



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:55 am GMT

PDB ID : 4V56
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with spectinomycin.
Authors : Borovinskaya, M.A.; Shoji, S.; Holton, J.M.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2007-07-21
Resolution : 3.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

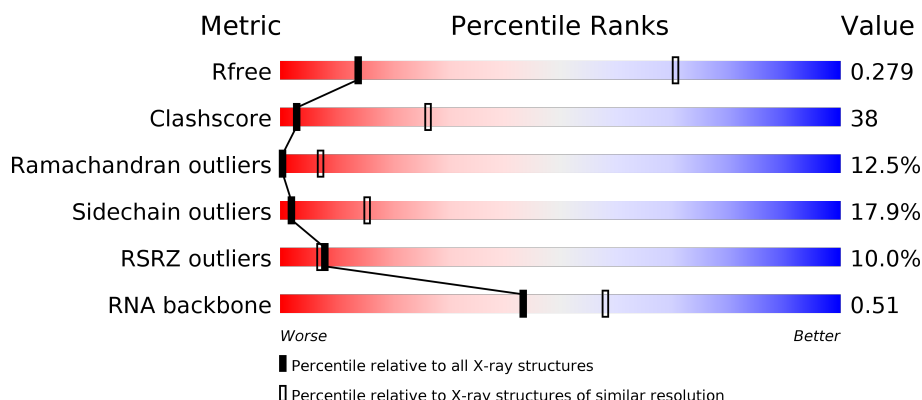
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.93 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1021 (4.28-3.60)
Clashscore	112137	1117 (4.28-3.60)
Ramachandran outliers	110173	1076 (4.28-3.60)
Sidechain outliers	110143	1067 (4.28-3.60)
RSRZ outliers	101464	1034 (4.28-3.60)
RNA backbone	2435	1018 (4.84-2.90)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	<div> <div>19%</div> <div>63%</div> <div>16%</div> <div>..</div> </div>
1	CA	1542	<div> <div>21%</div> <div>63%</div> <div>16%</div> <div>.</div> </div>
2	AC	232	<div> <div>6%</div> <div>19%</div> <div>46%</div> <div>22%</div> <div>11%</div> </div>
2	CC	232	<div> <div>13%</div> <div>22%</div> <div>48%</div> <div>18%</div> <div>11%</div> </div>

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	BB	3087	-	-	-	X
53	MG	CA	1612	-	-	-	X
53	MG	CA	1654	-	-	-	X
53	MG	DB	3026	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	BB	110	Total	Mg	0	0
			110	110		
53	CA	58	Total	Mg	0	0
			58	58		
53	AA	60	Total	Mg	0	0
			60	60		
53	CE	1	Total	Mg	0	0
			1	1		
53	DN	1	Total	Mg	0	0
			1	1		
53	DB	110	Total	Mg	0	0
			110	110		

- Molecule 54 is SPECTINOMYCIN (three-letter code: SCM) (formula: C₁₄H₂₄N₂O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	AA	1	Total 23	C 14	N 2	O 7	0	0
54	CA	1	Total 23	C 14	N 2	O 7	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	288	Total O 288 288	0	0
56	AE	3	Total O 3 3	0	0
56	AK	1	Total O 1 1	0	0
56	AL	4	Total O 4 4	0	0
56	AP	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AT	1	Total 1	O 1	0	0
56	AN	2	Total 2	O 2	0	0
56	BB	494	Total 494	O 494	0	0
56	BC	4	Total 4	O 4	0	0
56	BE	3	Total 3	O 3	0	0
56	BL	4	Total 4	O 4	0	0
56	BH	1	Total 1	O 1	0	0
56	BT	1	Total 1	O 1	0	0
56	CA	275	Total 275	O 275	0	0
56	CE	4	Total 4	O 4	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	5	Total 5	O 5	0	0
56	CP	1	Total 1	O 1	0	0
56	CT	2	Total 2	O 2	0	0
56	CN	5	Total 5	O 5	0	0
56	DB	500	Total 500	O 500	0	0
56	DC	3	Total 3	O 3	0	0
56	DD	1	Total 1	O 1	0	0
56	DP	1	Total 1	O 1	0	0
56	DE	1	Total 1	O 1	0	0
56	DL	3	Total 3	O 3	0	0

Continued on next page...

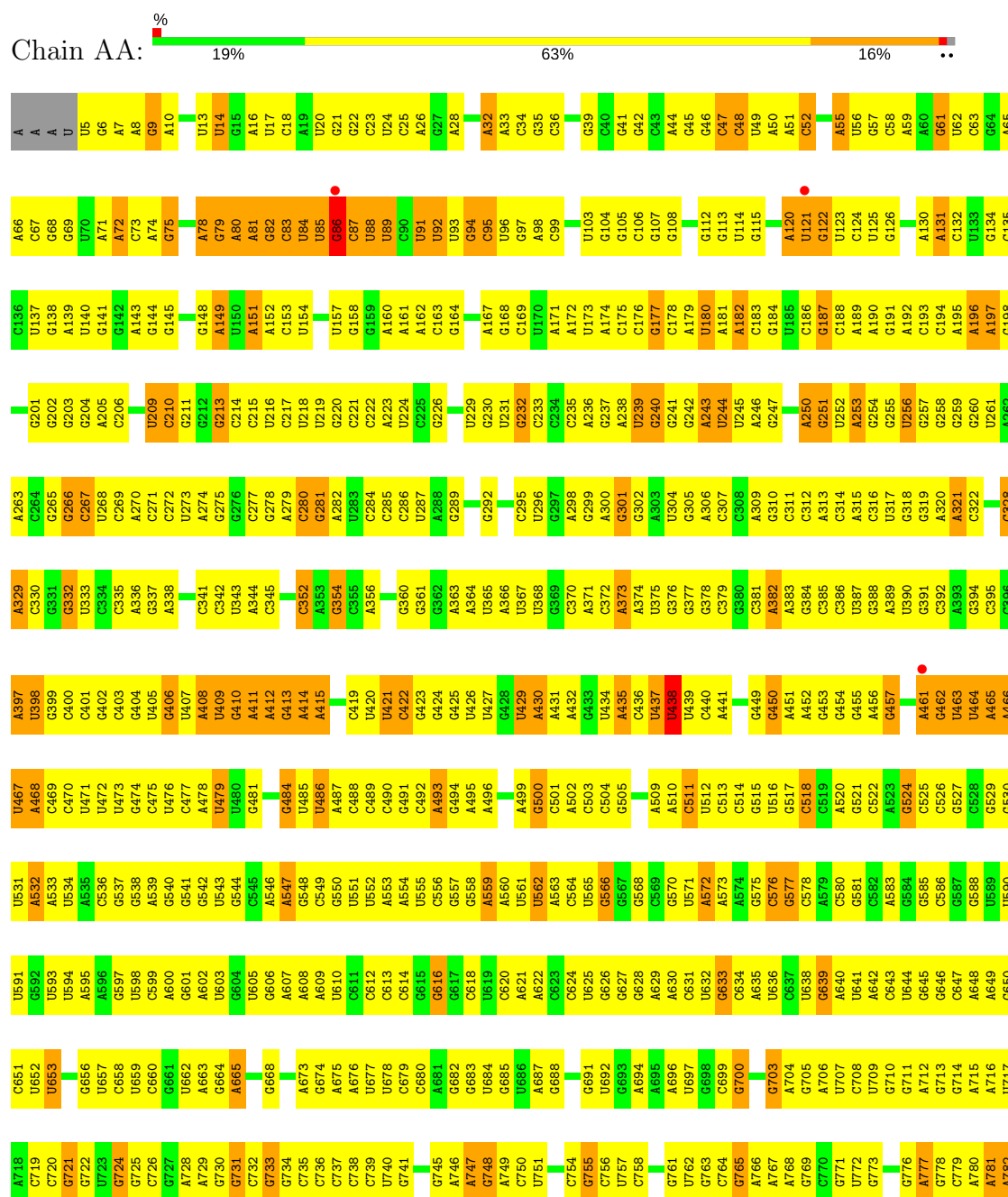
Continued from previous page...

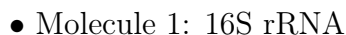
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DJ	1	Total 1	O 1	0	0
56	DN	2	Total 2	O 2	0	0
56	DR	1	Total 1	O 1	0	0

3 Residue-property plots

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

• Molecule 1: 16S rRNA

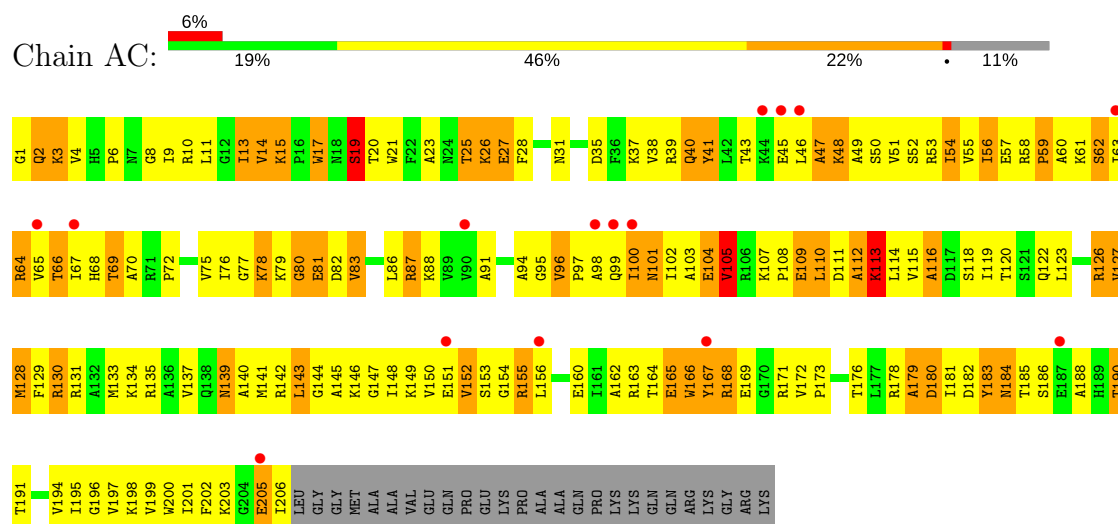




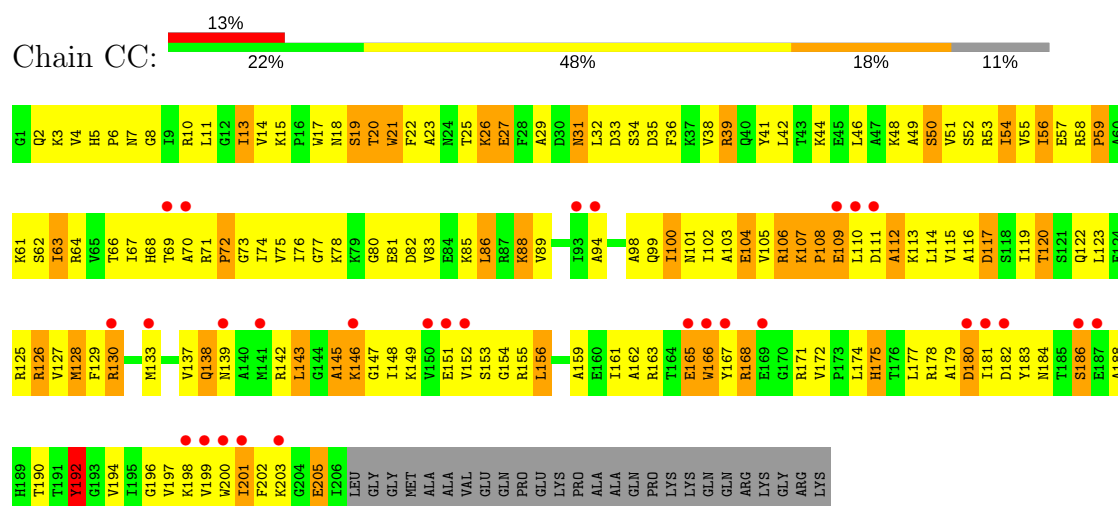
U133	A65	A
G134	A66	A
C135	C67	A
G136	G68	U
U137	G69	U5
G138	U70	G6
	A71	A7
A143	A72	A8
G144	C73	G9
G145	A74	A10
	G75	
G148	G76	U13
A149	A77	U14
U150	A78	G15
A151	G79	A16
A152	A80	U17
C153	A81	C18
U154	G82	A19
	C83	U20
U157	U84	G21
G158	U85	G22
G159	G86	G23
A160	C87	U24
A161	U88	C25
A162	U89	A26
C163	C90	G27
G164	U91	A28
	U92	
A167	U93	A32
G168	G94	A33
C169	C95	C34
		G35
	A98	C36
A174	C99	
C175	G100	G39
C176	A101	C40
G177	G102	G41
C178	U103	G42
U180	G104	C43
A181	C106	A44
A182	G105	G45
C183	G107	G46
G184	G108	C47
U185		C48
C186	G112	U49
G187	G113	A50
C188	U114	A51
A189	G115	C52
A190		A53
G191	A120	C54
A192	U121	A55
C193	G122	U56
C194	U123	G57
A195	C124	C58
A196	U125	A59
A197	G126	A60
G198		G61
	A130	U62
	C131	C63
	C132	C64
G201		
C202		

G1175	A1111	G1048	C985	G922	C857	A792	G724	G660	G597	G537	G474	G402	C335	G266	G203
A1176	C1112	U1049	U986	A923	G858	U793	G725	G661	U998	G538	C475	C403	A336	C267	G204
G1177	G1113	G1050	G987	C924	A860	A794	A728	U662	C599	A539	U476	G404	A337	U268	A205
G1178	C1114	G1051	G988	G925	A860	C795	A728	A663	A600	G540	C477	U405	A338	C269	C206
A1179	U1052	U1052	U989	G926	G861	C796	A729	G664	G601	G541	U479	G406	C341	A270	U209
A1180	U1116	G1053	C990	G927	C862	C797	G730	A665	A602	G542	U480	U407	C342	C271	C210
G1181	A1117	C1054	U991	G928	U863	U798	G731	G666	U603	U543	U480	U408	C343	C272	G211
U1182	U1118	A1055	U992	G929	A864	A802	G732	G667	G604	G544	U481	U409	C344	U273	G212
G1183	C1119	U1056	G993	C930	A865	G803	G733	G668	G606	C545	U482	U410	C345	U274	G213
G1184	U1121	G1057	A994	G931	C866	U804	C734	U672	G607	A547	C483	A411	C346	G275	C214
	U1122	G1058	C995	C932	G867	C805	C735	A673	A608	G548	U485	A412	G347		C215
G1190	U1123	C1059	A996	G933	C868	C806	C736	G674	A609	C549	U486	A414	C352	C280	U216
A1191	U1124	U1060	U997	C934	G869	A807	C737	A675		G550	U487	A415	C353	C281	C217
C1192	U1125	G1062	A1000	A935	G874	C808	C738		C612	U551	C488		C354	U282	U218
G1193	U1126	U1062	U997	A936	G875	G808	C739	A676	C613	U552	C489	U420	A355	U283	U219
A1196	U1126	C1063	C1001	A937	G876	C809	C740	U677	C614	A553	C490	U421	C356	C284	G220
G1197	C1127	G1064	G1002	A938	G877	C810	G741	U678	G615	A554	C491	U422	C357	C285	C221
U1198	G1128	U1065	G1003	G939	C878	C811		C679	G616	U555	C492	G423	C361	C286	C222
G1198	C1129	C1066	A1004	C940	A878	G812	G745	C680	G617	C556	A493	G424	C362	U287	A223
U1199	C1130	A1067	A1005	G941	C879	U813	A746	A681	G618	C557	G494	G425	C363	A288	U224
C1200	G1132	G1068	U1006	G942	C880	A814	A747	U682	C619	G558	C495	U426	A364	U289	G225
A1201	G1133	C1069	U1007	G950	A889	A815	G748	U683	U619	G559	A496	U427	C365	G292	G226
U1202	G1134	U1070	G881	U951	G890	A816	A749	U684	G620	A560	U499	U428	C366		U229
C1203	U1135	C1071	C882	U952	G891	A817		U685	G621	U561	A430	U429	C367	C295	G230
	C1136	G1072	U884	G954	C892	G818	C750	U686	A622	U562	A431	U430	C368	U296	U231
G1206	C1137	U1073	G885	A949	C893	A819	A753	A687	C623	U563	A432	U431	C369	G297	G232
G1207	G1138	G1074	U950	U950	A894	U820	C754	G688	U625	A563	A502	U432	C370	A298	C233
C1208	U1139	U1075	G889	G951	G895	G821	G755	U689		C575	C504	U433	C371	C299	C234
G1209	G1140	C1082	G890	U952	G896	U822	C756	U690	G626	U571	C505	U434	C372	A300	C235
C1210	C1141	G1083	C891	G953	C897	U823	C757	G691	G627	C572	C506	U435	C373	G301	A236
U1211	U1142	U1085	U892	G954	C898	G824	C758	U692	A629	A572	C507	U436	C374	G302	G237
G1212	G1143	A1080	C893	U955	C899	A825	G765	U693	A630	C573	C513	U437	C375	A303	U239
A1213	A1081	U1086	G894	U956	A900	C826	A766	A694	A631	C574	C514	U438	C376	G305	G240
C1214	A1145	U1087	G895	U957	A901	U827	A767	A695	C632	C575	G615	U439	C377	A306	G241
G1215	A1146	G1088	G896	U958	G902	U828	A768	A696	U638	C576	U516	U440	C378	G307	G242
A1216	G1147	U1089	C897	A959	G903	U836	C770	U697	G639	C577	C517	U441	C379	C309	A243
G1217	U1148	G1090	C898	U960	U904	U837	C771	G705	U641	A578	C518	U442	C380	G310	U244
U1218	C1149	U1091	G899	U961	U905	G838	U772	A706	A642	C580	C519	U443	C381	C311	U245
A1219	A1150	G1092	A900	U962	A906	C839	G773	U707	C643	C581	C520	U444	C382	C312	A246
G1220	U1151	G1093	G901	G962	A907	C840	G776	U708	U644	C582	C522	U445	C383	C313	G247
G1221	A1152	C1094	G902	G963	A908	C841	A777	U709	G645	A583	A523	U446	C384	G314	A250
C1222	U1153	G1095	G903	A964	A909	U842	C778	G710	G646	G584	C524	U447	C385	G315	G251
G1223	G1156	U1096	U904	U965	G904	U843	C779	G711	C647	G585	C525	U448	C386	G316	A252
U1224	A1157	U1097	U905	C967	U906	U844	C780	G712	A648	C586	C526	U449	C387	G317	A253
A1225	C1158	G1098	A906	A968	A907	A845	A781	G713	G649	G587	C527	U450	C388	G318	G254
C1226	U1159	U1099	A907	A969	A908	A846	A780	G714	G650	U588	C528	U451	C389	A321	U255
G1227	G1160	C1099	A908	C970	A909	C847	A777	G715	C651	G589	C529	U452	C390	C328	G256
C1228	A1163	C1098	A909	G971	A910	U847	C778	A716	U652	U590	C530	U453	C391	A329	G257
A1229	U1164	G1099	U911	G972	A911	G844	C779	A717	U653	U591	C531	U454	C392	C330	U261
G1230	G1165	U1099	C912	G973	U912	A845	A780	G718	G654	U592	C532	U455	C393	G331	G262
C1231	U1166	C1099	C913	A974	U913	A846	A781	G719	G655	U593	A533	U456	C394	C332	U263
U1232	G1167	G1100	A914	A975	A914	C847	A782	G720	G656	U594	C534	U457	C395	C333	A264
G1233	U1168	A1101	A915	G976	A915	C848	C783	A716	U657	U595	C535	U458	C396	A329	G265
C1234	U1169	C1103	A916	A977	U916	C849	A784	G721	U658	U596	C536	U459	C397	C334	C266
U1235	G1170	G1104	U917	A978	U917	G851	A785	G722	U659	U597	A537	U460	C398	C335	U267
A1236	A1171	U1099	C917	C979	U918	C852	G785	G723	G656	U598	C538	U461	C399	G336	A268
C1237	U1172	G1107	A918	C980	A918	C853	A789	G724	U657	U599	C539	U462	C400	C337	G269
A1238	C1173	C1109	U920	U981	A919	U854	A790	G725	U658	U600	C540	U463	C401	C338	U270
U1240	G1174	A1110	G1047	C984	U921	U855	G791	U723	U659	A596	C536	U473			G271

