



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 02:02 pm BST

PDB ID : 4V52
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with neomycin.
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-15
Resolution : 3.21 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

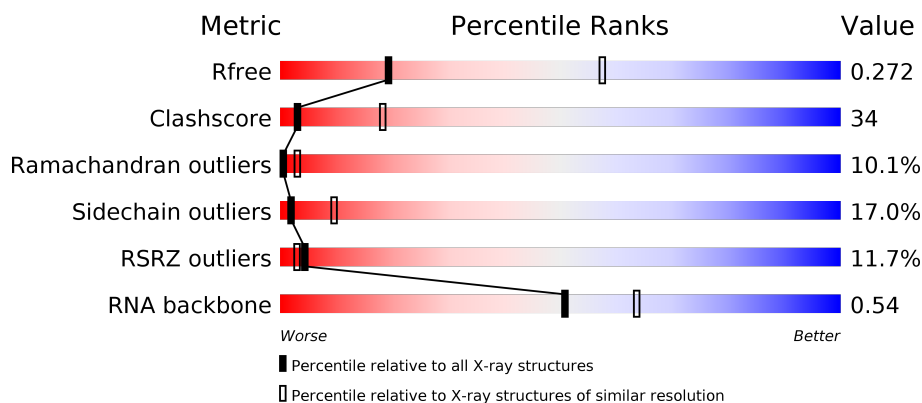
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)
RNA backbone	3102	1023 (3.54-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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>15%</div> <div>28%</div> <div>60%</div> <div>12%</div> <div>.</div> </div>
1	CA	1542	<div> <div>28%</div> <div>60%</div> <div>11%</div> <div>.</div> </div>
2	AC	232	<div> <div>15%</div> <div>32%</div> <div>44%</div> <div>13%</div> <div>11%</div> </div>
2	CC	232	<div> <div>12%</div> <div>31%</div> <div>46%</div> <div>12%</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	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	70	
21	CU	70	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	NMY	BB	3001	-	-	-	X
53	NMY	DB	3001	-	-	-	X
54	MG	DB	3059	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284172 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 S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

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

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

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

- 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			

- 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			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

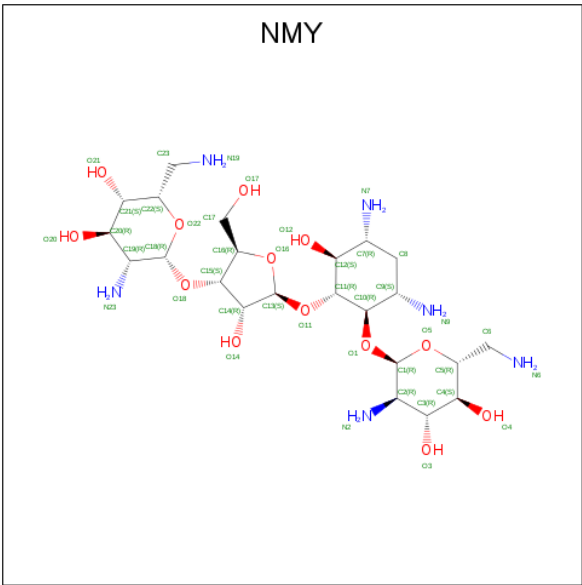
- Molecule 51 is a protein called 50S ribosomal protein L28.

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

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

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

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	110	Total	Mg	0	0
			110	110		
54	CN	1	Total	Mg	0	0
			1	1		
54	CA	60	Total	Mg	0	0
			60	60		
54	AA	60	Total	Mg	0	0
			60	60		
54	CE	1	Total	Mg	0	0
			1	1		
54	DB	111	Total	Mg	0	0
			111	111		

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

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

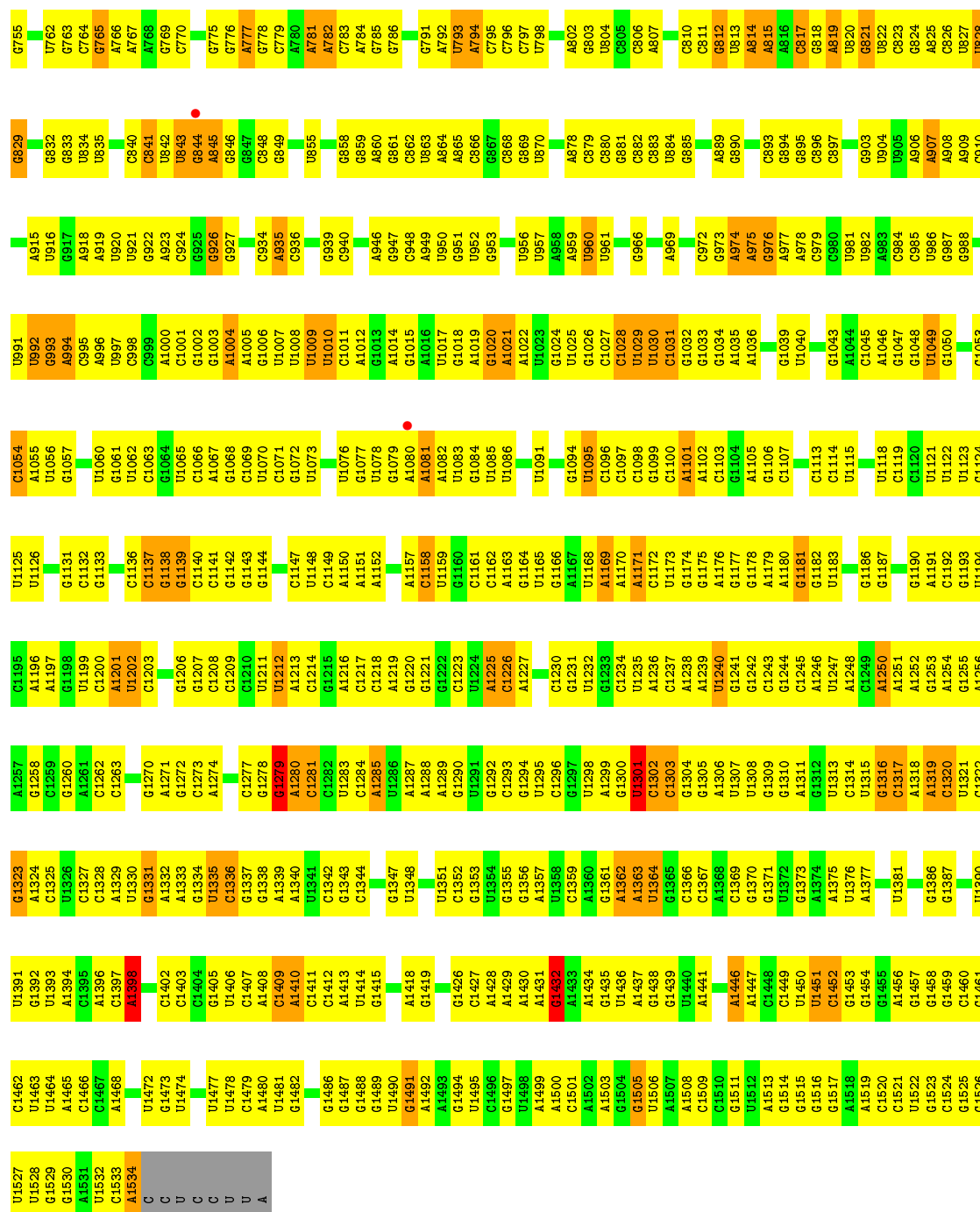
- Molecule 56 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	291	Total O 291 291	0	0
56	AL	4	Total O 4 4	0	0
56	AN	4	Total O 4 4	0	0
56	AT	1	Total O 1 1	0	0
56	BB	497	Total O 497 497	0	0
56	BC	5	Total O 5 5	0	0
56	BE	1	Total O 1 1	0	0
56	BL	1	Total O 1 1	0	0
56	BN	1	Total O 1 1	0	0
56	BR	1	Total O 1 1	0	0
56	CA	298	Total O 298 298	0	0
56	CE	3	Total O 3 3	0	0
56	CL	2	Total O 2 2	0	0
56	CN	4	Total O 4 4	0	0
56	CP	1	Total O 1 1	0	0
56	CT	1	Total O 1 1	0	0
56	DB	502	Total O 502 502	0	0
56	DC	6	Total O 6 6	0	0

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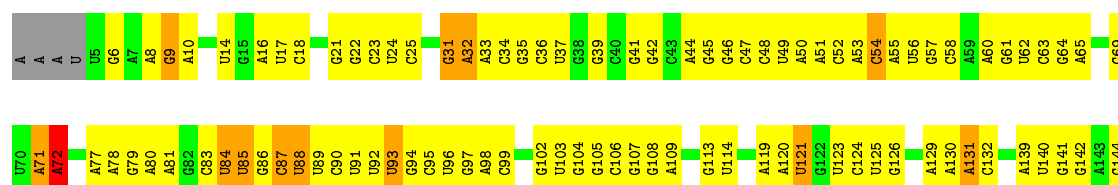
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DE	1	Total	O	0	0
			1	1		
56	DL	2	Total	O	0	0
			2	2		
56	DR	1	Total	O	0	0
			1	1		



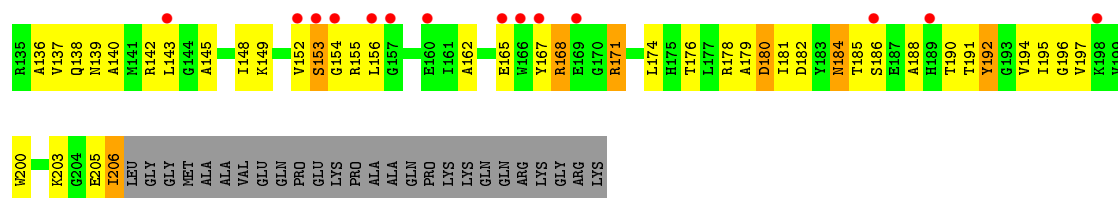
• Molecule 1: 16S rRNA

Chain CA: 28% 60% 11% .

