	3136	ERY	C25-C24-C23	-4.98	102.77	110.03
54	BA	3136	ERY	O7-C5-C6	-4.70	100.45	106.44
54	BA	3136	ERY	C3-C2-C1	-3.52	102.98	109.86
54	BA	3136	ERY	O2-C1-O1	-3.22	117.27	123.89
54	BA	3136	ERY	C15-C16-C17	-3.05	103.99	107.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	BA	3136	ERY	4	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	1533/1533 (100%)	-0.56	17 (1%) 82 66	21, 74, 188, 404	0
1	CA	1530/1533 (99%)	0.05	46 (3%) 54 29	38, 102, 287, 422	0
2	AB	218/218 (100%)	1.63	73 (33%) 0 0	72, 142, 202, 237	0
2	CB	218/218 (100%)	1.62	72 (33%) 0 0	98, 165, 222, 272	0
3	AC	206/206 (100%)	0.69	24 (11%) 6 2	54, 101, 149, 187	0
3	CC	206/206 (100%)	1.19	50 (24%) 1 0	80, 139, 210, 243	0
4	AD	205/205 (100%)	-0.04	8 (3%) 43 21	38, 80, 182, 310	0
4	CD	205/205 (100%)	-0.25	1 (0%) 91 83	29, 54, 103, 236	0
5	AE	150/150 (100%)	-0.08	3 (2%) 68 46	37, 70, 136, 207	0
5	CE	150/150 (100%)	0.36	3 (2%) 68 46	38, 87, 150, 253	0
6	AF	100/100 (100%)	-0.16	0 100 100	43, 85, 149, 174	0
6	CF	100/100 (100%)	0.05	4 (4%) 42 20	58, 109, 180, 202	0
7	AG	151/151 (100%)	0.26	9 (5%) 25 10	82, 155, 235, 286	0
7	CG	150/151 (99%)	2.39	69 (46%) 0 0	112, 196, 246, 272	0
8	AH	129/129 (100%)	-0.02	4 (3%) 52 28	41, 69, 120, 203	0
8	CH	129/129 (100%)	0.67	14 (10%) 7 2	52, 107, 161, 197	0
9	AI	127/127 (100%)	0.92	17 (13%) 4 2	68, 153, 256, 288	0
9	CI	127/127 (100%)	1.90	49 (38%) 0 0	102, 200, 285, 325	0
10	AJ	98/98 (100%)	0.65	18 (18%) 2 1	60, 119, 200, 251	0
10	CJ	98/98 (100%)	2.89	58 (59%) 0 0	102, 192, 267, 283	0
11	AK	117/117 (100%)	0.68	12 (10%) 9 3	38, 104, 176, 222	0
11	CK	117/117 (100%)	0.30	4 (3%) 49 24	53, 102, 161, 200	0
12	AL	123/123 (100%)	-0.33	2 (1%) 74 55	16, 49, 111, 187	0
12	CL	123/123 (100%)	0.22	3 (2%) 62 39	41, 81, 128, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.49	13 (11%) 7 2	69, 139, 213, 258	0
13	CM	114/114 (100%)	2.36	61 (53%) 0 0	190, 427, 522, 545	0
14	AN	96/100 (96%)	0.40	6 (6%) 23 9	68, 111, 199, 266	0
14	CN	95/100 (95%)	2.15	44 (46%) 0 0	112, 209, 319, 350	0
15	AO	88/88 (100%)	-0.40	0 100 100	34, 70, 111, 172	0
15	CO	88/88 (100%)	-0.12	1 (1%) 82 66	68, 112, 187, 286	0
16	AP	82/82 (100%)	0.73	10 (12%) 5 2	45, 68, 174, 288	0
16	CP	81/82 (98%)	0.75	10 (12%) 5 2	46, 97, 157, 229	0
17	AQ	80/80 (100%)	0.43	7 (8%) 12 4	35, 71, 134, 209	0
17	CQ	80/80 (100%)	0.85	12 (15%) 3 1	47, 103, 151, 188	0
18	AR	55/55 (100%)	0.13	3 (5%) 29 12	50, 80, 154, 211	0
18	CR	55/55 (100%)	-0.05	2 (3%) 46 23	51, 87, 157, 235	0
19	AS	79/79 (100%)	1.57	28 (35%) 0 0	81, 150, 212, 259	0
19	CS	79/79 (100%)	2.93	46 (58%) 0 0	217, 411, 508, 531	0
20	AT	85/85 (100%)	-0.31	0 100 100	35, 69, 129, 176	0
20	CT	85/85 (100%)	0.85	12 (14%) 4 2	66, 130, 204, 226	0
21	AU	51/51 (100%)	1.74	20 (39%) 0 0	90, 146, 226, 252	0
21	CU	51/51 (100%)	0.59	7 (13%) 4 2	54, 109, 189, 269	0
22	BA	2854/2904 (98%)	-0.48	39 (1%) 78 60	6, 25, 148, 390	0
22	DA	2841/2904 (97%)	0.25	96 (3%) 49 24	55, 116, 270, 526	0
23	BB	118/118 (100%)	-0.64	0 100 100	12, 40, 73, 109	0
23	DB	117/118 (99%)	-0.11	2 (1%) 73 52	88, 164, 221, 243	0