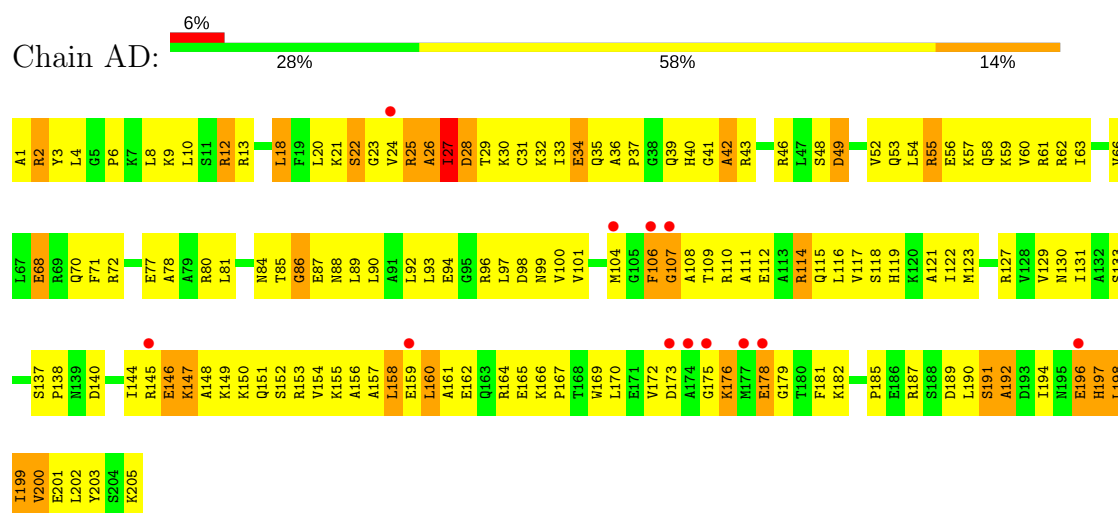
- Molecule 2: 30S ribosomal protein S3



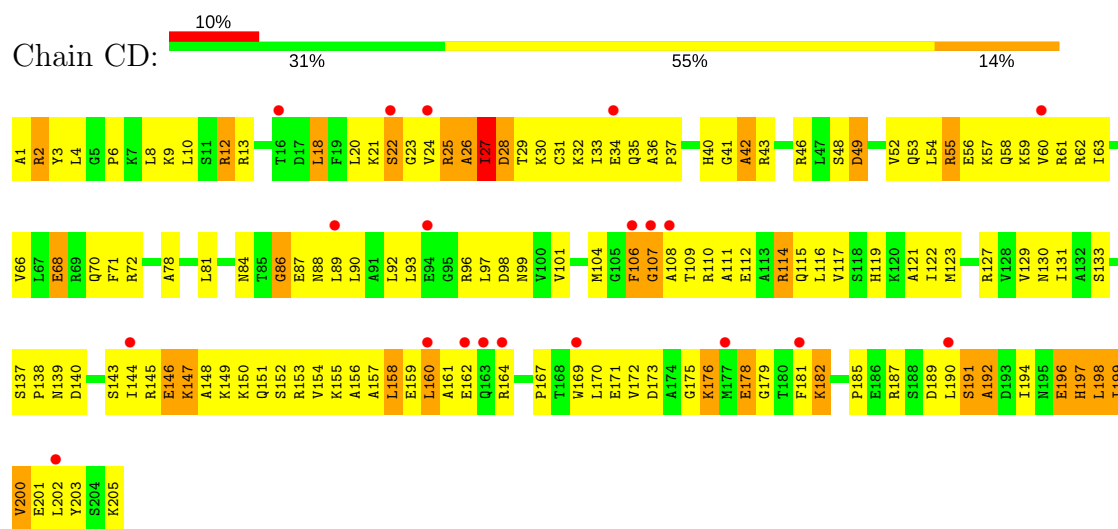
- Molecule 2: 30S ribosomal protein S3



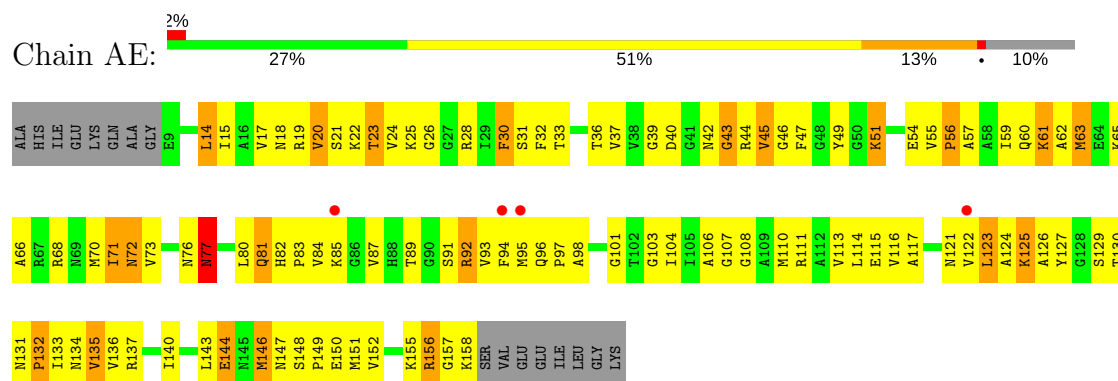
- Molecule 3: 30S ribosomal protein S4



• Molecule 3: 30S ribosomal protein S4

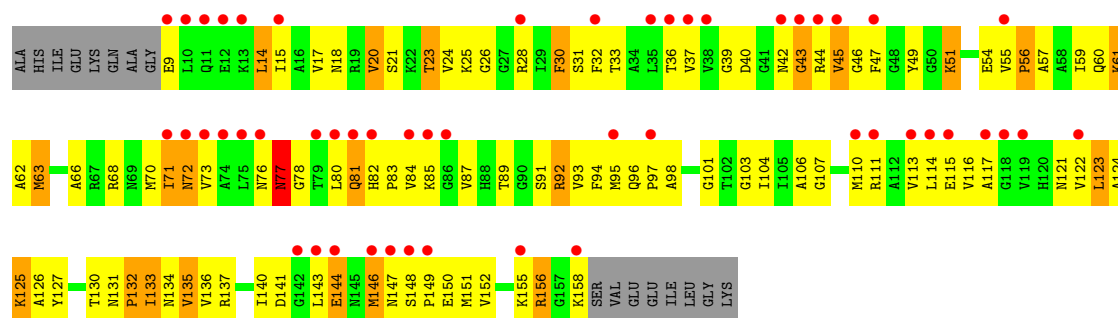


• Molecule 4: 30S ribosomal protein S5

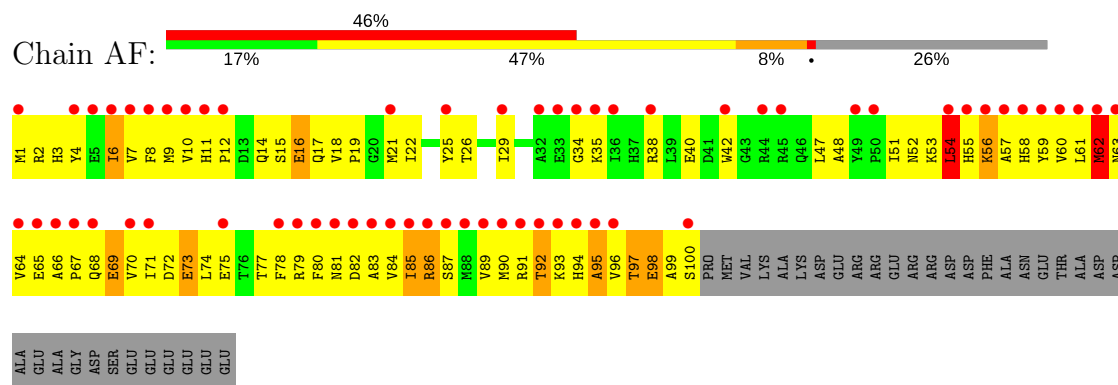


• Molecule 4: 30S ribosomal protein S5

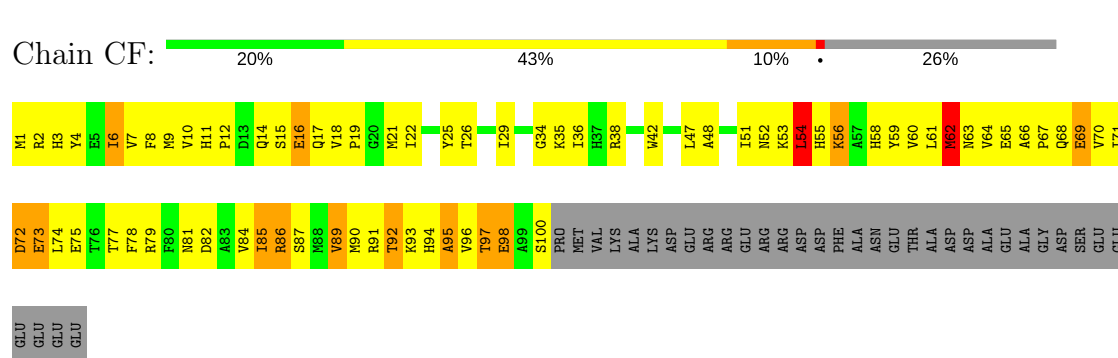




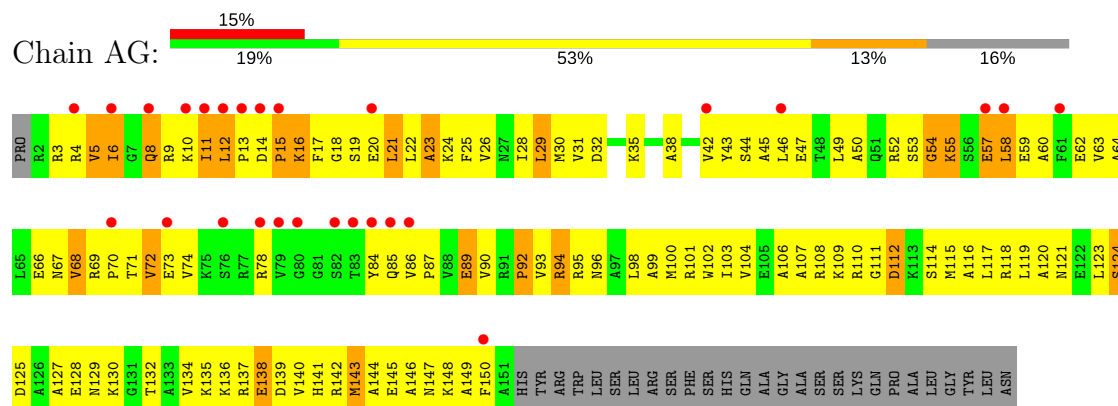
• Molecule 5: 30S ribosomal protein S6



• Molecule 5: 30S ribosomal protein S6



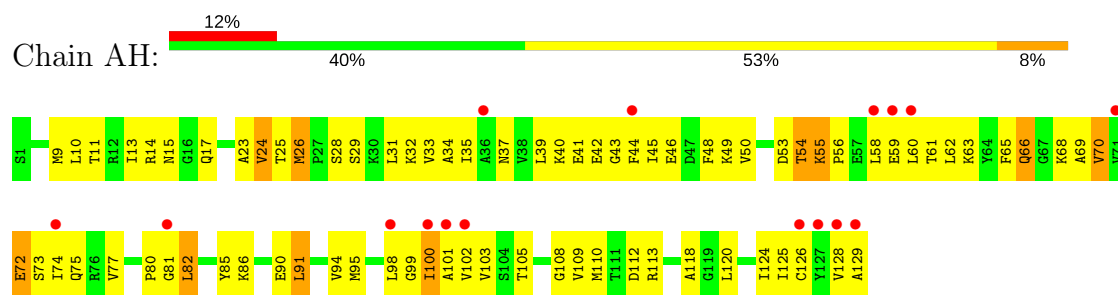
• Molecule 6: 30S ribosomal protein S7



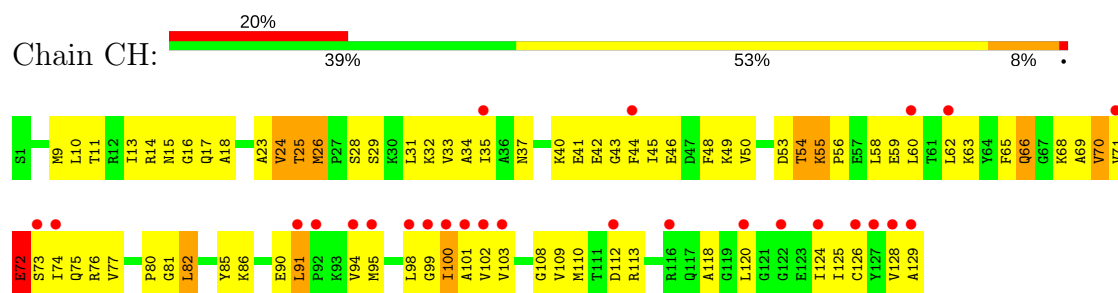
• Molecule 6: 30S ribosomal protein S7



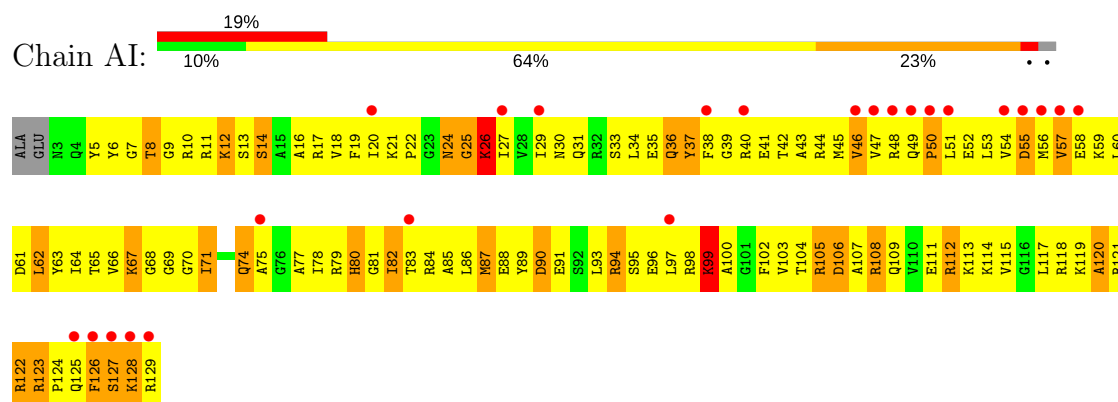
- Molecule 7: 30S ribosomal protein S8



- Molecule 7: 30S ribosomal protein S8

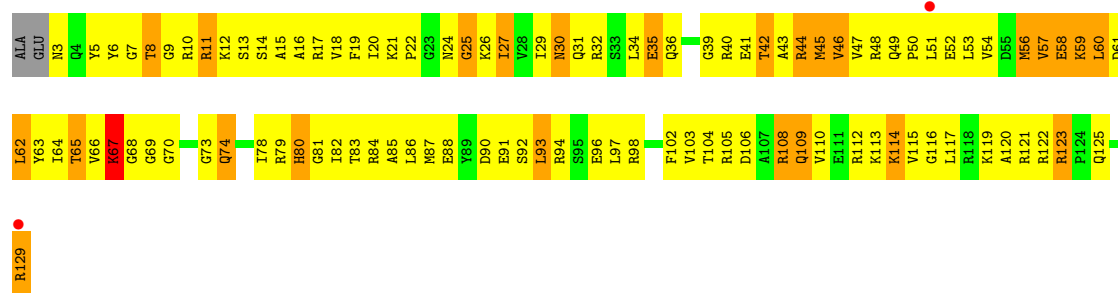


- Molecule 8: 30S ribosomal protein S9

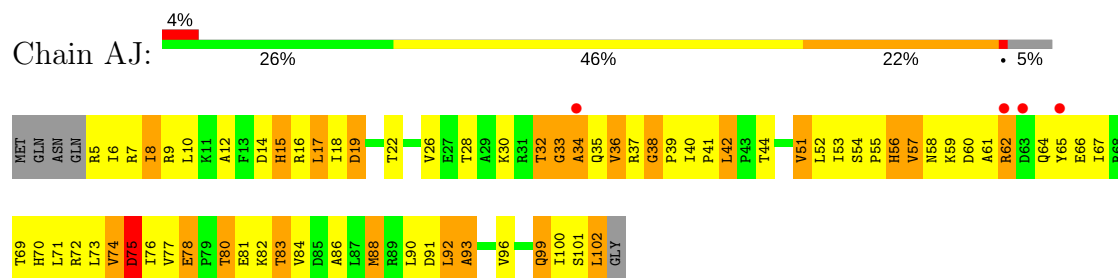


- Molecule 8: 30S ribosomal protein S9

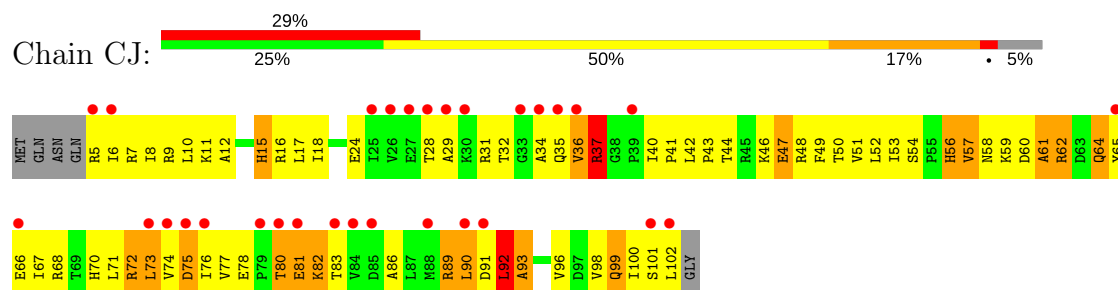




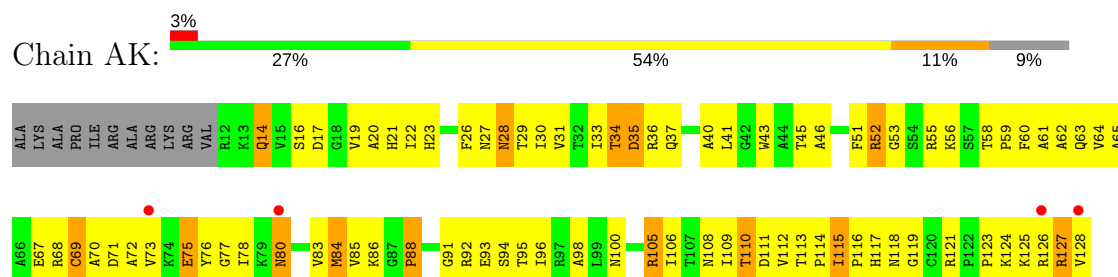
- Molecule 9: 30S ribosomal protein S10



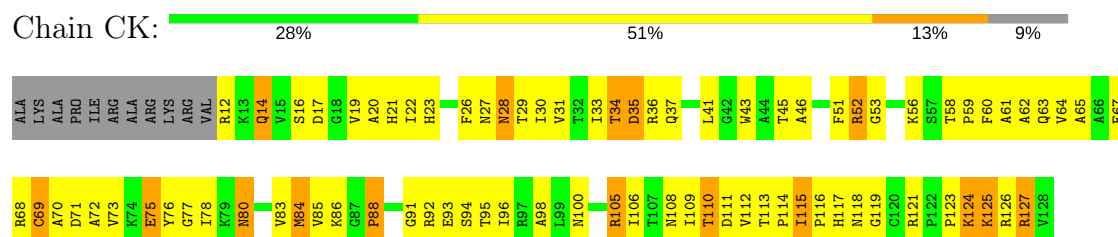
- Molecule 9: 30S ribosomal protein S10



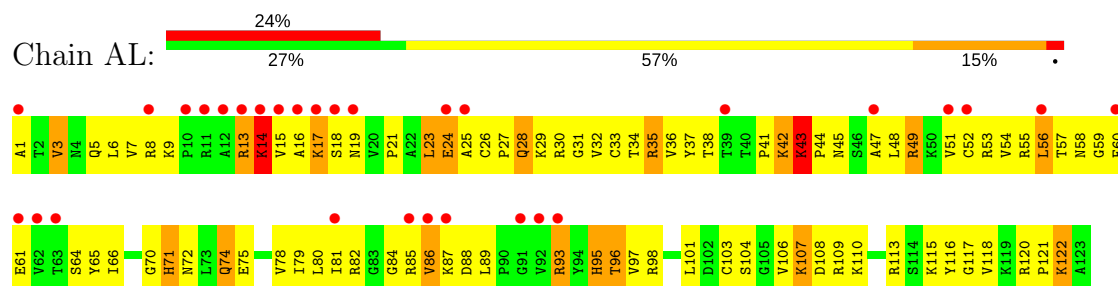
- Molecule 10: 30S ribosomal protein S11



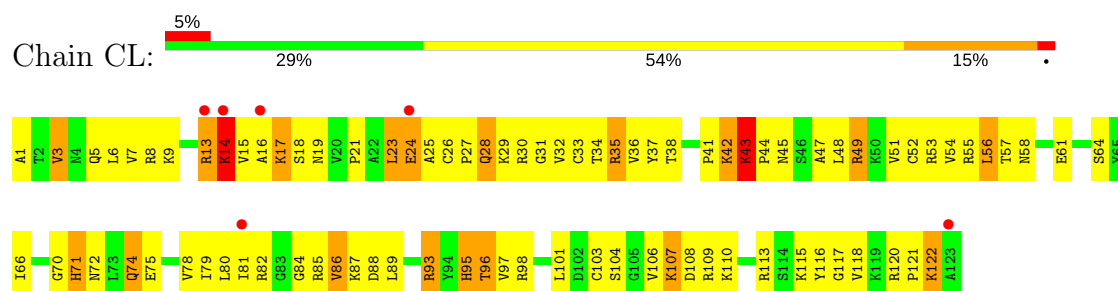
- Molecule 10: 30S ribosomal protein S11



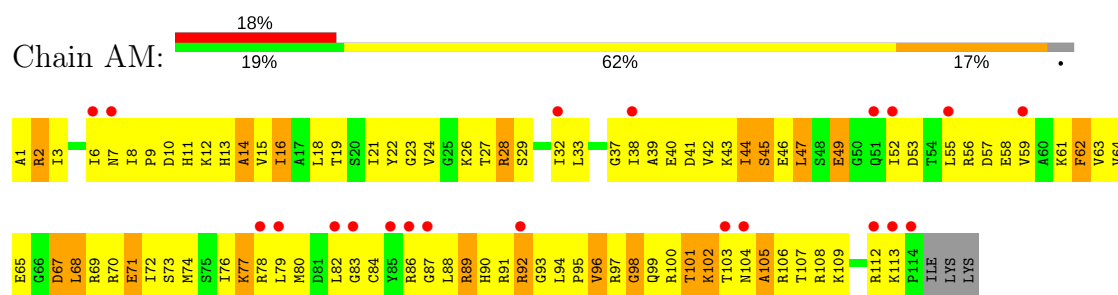
• Molecule 11: 30S ribosomal protein S12



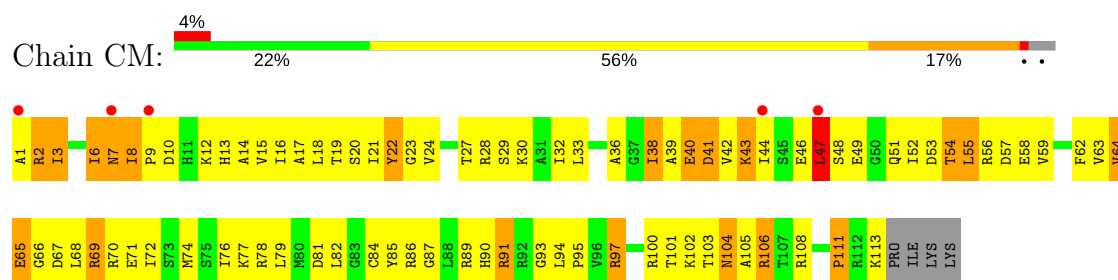
• Molecule 11: 30S ribosomal protein S12



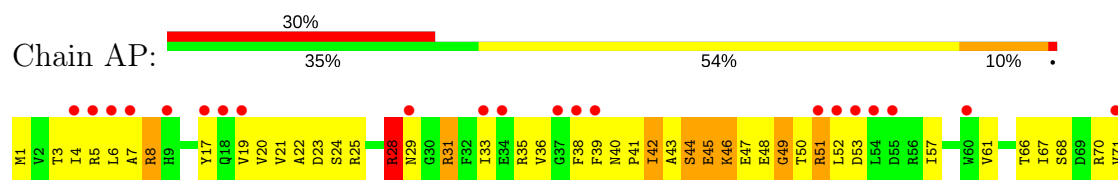
• Molecule 12: 30S ribosomal protein S13

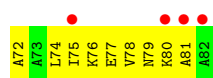


• Molecule 12: 30S ribosomal protein S13

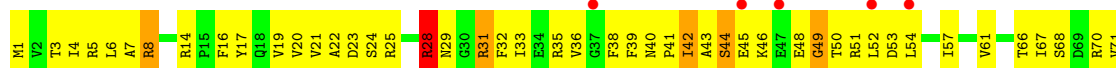


• Molecule 13: 30S ribosomal protein S16

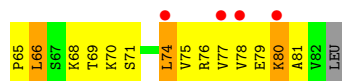
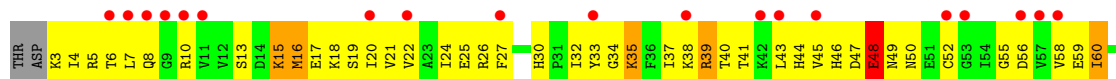




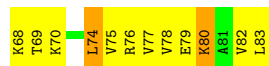
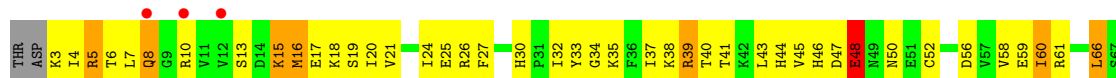
• Molecule 13: 30S ribosomal protein S16



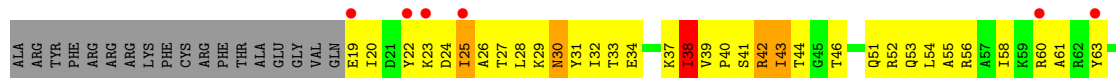
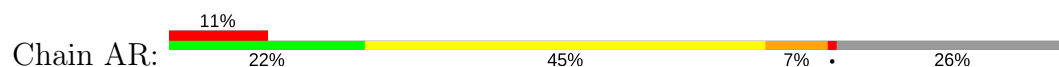
• Molecule 14: 30S ribosomal protein S17



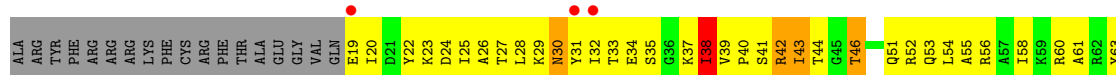
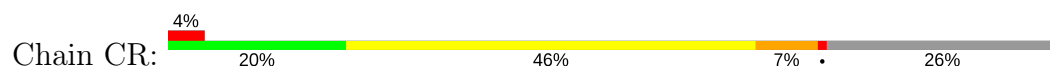
• Molecule 14: 30S ribosomal protein S17



• Molecule 15: 30S ribosomal protein S18

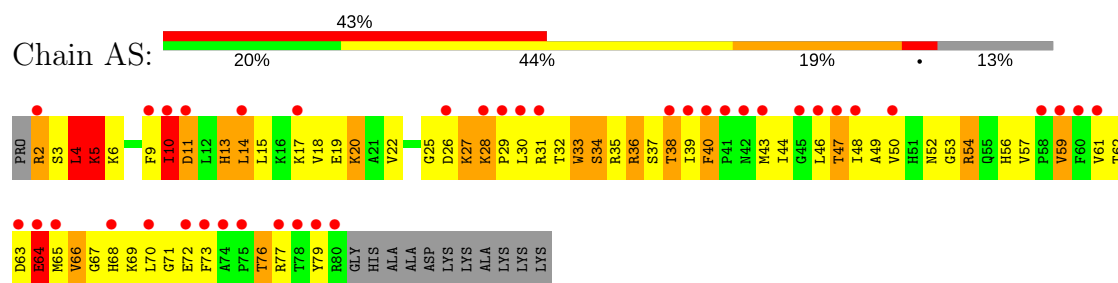


• Molecule 15: 30S ribosomal protein S18

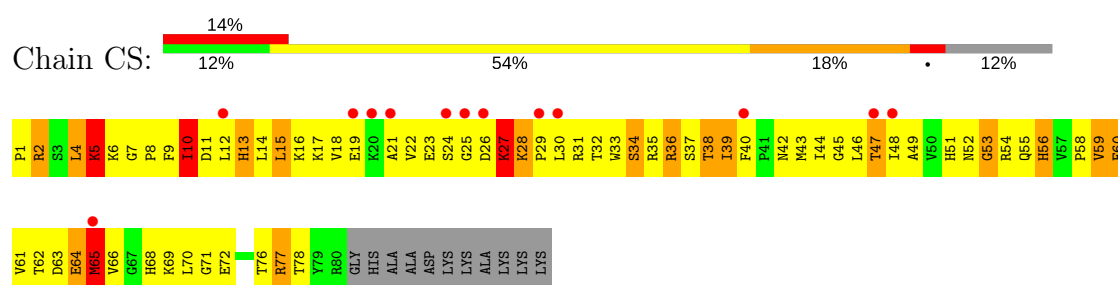




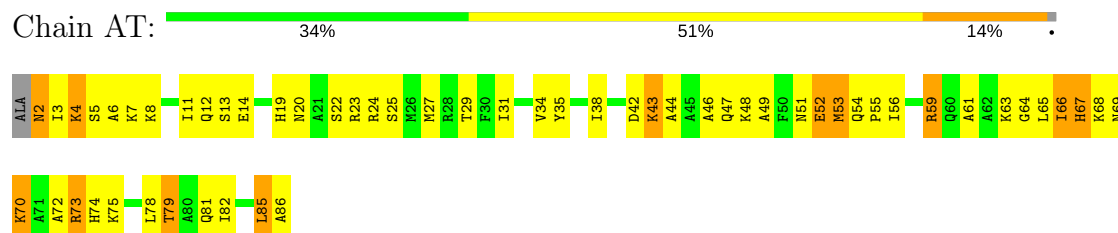
• Molecule 16: 30S ribosomal protein S19



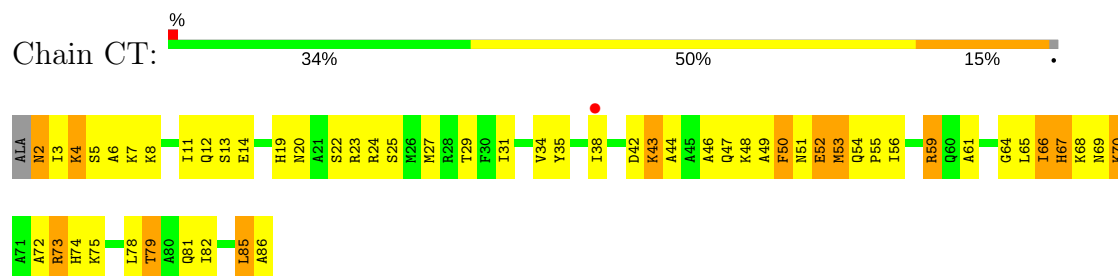
• Molecule 16: 30S ribosomal protein S19



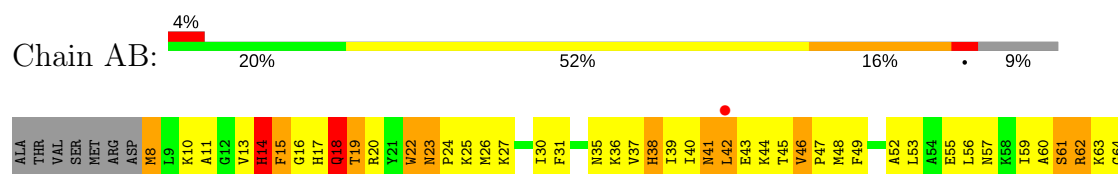
• Molecule 17: 30S ribosomal protein S20