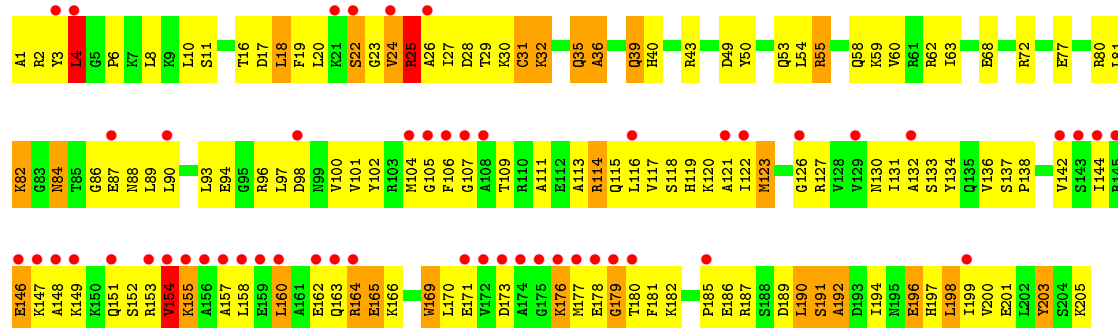


WORLDWIDE
PDB
PROTEIN DATA BANK

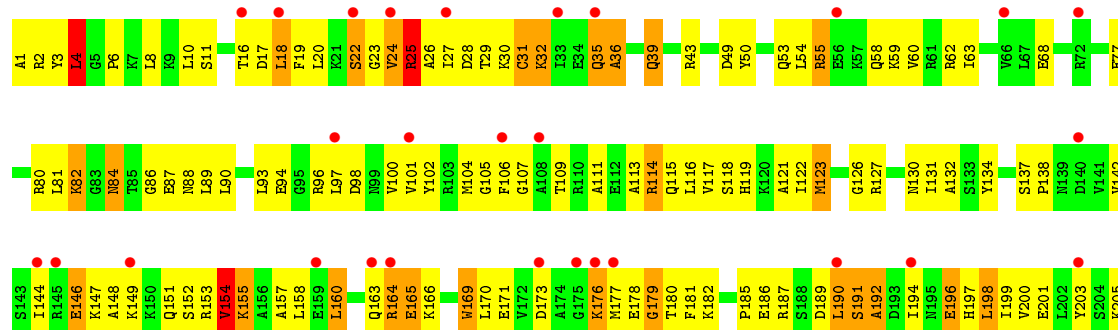




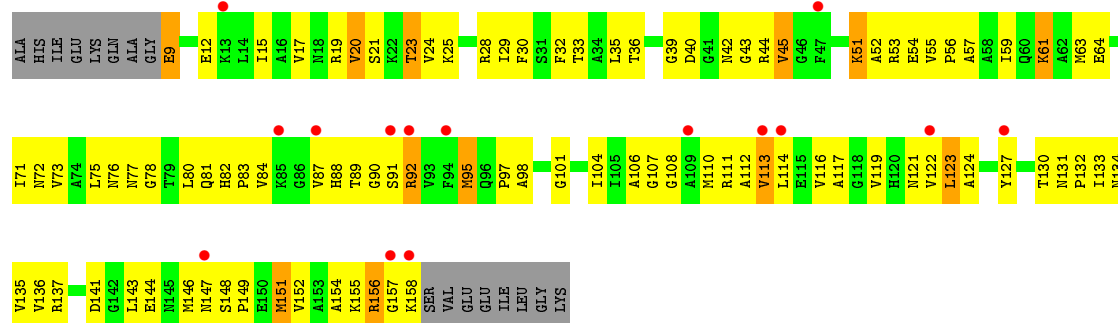
• Molecule 3: 30S ribosomal protein S4



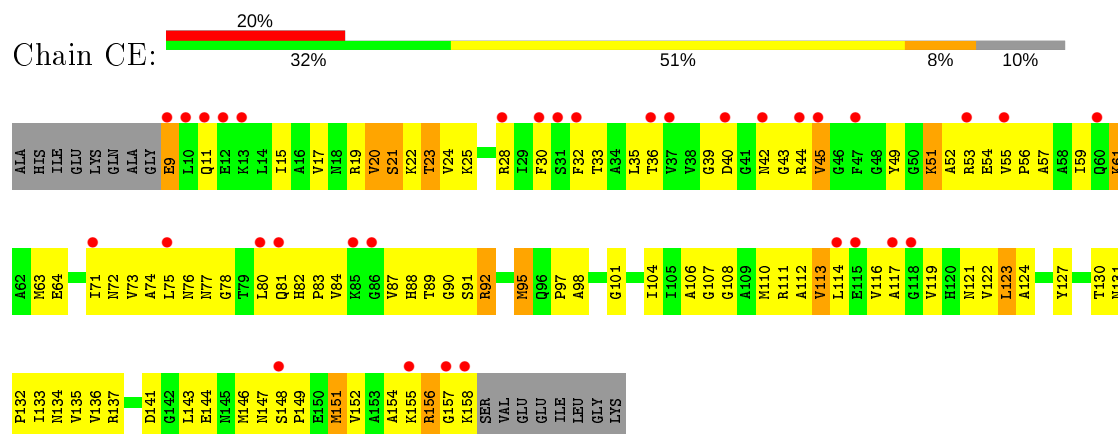
• Molecule 3: 30S ribosomal protein S4



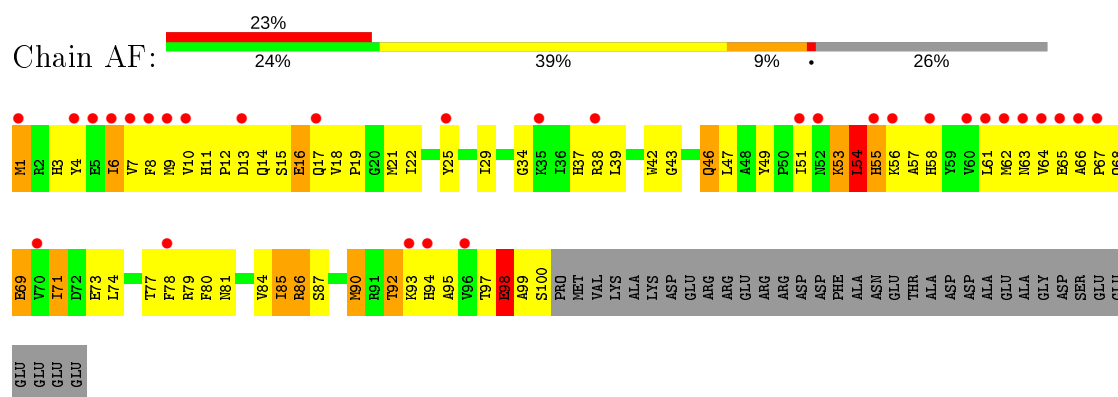
• Molecule 4: 30S ribosomal protein S5



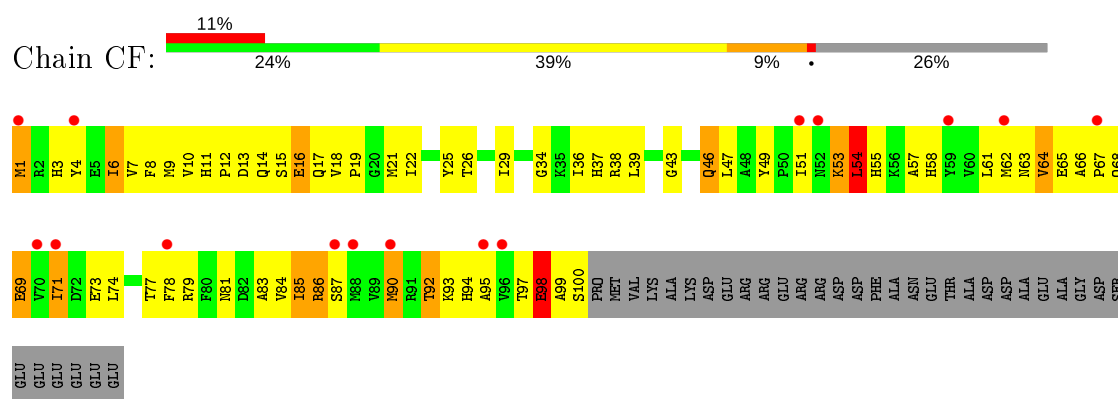
- Molecule 4: 30S ribosomal protein S5



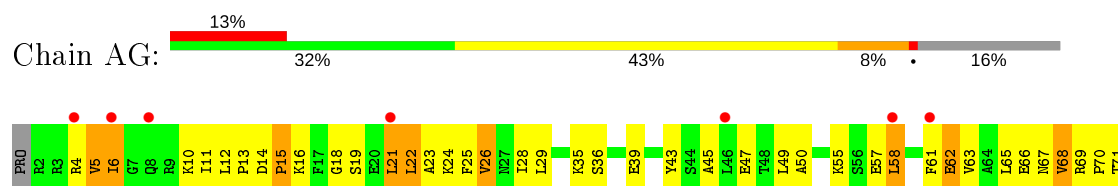
- Molecule 5: 30S ribosomal protein S6

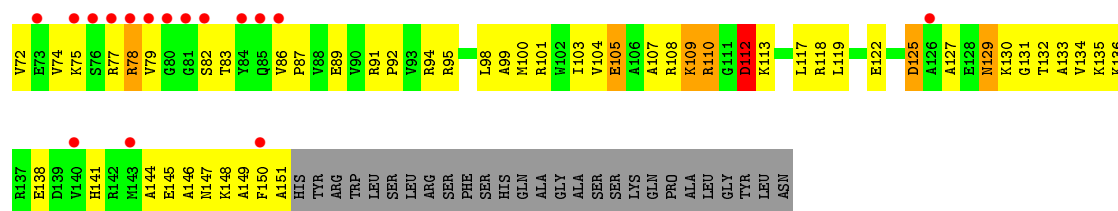


- Molecule 5: 30S ribosomal protein S6

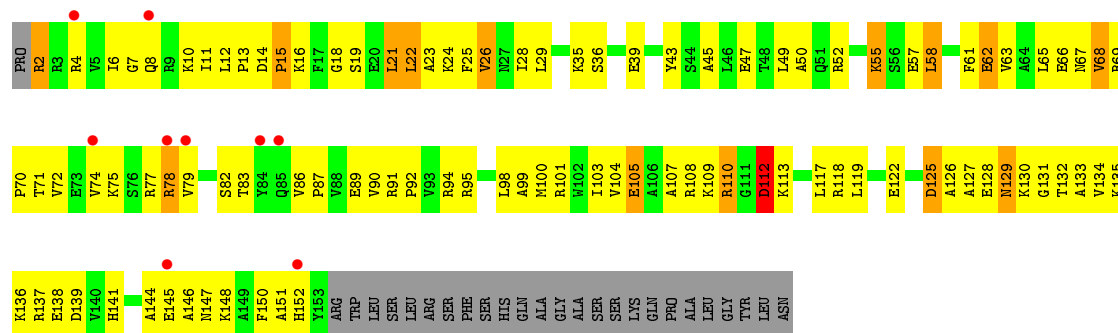


- Molecule 6: 30S ribosomal protein S7

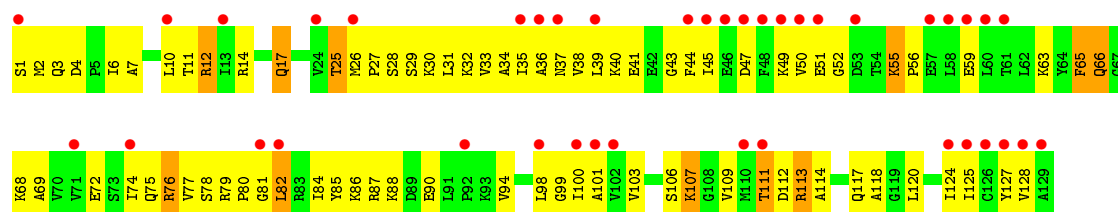




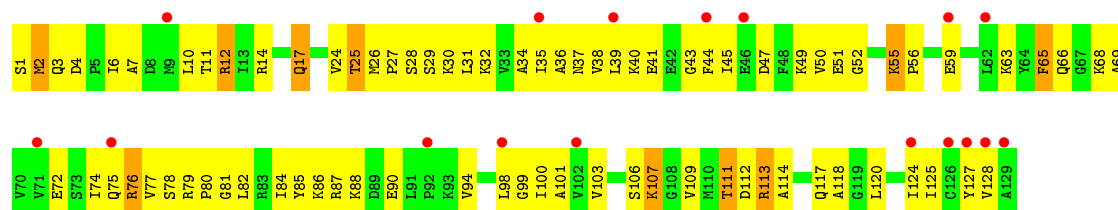
• Molecule 6: 30S ribosomal protein S7



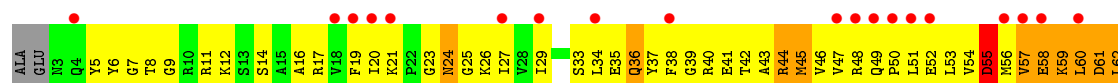
• Molecule 7: 30S ribosomal protein S8

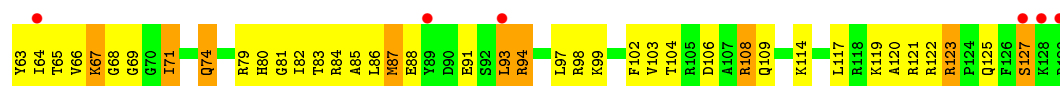


• Molecule 7: 30S ribosomal protein S8

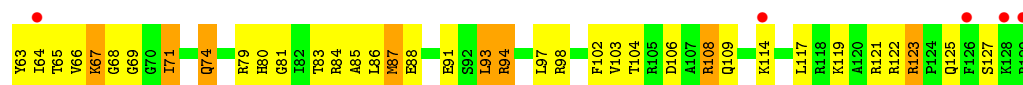
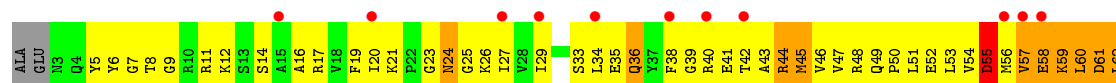


• Molecule 8: 30S ribosomal protein S9

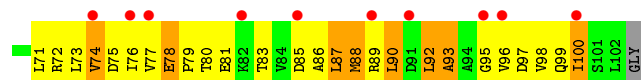
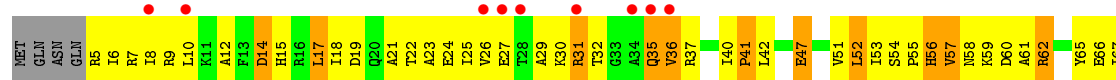




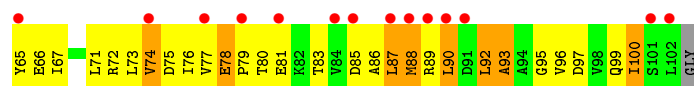
• Molecule 8: 30S ribosomal protein S9



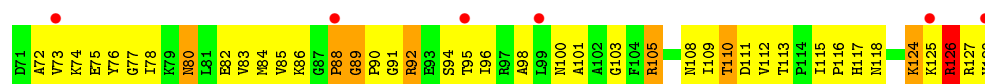
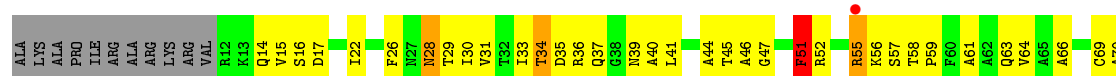
• Molecule 9: 30S ribosomal protein S10



• Molecule 9: 30S ribosomal protein S10

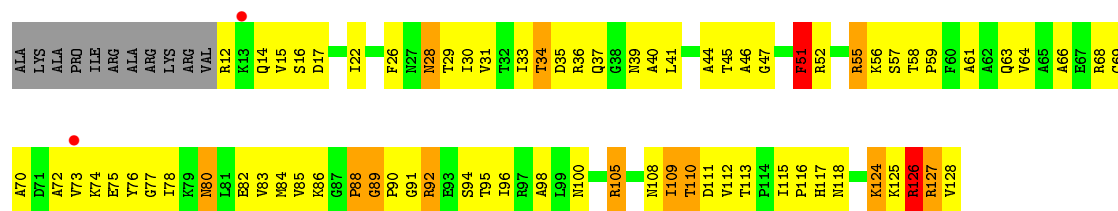


• Molecule 10: 30S ribosomal protein S11

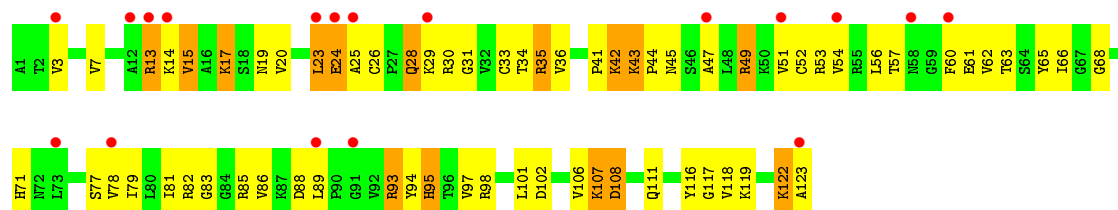


• Molecule 10: 30S ribosomal protein S11

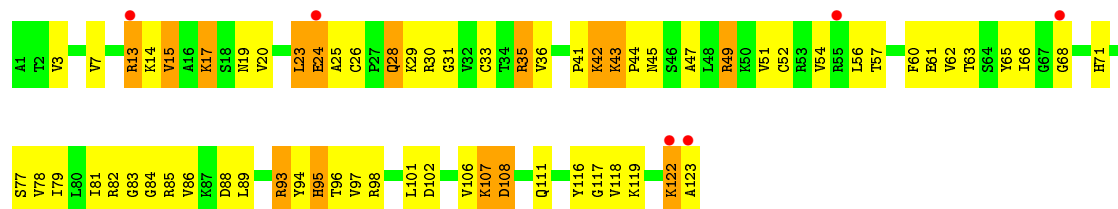




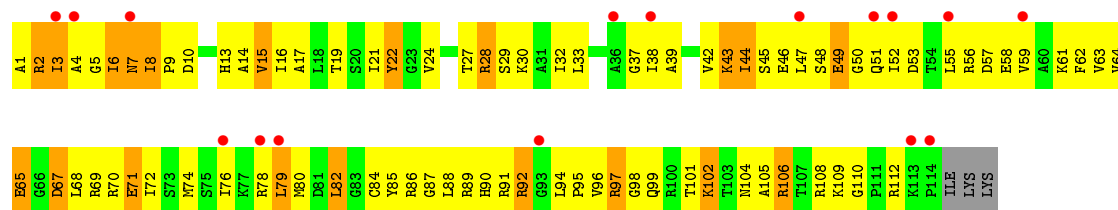
• Molecule 11: 30S ribosomal protein S12



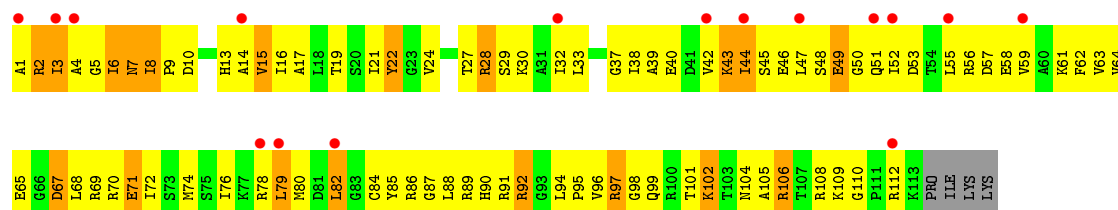
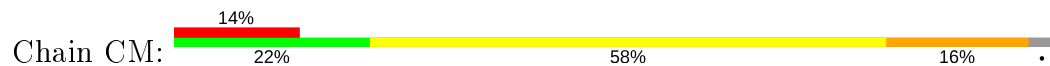
• Molecule 11: 30S ribosomal protein S12



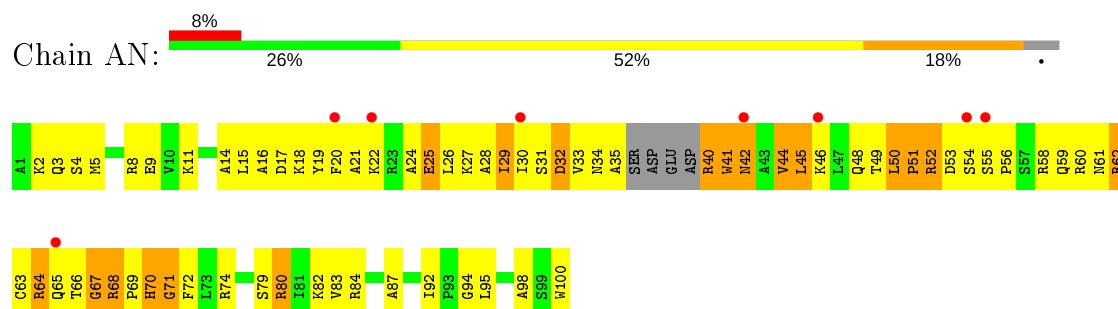
• Molecule 12: 30S ribosomal protein S13



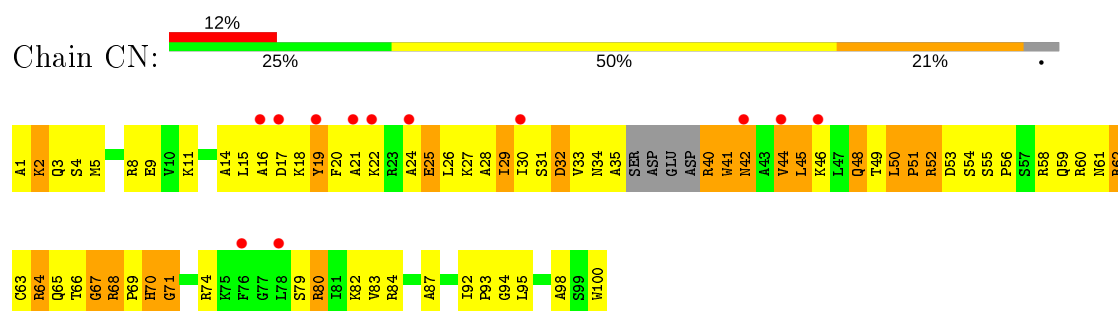
• Molecule 12: 30S ribosomal protein S13



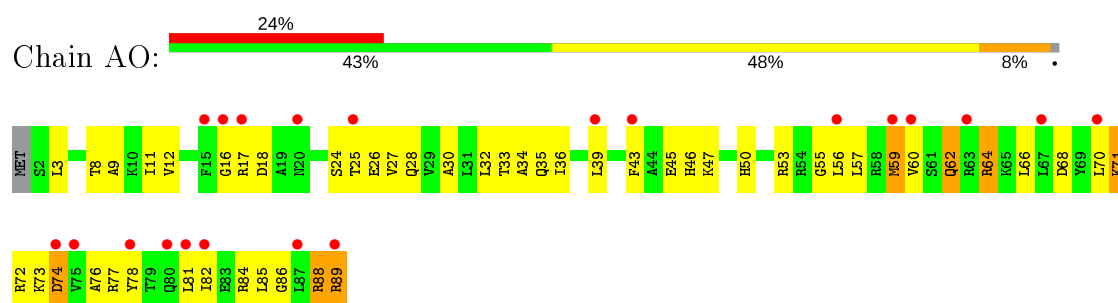
- Molecule 13: 30S ribosomal protein S14



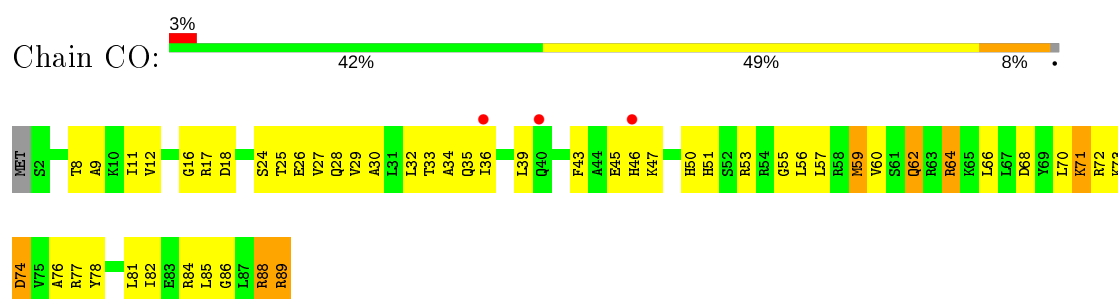
- Molecule 13: 30S ribosomal protein S14



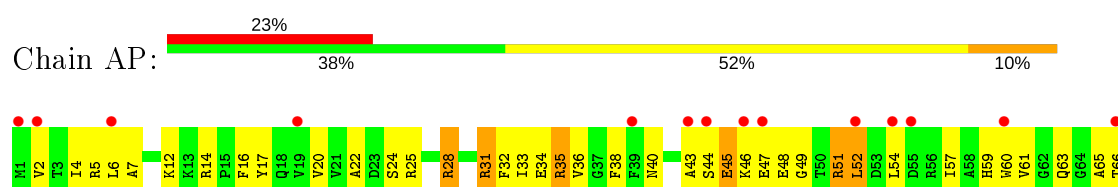
- Molecule 14: 30S ribosomal protein S15

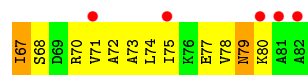


- Molecule 14: 30S ribosomal protein S15

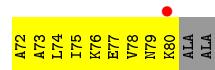


- Molecule 15: 30S ribosomal protein S16

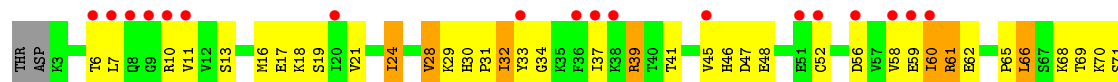
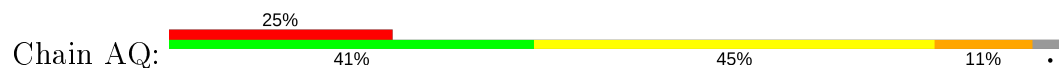




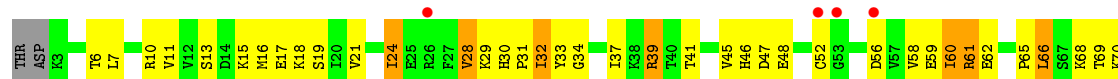
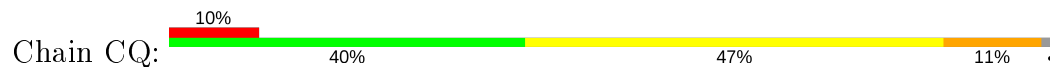
- Molecule 15: 30S ribosomal protein S16



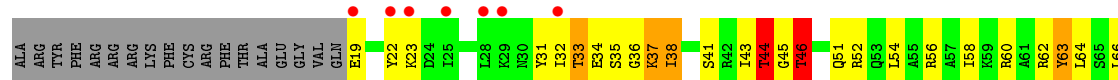
- Molecule 16: 30S ribosomal protein S17



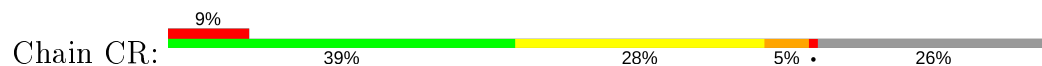
- Molecule 16: 30S ribosomal protein S17