24	BC	271/271 (100%)	-0.35	6 (2%) 65 42	8, 35, 82, 192	0
24	DC	271/271 (100%)	0.56	25 (9%) 11 4	42, 95, 151, 215	0
25	BD	209/209 (100%)	-0.44	0 100 100	6, 21, 69, 179	0
25	DD	209/209 (100%)	0.77	28 (13%) 4 2	55, 115, 199, 284	0
26	BE	201/201 (100%)	-0.43	0 100 100	7, 36, 86, 151	0
26	DE	201/201 (100%)	1.62	67 (33%) 0 0	61, 235, 398, 470	0
27	BF	178/178 (100%)	-0.02	3 (1%) 73 52	21, 63, 136, 167	0
27	DF	178/178 (100%)	2.25	90 (50%) 0 0	142, 219, 259, 301	0
28	BG	176/176 (100%)	-0.01	2 (1%) 82 66	20, 61, 131, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
28	DG	176/176 (100%)	1.54	54 (30%)	1	0	88, 239, 337, 389	0
29	BH	149/149 (100%)	3.09	64 (42%)	0	0	40, 171, 260, 304	0
29	DH	149/149 (100%)	2.65	63 (42%)	0	0	68, 188, 268, 298	0
30	BI	141/141 (100%)	2.45	63 (44%)	0	0	170, 245, 289, 301	0
30	DI	141/141 (100%)	3.24	97 (68%)	0	0	178, 312, 349, 370	0
31	BJ	142/142 (100%)	-0.55	1 (0%)	89	78	7, 16, 60, 137	0
31	DJ	142/142 (100%)	0.47	9 (6%)	23	9	50, 106, 169, 198	0
32	BK	122/122 (100%)	-0.39	1 (0%)	87	75	11, 24, 69, 242	0
32	DK	122/122 (100%)	0.62	13 (10%)	8	3	59, 97, 147, 210	0
33	BL	143/143 (100%)	-0.47	0	100	100	6, 30, 71, 123	0
33	DL	143/143 (100%)	1.37	31 (21%)	1	0	59, 164, 279, 354	0
34	BM	136/136 (100%)	-0.54	0	100	100	7, 22, 59, 147	0
34	DM	136/136 (100%)	0.82	17 (12%)	5	2	37, 112, 192, 250	0
35	BN	120/120 (100%)	-0.54	0	100	100	8, 17, 40, 149	0
35	DN	120/120 (100%)	1.42	32 (26%)	1	0	63, 131, 211, 305	0
36	BO	116/116 (100%)	-0.34	0	100	100	21, 41, 72, 113	0
36	DO	116/116 (100%)	1.50	33 (28%)	1	0	106, 172, 240, 273	0
37	BP	114/114 (100%)	-0.43	1 (0%)	85	72	12, 32, 87, 176	0
37	DP	114/114 (100%)	0.86	16 (14%)	4	2	50, 110, 175, 196	0
38	BQ	117/117 (100%)	-0.62	1 (0%)	85	72	6, 15, 39, 225	0
38	DQ	117/117 (100%)	0.95	19 (16%)	3	1	65, 113, 193, 331	0
39	BR	103/103 (100%)	-0.53	1 (0%)	84	69	6, 26, 67, 184	0
39	DR	103/103 (100%)	1.98	45 (43%)	0	0	73, 144, 238, 305	0
40	BS	110/110 (100%)	-0.56	0	100	100	7, 15, 48, 172	0
40	DS	110/110 (100%)	1.52	39 (35%)	0	0	71, 132, 214, 254	0
41	BT	93/93 (100%)	-0.00	3 (3%)	51	27	13, 43, 123, 233	0
41	DT	93/93 (100%)	2.43	48 (51%)	0	0	124, 265, 379, 423	0
42	BU	102/102 (100%)	-0.19	2 (1%)	68	46	21, 45, 131, 240	0
42	DU	102/102 (100%)	3.19	63 (61%)	0	0	148, 305, 420, 554	0
43	BV	94/94 (100%)	-0.29	0	100	100	14, 38, 78, 135	0
43	DV	94/94 (100%)	1.01	18 (19%)	2	1	88, 136, 193, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	79/79 (100%)	-0.13	2 (2%) 61 37	13, 29, 98, 213	0
44	DW	79/79 (100%)	2.15	35 (44%) 0 0	73, 169, 279, 323	0
45	BX	77/77 (100%)	-0.57	0 100 100	13, 37, 77, 108	0
45	DX	77/77 (100%)	0.80	11 (14%) 4 2	62, 118, 215, 280	0
46	BY	63/63 (100%)	-0.12	1 (1%) 74 55	27, 59, 126, 209	0
46	DY	63/63 (100%)	1.65	18 (28%) 1 0	152, 379, 492, 508	0
47	BZ	58/58 (100%)	-0.60	0 100 100	9, 16, 47, 61	0
47	DZ	58/58 (100%)	0.48	5 (8%) 13 4	68, 143, 251, 271	0
48	B0	56/56 (100%)	-0.68	0 100 100	6, 18, 71, 138	0
48	D0	56/56 (100%)	1.47	17 (30%) 1 0	63, 144, 246, 262	0
49	B1	50/50 (100%)	0.15	3 (6%) 25 10	27, 47, 93, 115	0