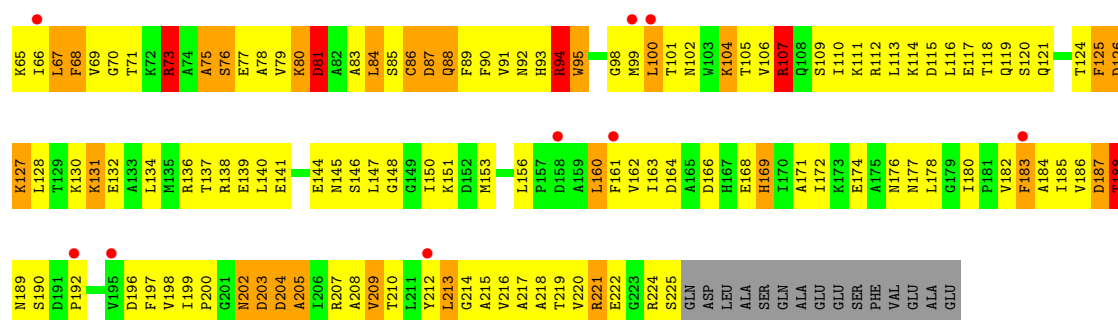


• Molecule 17: 30S ribosomal protein S20

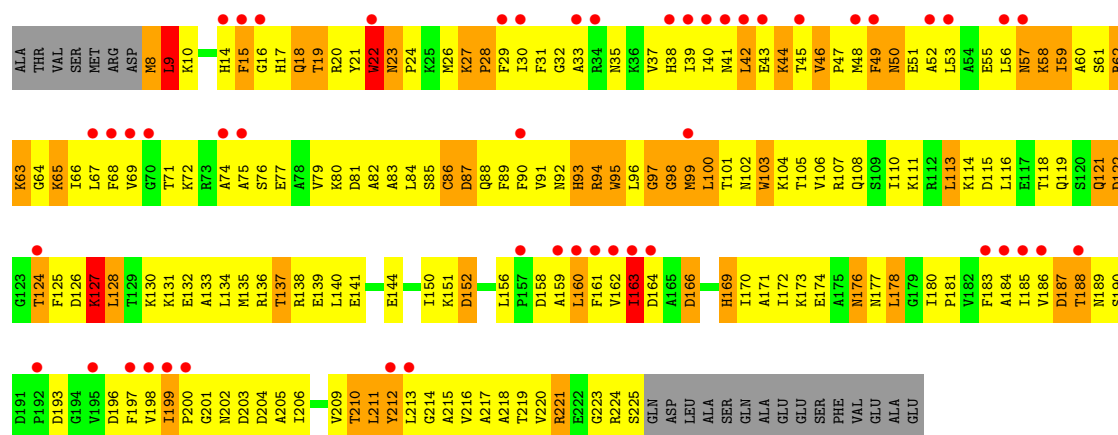
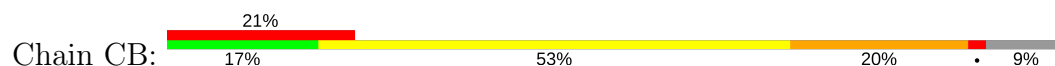


• Molecule 18: 30S ribosomal protein S2

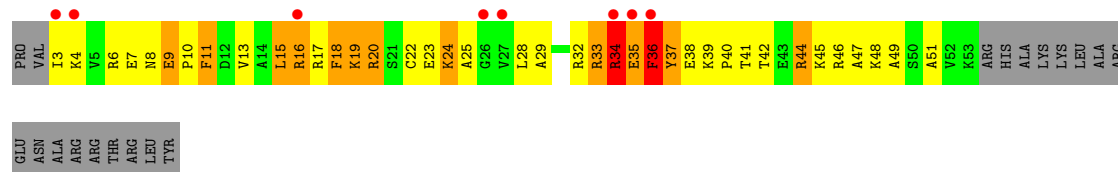
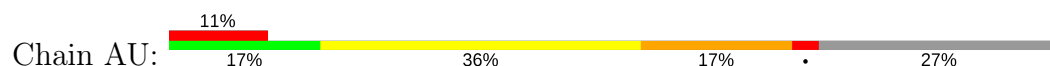




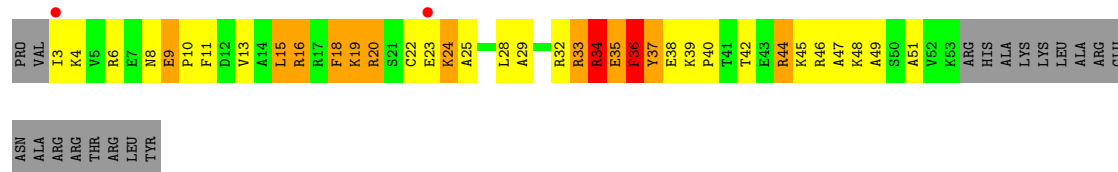
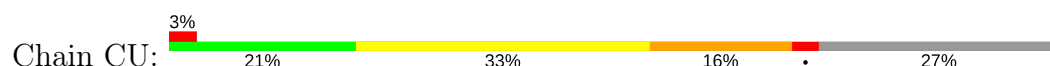
• Molecule 18: 30S ribosomal protein S2



• Molecule 19: 30S ribosomal protein S21

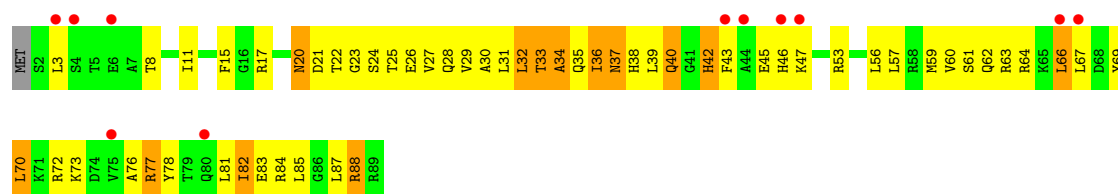


• Molecule 19: 30S ribosomal protein S21

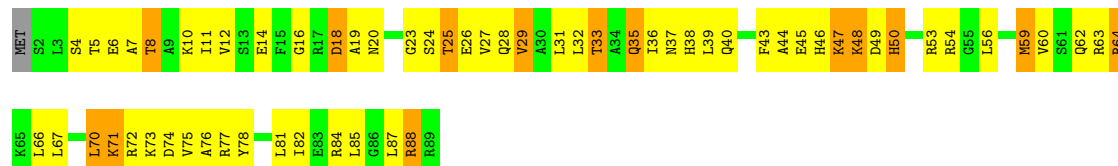


• Molecule 20: 30S ribosomal protein S15

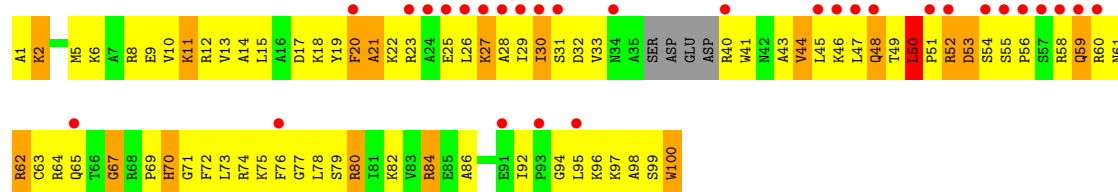




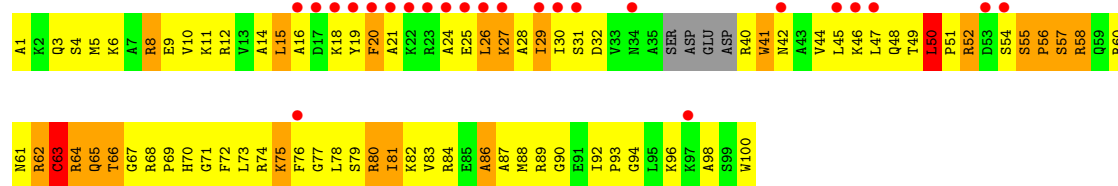
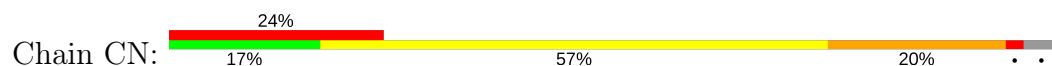
• Molecule 20: 30S ribosomal protein S15



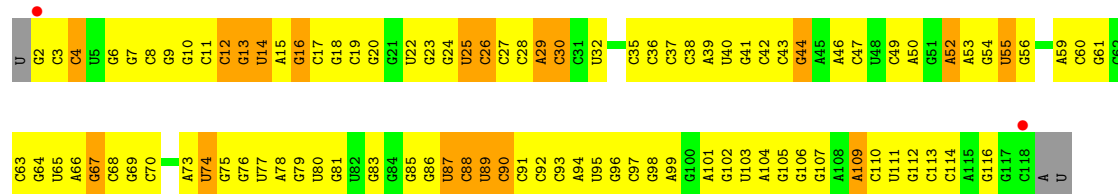
• Molecule 21: 30S ribosomal protein S14



• Molecule 21: 30S ribosomal protein S14

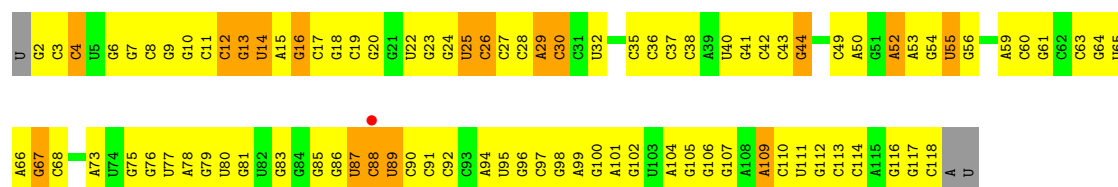


• Molecule 22: 5S rRNA

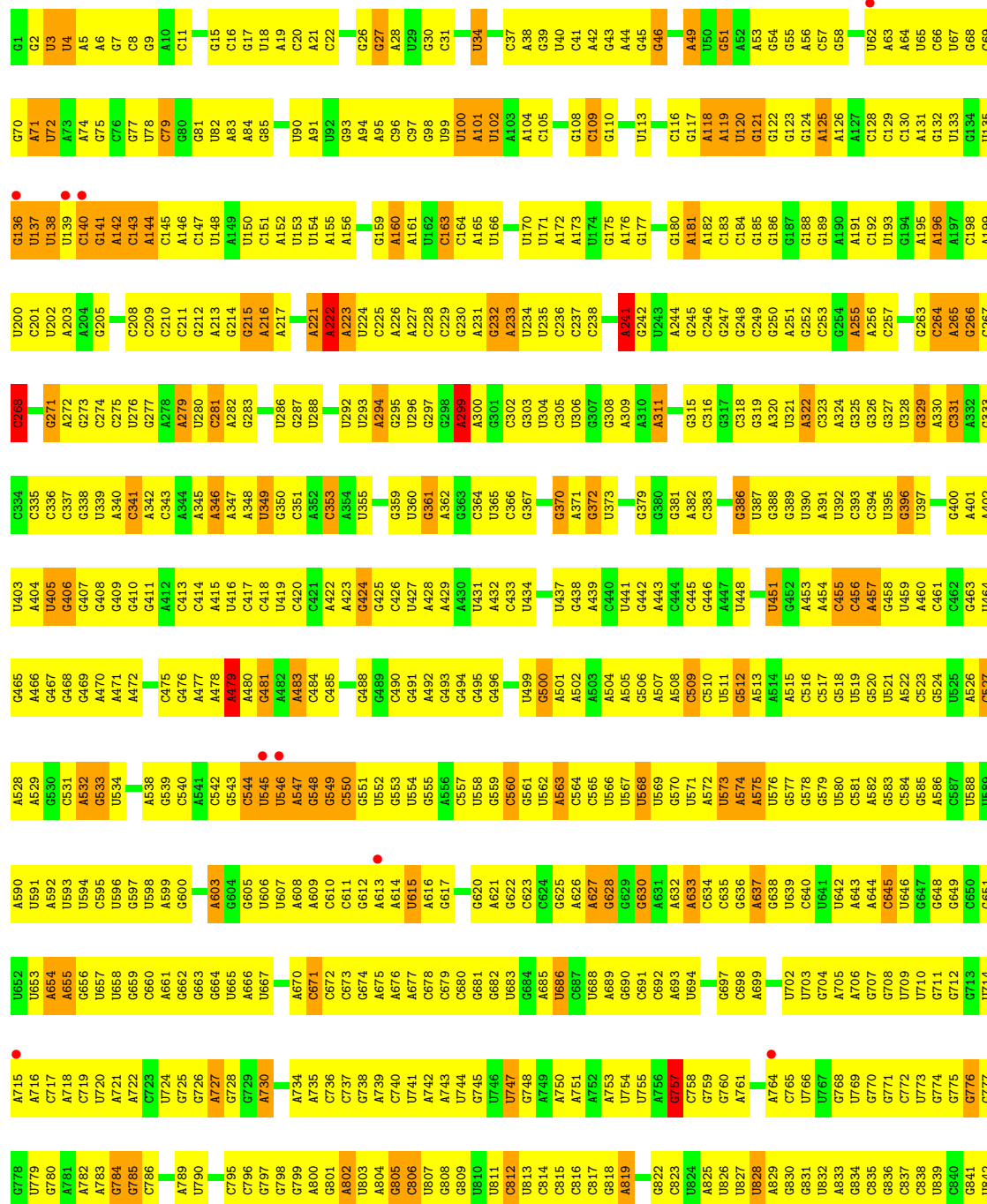


• Molecule 22: 5S rRNA





Molecule 23: 23S rRNA



G1749	G1684	G1619	U1486	G1424	G1360	C1293	C1229	G1160	U1097	U1033	G969	G907	G843
G1750	G1685	G1623	U1487	G1425	G1361	U1294	U1230	G1163	A1098	G1034	U970	G908	A844
G1751	G1686	G1624	C1488	G1426	G1362	G1295	U1231	G1164	G1099	U1035	G971	C908	A845
G1752	G1687	U1624	C1489	A1427	G1363	G1296	G1232	A1165	U1101	G1036	A972	A910	U846
G1753	G1688	C1625	A1490	C1428	A1365	C1297	U1234	G1165	U1102	G1037	A973	A911	U847
G1754	U1689	G1626	U1558	G1429	A1366	G1300	U1235	G1166	C1102	G1038	A974	A912	U848
G1755	A1690	U1627	G1559	G1430	A1367	A1301	G1236	C1167	A1103	A1040	A975	C912	A849
G1756	C1691	U1629	G1560	A1431	A1368	A1302	A1237	C1170	C1104	U1041	U974	G914	U850
G1757	U1692	U1630	U1562	A1495	G1369	A1301	G1238	G1171	U1105	G1042	U975	G915	C851
U1758	G1693	G1631	U1563	A1434	C1370	A1302	U1240	G1172	A979	G1043	A980	C916	U852
C1694	U1694	A1632	U1564	A1434	G1371	C1306	U1241	C1173	A981	C1044	A981	C917	C853
G1695	G1633	G1435	U1565	G1435	U1372	A1307	A1241	U1173	U1108	G1045	A982	A918	C854
C1760	A1501	G1436	A1502	G1436	A1373	A1308	U1242	U1174	C1109	A1046	A983	U919	C855
C1761	A1566	G1437	G1567	C1437	G1374	G1309	C1243	A1175	A984	G1047	A984	U920	C856
A1762	G1567	U1438	U1568	A1439	U1375	G1310	G1244	U1176	A1111	G1047	C985	C921	G857
G1763	G1568	U1438	U1569	A1439	U1376	G1311	G1245	G1177	G1112	A1050	C986	C922	U858
C1764	A1504	U1440	A1505	U1440	U1379	U1312	G1248	C1178	U1051	G1051	C987	G923	G859
C1765	U1506	G1441	U1507	G1441	U1380	U1313	U1249	G1179	G1115	G1052	C988	G924	U860
A1705	U1507	U1442	A1508	U1442	G1381	U1314	U1250	U1180	G1116	C1052	A988	A925	A861
C1706	A1508	U1443	A1509	U1443	G1382	C1315	G1251	U1181	C1117	C1053	A989	A926	G862
C1768	A1509	G1444	U1513	G1444	G1383	C1316	G1252	U1182	C1118	A1054	A990	G927	A863
G1771	U1514	G1445	A1515	G1445	A1384	G1317	G1253	U1183	U1119	G1056	C991	A928	G864
A1772	G1514	C1447	A1516	G1447	A1385	U1318	A1254	U1184	C1121	U1057	C992	G929	C865
C1773	U1515	G1448	G1517	G1448	C1386	C1319	U1255	G1187	U1058	G984	G993	U929	A866
C1774	G1517	U1449	G1518	G1449	G1387	C1320	U1256	U1188	G1124	U1059	C995	G930	U870
U1777	G1518	G1450	C1518	G1450	G1388	A1321	G1257	A1189	G1125	G1060	A996	U931	U871
G1778	G1519	U1451	A1523	U1451	G1389	G1324	U1258	A1190	U1061	U1061	A997	U932	U872
A1779	U1520	A1453	U1524	U1453	U1390	U1325	U1259	G1191	G1062	G1062	G997	A934	C873
U1780	G1521	C1454	U1525	C1454	U1391	U1326	A1260	G1192	G1063	G1063	C998	C935	G874
U1781	U1522	U1455	U1526	U1455	A1392	A1327	C1261	G1193	A1129	C1064	A1000	A936	G875
U1782	G1523	U1456	U1527	U1456	A1393	A1328	A1262	A1194	U1130	U1065	A1001	C937	C876
A1783	U1524	U1457	U1528	U1457	U1394	U1329	U1263	G1195	U1131	U1066	C1005	G938	A877
U1784	G1525	U1458	A1529	U1458	U1395	C1330	G1266	G1196	U1132	A1067	C1006	G939	A878
A1785	U1526	U1459	U1530	U1459	C1396	C1331	U1267	G1197	U1133	G1068	A941	G940	G
U1786	U1527	C1461	U1531	C1461	C1397	G1332	U1268	U1198	A1134	G1069	A942	G941	G
G1788	G1528	C1462	U1532	C1462	U1400	G1333	A1269	U1199	C1135	A1070	A943	G942	G
A1789	U1529	C1463	U1533	C1463	G1401	C1335	U1270	U1203	G1136	G1071	A1010	G943	G
C1790	G1530	G1464	U1534	G1464	U1402	A1336	G1271	U1204	G1137	C1072	G1011	C944	G
G1791	U1531	G1465	U1535	G1465	U1403	G1337	U1272	A1205	G1138	C1076	U1012	A945	U
C1792	U1532	U1466	U1536	U1466	C1404	G1338	U1273	G1206	C1140	A1077	C1013	C946	C
C1793	U1533	U1467	U1537	U1467	U1405	G1339	U1274	U1141	U1141	U1078	A1014	A947	A
A1794	U1534	U1468	U1538	U1468	U1406	U1340	A1275	U1142	U1142	C1079	U1015	C948	U
C1795	U1535	U1469	U1539	U1469	G1407	G1341	A1276	G1210	A1143	A1080	G1016	G949	C
U1796	U1536	U1470	U1540	U1470	G1408	U1344	A1277	C1211	A1144	U1081	G1017	G950	C
G1797	U1537	U1471	U1541	U1471	U1409	C1345	G1279	C1212	C1145	U1082	U1018	C951	C
U1798	U1538	C1472	U1542	C1472	G1410	G1346	U1280	A1213	C1146	U1083	U1019	G952	G
G1799	U1539	U1473	U1543	U1473	U1411	U1347	G1281	G1214	C1147	A1084	A1020	U955	A
C1800	U1540	G1474	U1544	G1474	U1412	C1348	U1282	G1215	U1148	U1085	G1022	G956	C
A1801	U1541	U1475	U1545	U1475	C1414	C1349	U1283	U1219	G1149	A1086	U1023	C957	U
A1802	U1542	U1476	U1546	U1476	U1415	C1350	A1284	G1220	C1150	G1087	G1024	U958	A
A1803	U1543	A1477	U1547	A1477	G1416	C1351	U1285	G1221	A1151	A1088	G1025	A959	C
C1804	U1544	U1478	U1548	U1478	C1417	U1352	A1286	C1221	C1152	A1089	A960	C961	C898
A1805	U1545	G1479	U1549	G1479	G1418	A1353	U1287	U1222	C1153	A1090	A1027	G962	A899
C1806	U1546	U1480	U1550	U1480	G1419	A1354	C1288	G1225	G1154	C1091	A1028	U963	A900
G1807	U1547	U1481	U1551	U1481	A1419	G1355	C1289	A1226	U1157	C1092	A1029	C964	C901
U1808	U1548	G1482	U1552	G1482	A1420	G1356	C1290	G1227	C1158	A1095	C1030	U967	C902
A1809	U1549	U1483	U1553	U1483	G1421	C1357	C1291	U1228	U1159	A1096	C1031	C968	G904
U1810	C1550	G1484	U1554	G1484	G1422	G1358	C1292						
C1748	A1551	U1485		U1485	G1423	A1359							

C2815	C2816	A2748	G2677	C2610	A2542	G2472	A2406	A2340	A2274	C2145	A2080	A2015	U1944	G1878	U1812
G2817	U2817	A2749	C2678	C2611	G2543	C2473	A2407	G2341	C2275	C2146	U2081	G2018	G1945	C1879	G1813
U2818	G2751	U2750	A2679	U2612	G2544	C2476	U2408	C2342	G2276	A2147	A2082	G2019	C1946	U1880	C1816
C2819	G2819	C2752	A2680	U2613	G2545	A2476	G2409	U2343	G2277	G2148		A2020	C1947	U1881	U1817
A2820	C2753	A2753	U2681	U2614	U2546	U2479	G2410	G2344	A2278	U2149	U2085	C2021	G1948	U1883	U1818
A2821	U2754	U2754	C2480	G2615	U2548	C2480	G2411	G2345	G2279	C2150	G2087	U2022	G1950	G1884	A1819
G2822				G2616	U2549		G2412	A2346	G2280	C2153	A2088	C2023	U1951	A1885	U1820
A2823				G2618	G2550	G2484	G2413	C2347	A2281	A2154	C2089	G2024	U1952	U1886	A1821
C2824					C2551	G2485	G2415	G2349	G2282			C2025	A1953	G1887	G1822
G2825				G2621	U2552	G2486	C2416	C2350	G2283	U2155	U2092	U2026	G1954	G1888	G1823
				U2622	G2553	G2487	C2417	G2351	A2284	G2157	G2093	G2027	U1955	A1889	G1824
G2828				G2623	U2554	G2488	A2418	A2352	G2285		A2094	U2028	U1956	U1825	U1825
A2829				G2624	U2555	U2489	U2419	G2353	A2287	G	A2095	G2029	C1957	G1826	G1826
G2830				G2625	C2556	G2490	C2420	G2354	G2288	C	C2096	A2030	G1958	G1897	U1827
G2831				G2626	G2557	U2491		G2355	G2289	C	A2097	A2031	G1959	U1898	G1828
				G2627	U2558	U2492		U2356	G2290	G	U2098	G2032	U1963	A1899	A1829
G2834				G2628	C2559	G2493	U2423	G2357	U2291		U2099	G2035	G1964	A1900	G1830
A2835				U2629	A2560	G2494	A2425	A2358	U2292	C	G2100	G2036	C1965	A1901	G1831
U2836				G2630		G2495	A2426	C2359	G2293	C	A2101	C2037	U1966	G1902	G1832
A2837					A2564		C2427	G2360	U2297	U		A2037	C1967	G1903	
G2838				G2632	A2565		G2428	G2361	A2297	U	U2102	G2038	A1968	G1904	G1838
G2839				G2633	A2566		G2429	C2362	A2298	U	C2103	U2039	C1967	G1905	G1839
C2840				A2634	A2567		A2430	G2363	U2299	G	C2104	G2040	G1968	G1906	G1840
C2841				A2635	U2568		U2431	G2364	C2300	A	U2105	U2041	A1970		U1841
G2842				C2636	G2569		A2432	G2365	C2301	A	U2106	A2042	U1971	G1909	G1842
G2843				U2637	U2570		A2433	A2366	G2239			A2043	U1972	G1910	G1843
U2844				G2638	G2571		G2437	G2367	U2240	U	G2110	G2046	G1973	U1911	C1844
G2845				A2639	A2572		U2438	G2368	G2242	C		C2047	C1974	A1912	G1845
U2846				G2640	C2573		U2439	G2370	U2243	C		G2048	A1977	G1914	G1846
U2847					G2574		A2440	G2371	G2244	C		G2049	A1978	A1847	A1847
U2848				G2641	C2575		U2441	U2372	U2245	C		C2050	U1915	A1848	A1848
U2849				C2646	U2576		U2449	C2380	G2246			G2056	A1916	G1849	G1849
U2850				U2647	G2578		A2450	G2383	C2247	G		A2051	G1983	U1917	G1850
A2851				G2648	C2579		A2451	A2376	C2248	U		A2052	G1984	A1918	U1851
G2852				C2649	U2580		C2452	A2377	U2249	U		G2053	C1985	A1919	U1852
C2853				U2650	G2581		A2453	C2378	G2250	U		A2054	C1986	C1920	A1853
G2854				C2651	G2582		U2454	G2379	G2251	A		C2055	A1987	G1921	A1854
				C2652			A2448	C2380	G2252			G2056	U1988	U1922	
				C2653	U2586		U2449	G2383	G2253	U		G2056	G1989	U1923	G1857
				U2647	A2587		A2450	G2384	C2254	U		A2060	C1990	C1924	A1858
				G2654			A2451	U2384	G2255	G		G2061	U1991	G1925	U1859
				U2655			C2452	C2385	G2256	U		A2062	U1992	U1926	G1860
				U2656	A2590		A2453	A2386	U2257	U		C2063	U1993	A1927	G1861
				C2657	G2591		G2454	U2387	C2258			C2064	C1994	A1928	G1862
				A2657	G2592		G2455	A2388	U2259			C2065	U1995	G1929	G1863
				G2658			U2456	G2389	C2260	C		C2066	C1996	U1930	U1864
				G2659	G2597		U2457	U2390	C2261	U		C2067	C1997	U1931	U1865
				A2733	U2526		G2458		U2262			U2068	A1998	A1932	A1866
				G2735	C2527		A2459	U2393	C2263			G2069	C1999	G1933	G1867
				G2736	U2528		U2460	U2394	C2264			A2070	C2000	G1868	C1868
				A2737	G2529		A2461	C2394	U2265	A		A2071	C2001	G1869	G1869
				G2738	A2530		C2462	C2395	U2266	A		C2072	C1935	A1870	C1870
				U2739	A2531		G2463	G2396	A2267			C2073	U1936	A1937	A1871
				A2740	G2532		G2463		A2268			C2074	A1938	A1872	G1872
				G2741	U2533				A2269			U2075	U1939	G1873	A1873
				U2742	A2534		C2466	U2400	G2270			U2076	U1940	C1874	C1874
				U2743	U2535		U2401	U2402	A2271			U2077	G1941	G1875	G1875
				G2744	C2536		A2463	A2403	G2272			A2078	A2013	A1876	A1876
				C2745	G2537		A2469	G2404	U2273			C2078	A2014	U1943	A1877
				U2746	C2538		G2470		A2274			U2079			
				G2747	U2539		A2471	G2405	A2275						

