



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 03:47 pm BST

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

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

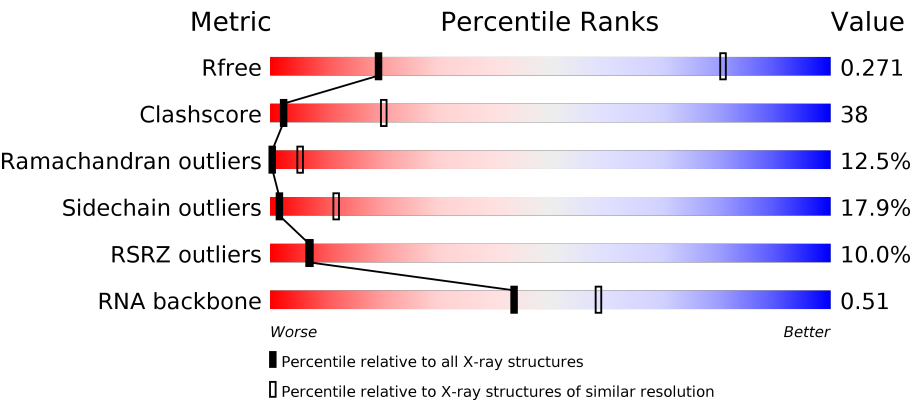
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance i

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}	130704	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)
RNA backbone	3102	1041 (4.84-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1542	<div><div>19%</div><div>63%</div><div>16%</div><div>2%</div></div>
1	CA	1542	<div><div>20%</div><div>63%</div><div>16%</div><div>1%</div></div>
2	AC	232	<div><div>6%</div><div>19%</div><div>46%</div><div>22%</div><div>7%</div></div>
2	CC	232	<div><div>12%</div><div>22%</div><div>48%</div><div>18%</div><div>11%</div></div>

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

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

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

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

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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

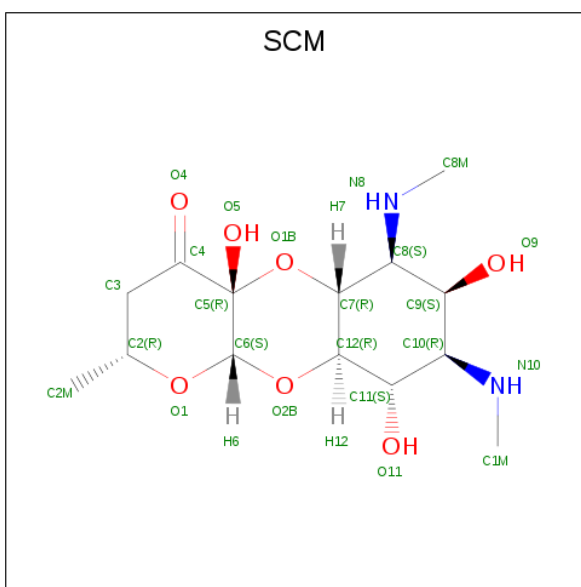
- Molecule 52 is a protein called 50S ribosomal protein L27.

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	C	N	O	0	0
			23	14	2	7		
54	CA	1	Total	C	N	O	0	0
			23	14	2	7		

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

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	288	Total	O	0	0
			288	288		
56	AE	3	Total	O	0	0
			3	3		
56	AK	1	Total	O	0	0
			1	1		
56	AL	4	Total	O	0	0
			4	4		
56	AP	1	Total	O	0	0
			1	1		

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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

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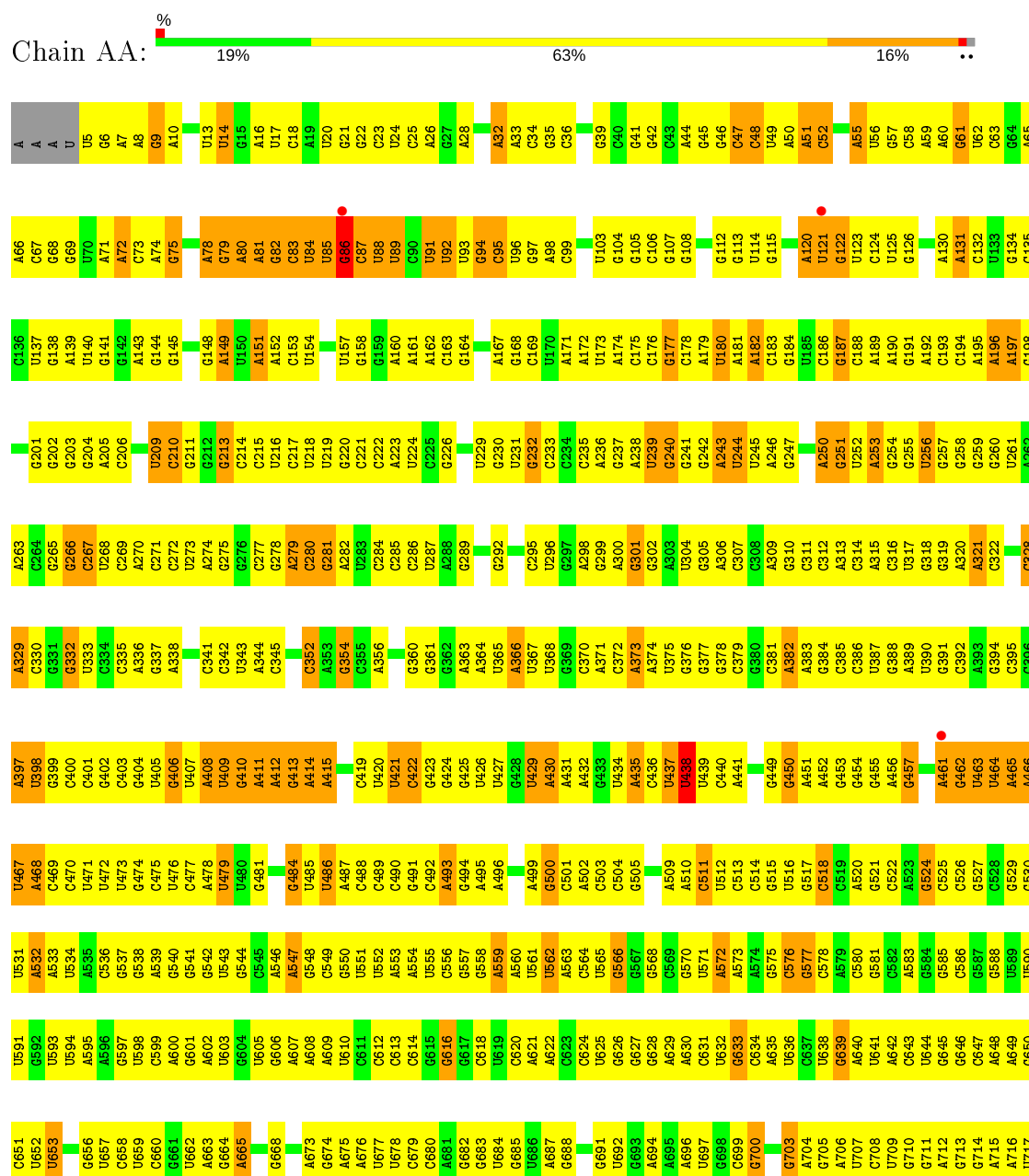
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DJ	1	Total 1	O 1	0	0
56	DN	2	Total 2	O 2	0	0
56	DR	1	Total 1	O 1	0	0

3 Residue-property plots

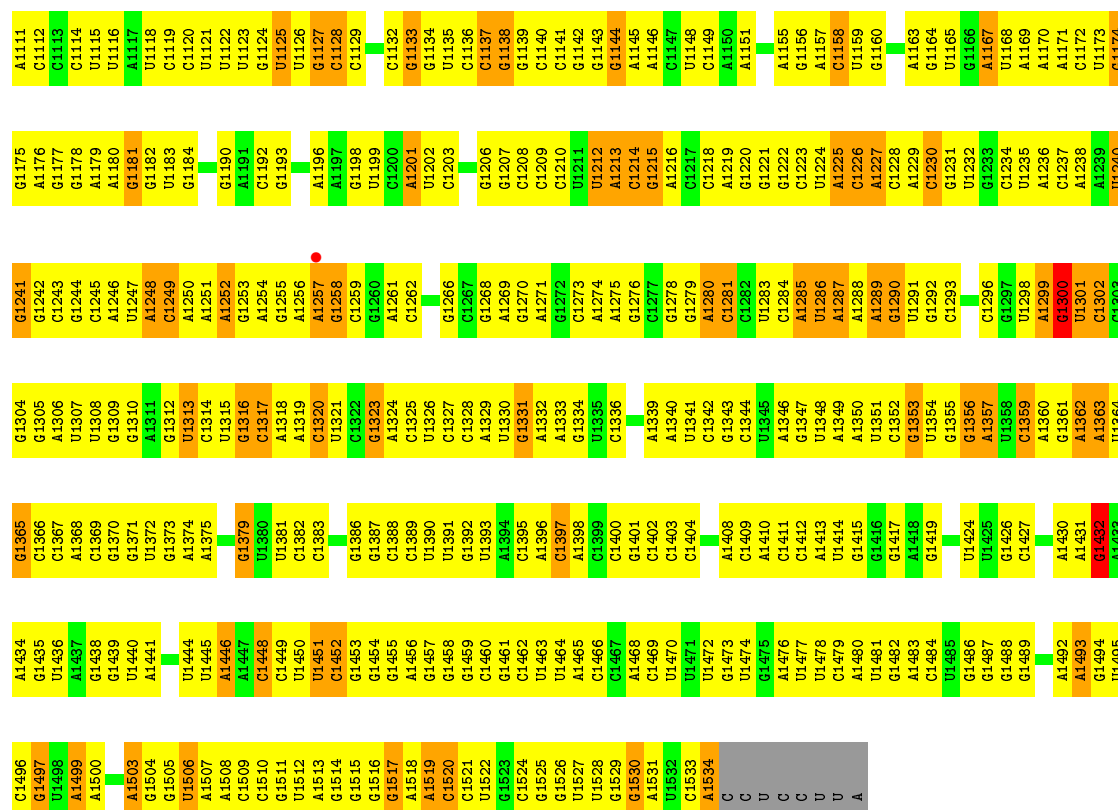
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

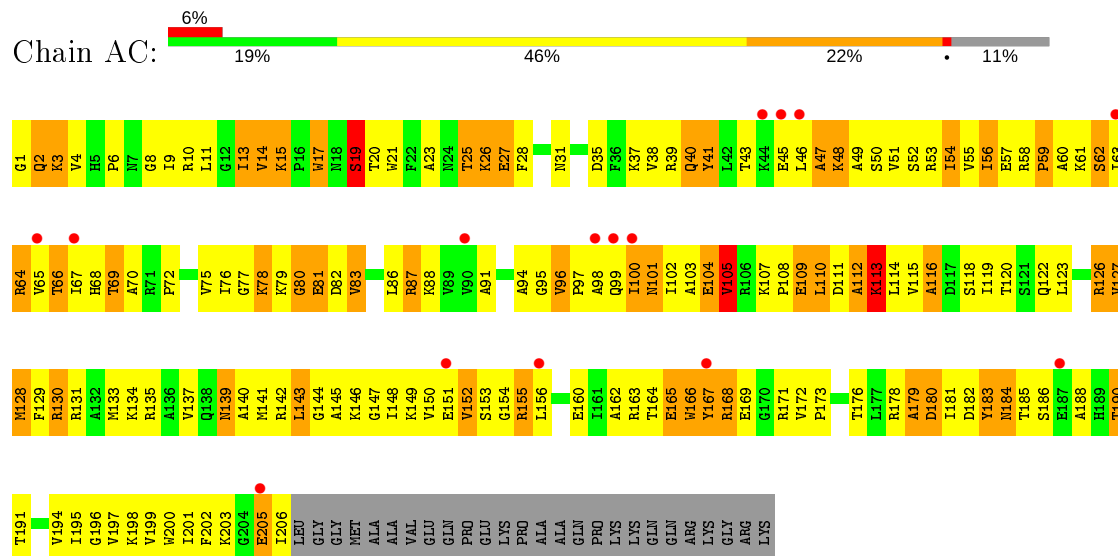




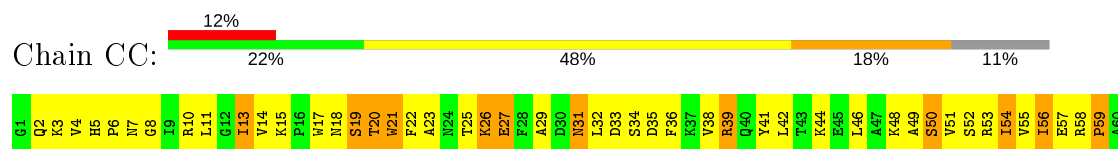
G1048	G1049	G985	G922	C857	A792	G724	C660	G597	G474	G402	C335	G266	G203	U133	A65
U986	U987	G858	A923	G859	U793	G725	G661	U598	C475	C403	A336	C267	G204	G134	A66
G988	G989	A860	C924	A861	A794	A728	U662	C599	U476	U405	A337	U268	C206	C136	G67
U989	U990	G861	G925	G862	C795	G729	A663	A600	U477	U406	A338	C269	G206	G137	G68
G990	G991	C862	G926	C863	C796	G730	G664	G601	A478	G407	C341	A270	U209	U138	G69
C1054	C1055	U863	G927	U864	C797	G731	G665	A602	U479	U408	C342	C271	C210	G138	U70
A1056	A1057	A864	G928	A865	U798	G732	G666	U603	U480	A408	U343	C272	C211	A143	A71
G993	G994	C866	C930	C867	C733	G733	G667	G604	C481	U409	U344	U273	G212	A144	A72
A994	A995	G867	G931	G868	C734	G734	A546	G606	C483	U410	C345	A274	G213	G145	C73
G996	G997	C868	C932	C869	U804	C735	U672	A607	U484	A411	G346	G275	C214	A74	G75
U1060	U1061	G869	G933	G870	C805	C736	A673	A608	U485	G413	G347	A279	C215	G148	G76
G1061	G1062	G870	C934	G871	C806	C737	G674	A609	U486	A414	C352	G280	U216	A149	A77
U1062	U1063	A874	A935	A875	A807	C738	A675	G550	A487	A415	C353	G281	C217	U150	A78
C1001	C1002	U875	G936	U876	C808	C739	A676	U551	C488	U420	A354	A282	U218	A151	G79
U1008	U1009	G880	G937	G881	G809	U740	A677	U552	C489	U421	U345	U273	U219	A152	A80
G1004	G1005	C882	G938	C883	C810	G741	U678	A614	C490	U422	C355	C284	G220	C153	A81
C1066	C1067	G877	G939	G878	C811	C742	G679	A554	C491	G423	A356	C285	C221	U154	G82
A1006	A1007	U878	G940	U879	G812	G745	G680	G616	C492	G424	C361	U287	C222	C83	G83
U1008	U1009	C879	G941	C880	U813	A746	A681	G617	C493	G425	G362	U288	C223	U157	U84
G1072	G1073	C880	G942	C881	A814	A747	G682	C618	A494	U426	A363	G289	U224	G158	U85
U1070	U1071	A815	G943	C882	A816	G748	U683	U619	U426	U427	A364	G290	C225	G159	G86
C1072	C1073	A817	G944	C883	A818	A749	U684	C620	A495	U427	A365	G291	G226	A160	C87
U1074	U1075	C750	G945	G884	C817	C750	G685	A621	A560	G428	U365	G292	C227	A161	U88
U1076	U1077	G751	G946	U885	U818	G752	U686	A622	U561	U429	A366	G300	C228	A162	U89
U1078	U1079	A753	G947	C885	A819	G753	A687	G623	U562	A430	U367	G301	G230	C163	C90
A1080	A1081	G754	G948	C886	U820	G754	G688	C624	A563	A431	U368	G302	U231	G164	U91
U1082	U1083	A755	G949	C887	G821	C755	U691	U632	U570	U432	G369	G303	G232	U92	U92
U1084	U1085	G756	G950	C888	A822	C756	U692	G633	U571	U433	C370	U304	C233	A167	U93
U1086	U1087	C757	G951	C889	U823	U757	U693	C634	A572	U434	A371	G305	C234	G168	G94
G1088	G1089	G758	G952	C890	G824	C758	G693	A629	U567	A435	C372	A300	C235	C169	C95
U1090	U1091	C759	G953	C891	A825	G759	A694	A630	G568	A436	A373	G304	G236	U174	A98
U1092	U1093	G760	G954	C892	A826	A766	A695	C631	U569	U437	A374	G305	A237	C175	C99
U1094	U1095	A767	G955	C893	U827	A767	U696	G632	U570	U438	U375	U304	U238	C176	G100
G1096	G1097	G768	G956	C894	U828	G768	U697	G633	C511	A441	G376	G306	G240	G177	A101
U1098	U1099	C769	G957	C895	G829	C769	G698	C634	U512	G449	G377	A306	G241	C178	G102
C1100	C1101	G770	G958	C896	G830	G770	C699	A635	C513	C514	C379	C307	G242	U103	U103
A1101	A1102	U837	G959	C897	U838	U772	C705	U641	U519	G454	C384	A312	G247	G184	G108
U1102	U1103	G838	G960	C898	G839	G773	A706	A642	C580	G455	C385	A313	G248	U185	G104
C1103	C1104	C839	G961	C899	C840	G773	U707	U643	U581	A456	C386	A314	G249	C186	G112
U1104	U1105	G840	G962	C900	U834	A767	A702	U638	C576	A451	C387	A315	G251	G187	G113
G1104	G1105	C841	G963	A901	U835	A768	G703	G639	U577	A452	U388	C316	U252	C188	U114
U1106	U1107	U842	G964	G902	U836	G769	A704	A640	C578	G453	A382	U317	G253	C189	G115
A1108	A1109	C843	G965	G903	G836	C770	G705	U641	U519	G454	A383	G311	G254	A190	A120
C1109	C1110	U844	G966	U904	U837	G771	A706	A642	C580	G455	C384	A312	G255	G191	U121
U1109	U1110	A845	G967	U905	G838	U772	U707	U643	U581	A456	C386	A314	U256	A192	U122
G1107	G1108	C846	G968	A906	C839	G773	C708	U644	C582	G457	U387	A315	G257	C193	G122
C1045	C1046	U847	G969	A907	C840	G774	U709	G645	A583	A461	U388	C316	U258	C194	U123
U1046	U1047	C841	G970	A908	C841	A777	G710	G646	G584	G462	U389	U317	G259	A195	C124
G1047	G1048	U842	G971	A909	U842	G778	G711	C647	G585	G463	U390	G318	G260	A196	U125
U1049	U1050	C843	G972	A910	U843	G779	A712	A648	C586	U464	U391	G319	U261	A197	U126
C1051	C1052	U844	G973	A911	C844	C779	G713	A649	G587	U465	C392	A321	G262	G198	G126
U1053	U1054	A845	G974	A912	A846	A780	G714	G650	U588	A466	A393	C322	G263	C201	A130
A1055	A1056	C846	G975	A913	U847	A781	G715	C651	U589	A467	U394	G328	G264	G202	G132
G1057	G1058	U847	G976	A914	C848	C783	A716	G652	U590	U467	C395	A329	C265	A131	A131
U1059	U1060	A848	G977	A915	C849	G783	G722	U653	U591	A468	C396	A330	G266	G199	G127
C1060	C1061	U849	G978	A916	U851	A784	C719	U654	U592	C469	A397	G331	U267	A132	A132
U1062	U1063	G851	G979	A917	G852	G785	G720	G656	A593	C470	U398	G332	G267	G203	G128
G1064	G1065	C852	G980	A918	C853	U789	G721	U657	U594	U471	U399	G333	C268	G204	G129
U1066	U1067	U854	G981	A919	U854	G791	U723	U659	A596	U473	C400	G334	G269	G205	G130
C1068	C1069	G855	G982	A920	U855	G792	U724	U660	A597	U474	C401	G335	G270	G206	G131
U1070	U1071	C856	G983	A921	C856	G793	U725	U661	A598	U475	C402	G336	G271	G207	G132
G1072	G1073	U856	G984	A922	C857	G794	U726	U662	A599	U476	C403	G337	G272	G208	G133
U1074	U1075	G857	G985	A923	C858	G795	U727	U663	A600	U477	C404	G338	G273	G209	G134
C1074	C1075	U858	G986	A924	C859	G796	U728	U664	A601	U478	C405	G339	G274	G210	G135
U1076	U1077	G859	G987	A925	C860	G797	U729	U665	A602	U479	C406	G340	G275	G211	G136
G1078	G1079	U860	G988	A926	C861	G798	U730	U666	A603	U480	C407	G341	G276	G212	G137
A1080	A1081	C862	G989	A927	C862	G799	U731	U667	A604	U481	C408	G342	G277	G213	G138
U1082	U1083	U863	G990	A928	C863	G800	U732	U668	A605	U482	C409	G343	G278	G214	G139
U1084	U1085	G864	G991	A929	C864	C801	U733	U669	A606	U483	C410	G344	G279	G215	G140
U1086	U1087	U865	G992	A930	C865	C802	U734	U670	A607	U484	C411	G345	G280	G216	G141
G1088	G1089	C866	G993	A931	C866	C803	U735	U671	A608	U485	C412	G346	G281	G217	G142
U1090	U1091	U866	G994	A932	C867	C804	U736	U672	A609	U486	C413	G347	G282	G218	G143
U1092	U1093	G867	G995	A933	C868	C805	U737	U673	A610	U487	C414	G348	G283	G219	G144
C1094	C1095	U868	G996	A934	C869	C806	U738	U674	A611	U488	C415	G349	G284	G220	G145
U1096	U1097	G869	G997	A935	C870	C807	U739	U675	A612	U489	C416	G350	G285	G221	G146
G1098	G1099	U870	G998	A936	C871	C808	U740	U676	A613	U490	C417	G351	G286	G222	G147
U1100	U1101	C872	G999	A937	C872	C809	U741	U677	A614	U491	C418	G352	G287	G223	G148
C1102	C1103	U871	G1000	A938	C873	C810	G741	U678	A615	U492	C419	G353	G288	G224	G149
U1104	U1105	G872	G1001	A939	C874	C811	G742	U679	A616	U493	C420	G354	G289	G225	G150
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G1107	G1108	C874	G1003	A941	C876	C813	G744	U681	A618	U495	C422	G356	G291	G227	G152
U1109	U1110	U874	G1004	A942	C877	C814	G745	U682	A619	U496	C423	G357	G292	G228	G153
C1109	C1110	G875	G1005	A943	C878	C815	G746	U683	A620	U497	C424	G358	G293	G229	G154
U1110	U1111	U876	G1006	A944	C879	C816	G747	U684	A621	U498	C425	G359	G294	G230	G155
G1110	G1111	C876	G1007	A945	C880	C817	G748	U685	A622	U499	C426	G360	G295	G231	G156
U1112	U1113	U877	G1008	A946	C881	C818	G749	U686	A623	U500	C427	G361	G296	G232	G157
C1112	C1113	G877	G1009	A947	C882	C819	G750	U687	A624	U501	C428	G362	G297	G233	G158
U1114	U1115	U878	G1010	A948	C883	C820	G751	U688	A625	U502	C429	G363	G298	G234	G159
G1115	G1116	C878	G1011	A949	C884										