49	D1	50/50 (100%)	1.61	15 (30%) 1 0	97, 154, 208, 231	0
50	B2	46/46 (100%)	-0.54	0 100 100	10, 19, 43, 195	0
50	D2	46/46 (100%)	1.29	8 (17%) 2 1	59, 119, 184, 211	0
51	B3	64/64 (100%)	-0.53	0 100 100	8, 22, 38, 65	0
51	D3	64/64 (100%)	1.15	12 (18%) 2 1	64, 122, 197, 255	0
52	B4	38/38 (100%)	0.31	2 (5%) 30 13	25, 49, 94, 97	0
52	D4	38/38 (100%)	3.16	26 (68%) 0 0	87, 173, 235, 241	0
All	All	20434/20562 (99%)	0.33	2089 (10%) 9 3	6, 93, 274, 554	0

The worst 5 of 2089 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DH	92	GLY	21.5
29	DH	124	THR	18.6
29	DH	91	PHE	16.6
29	BH	122	LEU	16.2
29	BH	118	PRO	16.1

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	MG	BA	3130	1/1	0.70	0.47	25.95	205,205,205,205	0
53	MG	CA	1628	1/1	0.57	1.57	23.15	236,236,236,236	0
53	MG	DA	3033	1/1	0.59	0.53	21.53	149,149,149,149	0
53	MG	DA	3079	1/1	0.81	0.63	20.91	150,150,150,150	0
53	MG	BA	3057	1/1	0.76	0.24	19.36	161,161,161,161	0
53	MG	BA	3036	1/1	0.94	0.38	17.15	169,169,169,169	0
53	MG	BA	3040	1/1	0.96	0.21	14.97	8,8,8,8	0
53	MG	BA	3070	1/1	0.95	0.24	14.48	134,134,134,134	0
53	MG	DA	3013	1/1	0.60	0.88	12.81	185,185,185,185	0
53	MG	DA	3082	1/1	0.51	0.36	11.85	189,189,189,189	0
53	MG	BA	3135	1/1	0.96	0.43	8.59	196,196,196,196	0
53	MG	BA	3100	1/1	0.95	0.21	8.54	24,24,24,24	0
53	MG	DA	3075	1/1	0.83	0.41	6.42	140,140,140,140	0
53	MG	BA	3123	1/1	0.92	0.44	6.04	118,118,118,118	0
53	MG	BA	3082	1/1	0.86	0.19	5.95	85,85,85,85	0
53	MG	CA	1625	1/1	0.89	0.30	5.66	91,91,91,91	0
53	MG	BA	3103	1/1	0.94	0.20	5.25	7,7,7,7	0
53	MG	DA	3108	1/1	0.81	0.41	4.89	172,172,172,172	0
53	MG	DA	3076	1/1	0.89	0.28	4.79	158,158,158,158	0
53	MG	DA	3002	1/1	0.67	0.32	4.53	160,160,160,160	0
53	MG	DA	3133	1/1	0.18	0.46	4.50	239,239,239,239	0
53	MG	BA	3063	1/1	0.99	0.18	3.91	13,13,13,13	0
53	MG	CA	1607	1/1	0.71	0.26	3.39	154,154,154,154	0
53	MG	DA	3129	1/1	0.90	0.74	3.28	203,203,203,203	0
53	MG	AA	1620	1/1	0.97	0.18	3.25	28,28,28,28	0
53	MG	BA	3104	1/1	0.95	0.19	3.04	12,12,12,12	0
53	MG	BA	3108	1/1	0.95	0.18	2.98	8,8,8,8	0
53	MG	CA	1618	1/1	0.80	0.30	2.97	139,139,139,139	0
53	MG	BA	3027	1/1	0.97	0.19	2.96	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BA	3047	1/1	0.56	0.16	2.78	152,152,152,152	0
53	MG	AA	1639	1/1	0.90	0.16	1.67	126,126,126,126	0
53	MG	DA	3115	1/1	0.83	0.24	1.60	139,139,139,139	0
53	MG	BA	3128	1/1	0.96	0.17	1.53	7,7,7,7	0
53	MG	CA	1621	1/1	0.94	0.21	1.44	55,55,55,55	0
53	MG	BA	3133	1/1	0.96	0.18	1.44	10,10,10,10	0
53	MG	BA	3111	1/1	0.96	0.16	1.33	74,74,74,74	0
53	MG	BA	3107	1/1	0.98	0.17	1.26	8,8,8,8	0
54	ERY	BA	3136	51/51	0.96	0.23	1.24	5,11,15,16	0
53	MG	DA	3051	1/1	0.78	0.21	0.94	124,124,124,124	0
53	MG	AA	1621	1/1	0.95	0.14	0.81	91,91,91,91	0
53	MG	BA	3013	1/1	0.99	0.17	0.78	9,9,9,9	0
53	MG	BA	3049	1/1	0.96	0.16	0.57	11,11,11,11	0
53	MG	AA	1616	1/1	0.88	0.16	0.52	78,78,78,78	0
53	MG	DA	3043	1/1	0.43	0.44	0.43	213,213,213,213	0
53	MG	DA	3120	1/1	0.83	0.23	0.41	76,76,76,76	0
53	MG	BA	3115	1/1	0.91	0.15	0.37	10,10,10,10	0
53	MG	CA	1631	1/1	0.86	0.22	0.01	88,88,88,88	0
53	MG	CA	1629	1/1	0.74	0.19	-0.09	217,217,217,217	0