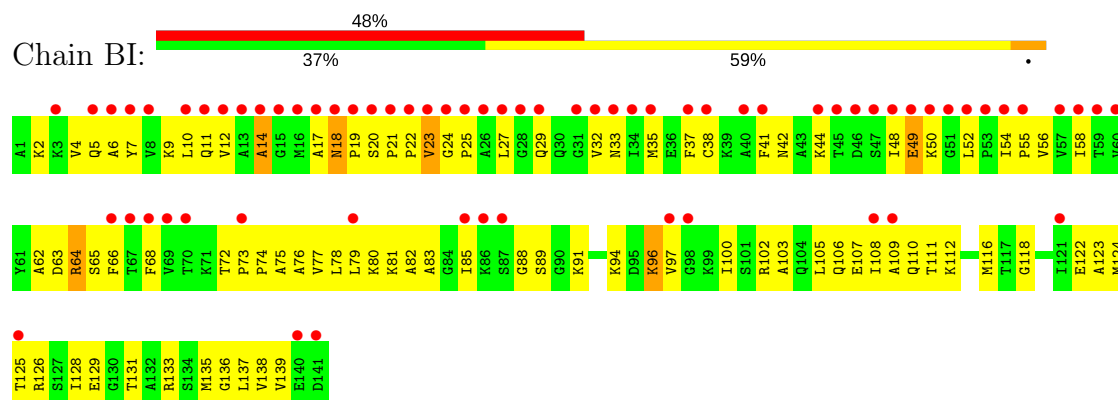


A1819	G1756	C1691	G1628	C1561	A1494	G1432	C1370	G1306	G1238	C1170	C1104	A1029	U967	C903
U1820	A1757	U1692	U1629	U1562	A1495	A1433	G1371	A1307	G1239	G1171	U1105	C1030	C968	G904
A1821	U1758	U1693	A1630	U1563	A1496	A1434	U1372	G1309	U1240	C1172	U1106	G1031	C969	G907
C1822	A1759	C1694	G1631	C1564	G1501	G1435	A1373	G1309	A1241	U1173	U1107	A1032	U970	C908
G1823	C1760	G1695	A1632	C1565	A1502	G1437	G1374	G1311	U1242	U1174	C1107	U1033	G971	A909
G1824	C1761	G1696	G1633	A1566	A1503	A1438	U1375	G1312	C1243	A1175	G1110	A1039	A972	A910
U1825	A1762	A1700	A1634	G1567	A1504	U1439	C1376	U1313	A1244	U1176	G1111	A1040	A973	A911
G1826	C1763	A1701	A1635	G1568	A1505	A1440	U1379	C1314	G1245	G1177	U1112	G1041	G974	C912
A1827	G1764	G1702	U1636	A1569	A1506	U1441	U1380	C1315	G1248	U1178	G1113	G1042	A975	U913
G1828	U1765	C1704	A1637	A1570	U1507	G1441	G1381	C1316	U1249	U1179	U1114	C1043	G978	G914
A1829	G1766	A1705	C1638	A1571	U1508	U1442	G1382	C1317	U1250	U1180	C1115	C1044	A979	C915
C1830	C1767	C1706	G1639	A1572	A1508	U1443	A1383	G1318	G1251	U1181	G1116	C1045	A980	G916
G1831	C1768	G1703	A1640	G1573	A1509	U1444	A1384	C1319	G1252	U1182	C1117	A1046	A981	A917
C1832	U1769	U1704	A1641	U1574	U1513	G1445	A1385	C1320	A1253	U1183	U1118	G1047	A982	A918
U1833	C1771	G1710	G1645	U1575	G1514	C1446	A1386	A1321	U1254	U1184	U1119	C1048	A983	A920
C1838	A1772	U1711	U1646	C1577	A1515	C1447	A1387	C1322	G1256	U1187	G1120	A1049	A984	C921
G1839	C1773	U1712	A1647	A1578	A1516	G1448	G1388	C1323	C1257	U1188	U1121	C1050	A985	C922
U1841	A1774	A1713	U1648	A1579	G1517	G1449	G1389	G1324	U1258	A1189	G1124	G1051	C986	G923
C1842	U1715	U1714	G1649	G1581	C1518	G1451	U1390	U1325	G1259	G1190	G1128	C1053	C987	G924
G1843	G1716	G1716	A1650	C1582	C1519	G1452	U1391	U1326	A1260	U1191	U1129	C1054	A988	A925
U1844	U1717	U1717	G1651	A1583	U1520	A1453	A1392	C1327	C1261	G1192	U1130	G1055	G989	G926
C1845	A1718	U1718	G1652	U1584	G1521	C1454	A1393	A1328	A1262	G1193	U1131	G1056	A990	A927
G1846	G1719	G1719	A1653	C1585	U1522	U1457	U1396	C1329	U1263	A1194	U1132	A1057	C991	A928
A1847	U1781	U1720	G1654	A1586	U1523	U1458	U1397	C1330	G1266	U1195	A1143	A1070	C992	U929
U1848	A1782	G1721	A1655	G1587	G1524	U1459	U1398	G1331	U1267	C1196	A1144	C1076	C993	G930
G1849	C1774	A1722	C1656	U1588	A1525	G1459	C1399	G1334	A1268	G1197	C1145	U1060	C994	U931
U1851	A1785	G1723	A1657	G1589	C1526	U1460	U1400	C1335	A1269	U1198	C1146	U1061	C995	U932
C1852	U1786	G1724	C1658	A1590	U1528	C1462	G1401	A1336	G1270	U1199	U1147	G1062	A996	A933
A1853	G1787	U1725	G1659	A1591	A1529	G1463	U1402	G1337	U1271	C1200	G1137	G1063	G997	U934
U1854	C1726	C1727	G1660	C1592	G1529	G1464	A1403	G1338	A1272	U1203	G1138	C1064	C998	C935
U1855	A1789	G1728	G1661	U1593	U1530	G1465	A1404	G1339	U1273	A1204	G1139	U1065	A936	A936
U1856	C1729	U1729	G1662	C1594	C1532	U1466	U1405	U1340	A1274	A1205	U1141	A1000	C937	C937
U1857	G1792	C1730	A1663	U1595	U1533	U1467	U1406	G1341	A1275	G1206	A1142	A1070	A1001	G938
G1858	A1794	G1731	A1665	A1597	U1534	U1468	G1407	U1344	A1276	U1210	A1143	C1076	C1005	G939
U1859	C1795	C1732	G1666	A1598	A1535	A1469	U1408	G1345	G1279	G1211	C1144	A1077	C1006	G940
G1860	U1796	G1733	A1669	U1599	C1536	A1470	U1409	G1346	U1280	G1212	C1145	C1007	C1007	A941
U1861	C1797	U1734	C1670	G1600	G1537	G1471	G1410	G1347	G1281	A1213	C1146	A1080	A1008	G942
G1862	U1798	A1735	A1670	U1601	U1538	C1472	U1411	A1347	U1282	A1214	U1147	A1081	A1009	A943
U1863	G1799	U1736	G1671	G1602	U1539	G1473	A1412	C1348	U1283	U1215	U1148	U1082	A1010	C944
U1864	C1800	G1737	A1672	U1603	G1540	U1474	A1413	C1349	U1284	U1219	G1149	U1083	G1011	A945
U1865	A1801	G1738	G1673	C1607	C1541	G1475	C1414	C1350	A1285	U1219	C1150	A1084	U1012	G946
G1866	U1802	U1739	A1674	A1608	U1542	U1476	U1415	C1351	A1286	G1220	A1151	A1085	C1013	A947
C1867	A1803	G1740	C1675	A1609	G1543	A1477	G1416	U1352	A1287	C1221	C1152	A1086	A1014	C948
U1868	C1804	U1741	G1681	C1617	U1544	G1478	G1417	A1353	U1288	U1222	C1153	G1087	U1015	G949
G1869	A1805	U1742	A1676	A1610	A1545	G1479	G1418	A1354	A1289	G1225	G1154	A1088	G1016	G950
C1870	C1806	G1743	A1677	G1613	U1546	C1480	A1419	A1355	C1290	U1226	U1157	A1089	G1017	C951
A1871	U1807	A1744	A1678	U1619	G1547	U1481	G1420	G1356	G1292	A1227	C1158	A1090	U1018	G952
A1872	G1807	U1745	U1680	G1623	A1548	G1482	G1421	A1359	G1293	G1227	C1161	G1091	U1019	U955
G1873	A1808	A1746	G1681	A1616	U1549	G1483	G1422	G1360	G1294	U1228	U1162	C1092	A1020	G956
C1874	A1809	U1747	C1682	C1617	C1550	U1484	G1423	G1361	U1294	C1229	G1163	G1093	A1021	C957
U1875	U1810	C1748	U1683	A1618	A1551	U1485	G1424	C1362	G1296	U1231	G1164	U1094	G1022	U958
A1876	G1811	U1749	G1684	G1619	U1486	U1486	G1425	A1365	G1296	U1231	A1165	U1097	U1023	A959
U1877	U1812	U1750	C1685	U1623	A1553	U1487	G1426	A1365	G1300	U1234	G1166	A1098	G1024	A960
G1878	G1813	U1751	C1686	G1624	U1554	C1488	A1427	A1366	A1301	G1235	G1167	G1099	G1025	C961
U1879	U1814	C1752	C1687	U1625	U1555	C1489	C1428	A1367	A1302	G1236	G1168	C1100	A1027	G962
U1880	A1815	U1753	G1688	C1626	U1559	A1490	G1429	G1368	U1302	U1237	G1169	U1101	A1028	C964
G1881	C1816	A1754	A1689	U1627	U1560	U1490	A1431	G1369	U1302	U1237	G1169	U1101	A1028	C964
U1882	U1817	U1755	A1690	G1627	G1560	C1493								

WORLDWIDE
PDB
PROTEIN DATA BANK

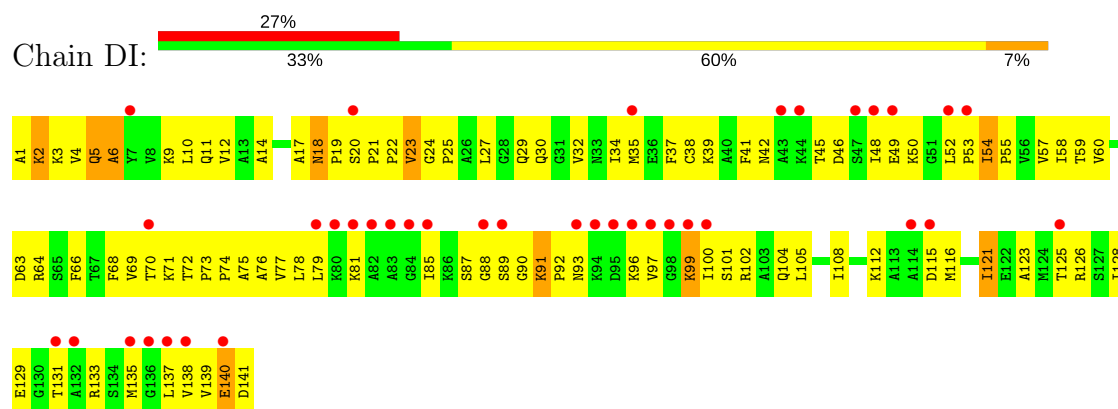
- Molecule 24: 50S ribosomal protein L11

Chain BI:



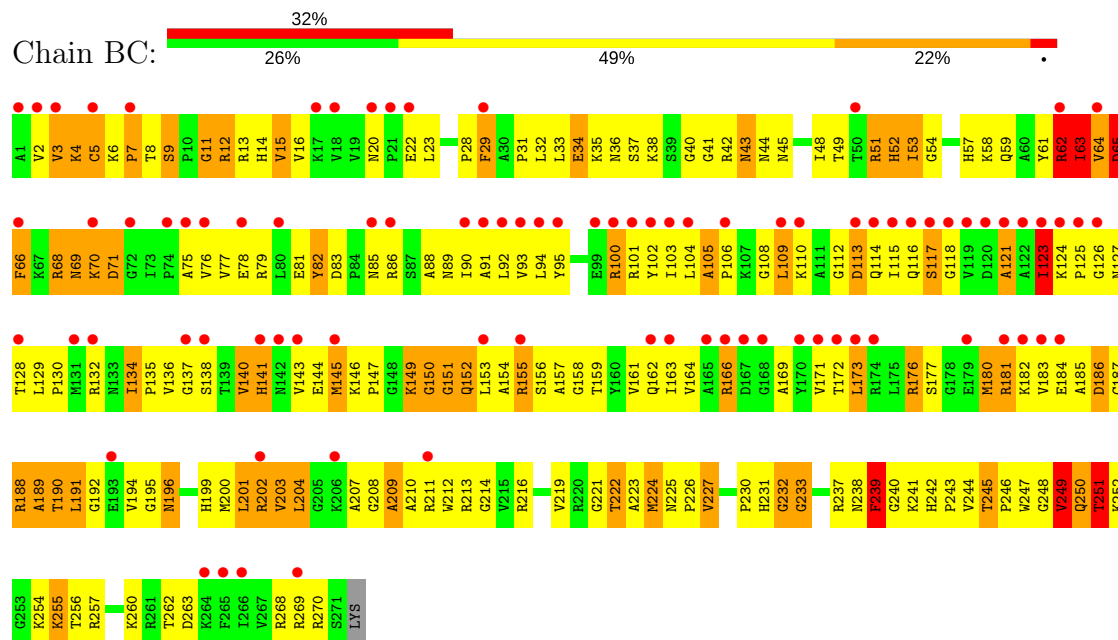
- Molecule 24: 50S ribosomal protein L11

Chain DI:

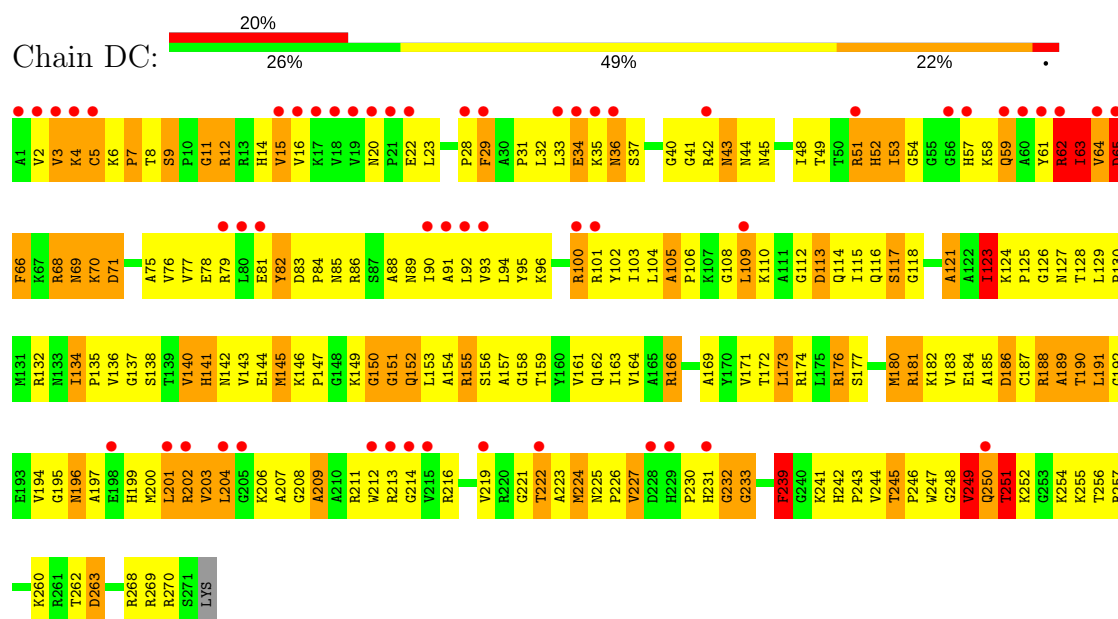


- Molecule 25: 50S ribosomal protein L2

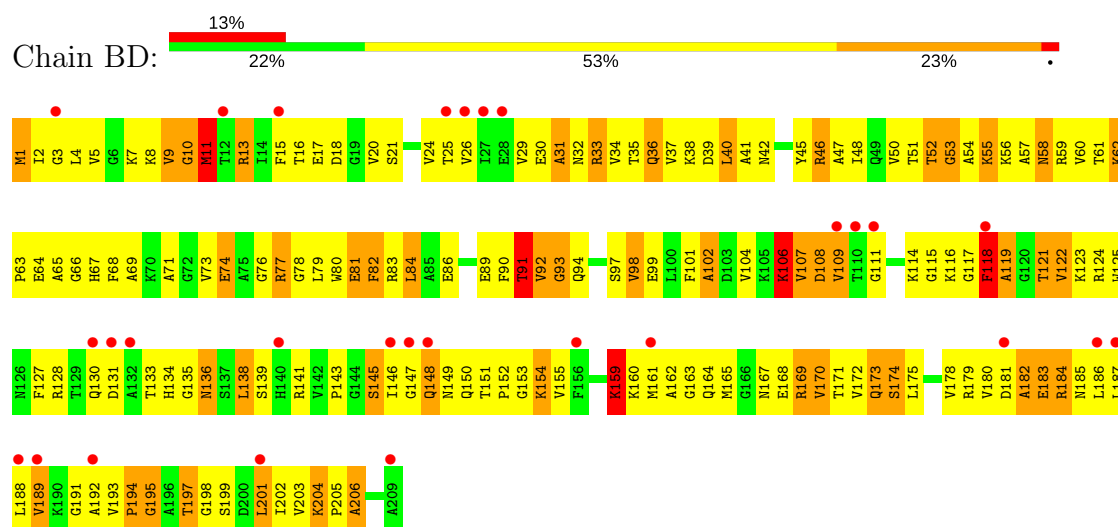
Chain BC:



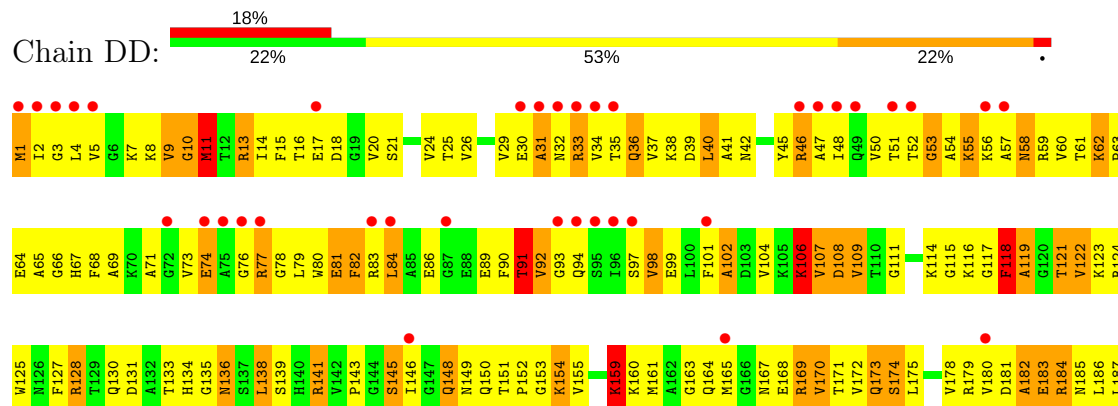
- Molecule 25: 50S ribosomal protein L2



• Molecule 26: 50S ribosomal protein L3

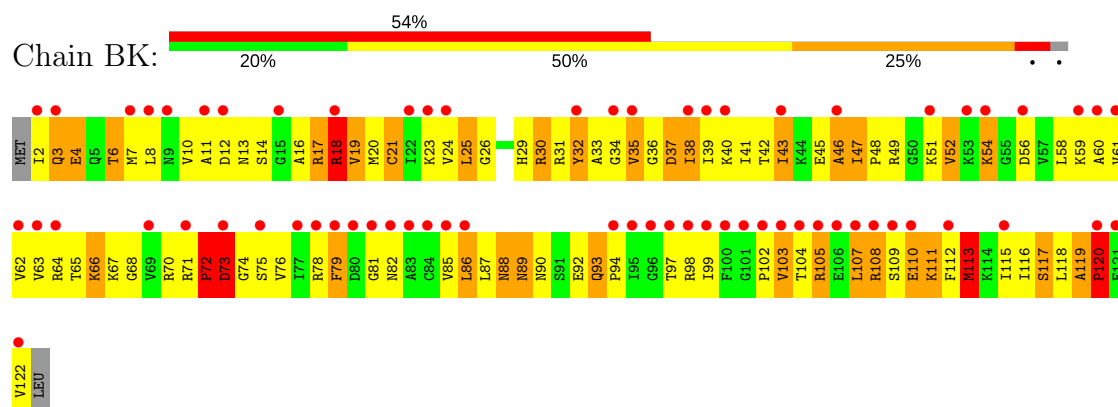


• Molecule 26: 50S ribosomal protein L3

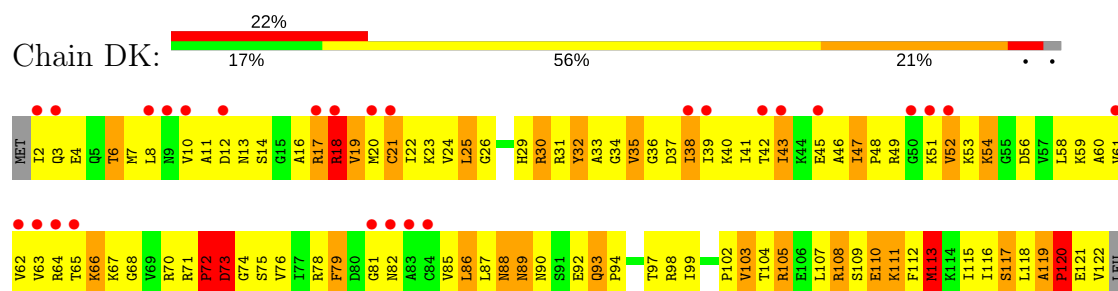




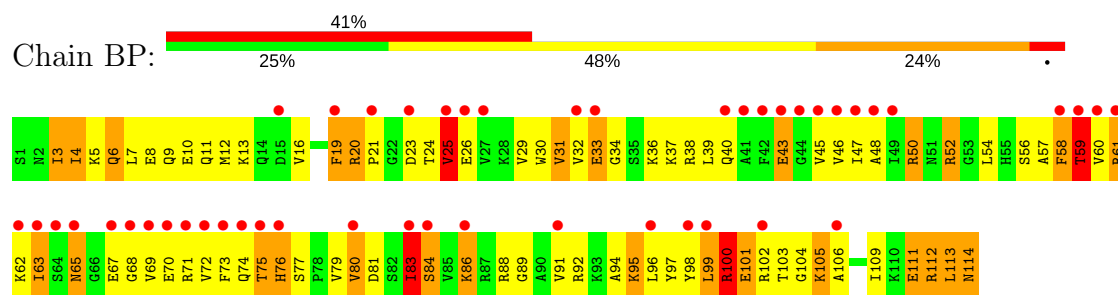
- Molecule 27: 50S ribosomal protein L14



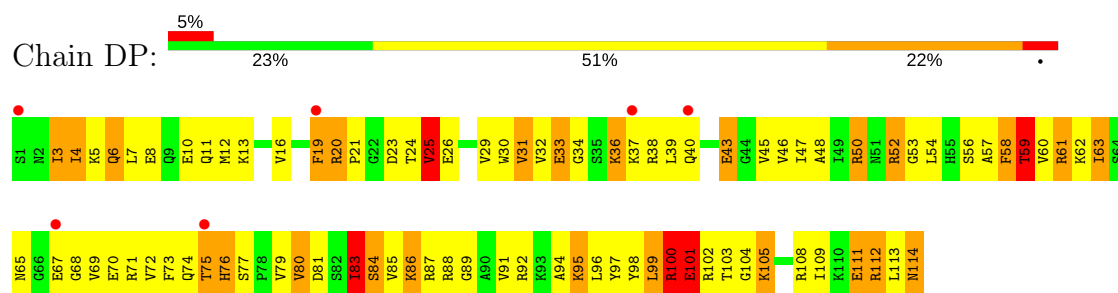
- Molecule 27: 50S ribosomal protein L14