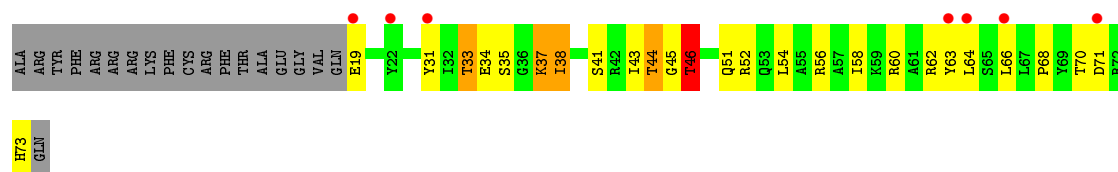


- Molecule 17: 30S ribosomal protein S18

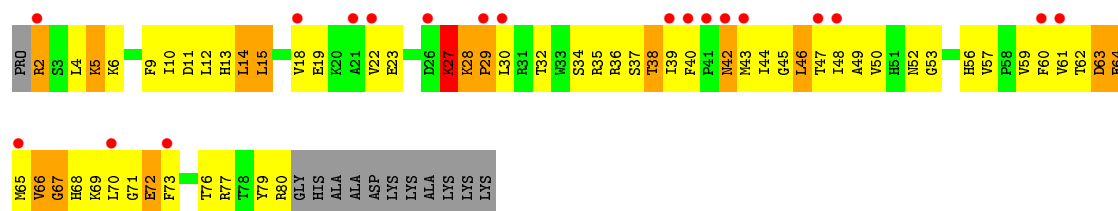


- Molecule 17: 30S ribosomal protein S18

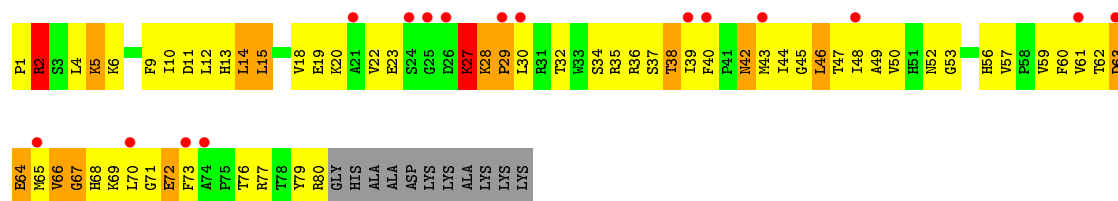




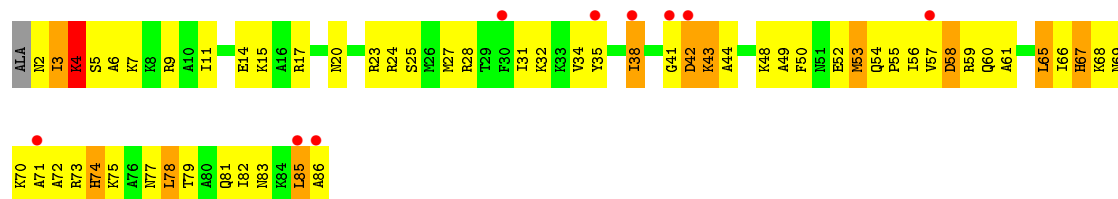
- Molecule 18: 30S ribosomal protein S19



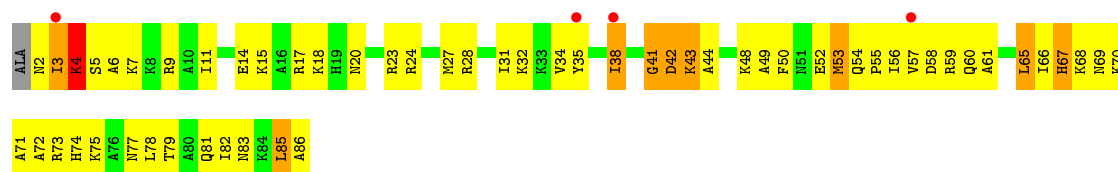
- Molecule 18: 30S ribosomal protein S19



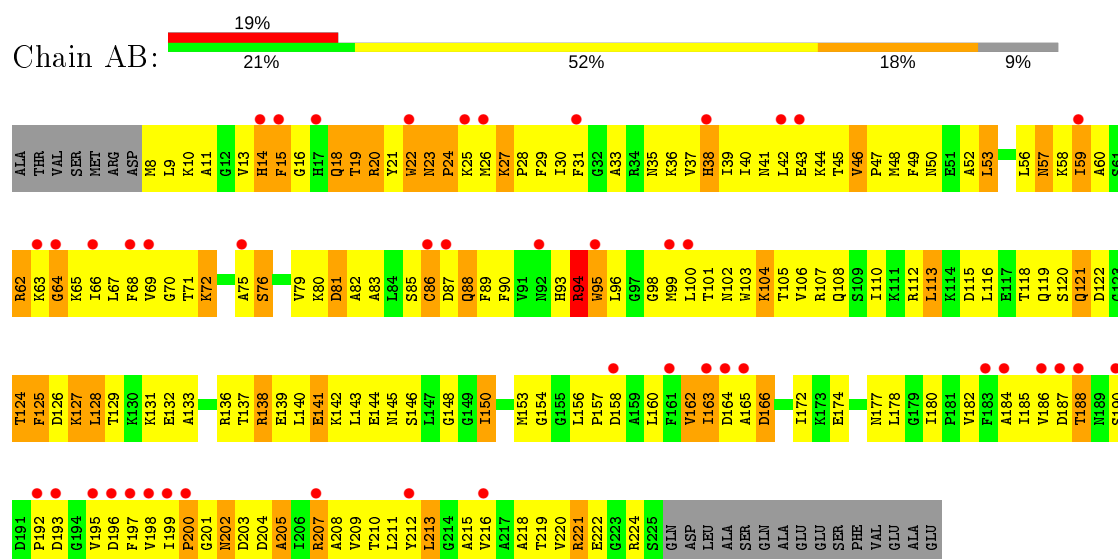
- Molecule 19: 30S ribosomal protein S20



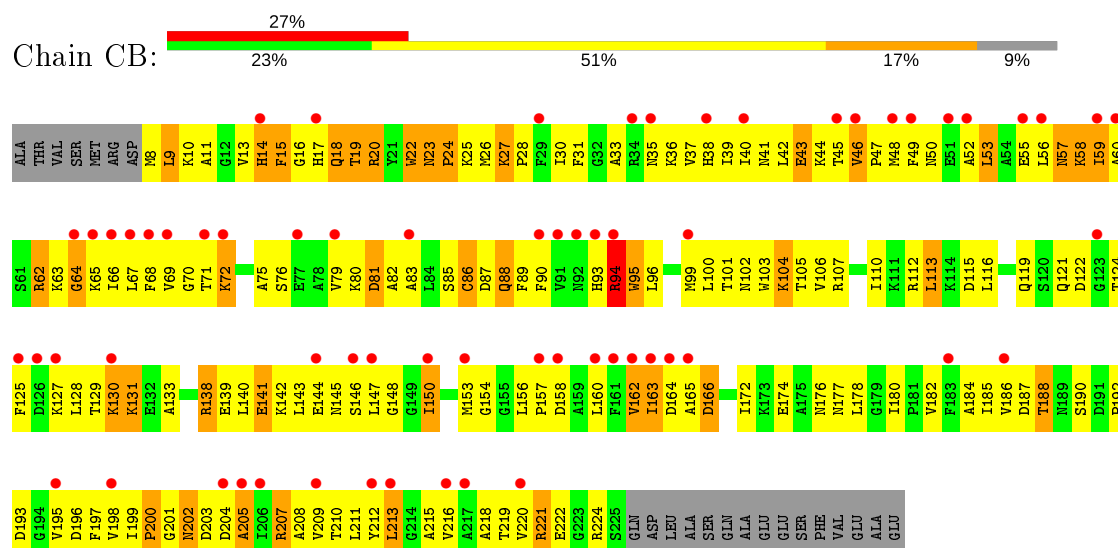
- Molecule 19: 30S ribosomal protein S20



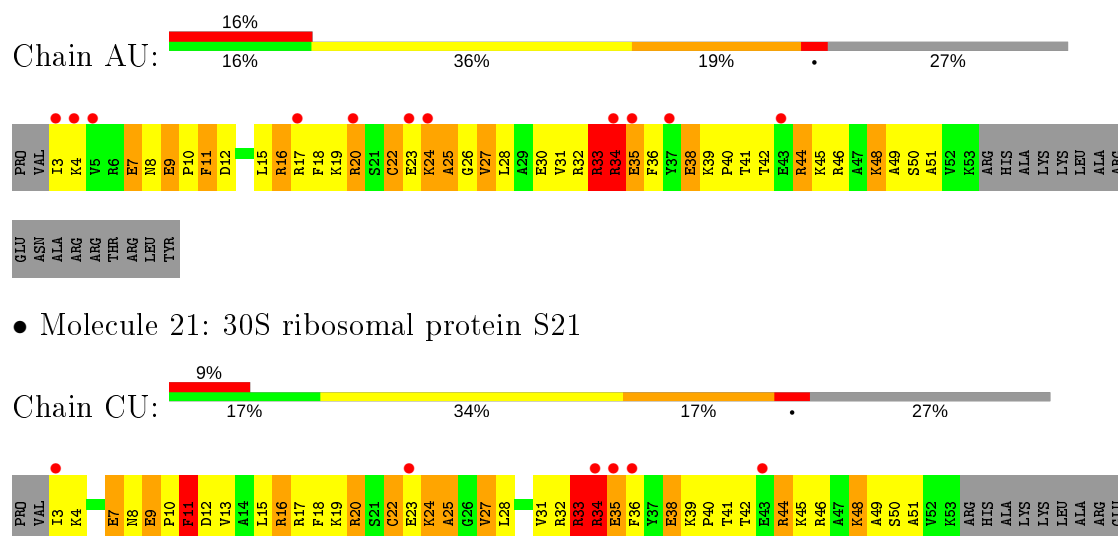
- Molecule 20: 30S ribosomal protein S2



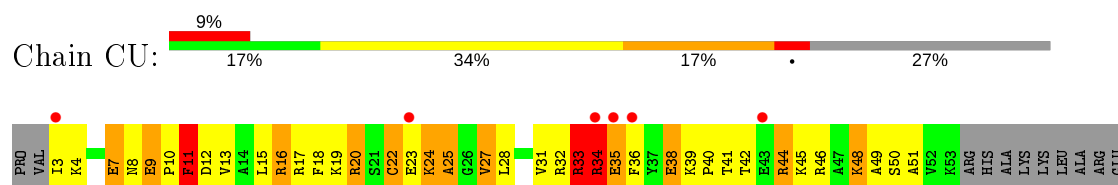
• Molecule 20: 30S ribosomal protein S2



• Molecule 21: 30S ribosomal protein S21



• Molecule 21: 30S ribosomal protein S21

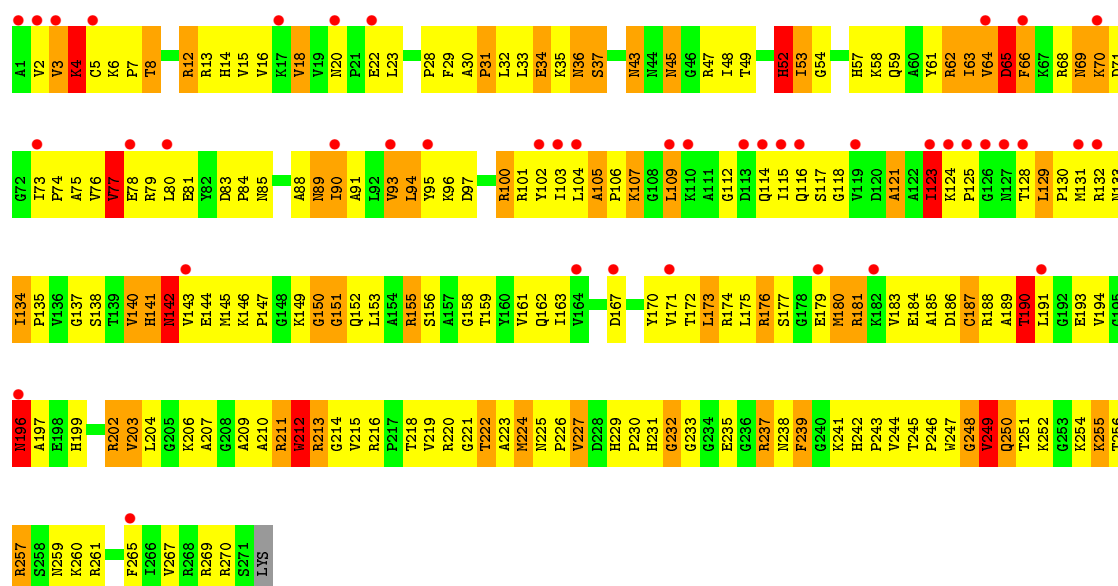


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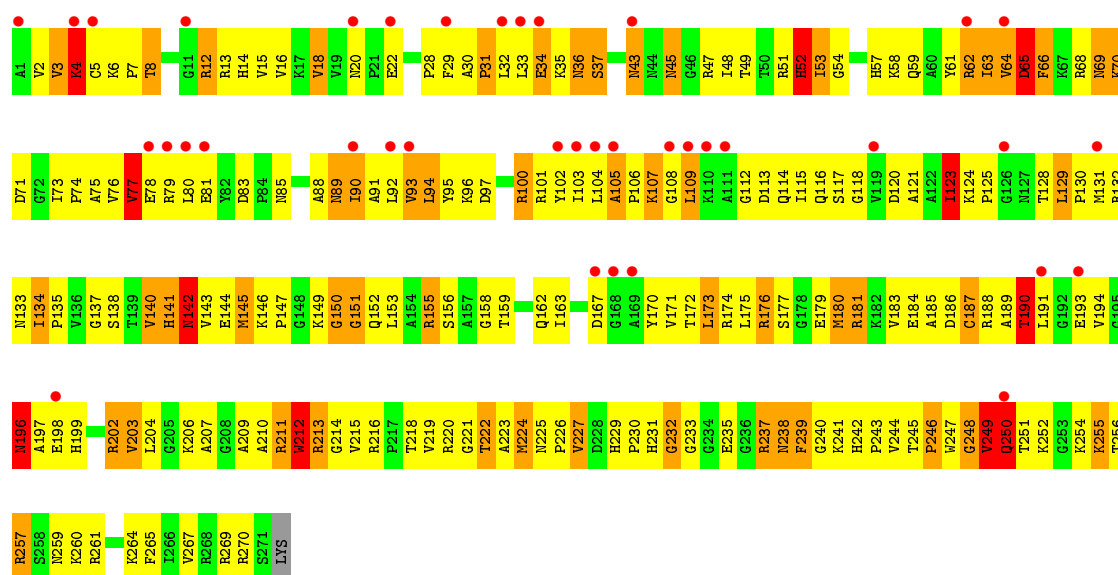


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U1572	U1434	C1297	G1368	C1297	G1223	A1155	A1088	A947	G	C817	A742	A670	A603
A1508	G1437	U1298	G1368	U1298	U1224	A1156	A1089	C948	G	G818	A743	C672	A608
G1510	U1438	G1299	U1372	G1299	C1229	U1159	G1017	G949	U	G819	U744	C673	A609
U1513	A1439	A1300	A1373	A1300	A1230	G1160	A1018	C950	G	U820	G745	C674	C610
U1576	G1440	G1301	G1374	G1301	U1231	C1161	U1019	C951	C	A821	U746	A675	C611
G1514	U1441	A1302	U1375	A1302	U1231	C1162	A1020	G952	A	G822	U747	A676	G612
A1515	U1442	G1303	C1376	G1303	G1236	G1163	A1021	U955	C	C823	C677	A677	A613
G1516	U1443	A1304	U1379	A1304	A1237	C1164	G1022	G956	C	U824	A751	C678	C614
G1517	G1444	C1305	U1380	C1305	G1238	A1165	U1023	C957	C	U826	A752	A678	G615
A1518	G1445	G1306	C1306	A1237	A1238	A1166	U1024	C958	C	U826	A753	C679	A614
G1519	C1446	A1307	G1381	A1307	G1238	G1166	G1025	U958	G	U826	A753	C679	A614