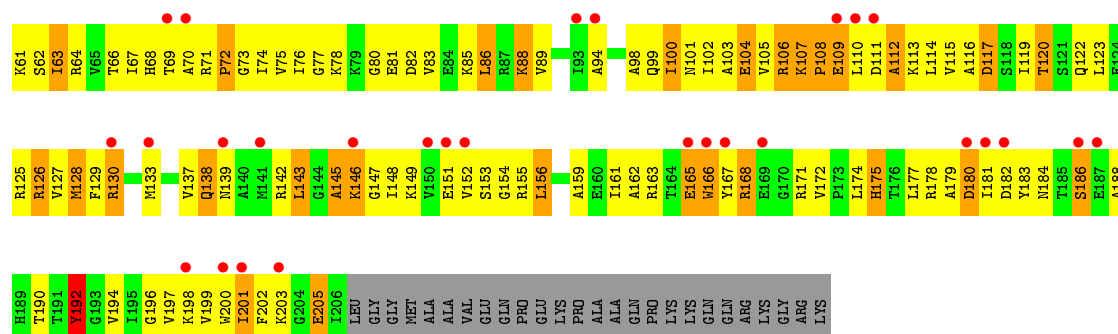


• Molecule 2: 30S ribosomal protein S3

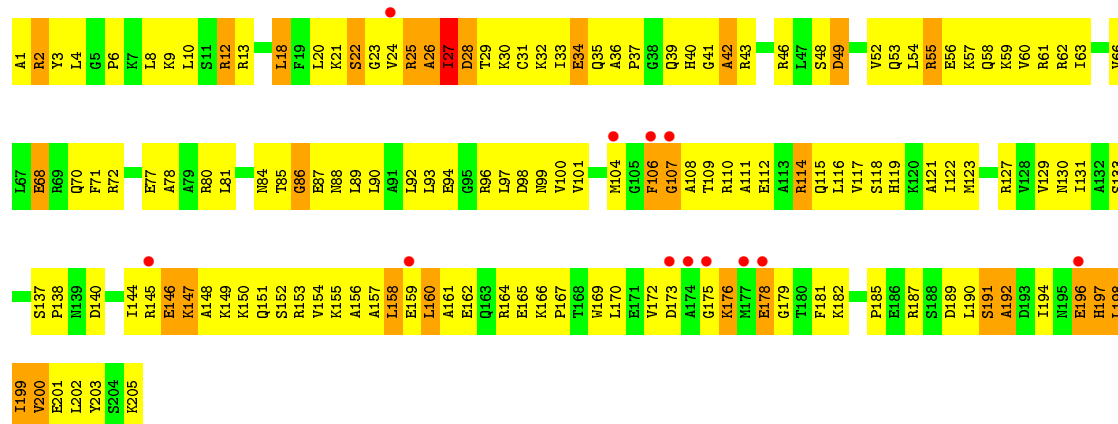


• Molecule 2: 30S ribosomal protein S3

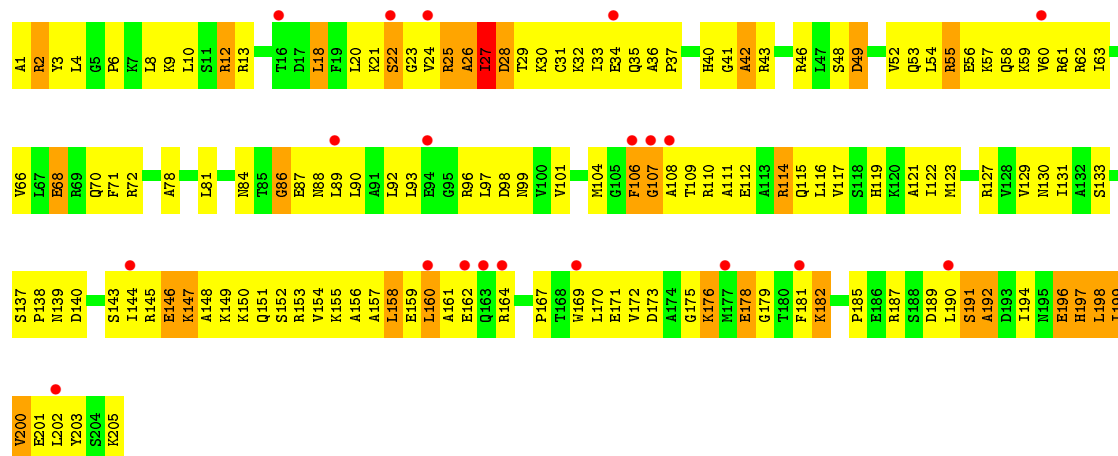




• Molecule 3: 30S ribosomal protein S4

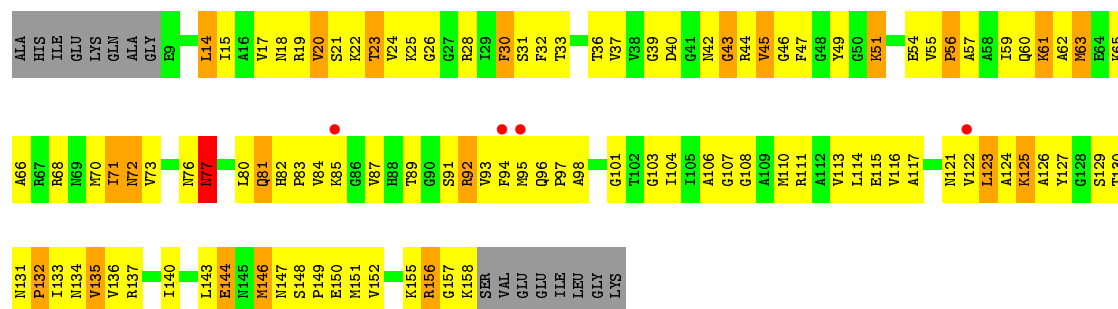


• Molecule 3: 30S ribosomal protein S4

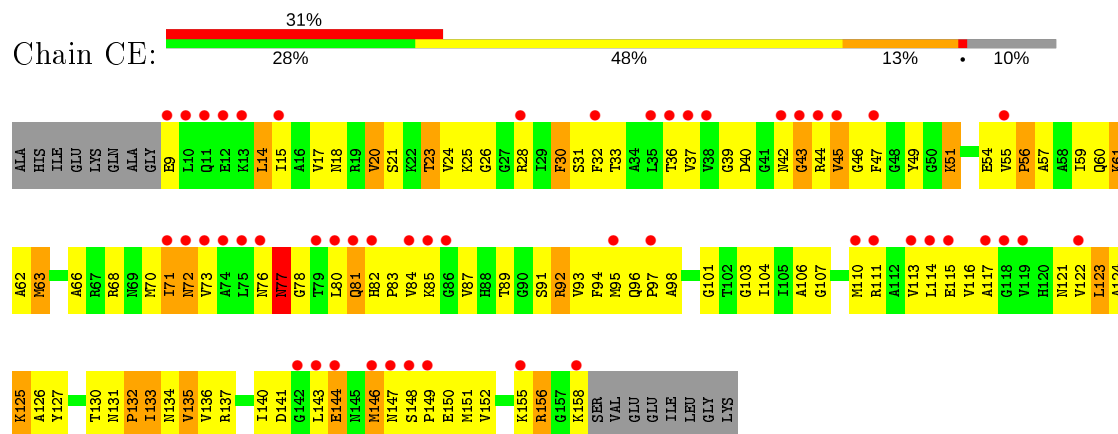


• Molecule 4: 30S ribosomal protein S5

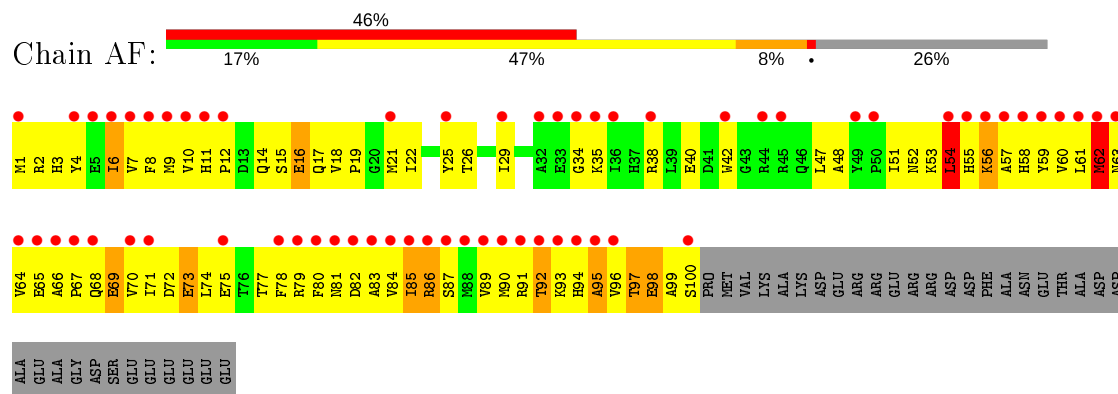




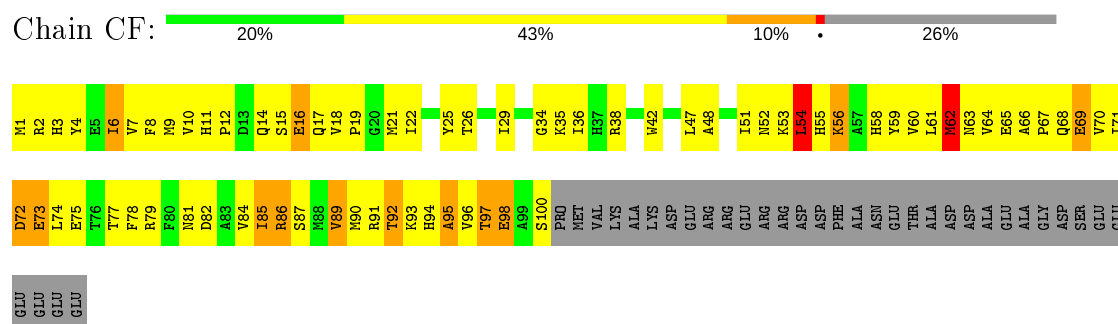
• Molecule 4: 30S ribosomal protein S5



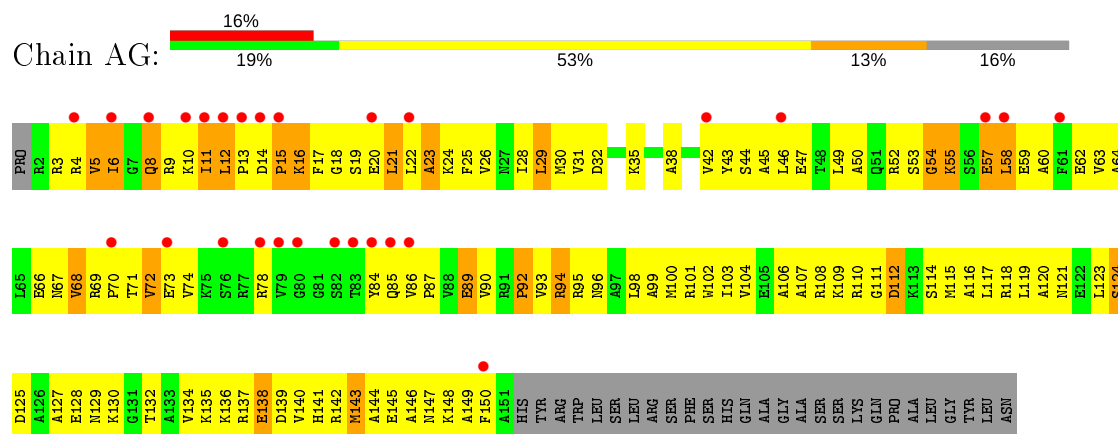
• Molecule 5: 30S ribosomal protein S6



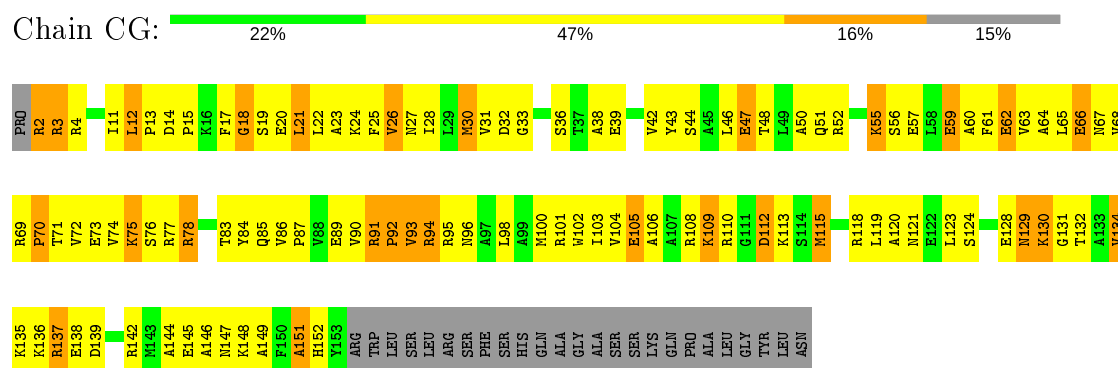
• Molecule 5: 30S ribosomal protein S6



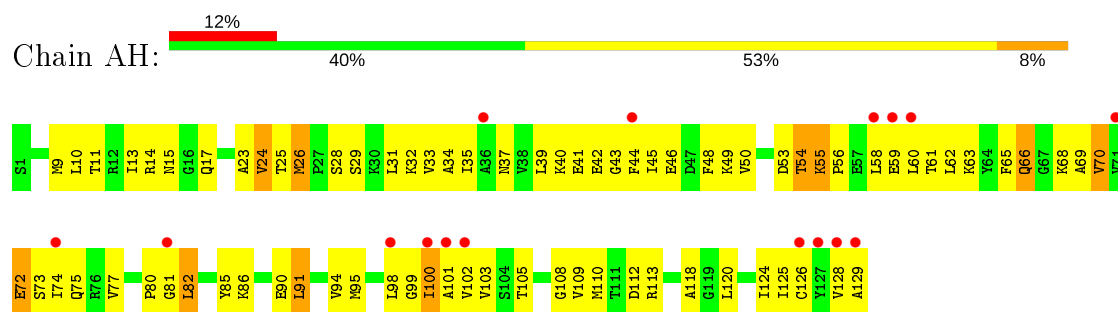
- Molecule 6: 30S ribosomal protein S7



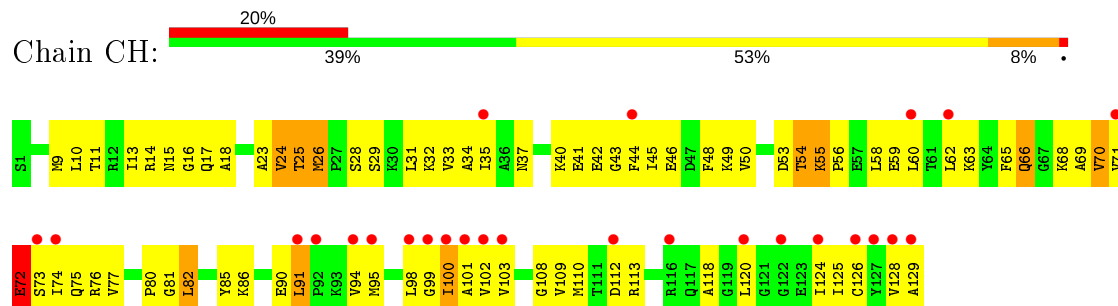
- Molecule 6: 30S ribosomal protein S7



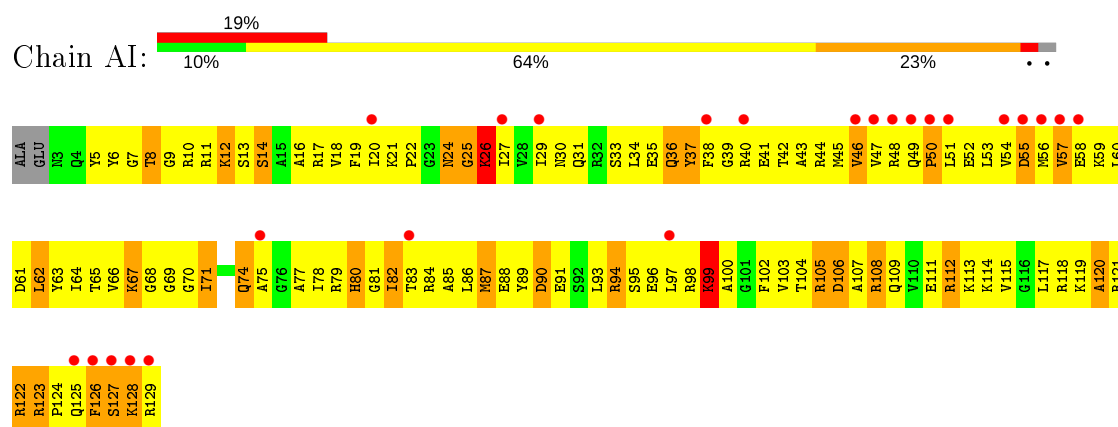
- Molecule 7: 30S ribosomal protein S8



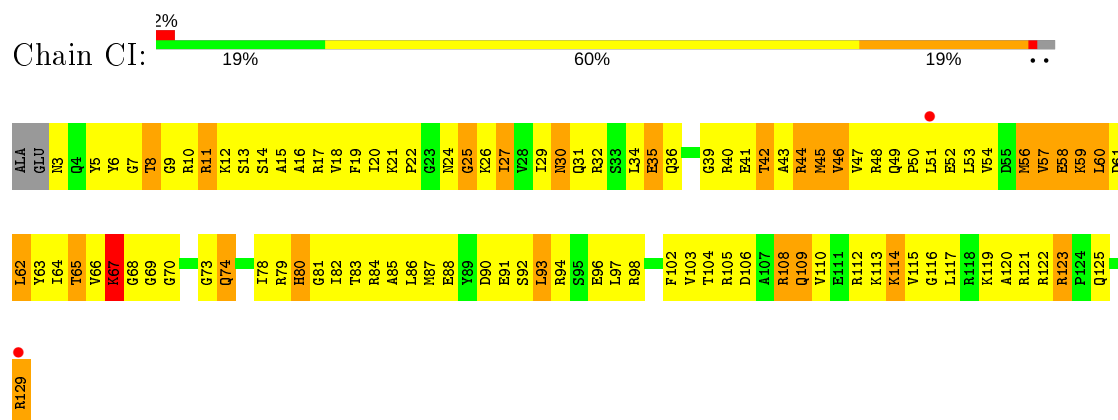
- Molecule 7: 30S ribosomal protein S8



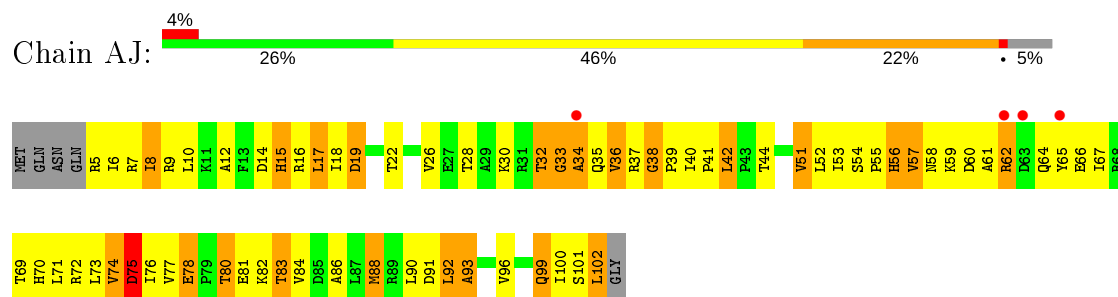
- Molecule 8: 30S ribosomal protein S9



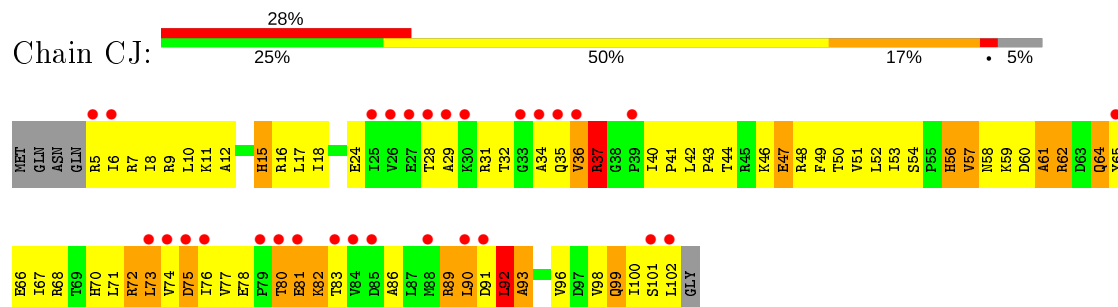
• Molecule 8: 30S ribosomal protein S9



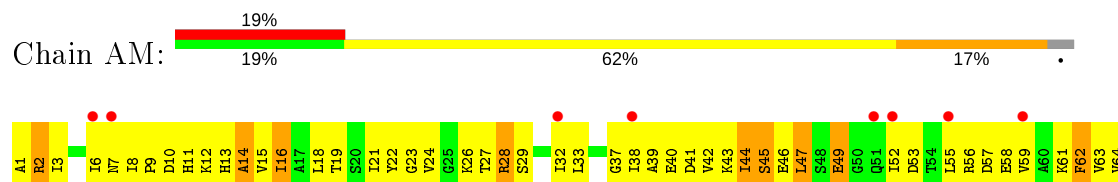
• Molecule 9: 30S ribosomal protein S10

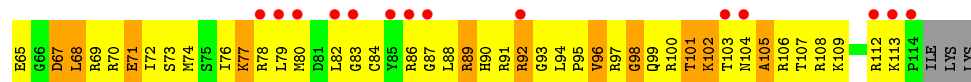


• Molecule 9: 30S ribosomal protein S10

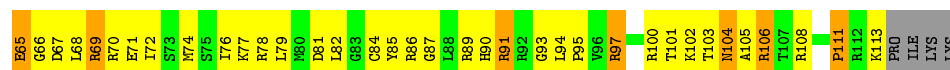


• Molecule 10: 30S ribosomal protein S11

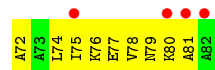
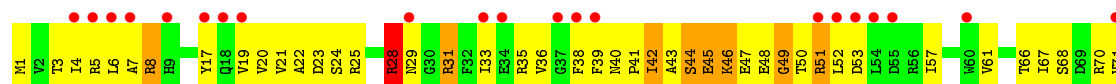




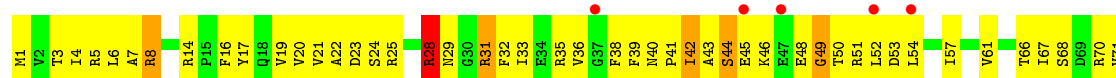
- Molecule 12: 30S ribosomal protein S13



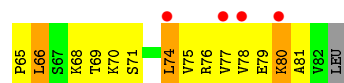