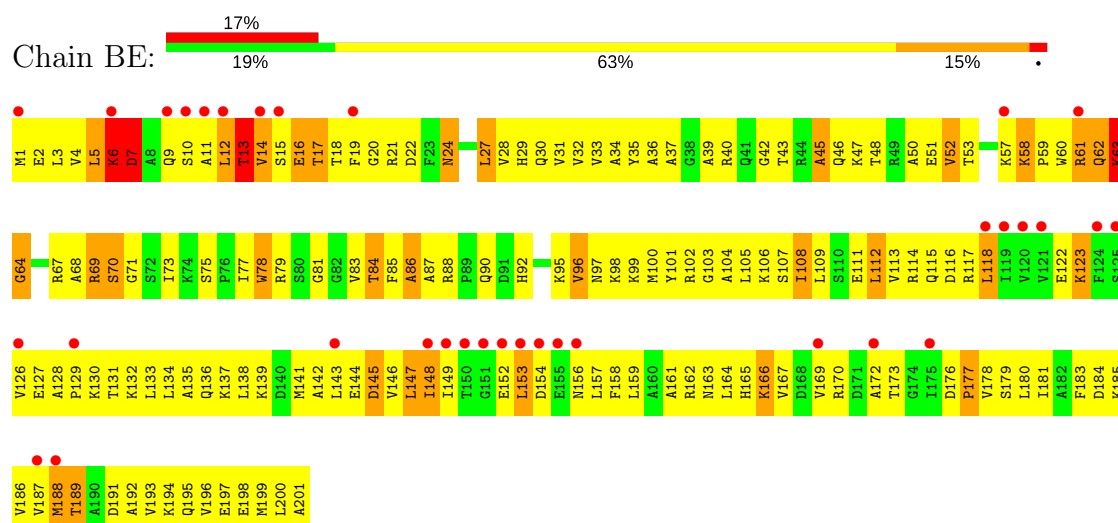
- Molecule 28: 50S ribosomal protein L19



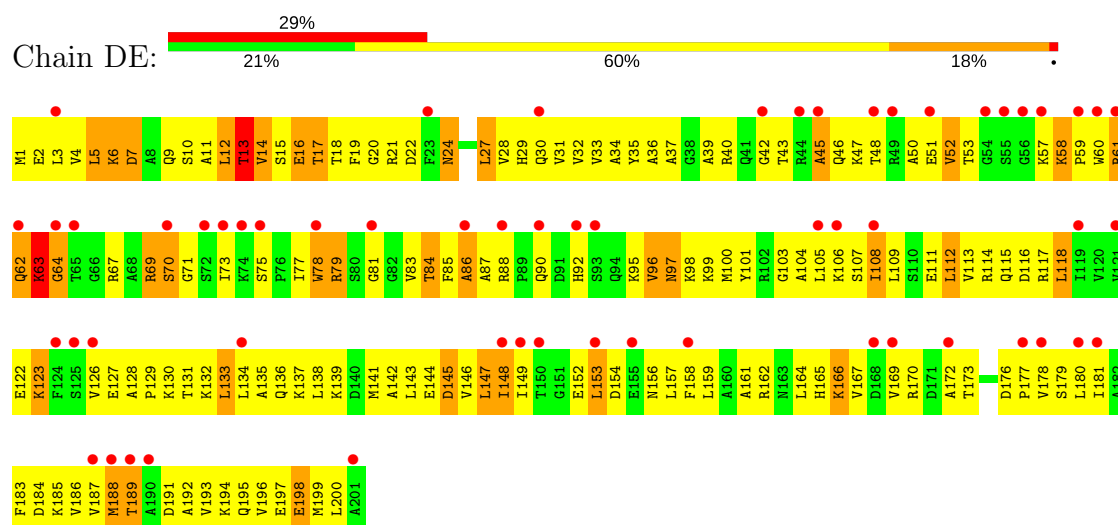
- Molecule 28: 50S ribosomal protein L19



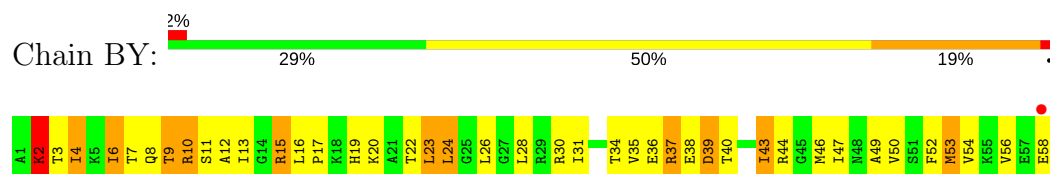
- Molecule 29: 50S ribosomal protein L4



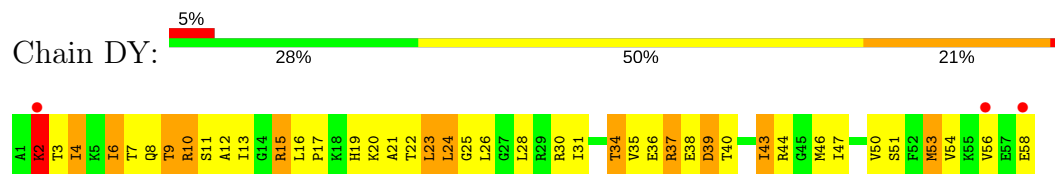
• Molecule 29: 50S ribosomal protein L4



• Molecule 30: 50S ribosomal protein L30



• Molecule 30: 50S ribosomal protein L30

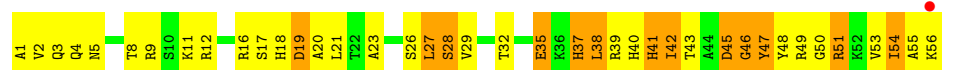


• Molecule 31: 50S ribosomal protein L32





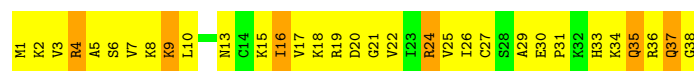
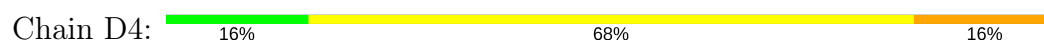
- Molecule 31: 50S ribosomal protein L32



- Molecule 32: 50S ribosomal protein L36



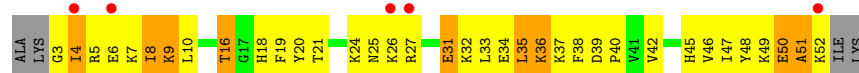
- Molecule 32: 50S ribosomal protein L36



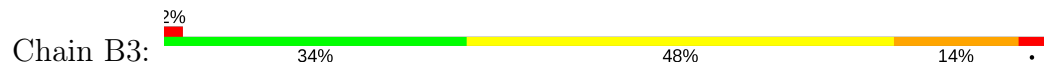
- Molecule 33: 50S ribosomal protein L33



- Molecule 33: 50S ribosomal protein L33

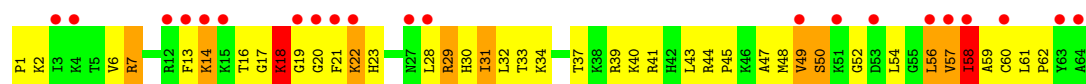


- Molecule 34: 50S ribosomal protein L35



- Molecule 34: 50S ribosomal protein L35

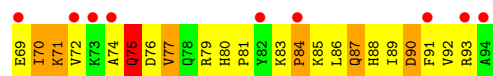
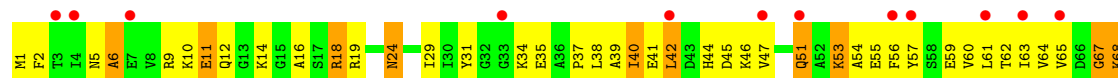




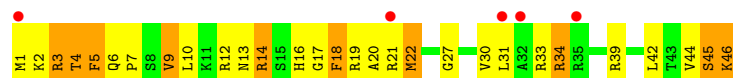
• Molecule 35: 50S ribosomal protein L25



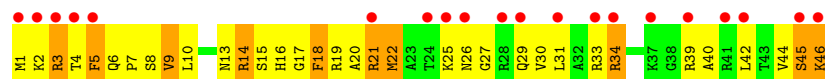
• Molecule 35: 50S ribosomal protein L25



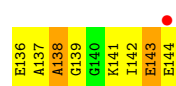
• Molecule 36: 50S ribosomal protein L34



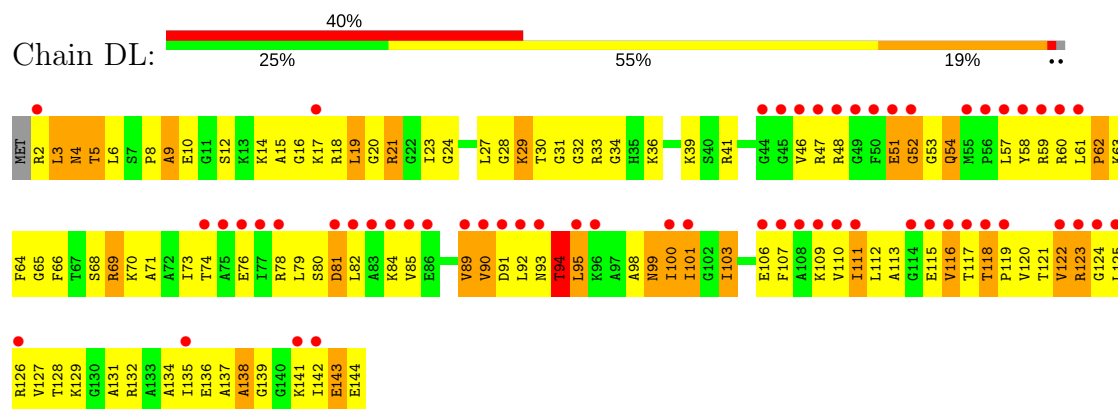
• Molecule 36: 50S ribosomal protein L34



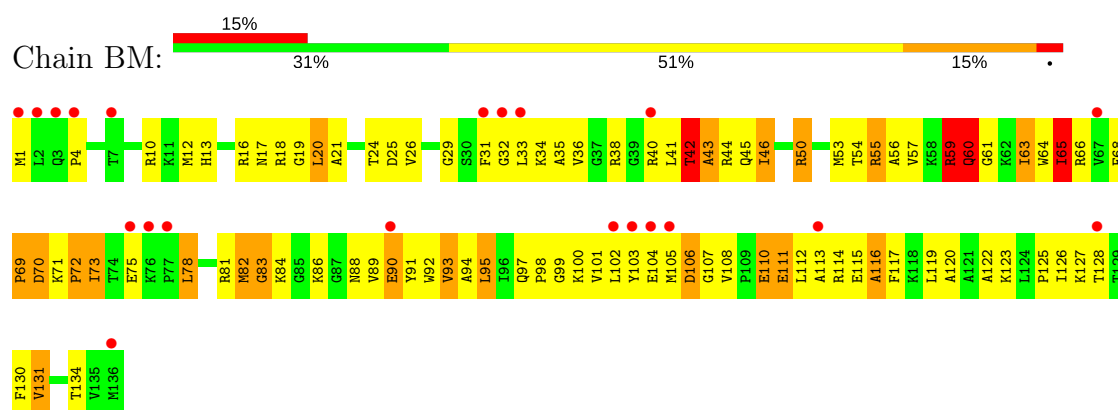
• Molecule 37: 50S ribosomal protein L15



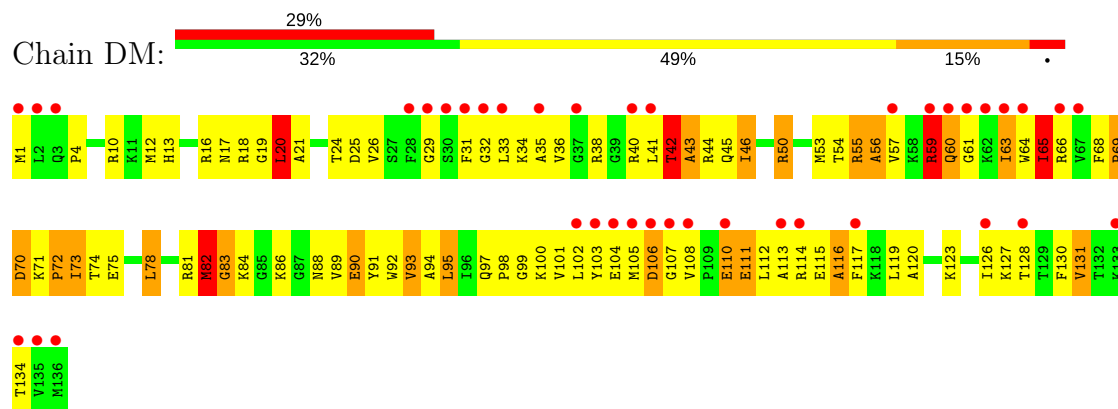
- Molecule 37: 50S ribosomal protein L15



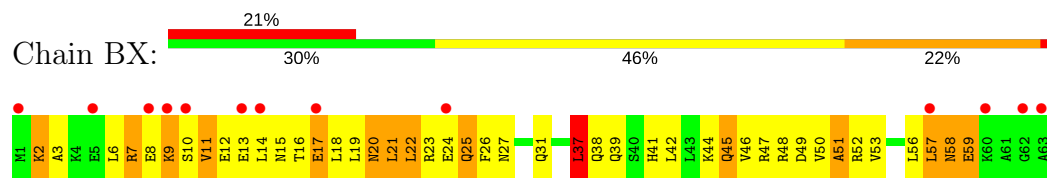
- Molecule 38: 50S ribosomal protein L16



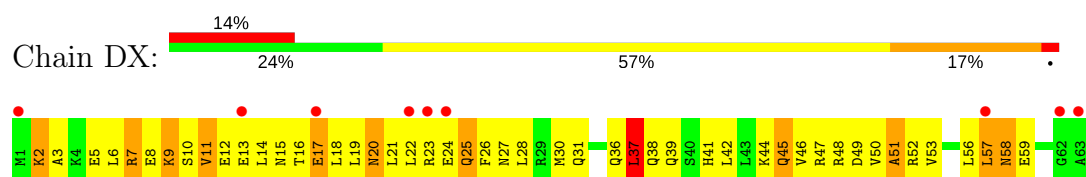
- Molecule 38: 50S ribosomal protein L16



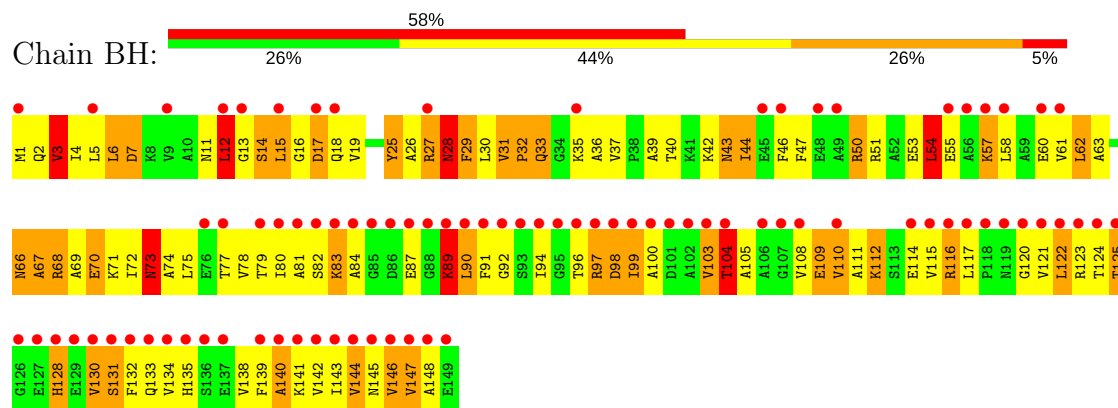
- Molecule 39: 50S ribosomal protein L29



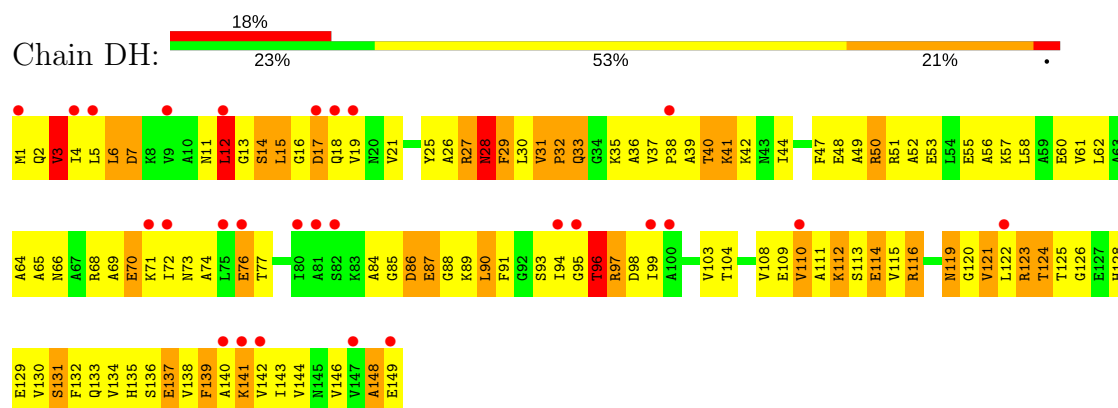
- Molecule 39: 50S ribosomal protein L29



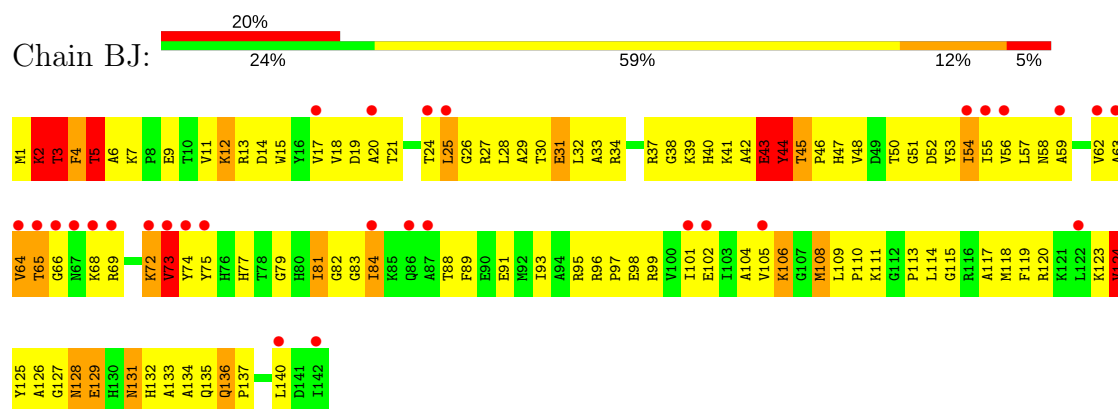
• Molecule 40: 50S ribosomal protein L9



• Molecule 40: 50S ribosomal protein L9

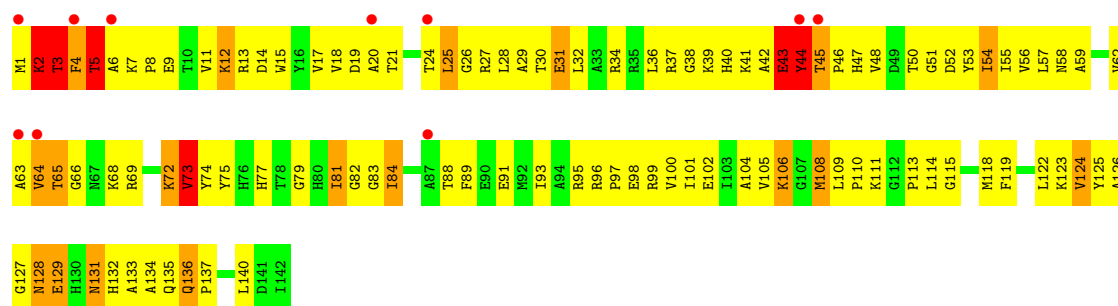


• Molecule 41: 50S ribosomal protein L13

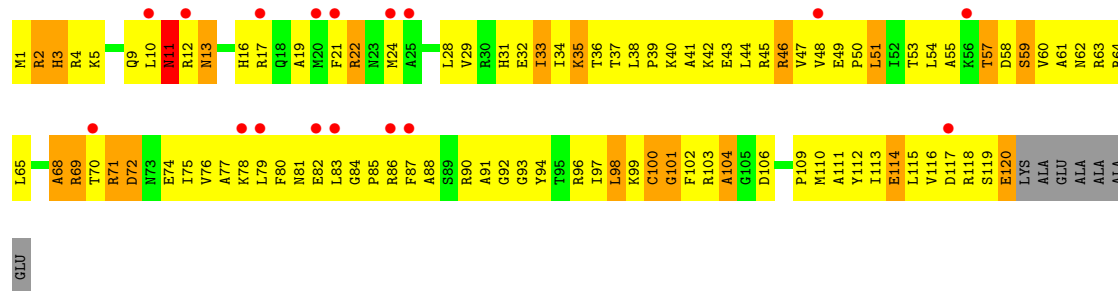


• Molecule 41: 50S ribosomal protein L13

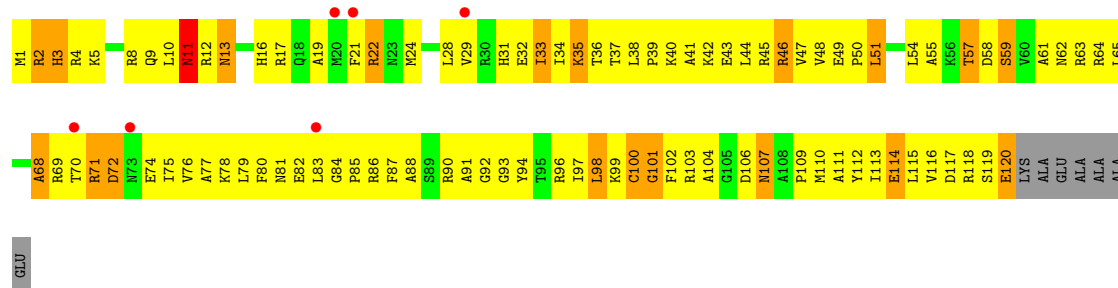




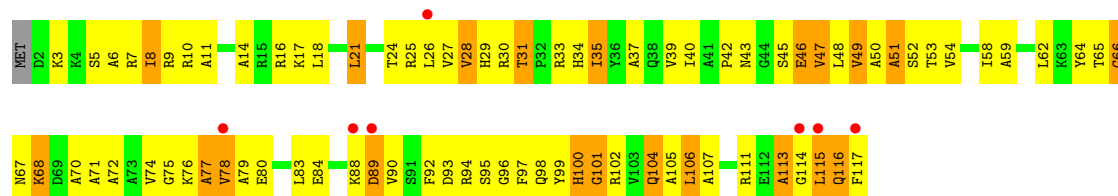
• Molecule 42: 50S ribosomal protein L17



• Molecule 42: 50S ribosomal protein L17

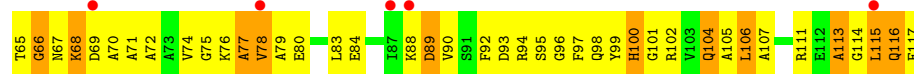


• Molecule 43: 50S ribosomal protein L18



• Molecule 43: 50S ribosomal protein L18

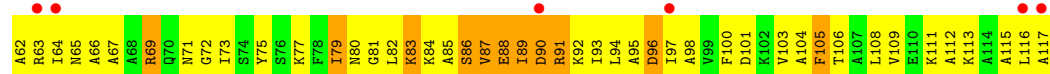
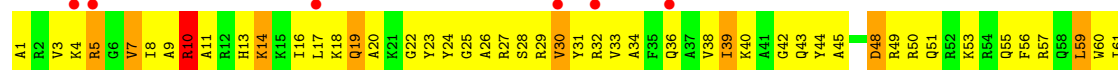




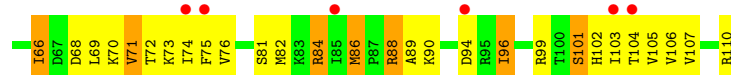
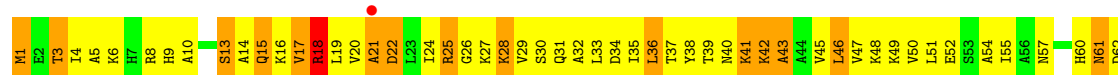
• Molecule 44: 50S ribosomal protein L20



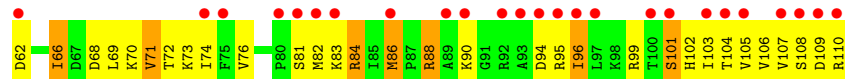
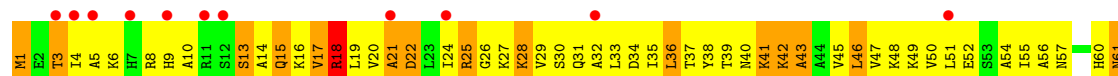
• Molecule 44: 50S ribosomal protein L20



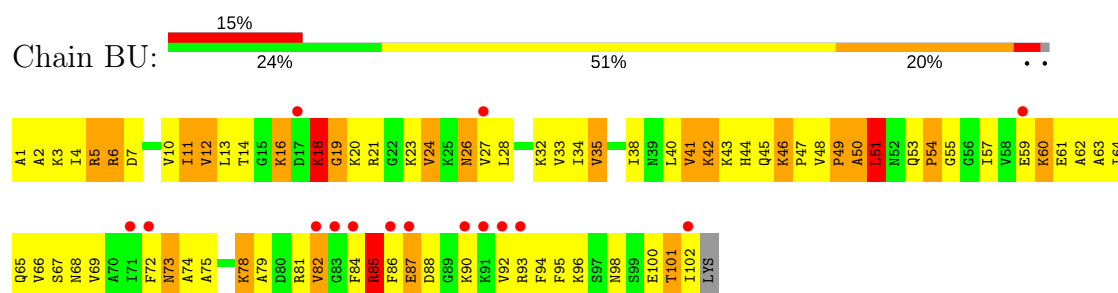
• Molecule 45: 50S ribosomal protein L22



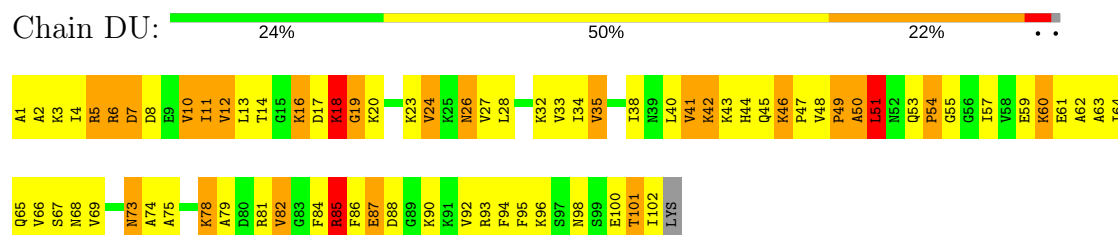
• Molecule 45: 50S ribosomal protein L22