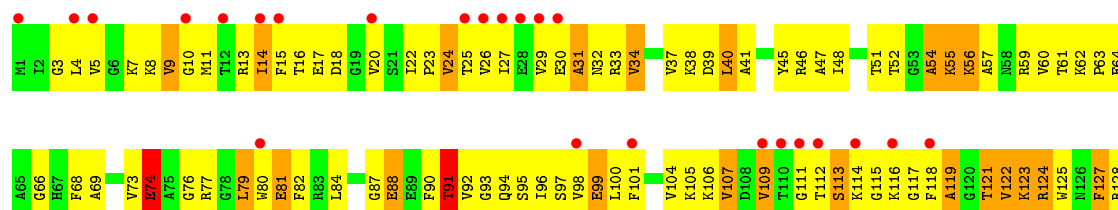


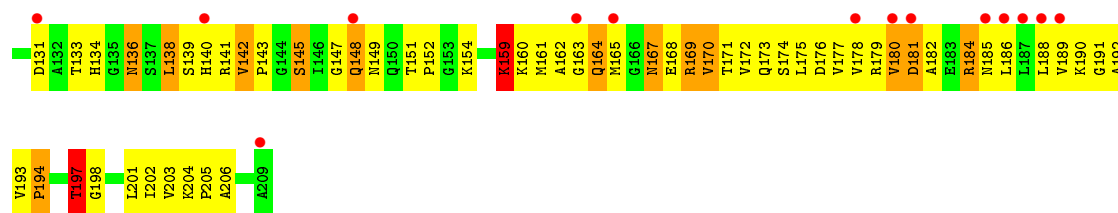


• Molecule 25: 50S ribosomal protein L2

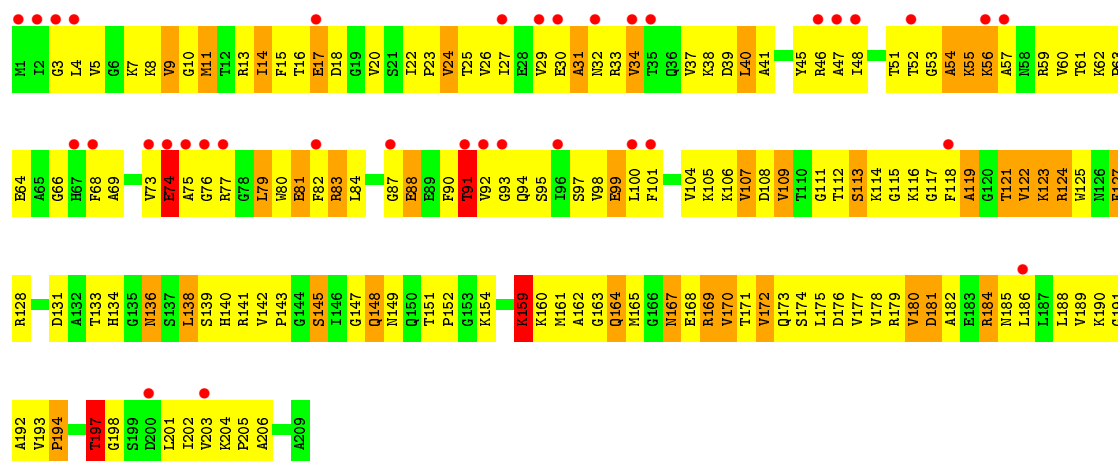


• Molecule 26: 50S ribosomal protein L3

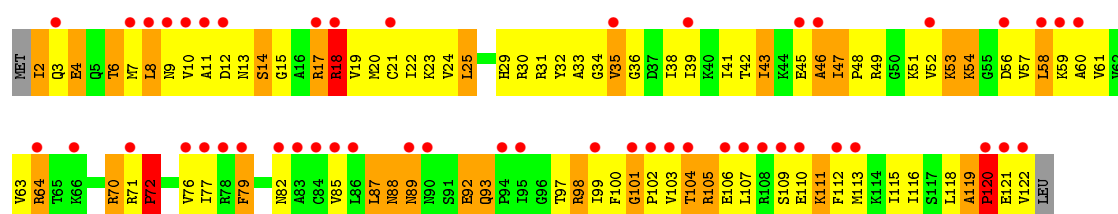




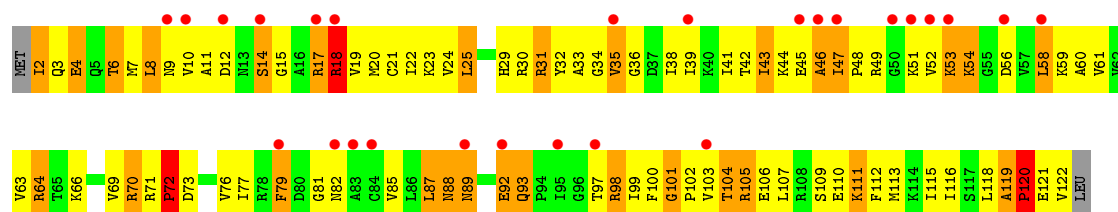
• Molecule 26: 50S ribosomal protein L3



• Molecule 27: 50S ribosomal protein L14

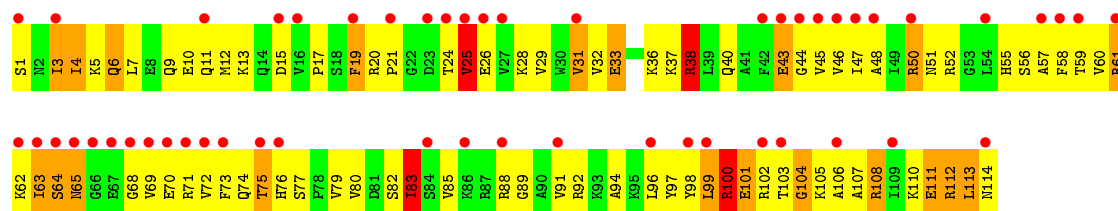


• Molecule 27: 50S ribosomal protein L14

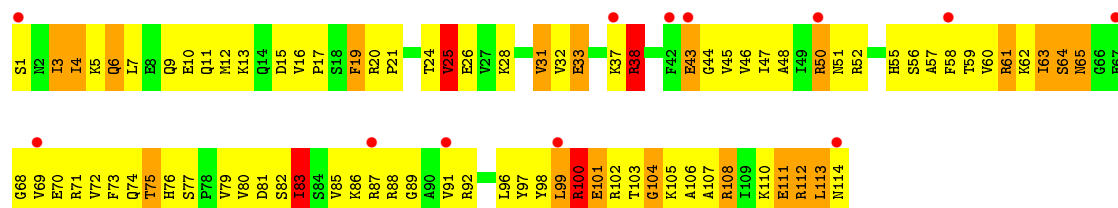


• Molecule 28: 50S ribosomal protein L19

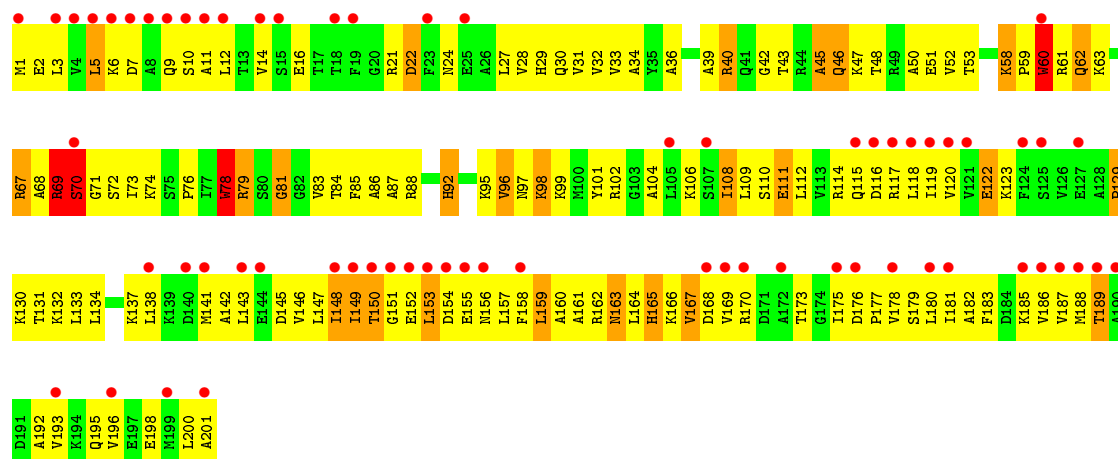




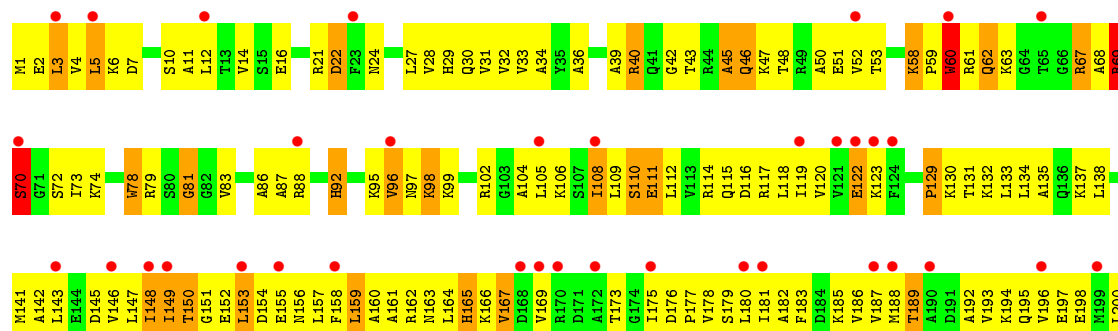
• Molecule 28: 50S ribosomal protein L19



• Molecule 29: 50S ribosomal protein L4

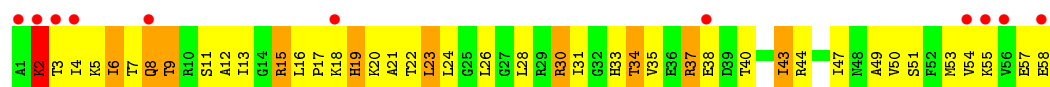


• Molecule 29: 50S ribosomal protein L4

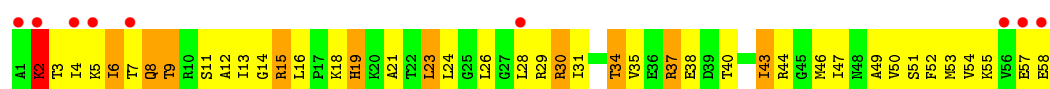




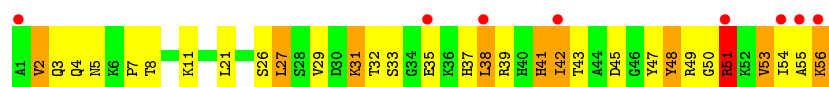
- Molecule 30: 50S ribosomal protein L30



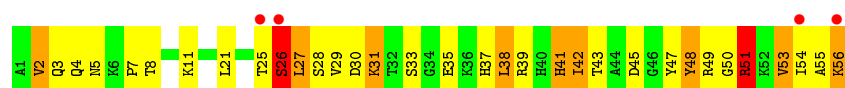
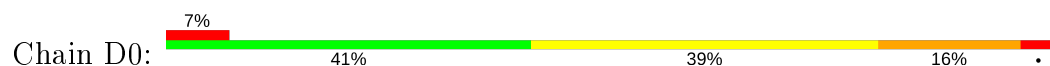
- Molecule 30: 50S ribosomal protein L30



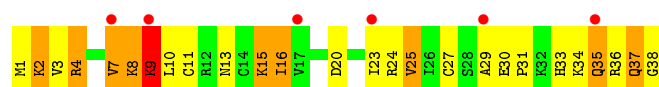
- Molecule 31: 50S ribosomal protein L32



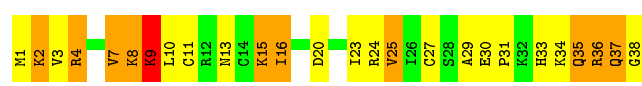
- Molecule 31: 50S ribosomal protein L32



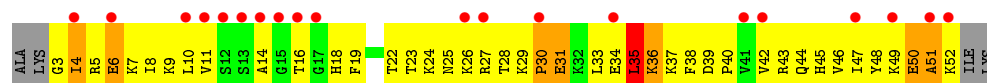
- Molecule 32: 50S ribosomal protein L36



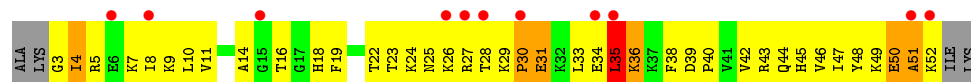
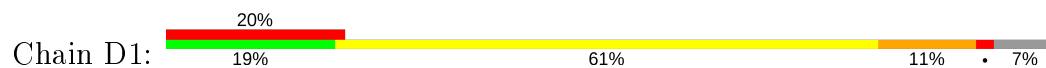
- Molecule 32: 50S ribosomal protein L36



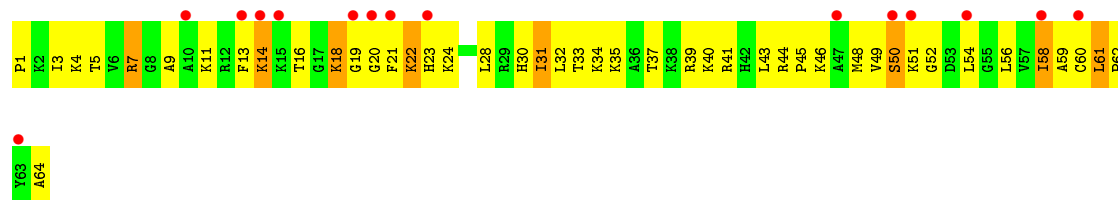
- Molecule 33: 50S ribosomal protein L33



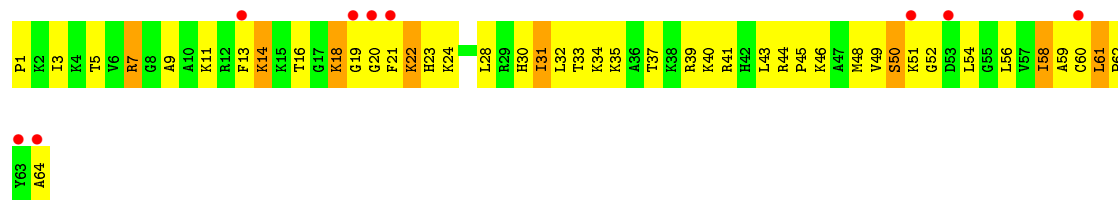
• Molecule 33: 50S ribosomal protein L33



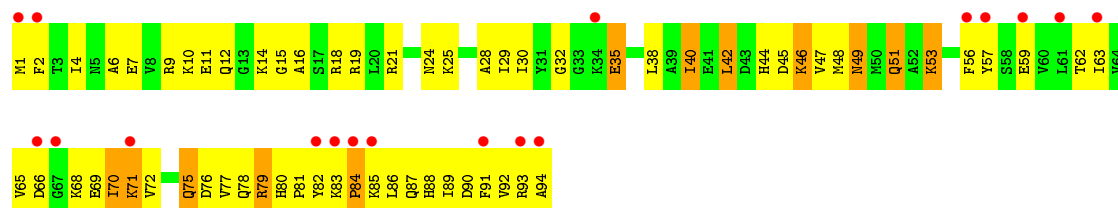
• Molecule 34: 50S ribosomal protein L35



• Molecule 34: 50S ribosomal protein L35

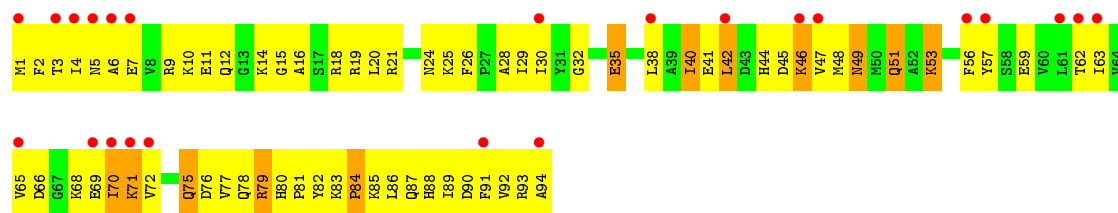


• Molecule 35: 50S ribosomal protein L25

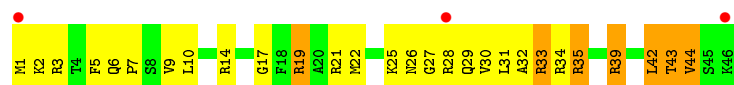


• Molecule 35: 50S ribosomal protein L25

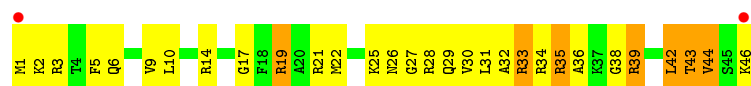




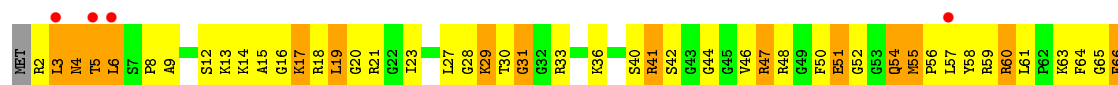
• Molecule 36: 50S ribosomal protein L34



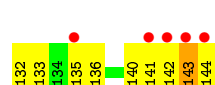
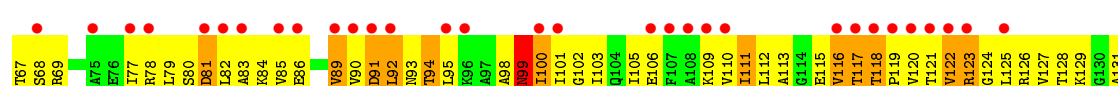
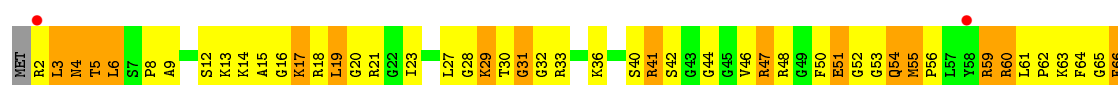
• Molecule 36: 50S ribosomal protein L34



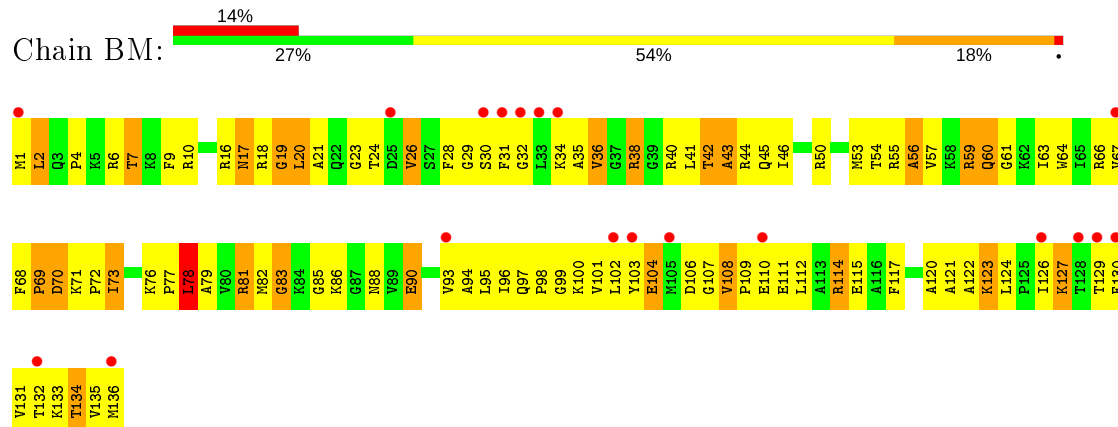
• Molecule 37: 50S ribosomal protein L15



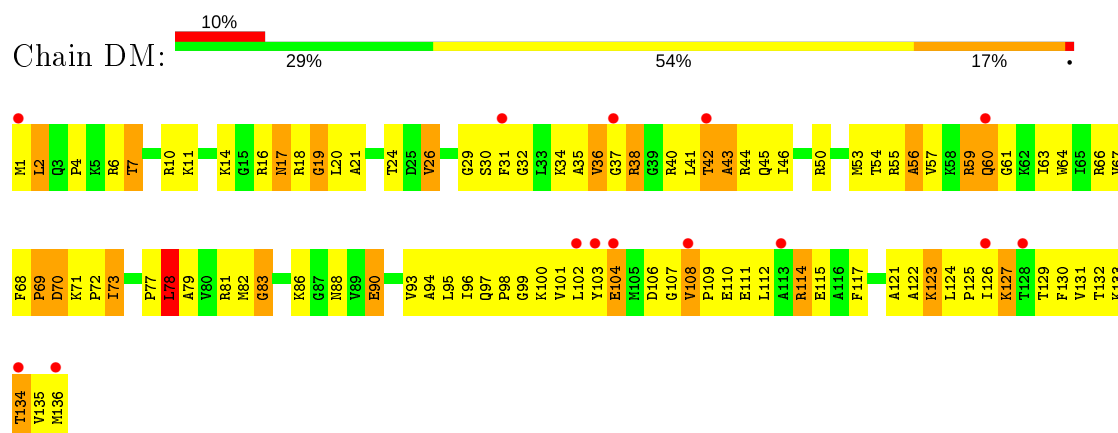
• Molecule 37: 50S ribosomal protein L15



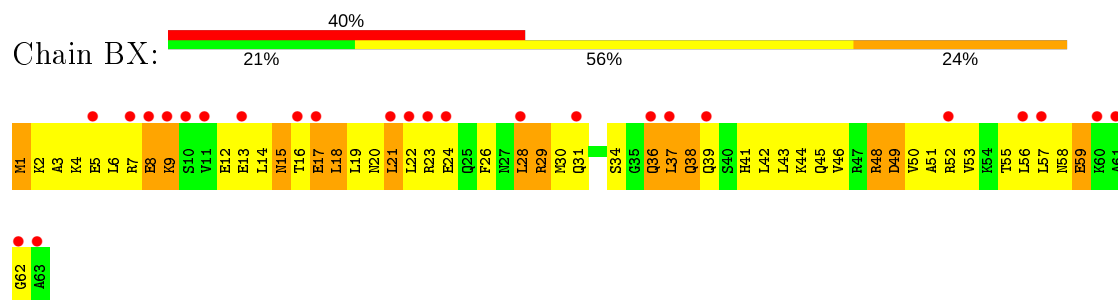
- Molecule 38: 50S ribosomal protein L16