53	MG	DA	3128	1/1	0.93	0.24	-0.10	123,123,123,123	0
53	MG	AA	1631	1/1	0.97	0.13	-0.15	69,69,69,69	0
53	MG	BA	3008	1/1	0.97	0.14	-0.18	13,13,13,13	0
53	MG	DA	3065	1/1	0.92	0.22	-0.20	83,83,83,83	0
53	MG	CA	1616	1/1	0.87	0.35	-0.22	232,232,232,232	0
53	MG	BA	3106	1/1	0.96	0.15	-0.33	25,25,25,25	0
53	MG	DA	3084	1/1	0.62	0.18	-0.35	182,182,182,182	0
53	MG	DA	3048	1/1	0.92	0.18	-0.36	132,132,132,132	0
53	MG	AN	202	1/1	0.93	0.15	-0.43	169,169,169,169	0
53	MG	DA	3083	1/1	0.55	0.20	-0.48	224,224,224,224	0
53	MG	DA	3095	1/1	0.74	0.21	-0.48	116,116,116,116	0
53	MG	AA	1622	1/1	0.90	0.13	-0.51	97,97,97,97	0
53	MG	BA	3062	1/1	0.92	0.15	-0.60	15,15,15,15	0
53	MG	DA	3037	1/1	0.91	0.14	-0.62	81,81,81,81	0
53	MG	DA	3069	1/1	0.87	0.19	-0.65	202,202,202,202	0
53	MG	DA	3104	1/1	0.86	0.17	-0.69	34,34,34,34	0
53	MG	BA	3131	1/1	0.92	0.11	-0.74	140,140,140,140	0
53	MG	CA	1609	1/1	0.92	0.20	-0.84	80,80,80,80	0
53	MG	AA	1606	1/1	0.91	0.11	-0.90	58,58,58,58	0
53	MG	CA	1617	1/1	0.74	0.16	-0.93	280,280,280,280	0
53	MG	DA	3103	1/1	0.91	0.16	-0.96	98,98,98,98	0
53	MG	DA	3101	1/1	0.84	0.21	-0.96	104,104,104,104	0
53	MG	AA	1607	1/1	0.81	0.15	-0.97	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BA	3071	1/1	0.96	0.15	-1.03	112,112,112,112	0
53	MG	DB	201	1/1	0.80	0.09	-1.19	114,114,114,114	0
53	MG	DA	3100	1/1	0.92	0.19	-1.21	93,93,93,93	0
53	MG	AA	1633	1/1	0.90	0.08	-1.31	75,75,75,75	0
53	MG	BA	3037	1/1	0.98	0.13	-1.31	17,17,17,17	0
53	MG	DA	3044	1/1	0.92	0.17	-1.31	83,83,83,83	0
53	MG	DA	3112	1/1	0.91	0.14	-1.33	66,66,66,66	0
55	ZN	D4	101	1/1	0.93	0.09	-1.38	151,151,151,151	0
53	MG	BA	3012	1/1	0.97	0.15	-1.42	6,6,6,6	0
53	MG	CA	1641	1/1	0.91	0.14	-1.63	80,80,80,80	0
53	MG	BA	3017	1/1	0.97	0.09	-1.64	30,30,30,30	0
53	MG	BA	3016	1/1	0.96	0.13	-1.73	7,7,7,7	0
55	ZN	B4	101	1/1	0.99	0.10	-1.74	84,84,84,84	0
53	MG	DA	3131	1/1	0.86	0.15	-1.88	70,70,70,70	0
53	MG	CA	1606	1/1	0.93	0.14	-1.89	63,63,63,63	0
53	MG	AA	1632	1/1	0.99	0.11	-1.91	31,31,31,31	0
53	MG	DA	3061	1/1	0.84	0.11	-1.92	134,134,134,134	0
53	MG	DA	3105	1/1	0.94	0.14	-2.11	51,51,51,51	0
53	MG	DA	3040	1/1	0.91	0.17	-2.18	52,52,52,52	0
53	MG	CA	1604	1/1	0.96	0.07	-2.21	60,60,60,60	0
53	MG	DA	3068	1/1	0.89	0.11	-2.28	78,78,78,78	0
53	MG	BA	3022	1/1	0.97	0.14	-2.32	9,9,9,9	0
53	MG	BA	3113	1/1	0.96	0.09	-2.33	21,21,21,21	0
53	MG	DA	3038	1/1	0.63	0.12	-2.33	204,204,204,204	0
53	MG	DA	3024	1/1	0.88	0.15	-2.42	106,106,106,106	0
53	MG	AA	1641	1/1	0.97	0.11	-2.49	39,39,39,39	0
53	MG	DA	3106	1/1	0.64	0.15	-2.50	205,205,205,205	0
53	MG	BA	3078	1/1	0.91	0.08	-2.55	41,41,41,41	0
53	MG	CA	1642	1/1	0.97	0.05	-2.59	58,58,58,58	0
53	MG	DA	3025	1/1	0.88	0.12	-2.62	110,110,110,110	0
53	MG	DA	3052	1/1	0.93	0.10	-2.76	49,49,49,49	0
53	MG	AA	1613	1/1	0.95	0.08	-2.91	57,57,57,57	0
53	MG	DA	3050	1/1	0.74	0.13	-2.95	125,125,125,125	0
53	MG	DA	3027	1/1	0.73	0.10	-3.04	144,144,144,144	0
53	MG	BA	3005	1/1	0.95	0.10	-3.09	93,93,93,93	0
53	MG	AA	1629	1/1	0.93	0.07	-3.14	183,183,183,183	0
53	MG	BA	3002	1/1	0.86	0.11	-3.15	77,77,77,77	0
53	MG	CA	1639	1/1	0.84	0.10	-3.30	226,226,226,226	0