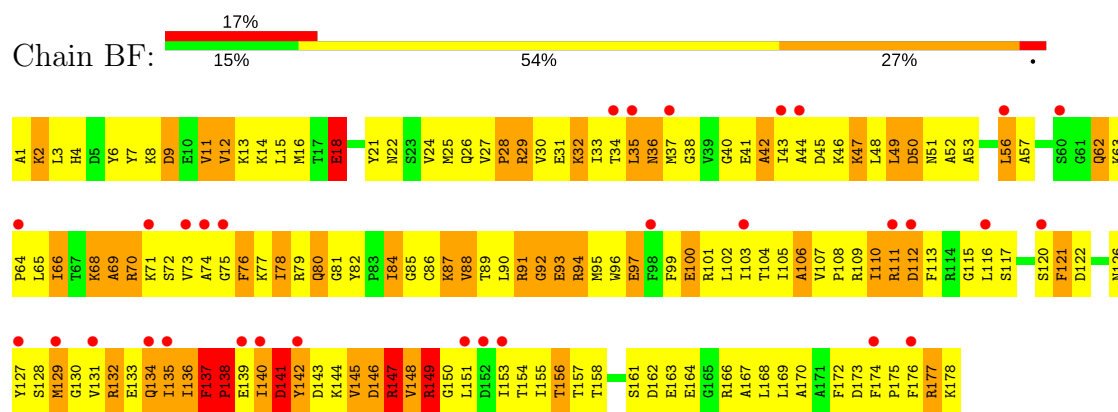
• Molecule 46: 50S ribosomal protein L24



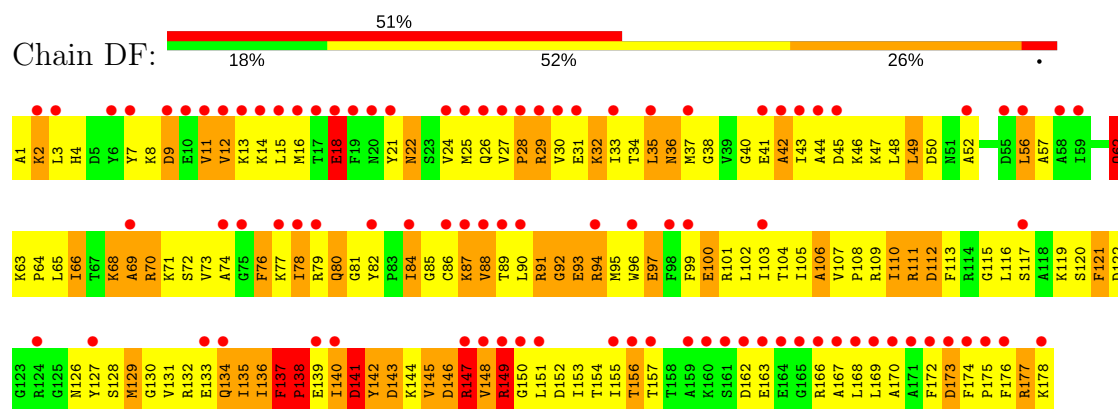
• Molecule 46: 50S ribosomal protein L24



• Molecule 47: 50S ribosomal protein L5

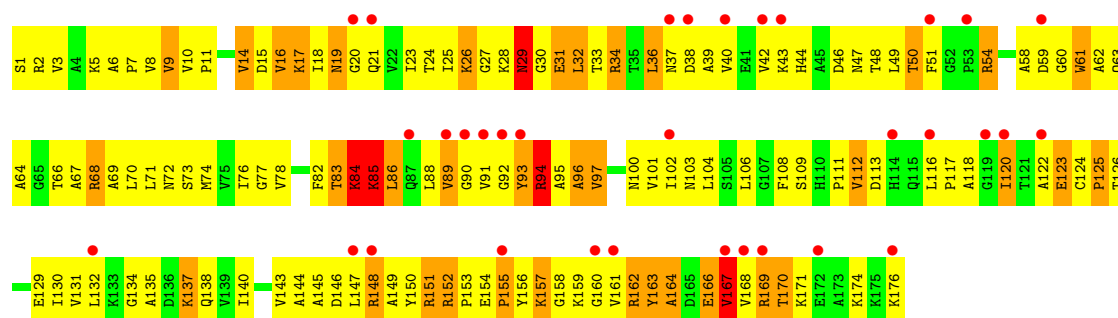


• Molecule 47: 50S ribosomal protein L5

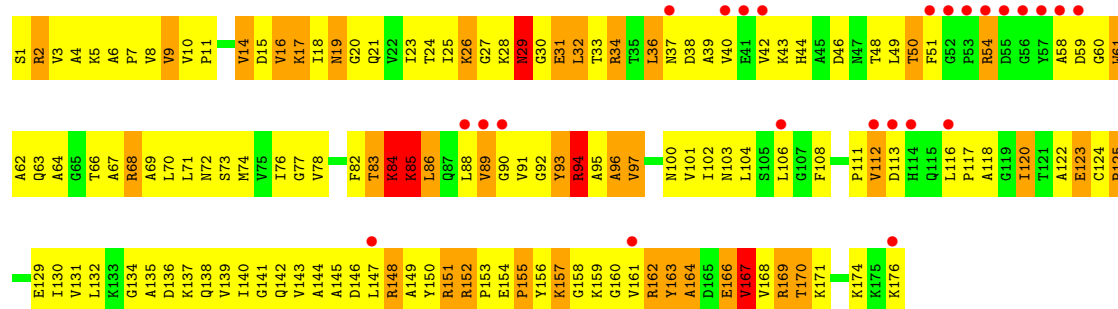


• Molecule 48: 50S ribosomal protein L6

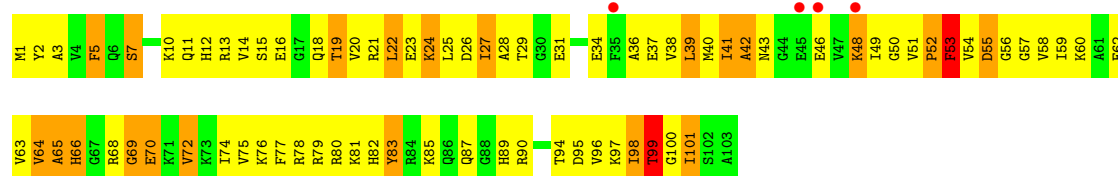




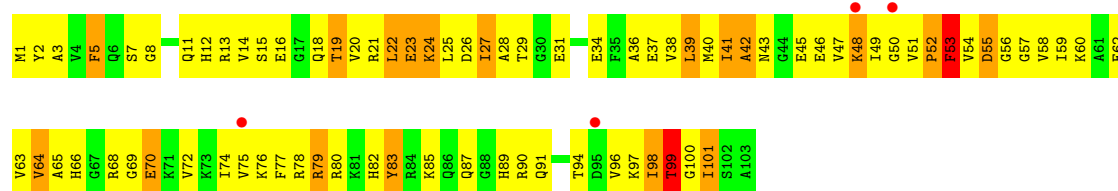
• Molecule 48: 50S ribosomal protein L6



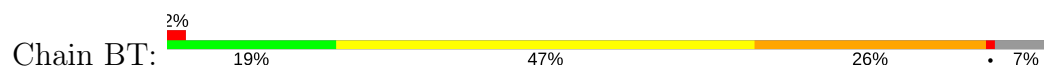
• Molecule 49: 50S ribosomal protein L21

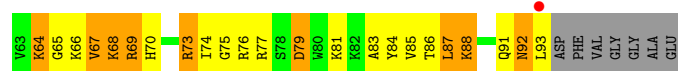


• Molecule 49: 50S ribosomal protein L21

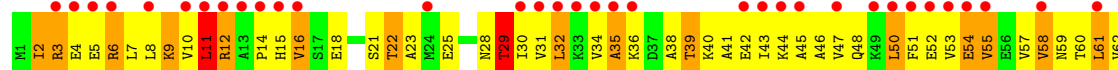
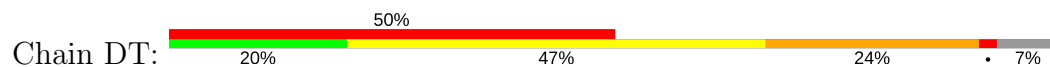


• Molecule 50: 50S ribosomal protein L23

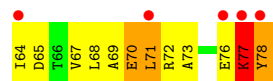




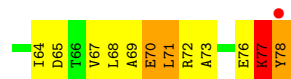
- Molecule 50: 50S ribosomal protein L23



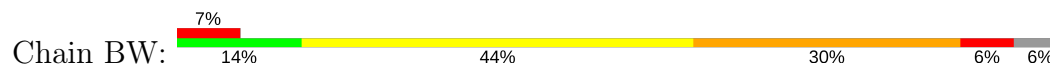
- Molecule 51: 50S ribosomal protein L28



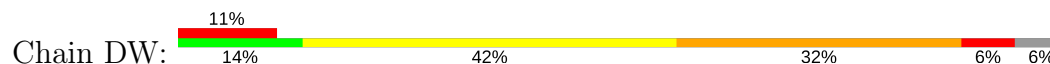
- Molecule 51: 50S ribosomal protein L28

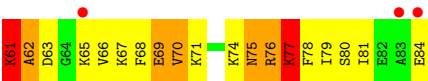


- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.93 182.94 – 3.94	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.93) 75.9 (182.94-3.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.311 0.231 , 0.279	Depositor DCC
R_{free} test set	19247 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	149.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284033	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.27	2/36762 (0.0%)	0.76	12/57350 (0.0%)
1	CA	0.31	1/36762 (0.0%)	0.77	11/57350 (0.0%)
2	AC	0.23	0/1651	0.45	0/2225
2	CC	0.23	0/1651	0.46	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.23	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.45	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.44	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.22	0/796	0.48	0/1077
10	AK	0.24	0/893	0.44	0/1205
10	CK	0.24	0/893	0.44	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.45	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AP	0.25	0/659	0.45	0/884
13	CP	0.25	0/648	0.44	0/870
14	AQ	0.23	0/657	0.46	0/881
14	CQ	0.24	0/666	0.46	0/892
15	AR	0.23	0/462	0.46	0/621
15	CR	0.23	0/462	0.46	0/621
16	AS	0.25	0/652	0.46	0/877
16	CS	0.25	0/660	0.49	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.23	0/671	0.40	0/888
17	CT	0.23	0/671	0.40	0/888
18	AB	0.25	0/1735	0.45	0/2338
18	CB	0.25	0/1735	0.45	0/2338
19	AU	0.26	0/430	0.46	0/570
19	CU	0.25	0/430	0.46	0/570
20	AO	0.22	0/722	0.45	0/964
20	CO	0.23	0/722	0.44	0/964
21	AN	0.24	0/785	0.44	0/1043
21	CN	0.24	0/785	0.46	0/1043
22	BA	0.23	0/2803	0.74	1/4371 (0.0%)
22	DA	0.24	0/2803	0.75	1/4371 (0.0%)
23	BB	0.28	5/68314 (0.0%)	0.77	33/106569 (0.0%)
23	DB	0.28	5/68314 (0.0%)	0.77	33/106569 (0.0%)
24	BI	0.24	0/1046	0.46	0/1410
24	DI	0.25	0/1046	0.47	0/1410
25	BC	0.22	0/2121	0.47	0/2852
25	DC	0.22	0/2121	0.47	0/2852
26	BD	0.24	0/1586	0.48	0/2134
26	DD	0.24	0/1586	0.48	0/2134
27	BK	0.24	0/939	0.53	0/1258
27	DK	0.24	0/939	0.53	0/1258
28	BP	0.24	0/929	0.49	0/1242
28	DP	0.24	0/929	0.49	0/1242
29	BE	0.24	0/1571	0.48	0/2113
29	DE	0.24	0/1571	0.48	0/2113
30	BY	0.24	0/453	0.49	0/605
30	DY	0.23	0/453	0.49	0/605
31	B0	0.23	0/450	0.51	0/599
31	D0	0.23	0/450	0.51	0/599
32	B4	0.22	0/303	0.49	0/397
32	D4	0.23	0/303	0.49	0/397
33	B1	0.27	0/416	0.48	0/554
33	D1	0.27	0/416	0.48	0/554
34	B3	0.24	0/513	0.46	0/676
34	D3	0.24	0/513	0.46	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.26	0/380	0.47	0/498
36	D2	0.26	0/380	0.47	0/498
37	BL	0.24	0/1054	0.48	0/1403
37	DL	0.24	0/1054	0.48	0/1403
38	BM	0.25	0/1093	0.47	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.47	0/1460
39	BX	0.24	0/510	0.50	0/677
39	DX	0.23	0/510	0.50	0/677
40	BH	0.25	0/1122	0.47	0/1515
40	DH	0.25	0/1122	0.47	0/1515
41	BJ	0.23	0/1152	0.47	0/1551
41	DJ	0.23	0/1152	0.47	0/1551
42	BN	0.24	0/973	0.49	0/1301
42	DN	0.24	0/973	0.49	0/1301
43	BO	0.23	0/902	0.47	0/1209
43	DO	0.23	0/902	0.47	0/1209
44	BQ	0.25	0/960	0.47	0/1278
44	DQ	0.25	0/960	0.47	0/1278
45	BS	0.22	0/864	0.50	0/1156
45	DS	0.22	0/864	0.50	0/1156
46	BU	0.25	0/787	0.45	0/1051
46	DU	0.25	0/787	0.45	0/1051
47	BF	0.26	0/1444	0.49	0/1937
47	DF	0.26	0/1444	0.49	0/1937
48	BG	0.23	0/1343	0.47	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.26	0/829	0.48	0/1107
49	DR	0.25	0/829	0.48	0/1107
50	BT	0.23	0/744	0.51	0/994
50	DT	0.23	0/744	0.51	0/994
51	BZ	0.25	0/635	0.49	0/848
51	DZ	0.25	0/635	0.50	0/848
52	BW	0.28	0/603	0.49	0/797
52	DW	0.28	0/603	0.49	0/797
All	All	0.27	13/306360 (0.0%)	0.70	91/457969 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	15
1	CA	0	19
23	BB	0	37
23	DB	0	37
All	All	0	108

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-16.20	1.26	1.41
23	BB	1086	A	C5-C6	-16.10	1.26	1.41
23	DB	1088	A	C6-N1	-10.51	1.28	1.35
23	BB	1088	A	C6-N1	-10.50	1.28	1.35
23	BB	1060	U	C2-N3	7.92	1.43	1.37

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-30.02	74.68	110.70
23	BB	2204	G	O5'-P-OP2	-28.49	76.52	110.70
23	DB	2791	G	O5'-P-OP2	-28.43	76.59	110.70
23	BB	2791	G	O5'-P-OP1	-27.42	77.80	110.70
23	DB	2204	G	O5'-P-OP2	17.65	131.88	110.70

There are no chirality outliers.

5 of 108 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	437	U	Sidechain
1	AA	438	U	Sidechain
1	AA	450	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1458	0
1	CA	32831	0	16521	1414	0
2	AC	1624	0	1699	205	0
2	CC	1624	0	1699	191	0
3	AD	1643	0	1710	179	0
3	CD	1643	0	1710	177	0
4	AE	1105	0	1148	129	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CE	1105	0	1148	121	0
5	AF	817	0	808	89	0
5	CF	817	0	808	91	0
6	AG	1174	0	1230	146	0
6	CG	1196	0	1246	133	0
7	AH	979	0	1034	89	0
7	CH	979	0	1034	91	0
8	AI	1022	0	1070	180	0
8	CI	1022	0	1070	146	0
9	AJ	786	0	828	85	0
9	CJ	786	0	828	103	0
10	AK	877	0	887	110	0
10	CK	877	0	887	100	0
11	AL	955	0	1019	96	0
11	CL	955	0	1019	97	0
12	AM	883	0	944	135	0
12	CM	876	0	937	138	0
13	AP	649	0	666	65	0
13	CP	638	0	656	66	0
14	AQ	648	0	691	63	0
14	CQ	657	0	702	62	0
15	AR	455	0	478	35	0
15	CR	455	0	478	37	0
16	AS	637	0	665	97	0
16	CS	644	0	675	115	0
17	AT	665	0	714	60	0
17	CT	665	0	714	61	0
18	AB	1704	0	1732	209	0
18	CB	1704	0	1732	229	0
19	AU	425	0	449	57	0
19	CU	425	0	449	54	0
20	AO	714	0	734	63	0
20	CO	714	0	734	62	0
21	AN	774	0	827	102	0
21	CN	774	0	827	114	0
22	BA	2507	0	1270	116	0
22	DA	2507	0	1270	111	0
23	BB	60995	0	30679	2412	0
23	DB	60995	0	30678	2455	0
24	BI	1032	0	1088	109	0
24	DI	1032	0	1088	168	0
25	BC	2082	0	2157	234	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DC	2082	0	2157	239	0
26	BD	1565	0	1616	234	0
26	DD	1565	0	1616	239	0
27	BK	930	0	1000	153	0
27	DK	930	0	1000	154	0
28	BP	917	0	965	126	0
28	DP	917	0	965	132	0
29	BE	1552	0	1619	208	0
29	DE	1552	0	1619	202	0
30	BY	449	0	491	59	0
30	DY	449	0	491	53	0
31	B0	444	0	461	48	0
31	D0	444	0	461	44	0
32	B4	302	0	340	42	0
32	D4	302	0	340	43	0
33	B1	409	0	440	54	0
33	D1	409	0	440	50	0
34	B3	504	0	574	47	0
34	D3	504	0	574	52	0
35	BV	753	0	780	83	0
35	DV	753	0	780	86	0
36	B2	377	0	418	37	0
36	D2	377	0	418	43	0
37	BL	1045	0	1117	138	0
37	DL	1045	0	1117	144	0
38	BM	1074	0	1157	123	0
38	DM	1074	0	1157	119	0
39	BX	509	0	543	46	0
39	DX	509	0	543	50	0
40	BH	1111	0	1148	172	0
40	DH	1111	0	1148	147	0
41	BJ	1129	0	1162	134	0
41	DJ	1129	0	1162	141	0
42	BN	960	0	1000	137	0
42	DN	960	0	1000	133	0
43	BO	892	0	923	91	0
43	DO	892	0	923	94	0
44	BQ	947	0	1022	150	0
44	DQ	947	0	1022	143	0
45	BS	857	0	922	97	0
45	DS	857	0	922	98	0
46	BU	779	0	834	116	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DU	779	0	834	114	0
47	BF	1420	0	1460	264	0
47	DF	1420	0	1460	249	0
48	BG	1323	0	1374	187	0
48	DG	1323	0	1374	178	0
49	BR	816	0	839	105	0
49	DR	816	0	839	112	0
50	BT	738	0	807	115	0
50	DT	738	0	807	110	0
51	BZ	625	0	652	75	0
51	DZ	625	0	652	71	0
52	BW	596	0	610	122	0
52	DW	596	0	610	130	0
53	AA	60	0	0	0	0
53	BB	110	0	0	0	0
53	CA	58	0	0	0	0
53	CE	1	0	0	0	0
53	DB	110	0	0	0	0
53	DN	1	0	0	0	0
54	AA	23	0	24	2	0
54	CA	23	0	24	1	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	288	0	0	6	0
56	AE	3	0	0	1	0
56	AK	1	0	0	0	0
56	AL	4	0	0	0	0
56	AN	2	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	BB	494	0	0	4	0
56	BC	4	0	0	0	0
56	BE	3	0	0	0	0
56	BH	1	0	0	0	0
56	BL	4	0	0	0	0
56	BT	1	0	0	0	0
56	CA	275	0	0	4	0
56	CE	4	0	0	0	0
56	CK	1	0	0	0	0
56	CL	5	0	0	0	0
56	CN	5	0	0	0	0
56	CP	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CT	2	0	0	0	0
56	DB	500	0	0	9	0
56	DC	3	0	0	0	0
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DJ	1	0	0	0	0
56	DL	3	0	0	0	0
56	DN	2	0	0	0	0
56	DP	1	0	0	0	0
56	DR	1	0	0	0	0
All	All	284033	0	190711	17874	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

The worst 5 of 17874 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.36	1.21
23:BB:855:G:H21	52:BW:23:LYS:HG2	1.11	1.13
23:DB:322:A:H5'	23:DB:340:A:H1'	1.32	1.12
2:AC:70:ALA:HA	2:AC:105:VAL:HG21	1.26	1.11
23:BB:1205:A:H62	29:BE:165:HIS:HB2	1.11	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AC	204/232 (88%)	112 (55%)	56 (28%)	36 (18%)	0 3
2	CC	204/232 (88%)	134 (66%)	48 (24%)	22 (11%)	0 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	133 (66%)	58 (29%)	12 (6%)	2	25
3	CD	203/205 (99%)	132 (65%)	58 (29%)	13 (6%)	1	24
4	AE	148/166 (89%)	109 (74%)	30 (20%)	9 (6%)	2	25
4	CE	148/166 (89%)	108 (73%)	31 (21%)	9 (6%)	2	25
5	AF	98/135 (73%)	62 (63%)	27 (28%)	9 (9%)	1	15
5	CF	98/135 (73%)	64 (65%)	25 (26%)	9 (9%)	1	15
6	AG	148/178 (83%)	98 (66%)	44 (30%)	6 (4%)	3	33
6	CG	150/178 (84%)	101 (67%)	36 (24%)	13 (9%)	1	15
7	AH	127/129 (98%)	86 (68%)	35 (28%)	6 (5%)	3	30
7	CH	127/129 (98%)	85 (67%)	36 (28%)	6 (5%)	3	30
8	AI	125/129 (97%)	84 (67%)	25 (20%)	16 (13%)	0	7
8	CI	125/129 (97%)	89 (71%)	30 (24%)	6 (5%)	2	29
9	AJ	96/103 (93%)	61 (64%)	18 (19%)	17 (18%)	0	3
9	CJ	96/103 (93%)	62 (65%)	21 (22%)	13 (14%)	0	5
10	AK	115/128 (90%)	85 (74%)	26 (23%)	4 (4%)	4	38
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	2	28
11	AL	121/123 (98%)	71 (59%)	34 (28%)	16 (13%)	0	6
11	CL	121/123 (98%)	72 (60%)	33 (27%)	16 (13%)	0	6
12	AM	112/117 (96%)	69 (62%)	36 (32%)	7 (6%)	1	24
12	CM	111/117 (95%)	77 (69%)	23 (21%)	11 (10%)	1	12
13	AP	80/82 (98%)	53 (66%)	18 (22%)	9 (11%)	0	9
13	CP	78/82 (95%)	53 (68%)	19 (24%)	6 (8%)	1	18
14	AQ	78/83 (94%)	61 (78%)	14 (18%)	3 (4%)	4	35
14	CQ	79/83 (95%)	62 (78%)	15 (19%)	2 (2%)	6	44
15	AR	53/74 (72%)	33 (62%)	17 (32%)	3 (6%)	2	26
15	CR	53/74 (72%)	33 (62%)	16 (30%)	4 (8%)	1	19
16	AS	77/91 (85%)	49 (64%)	21 (27%)	7 (9%)	1	15
16	CS	78/91 (86%)	51 (65%)	20 (26%)	7 (9%)	1	15
17	AT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	2	25
17	CT	83/86 (96%)	63 (76%)	14 (17%)	6 (7%)	1	21
18	AB	216/240 (90%)	140 (65%)	53 (24%)	23 (11%)	0	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CB	216/240 (90%)	135 (62%)	59 (27%)	22 (10%)	1	12
19	AU	49/70 (70%)	29 (59%)	13 (26%)	7 (14%)	0	5
19	CU	49/70 (70%)	29 (59%)	15 (31%)	5 (10%)	1	12
20	AO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	17
20	CO	86/89 (97%)	50 (58%)	29 (34%)	7 (8%)	1	17
21	AN	92/100 (92%)	54 (59%)	29 (32%)	9 (10%)	1	13
21	CN	92/100 (92%)	45 (49%)	31 (34%)	16 (17%)	0	3
24	BI	139/141 (99%)	118 (85%)	16 (12%)	5 (4%)	4	37
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	4	37
25	BC	269/272 (99%)	149 (55%)	68 (25%)	52 (19%)	0	2
25	DC	269/272 (99%)	147 (55%)	70 (26%)	52 (19%)	0	2
26	BD	207/209 (99%)	113 (55%)	58 (28%)	36 (17%)	0	3
26	DD	207/209 (99%)	114 (55%)	58 (28%)	35 (17%)	0	4
27	BK	119/123 (97%)	73 (61%)	24 (20%)	22 (18%)	0	3
27	DK	119/123 (97%)	73 (61%)	25 (21%)	21 (18%)	0	3
28	BP	112/114 (98%)	67 (60%)	28 (25%)	17 (15%)	0	4
28	DP	112/114 (98%)	66 (59%)	31 (28%)	15 (13%)	0	5
29	BE	199/201 (99%)	120 (60%)	49 (25%)	30 (15%)	0	4
29	DE	199/201 (99%)	123 (62%)	47 (24%)	29 (15%)	0	5
30	BY	56/58 (97%)	36 (64%)	16 (29%)	4 (7%)	1	21
30	DY	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	0	10
31	B0	54/56 (96%)	34 (63%)	10 (18%)	10 (18%)	0	3
31	D0	54/56 (96%)	35 (65%)	9 (17%)	10 (18%)	0	3
32	B4	36/38 (95%)	19 (53%)	13 (36%)	4 (11%)	0	9
32	D4	36/38 (95%)	19 (53%)	13 (36%)	4 (11%)	0	9
33	B1	48/54 (89%)	36 (75%)	8 (17%)	4 (8%)	1	16
33	D1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	16
34	B3	62/64 (97%)	34 (55%)	20 (32%)	8 (13%)	0	6
34	D3	62/64 (97%)	35 (56%)	19 (31%)	8 (13%)	0	6
35	BV	92/94 (98%)	60 (65%)	25 (27%)	7 (8%)	1	19
35	DV	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	1	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	B2	44/46 (96%)	23 (52%)	16 (36%)	5 (11%)	0	9
36	D2	44/46 (96%)	23 (52%)	12 (27%)	9 (20%)	0	2
37	BL	141/144 (98%)	76 (54%)	37 (26%)	28 (20%)	0	2
37	DL	141/144 (98%)	76 (54%)	39 (28%)	26 (18%)	0	3
38	BM	134/136 (98%)	79 (59%)	39 (29%)	16 (12%)	0	8
38	DM	134/136 (98%)	82 (61%)	35 (26%)	17 (13%)	0	7
39	BX	61/63 (97%)	35 (57%)	20 (33%)	6 (10%)	1	13
39	DX	61/63 (97%)	35 (57%)	20 (33%)	6 (10%)	1	13
40	BH	147/149 (99%)	78 (53%)	42 (29%)	27 (18%)	0	3
40	DH	147/149 (99%)	91 (62%)	30 (20%)	26 (18%)	0	3
41	BJ	140/142 (99%)	85 (61%)	37 (26%)	18 (13%)	0	6
41	DJ	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	5
42	BN	118/127 (93%)	73 (62%)	33 (28%)	12 (10%)	1	12
42	DN	118/127 (93%)	74 (63%)	33 (28%)	11 (9%)	1	14
43	BO	114/117 (97%)	68 (60%)	28 (25%)	18 (16%)	0	4
43	DO	114/117 (97%)	66 (58%)	30 (26%)	18 (16%)	0	4
44	BQ	115/117 (98%)	76 (66%)	29 (25%)	10 (9%)	1	15
44	DQ	115/117 (98%)	76 (66%)	30 (26%)	9 (8%)	1	18
45	BS	108/110 (98%)	59 (55%)	34 (32%)	15 (14%)	0	5
45	DS	108/110 (98%)	60 (56%)	33 (31%)	15 (14%)	0	5
46	BU	100/103 (97%)	58 (58%)	25 (25%)	17 (17%)	0	4
46	DU	100/103 (97%)	57 (57%)	24 (24%)	19 (19%)	0	2
47	BF	176/178 (99%)	91 (52%)	51 (29%)	34 (19%)	0	2
47	DF	176/178 (99%)	93 (53%)	49 (28%)	34 (19%)	0	2
48	BG	174/176 (99%)	100 (58%)	42 (24%)	32 (18%)	0	3
48	DG	174/176 (99%)	101 (58%)	42 (24%)	31 (18%)	0	3
49	BR	101/103 (98%)	57 (56%)	26 (26%)	18 (18%)	0	3
49	DR	101/103 (98%)	58 (57%)	26 (26%)	17 (17%)	0	4
50	BT	91/100 (91%)	40 (44%)	40 (44%)	11 (12%)	0	7
50	DT	91/100 (91%)	41 (45%)	39 (43%)	11 (12%)	0	7
51	BZ	75/78 (96%)	53 (71%)	16 (21%)	6 (8%)	1	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DZ	75/78 (96%)	54 (72%)	14 (19%)	7 (9%)	1	14
52	BW	77/84 (92%)	29 (38%)	24 (31%)	24 (31%)	0	0
52	DW	77/84 (92%)	27 (35%)	26 (34%)	24 (31%)	0	0
All	All	11241/11914 (94%)	6932 (62%)	2908 (26%)	1401 (12%)	0	7