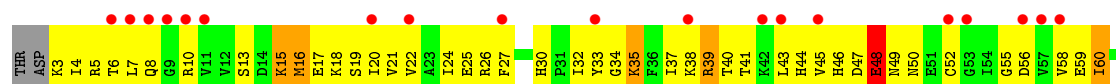
- Molecule 13: 30S ribosomal protein S16



- Molecule 13: 30S ribosomal protein S16

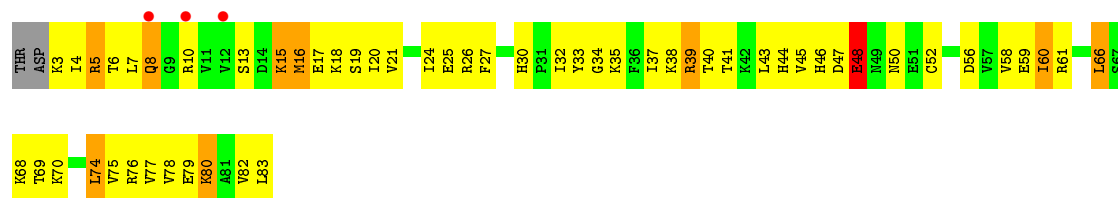


- Molecule 14: 30S ribosomal protein S17

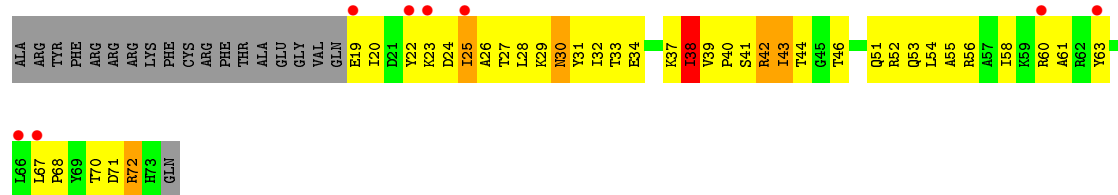
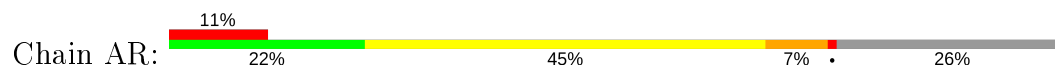


- Molecule 14: 30S ribosomal protein S17

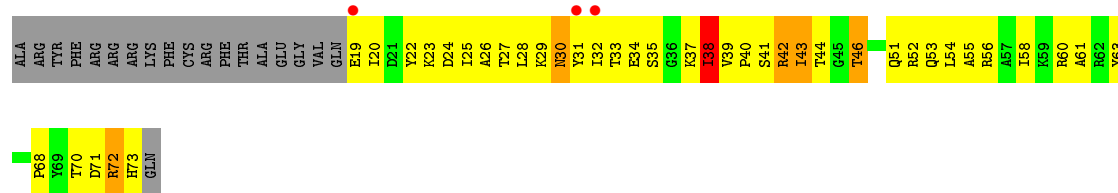
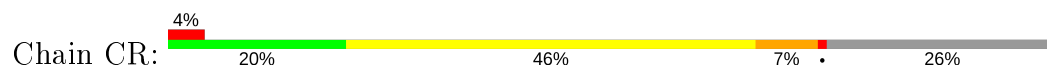




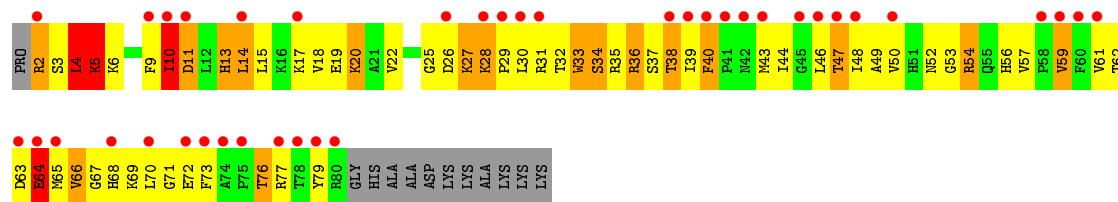
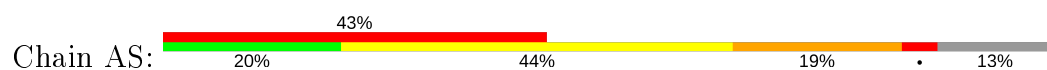
- Molecule 15: 30S ribosomal protein S18



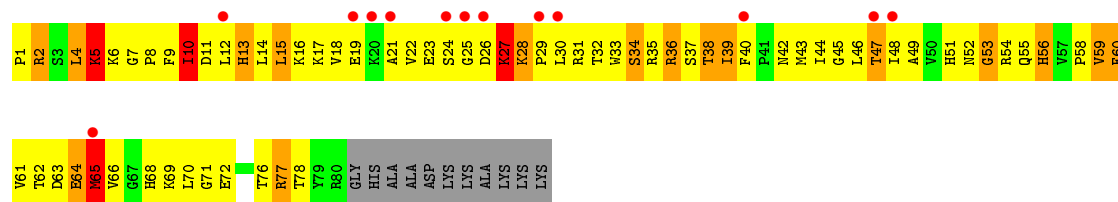
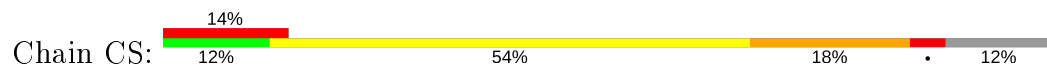
- Molecule 15: 30S ribosomal protein S18



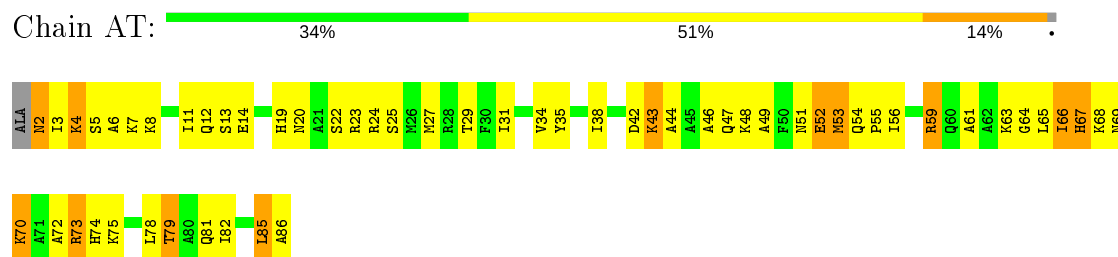
- Molecule 16: 30S ribosomal protein S19



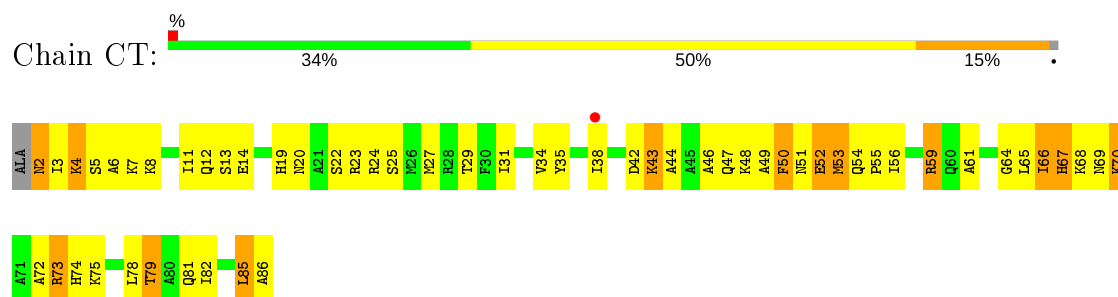
- Molecule 16: 30S ribosomal protein S19



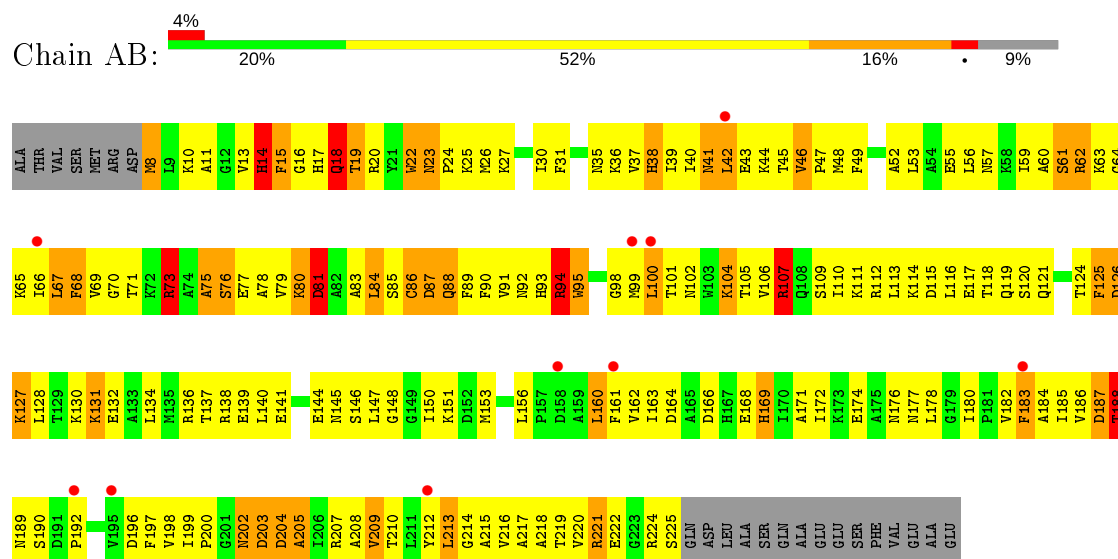
- Molecule 17: 30S ribosomal protein S20



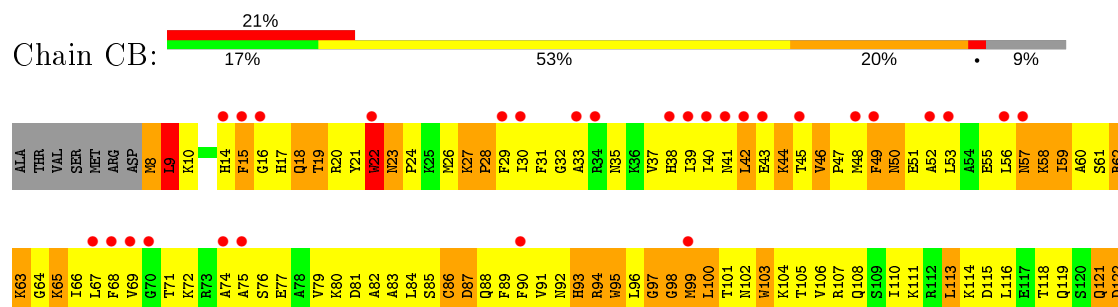
• Molecule 17: 30S ribosomal protein S20

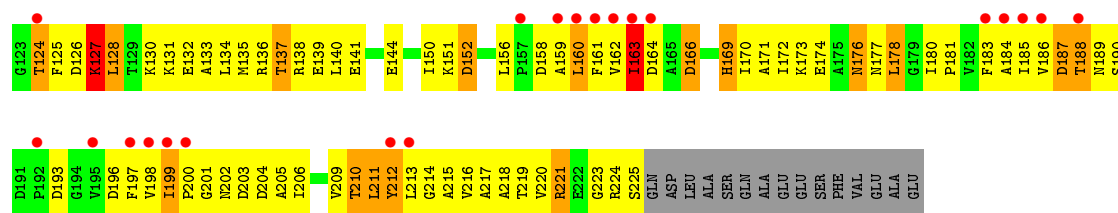


• Molecule 18: 30S ribosomal protein S2

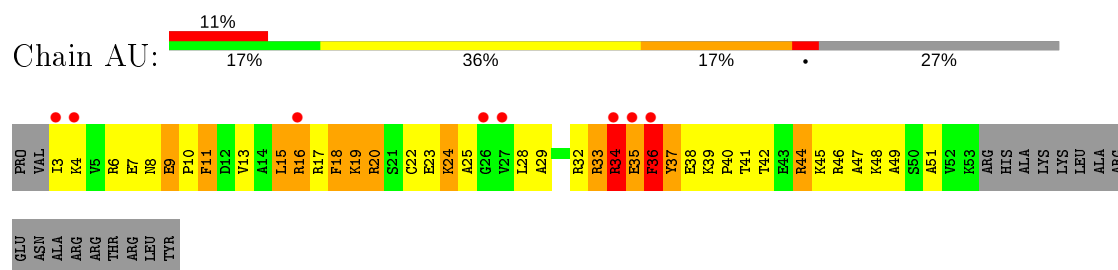


• Molecule 18: 30S ribosomal protein S2

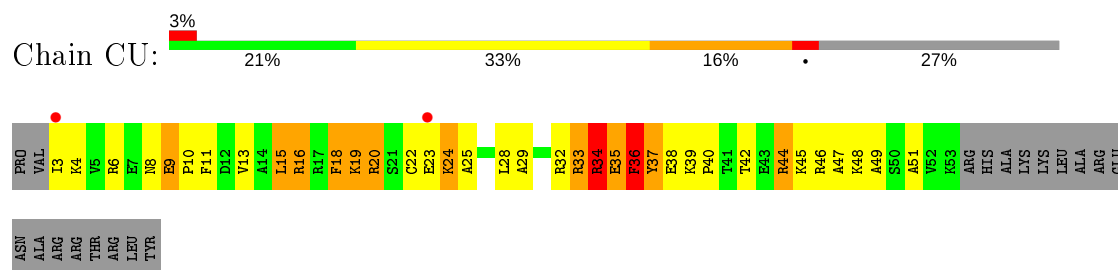




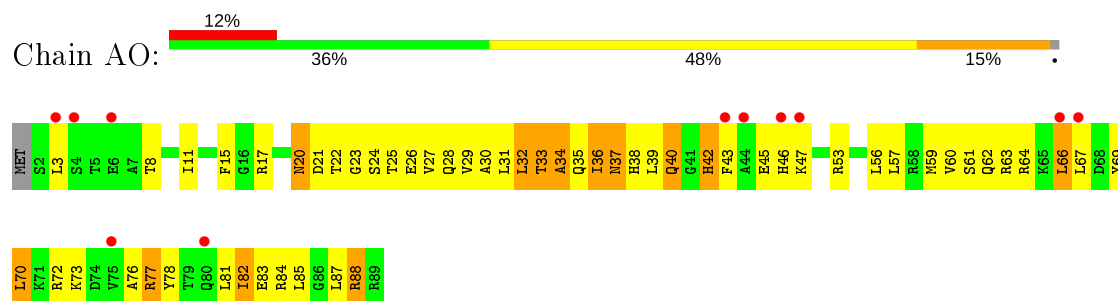
• Molecule 19: 30S ribosomal protein S21



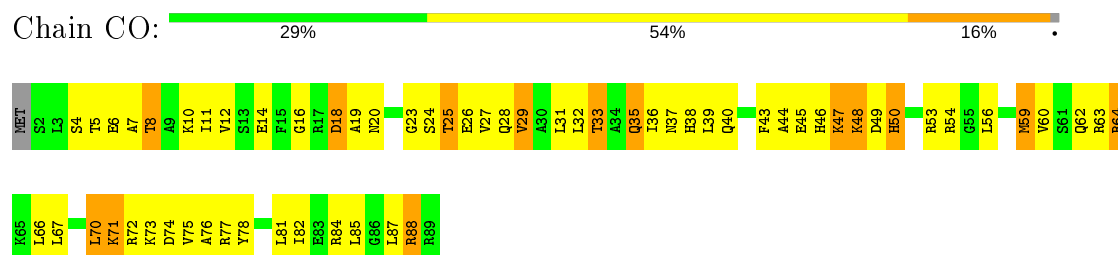
• Molecule 19: 30S ribosomal protein S21



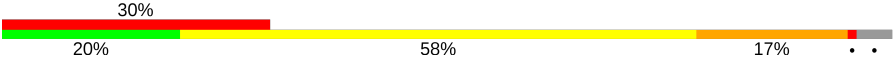
• Molecule 20: 30S ribosomal protein S15

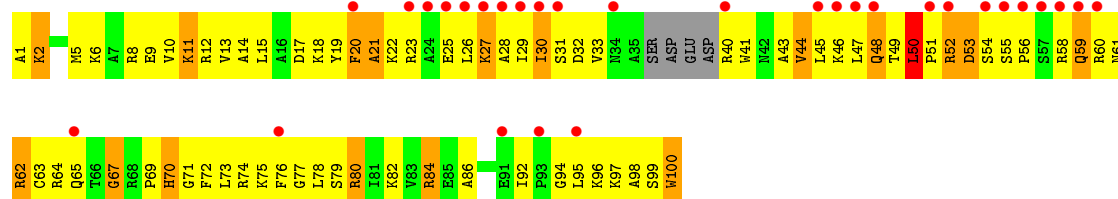


• Molecule 20: 30S ribosomal protein S15



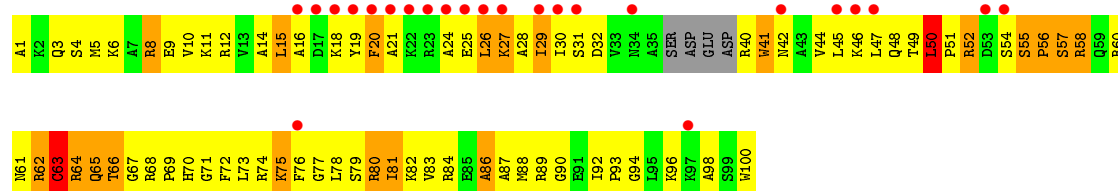
• Molecule 21: 30S ribosomal protein S14