53	MG	DA	3012	1/1	0.93	0.09	-3.40	51,51,51,51	0
53	MG	AN	201	1/1	0.96	0.07	-3.45	105,105,105,105	0
53	MG	AA	1623	1/1	0.92	0.09	-3.57	72,72,72,72	0
53	MG	DA	3017	1/1	0.84	0.13	-3.58	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DA	3055	1/1	0.95	0.10	-3.84	84,84,84,84	0
53	MG	DA	3023	1/1	0.82	0.13	-3.92	78,78,78,78	0
53	MG	BA	3096	1/1	0.96	0.11	-3.94	45,45,45,45	0
53	MG	BA	3129	1/1	0.97	0.12	-4.13	14,14,14,14	0
53	MG	BA	3021	1/1	0.96	0.08	-4.29	43,43,43,43	0
53	MG	BA	3053	1/1	0.99	0.09	-4.41	9,9,9,9	0
53	MG	DA	3124	1/1	0.96	0.12	-4.42	48,48,48,48	0
53	MG	AA	1627	1/1	0.95	0.06	-4.63	78,78,78,78	0
53	MG	BA	3119	1/1	0.88	0.11	-4.72	12,12,12,12	0
53	MG	DA	3066	1/1	0.97	0.08	-4.79	48,48,48,48	0
53	MG	BB	202	1/1	0.93	0.07	-5.27	43,43,43,43	0
53	MG	BA	3068	1/1	0.99	0.10	-5.37	20,20,20,20	0
53	MG	BA	3092	1/1	0.89	0.07	-5.40	38,38,38,38	0
53	MG	BA	3024	1/1	0.98	0.11	-5.49	17,17,17,17	0
53	MG	BA	3095	1/1	0.98	0.10	-5.59	22,22,22,22	0
53	MG	BA	3065	1/1	0.97	0.09	-5.89	7,7,7,7	0
53	MG	AA	1609	1/1	0.94	0.06	-6.40	28,28,28,28	0
53	MG	BA	3117	1/1	0.94	0.08	-6.94	83,83,83,83	0
53	MG	BA	3023	1/1	0.96	0.10	-7.45	7,7,7,7	0
53	MG	BA	3109	1/1	0.98	0.06	-8.11	57,57,57,57	0
53	MG	BA	3058	1/1	0.97	0.07	-13.22	35,35,35,35	0
53	MG	CA	1613	1/1	0.84	0.11	-13.26	114,114,114,114	0
53	MG	BA	3038	1/1	0.97	0.13	-	7,7,7,7	0
53	MG	AA	1615	1/1	0.94	0.05	-	128,128,128,128	0
53	MG	BA	3033	1/1	0.88	0.16	-	10,10,10,10	0
53	MG	BA	3118	1/1	0.95	0.38	-	168,168,168,168	0
53	MG	BA	3073	1/1	0.89	0.18	-	135,135,135,135	0
53	MG	DA	3110	1/1	0.32	0.17	-	183,183,183,183	0
53	MG	BA	3120	1/1	0.95	0.10	-	53,53,53,53	0
53	MG	CA	1636	1/1	0.28	0.18	-	155,155,155,155	0
53	MG	DA	3036	1/1	0.79	0.16	-	211,211,211,211	0
53	MG	DA	3026	1/1	0.71	0.97	-	244,244,244,244	0
53	MG	DA	3046	1/1	0.90	0.10	-	76,76,76,76	0
53	MG	BA	3064	1/1	0.97	0.10	-	6,6,6,6	0
53	MG	DA	3003	1/1	0.08	1.80	-	268,268,268,268	0
53	MG	DA	3073	1/1	0.78	0.11	-	162,162,162,162	0
53	MG	BA	3094	1/1	0.98	0.09	-	24,24,24,24	0
53	MG	DA	3072	1/1	0.87	0.13	-	132,132,132,132	0
53	MG	CA	1624	1/1	0.91	0.69	-	179,179,179,179	0
53	MG	DA	3019	1/1	0.94	0.21	-	224,224,224,224	0
53	MG	AA	1614	1/1	0.91	0.15	-	197,197,197,197	0
53	MG	DA	3094	1/1	0.83	0.09	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	1626	1/1	0.92	0.26	-	29,29,29,29	0
53	MG	BA	3112	1/1	0.84	0.28	-	89,89,89,89	0
53	MG	CA	1640	1/1	0.67	0.21	-	149,149,149,149	0
53	MG	BA	3132	1/1	0.76	0.23	-	165,165,165,165	0
53	MG	DA	3107	1/1	0.93	0.18	-	121,121,121,121	0
53	MG	CA	1638	1/1	0.88	0.15	-	139,139,139,139	0
53	MG	DA	3016	1/1	-0.03	0.67	-	231,231,231,231	0
53	MG	BA	3059	1/1	0.87	0.22	-	109,109,109,109	0
53	MG	BA	3042	1/1	0.93	0.14	-	18,18,18,18	0
53	MG	BA	3025	1/1	0.92	0.46	-	119,119,119,119	0
53	MG	DA	3032	1/1	0.74	0.14	-	100,100,100,100	0
53	MG	BA	3101	1/1	0.95	0.12	-	64,64,64,64	0
53	MG	DA	3041	1/1	0.94	0.13	-	122,122,122,122	0
53	MG	AA	1625	1/1	0.95	0.31	-	121,121,121,121	0
53	MG	DA	3029	1/1	0.86	0.47	-	151,151,151,151	0
53	MG	DA	3099	1/1	0.00	0.23	-	180,180,180,180	0