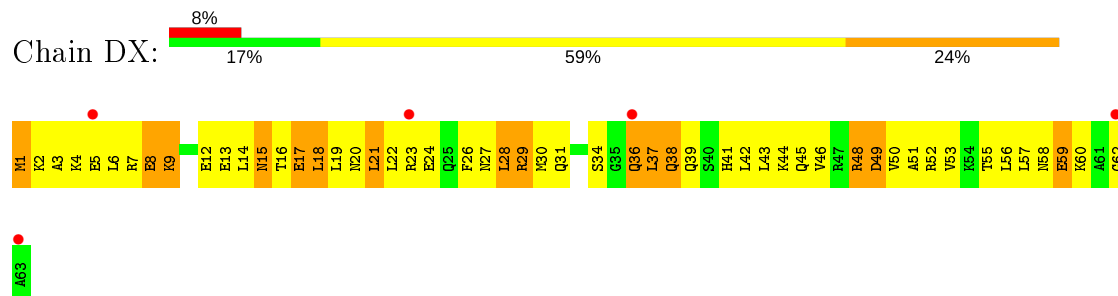
- Molecule 38: 50S ribosomal protein L16



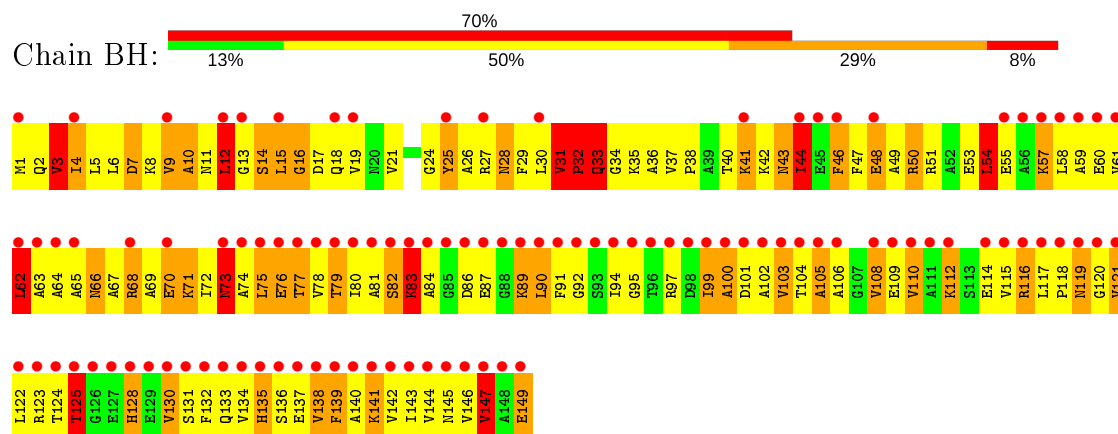
- Molecule 39: 50S ribosomal protein L29



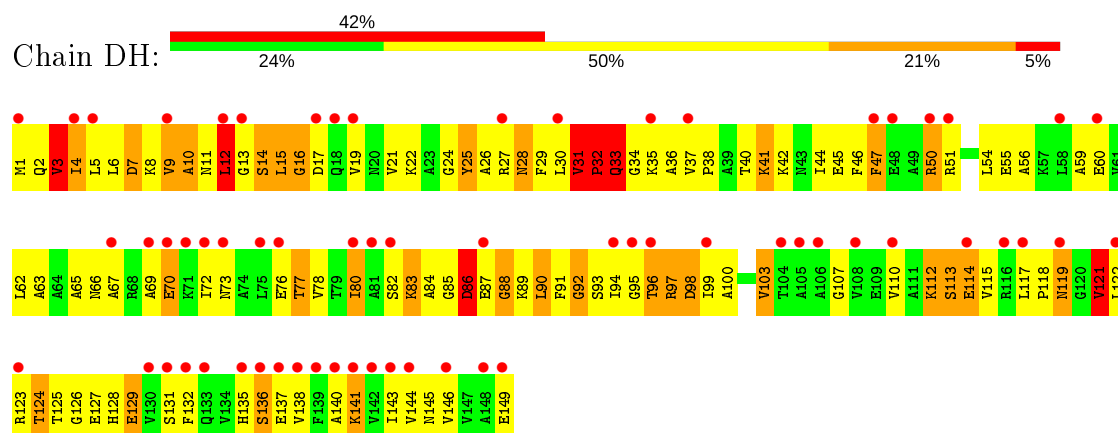
- Molecule 39: 50S ribosomal protein L29



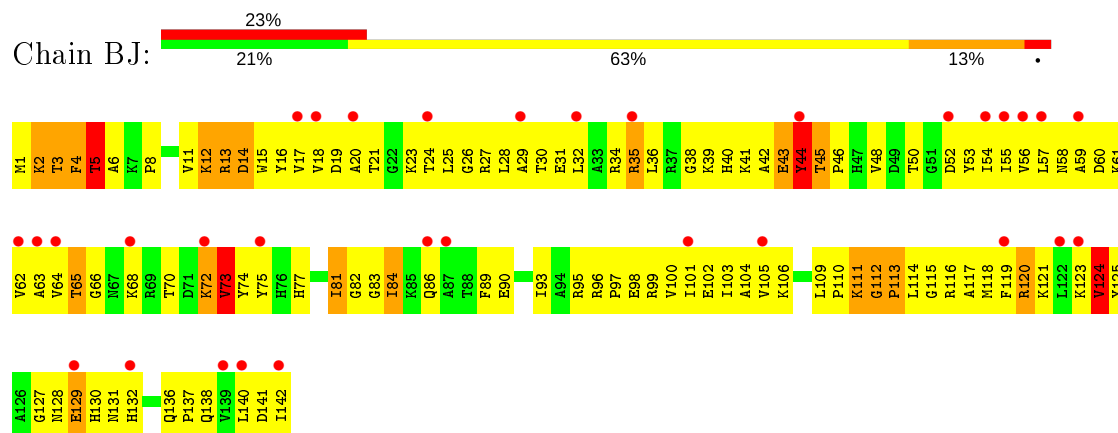
- Molecule 40: 50S ribosomal protein L9



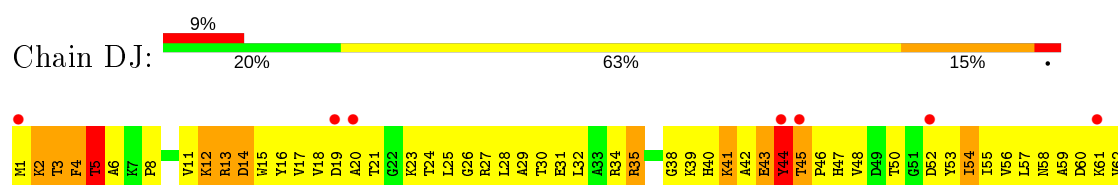
- Molecule 40: 50S ribosomal protein L9



- Molecule 41: 50S ribosomal protein L13

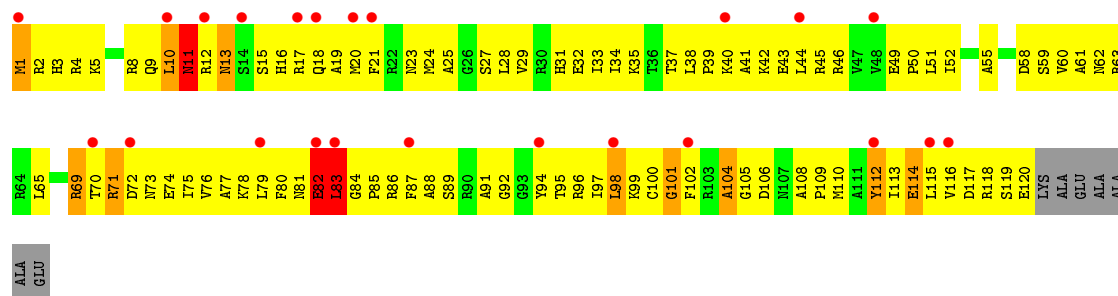


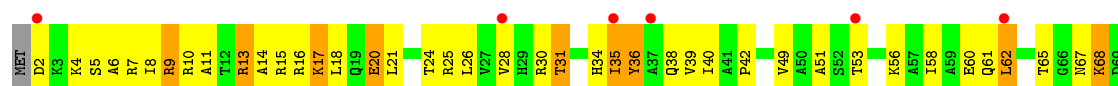
- Molecule 41: 50S ribosomal protein L13



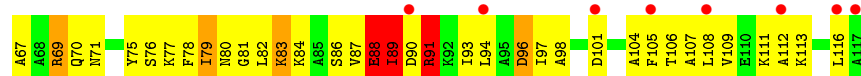


• Molecule 42: 50S ribosomal protein L17

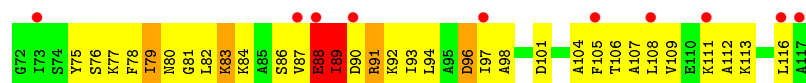
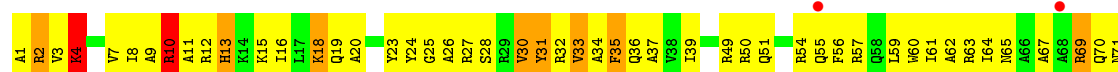




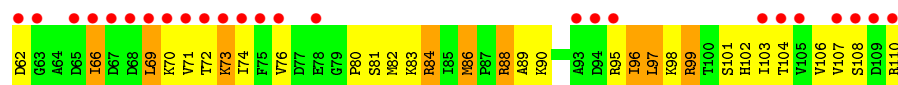
• Molecule 44: 50S ribosomal protein L20



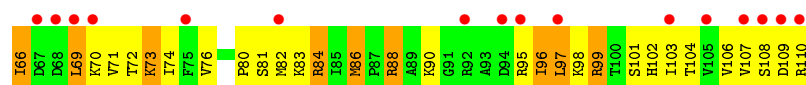
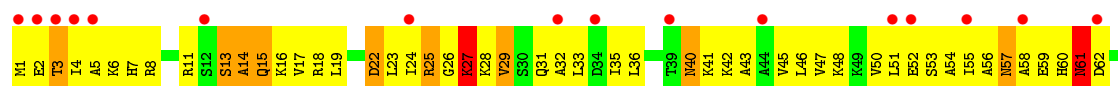
• Molecule 44: 50S ribosomal protein L20



• Molecule 45: 50S ribosomal protein L22



• Molecule 45: 50S ribosomal protein L22



Chain BU:

Chain DU:

Category	Percentage
8%	8%
18%	18%
55%	55%
22%	22%

Chain BF:

29%

20%

52%

26%

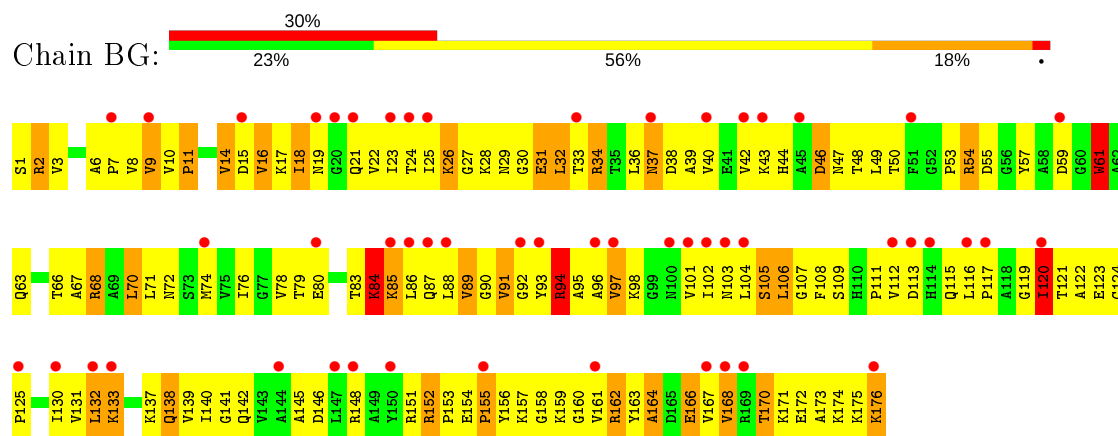
A1
K2
L3
H4
Y7
K8
D9
E10
V11
V12
K13
K14
L15
E18
F19
E20
Y21
V24
V27
F28
E29
V30
E31
K32
I33
T34
L35
N36
M37
G38
V39
G40
E41
A42
I43
A44
D45
K46
K47
L48
L49
D50
N51
A52
A53
A54
D55
L56
I59
S60
G61
Q62
K63
P64
I65
T66
T67
X68
A69
R70
K71
S72
V73
A74
G75
F76
K77
I78
R79
Q80
G81
X82
P83
I84
S85
C86
K87
V88
T89
I90
R91
G92
E93
R94
I95
N96
E97
F98
F99
E100
L101
L102
I103
T104
I105
A106
V107
P108
R109
T110
R111
D112
F113
R114
G115
L116
S117
A118
K119
S120
F121
R124
G125
N126
Y127
S128
M129
G130
V131
K132
E133
Q134
I135
L136
F137
F138
E139
I140
D141
Y142
D143
K144
V145
D146
R147
K148
R149
L150
L151
D152
I153
T154
I155
T156
T157
T158
A159
K160
S161
D162
E163
E164
G165
R166
A167
L168
L169
F170
D171
D173
F174
P175
F176
R177
K178

Chain DF:

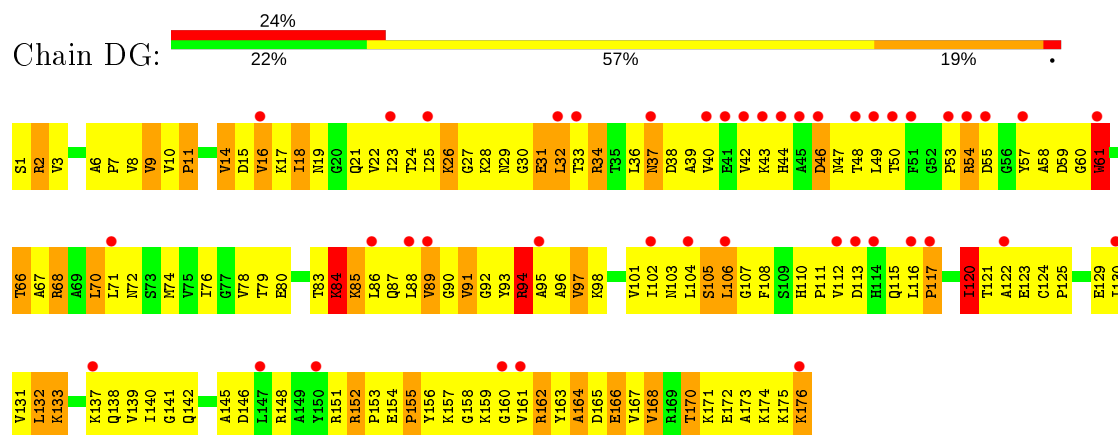
34% 20% 53% 25%

A1 K2 L3 H4 D5 Y6 Y7 K8 D9 E10 V11 V12 K13 L14 L15 M16 T17 E18 F19 N20 Y21 V24 V27 P28 R29 V30 E31 K32 I33 T34 L35 N36 K37 G38 V39 G40 E41 A42 I43 A44 K45 K46 K47 L48 L49 D50 S51 A52 A53 A54 D55 L56 I59 S90 G61 Q62 Y63 P64 L65 L66 T67 K68 A69 K70 K71 S72 V73 A74 G75 F76 K77 P78 R79 Q80 G81 Y82 P83 L84 G85 G86 K87 H88 T89 L90 R91 G92 S93 R94 N95 Y96 E97 F98 F99 E100 R101 L102 E103 T104 I105 A106 V107 P108 R109 L110 R111 D112 F113 R114 L115 G116 L117 S117 A118 K119 S120 F121 D122 G123 R124 G125 N126 Y127 S128 M129 G130 V131 R132 E133 Q134 K135 L136 F137 P138 L140 D141 Y142 D143 K144 V145 D146 L147 V148 R149 G150 L151 D152 I153 T154 L155 T156 T157 L158 A159 K160 S161 D162 E163 E164 G165 R166 A167 L168 L169 A170 A171 F172 D173 F174 P175 F176 R177 K178

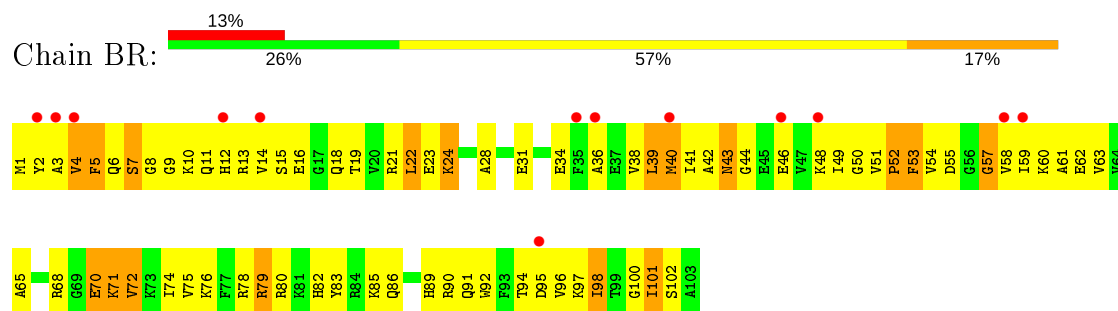
- Molecule 48: 50S ribosomal protein L6



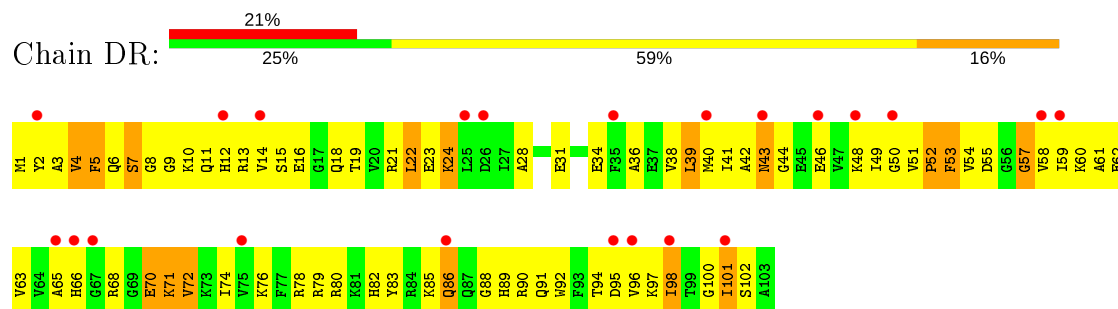
- Molecule 48: 50S ribosomal protein L6



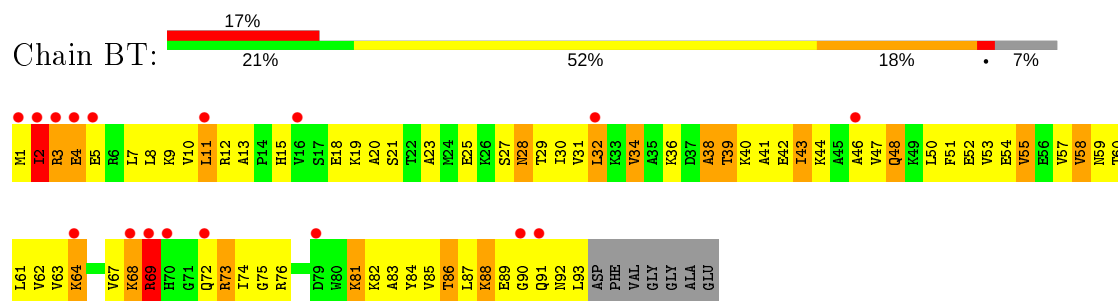
- Molecule 49: 50S ribosomal protein L21