Chain AN: 



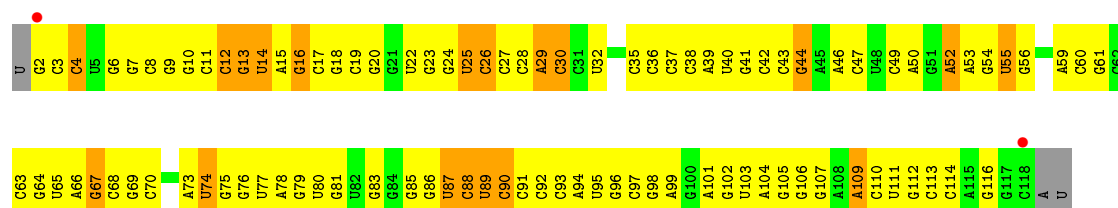
- Molecule 21: 30S ribosomal protein S14

Chain CN: 



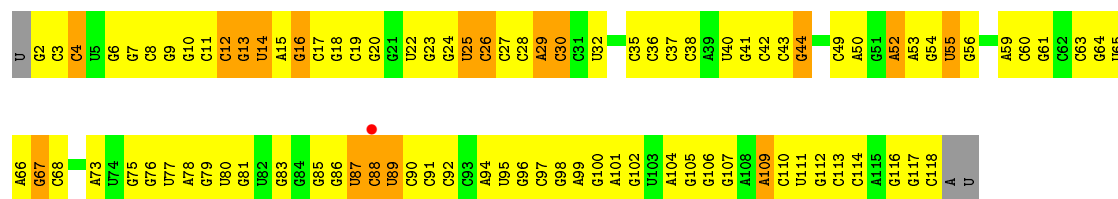
- Molecule 22: 5S rRNA

Chain BA: 



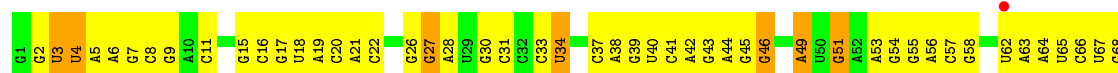
- Molecule 22: 5S rRNA

Chain DA: 



- Molecule 23: 23S rRNA

Chain BB: 

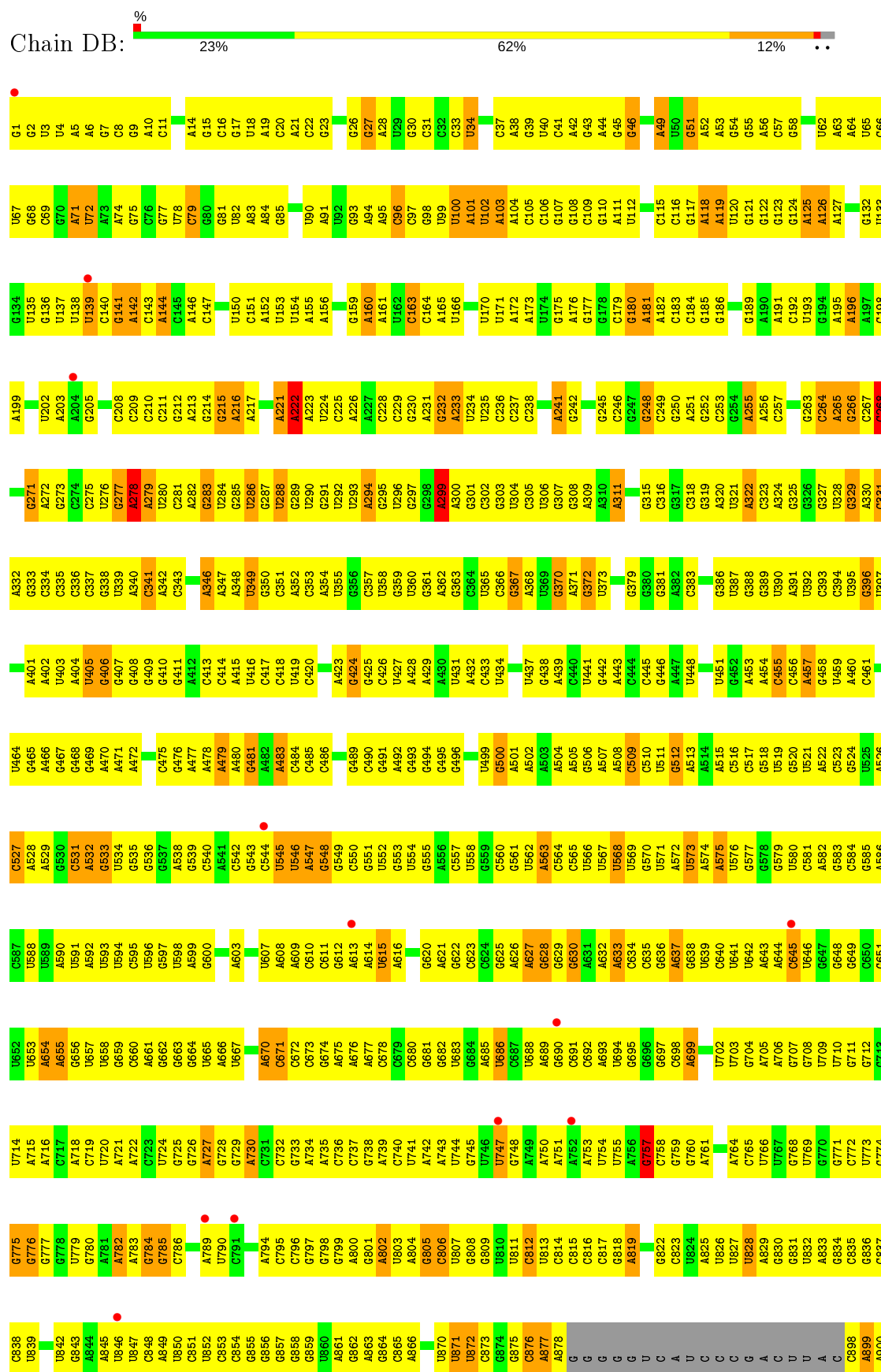


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	G914	C851	C786	G723	C860	U598	A538	C475	A412	A342	U277	C209	C144	U78
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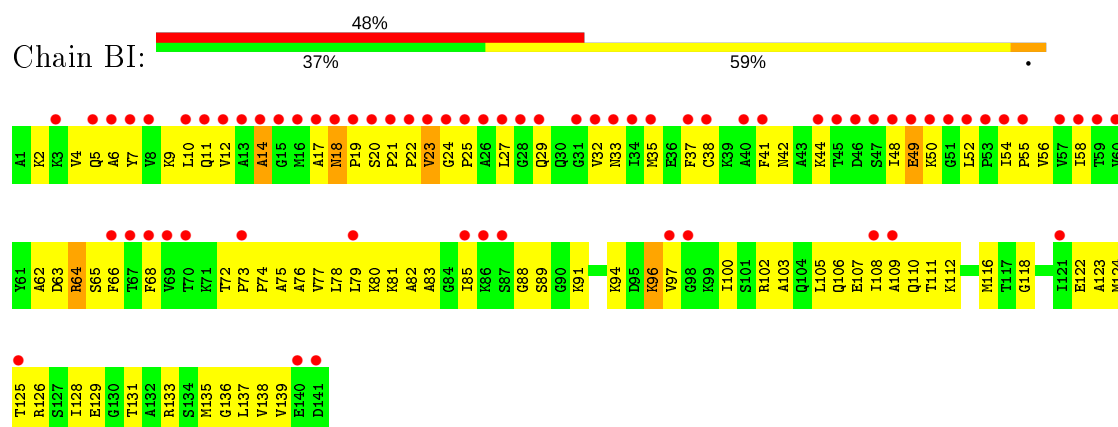


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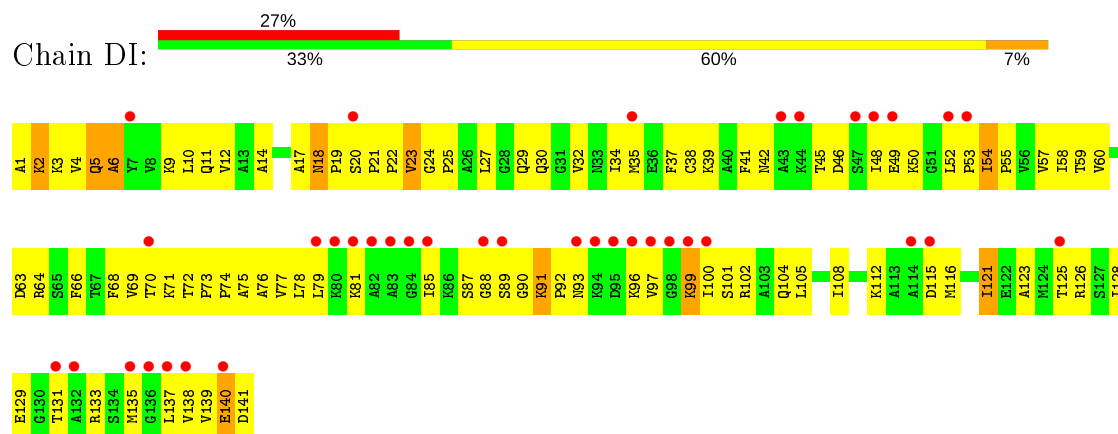
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A2748	G2665	G2665	U2532	U2526	U2463	C2395	G2332	G2269	C2207	G2145	C2078	G2012	A1938	A1872
G2749	G2666	G2666	U2533	U2527	U2464	C2396	A2333	A2270	U2210	C2146	U2079	G2013	U1939	G1873
U2751	G2667	G2667	U2534	U2528	U2465	C2397	U2334	G2271	A2211	A2147	A2080	A2014	U1940	C1874
G2752	G2668	G2668	U2535	U2529	U2466	C2398	A2335	U2272	A2212	G2148	U2081	A2015	U1941	G1875
A2753	G2669	G2669	U2536	U2530	U2467	C2399	A2336	A2273	A2213	U2149	A2082	G2016	U1942	A1876
U2754	G2670	G2670	U2537	U2531	U2468	C2400	U2337	G2274	C2214	U2150	U2085	G2017	U1943	A1877
G2755	G2671	G2671	U2538	U2532	U2469	C2401	A2338	G2275	G2215	U2151	U2086	A2018	G1945	G1878
A2756	G2672	G2672	U2539	U2533	U2470	C2402	U2339	G2276	G2216	G2152	U2087	C2021	U1946	C1879
U2757	G2673	G2673	U2540	U2534	U2471	C2403	A2340	G2277	G2217	C2153	A2088	U2022	G1947	G1884
G2758	G2674	G2674	U2541	U2535	U2472	C2404	U2341	G2278	G2218	A2154				
A2759	G2675	G2675	U2542	U2536	U2473	C2405	U2342	G2279						
G2760	G2676	G2676	U2543	U2537	U2474	C2406	U2343	G2280						
U2761	G2677	G2677	U2544	U2538	U2475	C2407	U2344							
A2762	G2678	G2678	U2545	U2539	U2476	U2408	U2345							



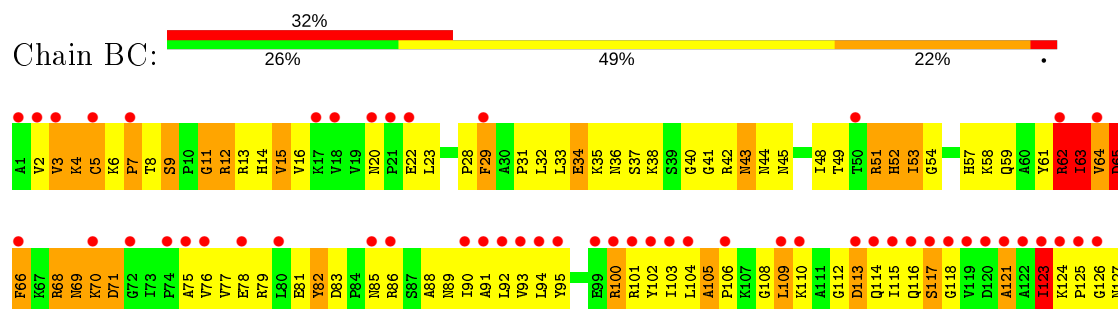
• Molecule 24: 50S ribosomal protein L11

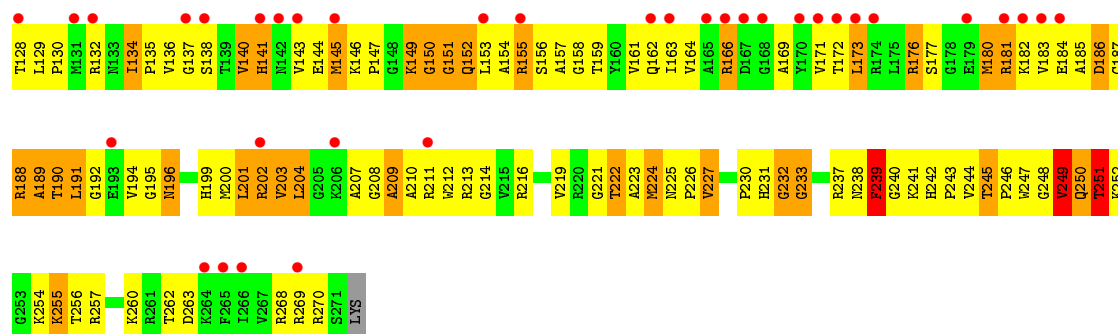


• Molecule 24: 50S ribosomal protein L11

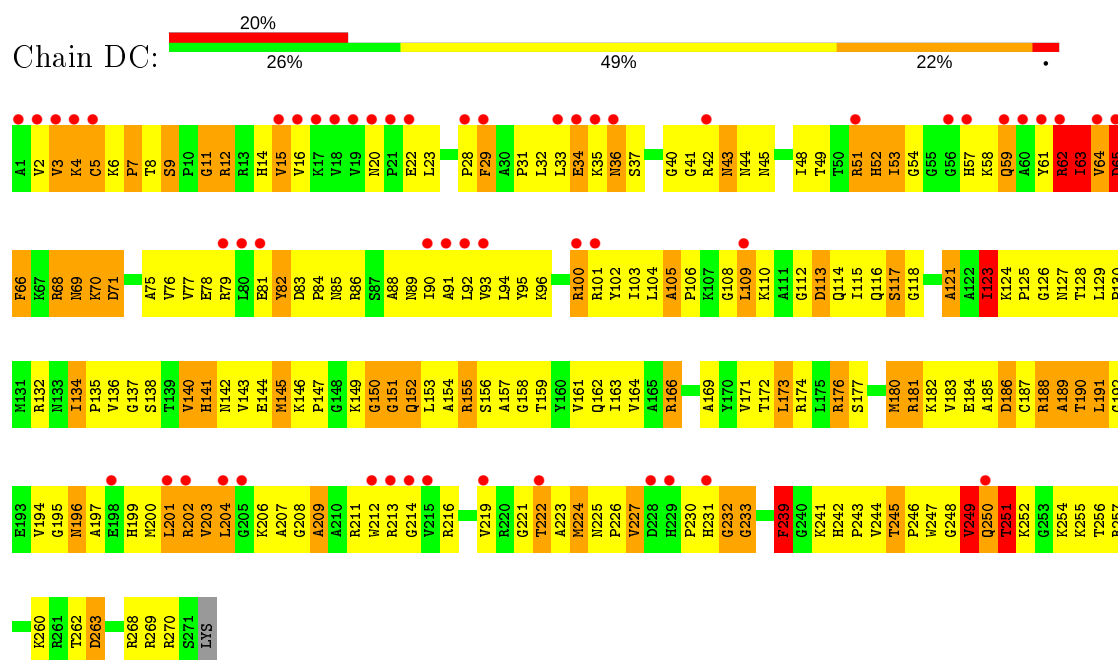


• Molecule 25: 50S ribosomal protein L2

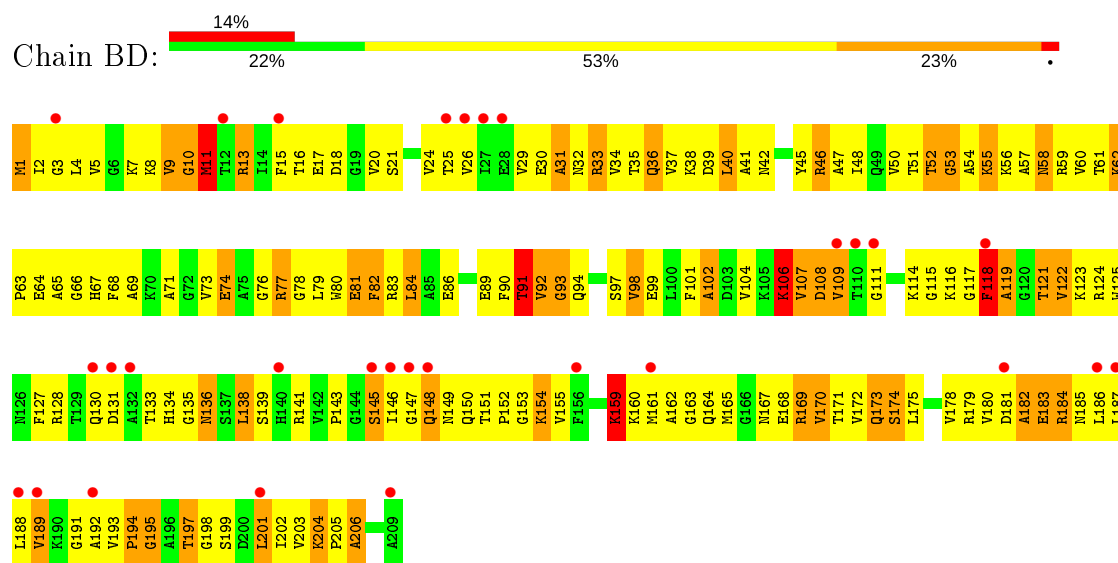




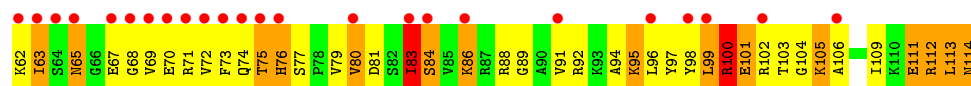
• Molecule 25: 50S ribosomal protein L2



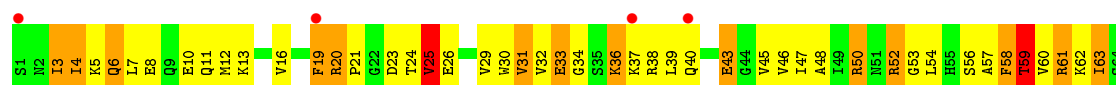
• Molecule 26: 50S ribosomal protein L3



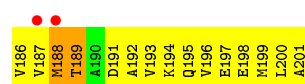
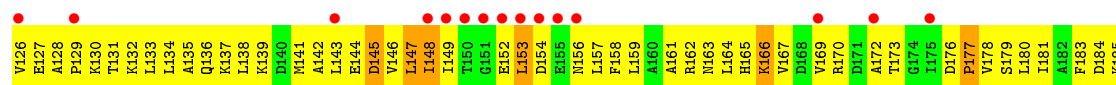
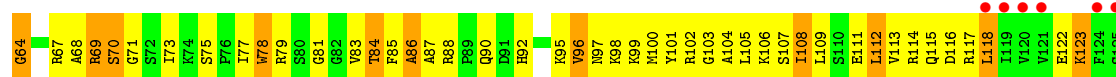
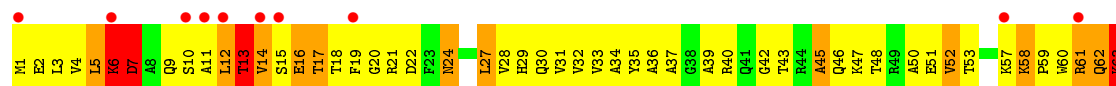
• Molecule 26: 50S ribosomal protein L3