53	MG	BB	204	1/1	0.97	0.09	-	20,20,20,20	0
53	MG	BA	3072	1/1	0.97	0.12	-	10,10,10,10	0
53	MG	DA	3006	1/1	0.67	0.21	-	267,267,267,267	0
53	MG	DA	3005	1/1	0.88	1.08	-	309,309,309,309	0
53	MG	BA	3050	1/1	0.95	0.12	-	37,37,37,37	0
53	MG	BA	3034	1/1	0.93	0.30	-	154,154,154,154	0
53	MG	DA	3030	1/1	0.92	0.17	-	111,111,111,111	0
53	MG	AA	1637	1/1	0.95	0.09	-	104,104,104,104	0
53	MG	DA	3132	1/1	0.68	0.10	-	175,175,175,175	0
53	MG	CA	1603	1/1	0.80	0.32	-	165,165,165,165	0
53	MG	DA	3121	1/1	0.93	0.23	-	119,119,119,119	0
53	MG	DA	3062	1/1	0.30	1.12	-	193,193,193,193	0
53	MG	DA	3031	1/1	0.90	0.10	-	79,79,79,79	0
53	MG	DA	3047	1/1	0.62	0.19	-	136,136,136,136	0
53	MG	BA	3088	1/1	0.98	0.05	-	11,11,11,11	0
53	MG	BA	3121	1/1	0.96	0.18	-	10,10,10,10	0
53	MG	BA	3116	1/1	0.97	0.07	-	17,17,17,17	0
53	MG	DA	3008	1/1	0.81	0.14	-	142,142,142,142	0
53	MG	BA	3084	1/1	0.86	0.20	-	50,50,50,50	0
53	MG	CA	1623	1/1	0.88	0.13	-	120,120,120,120	0
53	MG	DA	3039	1/1	0.62	0.13	-	99,99,99,99	0
53	MG	BA	3004	1/1	0.86	0.24	-	147,147,147,147	0
53	MG	CA	1608	1/1	0.89	0.15	-	51,51,51,51	0
53	MG	CA	1622	1/1	0.21	0.08	-	208,208,208,208	0
53	MG	AA	1608	1/1	0.96	0.15	-	32,32,32,32	0
53	MG	BA	3007	1/1	0.87	0.10	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	1636	1/1	0.92	0.08	-	25,25,25,25	0
53	MG	DA	3028	1/1	0.04	1.00	-	262,262,262,262	0
53	MG	BA	3087	1/1	0.89	0.18	-	125,125,125,125	0
53	MG	BA	3006	1/1	0.98	0.06	-	31,31,31,31	0
53	MG	BA	3056	1/1	0.97	0.24	-	233,233,233,233	0
53	MG	DA	3125	1/1	0.72	0.31	-	163,163,163,163	0
53	MG	DA	3089	1/1	0.86	0.24	-	69,69,69,69	0
53	MG	AA	1624	1/1	0.97	0.24	-	31,31,31,31	0
53	MG	DA	3123	1/1	0.86	0.20	-	165,165,165,165	0
53	MG	DA	3021	1/1	0.96	0.19	-	41,41,41,41	0
53	MG	AA	1626	1/1	0.89	0.18	-	106,106,106,106	0
53	MG	AA	1619	1/1	0.80	0.15	-	125,125,125,125	0
53	MG	BA	3003	1/1	0.94	0.12	-	42,42,42,42	0
53	MG	BA	3066	1/1	0.96	0.15	-	11,11,11,11	0
53	MG	BA	3098	1/1	0.87	0.16	-	51,51,51,51	0
53	MG	BA	3110	1/1	0.94	0.20	-	102,102,102,102	0
53	MG	DA	3022	1/1	0.82	0.27	-	162,162,162,162	0
53	MG	DA	3090	1/1	0.90	0.10	-	91,91,91,91	0
53	MG	DA	3060	1/1	0.89	0.50	-	161,161,161,161	0
53	MG	DA	3093	1/1	0.91	0.16	-	228,228,228,228	0
53	MG	CA	1610	1/1	0.74	0.09	-	175,175,175,175	0
53	MG	DA	3011	1/1	0.87	0.17	-	152,152,152,152	0
53	MG	BA	3075	1/1	0.89	0.19	-	69,69,69,69	0
53	MG	BA	3086	1/1	0.88	0.18	-	88,88,88,88	0
53	MG	CA	1615	1/1	0.90	0.09	-	124,124,124,124	0
53	MG	BA	3020	1/1	0.98	0.15	-	35,35,35,35	0
53	MG	AA	1612	1/1	0.91	0.21	-	104,104,104,104	0
53	MG	BA	3055	1/1	0.89	0.32	-	191,191,191,191	0
53	MG	BA	3060	1/1	0.90	0.48	-	174,174,174,174	0
53	MG	DA	3078	1/1	0.38	1.02	-	210,210,210,210	0
53	MG	DA	3119	1/1	0.91	0.14	-	88,88,88,88	0
53	MG	BA	3054	1/1	0.98	0.10	-	25,25,25,25	0
53	MG	BA	3074	1/1	0.98	0.15	-	18,18,18,18	0
53	MG	BA	3134	1/1	0.93	0.22	-	143,143,143,143	0
53	MG	CA	1627	1/1	0.68	0.21	-	198,198,198,198	0
53	MG	DA	3057	1/1	0.80	0.51	-	212,212,212,212	0
53	MG	DA	3007	1/1	0.73	0.44	-	253,253,253,253	0
53	MG	DA	3085	1/1	0.90	0.28	-	148,148,148,148	0
53	MG	BA	3093	1/1	0.96	0.07	-	45,45,45,45	0