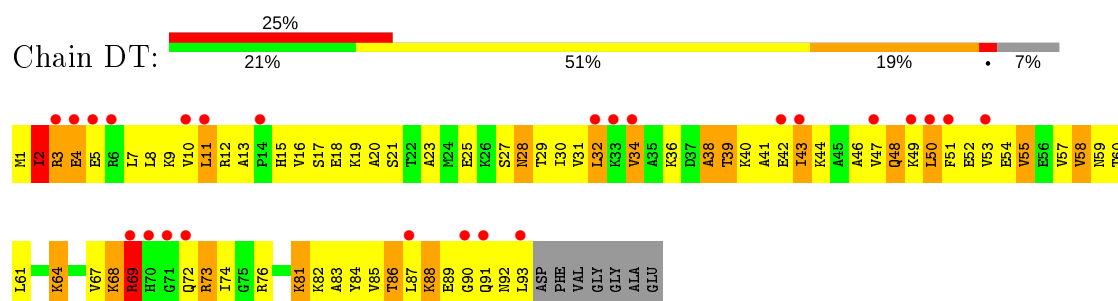
- Molecule 49: 50S ribosomal protein L21



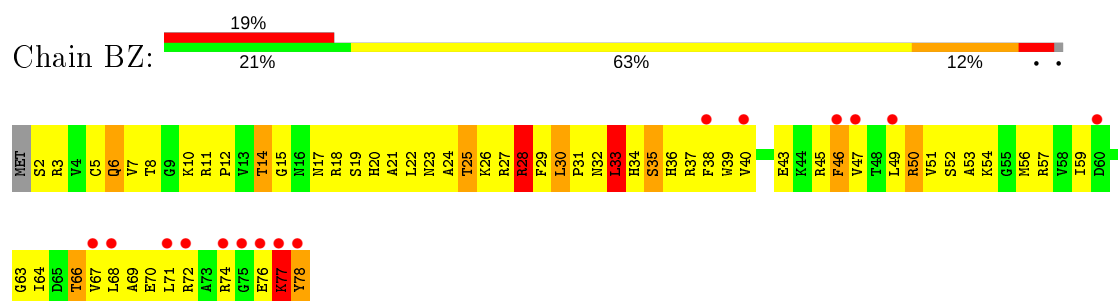
- Molecule 50: 50S ribosomal protein L23



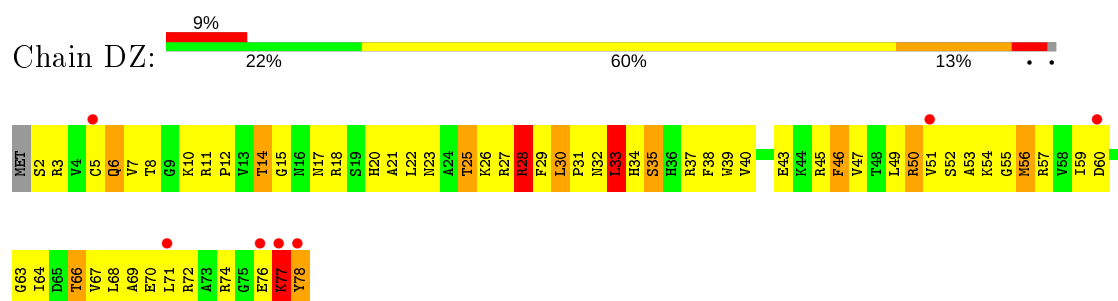
- Molecule 50: 50S ribosomal protein L23



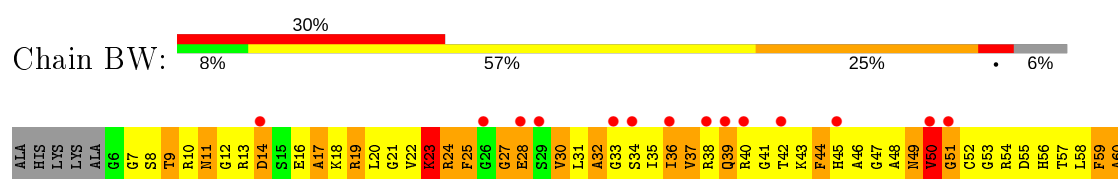
- Molecule 51: 50S ribosomal protein L28

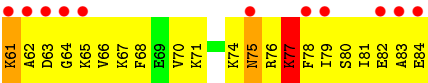


- Molecule 51: 50S ribosomal protein L28

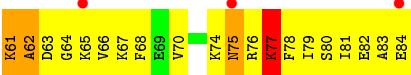
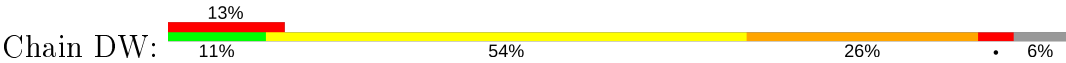


- Molecule 52: 50S ribosomal protein L27





● 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 – 3.21 138.41 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.21) 66.7 (138.41-3.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.309 0.240 , 0.272	Depositor DCC
R_{free} test set	30053 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	284172	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.25	1/36762 (0.0%)	0.75	12/57350 (0.0%)
1	CA	0.26	1/36762 (0.0%)	0.75	16/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.24	0/1118	0.46	0/1504
4	CE	0.23	0/1118	0.46	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	0.45	0/1326
7	CH	0.23	0/989	0.45	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.49	0/1077
10	AK	0.24	0/893	0.47	0/1205
10	CK	0.24	0/893	0.47	0/1205
11	AL	0.22	0/969	0.49	0/1300
11	CL	0.22	0/969	0.49	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.48	0/1043
13	CN	0.24	0/785	0.48	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.23	0/722	0.47	0/964
15	AP	0.25	0/659	0.46	0/884
15	CP	0.25	0/648	0.46	0/870
16	AQ	0.23	0/657	0.47	0/881
16	CQ	0.23	0/666	0.48	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.45	0/621
17	CR	0.23	0/462	0.45	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.48	0/888
19	AT	0.24	0/671	0.40	0/888
19	CT	0.24	0/671	0.40	0/888
20	AB	0.25	0/1735	0.45	0/2338
20	CB	0.25	0/1735	0.45	0/2338
21	AU	0.26	0/430	0.48	0/570
21	CU	0.26	0/430	0.48	0/570
22	BA	0.24	0/2803	0.75	1/4371 (0.0%)
22	DA	0.24	0/2803	0.75	1/4371 (0.0%)
23	BB	0.28	8/68314 (0.0%)	0.77	42/106569 (0.0%)
23	DB	0.28	9/68314 (0.0%)	0.77	48/106569 (0.0%)
24	BI	0.24	0/1046	0.47	0/1410
24	DI	0.25	0/1046	0.49	0/1410
25	BC	0.22	0/2121	0.48	0/2852
25	DC	0.22	0/2121	0.48	0/2852
26	BD	0.24	0/1586	0.49	0/2134
26	DD	0.24	0/1586	0.49	0/2134
27	BK	0.24	0/939	0.56	0/1258
27	DK	0.24	0/939	0.56	0/1258
28	BP	0.24	0/929	0.51	0/1242
28	DP	0.24	0/929	0.51	0/1242
29	BE	0.24	0/1571	0.51	0/2113
29	DE	0.24	0/1571	0.51	0/2113
30	BY	0.23	0/453	0.50	0/605
30	DY	0.23	0/453	0.50	0/605
31	B0	0.22	0/450	0.56	0/599
31	D0	0.22	0/450	0.56	0/599
32	B4	0.23	0/303	0.48	0/397
32	D4	0.23	0/303	0.47	0/397
33	B1	0.27	0/416	0.49	0/554
33	D1	0.27	0/416	0.49	0/554
34	B3	0.24	0/513	0.48	0/676
34	D3	0.24	0/513	0.48	0/676
35	BV	0.25	0/766	0.42	0/1025
35	DV	0.25	0/766	0.42	0/1025
36	B2	0.26	0/380	0.47	0/498
36	D2	0.26	0/380	0.47	0/498
37	BL	0.23	0/1054	0.48	0/1403
37	DL	0.24	0/1054	0.49	0/1403
38	BM	0.25	0/1093	0.49	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.48	0/1460
39	BX	0.24	0/510	0.53	0/677
39	DX	0.24	0/510	0.53	0/677
40	BH	0.25	0/1122	0.48	0/1515
40	DH	0.25	0/1122	0.49	0/1515
41	BJ	0.23	0/1152	0.48	0/1551
41	DJ	0.23	0/1152	0.48	0/1551
42	BN	0.24	0/973	0.52	0/1301
42	DN	0.24	0/973	0.52	0/1301
43	BO	0.23	0/902	0.49	0/1209
43	DO	0.23	0/902	0.49	0/1209
44	BQ	0.26	0/960	0.50	0/1278
44	DQ	0.26	0/960	0.50	0/1278
45	BS	0.22	0/864	0.52	0/1156
45	DS	0.22	0/864	0.52	0/1156
46	BU	0.25	0/787	0.47	0/1051
46	DU	0.25	0/787	0.48	0/1051
47	BF	0.26	0/1444	0.52	0/1937
47	DF	0.26	0/1444	0.52	0/1937
48	BG	0.23	0/1343	0.47	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.25	0/829	0.49	0/1107
49	DR	0.25	0/829	0.49	0/1107
50	BT	0.23	0/744	0.57	0/994
50	DT	0.23	0/744	0.57	0/994
51	BZ	0.25	0/635	0.52	0/848
51	DZ	0.25	0/635	0.52	0/848
52	BW	0.28	0/603	0.53	0/797
52	DW	0.28	0/603	0.53	0/797
All	All	0.26	19/306360 (0.0%)	0.70	120/457969 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	13
1	CA	0	11
23	BB	0	43
23	DB	0	42
All	All	0	109

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-16.27	1.26	1.41
23	BB	1086	A	C5-C6	-16.18	1.26	1.41
23	BB	1088	A	C6-N1	-10.58	1.28	1.35
23	DB	1088	A	C6-N1	-10.47	1.28	1.35
23	DB	2323	G	O3'-P	9.74	1.72	1.61

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-29.64	75.14	110.70
23	BB	2204	G	O5'-P-OP2	-28.20	76.86	110.70
23	BB	2791	G	O5'-P-OP1	-27.64	77.53	110.70
23	DB	2791	G	O5'-P-OP2	-26.90	78.42	110.70
23	BB	2791	G	O5'-P-OP2	18.64	133.06	110.70

There are no chirality outliers.

5 of 109 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	78	A	Sidechain
1	AA	86	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1156	0
1	CA	32831	0	16521	1152	0
2	AC	1624	0	1699	127	0
2	CC	1624	0	1699	127	0
3	AD	1643	0	1710	158	0
3	CD	1643	0	1710	151	0
4	AE	1105	0	1148	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CE	1105	0	1148	95	0
5	AF	817	0	808	83	0
5	CF	817	0	808	79	0
6	AG	1174	0	1230	89	0
6	CG	1196	0	1246	88	0
7	AH	979	0	1034	83	0
7	CH	979	0	1034	82	0
8	AI	1022	0	1070	128	0
8	CI	1022	0	1070	118	0
9	AJ	786	0	828	85	0
9	CJ	786	0	828	89	0
10	AK	877	0	887	94	0
10	CK	877	0	887	93	0
11	AL	955	0	1019	75	0
11	CL	955	0	1019	73	0
12	AM	883	0	944	116	0
12	CM	876	0	937	115	0
13	AN	774	0	827	101	0
13	CN	774	0	827	105	0
14	AO	714	0	734	57	0
14	CO	714	0	734	52	0
15	AP	649	0	666	54	0
15	CP	638	0	656	51	0
16	AQ	648	0	691	42	0
16	CQ	657	0	702	45	0
17	AR	455	0	478	28	0
17	CR	455	0	478	26	0
18	AS	637	0	665	86	0
18	CS	644	0	675	89	0
19	AT	665	0	714	55	0
19	CT	665	0	714	52	0
20	AB	1704	0	1732	199	0
20	CB	1704	0	1732	199	0
21	AU	425	0	449	61	0
21	CU	425	0	449	59	0
22	BA	2507	0	1270	96	0
22	DA	2507	0	1270	89	0
23	BB	60995	0	30678	2146	0
23	DB	60995	0	30677	2248	0
24	BI	1032	0	1088	111	0
24	DI	1032	0	1088	196	0
25	BC	2082	0	2157	259	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DC	2082	0	2157	244	0
26	BD	1565	0	1616	204	0
26	DD	1565	0	1616	214	0
27	BK	930	0	1000	117	0
27	DK	930	0	1000	121	0
28	BP	917	0	965	119	0
28	DP	917	0	965	117	0
29	BE	1552	0	1619	185	0
29	DE	1552	0	1619	165	0
30	BY	449	0	491	52	0
30	DY	449	0	491	47	0
31	B0	444	0	461	45	0
31	D0	444	0	461	46	0
32	B4	302	0	340	30	0
32	D4	302	0	341	28	0
33	B1	409	0	440	51	0
33	D1	409	0	440	42	0
34	B3	504	0	574	56	0
34	D3	504	0	574	51	0
35	BV	753	0	780	80	0
35	DV	753	0	780	83	0
36	B2	377	0	418	44	0
36	D2	377	0	418	47	0
37	BL	1045	0	1117	142	0
37	DL	1045	0	1117	152	0
38	BM	1074	0	1157	115	0
38	DM	1074	0	1157	114	0
39	BX	509	0	543	62	0
39	DX	509	0	543	58	0
40	BH	1111	0	1148	196	0
40	DH	1111	0	1148	153	0
41	BJ	1129	0	1162	146	0
41	DJ	1129	0	1162	148	0
42	BN	960	0	1000	116	0
42	DN	960	0	1000	116	0
43	BO	892	0	923	79	0
43	DO	892	0	923	91	0
44	BQ	947	0	1022	142	0
44	DQ	947	0	1022	147	0
45	BS	857	0	922	103	0
45	DS	857	0	922	100	0
46	BU	779	0	834	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DU	779	0	834	118	0
47	BF	1420	0	1460	231	0
47	DF	1420	0	1460	237	0
48	BG	1323	0	1374	187	0
48	DG	1323	0	1374	189	0
49	BR	816	0	839	97	0
49	DR	816	0	839	102	0
50	BT	738	0	807	129	0
50	DT	738	0	807	122	0
51	BZ	625	0	652	82	0
51	DZ	625	0	652	83	0
52	BW	596	0	610	136	0
52	DW	596	0	610	143	0
53	AA	42	0	46	2	0
53	BB	42	0	46	0	0
53	CA	42	0	46	0	0
53	DB	42	0	46	1	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	60	0	0	0	0
54	CE	1	0	0	0	0
54	CN	1	0	0	0	0
54	DB	111	0	0	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	291	0	0	2	0
56	AL	4	0	0	0	0
56	AN	4	0	0	0	0
56	AT	1	0	0	0	0
56	BB	497	0	0	8	0
56	BC	5	0	0	0	0
56	BE	1	0	0	0	0
56	BL	1	0	0	0	0
56	BN	1	0	0	0	0
56	BR	1	0	0	0	0
56	CA	298	0	0	1	0
56	CE	3	0	0	0	0
56	CL	2	0	0	0	0
56	CN	4	0	0	0	0
56	CP	1	0	0	0	0
56	CT	1	0	0	0	0
56	DB	502	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DC	6	0	0	0	0
56	DE	1	0	0	0	0
56	DL	2	0	0	0	0
56	DR	1	0	0	0	0
All	All	284172	0	190846	16001	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 34.