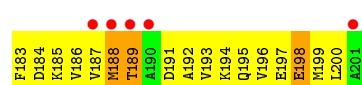
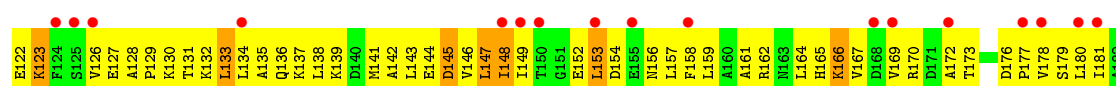
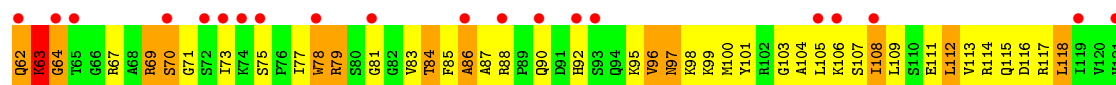
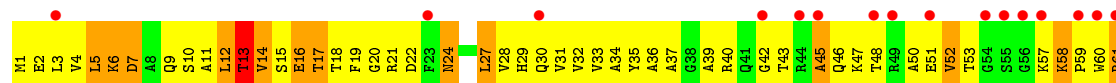
• Molecule 28: 50S ribosomal protein L19



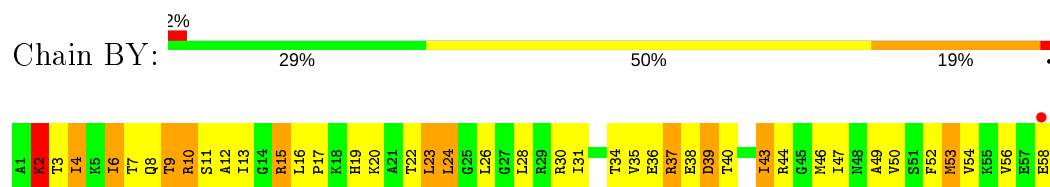
• Molecule 29: 50S ribosomal protein L4



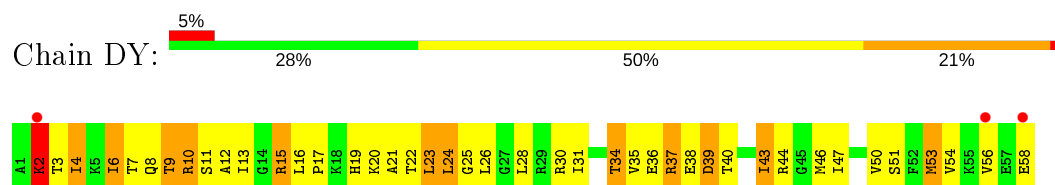
• Molecule 29: 50S ribosomal protein L4



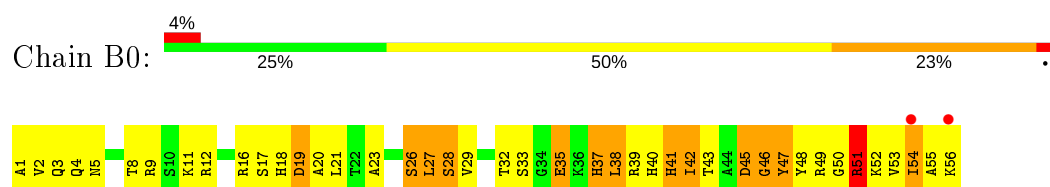
- Molecule 30: 50S ribosomal protein L30



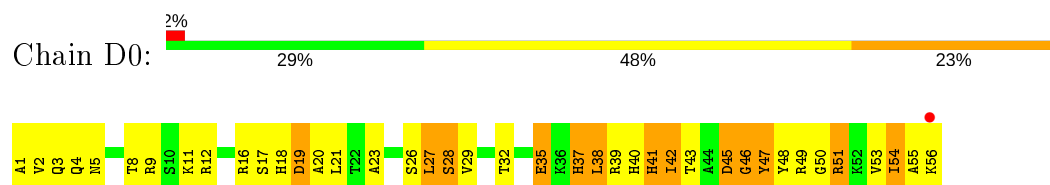
- Molecule 30: 50S ribosomal protein L30



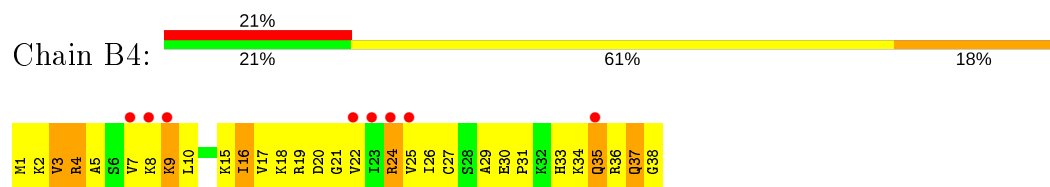
- Molecule 31: 50S ribosomal protein L32



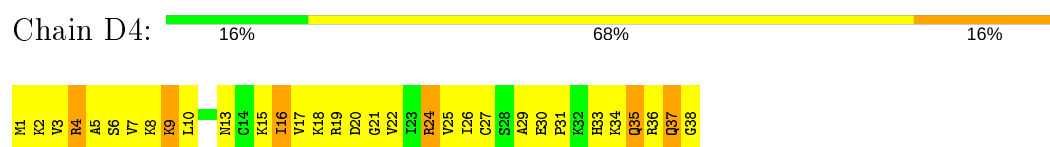
- Molecule 31: 50S ribosomal protein L32



- 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

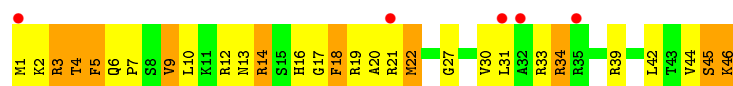


- Molecule 35: 50S ribosomal protein L25

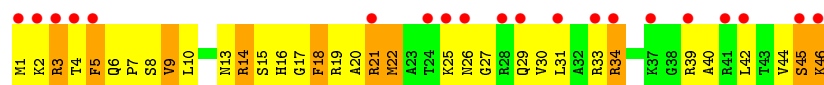


- Molecule 36: 50S ribosomal protein L34

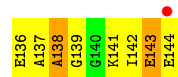
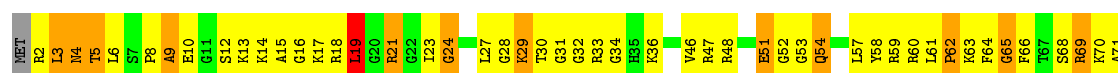




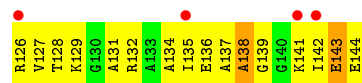
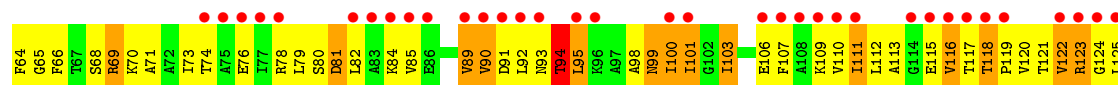
• Molecule 36: 50S ribosomal protein L34



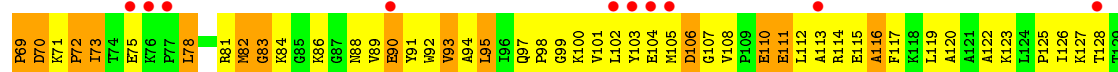
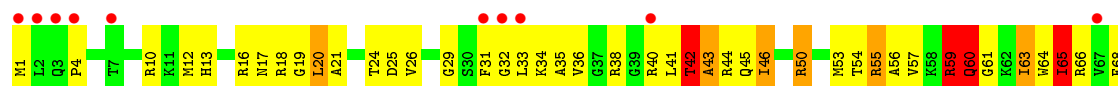
• Molecule 37: 50S ribosomal protein L15

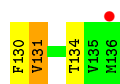


• Molecule 37: 50S ribosomal protein L15

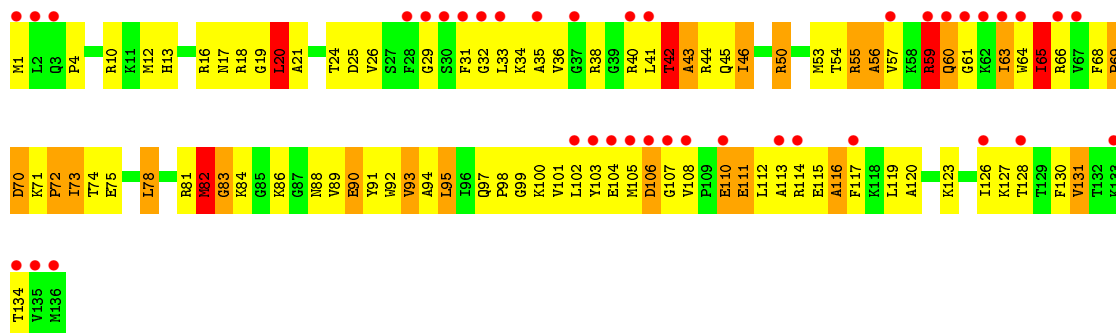


• Molecule 38: 50S ribosomal protein L16





• Molecule 38: 50S ribosomal protein L16



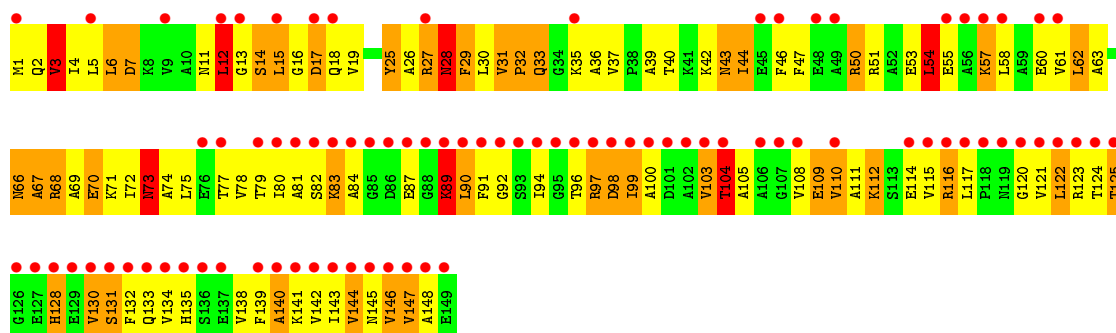
• Molecule 39: 50S ribosomal protein L29



• Molecule 39: 50S ribosomal protein L29

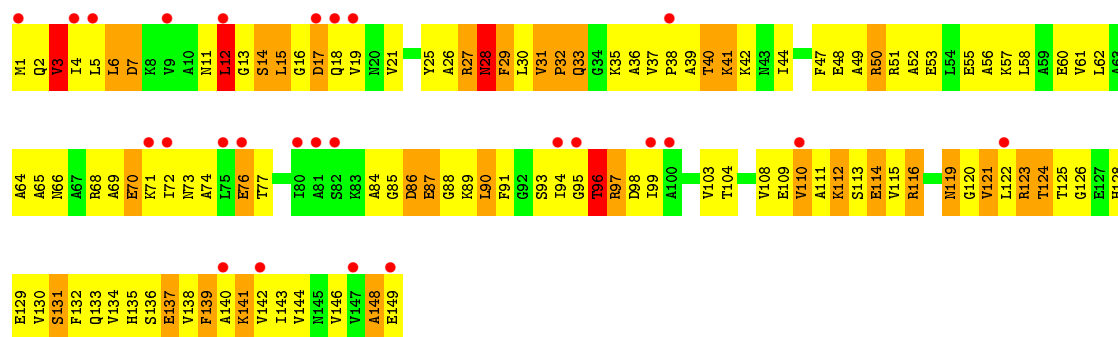


• Molecule 40: 50S ribosomal protein L9

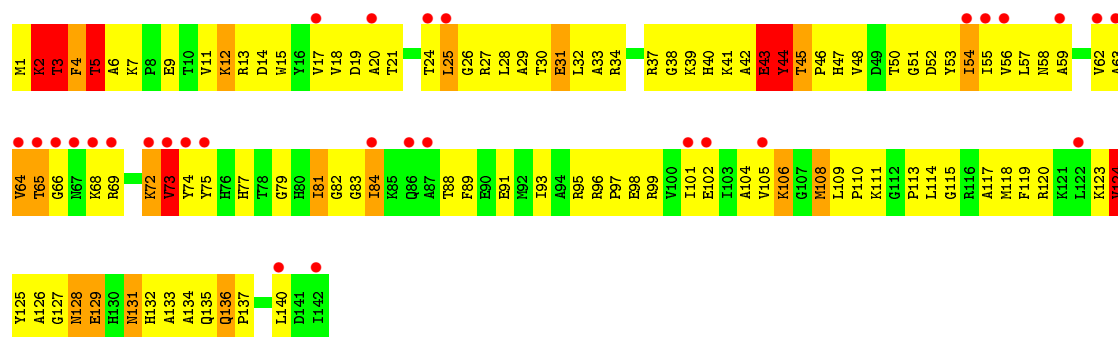


• Molecule 40: 50S ribosomal protein L9

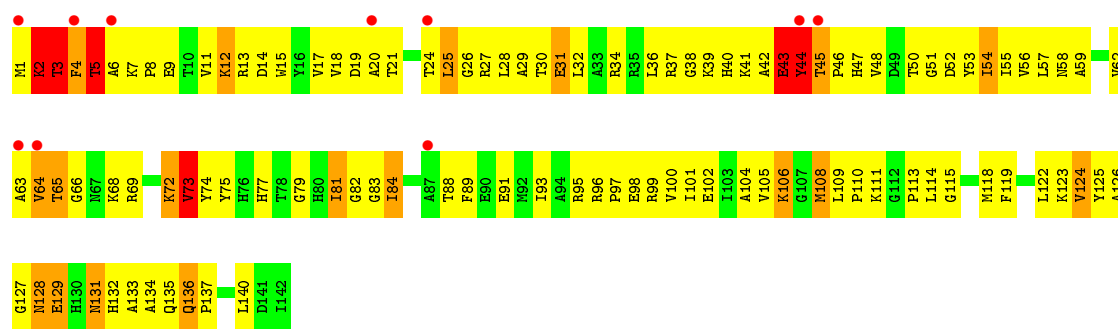




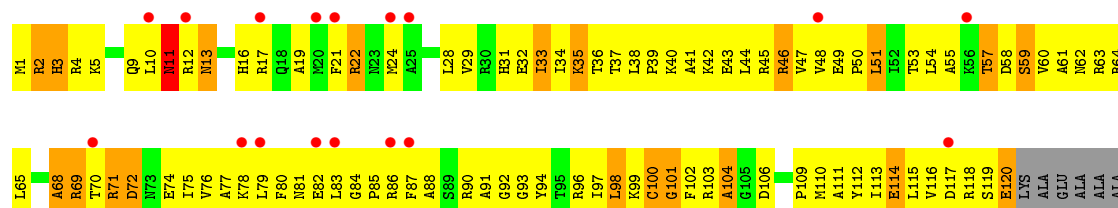
● Molecule 41: 50S ribosomal protein L13



● Molecule 41: 50S ribosomal protein L13



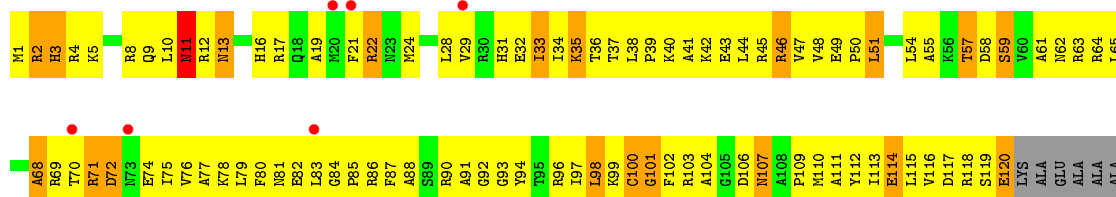
● Molecule 42: 50S ribosomal protein L17



GLU

- Molecule 42: 50S ribosomal protein L17

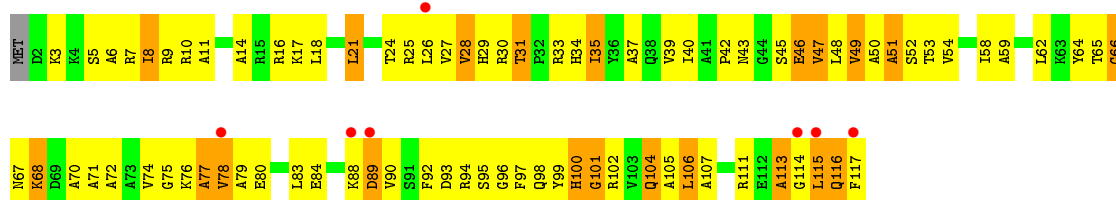
Chain DN: 5% 17% 61% 15% 6%



GLU

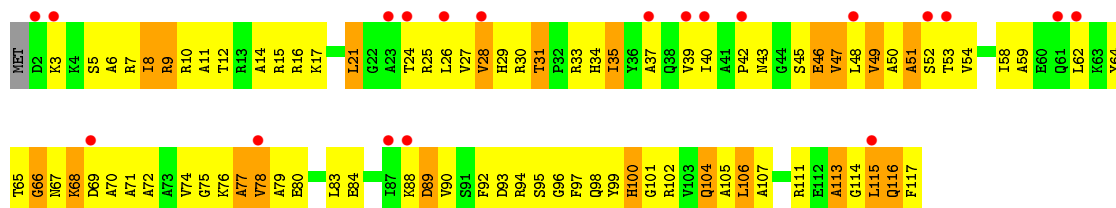
- Molecule 43: 50S ribosomal protein L18

Chain BO: 6% 28% 53% 18%



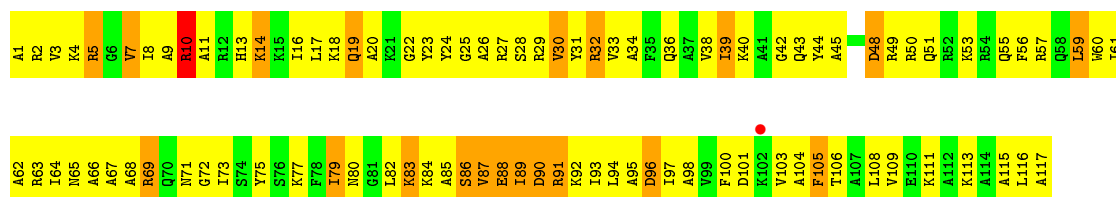
- Molecule 43: 50S ribosomal protein L18

Chain DO: 17% 26% 55% 18%

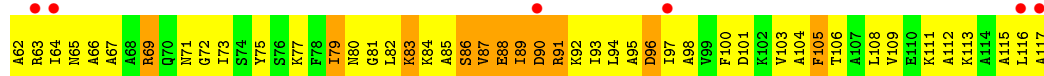
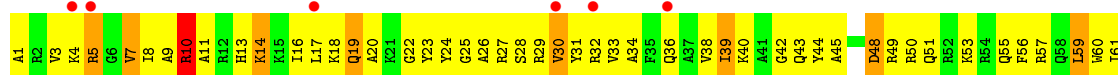


- Molecule 44: 50S ribosomal protein L20

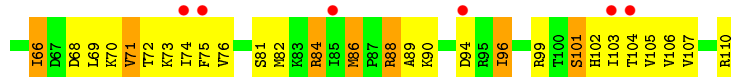
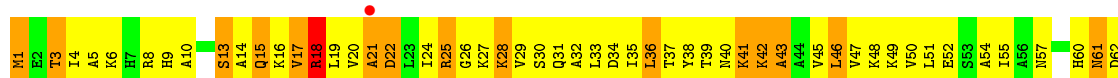
Chain BQ: 20% 62% 17%



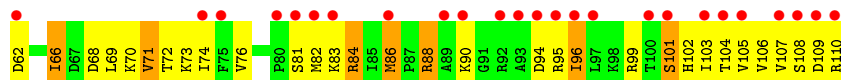
- Molecule 44: 50S ribosomal protein L20



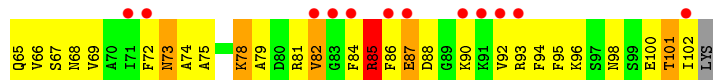
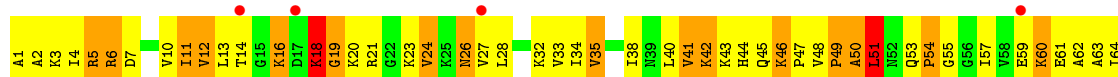
• Molecule 45: 50S ribosomal protein L22



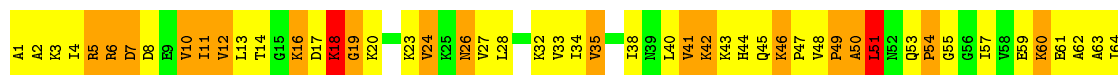
• Molecule 45: 50S ribosomal protein L22