53	MG	AA	1603	1/1	0.91	0.17	-	121,121,121,121	0
53	MG	BB	203	1/1	0.93	0.12	-	17,17,17,17	0
53	MG	BA	3044	1/1	0.99	0.22	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DA	3091	1/1	0.91	0.38	-	200,200,200,200	0
53	MG	DA	3102	1/1	0.95	0.06	-	62,62,62,62	0
53	MG	BA	3124	1/1	0.98	0.16	-	16,16,16,16	0
53	MG	AA	1617	1/1	0.83	0.69	-	203,203,203,203	0
53	MG	DC	301	1/1	0.88	0.12	-	124,124,124,124	0
53	MG	DA	3004	1/1	0.88	0.12	-	80,80,80,80	0
53	MG	BA	3011	1/1	0.84	0.30	-	131,131,131,131	0
53	MG	CA	1605	1/1	0.95	0.21	-	40,40,40,40	0
53	MG	CA	1630	1/1	0.84	0.09	-	123,123,123,123	0
53	MG	BA	3051	1/1	0.99	0.12	-	10,10,10,10	0
53	MG	CA	1633	1/1	0.83	0.10	-	77,77,77,77	0
53	MG	BA	3026	1/1	0.98	0.07	-	19,19,19,19	0
53	MG	DA	3067	1/1	0.97	0.10	-	38,38,38,38	0
53	MG	DA	3070	1/1	0.81	0.11	-	56,56,56,56	0
53	MG	BA	3081	1/1	0.98	0.08	-	39,39,39,39	0
53	MG	AA	1610	1/1	0.87	0.12	-	210,210,210,210	0
53	MG	DA	3118	1/1	0.89	0.12	-	70,70,70,70	0
53	MG	BA	3089	1/1	0.89	0.09	-	30,30,30,30	0
53	MG	DA	3045	1/1	0.60	0.49	-	233,233,233,233	0
53	MG	AA	1634	1/1	0.72	0.15	-	199,199,199,199	0
53	MG	AA	1630	1/1	0.89	0.14	-	87,87,87,87	0
53	MG	DA	3035	1/1	0.86	0.17	-	84,84,84,84	0
53	MG	DA	3097	1/1	0.66	0.25	-	116,116,116,116	0
53	MG	CA	1620	1/1	0.66	0.10	-	170,170,170,170	0
53	MG	DA	3010	1/1	0.60	0.51	-	171,171,171,171	0
53	MG	DA	3086	1/1	0.88	0.16	-	94,94,94,94	0
53	MG	BA	3014	1/1	0.94	0.21	-	42,42,42,42	0
53	MG	DA	3114	1/1	0.81	0.16	-	123,123,123,123	0
53	MG	AA	1618	1/1	0.74	0.09	-	164,164,164,164	0
53	MG	DA	3127	1/1	0.58	0.57	-	199,199,199,199	0
53	MG	DA	3111	1/1	0.22	0.41	-	127,127,127,127	0
53	MG	BA	3009	1/1	0.95	0.13	-	13,13,13,13	0
53	MG	BA	3031	1/1	0.95	0.09	-	34,34,34,34	0
53	MG	AA	1611	1/1	0.96	0.06	-	54,54,54,54	0
53	MG	DA	3018	1/1	0.63	0.25	-	232,232,232,232	0
53	MG	DA	3058	1/1	0.57	0.49	-	235,235,235,235	0
53	MG	BA	3076	1/1	0.95	0.06	-	32,32,32,32	0
53	MG	CA	1637	1/1	0.72	0.13	-	63,63,63,63	0
53	MG	DA	3096	1/1	0.89	0.09	-	92,92,92,92	0
53	MG	BA	3019	1/1	0.96	0.31	-	10,10,10,10	0
53	MG	BA	3083	1/1	0.80	0.20	-	113,113,113,113	0
53	MG	AA	1605	1/1	0.96	0.16	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BA	3043	1/1	0.97	0.12	-	29,29,29,29	0
53	MG	AA	1604	1/1	0.82	0.14	-	120,120,120,120	0
53	MG	AA	1628	1/1	0.84	0.18	-	183,183,183,183	0
53	MG	CA	1614	1/1	0.51	1.07	-	231,231,231,231	0
53	MG	DA	3113	1/1	0.94	0.07	-	96,96,96,96	0
53	MG	BA	3127	1/1	0.97	0.15	-	15,15,15,15	0
53	MG	DA	3122	1/1	0.77	0.11	-	72,72,72,72	0
53	MG	BA	3114	1/1	0.91	0.16	-	144,144,144,144	0
53	MG	DA	3098	1/1	0.82	0.15	-	118,118,118,118	0
53	MG	DA	3117	1/1	0.94	0.17	-	71,71,71,71	0
53	MG	BA	3010	1/1	0.95	0.08	-	19,19,19,19	0
53	MG	BA	3028	1/1	0.91	0.11	-	32,32,32,32	0
53	MG	DA	3081	1/1	0.97	0.10	-	92,92,92,92	0
53	MG	CA	1634	1/1	0.93	0.12	-	153,153,153,153	0
53	MG	BA	3105	1/1	0.98	0.14	-	9,9,9,9	0
53	MG	BA	3122	1/1	0.93	0.10	-	21,21,21,21	0
53	MG	DA	3109	1/1	0.10	0.71	-	176,176,176,176	0
53	MG	BA	3041	1/1	0.98	0.19	-	13,13,13,13	0
53	MG	DA	3080	1/1	0.91	0.15	-	137,137,137,137	0
53	MG	DA	3015	1/1	0.62	0.41	-	145,145,145,145	0