5 of 1401 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	19	SER
2	AC	26	LYS
2	AC	47	ALA
2	AC	54	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	139 (82%)	31 (18%)	2	15
2	CC	170/189 (90%)	134 (79%)	36 (21%)	1	9
3	AD	172/172 (100%)	145 (84%)	27 (16%)	3	22
3	CD	172/172 (100%)	146 (85%)	26 (15%)	3	23
4	AE	113/125 (90%)	93 (82%)	20 (18%)	2	16
4	CE	113/125 (90%)	93 (82%)	20 (18%)	2	16
5	AF	87/116 (75%)	76 (87%)	11 (13%)	5	29
5	CF	87/116 (75%)	75 (86%)	12 (14%)	4	27
6	AG	123/146 (84%)	102 (83%)	21 (17%)	2	18
6	CG	125/146 (86%)	98 (78%)	27 (22%)	1	9
7	AH	104/104 (100%)	95 (91%)	9 (9%)	12	45
7	CH	104/104 (100%)	95 (91%)	9 (9%)	12	45
8	AI	105/106 (99%)	78 (74%)	27 (26%)	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	79 (75%)	26 (25%)	1	6
9	AJ	86/90 (96%)	73 (85%)	13 (15%)	3	23
9	CJ	86/90 (96%)	72 (84%)	14 (16%)	3	20
10	AK	90/98 (92%)	73 (81%)	17 (19%)	2	13
10	CK	90/98 (92%)	73 (81%)	17 (19%)	2	13
11	AL	103/103 (100%)	87 (84%)	16 (16%)	3	22
11	CL	103/103 (100%)	87 (84%)	16 (16%)	3	22
12	AM	92/95 (97%)	72 (78%)	20 (22%)	1	9
12	CM	91/95 (96%)	75 (82%)	16 (18%)	2	16
13	AP	65/65 (100%)	61 (94%)	4 (6%)	21	58
13	CP	65/65 (100%)	61 (94%)	4 (6%)	21	58
14	AQ	74/77 (96%)	63 (85%)	11 (15%)	3	24
14	CQ	75/77 (97%)	63 (84%)	12 (16%)	3	21
15	AR	48/64 (75%)	41 (85%)	7 (15%)	3	24
15	CR	48/64 (75%)	40 (83%)	8 (17%)	2	19
16	AS	70/78 (90%)	49 (70%)	21 (30%)	0	3
16	CS	71/78 (91%)	51 (72%)	20 (28%)	0	4
17	AT	65/65 (100%)	51 (78%)	14 (22%)	1	9
17	CT	65/65 (100%)	51 (78%)	14 (22%)	1	9
18	AB	180/198 (91%)	141 (78%)	39 (22%)	1	9
18	CB	180/198 (91%)	133 (74%)	47 (26%)	0	5
19	AU	44/60 (73%)	31 (70%)	13 (30%)	0	3
19	CU	44/60 (73%)	32 (73%)	12 (27%)	0	4
20	AO	76/77 (99%)	65 (86%)	11 (14%)	4	25
20	CO	76/77 (99%)	61 (80%)	15 (20%)	1	12
21	AN	79/83 (95%)	63 (80%)	16 (20%)	1	11
21	CN	79/83 (95%)	64 (81%)	15 (19%)	2	13
24	BI	109/109 (100%)	108 (99%)	1 (1%)	82	92
24	DI	109/109 (100%)	103 (94%)	6 (6%)	25	62
25	BC	216/217 (100%)	180 (83%)	36 (17%)	2	19
25	DC	216/217 (100%)	181 (84%)	35 (16%)	3	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	134 (82%)	30 (18%)	2	14
26	DD	164/164 (100%)	133 (81%)	31 (19%)	2	13
27	BK	102/104 (98%)	76 (74%)	26 (26%)	0	6
27	DK	102/104 (98%)	78 (76%)	24 (24%)	1	7
28	BP	99/99 (100%)	77 (78%)	22 (22%)	1	8
28	DP	99/99 (100%)	77 (78%)	22 (22%)	1	8
29	BE	165/165 (100%)	143 (87%)	22 (13%)	4	28
29	DE	165/165 (100%)	143 (87%)	22 (13%)	4	28
30	BY	48/48 (100%)	39 (81%)	9 (19%)	2	14
30	DY	48/48 (100%)	39 (81%)	9 (19%)	2	14
31	B0	47/47 (100%)	36 (77%)	11 (23%)	1	7
31	D0	47/47 (100%)	37 (79%)	10 (21%)	1	9
32	B4	34/34 (100%)	30 (88%)	4 (12%)	6	32
32	D4	34/34 (100%)	31 (91%)	3 (9%)	12	44
33	B1	45/48 (94%)	39 (87%)	6 (13%)	4	28
33	D1	45/48 (94%)	39 (87%)	6 (13%)	4	28
34	B3	51/51 (100%)	45 (88%)	6 (12%)	6	32
34	D3	51/51 (100%)	45 (88%)	6 (12%)	6	32
35	BV	78/78 (100%)	64 (82%)	14 (18%)	2	15
35	DV	78/78 (100%)	64 (82%)	14 (18%)	2	15
36	B2	38/38 (100%)	32 (84%)	6 (16%)	3	22
36	D2	38/38 (100%)	33 (87%)	5 (13%)	5	28
37	BL	102/103 (99%)	89 (87%)	13 (13%)	5	29
37	DL	102/103 (99%)	90 (88%)	12 (12%)	6	32
38	BM	109/109 (100%)	86 (79%)	23 (21%)	1	10
38	DM	109/109 (100%)	86 (79%)	23 (21%)	1	10
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	9
39	DX	55/55 (100%)	45 (82%)	10 (18%)	2	15
40	BH	114/114 (100%)	81 (71%)	33 (29%)	0	3
40	DH	114/114 (100%)	89 (78%)	25 (22%)	1	9
41	BJ	116/116 (100%)	95 (82%)	21 (18%)	2	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DJ	116/116 (100%)	96 (83%)	20 (17%)	2	17
42	BN	100/103 (97%)	87 (87%)	13 (13%)	5	28
42	DN	100/103 (97%)	87 (87%)	13 (13%)	5	28
43	BO	86/87 (99%)	72 (84%)	14 (16%)	3	20
43	DO	86/87 (99%)	72 (84%)	14 (16%)	3	20
44	BQ	89/89 (100%)	74 (83%)	15 (17%)	2	18
44	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	18
45	BS	93/93 (100%)	80 (86%)	13 (14%)	4	27
45	DS	93/93 (100%)	80 (86%)	13 (14%)	4	27
46	BU	83/84 (99%)	69 (83%)	14 (17%)	2	18
46	DU	83/84 (99%)	69 (83%)	14 (17%)	2	18
47	BF	149/149 (100%)	117 (78%)	32 (22%)	1	9
47	DF	149/149 (100%)	116 (78%)	33 (22%)	1	8
48	BG	137/137 (100%)	112 (82%)	25 (18%)	2	15
48	DG	137/137 (100%)	112 (82%)	25 (18%)	2	15
49	BR	84/84 (100%)	71 (84%)	13 (16%)	3	22
49	DR	84/84 (100%)	73 (87%)	11 (13%)	5	28
50	BT	80/84 (95%)	59 (74%)	21 (26%)	0	5
50	DT	80/84 (95%)	60 (75%)	20 (25%)	1	6
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	10
51	DZ	67/68 (98%)	53 (79%)	14 (21%)	1	10
52	BW	59/62 (95%)	42 (71%)	17 (29%)	0	3
52	DW	59/62 (95%)	42 (71%)	17 (29%)	0	3
All	All	9333/9700 (96%)	7661 (82%)	1672 (18%)	2	15

5 of 1672 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BG	84	LYS
13	CP	28	ARG
46	DU	51	LEU
49	BR	66	HIS
3	CD	147	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 332 such sidechains are listed below:

Mol	Chain	Res	Type
47	BF	126	ASN
5	CF	17	GLN
46	DU	26	ASN
48	BG	127	GLN
3	CD	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	292 (19%)	0
1	CA	1529/1542 (99%)	282 (18%)	0
22	BA	116/120 (96%)	21 (18%)	0
22	DA	116/120 (96%)	19 (16%)	0
23	BB	2837/2904 (97%)	456 (16%)	0
23	DB	2837/2904 (97%)	469 (16%)	0
All	All	8964/9132 (98%)	1539 (17%)	0

5 of 1539 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 344 ligands modelled in this entry, 342 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
54	SCM	AA	1661	-	22,25,25	1.69	8 (36%)	25,39,39	0.88	1 (4%)
54	SCM	CA	1659	-	22,25,25	1.63	6 (27%)	25,39,39	0.94	1 (4%)

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	SCM	AA	1661	-	-	0/4/57/57	0/3/3/3
54	SCM	CA	1659	-	-	0/4/57/57	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	AA	1661	SCM	C10-N10	-2.01	1.44	1.47
54	CA	1659	SCM	O2B-C12	2.07	1.47	1.43
54	AA	1661	SCM	O5-C5	2.10	1.43	1.39
54	CA	1659	SCM	C12-C7	2.22	1.57	1.52
54	AA	1661	SCM	O2B-C12	2.26	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	1659	SCM	C2M-C2-C3	-2.64	108.11	113.27
54	AA	1661	SCM	C2M-C2-C3	-2.44	108.49	113.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	AA	1661	SCM	2	0
54	CA	1659	SCM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.77	9 (0%) 89 84	12, 77, 142, 179	0
1	CA	1530/1542 (99%)	-0.76	2 (0%) 95 94	5, 57, 124, 180	0
2	AC	206/232 (88%)	0.22	15 (7%) 16 12	5, 70, 115, 162	0
2	CC	206/232 (88%)	0.53	29 (14%) 3 4	5, 71, 111, 150	0
3	AD	205/205 (100%)	-0.05	12 (5%) 23 17	5, 79, 127, 173	0
3	CD	205/205 (100%)	0.57	20 (9%) 8 7	5, 66, 125, 166	0
4	AE	150/166 (90%)	0.06	4 (2%) 55 45	5, 68, 122, 157	0
4	CE	150/166 (90%)	1.48	51 (34%) 0 1	5, 67, 121, 180	0
5	AF	100/135 (74%)	2.52	62 (62%) 0 1	10, 81, 133, 147	0
5	CF	100/135 (74%)	-0.47	0 100 100	5, 73, 131, 172	0
6	AG	150/178 (84%)	0.74	27 (18%) 2 2	16, 89, 125, 143	0
6	CG	152/178 (85%)	-0.54	0 100 100	6, 79, 125, 172	0
7	AH	129/129 (100%)	0.37	16 (12%) 4 5	19, 77, 130, 158	0
7	CH	129/129 (100%)	0.75	26 (20%) 1 2	5, 62, 116, 158	0
8	AI	127/129 (98%)	0.76	24 (18%) 1 2	6, 83, 117, 155	0
8	CI	127/129 (98%)	0.02	2 (1%) 72 62	5, 80, 122, 157	0
9	AJ	98/103 (95%)	0.49	4 (4%) 38 30	9, 79, 126, 147	0
9	CJ	98/103 (95%)	1.28	30 (30%) 0 1	16, 82, 113, 137	0
10	AK	117/128 (91%)	0.23	4 (3%) 46 36	5, 72, 117, 155	0
10	CK	117/128 (91%)	-0.54	0 100 100	5, 67, 123, 136	0
11	AL	123/123 (100%)	1.01	30 (24%) 1 1	6, 79, 123, 158	0
11	CL	123/123 (100%)	0.26	6 (4%) 30 24	5, 54, 103, 151	0
12	AM	114/117 (97%)	0.95	21 (18%) 1 2	23, 96, 137, 169	0
12	CM	113/117 (96%)	-0.21	5 (4%) 35 27	22, 96, 142, 162	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	82/82 (100%)	1.48	25 (30%) 0 1	15, 82, 130, 163	0
13	CP	80/82 (97%)	0.05	5 (6%) 21 15	5, 58, 126, 180	0
14	AQ	80/83 (96%)	1.25	23 (28%) 1 1	15, 92, 145, 154	0
14	CQ	81/83 (97%)	0.25	3 (3%) 42 33	5, 72, 119, 149	0
15	AR	55/74 (74%)	0.81	8 (14%) 3 3	5, 73, 129, 164	0
15	CR	55/74 (74%)	0.23	3 (5%) 26 20	5, 66, 127, 143	0
16	AS	79/91 (86%)	1.98	39 (49%) 0 1	52, 98, 142, 167	0
16	CS	80/91 (87%)	0.51	13 (16%) 2 3	41, 95, 133, 159	0
17	AT	85/86 (98%)	-0.68	0 100 100	19, 88, 126, 156	0
17	CT	85/86 (98%)	-0.28	1 (1%) 79 70	5, 66, 113, 154	0
18	AB	218/240 (90%)	-0.07	10 (4%) 33 26	12, 81, 120, 160	0
18	CB	218/240 (90%)	0.92	50 (22%) 1 1	5, 87, 133, 163	0
19	AU	51/70 (72%)	0.78	8 (15%) 2 3	20, 94, 139, 153	0
19	CU	51/70 (72%)	0.11	2 (3%) 40 31	57, 96, 137, 171	0
20	AO	88/89 (98%)	1.00	11 (12%) 4 5	5, 73, 118, 177	0
20	CO	88/89 (98%)	-0.48	0 100 100	5, 56, 108, 135	0
21	AN	96/100 (96%)	1.33	30 (31%) 0 1	5, 84, 128, 155	0
21	CN	96/100 (96%)	1.13	24 (25%) 1 1	5, 75, 129, 145	0
22	BA	117/120 (97%)	0.07	2 (1%) 70 61	35, 77, 125, 167	0
22	DA	117/120 (97%)	-0.56	1 (0%) 84 76	31, 87, 133, 176	0
23	BB	2841/2904 (97%)	-0.46	23 (0%) 86 79	5, 60, 136, 180	0
23	DB	2841/2904 (97%)	-0.52	23 (0%) 86 79	5, 51, 136, 180	0
24	BI	141/141 (100%)	2.65	68 (48%) 0 1	60, 135, 178, 180	0
24	DI	141/141 (100%)	1.29	38 (26%) 1 1	66, 135, 180, 180	0
25	BC	271/272 (99%)	1.41	88 (32%) 0 1	5, 61, 109, 132	0
25	DC	271/272 (99%)	0.81	54 (19%) 1 2	5, 45, 99, 144	0
26	BD	209/209 (100%)	0.50	28 (13%) 4 4	5, 71, 118, 148	0
26	DD	209/209 (100%)	0.91	38 (18%) 1 2	5, 60, 110, 168	0
27	BK	121/123 (98%)	2.08	66 (54%) 0 1	5, 75, 125, 159	0
27	DK	121/123 (98%)	1.05	27 (22%) 1 1	5, 45, 112, 150	0
28	BP	114/114 (100%)	1.54	47 (41%) 0 1	7, 82, 125, 155	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.40	6 (5%)	27 22	5, 64, 118, 139	0
29	BE	201/201 (100%)	0.81	34 (16%)	2 3	5, 65, 128, 164	0
29	DE	201/201 (100%)	1.23	58 (28%)	1 1	5, 73, 123, 160	0
30	BY	58/58 (100%)	-0.26	1 (1%)	70 61	5, 75, 129, 160	0
30	DY	58/58 (100%)	-0.23	3 (5%)	28 22	5, 72, 116, 147	0
31	B0	56/56 (100%)	0.04	2 (3%)	43 34	5, 78, 118, 147	0
31	D0	56/56 (100%)	0.18	1 (1%)	69 59	5, 62, 129, 153	0
32	B4	38/38 (100%)	0.95	8 (21%)	1 2	27, 81, 131, 145	0
32	D4	38/38 (100%)	-0.34	0	100 100	5, 67, 106, 117	0
33	B1	50/54 (92%)	0.62	4 (8%)	13 11	17, 70, 120, 134	0
33	D1	50/54 (92%)	0.34	5 (10%)	8 7	17, 73, 116, 137	0
34	B3	64/64 (100%)	-0.23	1 (1%)	72 62	5, 68, 103, 129	0
34	D3	64/64 (100%)	1.36	21 (32%)	0 1	5, 55, 86, 122	0
35	BV	94/94 (100%)	0.63	13 (13%)	3 4	5, 81, 126, 152	0
35	DV	94/94 (100%)	0.94	21 (22%)	1 1	5, 88, 120, 160	0
36	B2	46/46 (100%)	0.77	5 (10%)	6 6	5, 53, 104, 141	0
36	D2	46/46 (100%)	1.65	20 (43%)	0 1	9, 48, 110, 141	0
37	BL	143/144 (99%)	-0.16	2 (1%)	75 66	5, 67, 121, 145	0
37	DL	143/144 (99%)	1.63	58 (40%)	0 1	5, 63, 111, 145	0
38	BM	136/136 (100%)	0.91	21 (15%)	2 3	7, 68, 121, 179	0
38	DM	136/136 (100%)	1.31	39 (28%)	1 1	5, 65, 117, 144	0
39	BX	63/63 (100%)	0.99	13 (20%)	1 2	16, 79, 128, 159	0
39	DX	63/63 (100%)	1.08	9 (14%)	3 4	16, 91, 144, 169	0
40	BH	149/149 (100%)	3.05	87 (58%)	0 1	7, 104, 149, 180	0
40	DH	149/149 (100%)	0.86	27 (18%)	1 2	5, 91, 131, 162	0
41	BJ	142/142 (100%)	0.94	29 (20%)	1 2	5, 77, 118, 140	0
41	DJ	142/142 (100%)	0.27	10 (7%)	17 13	5, 70, 119, 173	0
42	BN	120/127 (94%)	0.84	17 (14%)	3 4	5, 69, 111, 154	0
42	DN	120/127 (94%)	0.02	6 (5%)	30 23	5, 51, 94, 163	0
43	BO	116/117 (99%)	-0.08	7 (6%)	23 16	6, 80, 109, 172	0
43	DO	116/117 (99%)	0.90	20 (17%)	2 2	5, 83, 136, 158	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	-0.62	1 (0%) 84 76	5, 62, 115, 144	0
44	DQ	117/117 (100%)	0.46	12 (10%) 7 7	5, 60, 111, 154	0
45	BS	110/110 (100%)	0.39	7 (6%) 20 14	5, 62, 121, 148	0
45	DS	110/110 (100%)	1.42	36 (32%) 0 1	5, 64, 127, 156	0
46	BU	102/103 (99%)	0.84	15 (14%) 3 3	12, 80, 125, 157	0
46	DU	102/103 (99%)	-0.41	0 100 100	8, 94, 127, 149	0
47	BF	178/178 (100%)	0.73	31 (17%) 2 2	29, 100, 146, 180	0
47	DF	178/178 (100%)	2.23	90 (50%) 0 1	12, 93, 142, 163	0
48	BG	176/176 (100%)	0.77	33 (18%) 1 2	18, 94, 133, 171	0
48	DG	176/176 (100%)	0.39	24 (13%) 3 4	8, 90, 136, 166	0
49	BR	103/103 (100%)	-0.03	4 (3%) 40 31	5, 83, 123, 133	0
49	DR	103/103 (100%)	0.13	4 (3%) 40 31	10, 76, 135, 149	0
50	BT	93/100 (93%)	-0.08	2 (2%) 62 53	8, 83, 130, 165	0
50	DT	93/100 (93%)	2.28	50 (53%) 0 1	5, 84, 144, 172	0
51	BZ	77/78 (98%)	0.57	12 (15%) 2 3	5, 63, 120, 142	0
51	DZ	77/78 (98%)	0.01	1 (1%) 77 68	5, 56, 106, 120	0
52	BW	79/84 (94%)	0.45	6 (7%) 15 11	5, 75, 124, 180	0
52	DW	79/84 (94%)	0.69	9 (11%) 6 6	5, 71, 121, 166	0
All	All	20417/21046 (97%)	0.14	2042 (10%) 8 7	5, 70, 134, 180	0

The worst 5 of 2042 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	BI	17	ALA	14.5
23	BB	546	U	12.7
24	BI	18	ASN	12.4
40	BH	124	THR	12.3
24	BI	51	GLY	12.2