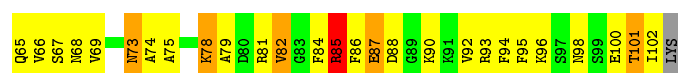


• Molecule 46: 50S ribosomal protein L24

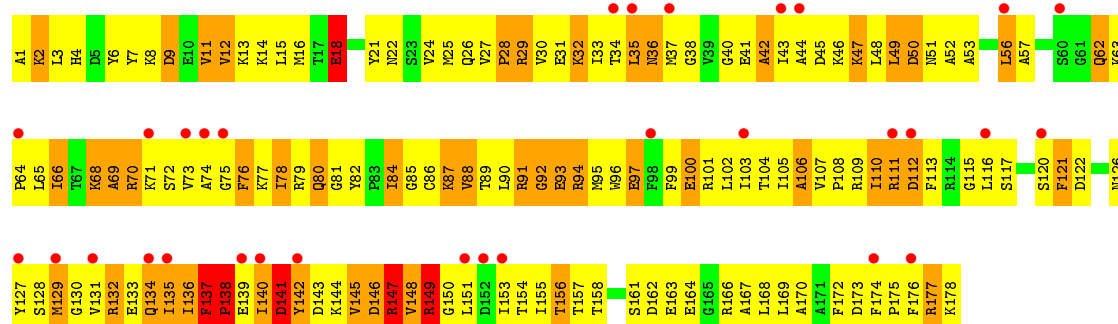
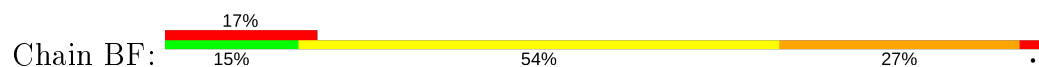


• Molecule 46: 50S ribosomal protein L24

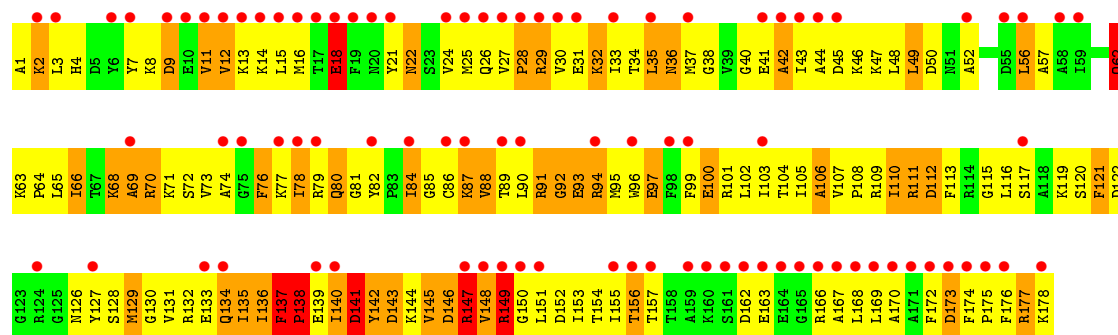
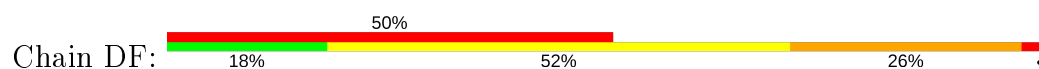




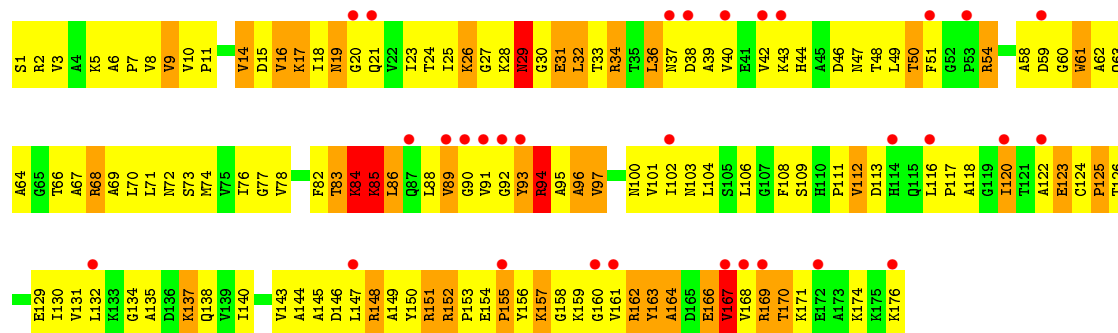
• Molecule 47: 50S ribosomal protein L5



• Molecule 47: 50S ribosomal protein L5

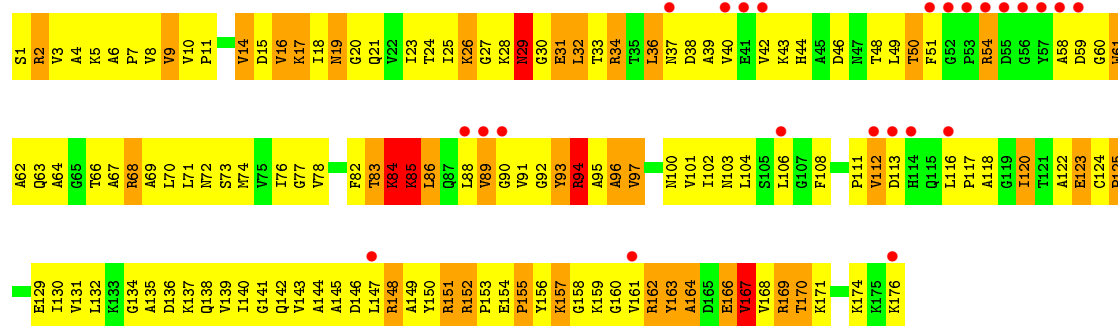


• Molecule 48: 50S ribosomal protein L6

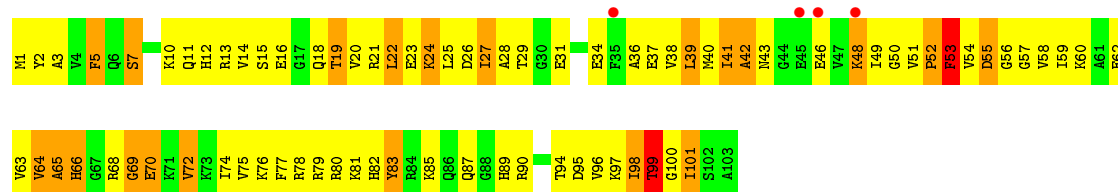


• Molecule 48: 50S ribosomal protein L6

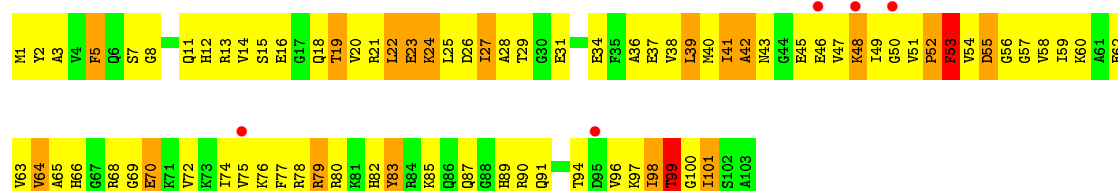




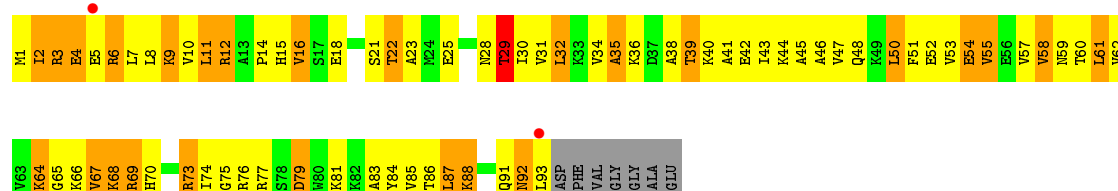
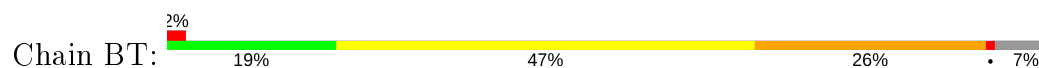
• Molecule 49: 50S ribosomal protein L21



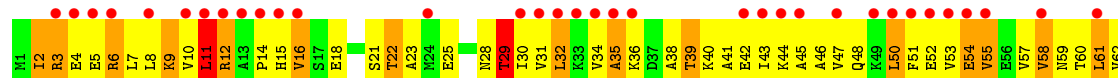
• Molecule 49: 50S ribosomal protein L21



• Molecule 50: 50S ribosomal protein L23

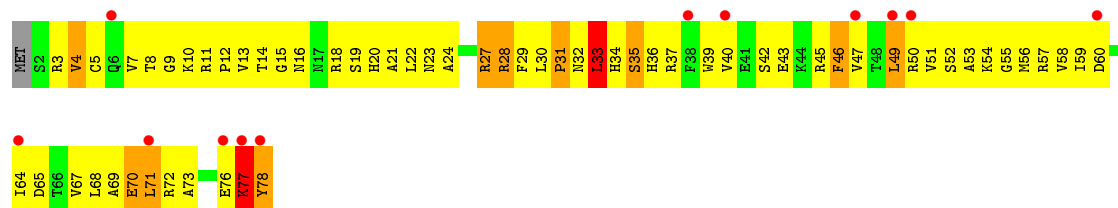


• Molecule 50: 50S ribosomal protein L23

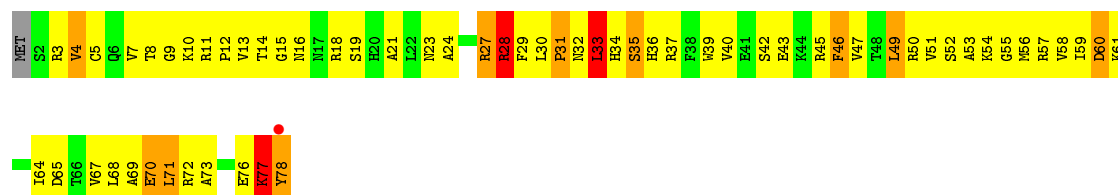




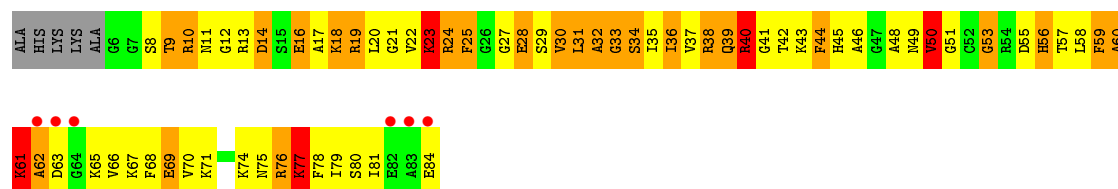
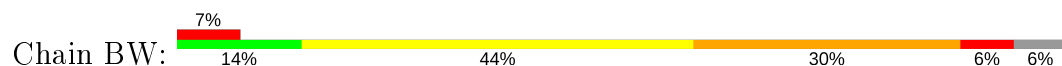
- Molecule 51: 50S ribosomal protein L28



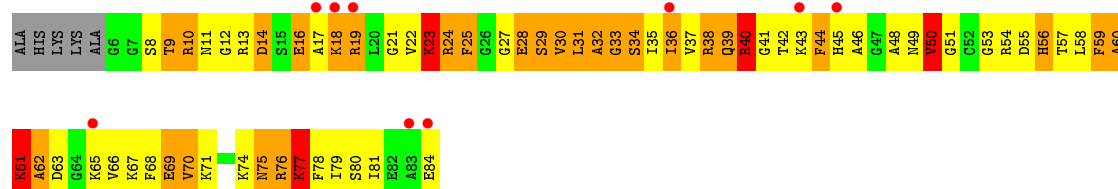
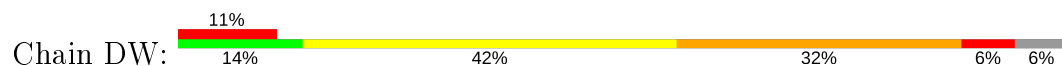
- Molecule 51: 50S ribosomal protein L28



- 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 0.224 , 0.271	Depositor DCC
R_{free} test set	19247 reflections (4.92%)	wwPDB-VP
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

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

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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

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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

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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

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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 2
2	CC	204/232 (88%)	134 (66%)	48 (24%)	22 (11%)	0 8

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DZ	75/78 (96%)	54 (72%)	14 (19%)	7 (9%)	0	11
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	5

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%)	1	11
2	CC	170/189 (90%)	134 (79%)	36 (21%)	1	6
3	AD	172/172 (100%)	145 (84%)	27 (16%)	2	16
3	CD	172/172 (100%)	146 (85%)	26 (15%)	3	17
4	AE	113/125 (90%)	93 (82%)	20 (18%)	2	12
4	CE	113/125 (90%)	93 (82%)	20 (18%)	2	12
5	AF	87/116 (75%)	76 (87%)	11 (13%)	4	22
5	CF	87/116 (75%)	75 (86%)	12 (14%)	3	21
6	AG	123/146 (84%)	102 (83%)	21 (17%)	2	13
6	CG	125/146 (86%)	98 (78%)	27 (22%)	1	6
7	AH	104/104 (100%)	95 (91%)	9 (9%)	10	35
7	CH	104/104 (100%)	95 (91%)	9 (9%)	10	35
8	AI	105/106 (99%)	78 (74%)	27 (26%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	79 (75%)	26 (25%)	0	4
9	AJ	86/90 (96%)	73 (85%)	13 (15%)	3	17
9	CJ	86/90 (96%)	72 (84%)	14 (16%)	2	15
10	AK	90/98 (92%)	73 (81%)	17 (19%)	1	10
10	CK	90/98 (92%)	73 (81%)	17 (19%)	1	10
11	AL	103/103 (100%)	87 (84%)	16 (16%)	2	17
11	CL	103/103 (100%)	87 (84%)	16 (16%)	2	17
12	AM	92/95 (97%)	72 (78%)	20 (22%)	1	6
12	CM	91/95 (96%)	75 (82%)	16 (18%)	2	12
13	AP	65/65 (100%)	61 (94%)	4 (6%)	18	46
13	CP	65/65 (100%)	61 (94%)	4 (6%)	18	46
14	AQ	74/77 (96%)	63 (85%)	11 (15%)	3	18
14	CQ	75/77 (97%)	63 (84%)	12 (16%)	2	16
15	AR	48/64 (75%)	41 (85%)	7 (15%)	3	18
15	CR	48/64 (75%)	40 (83%)	8 (17%)	2	14
16	AS	70/78 (90%)	49 (70%)	21 (30%)	0	2
16	CS	71/78 (91%)	51 (72%)	20 (28%)	0	2
17	AT	65/65 (100%)	51 (78%)	14 (22%)	1	6
17	CT	65/65 (100%)	51 (78%)	14 (22%)	1	6
18	AB	180/198 (91%)	141 (78%)	39 (22%)	1	6
18	CB	180/198 (91%)	133 (74%)	47 (26%)	0	4
19	AU	44/60 (73%)	31 (70%)	13 (30%)	0	2
19	CU	44/60 (73%)	32 (73%)	12 (27%)	0	3
20	AO	76/77 (99%)	65 (86%)	11 (14%)	3	19
20	CO	76/77 (99%)	61 (80%)	15 (20%)	1	8
21	AN	79/83 (95%)	63 (80%)	16 (20%)	1	7
21	CN	79/83 (95%)	64 (81%)	15 (19%)	1	9
24	BI	109/109 (100%)	108 (99%)	1 (1%)	78	87
24	DI	109/109 (100%)	103 (94%)	6 (6%)	21	50
25	BC	216/217 (100%)	180 (83%)	36 (17%)	2	14
25	DC	216/217 (100%)	181 (84%)	35 (16%)	2	15

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DJ	116/116 (100%)	96 (83%)	20 (17%)	2	13
42	BN	100/103 (97%)	87 (87%)	13 (13%)	4	22
42	DN	100/103 (97%)	87 (87%)	13 (13%)	4	22
43	BO	86/87 (99%)	72 (84%)	14 (16%)	2	15
43	DO	86/87 (99%)	72 (84%)	14 (16%)	2	15
44	BQ	89/89 (100%)	74 (83%)	15 (17%)	2	14
44	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	14
45	BS	93/93 (100%)	80 (86%)	13 (14%)	3	20
45	DS	93/93 (100%)	80 (86%)	13 (14%)	3	20
46	BU	83/84 (99%)	69 (83%)	14 (17%)	2	14
46	DU	83/84 (99%)	69 (83%)	14 (17%)	2	14
47	BF	149/149 (100%)	117 (78%)	32 (22%)	1	6
47	DF	149/149 (100%)	116 (78%)	33 (22%)	1	6
48	BG	137/137 (100%)	112 (82%)	25 (18%)	1	11
48	DG	137/137 (100%)	112 (82%)	25 (18%)	1	11
49	BR	84/84 (100%)	71 (84%)	13 (16%)	2	17
49	DR	84/84 (100%)	73 (87%)	11 (13%)	4	22
50	BT	80/84 (95%)	59 (74%)	21 (26%)	0	4
50	DT	80/84 (95%)	60 (75%)	20 (25%)	0	4
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	7
51	DZ	67/68 (98%)	53 (79%)	14 (21%)	1	7
52	BW	59/62 (95%)	42 (71%)	17 (29%)	0	2
52	DW	59/62 (95%)	42 (71%)	17 (29%)	0	2
All	All	9333/9700 (96%)	7661 (82%)	1672 (18%)	2	12

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%)	25 (1%)
1	CA	1529/1542 (99%)	282 (18%)	21 (1%)
22	BA	116/120 (96%)	21 (18%)	1 (0%)
22	DA	116/120 (96%)	19 (16%)	1 (0%)
23	BB	2837/2904 (97%)	456 (16%)	18 (0%)
23	DB	2837/2904 (97%)	469 (16%)	20 (0%)
All	All	8964/9132 (98%)	1539 (17%)	86 (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

5 of 86 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2425	A
1	CA	279	A
23	DB	2336	A
23	BB	2430	A
23	BB	2894	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	CA	1659	-	23,25,25	1.61	6 (26%)	26,39,39	1.32	2 (7%)
54	SCM	AA	1661	-	23,25,25	1.66	8 (34%)	26,39,39	1.32	2 (7%)

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	CA	1659	-	-	2/4/57/57	0/3/3/3
54	SCM	AA	1661	-	-	2/4/57/57	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	CA	1659	SCM	C9-C8	3.10	1.59	1.53
54	AA	1661	SCM	C3-C2	3.03	1.58	1.51
54	AA	1661	SCM	C9-C8	2.91	1.58	1.53
54	CA	1659	SCM	C3-C2	2.82	1.57	1.51
54	AA	1661	SCM	C3-C4	2.56	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	1661	SCM	C1M-N10-C10	-4.88	107.28	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	1659	SCM	C1M-N10-C10	-4.55	107.76	114.38
54	CA	1659	SCM	C2M-C2-C3	-2.62	108.11	113.22
54	AA	1661	SCM	C2M-C2-C3	-2.42	108.49	113.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	AA	1661	SCM	C9-C10-N10-C1M
54	AA	1661	SCM	C11-C10-N10-C1M
54	CA	1659	SCM	C11-C10-N10-C1M
54	CA	1659	SCM	C9-C10-N10-C1M

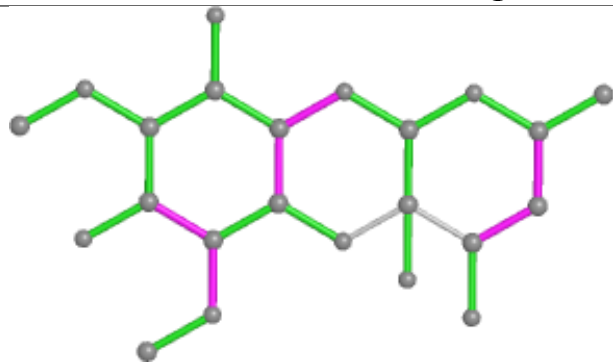
There are no ring outliers.