53	MG	BA	3090	1/1	0.85	0.07	-	73,73,73,73	0
53	MG	DA	3074	1/1	0.60	1.19	-	240,240,240,240	0
53	MG	BA	3035	1/1	0.97	0.12	-	11,11,11,11	0
53	MG	DA	3042	1/1	0.83	0.17	-	94,94,94,94	0
53	MG	BA	3001	1/1	0.92	0.14	-	110,110,110,110	0
53	MG	DA	3092	1/1	0.70	0.12	-	121,121,121,121	0
53	MG	BA	3125	1/1	0.89	0.18	-	41,41,41,41	0
53	MG	DJ	201	1/1	-0.32	3.06	-	284,284,284,284	0
53	MG	DC	302	1/1	0.88	0.27	-	121,121,121,121	0
53	MG	BA	3067	1/1	0.96	0.12	-	10,10,10,10	0
53	MG	BA	3029	1/1	0.98	0.09	-	66,66,66,66	0
53	MG	BA	3018	1/1	0.95	0.16	-	40,40,40,40	0
53	MG	BA	3079	1/1	0.93	0.18	-	30,30,30,30	0
53	MG	AA	1635	1/1	0.90	0.10	-	88,88,88,88	0
53	MG	BA	3077	1/1	0.97	0.15	-	121,121,121,121	0
53	MG	DA	3126	1/1	0.86	0.10	-	76,76,76,76	0
53	MG	BA	3039	1/1	0.99	0.17	-	20,20,20,20	0
53	MG	BA	3080	1/1	0.96	0.13	-	11,11,11,11	0
53	MG	DA	3053	1/1	0.86	0.12	-	80,80,80,80	0
53	MG	DA	3130	1/1	0.12	2.60	-	279,279,279,279	0
53	MG	DA	3001	1/1	0.76	0.12	-	130,130,130,130	0
53	MG	CA	1601	1/1	0.71	0.12	-	179,179,179,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DA	3054	1/1	0.88	0.08	-	71,71,71,71	0
53	MG	BA	3102	1/1	0.95	0.13	-	23,23,23,23	0
53	MG	AA	1640	1/1	0.98	0.18	-	17,17,17,17	0
53	MG	CA	1632	1/1	0.82	0.16	-	163,163,163,163	0
53	MG	BA	3126	1/1	0.99	0.11	-	18,18,18,18	0
53	MG	DA	3087	1/1	0.53	0.17	-	164,164,164,164	0
53	MG	DA	3064	1/1	0.31	1.25	-	230,230,230,230	0
53	MG	DA	3071	1/1	0.89	0.19	-	52,52,52,52	0
53	MG	BA	3030	1/1	0.98	0.22	-	15,15,15,15	0
53	MG	DA	3009	1/1	0.76	0.17	-	101,101,101,101	0
53	MG	BA	3046	1/1	0.96	0.15	-	16,16,16,16	0
53	MG	BA	3099	1/1	0.93	0.10	-	18,18,18,18	0
53	MG	CA	1602	1/1	0.58	0.20	-	175,175,175,175	0
53	MG	DA	3116	1/1	0.80	0.18	-	66,66,66,66	0
53	MG	BA	3048	1/1	0.76	0.18	-	104,104,104,104	0
53	MG	BA	3032	1/1	0.98	0.13	-	16,16,16,16	0
53	MG	DA	3049	1/1	0.78	0.32	-	235,235,235,235	0
53	MG	BA	3085	1/1	0.98	0.13	-	6,6,6,6	0
53	MG	AA	1638	1/1	0.79	0.11	-	102,102,102,102	0
53	MG	BB	201	1/1	0.71	0.32	-	236,236,236,236	0
53	MG	DA	3059	1/1	0.59	0.22	-	183,183,183,183	0
53	MG	CA	1611	1/1	0.88	0.20	-	122,122,122,122	0
53	MG	CA	1635	1/1	0.97	0.08	-	85,85,85,85	0
53	MG	DA	3056	1/1	0.94	0.13	-	112,112,112,112	0
53	MG	BA	3097	1/1	0.95	0.14	-	80,80,80,80	0
53	MG	CA	1612	1/1	0.86	0.39	-	120,120,120,120	0
53	MG	BA	3045	1/1	0.99	0.13	-	17,17,17,17	0
53	MG	BA	3052	1/1	0.94	0.12	-	25,25,25,25	0
53	MG	DA	3014	1/1	0.56	0.29	-	128,128,128,128	0
53	MG	CA	1619	1/1	0.89	0.16	-	201,201,201,201	0
53	MG	DA	3077	1/1	0.95	0.27	-	114,114,114,114	0
53	MG	DA	3034	1/1	0.91	0.09	-	89,89,89,89	0
53	MG	DA	3063	1/1	0.73	2.08	-	192,192,192,192	0
53	MG	BA	3015	1/1	0.94	0.13	-	38,38,38,38	0
53	MG	DA	3088	1/1	0.86	0.14	-	141,141,141,141	0
53	MG	AA	1602	1/1	0.89	0.12	-	119,119,119,119	0
53	MG	BA	3069	1/1	0.91	0.10	-	176,176,176,176	0
53	MG	DA	3020	1/1	0.67	0.52	-	218,218,218,218	0
53	MG	BA	3091	1/1	0.82	0.26	-	113,113,113,113	0
53	MG	AA	1601	1/1	0.96	0.13	-	78,78,78,78	0
53	MG	BA	3061	1/1	0.85	0.28	-	223,223,223,223	0

6.5 Other polymers [i](#)

There are no such residues in this entry.