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	CA	1612	1/1	0.84	0.28	10.75	93,93,93,93	0
53	MG	BB	3087	1/1	0.98	0.25	10.45	80,80,80,80	0
53	MG	CA	1654	1/1	0.91	0.22	4.60	105,105,105,105	0
53	MG	DB	3026	1/1	0.99	0.23	4.22	45,45,45,45	0
53	MG	CA	1656	1/1	0.99	0.14	2.00	38,38,38,38	0
53	MG	DB	3071	1/1	0.94	0.16	1.69	57,57,57,57	0
53	MG	DB	3097	1/1	0.99	0.17	1.63	41,41,41,41	0
53	MG	DB	3035	1/1	0.92	0.22	1.29	79,79,79,79	0
53	MG	BB	3001	1/1	0.92	0.19	1.19	5,5,5,5	0
53	MG	BB	3110	1/1	0.96	0.13	0.87	80,80,80,80	0
53	MG	DB	3030	1/1	0.97	0.19	0.72	47,47,47,47	0
53	MG	CA	1610	1/1	0.98	0.14	0.72	5,5,5,5	0
53	MG	DB	3095	1/1	0.98	0.15	0.49	92,92,92,92	0
53	MG	DB	3089	1/1	0.96	0.13	0.46	79,79,79,79	0
54	SCM	CA	1659	23/23	0.91	0.16	0.44	18,18,18,18	0
53	MG	DB	3088	1/1	0.98	0.17	0.39	87,87,87,87	0
53	MG	CA	1621	1/1	0.98	0.16	0.36	80,80,80,80	0
53	MG	BB	3098	1/1	0.97	0.15	0.24	14,14,14,14	0
53	MG	BB	3049	1/1	0.84	0.19	0.17	67,67,67,67	0
53	MG	BB	3011	1/1	0.98	0.15	0.07	5,5,5,5	0
53	MG	AA	1635	1/1	0.77	0.15	-0.02	80,80,80,80	0
54	SCM	AA	1661	23/23	0.97	0.10	-0.33	13,13,13,13	0
53	MG	DB	3069	1/1	0.97	0.23	-0.35	64,64,64,64	0
53	MG	DB	3010	1/1	0.97	0.14	-0.42	5,5,5,5	0
53	MG	DB	3077	1/1	0.98	0.13	-0.66	45,45,45,45	0
53	MG	AA	1643	1/1	0.98	0.09	-0.77	40,40,40,40	0
53	MG	DB	3102	1/1	0.99	0.23	-0.78	28,28,28,28	0
53	MG	DB	3007	1/1	0.97	0.12	-0.90	62,62,62,62	0
53	MG	DB	3047	1/1	0.98	0.15	-0.98	43,43,43,43	0
53	MG	DB	3109	1/1	0.94	0.04	-0.99	9,9,9,9	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3012	1/1	0.99	0.12	-1.02	9,9,9,9	0
53	MG	BB	3083	1/1	0.99	0.14	-1.03	30,30,30,30	0
53	MG	AA	1652	1/1	0.86	0.08	-1.08	84,84,84,84	0
53	MG	BB	3059	1/1	0.99	0.13	-1.08	10,10,10,10	0
53	MG	DB	3055	1/1	0.96	0.16	-1.09	44,44,44,44	0
53	MG	AA	1651	1/1	0.97	0.06	-1.12	35,35,35,35	0
53	MG	DB	3014	1/1	1.00	0.05	-1.12	21,21,21,21	0
53	MG	BB	3090	1/1	0.95	0.10	-1.12	88,88,88,88	0
53	MG	BB	3021	1/1	0.96	0.13	-1.12	52,52,52,52	0
53	MG	AA	1607	1/1	0.99	0.08	-1.17	57,57,57,57	0
53	MG	BB	3040	1/1	0.98	0.08	-1.23	12,12,12,12	0
53	MG	BB	3005	1/1	0.94	0.11	-1.23	5,5,5,5	0
53	MG	DB	3068	1/1	0.99	0.15	-1.24	5,5,5,5	0
53	MG	DB	3098	1/1	0.98	0.10	-1.24	5,5,5,5	0
55	ZN	D4	101	1/1	0.93	0.05	-1.26	62,62,62,62	0
53	MG	BB	3050	1/1	0.98	0.12	-1.29	53,53,53,53	0
53	MG	BB	3019	1/1	0.98	0.12	-1.40	21,21,21,21	0
53	MG	AA	1613	1/1	0.96	0.04	-1.46	58,58,58,58	0
53	MG	BB	3086	1/1	0.98	0.10	-1.54	5,5,5,5	0
53	MG	CA	1652	1/1	0.97	0.07	-1.57	49,49,49,49	0
55	ZN	B4	101	1/1	0.94	0.07	-1.64	67,67,67,67	0
53	MG	BB	3012	1/1	0.99	0.06	-1.65	67,67,67,67	0
53	MG	AA	1601	1/1	0.96	0.09	-1.68	36,36,36,36	0
53	MG	AA	1603	1/1	0.96	0.10	-1.75	57,57,57,57	0
53	MG	AA	1653	1/1	0.98	0.09	-1.75	21,21,21,21	0
53	MG	DB	3091	1/1	0.94	0.11	-1.86	90,90,90,90	0
53	MG	BB	3023	1/1	0.95	0.10	-1.89	5,5,5,5	0
53	MG	DB	3003	1/1	0.95	0.05	-1.98	30,30,30,30	0
53	MG	AA	1638	1/1	0.97	0.07	-2.00	51,51,51,51	0
53	MG	CA	1604	1/1	0.95	0.10	-2.03	20,20,20,20	0
53	MG	DB	3084	1/1	0.99	0.09	-2.04	29,29,29,29	0
53	MG	DB	3006	1/1	0.98	0.11	-2.09	10,10,10,10	0
53	MG	AA	1630	1/1	0.98	0.04	-2.16	88,88,88,88	0
53	MG	BB	3069	1/1	0.95	0.07	-2.22	5,5,5,5	0
53	MG	CA	1605	1/1	0.95	0.05	-2.27	12,12,12,12	0
53	MG	DB	3075	1/1	0.98	0.11	-2.27	44,44,44,44	0
53	MG	CA	1611	1/1	0.99	0.07	-2.29	28,28,28,28	0
53	MG	AA	1633	1/1	0.92	0.05	-2.30	65,65,65,65	0
53	MG	CA	1633	1/1	0.96	0.06	-2.30	23,23,23,23	0
53	MG	DB	3083	1/1	0.98	0.08	-2.30	27,27,27,27	0
53	MG	DB	3086	1/1	0.98	0.12	-2.32	18,18,18,18	0
53	MG	DB	3051	1/1	0.95	0.11	-2.35	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	1629	1/1	0.97	0.06	-2.43	12,12,12,12	0
53	MG	AA	1609	1/1	0.98	0.06	-2.46	40,40,40,40	0
53	MG	BB	3085	1/1	0.99	0.07	-2.51	34,34,34,34	0
53	MG	BB	3035	1/1	0.88	0.07	-2.54	13,13,13,13	0
53	MG	BB	3062	1/1	0.98	0.08	-2.54	7,7,7,7	0
53	MG	CA	1636	1/1	1.00	0.04	-2.57	5,5,5,5	0
53	MG	BB	3096	1/1	0.97	0.07	-2.78	58,58,58,58	0
53	MG	DB	3067	1/1	0.94	0.06	-2.78	5,5,5,5	0
53	MG	DB	3107	1/1	0.99	0.04	-2.79	5,5,5,5	0
53	MG	BB	3079	1/1	0.94	0.07	-2.84	38,38,38,38	0
53	MG	DB	3044	1/1	0.98	0.05	-2.85	18,18,18,18	0
53	MG	DB	3056	1/1	0.98	0.06	-2.91	5,5,5,5	0
53	MG	BB	3081	1/1	0.92	0.10	-3.02	30,30,30,30	0
53	MG	CA	1624	1/1	0.99	0.07	-3.15	38,38,38,38	0
53	MG	DB	3087	1/1	0.98	0.08	-3.22	5,5,5,5	0
53	MG	BB	3066	1/1	0.99	0.04	-3.30	5,5,5,5	0
53	MG	BB	3094	1/1	0.98	0.06	-3.37	36,36,36,36	0
53	MG	BB	3065	1/1	0.97	0.06	-3.39	32,32,32,32	0
53	MG	BB	3013	1/1	0.97	0.10	-3.40	45,45,45,45	0
53	MG	BB	3103	1/1	0.98	0.08	-3.51	11,11,11,11	0
53	MG	CA	1655	1/1	0.99	0.03	-3.64	32,32,32,32	0
53	MG	BB	3108	1/1	0.93	0.06	-3.77	10,10,10,10	0
53	MG	BB	3088	1/1	0.96	0.06	-3.80	11,11,11,11	0
53	MG	DB	3009	1/1	0.98	0.07	-4.08	9,9,9,9	0
53	MG	CA	1627	1/1	0.92	0.07	-4.29	27,27,27,27	0
53	MG	DB	3019	1/1	0.98	0.06	-4.46	5,5,5,5	0
53	MG	AA	1654	1/1	0.95	0.07	-4.58	67,67,67,67	0
53	MG	BB	3002	1/1	0.98	0.06	-4.59	23,23,23,23	0
53	MG	BB	3056	1/1	0.98	0.03	-4.65	5,5,5,5	0
53	MG	DB	3002	1/1	0.98	0.05	-4.72	11,11,11,11	0
53	MG	DB	3034	1/1	0.91	0.08	-4.78	57,57,57,57	0
53	MG	DB	3079	1/1	0.97	0.06	-4.90	7,7,7,7	0
53	MG	CA	1601	1/1	0.98	0.06	-4.90	5,5,5,5	0
53	MG	AA	1610	1/1	0.99	0.06	-5.07	78,78,78,78	0
53	MG	CA	1635	1/1	0.98	0.06	-5.10	30,30,30,30	0
53	MG	AA	1619	1/1	0.97	0.04	-5.42	111,111,111,111	0
53	MG	AA	1641	1/1	0.99	0.02	-5.59	32,32,32,32	0
53	MG	BB	3074	1/1	0.98	0.06	-5.61	10,10,10,10	0
53	MG	BB	3029	1/1	0.99	0.05	-5.67	5,5,5,5	0
53	MG	BB	3048	1/1	0.98	0.04	-6.58	12,12,12,12	0
53	MG	BB	3032	1/1	0.96	0.07	-9.10	22,22,22,22	0
53	MG	DB	3001	1/1	0.96	0.06	-10.06	5,5,5,5	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3064	1/1	0.94	0.19	-	78,78,78,78	0
53	MG	DB	3096	1/1	0.95	0.11	-	26,26,26,26	0
53	MG	DB	3060	1/1	0.95	0.12	-	83,83,83,83	0
53	MG	DB	3070	1/1	0.98	0.06	-	33,33,33,33	0
53	MG	DB	3020	1/1	0.98	0.09	-	5,5,5,5	0
53	MG	BB	3076	1/1	0.96	0.12	-	35,35,35,35	0
53	MG	DB	3072	1/1	0.98	0.07	-	20,20,20,20	0
53	MG	DB	3101	1/1	0.99	0.10	-	26,26,26,26	0
53	MG	BB	3101	1/1	1.00	0.05	-	19,19,19,19	0
53	MG	BB	3099	1/1	0.95	0.06	-	41,41,41,41	0
53	MG	DB	3018	1/1	0.95	0.09	-	7,7,7,7	0
53	MG	BB	3106	1/1	0.98	0.12	-	10,10,10,10	0
53	MG	BB	3057	1/1	0.96	0.16	-	53,53,53,53	0
53	MG	DB	3046	1/1	0.98	0.04	-	23,23,23,23	0
53	MG	CA	1631	1/1	0.95	0.04	-	41,41,41,41	0
53	MG	BB	3037	1/1	0.87	0.13	-	45,45,45,45	0
53	MG	CE	201	1/1	0.92	0.08	-	109,109,109,109	0
53	MG	AA	1636	1/1	0.98	0.04	-	64,64,64,64	0
53	MG	CA	1637	1/1	0.94	0.17	-	98,98,98,98	0
53	MG	BB	3073	1/1	0.99	0.10	-	44,44,44,44	0
53	MG	AA	1602	1/1	0.93	0.13	-	85,85,85,85	0
53	MG	BB	3063	1/1	0.99	0.05	-	33,33,33,33	0
53	MG	DB	3100	1/1	0.96	0.17	-	19,19,19,19	0
53	MG	DB	3066	1/1	0.89	0.33	-	65,65,65,65	0
53	MG	DB	3008	1/1	0.98	0.06	-	13,13,13,13	0
53	MG	BB	3053	1/1	0.97	0.09	-	60,60,60,60	0
53	MG	DB	3092	1/1	0.98	0.15	-	10,10,10,10	0
53	MG	AA	1627	1/1	0.91	0.07	-	63,63,63,63	0
53	MG	AA	1655	1/1	0.89	0.14	-	88,88,88,88	0
53	MG	DB	3028	1/1	0.95	0.18	-	70,70,70,70	0
53	MG	AA	1648	1/1	0.99	0.06	-	6,6,6,6	0
53	MG	BB	3003	1/1	0.95	0.06	-	53,53,53,53	0
53	MG	DB	3062	1/1	0.98	0.23	-	58,58,58,58	0
53	MG	DB	3064	1/1	0.93	0.39	-	49,49,49,49	0
53	MG	AA	1615	1/1	0.96	0.35	-	96,96,96,96	0
53	MG	BB	3093	1/1	0.88	0.10	-	108,108,108,108	0
53	MG	DB	3054	1/1	0.97	0.15	-	21,21,21,21	0
53	MG	CA	1625	1/1	0.94	0.05	-	70,70,70,70	0
53	MG	DB	3073	1/1	0.99	0.07	-	50,50,50,50	0
53	MG	AA	1622	1/1	0.70	0.34	-	130,130,130,130	0
53	MG	DB	3057	1/1	0.97	0.05	-	48,48,48,48	0
53	MG	BB	3084	1/1	0.97	0.06	-	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3065	1/1	0.95	0.07	-	128,128,128,128	0
53	MG	AA	1625	1/1	0.82	0.39	-	79,79,79,79	1
53	MG	AA	1659	1/1	0.97	0.39	-	108,108,108,108	0
53	MG	AA	1616	1/1	0.97	0.09	-	5,5,5,5	0
53	MG	AA	1644	1/1	0.98	0.05	-	75,75,75,75	0
53	MG	DB	3090	1/1	0.98	0.09	-	14,14,14,14	0
53	MG	BB	3042	1/1	0.60	0.23	-	92,92,92,92	0
53	MG	BB	3100	1/1	0.97	0.20	-	116,116,116,116	0
53	MG	DB	3017	1/1	0.98	0.23	-	5,5,5,5	0
53	MG	DB	3032	1/1	0.90	0.16	-	73,73,73,73	0
53	MG	DB	3045	1/1	0.88	0.11	-	110,110,110,110	0
53	MG	DB	3022	1/1	0.94	0.06	-	11,11,11,11	0
53	MG	CA	1649	1/1	0.90	0.27	-	123,123,123,123	0
53	MG	BB	3022	1/1	0.98	0.12	-	32,32,32,32	0
53	MG	CA	1650	1/1	0.83	0.09	-	105,105,105,105	0
53	MG	BB	3039	1/1	0.97	0.15	-	41,41,41,41	0
53	MG	DB	3025	1/1	0.99	0.07	-	44,44,44,44	0
53	MG	CA	1617	1/1	0.93	0.18	-	88,88,88,88	0
53	MG	DB	3027	1/1	0.96	0.07	-	13,13,13,13	0
53	MG	DB	3104	1/1	0.92	0.12	-	29,29,29,29	0
53	MG	BB	3030	1/1	0.97	0.07	-	51,51,51,51	0
53	MG	BB	3007	1/1	0.98	0.14	-	68,68,68,68	0
53	MG	BB	3071	1/1	0.94	0.18	-	68,68,68,68	0
53	MG	CA	1645	1/1	0.92	0.10	-	55,55,55,55	0
53	MG	DB	3043	1/1	0.98	0.06	-	7,7,7,7	0
53	MG	AA	1647	1/1	0.85	0.82	-	113,113,113,113	0
53	MG	DB	3037	1/1	0.99	0.16	-	8,8,8,8	0
53	MG	BB	3051	1/1	0.91	0.13	-	107,107,107,107	0
53	MG	CA	1614	1/1	0.98	0.16	-	83,83,83,83	0
53	MG	BB	3058	1/1	0.99	0.06	-	15,15,15,15	0
53	MG	DB	3016	1/1	0.94	0.08	-	5,5,5,5	0
53	MG	BB	3041	1/1	0.99	0.08	-	5,5,5,5	0
53	MG	BB	3070	1/1	0.96	0.05	-	74,74,74,74	0
53	MG	CA	1638	1/1	0.97	0.10	-	86,86,86,86	0
53	MG	DB	3033	1/1	0.98	0.04	-	11,11,11,11	0
53	MG	BB	3044	1/1	0.98	0.09	-	45,45,45,45	0
53	MG	DB	3082	1/1	0.97	0.11	-	83,83,83,83	0
53	MG	CA	1623	1/1	0.96	0.10	-	11,11,11,11	0
53	MG	CA	1619	1/1	0.98	0.09	-	36,36,36,36	0
53	MG	DB	3052	1/1	0.77	0.29	-	105,105,105,105	0
53	MG	BB	3010	1/1	0.90	0.16	-	53,53,53,53	0
53	MG	AA	1618	1/1	0.95	0.08	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3094	1/1	0.79	0.14	-	100,100,100,100	0
53	MG	BB	3016	1/1	0.99	0.04	-	55,55,55,55	0
53	MG	BB	3061	1/1	0.98	0.08	-	24,24,24,24	0
53	MG	AA	1657	1/1	0.91	0.34	-	91,91,91,91	0
53	MG	DB	3105	1/1	0.99	0.04	-	40,40,40,40	0
53	MG	CA	1642	1/1	0.99	0.07	-	79,79,79,79	0
53	MG	DB	3074	1/1	0.98	0.07	-	26,26,26,26	0
53	MG	DB	3059	1/1	0.81	0.11	-	99,99,99,99	0
53	MG	DB	3011	1/1	0.99	0.10	-	5,5,5,5	0
53	MG	DB	3063	1/1	0.90	0.16	-	72,72,72,72	0
53	MG	AA	1639	1/1	0.98	0.04	-	93,93,93,93	0
53	MG	BB	3047	1/1	0.98	0.11	-	104,104,104,104	0
53	MG	AA	1631	1/1	0.97	0.12	-	5,5,5,5	0
53	MG	BB	3008	1/1	0.94	0.12	-	82,82,82,82	0
53	MG	BB	3036	1/1	0.96	0.20	-	51,51,51,51	0
53	MG	DB	3038	1/1	0.99	0.07	-	5,5,5,5	0
53	MG	AA	1604	1/1	0.99	0.09	-	38,38,38,38	0
53	MG	DB	3106	1/1	0.97	0.05	-	61,61,61,61	0
53	MG	CA	1613	1/1	0.88	0.49	-	126,126,126,126	0
53	MG	BB	3055	1/1	0.99	0.12	-	6,6,6,6	0
53	MG	BB	3034	1/1	0.96	0.12	-	86,86,86,86	0
53	MG	DB	3076	1/1	0.99	0.10	-	33,33,33,33	0
53	MG	CA	1644	1/1	0.86	0.14	-	57,57,57,57	0
53	MG	BB	3009	1/1	0.89	0.10	-	98,98,98,98	0
53	MG	DB	3050	1/1	0.93	0.11	-	80,80,80,80	0
53	MG	BB	3006	1/1	0.96	0.15	-	61,61,61,61	0
53	MG	BB	3068	1/1	0.90	0.19	-	13,13,13,13	0
53	MG	AA	1649	1/1	0.90	0.04	-	89,89,89,89	0
53	MG	CA	1646	1/1	0.82	0.11	-	139,139,139,139	0
53	MG	AA	1640	1/1	0.98	0.15	-	46,46,46,46	0
53	MG	AA	1612	1/1	0.91	0.08	-	61,61,61,61	0
53	MG	BB	3045	1/1	0.98	0.14	-	72,72,72,72	0
53	MG	CA	1634	1/1	0.91	0.11	-	74,74,74,74	0
53	MG	BB	3102	1/1	0.97	0.12	-	43,43,43,43	0
53	MG	AA	1634	1/1	0.99	0.03	-	72,72,72,72	0
53	MG	CA	1603	1/1	0.99	0.03	-	56,56,56,56	0
53	MG	BB	3015	1/1	0.95	0.10	-	25,25,25,25	0
53	MG	CA	1615	1/1	0.95	0.06	-	13,13,13,13	0
53	MG	CA	1626	1/1	0.98	0.08	-	8,8,8,8	0
53	MG	DB	3024	1/1	0.98	0.05	-	40,40,40,40	0
53	MG	BB	3107	1/1	0.99	0.21	-	46,46,46,46	0
53	MG	DB	3031	1/1	0.97	0.09	-	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	1658	1/1	0.96	0.08	-	37,37,37,37	0
53	MG	DB	3041	1/1	0.96	0.08	-	40,40,40,40	0
53	MG	BB	3077	1/1	0.98	0.11	-	53,53,53,53	0
53	MG	AA	1645	1/1	0.94	0.20	-	70,70,70,70	0
53	MG	CA	1618	1/1	0.84	0.13	-	73,73,73,73	0
53	MG	DB	3015	1/1	0.99	0.06	-	42,42,42,42	0
53	MG	DB	3029	1/1	0.86	0.70	-	87,87,87,87	0
53	MG	BB	3072	1/1	0.99	0.10	-	35,35,35,35	0
53	MG	CA	1643	1/1	0.98	0.06	-	36,36,36,36	0
53	MG	BB	3075	1/1	0.97	0.09	-	40,40,40,40	0
53	MG	BB	3046	1/1	0.91	0.10	-	89,89,89,89	0
53	MG	BB	3078	1/1	0.95	0.19	-	27,27,27,27	0
53	MG	DB	3023	1/1	0.99	0.04	-	69,69,69,69	0
53	MG	CA	1606	1/1	0.88	0.14	-	106,106,106,106	0
53	MG	BB	3095	1/1	0.97	0.07	-	62,62,62,62	0
53	MG	DB	3021	1/1	0.99	0.04	-	16,16,16,16	0
53	MG	DB	3036	1/1	0.98	0.04	-	87,87,87,87	0
53	MG	CA	1608	1/1	0.91	0.05	-	76,76,76,76	0
53	MG	CA	1647	1/1	0.97	0.06	-	75,75,75,75	0
53	MG	DB	3080	1/1	0.99	0.10	-	62,62,62,62	0
53	MG	AA	1623	1/1	0.83	0.36	-	33,33,33,33	1
53	MG	BB	3026	1/1	0.98	0.10	-	65,65,65,65	0
53	MG	BB	3025	1/1	0.95	0.15	-	30,30,30,30	0
53	MG	BB	3020	1/1	0.94	0.31	-	6,6,6,6	0
53	MG	DB	3048	1/1	0.98	0.11	-	38,38,38,38	0
53	MG	DB	3040	1/1	0.99	0.05	-	5,5,5,5	0
53	MG	DB	3085	1/1	0.98	0.05	-	38,38,38,38	0
53	MG	DB	3099	1/1	0.98	0.13	-	58,58,58,58	0
53	MG	CA	1632	1/1	0.93	0.24	-	76,76,76,76	0
53	MG	AA	1646	1/1	0.85	0.10	-	84,84,84,84	0
53	MG	AA	1628	1/1	0.94	0.18	-	70,70,70,70	0
53	MG	AA	1642	1/1	0.90	0.13	-	49,49,49,49	0
53	MG	AA	1621	1/1	0.94	0.17	-	36,36,36,36	0
53	MG	DB	3053	1/1	0.95	0.07	-	65,65,65,65	0
53	MG	AA	1660	1/1	0.96	0.03	-	56,56,56,56	0
53	MG	DB	3061	1/1	0.98	0.04	-	66,66,66,66	0
53	MG	DB	3058	1/1	0.77	0.09	-	139,139,139,139	0
53	MG	DB	3004	1/1	0.98	0.08	-	8,8,8,8	0
53	MG	AA	1611	1/1	0.99	0.05	-	43,43,43,43	0
53	MG	DB	3049	1/1	1.00	0.14	-	42,42,42,42	0
53	MG	BB	3017	1/1	0.96	0.13	-	50,50,50,50	0
53	MG	BB	3067	1/1	0.97	0.17	-	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	1641	1/1	0.96	0.10	-	42,42,42,42	0
53	MG	BB	3080	1/1	0.88	0.16	-	53,53,53,53	0
53	MG	CA	1629	1/1	0.91	0.17	-	67,67,67,67	0
53	MG	AA	1656	1/1	0.92	0.14	-	87,87,87,87	0
53	MG	BB	3038	1/1	0.96	0.07	-	92,92,92,92	0
53	MG	BB	3097	1/1	0.59	0.07	-	113,113,113,113	0
53	MG	BB	3089	1/1	0.98	0.12	-	72,72,72,72	0
53	MG	AA	1617	1/1	0.89	0.09	-	112,112,112,112	0
53	MG	DB	3110	1/1	0.95	0.12	-	84,84,84,84	0
53	MG	CA	1602	1/1	0.99	0.12	-	5,5,5,5	0
53	MG	CA	1609	1/1	0.92	0.10	-	85,85,85,85	0
53	MG	CA	1639	1/1	0.98	0.05	-	35,35,35,35	0
53	MG	CA	1657	1/1	0.99	0.05	-	73,73,73,73	0
53	MG	CA	1653	1/1	0.97	0.07	-	48,48,48,48	0
53	MG	AA	1608	1/1	0.56	0.13	-	123,123,123,123	0
53	MG	DB	3078	1/1	0.97	0.04	-	25,25,25,25	0
53	MG	AA	1624	1/1	0.70	0.24	-	83,83,83,83	0
53	MG	BB	3033	1/1	0.80	0.34	-	102,102,102,102	0
53	MG	AA	1632	1/1	0.96	0.22	-	96,96,96,96	0
53	MG	BB	3092	1/1	0.95	0.09	-	46,46,46,46	0
53	MG	CA	1640	1/1	0.84	0.11	-	62,62,62,62	0
53	MG	DN	201	1/1	0.92	0.51	-	145,145,145,145	0
53	MG	BB	3014	1/1	0.92	0.07	-	37,37,37,37	0
53	MG	CA	1630	1/1	0.99	0.10	-	37,37,37,37	0
53	MG	BB	3018	1/1	0.98	0.12	-	39,39,39,39	0
53	MG	BB	3031	1/1	0.97	0.18	-	60,60,60,60	0
53	MG	BB	3043	1/1	0.92	0.12	-	107,107,107,107	0
53	MG	CA	1651	1/1	0.85	0.08	-	101,101,101,101	0
53	MG	CA	1622	1/1	0.99	0.18	-	5,5,5,5	0
53	MG	CA	1648	1/1	0.88	0.07	-	104,104,104,104	0
53	MG	DB	3108	1/1	0.95	0.10	-	43,43,43,43	0
53	MG	BB	3105	1/1	0.99	0.18	-	5,5,5,5	0
53	MG	DB	3005	1/1	0.93	0.17	-	25,25,25,25	0
53	MG	BB	3082	1/1	0.97	0.15	-	18,18,18,18	0
53	MG	AA	1637	1/1	0.88	0.32	-	99,99,99,99	0
53	MG	CA	1628	1/1	0.92	0.11	-	52,52,52,52	0
53	MG	AA	1620	1/1	0.79	0.06	-	60,60,60,60	0
53	MG	DB	3081	1/1	0.99	0.06	-	41,41,41,41	0
53	MG	BB	3004	1/1	0.92	0.05	-	80,80,80,80	0
53	MG	DB	3039	1/1	0.98	0.08	-	62,62,62,62	0
53	MG	DB	3013	1/1	0.88	0.08	-	52,52,52,52	0
53	MG	AA	1614	1/1	0.84	0.18	-	119,119,119,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	1607	1/1	0.97	0.06	-	5,5,5,5	0
53	MG	DB	3042	1/1	0.99	0.04	-	37,37,37,37	0
53	MG	BB	3028	1/1	0.99	0.24	-	9,9,9,9	0
53	MG	DB	3103	1/1	0.96	0.06	-	36,36,36,36	0
53	MG	AA	1605	1/1	0.92	0.10	-	50,50,50,50	0
53	MG	BB	3024	1/1	0.96	0.09	-	55,55,55,55	0
53	MG	BB	3091	1/1	0.98	0.10	-	5,5,5,5	0
53	MG	AA	1606	1/1	0.89	0.06	-	82,82,82,82	0
53	MG	BB	3109	1/1	0.98	0.10	-	11,11,11,11	0
53	MG	BB	3060	1/1	0.99	0.17	-	30,30,30,30	0
53	MG	CA	1620	1/1	0.99	0.10	-	72,72,72,72	0
53	MG	BB	3054	1/1	0.96	0.13	-	49,49,49,49	0
53	MG	AA	1658	1/1	0.94	0.04	-	120,120,120,120	0
53	MG	BB	3052	1/1	0.96	0.10	-	71,71,71,71	0
53	MG	DB	3093	1/1	0.98	0.05	-	59,59,59,59	0
53	MG	CA	1616	1/1	0.90	0.33	-	58,58,58,58	1
53	MG	BB	3104	1/1	0.95	0.17	-	26,26,26,26	0
53	MG	BB	3027	1/1	0.97	0.06	-	50,50,50,50	0
53	MG	AA	1626	1/1	0.88	0.20	-	36,36,36,36	1
53	MG	AA	1650	1/1	0.92	0.08	-	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.