2 monomers are involved in 3 short contacts:

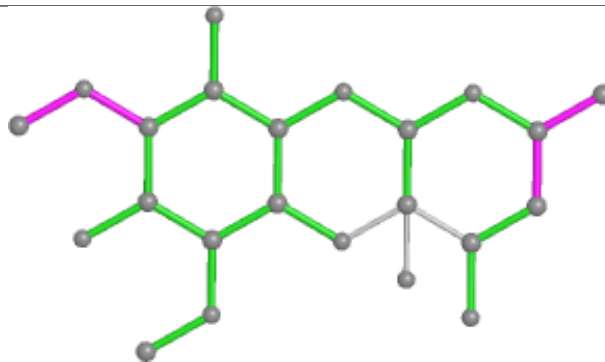
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	CA	1659	SCM	1	0
54	AA	1661	SCM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

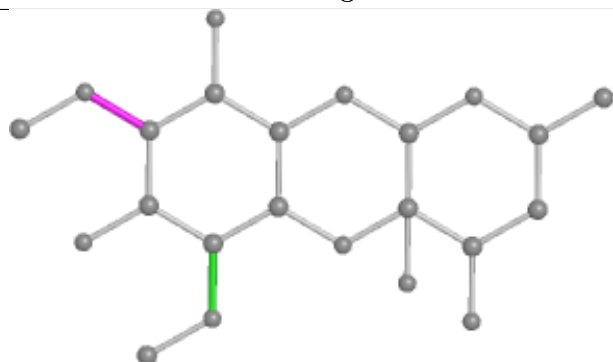
Ligand SCM CA 1659



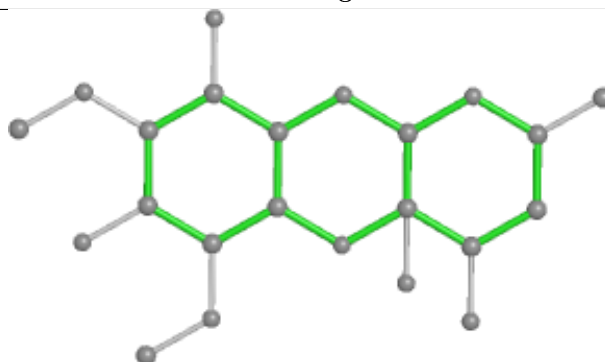
Bond lengths



Bond angles

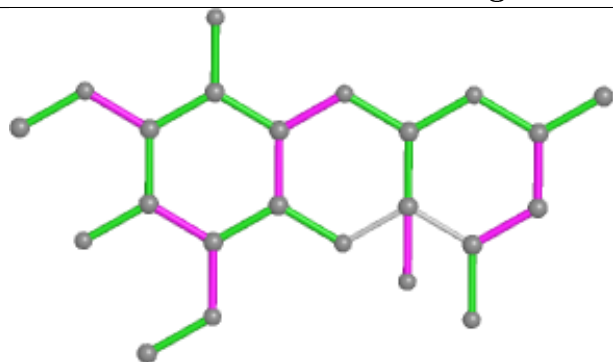


Torsions

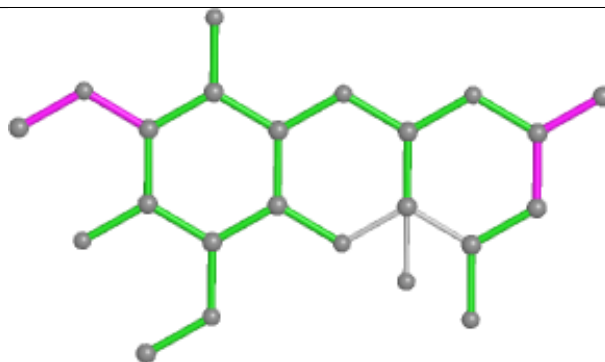


Rings

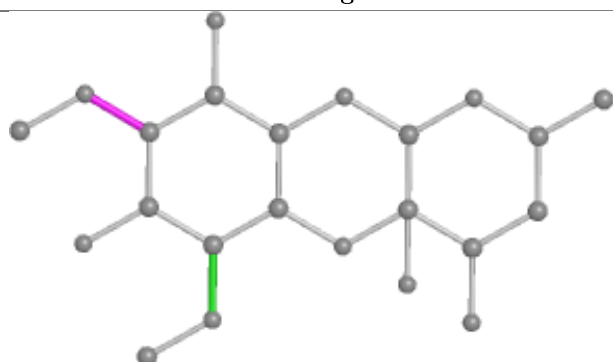
Ligand SCM AA 1661



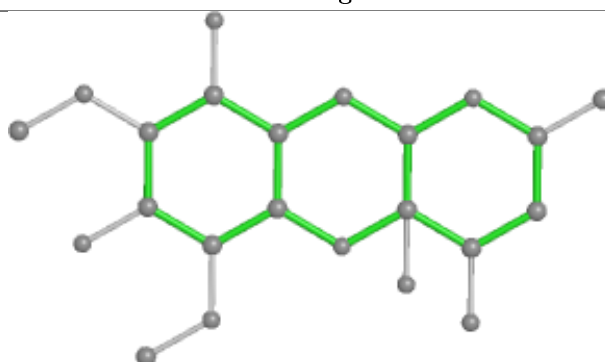
Bond lengths



Bond angles



Torsions



Rings

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%) 15 12	5, 70, 115, 162	0
2	CC	206/232 (88%)	0.53	28 (13%) 3 3	5, 71, 111, 150	0
3	AD	205/205 (100%)	-0.05	12 (5%) 22 18	5, 79, 127, 173	0
3	CD	205/205 (100%)	0.57	20 (9%) 7 7	5, 66, 125, 166	0
4	AE	150/166 (90%)	0.06	4 (2%) 54 44	5, 68, 122, 157	0
4	CE	150/166 (90%)	1.49	51 (34%) 0 0	5, 67, 121, 180	0
5	AF	100/135 (74%)	2.52	62 (62%) 0 0	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	28 (18%) 1 1	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 1	5, 62, 116, 158	0
8	AI	127/129 (98%)	0.76	24 (18%) 1 1	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%) 37 30	9, 79, 126, 147	0
9	CJ	98/103 (95%)	1.28	29 (29%) 0 0	16, 82, 113, 137	0
10	AK	117/128 (91%)	0.23	4 (3%) 45 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%) 0 0	6, 79, 123, 158	0
11	CL	123/123 (100%)	0.26	6 (4%) 29 25	5, 54, 103, 151	0
12	AM	114/117 (97%)	0.95	22 (19%) 1 1	23, 96, 137, 169	0
12	CM	113/117 (96%)	-0.21	5 (4%) 34 29	22, 96, 142, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	82/82 (100%)	1.48	25 (30%) 0 0	15, 82, 130, 163	0
13	CP	80/82 (97%)	0.05	5 (6%) 20 16	5, 58, 126, 180	0
14	AQ	80/83 (96%)	1.25	23 (28%) 0 0	15, 92, 145, 154	0
14	CQ	81/83 (97%)	0.26	3 (3%) 41 33	5, 72, 119, 149	0
15	AR	55/74 (74%)	0.81	8 (14%) 2 3	5, 73, 129, 164	0
15	CR	55/74 (74%)	0.23	3 (5%) 25 22	5, 66, 127, 143	0
16	AS	79/91 (86%)	1.98	39 (49%) 0 0	52, 98, 142, 167	0
16	CS	80/91 (87%)	0.50	13 (16%) 1 2	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%) 32 27	12, 81, 120, 160	0
18	CB	218/240 (90%)	0.92	50 (22%) 0 0	5, 87, 133, 163	0
19	AU	51/70 (72%)	0.78	8 (15%) 2 2	20, 94, 139, 153	0
19	CU	51/70 (72%)	0.11	2 (3%) 39 31	57, 96, 137, 171	0
20	AO	88/89 (98%)	1.00	11 (12%) 3 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 0	5, 84, 128, 155	0
21	CN	96/100 (96%)	1.13	24 (25%) 0 0	5, 75, 129, 145	0
22	BA	117/120 (97%)	0.07	2 (1%) 70 60	35, 77, 125, 167	0
22	DA	117/120 (97%)	-0.56	1 (0%) 84 77	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 0	60, 135, 178, 180	0
24	DI	141/141 (100%)	1.29	38 (26%) 0 0	66, 135, 180, 180	0
25	BC	271/272 (99%)	1.41	88 (32%) 0 0	5, 61, 109, 132	0
25	DC	271/272 (99%)	0.80	54 (19%) 1 1	5, 45, 99, 144	0
26	BD	209/209 (100%)	0.49	29 (13%) 2 3	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	65 (53%) 0 0	5, 75, 125, 159	0
27	DK	121/123 (98%)	1.05	27 (22%) 0 1	5, 45, 112, 150	0
28	BP	114/114 (100%)	1.54	47 (41%) 0 0	7, 82, 125, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.40	6 (5%) 26 23	5, 64, 118, 139	0
29	BE	201/201 (100%)	0.81	33 (16%) 1 2	5, 65, 128, 164	0
29	DE	201/201 (100%)	1.23	58 (28%) 0 0	5, 73, 123, 160	0
30	BY	58/58 (100%)	-0.26	1 (1%) 70 60	5, 75, 129, 160	0
30	DY	58/58 (100%)	-0.23	3 (5%) 27 24	5, 72, 116, 147	0
31	B0	56/56 (100%)	0.04	2 (3%) 42 34	5, 78, 118, 147	0
31	D0	56/56 (100%)	0.18	1 (1%) 68 60	5, 62, 129, 153	0
32	B4	38/38 (100%)	0.95	8 (21%) 1 1	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%) 12 11	17, 70, 120, 134	0
33	D1	50/54 (92%)	0.34	5 (10%) 7 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	22 (34%) 0 0	5, 55, 86, 122	0
35	BV	94/94 (100%)	0.64	14 (14%) 2 3	5, 81, 126, 152	0
35	DV	94/94 (100%)	0.94	21 (22%) 0 1	5, 88, 120, 160	0
36	B2	46/46 (100%)	0.77	5 (10%) 5 5	5, 53, 104, 141	0
36	D2	46/46 (100%)	1.64	20 (43%) 0 0	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	57 (39%) 0 0	5, 63, 111, 145	0
38	BM	136/136 (100%)	0.91	21 (15%) 2 2	7, 68, 121, 179	0
38	DM	136/136 (100%)	1.31	39 (28%) 0 0	5, 65, 117, 144	0
39	BX	63/63 (100%)	1.00	13 (20%) 1 1	16, 79, 128, 159	0
39	DX	63/63 (100%)	1.09	9 (14%) 2 3	16, 91, 144, 169	0
40	BH	149/149 (100%)	3.05	87 (58%) 0 0	7, 104, 149, 180	0
40	DH	149/149 (100%)	0.85	26 (17%) 1 2	5, 91, 131, 162	0
41	BJ	142/142 (100%)	0.94	29 (20%) 1 1	5, 77, 118, 140	0
41	DJ	142/142 (100%)	0.27	10 (7%) 16 13	5, 70, 119, 173	0
42	BN	120/127 (94%)	0.84	17 (14%) 2 3	5, 69, 111, 154	0
42	DN	120/127 (94%)	0.02	6 (5%) 28 25	5, 51, 94, 163	0
43	BO	116/117 (99%)	-0.08	7 (6%) 21 17	6, 80, 109, 172	0
43	DO	116/117 (99%)	0.90	20 (17%) 1 2	5, 83, 136, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	-0.62	1 (0%) 84 77	5, 62, 115, 144	0
44	DQ	117/117 (100%)	0.46	12 (10%) 6 6	5, 60, 111, 154	0
45	BS	110/110 (100%)	0.39	7 (6%) 19 15	5, 62, 121, 148	0
45	DS	110/110 (100%)	1.42	36 (32%) 0 0	5, 64, 127, 156	0
46	BU	102/103 (99%)	0.84	16 (15%) 2 2	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%) 1 2	29, 100, 146, 180	0
47	DF	178/178 (100%)	2.23	89 (50%) 0 0	12, 93, 142, 163	0
48	BG	176/176 (100%)	0.76	31 (17%) 1 2	18, 94, 133, 171	0
48	DG	176/176 (100%)	0.40	24 (13%) 3 3	8, 90, 136, 166	0
49	BR	103/103 (100%)	-0.03	4 (3%) 39 31	5, 83, 123, 133	0
49	DR	103/103 (100%)	0.13	5 (4%) 29 25	10, 76, 135, 149	0
50	BT	93/100 (93%)	-0.07	2 (2%) 62 52	8, 83, 130, 165	0
50	DT	93/100 (93%)	2.27	51 (54%) 0 0	5, 84, 144, 172	0
51	BZ	77/78 (98%)	0.57	12 (15%) 2 2	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%) 13 12	5, 75, 124, 180	0
52	DW	79/84 (94%)	0.69	9 (11%) 5 5	5, 71, 121, 166	0
All	All	20417/21046 (97%)	0.14	2041 (9%) 7 7	5, 70, 134, 180	0