The worst 5 of 16001 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	1.38	1.21
21:CU:36:PHE:HB3	21:CU:40:PRO:HD3	1.32	1.11
40:DH:31:VAL:HB	40:DH:32:PRO:HD2	1.30	1.11
6:CG:2:ARG:HH11	6:CG:2:ARG:HB3	1.10	1.11
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.29	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%)	155 (76%)	35 (17%)	14 (7%)	1	8
2	CC	204/232 (88%)	155 (76%)	36 (18%)	13 (6%)	1	9
3	AD	203/205 (99%)	154 (76%)	34 (17%)	15 (7%)	1	7
3	CD	203/205 (99%)	151 (74%)	37 (18%)	15 (7%)	1	7
4	AE	148/166 (89%)	120 (81%)	25 (17%)	3 (2%)	7	36
4	CE	148/166 (89%)	120 (81%)	24 (16%)	4 (3%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AF	98/135 (73%)	67 (68%)	26 (26%)	5 (5%)	2	15
5	CF	98/135 (73%)	65 (66%)	28 (29%)	5 (5%)	2	15
6	AG	148/178 (83%)	124 (84%)	18 (12%)	6 (4%)	3	19
6	CG	150/178 (84%)	127 (85%)	18 (12%)	5 (3%)	4	24
7	AH	127/129 (98%)	98 (77%)	25 (20%)	4 (3%)	4	26
7	CH	127/129 (98%)	97 (76%)	27 (21%)	3 (2%)	6	32
8	AI	125/129 (97%)	95 (76%)	20 (16%)	10 (8%)	1	5
8	CI	125/129 (97%)	97 (78%)	19 (15%)	9 (7%)	1	7
9	AJ	96/103 (93%)	73 (76%)	15 (16%)	8 (8%)	1	5
9	CJ	96/103 (93%)	74 (77%)	13 (14%)	9 (9%)	0	3
10	AK	115/128 (90%)	88 (76%)	22 (19%)	5 (4%)	2	19
10	CK	115/128 (90%)	85 (74%)	25 (22%)	5 (4%)	2	19
11	AL	121/123 (98%)	79 (65%)	33 (27%)	9 (7%)	1	7
11	CL	121/123 (98%)	80 (66%)	32 (26%)	9 (7%)	1	7
12	AM	112/117 (96%)	76 (68%)	27 (24%)	9 (8%)	1	5
12	CM	111/117 (95%)	77 (69%)	26 (23%)	8 (7%)	1	7
13	AN	92/100 (92%)	58 (63%)	24 (26%)	10 (11%)	0	2
13	CN	92/100 (92%)	58 (63%)	23 (25%)	11 (12%)	0	2
14	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	3	23
14	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	3	23
15	AP	80/82 (98%)	60 (75%)	14 (18%)	6 (8%)	1	6
15	CP	78/82 (95%)	58 (74%)	14 (18%)	6 (8%)	1	6
16	AQ	78/83 (94%)	58 (74%)	16 (20%)	4 (5%)	2	15
16	CQ	79/83 (95%)	59 (75%)	16 (20%)	4 (5%)	2	15
17	AR	53/74 (72%)	43 (81%)	8 (15%)	2 (4%)	3	21
17	CR	53/74 (72%)	43 (81%)	9 (17%)	1 (2%)	8	38
18	AS	77/91 (85%)	54 (70%)	17 (22%)	6 (8%)	1	6
18	CS	78/91 (86%)	54 (69%)	17 (22%)	7 (9%)	1	4
19	AT	83/86 (96%)	65 (78%)	12 (14%)	6 (7%)	1	7
19	CT	83/86 (96%)	66 (80%)	11 (13%)	6 (7%)	1	7
20	AB	216/240 (90%)	150 (69%)	44 (20%)	22 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	CB	216/240 (90%)	147 (68%)	48 (22%)	21 (10%)	0	3
21	AU	49/70 (70%)	28 (57%)	11 (22%)	10 (20%)	0	0
21	CU	49/70 (70%)	28 (57%)	10 (20%)	11 (22%)	0	0
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	3	22
24	DI	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	3	22
25	BC	269/272 (99%)	174 (65%)	49 (18%)	46 (17%)	0	0
25	DC	269/272 (99%)	174 (65%)	47 (18%)	48 (18%)	0	0
26	BD	207/209 (99%)	112 (54%)	63 (30%)	32 (16%)	0	1
26	DD	207/209 (99%)	114 (55%)	58 (28%)	35 (17%)	0	0
27	BK	119/123 (97%)	75 (63%)	28 (24%)	16 (13%)	0	1
27	DK	119/123 (97%)	75 (63%)	27 (23%)	17 (14%)	0	1
28	BP	112/114 (98%)	62 (55%)	35 (31%)	15 (13%)	0	1
28	DP	112/114 (98%)	63 (56%)	34 (30%)	15 (13%)	0	1
29	BE	199/201 (99%)	131 (66%)	51 (26%)	17 (8%)	1	4
29	DE	199/201 (99%)	130 (65%)	53 (27%)	16 (8%)	1	5
30	BY	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	0	2
30	DY	56/58 (97%)	37 (66%)	13 (23%)	6 (11%)	0	2
31	B0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	0	3
31	D0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	0	3
32	B4	36/38 (95%)	21 (58%)	7 (19%)	8 (22%)	0	0
32	D4	36/38 (95%)	20 (56%)	7 (19%)	9 (25%)	0	0
33	B1	48/54 (89%)	37 (77%)	5 (10%)	6 (12%)	0	1
33	D1	48/54 (89%)	37 (77%)	5 (10%)	6 (12%)	0	1
34	B3	62/64 (97%)	44 (71%)	13 (21%)	5 (8%)	1	5
34	D3	62/64 (97%)	44 (71%)	13 (21%)	5 (8%)	1	5
35	BV	92/94 (98%)	65 (71%)	23 (25%)	4 (4%)	2	19
35	DV	92/94 (98%)	65 (71%)	23 (25%)	4 (4%)	2	19
36	B2	44/46 (96%)	29 (66%)	14 (32%)	1 (2%)	6	33
36	D2	44/46 (96%)	28 (64%)	15 (34%)	1 (2%)	6	33
37	BL	141/144 (98%)	88 (62%)	30 (21%)	23 (16%)	0	1
37	DL	141/144 (98%)	88 (62%)	29 (21%)	24 (17%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BM	134/136 (98%)	86 (64%)	31 (23%)	17 (13%)	0	1
38	DM	134/136 (98%)	86 (64%)	32 (24%)	16 (12%)	0	2
39	BX	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	1	5
39	DX	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	1	5
40	BH	147/149 (99%)	77 (52%)	41 (28%)	29 (20%)	0	0
40	DH	147/149 (99%)	85 (58%)	39 (26%)	23 (16%)	0	1
41	BJ	140/142 (99%)	88 (63%)	36 (26%)	16 (11%)	0	2
41	DJ	140/142 (99%)	89 (64%)	33 (24%)	18 (13%)	0	1
42	BN	118/127 (93%)	72 (61%)	34 (29%)	12 (10%)	0	3
42	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	0	3
43	BO	114/117 (97%)	84 (74%)	25 (22%)	5 (4%)	2	18
43	DO	114/117 (97%)	83 (73%)	25 (22%)	6 (5%)	2	14
44	BQ	115/117 (98%)	73 (64%)	34 (30%)	8 (7%)	1	7
44	DQ	115/117 (98%)	70 (61%)	38 (33%)	7 (6%)	1	11
45	BS	108/110 (98%)	69 (64%)	28 (26%)	11 (10%)	0	3
45	DS	108/110 (98%)	69 (64%)	29 (27%)	10 (9%)	0	3
46	BU	100/103 (97%)	53 (53%)	25 (25%)	22 (22%)	0	0
46	DU	100/103 (97%)	54 (54%)	23 (23%)	23 (23%)	0	0
47	BF	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0	1
47	DF	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0	1
48	BG	174/176 (99%)	100 (58%)	48 (28%)	26 (15%)	0	1
48	DG	174/176 (99%)	101 (58%)	48 (28%)	25 (14%)	0	1
49	BR	101/103 (98%)	65 (64%)	25 (25%)	11 (11%)	0	2
49	DR	101/103 (98%)	64 (63%)	28 (28%)	9 (9%)	1	4
50	BT	91/100 (91%)	50 (55%)	31 (34%)	10 (11%)	0	2
50	DT	91/100 (91%)	51 (56%)	30 (33%)	10 (11%)	0	2
51	BZ	75/78 (96%)	53 (71%)	18 (24%)	4 (5%)	2	14
51	DZ	75/78 (96%)	50 (67%)	21 (28%)	4 (5%)	2	14
52	BW	77/84 (92%)	29 (38%)	27 (35%)	21 (27%)	0	0
52	DW	77/84 (92%)	29 (38%)	26 (34%)	22 (29%)	0	0
All	All	11241/11914 (94%)	7579 (67%)	2528 (22%)	1134 (10%)	0	3

5 of 1134 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	54	ILE
2	AC	153	SER
2	AC	205	GLU
5	AF	92	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	137 (81%)	33 (19%)	1	7
2	CC	170/189 (90%)	137 (81%)	33 (19%)	1	7
3	AD	172/172 (100%)	148 (86%)	24 (14%)	3	15
3	CD	172/172 (100%)	148 (86%)	24 (14%)	3	15
4	AE	113/125 (90%)	95 (84%)	18 (16%)	2	11
4	CE	113/125 (90%)	95 (84%)	18 (16%)	2	11
5	AF	87/116 (75%)	71 (82%)	16 (18%)	1	8
5	CF	87/116 (75%)	70 (80%)	17 (20%)	1	7
6	AG	123/146 (84%)	104 (85%)	19 (15%)	2	12
6	CG	125/146 (86%)	103 (82%)	22 (18%)	2	9
7	AH	104/104 (100%)	95 (91%)	9 (9%)	10	36
7	CH	104/104 (100%)	94 (90%)	10 (10%)	8	31
8	AI	105/106 (99%)	88 (84%)	17 (16%)	2	11
8	CI	105/106 (99%)	87 (83%)	18 (17%)	2	9
9	AJ	86/90 (96%)	71 (83%)	15 (17%)	2	9
9	CJ	86/90 (96%)	71 (83%)	15 (17%)	2	9
10	AK	90/98 (92%)	76 (84%)	14 (16%)	2	11
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2	9
11	AL	103/103 (100%)	88 (85%)	15 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	CL	103/103 (100%)	88 (85%)	15 (15%)	3	14
12	AM	92/95 (97%)	76 (83%)	16 (17%)	2	9
12	CM	91/95 (96%)	75 (82%)	16 (18%)	2	9
13	AN	79/83 (95%)	65 (82%)	14 (18%)	2	9
13	CN	79/83 (95%)	65 (82%)	14 (18%)	2	9
14	AO	76/77 (99%)	70 (92%)	6 (8%)	12	42
14	CO	76/77 (99%)	70 (92%)	6 (8%)	12	42
15	AP	65/65 (100%)	58 (89%)	7 (11%)	6	26
15	CP	65/65 (100%)	59 (91%)	6 (9%)	9	33
16	AQ	74/77 (96%)	65 (88%)	9 (12%)	5	21
16	CQ	75/77 (97%)	66 (88%)	9 (12%)	5	21
17	AR	48/64 (75%)	40 (83%)	8 (17%)	2	10
17	CR	48/64 (75%)	41 (85%)	7 (15%)	3	14
18	AS	70/78 (90%)	56 (80%)	14 (20%)	1	6
18	CS	71/78 (91%)	57 (80%)	14 (20%)	1	6
19	AT	65/65 (100%)	54 (83%)	11 (17%)	2	10
19	CT	65/65 (100%)	54 (83%)	11 (17%)	2	10
20	AB	180/198 (91%)	148 (82%)	32 (18%)	2	9
20	CB	180/198 (91%)	150 (83%)	30 (17%)	2	10
21	AU	44/60 (73%)	30 (68%)	14 (32%)	0	0
21	CU	44/60 (73%)	30 (68%)	14 (32%)	0	0
24	BI	109/109 (100%)	107 (98%)	2 (2%)	59	81
24	DI	109/109 (100%)	104 (95%)	5 (5%)	27	62
25	BC	216/217 (100%)	176 (82%)	40 (18%)	1	8
25	DC	216/217 (100%)	176 (82%)	40 (18%)	1	8
26	BD	164/164 (100%)	142 (87%)	22 (13%)	4	17
26	DD	164/164 (100%)	141 (86%)	23 (14%)	3	15
27	BK	102/104 (98%)	79 (78%)	23 (22%)	1	4
27	DK	102/104 (98%)	79 (78%)	23 (22%)	1	4
28	BP	99/99 (100%)	81 (82%)	18 (18%)	1	8
28	DP	99/99 (100%)	81 (82%)	18 (18%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BE	165/165 (100%)	136 (82%)	29 (18%)	2	9
29	DE	165/165 (100%)	137 (83%)	28 (17%)	2	9
30	BY	48/48 (100%)	38 (79%)	10 (21%)	1	5
30	DY	48/48 (100%)	38 (79%)	10 (21%)	1	5
31	B0	47/47 (100%)	36 (77%)	11 (23%)	1	3
31	D0	47/47 (100%)	35 (74%)	12 (26%)	0	2
32	B4	34/34 (100%)	28 (82%)	6 (18%)	2	9
32	D4	34/34 (100%)	28 (82%)	6 (18%)	2	9
33	B1	45/48 (94%)	40 (89%)	5 (11%)	6	25
33	D1	45/48 (94%)	41 (91%)	4 (9%)	9	35
34	B3	51/51 (100%)	47 (92%)	4 (8%)	12	42
34	D3	51/51 (100%)	47 (92%)	4 (8%)	12	42
35	BV	78/78 (100%)	62 (80%)	16 (20%)	1	6
35	DV	78/78 (100%)	62 (80%)	16 (20%)	1	6
36	B2	38/38 (100%)	32 (84%)	6 (16%)	2	11
36	D2	38/38 (100%)	32 (84%)	6 (16%)	2	11
37	BL	102/103 (99%)	89 (87%)	13 (13%)	4	19
37	DL	102/103 (99%)	88 (86%)	14 (14%)	3	16
38	BM	109/109 (100%)	91 (84%)	18 (16%)	2	10
38	DM	109/109 (100%)	91 (84%)	18 (16%)	2	10
39	BX	55/55 (100%)	40 (73%)	15 (27%)	0	1
39	DX	55/55 (100%)	40 (73%)	15 (27%)	0	1
40	BH	114/114 (100%)	64 (56%)	50 (44%)	0	0
40	DH	114/114 (100%)	86 (75%)	28 (25%)	0	2
41	BJ	116/116 (100%)	101 (87%)	15 (13%)	4	19
41	DJ	116/116 (100%)	100 (86%)	16 (14%)	3	16
42	BN	100/103 (97%)	87 (87%)	13 (13%)	4	18
42	DN	100/103 (97%)	87 (87%)	13 (13%)	4	18
43	BO	86/87 (99%)	70 (81%)	16 (19%)	1	8
43	DO	86/87 (99%)	70 (81%)	16 (19%)	1	8
44	BQ	89/89 (100%)	74 (83%)	15 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	10
45	BS	93/93 (100%)	79 (85%)	14 (15%)	3	13
45	DS	93/93 (100%)	79 (85%)	14 (15%)	3	13
46	BU	83/84 (99%)	68 (82%)	15 (18%)	1	8
46	DU	83/84 (99%)	68 (82%)	15 (18%)	1	8
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1	3
47	DF	149/149 (100%)	115 (77%)	34 (23%)	1	4
48	BG	137/137 (100%)	113 (82%)	24 (18%)	2	9
48	DG	137/137 (100%)	113 (82%)	24 (18%)	2	9
49	BR	84/84 (100%)	73 (87%)	11 (13%)	4	18
49	DR	84/84 (100%)	73 (87%)	11 (13%)	4	18
50	BT	80/84 (95%)	66 (82%)	14 (18%)	2	9
50	DT	80/84 (95%)	65 (81%)	15 (19%)	1	8
51	BZ	67/68 (98%)	52 (78%)	15 (22%)	1	4
51	DZ	67/68 (98%)	52 (78%)	15 (22%)	1	4
52	BW	59/62 (95%)	45 (76%)	14 (24%)	1	3
52	DW	59/62 (95%)	45 (76%)	14 (24%)	1	3
All	All	9333/9700 (96%)	7746 (83%)	1587 (17%)	2	9

5 of 1587 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BF	168	LEU
5	CF	86	ARG
46	DU	51	LEU
48	BG	120	ILE
2	CC	27	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 343 such sidechains are listed below:

Mol	Chain	Res	Type
48	BG	63	GLN
4	CE	81	GLN
46	DU	45	GLN
48	BG	114	HIS

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Mol	Chain	Res	Type
52	BW	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	239 (15%)	16 (1%)
1	CA	1529/1542 (99%)	229 (14%)	17 (1%)
22	BA	116/120 (96%)	17 (14%)	1 (0%)
22	DA	116/120 (96%)	17 (14%)	1 (0%)
23	BB	2837/2904 (97%)	435 (15%)	18 (0%)
23	DB	2837/2904 (97%)	433 (15%)	20 (0%)
All	All	8964/9132 (98%)	1370 (15%)	73 (0%)

5 of 1370 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	31	G
1	AA	32	A

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2894	G
1	CA	366	A
23	DB	2336	A
1	CA	243	A
1	CA	428	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	NMY	BB	3001	-	45,45,45	2.05	13 (28%)	63,67,67	1.20	7 (11%)
53	NMY	AA	1601	-	45,45,45	2.03	13 (28%)	63,67,67	1.18	5 (7%)
53	NMY	CA	1601	-	45,45,45	2.02	12 (26%)	63,67,67	1.29	8 (12%)
53	NMY	DB	3001	-	45,45,45	2.10	13 (28%)	63,67,67	1.30	7 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	NMY	BB	3001	-	-	4/18/94/94	0/4/4/4
53	NMY	AA	1601	-	-	4/18/94/94	0/4/4/4
53	NMY	CA	1601	-	-	5/18/94/94	0/4/4/4
53	NMY	DB	3001	-	-	4/18/94/94	0/4/4/4

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	DB	3001	NMY	C23-C22	5.27	1.59	1.52
53	BB	3001	NMY	C23-C22	5.17	1.59	1.52
53	AA	1601	NMY	C23-C22	5.06	1.58	1.52
53	CA	1601	NMY	C23-C22	4.92	1.58	1.52
53	CA	1601	NMY	O22-C18	4.78	1.54	1.41

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DB	3001	NMY	O11-C13-O16	4.60	116.41	111.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DB	3001	NMY	O18-C18-C19	4.01	115.12	108.22
53	CA	1601	NMY	O18-C18-C19	3.75	114.67	108.22
53	BB	3001	NMY	O18-C18-C19	3.63	114.46	108.22
53	AA	1601	NMY	O18-C18-C19	3.50	114.24	108.22

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	AA	1601	NMY	O16-C16-C17-O17
53	BB	3001	NMY	C19-C18-O18-C15
53	CA	1601	NMY	C14-C13-O11-C11
53	DB	3001	NMY	C19-C18-O18-C15
53	CA	1601	NMY	O16-C16-C17-O17

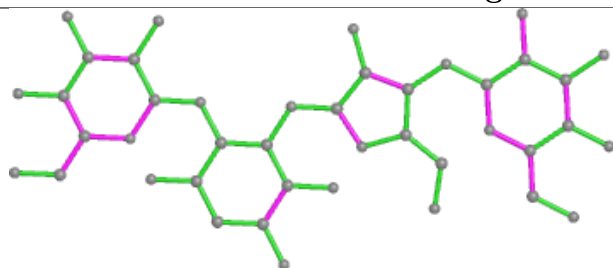
There are no ring outliers.

2 monomers are involved in 3 short contacts:

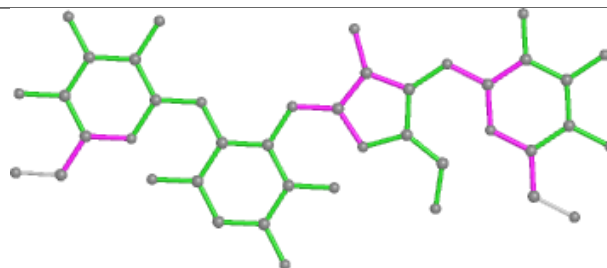
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	AA	1601	NMY	2	0
53	DB	3001	NMY	1	0

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.