The worst 5 of 2041 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	BI	17	ALA	14.4
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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	AA	1608	1/1	0.56	0.13	123,123,123,123	0
53	MG	BB	3042	1/1	0.60	0.23	92,92,92,92	0
53	MG	BB	3097	1/1	0.60	0.07	113,113,113,113	0
53	MG	AA	1622	1/1	0.70	0.34	130,130,130,130	0
53	MG	AA	1624	1/1	0.70	0.24	83,83,83,83	0
53	MG	DB	3052	1/1	0.77	0.29	105,105,105,105	0
53	MG	DB	3058	1/1	0.77	0.09	139,139,139,139	0
53	MG	AA	1635	1/1	0.77	0.15	80,80,80,80	0
53	MG	AA	1620	1/1	0.79	0.06	60,60,60,60	0
53	MG	DB	3094	1/1	0.79	0.14	100,100,100,100	0
53	MG	BB	3033	1/1	0.79	0.34	102,102,102,102	0
53	MG	DB	3059	1/1	0.81	0.11	99,99,99,99	0
53	MG	CA	1646	1/1	0.82	0.11	139,139,139,139	0
53	MG	AA	1625	1/1	0.82	0.39	79,79,79,79	1
53	MG	AA	1623	1/1	0.83	0.37	33,33,33,33	1
53	MG	CA	1650	1/1	0.83	0.10	105,105,105,105	0
53	MG	CA	1612	1/1	0.84	0.28	93,93,93,93	0
53	MG	CA	1618	1/1	0.84	0.13	73,73,73,73	0
53	MG	BB	3049	1/1	0.84	0.19	67,67,67,67	0
53	MG	AA	1614	1/1	0.84	0.18	119,119,119,119	0
53	MG	CA	1651	1/1	0.85	0.08	101,101,101,101	0
53	MG	AA	1647	1/1	0.85	0.81	113,113,113,113	0
53	MG	CA	1640	1/1	0.85	0.11	62,62,62,62	0
53	MG	AA	1646	1/1	0.85	0.10	84,84,84,84	0
53	MG	CA	1644	1/1	0.86	0.14	57,57,57,57	0
53	MG	AA	1652	1/1	0.86	0.08	84,84,84,84	0
53	MG	DB	3029	1/1	0.86	0.70	87,87,87,87	0
53	MG	BB	3037	1/1	0.87	0.13	45,45,45,45	0
53	MG	CA	1613	1/1	0.88	0.49	126,126,126,126	0
53	MG	BB	3080	1/1	0.88	0.15	53,53,53,53	0
53	MG	BB	3093	1/1	0.88	0.11	108,108,108,108	0
53	MG	DB	3013	1/1	0.88	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3035	1/1	0.88	0.07	13,13,13,13	0
53	MG	DB	3045	1/1	0.88	0.11	110,110,110,110	0
53	MG	CA	1648	1/1	0.88	0.07	104,104,104,104	0
53	MG	CA	1606	1/1	0.88	0.14	106,106,106,106	0
53	MG	AA	1626	1/1	0.88	0.20	36,36,36,36	1
53	MG	DB	3066	1/1	0.89	0.33	65,65,65,65	0
53	MG	AA	1655	1/1	0.89	0.14	88,88,88,88	0
53	MG	BB	3009	1/1	0.89	0.10	98,98,98,98	0
53	MG	AA	1606	1/1	0.89	0.07	82,82,82,82	0
53	MG	AA	1637	1/1	0.89	0.32	99,99,99,99	0
53	MG	AA	1617	1/1	0.89	0.09	112,112,112,112	0
53	MG	DB	3063	1/1	0.90	0.17	72,72,72,72	0
53	MG	BB	3010	1/1	0.90	0.16	53,53,53,53	0
53	MG	CA	1649	1/1	0.90	0.27	123,123,123,123	0
53	MG	BB	3068	1/1	0.90	0.19	13,13,13,13	0
53	MG	AA	1642	1/1	0.90	0.14	49,49,49,49	0
53	MG	AA	1649	1/1	0.90	0.04	89,89,89,89	0
53	MG	CA	1616	1/1	0.90	0.33	58,58,58,58	1
53	MG	DB	3032	1/1	0.90	0.16	73,73,73,73	0
53	MG	DB	3034	1/1	0.91	0.08	57,57,57,57	0
53	MG	BB	3051	1/1	0.91	0.12	107,107,107,107	0
53	MG	CA	1629	1/1	0.91	0.17	67,67,67,67	0
53	MG	AA	1612	1/1	0.91	0.08	61,61,61,61	0
53	MG	AA	1627	1/1	0.91	0.07	63,63,63,63	0
53	MG	CA	1634	1/1	0.91	0.11	74,74,74,74	0
53	MG	AA	1657	1/1	0.91	0.34	91,91,91,91	0
53	MG	CA	1608	1/1	0.91	0.05	76,76,76,76	0
53	MG	BB	3046	1/1	0.91	0.10	89,89,89,89	0
53	MG	CA	1654	1/1	0.91	0.22	105,105,105,105	0
54	SCM	CA	1659	23/23	0.91	0.16	18,18,18,18	0
53	MG	AA	1656	1/1	0.92	0.14	87,87,87,87	0
53	MG	BB	3081	1/1	0.92	0.10	30,30,30,30	0
53	MG	AA	1605	1/1	0.92	0.10	50,50,50,50	0
53	MG	CA	1609	1/1	0.92	0.10	85,85,85,85	0
53	MG	DB	3035	1/1	0.92	0.22	79,79,79,79	0
53	MG	BB	3014	1/1	0.92	0.07	37,37,37,37	0
53	MG	BB	3001	1/1	0.92	0.19	5,5,5,5	0
53	MG	DN	201	1/1	0.92	0.51	145,145,145,145	0
53	MG	BB	3043	1/1	0.92	0.12	107,107,107,107	0
53	MG	CE	201	1/1	0.92	0.08	109,109,109,109	0
53	MG	CA	1628	1/1	0.92	0.11	52,52,52,52	0
53	MG	BB	3004	1/1	0.92	0.05	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	DB	3104	1/1	0.92	0.12	29,29,29,29	0
53	MG	CA	1627	1/1	0.92	0.07	27,27,27,27	0
53	MG	DB	3050	1/1	0.92	0.11	80,80,80,80	0
53	MG	AA	1633	1/1	0.92	0.05	65,65,65,65	0
53	MG	AA	1650	1/1	0.92	0.08	94,94,94,94	0
55	ZN	D4	101	1/1	0.93	0.05	62,62,62,62	0
53	MG	BB	3108	1/1	0.93	0.06	10,10,10,10	0
53	MG	CA	1645	1/1	0.93	0.10	55,55,55,55	0
53	MG	DB	3064	1/1	0.93	0.39	49,49,49,49	0
53	MG	CA	1617	1/1	0.93	0.18	88,88,88,88	0
53	MG	CA	1632	1/1	0.93	0.24	76,76,76,76	0
53	MG	DB	3005	1/1	0.93	0.17	25,25,25,25	0
53	MG	AA	1621	1/1	0.94	0.17	36,36,36,36	0
53	MG	BB	3064	1/1	0.94	0.19	78,78,78,78	0
53	MG	DB	3028	1/1	0.94	0.18	70,70,70,70	0
53	MG	DB	3067	1/1	0.94	0.06	5,5,5,5	0
53	MG	DB	3022	1/1	0.94	0.06	11,11,11,11	0
53	MG	DB	3109	1/1	0.94	0.04	9,9,9,9	0
53	MG	AA	1645	1/1	0.94	0.20	70,70,70,70	0
53	MG	BB	3020	1/1	0.94	0.31	6,6,6,6	0
53	MG	CA	1625	1/1	0.94	0.05	70,70,70,70	0
55	ZN	B4	101	1/1	0.94	0.07	67,67,67,67	0
53	MG	BB	3071	1/1	0.94	0.18	68,68,68,68	0
53	MG	BB	3008	1/1	0.94	0.12	82,82,82,82	0
53	MG	CA	1637	1/1	0.94	0.17	98,98,98,98	0
53	MG	BB	3079	1/1	0.94	0.07	38,38,38,38	0
53	MG	AA	1628	1/1	0.94	0.18	70,70,70,70	0
53	MG	AA	1602	1/1	0.94	0.12	85,85,85,85	0
53	MG	DB	3091	1/1	0.94	0.11	90,90,90,90	0
53	MG	AA	1658	1/1	0.94	0.04	120,120,120,120	0
53	MG	BB	3005	1/1	0.94	0.11	5,5,5,5	0
53	MG	DB	3016	1/1	0.94	0.08	5,5,5,5	0
53	MG	DB	3071	1/1	0.94	0.17	57,57,57,57	0
53	MG	BB	3092	1/1	0.95	0.09	46,46,46,46	0
53	MG	CA	1615	1/1	0.95	0.06	13,13,13,13	0
53	MG	BB	3104	1/1	0.95	0.17	26,26,26,26	0
53	MG	DB	3096	1/1	0.95	0.11	26,26,26,26	0
53	MG	DB	3110	1/1	0.95	0.12	84,84,84,84	0
53	MG	BB	3003	1/1	0.95	0.06	53,53,53,53	0
53	MG	DB	3060	1/1	0.95	0.12	83,83,83,83	0
53	MG	AA	1618	1/1	0.95	0.08	38,38,38,38	0
53	MG	CA	1604	1/1	0.95	0.10	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3015	1/1	0.95	0.10	25,25,25,25	0
53	MG	BB	3090	1/1	0.95	0.10	88,88,88,88	0
53	MG	BB	3099	1/1	0.95	0.06	41,41,41,41	0
53	MG	DB	3065	1/1	0.95	0.07	128,128,128,128	0
53	MG	BB	3025	1/1	0.95	0.15	30,30,30,30	0
53	MG	DB	3108	1/1	0.95	0.10	43,43,43,43	0
53	MG	BB	3078	1/1	0.95	0.19	27,27,27,27	0
53	MG	BB	3023	1/1	0.95	0.10	5,5,5,5	0
53	MG	DB	3003	1/1	0.95	0.05	30,30,30,30	0
53	MG	DB	3051	1/1	0.95	0.11	75,75,75,75	0
53	MG	DB	3018	1/1	0.95	0.09	7,7,7,7	0
53	MG	CA	1631	1/1	0.95	0.04	41,41,41,41	0
53	MG	AA	1654	1/1	0.95	0.07	67,67,67,67	0
53	MG	DB	3053	1/1	0.95	0.07	65,65,65,65	0
53	MG	CA	1605	1/1	0.95	0.05	12,12,12,12	0
53	MG	BB	3069	1/1	0.95	0.07	5,5,5,5	0
53	MG	BB	3017	1/1	0.96	0.13	50,50,50,50	0
53	MG	BB	3034	1/1	0.96	0.12	86,86,86,86	0
53	MG	DB	3089	1/1	0.96	0.13	79,79,79,79	0
53	MG	AA	1613	1/1	0.96	0.04	58,58,58,58	0
53	MG	BB	3054	1/1	0.96	0.13	49,49,49,49	0
53	MG	BB	3006	1/1	0.96	0.15	61,61,61,61	0
53	MG	BB	3088	1/1	0.96	0.06	11,11,11,11	0
53	MG	DB	3055	1/1	0.96	0.16	44,44,44,44	0
53	MG	AA	1603	1/1	0.96	0.10	57,57,57,57	0
53	MG	BB	3070	1/1	0.96	0.05	74,74,74,74	0
53	MG	BB	3110	1/1	0.96	0.13	80,80,80,80	0
53	MG	AA	1632	1/1	0.96	0.21	96,96,96,96	0
53	MG	BB	3021	1/1	0.96	0.13	52,52,52,52	0
53	MG	BB	3032	1/1	0.96	0.07	22,22,22,22	0
53	MG	DB	3041	1/1	0.96	0.08	40,40,40,40	0
53	MG	DB	3027	1/1	0.96	0.07	13,13,13,13	0
53	MG	BB	3036	1/1	0.96	0.20	51,51,51,51	0
53	MG	AA	1615	1/1	0.96	0.35	96,96,96,96	0
53	MG	BB	3076	1/1	0.96	0.12	35,35,35,35	0
53	MG	BB	3038	1/1	0.96	0.08	92,92,92,92	0
53	MG	DB	3100	1/1	0.96	0.17	19,19,19,19	0
53	MG	CA	1623	1/1	0.96	0.10	11,11,11,11	0
53	MG	DB	3103	1/1	0.96	0.06	36,36,36,36	0
53	MG	BB	3024	1/1	0.96	0.09	55,55,55,55	0
53	MG	AA	1601	1/1	0.96	0.09	36,36,36,36	0
53	MG	CA	1658	1/1	0.96	0.08	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	DB	3001	1/1	0.96	0.06	5,5,5,5	0
53	MG	BB	3052	1/1	0.96	0.10	71,71,71,71	0
53	MG	BB	3057	1/1	0.96	0.16	53,53,53,53	0
53	MG	CA	1641	1/1	0.96	0.10	42,42,42,42	0
53	MG	CA	1633	1/1	0.96	0.06	23,23,23,23	0
53	MG	AA	1619	1/1	0.97	0.04	111,111,111,111	0
53	MG	DB	3069	1/1	0.97	0.23	64,64,64,64	0
53	MG	BB	3067	1/1	0.97	0.17	63,63,63,63	0
53	MG	BB	3031	1/1	0.97	0.18	60,60,60,60	0
53	MG	BB	3065	1/1	0.97	0.06	32,32,32,32	0
53	MG	AA	1638	1/1	0.97	0.07	51,51,51,51	0
53	MG	DB	3030	1/1	0.97	0.19	47,47,47,47	0
53	MG	CA	1652	1/1	0.97	0.07	49,49,49,49	0
53	MG	DB	3057	1/1	0.97	0.05	48,48,48,48	0
53	MG	AA	1659	1/1	0.97	0.39	108,108,108,108	0
53	MG	CA	1653	1/1	0.97	0.07	48,48,48,48	0
53	MG	CA	1638	1/1	0.97	0.10	86,86,86,86	0
53	MG	DB	3078	1/1	0.97	0.04	25,25,25,25	0
53	MG	AA	1616	1/1	0.97	0.09	5,5,5,5	0
53	MG	BB	3102	1/1	0.97	0.12	43,43,43,43	0
53	MG	DB	3082	1/1	0.97	0.11	83,83,83,83	0
53	MG	BB	3096	1/1	0.97	0.07	58,58,58,58	0
53	MG	BB	3084	1/1	0.97	0.06	32,32,32,32	0
53	MG	BB	3100	1/1	0.97	0.20	116,116,116,116	0
53	MG	DB	3010	1/1	0.97	0.14	5,5,5,5	0
53	MG	BB	3053	1/1	0.97	0.10	60,60,60,60	0
53	MG	DB	3031	1/1	0.97	0.09	46,46,46,46	0
53	MG	BB	3075	1/1	0.97	0.09	40,40,40,40	0
54	SCM	AA	1661	23/23	0.97	0.10	13,13,13,13	0
53	MG	BB	3082	1/1	0.97	0.15	18,18,18,18	0
53	MG	DB	3007	1/1	0.97	0.12	62,62,62,62	0
53	MG	DB	3054	1/1	0.97	0.15	21,21,21,21	0
53	MG	BB	3095	1/1	0.97	0.07	62,62,62,62	0
53	MG	CA	1607	1/1	0.97	0.06	5,5,5,5	0
53	MG	BB	3039	1/1	0.97	0.15	41,41,41,41	0
53	MG	DB	3079	1/1	0.97	0.06	7,7,7,7	0
53	MG	CA	1647	1/1	0.97	0.06	75,75,75,75	0
53	MG	AA	1631	1/1	0.97	0.12	5,5,5,5	0
53	MG	BB	3013	1/1	0.97	0.09	45,45,45,45	0
53	MG	AA	1629	1/1	0.97	0.06	12,12,12,12	0
53	MG	AA	1651	1/1	0.97	0.06	35,35,35,35	0
53	MG	DB	3106	1/1	0.97	0.05	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3027	1/1	0.97	0.06	50,50,50,50	0
53	MG	AA	1660	1/1	0.97	0.03	56,56,56,56	0
53	MG	BB	3030	1/1	0.97	0.07	51,51,51,51	0
53	MG	DB	3046	1/1	0.98	0.04	23,23,23,23	0
53	MG	BB	3077	1/1	0.98	0.11	53,53,53,53	0
53	MG	DB	3061	1/1	0.98	0.04	66,66,66,66	0
53	MG	BB	3007	1/1	0.98	0.14	68,68,68,68	0
53	MG	BB	3062	1/1	0.98	0.08	7,7,7,7	0
53	MG	AA	1639	1/1	0.98	0.04	93,93,93,93	0
53	MG	DB	3004	1/1	0.98	0.08	8,8,8,8	0
53	MG	DB	3043	1/1	0.98	0.06	7,7,7,7	0
53	MG	AA	1636	1/1	0.98	0.04	64,64,64,64	0
53	MG	BB	3002	1/1	0.98	0.06	23,23,23,23	0
53	MG	DB	3017	1/1	0.98	0.23	5,5,5,5	0
53	MG	CA	1614	1/1	0.98	0.15	83,83,83,83	0
53	MG	CA	1635	1/1	0.98	0.06	30,30,30,30	0
53	MG	BB	3026	1/1	0.98	0.10	65,65,65,65	0
53	MG	DB	3047	1/1	0.98	0.15	43,43,43,43	0
53	MG	BB	3098	1/1	0.98	0.15	14,14,14,14	0
53	MG	DB	3048	1/1	0.98	0.11	38,38,38,38	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	BB	3089	1/1	0.98	0.12	72,72,72,72	0
53	MG	DB	3008	1/1	0.98	0.06	13,13,13,13	0
53	MG	BB	3087	1/1	0.98	0.25	80,80,80,80	0
53	MG	DB	3033	1/1	0.98	0.04	11,11,11,11	0
53	MG	BB	3056	1/1	0.98	0.03	5,5,5,5	0
53	MG	BB	3019	1/1	0.98	0.12	21,21,21,21	0
53	MG	DB	3092	1/1	0.98	0.15	10,10,10,10	0
53	MG	CA	1610	1/1	0.98	0.14	5,5,5,5	0
53	MG	DB	3107	1/1	0.98	0.04	5,5,5,5	0
53	MG	DB	3077	1/1	0.98	0.13	45,45,45,45	0
53	MG	CA	1619	1/1	0.98	0.09	36,36,36,36	0
53	MG	BB	3086	1/1	0.98	0.10	5,5,5,5	0
53	MG	BB	3044	1/1	0.98	0.09	45,45,45,45	0
53	MG	DB	3019	1/1	0.98	0.06	5,5,5,5	0
53	MG	AA	1609	1/1	0.98	0.06	40,40,40,40	0
53	MG	DB	3088	1/1	0.98	0.17	87,87,87,87	0
53	MG	BB	3103	1/1	0.98	0.08	11,11,11,11	0
53	MG	DB	3062	1/1	0.98	0.23	58,58,58,58	0
53	MG	BB	3061	1/1	0.98	0.08	24,24,24,24	0
53	MG	CA	1639	1/1	0.98	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	DB	3074	1/1	0.98	0.07	26,26,26,26	0
53	MG	AA	1630	1/1	0.98	0.04	88,88,88,88	0
53	MG	BB	3074	1/1	0.98	0.06	10,10,10,10	0
53	MG	CA	1643	1/1	0.98	0.06	36,36,36,36	0
53	MG	DB	3090	1/1	0.98	0.09	14,14,14,14	0
53	MG	BB	3047	1/1	0.98	0.11	104,104,104,104	0
53	MG	DB	3036	1/1	0.98	0.04	87,87,87,87	0
53	MG	BB	3091	1/1	0.98	0.10	5,5,5,5	0
53	MG	DB	3087	1/1	0.98	0.08	5,5,5,5	0
53	MG	BB	3050	1/1	0.98	0.12	53,53,53,53	0
53	MG	BB	3048	1/1	0.98	0.04	12,12,12,12	0
53	MG	DB	3083	1/1	0.98	0.08	27,27,27,27	0
53	MG	BB	3018	1/1	0.98	0.12	39,39,39,39	0
53	MG	AA	1643	1/1	0.98	0.09	40,40,40,40	0
53	MG	DB	3056	1/1	0.98	0.06	5,5,5,5	0
53	MG	CA	1601	1/1	0.98	0.06	5,5,5,5	0
53	MG	BB	3040	1/1	0.98	0.08	12,12,12,12	0
53	MG	BB	3045	1/1	0.98	0.14	72,72,72,72	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	DB	3095	1/1	0.98	0.15	92,92,92,92	0
53	MG	DB	3006	1/1	0.98	0.11	10,10,10,10	0
53	MG	DB	3086	1/1	0.98	0.12	18,18,18,18	0
53	MG	DB	3072	1/1	0.98	0.07	20,20,20,20	0
53	MG	DB	3039	1/1	0.98	0.08	62,62,62,62	0
53	MG	CA	1626	1/1	0.98	0.08	8,8,8,8	0
53	MG	BB	3094	1/1	0.98	0.06	36,36,36,36	0
53	MG	AA	1640	1/1	0.98	0.15	46,46,46,46	0
53	MG	DB	3044	1/1	0.98	0.05	18,18,18,18	0
53	MG	BB	3011	1/1	0.98	0.15	5,5,5,5	0
53	MG	BB	3022	1/1	0.98	0.12	32,32,32,32	0
53	MG	BB	3109	1/1	0.98	0.10	11,11,11,11	0
53	MG	AA	1644	1/1	0.98	0.05	75,75,75,75	0
53	MG	DB	3009	1/1	0.98	0.07	9,9,9,9	0
53	MG	BB	3106	1/1	0.98	0.12	10,10,10,10	0
53	MG	DB	3002	1/1	0.98	0.05	11,11,11,11	0
53	MG	DB	3093	1/1	0.98	0.05	59,59,59,59	0
53	MG	DB	3098	1/1	0.98	0.10	5,5,5,5	0
53	MG	DB	3075	1/1	0.98	0.11	44,44,44,44	0
53	MG	DB	3024	1/1	0.98	0.05	40,40,40,40	0
53	MG	AA	1653	1/1	0.98	0.09	21,21,21,21	0
53	MG	CA	1621	1/1	0.98	0.16	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	AA	1641	1/1	0.99	0.02	32,32,32,32	0
53	MG	DB	3073	1/1	0.99	0.07	50,50,50,50	0
53	MG	DB	3015	1/1	0.99	0.06	42,42,42,42	0
53	MG	CA	1602	1/1	0.99	0.12	5,5,5,5	0
53	MG	CA	1611	1/1	0.99	0.07	28,28,28,28	0
53	MG	BB	3072	1/1	0.99	0.10	35,35,35,35	0
53	MG	CA	1657	1/1	0.99	0.05	73,73,73,73	0
53	MG	DB	3076	1/1	0.99	0.10	33,33,33,33	0
53	MG	BB	3083	1/1	0.99	0.14	30,30,30,30	0
53	MG	DB	3026	1/1	0.99	0.23	45,45,45,45	0
53	MG	BB	3012	1/1	0.99	0.06	67,67,67,67	0
53	MG	DB	3023	1/1	0.99	0.04	69,69,69,69	0
53	MG	AA	1604	1/1	0.99	0.09	38,38,38,38	0
53	MG	BB	3059	1/1	0.99	0.13	10,10,10,10	0
53	MG	DB	3021	1/1	0.99	0.04	16,16,16,16	0
53	MG	BB	3073	1/1	0.99	0.10	44,44,44,44	0
53	MG	DB	3102	1/1	0.99	0.23	28,28,28,28	0
53	MG	CA	1630	1/1	0.99	0.10	37,37,37,37	0
53	MG	CA	1624	1/1	0.99	0.07	38,38,38,38	0
53	MG	DB	3097	1/1	0.99	0.17	41,41,41,41	0
53	MG	DB	3080	1/1	0.99	0.10	62,62,62,62	0
53	MG	BB	3063	1/1	0.99	0.05	33,33,33,33	0
53	MG	BB	3041	1/1	0.99	0.09	5,5,5,5	0
53	MG	DB	3068	1/1	0.99	0.15	5,5,5,5	0
53	MG	DB	3037	1/1	0.99	0.16	8,8,8,8	0
53	MG	BB	3105	1/1	0.99	0.18	5,5,5,5	0
53	MG	BB	3058	1/1	0.99	0.06	15,15,15,15	0
53	MG	DB	3040	1/1	0.99	0.05	5,5,5,5	0
53	MG	DB	3012	1/1	0.99	0.12	9,9,9,9	0
53	MG	CA	1655	1/1	0.99	0.03	32,32,32,32	0
53	MG	CA	1656	1/1	0.99	0.14	38,38,38,38	0
53	MG	DB	3081	1/1	0.99	0.06	41,41,41,41	0
53	MG	CA	1620	1/1	0.99	0.10	72,72,72,72	0
53	MG	BB	3107	1/1	0.99	0.21	46,46,46,46	0
53	MG	AA	1607	1/1	0.99	0.09	57,57,57,57	0
53	MG	BB	3085	1/1	0.99	0.07	34,34,34,34	0
53	MG	AA	1648	1/1	0.99	0.06	6,6,6,6	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	BB	3029	1/1	0.99	0.05	5,5,5,5	0
53	MG	DB	3038	1/1	0.99	0.07	5,5,5,5	0
53	MG	BB	3016	1/1	0.99	0.04	55,55,55,55	0

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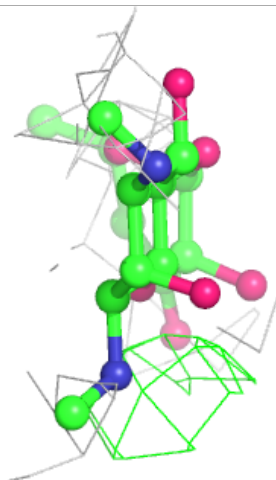
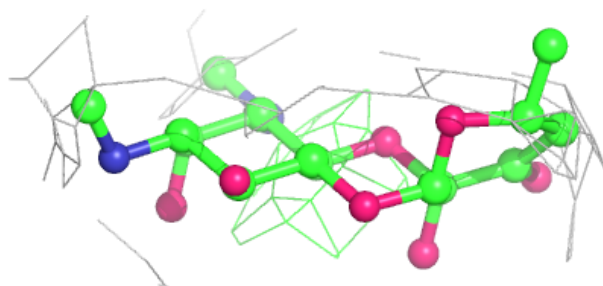
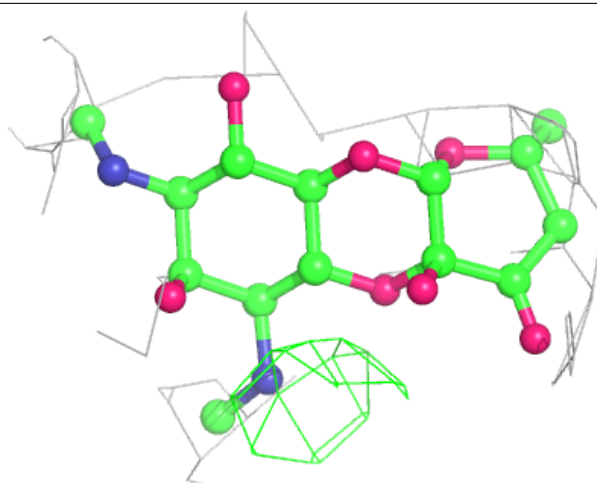
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	AA	1634	1/1	0.99	0.03	72,72,72,72	0
53	MG	BB	3066	1/1	0.99	0.04	5,5,5,5	0
53	MG	CA	1603	1/1	0.99	0.03	56,56,56,56	0
53	MG	BB	3060	1/1	0.99	0.17	30,30,30,30	0
53	MG	DB	3025	1/1	0.99	0.07	44,44,44,44	0
53	MG	AA	1611	1/1	0.99	0.05	43,43,43,43	0
53	MG	BB	3055	1/1	0.99	0.12	6,6,6,6	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	AA	1610	1/1	0.99	0.06	78,78,78,78	0
53	MG	CA	1622	1/1	0.99	0.17	5,5,5,5	0
53	MG	DB	3084	1/1	0.99	0.09	29,29,29,29	0
53	MG	DB	3011	1/1	0.99	0.10	5,5,5,5	0
53	MG	DB	3101	1/1	0.99	0.10	26,26,26,26	0
53	MG	DB	3014	1/1	1.00	0.05	21,21,21,21	0
53	MG	BB	3101	1/1	1.00	0.05	19,19,19,19	0
53	MG	CA	1636	1/1	1.00	0.04	5,5,5,5	0
53	MG	DB	3049	1/1	1.00	0.14	42,42,42,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

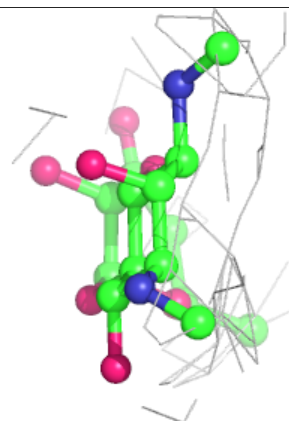
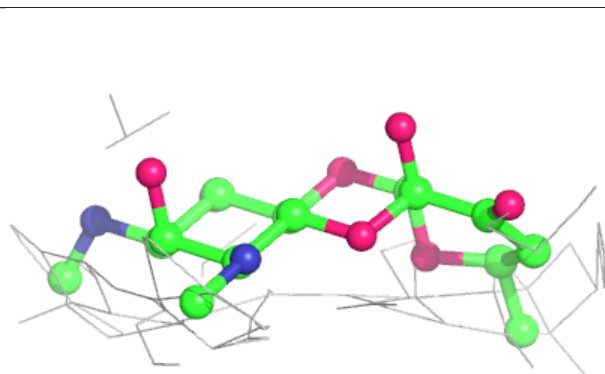
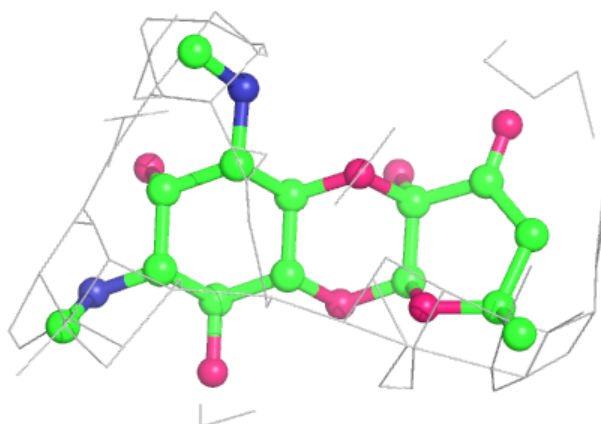
Electron density around SCM CA 1659:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SCM AA 1661:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.