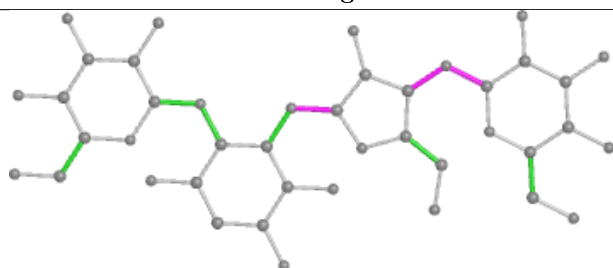
Ligand NMY BB 3001



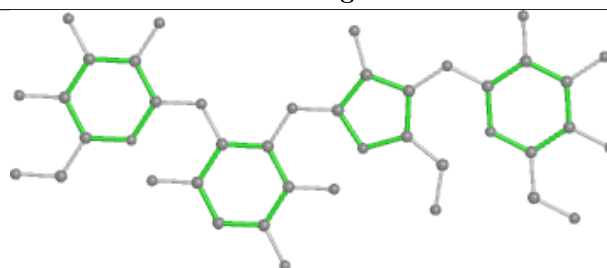
Bond lengths



Bond angles

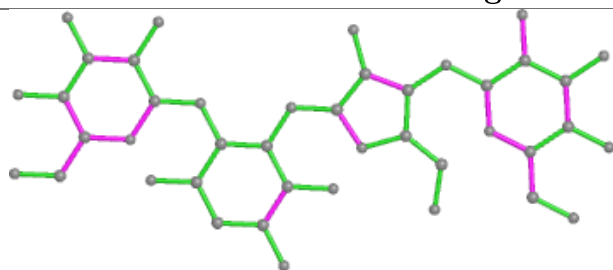


Torsions

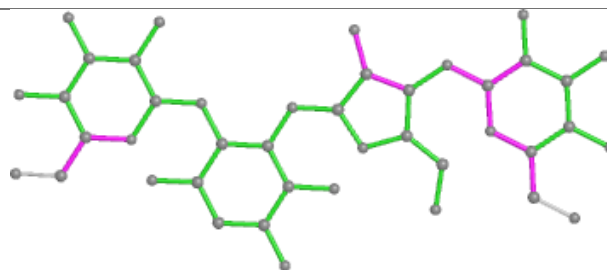


Rings

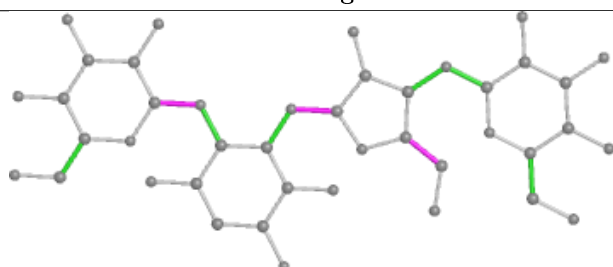
Ligand NMY AA 1601



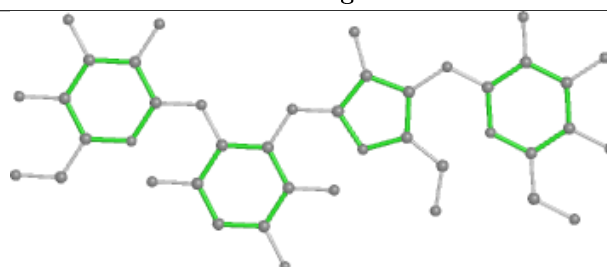
Bond lengths



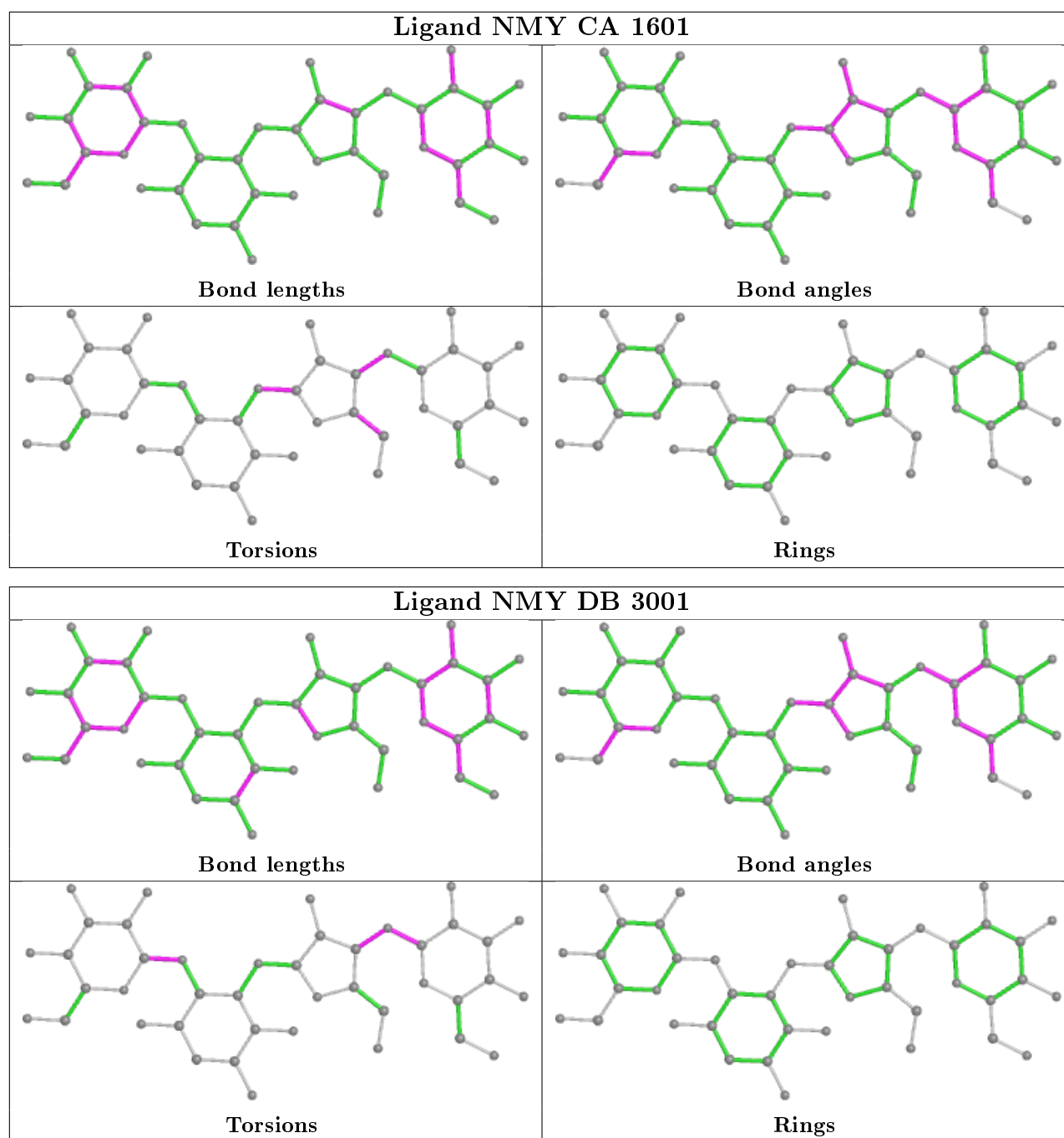
Bond angles



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%)	-0.62	11 (0%) 87 82	22, 76, 152, 180	0
1	CA	1530/1542 (99%)	-0.63	3 (0%) 95 94	12, 57, 136, 180	0
2	AC	206/232 (88%)	0.76	34 (16%) 1 1	16, 66, 135, 180	0
2	CC	206/232 (88%)	0.73	28 (13%) 3 2	14, 74, 124, 180	0
3	AD	205/205 (100%)	1.28	52 (25%) 0 0	8, 84, 155, 180	0
3	CD	205/205 (100%)	0.85	28 (13%) 3 2	15, 62, 135, 180	0
4	AE	150/166 (90%)	0.71	15 (10%) 7 4	7, 67, 122, 158	0
4	CE	150/166 (90%)	1.10	33 (22%) 0 0	10, 59, 122, 180	0
5	AF	100/135 (74%)	1.48	31 (31%) 0 0	32, 80, 148, 180	0
5	CF	100/135 (74%)	0.97	15 (15%) 2 1	23, 69, 138, 180	0
6	AG	150/178 (84%)	0.70	23 (15%) 2 1	39, 105, 151, 180	0
6	CG	152/178 (85%)	0.22	9 (5%) 22 13	32, 89, 152, 180	0
7	AH	129/129 (100%)	1.30	40 (31%) 0 0	29, 79, 133, 180	0
7	CH	129/129 (100%)	0.61	17 (13%) 3 2	7, 55, 120, 148	0
8	AI	127/129 (98%)	0.80	25 (19%) 1 0	37, 90, 164, 180	0
8	CI	127/129 (98%)	0.59	16 (12%) 3 2	32, 95, 162, 180	0
9	AJ	98/103 (95%)	0.96	19 (19%) 1 0	17, 85, 158, 180	0
9	CJ	98/103 (95%)	1.06	22 (22%) 0 0	22, 89, 150, 180	0
10	AK	117/128 (91%)	0.47	7 (5%) 21 13	17, 63, 128, 162	0
10	CK	117/128 (91%)	0.14	2 (1%) 70 58	10, 51, 116, 164	0
11	AL	123/123 (100%)	0.85	18 (14%) 2 1	19, 74, 135, 180	0
11	CL	123/123 (100%)	0.58	6 (4%) 29 18	6, 50, 127, 180	0
12	AM	114/117 (97%)	0.64	16 (14%) 2 2	52, 119, 180, 180	0
12	CM	113/117 (96%)	0.70	16 (14%) 2 2	53, 105, 167, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.56	8 (8%) 11 6	24, 79, 118, 152	0
13	CN	96/100 (96%)	0.61	12 (12%) 3 2	26, 82, 119, 139	0
14	AO	88/89 (98%)	1.20	21 (23%) 0 0	39, 76, 123, 180	0
14	CO	88/89 (98%)	0.35	3 (3%) 45 31	15, 55, 123, 154	0
15	AP	82/82 (100%)	1.47	19 (23%) 0 0	30, 87, 150, 180	0
15	CP	80/82 (97%)	0.58	10 (12%) 3 2	8, 56, 135, 180	0
16	AQ	80/83 (96%)	1.20	21 (26%) 0 0	49, 96, 155, 180	0
16	CQ	81/83 (97%)	0.56	8 (9%) 7 5	25, 66, 128, 180	0
17	AR	55/74 (74%)	0.98	8 (14%) 2 1	15, 74, 125, 165	0
17	CR	55/74 (74%)	0.65	7 (12%) 3 2	19, 63, 119, 170	0
18	AS	79/91 (86%)	0.96	19 (24%) 0 0	73, 121, 176, 180	0
18	CS	80/91 (87%)	0.97	16 (20%) 1 0	58, 109, 168, 180	0
19	AT	85/86 (98%)	0.45	9 (10%) 6 4	52, 104, 164, 180	0
19	CT	85/86 (98%)	0.05	4 (4%) 31 20	22, 62, 125, 179	0
20	AB	218/240 (90%)	0.89	45 (20%) 1 0	29, 99, 155, 180	0
20	CB	218/240 (90%)	1.28	65 (29%) 0 0	31, 102, 160, 180	0
21	AU	51/70 (72%)	1.03	11 (21%) 0 0	43, 92, 146, 180	0
21	CU	51/70 (72%)	0.71	6 (11%) 4 3	40, 85, 133, 166	0
22	BA	117/120 (97%)	-0.68	1 (0%) 84 76	49, 83, 138, 174	0
22	DA	117/120 (97%)	-0.58	1 (0%) 84 76	36, 75, 124, 180	0
23	BB	2841/2904 (97%)	-0.38	27 (0%) 82 73	16, 60, 154, 180	0
23	DB	2841/2904 (97%)	-0.41	10 (0%) 92 89	6, 47, 151, 180	0
24	BI	141/141 (100%)	3.62	97 (68%) 0 0	93, 176, 180, 180	0
24	DI	141/141 (100%)	1.95	60 (42%) 0 0	101, 177, 180, 180	0
25	BC	271/272 (99%)	0.91	43 (15%) 1 1	9, 50, 104, 180	0
25	DC	271/272 (99%)	0.84	38 (14%) 2 2	5, 35, 87, 135	0
26	BD	209/209 (100%)	0.91	38 (18%) 1 1	20, 76, 135, 180	0
26	DD	209/209 (100%)	1.00	36 (17%) 1 1	5, 50, 126, 180	0
27	BK	121/123 (98%)	1.90	50 (41%) 0 0	14, 72, 133, 180	0
27	DK	121/123 (98%)	1.25	26 (21%) 0 0	6, 43, 104, 164	0
28	BP	114/114 (100%)	1.94	52 (45%) 0 0	35, 86, 151, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.68	12 (10%) 6 4	6, 49, 113, 160	0
29	BE	201/201 (100%)	1.42	65 (32%) 0 0	10, 67, 144, 180	0
29	DE	201/201 (100%)	0.99	37 (18%) 1 0	5, 72, 137, 180	0
30	BY	58/58 (100%)	0.83	11 (18%) 1 0	34, 74, 139, 180	0
30	DY	58/58 (100%)	0.60	9 (15%) 2 1	21, 60, 141, 177	0
31	B0	56/56 (100%)	0.84	8 (14%) 2 2	15, 74, 151, 180	0
31	D0	56/56 (100%)	0.49	4 (7%) 16 10	9, 49, 124, 180	0
32	B4	38/38 (100%)	0.78	6 (15%) 2 1	35, 91, 145, 151	0
32	D4	38/38 (100%)	-0.13	0 100 100	18, 68, 129, 150	0
33	B1	50/54 (92%)	2.09	20 (40%) 0 0	52, 90, 134, 174	0
33	D1	50/54 (92%)	1.17	11 (22%) 0 0	14, 76, 127, 175	0
34	B3	64/64 (100%)	1.02	15 (23%) 0 0	26, 59, 87, 158	0
34	D3	64/64 (100%)	0.79	9 (14%) 2 2	9, 49, 112, 156	0
35	BV	94/94 (100%)	0.90	18 (19%) 1 0	29, 97, 155, 178	0
35	DV	94/94 (100%)	1.02	23 (24%) 0 0	21, 89, 153, 167	0
36	B2	46/46 (100%)	0.55	3 (6%) 18 11	14, 50, 83, 144	0
36	D2	46/46 (100%)	0.48	2 (4%) 35 23	5, 38, 76, 180	0
37	BL	143/144 (99%)	0.87	26 (18%) 1 1	25, 70, 133, 180	0
37	DL	143/144 (99%)	1.21	38 (26%) 0 0	9, 59, 117, 147	0
38	BM	136/136 (100%)	1.00	19 (13%) 2 2	21, 68, 136, 180	0
38	DM	136/136 (100%)	0.65	14 (10%) 6 4	13, 54, 118, 167	0
39	BX	63/63 (100%)	1.59	25 (39%) 0 0	21, 81, 149, 175	0
39	DX	63/63 (100%)	0.52	5 (7%) 12 7	38, 97, 156, 180	0
40	BH	149/149 (100%)	4.15	104 (69%) 0 0	31, 134, 180, 180	0
40	DH	149/149 (100%)	1.89	63 (42%) 0 0	32, 110, 160, 180	0
41	BJ	142/142 (100%)	1.05	32 (22%) 0 0	23, 82, 140, 169	0
41	DJ	142/142 (100%)	0.75	13 (9%) 9 5	17, 61, 126, 180	0
42	BN	120/127 (94%)	0.91	23 (19%) 1 0	24, 71, 139, 180	0
42	DN	120/127 (94%)	0.33	5 (4%) 36 24	7, 43, 91, 172	0
43	BO	116/117 (99%)	1.00	28 (24%) 0 0	35, 83, 145, 180	0
43	DO	116/117 (99%)	0.50	7 (6%) 21 13	19, 73, 135, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.29	8 (6%) 17 10	10, 66, 129, 167	0
44	DQ	117/117 (100%)	0.76	12 (10%) 6 4	8, 50, 104, 180	0
45	BS	110/110 (100%)	1.58	40 (36%) 0 0	6, 62, 123, 152	0
45	DS	110/110 (100%)	1.55	32 (29%) 0 0	12, 48, 129, 180	0
46	BU	102/103 (99%)	1.58	32 (31%) 0 0	21, 77, 140, 180	0
46	DU	102/103 (99%)	0.29	8 (7%) 13 7	22, 94, 154, 180	0
47	BF	178/178 (100%)	1.32	51 (28%) 0 0	56, 128, 177, 180	0
47	DF	178/178 (100%)	1.81	61 (34%) 0 0	30, 107, 168, 180	0
48	BG	176/176 (100%)	1.36	52 (29%) 0 0	49, 112, 163, 180	0
48	DG	176/176 (100%)	1.18	43 (24%) 0 0	35, 97, 161, 180	0
49	BR	103/103 (100%)	0.59	13 (12%) 3 2	25, 87, 151, 176	0
49	DR	103/103 (100%)	1.09	22 (21%) 0 0	23, 76, 139, 161	0
50	BT	93/100 (93%)	1.06	17 (18%) 1 0	22, 77, 159, 180	0
50	DT	93/100 (93%)	1.07	25 (26%) 0 0	24, 64, 156, 179	0
51	BZ	77/78 (98%)	0.93	15 (19%) 1 0	12, 51, 112, 143	0
51	DZ	77/78 (98%)	0.56	7 (9%) 9 5	9, 48, 94, 128	0
52	BW	79/84 (94%)	1.57	25 (31%) 0 0	18, 85, 141, 159	0
52	DW	79/84 (94%)	0.86	11 (13%) 2 2	20, 71, 134, 180	0
All	All	20417/21046 (97%)	0.37	2386 (11%) 4 3	5, 69, 156, 180	0

The worst 5 of 2386 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
40	BH	84	ALA	19.9
40	BH	85	GLY	18.2
40	BH	142	VAL	14.1
40	BH	130	VAL	14.0
40	BH	86	ASP	13.4

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(Å ²)	Q<0.9
54	MG	DB	3067	1/1	0.11	0.13	178,178,178,178	0
54	MG	AA	1660	1/1	0.24	0.35	163,163,163,163	0
54	MG	AA	1603	1/1	0.41	0.15	133,133,133,133	0
54	MG	AA	1615	1/1	0.46	0.08	110,110,110,110	0
54	MG	DB	3061	1/1	0.48	0.08	115,115,115,115	0
54	MG	BB	3101	1/1	0.54	0.12	138,138,138,138	0
54	MG	AA	1626	1/1	0.55	0.19	64,64,64,64	1
54	MG	AA	1638	1/1	0.56	0.36	147,147,147,147	0
53	NMY	BB	3001	42/42	0.59	0.49	100,100,100,100	42
54	MG	BB	3011	1/1	0.65	0.13	66,66,66,66	0
54	MG	BB	3098	1/1	0.67	0.12	80,80,80,80	0
54	MG	CA	1635	1/1	0.68	0.09	96,96,96,96	0
53	NMY	DB	3001	42/42	0.68	0.53	88,88,88,88	42
54	MG	AA	1623	1/1	0.68	0.28	129,129,129,129	0
54	MG	CA	1657	1/1	0.70	0.15	91,91,91,91	0
54	MG	DB	3053	1/1	0.70	0.09	102,102,102,102	0
54	MG	AA	1636	1/1	0.70	0.12	88,88,88,88	0
54	MG	DB	3096	1/1	0.72	0.11	127,127,127,127	0
54	MG	CA	1619	1/1	0.72	0.09	59,59,59,59	0
54	MG	BB	3034	1/1	0.73	0.23	136,136,136,136	0
54	MG	DB	3084	1/1	0.74	0.20	92,92,92,92	0
54	MG	AA	1650	1/1	0.74	0.06	114,114,114,114	0
54	MG	CA	1612	1/1	0.76	0.10	84,84,84,84	0
54	MG	CA	1609	1/1	0.76	0.13	121,121,121,121	0
54	MG	BB	3044	1/1	0.77	0.12	108,108,108,108	0
54	MG	DB	3059	1/1	0.77	1.44	180,180,180,180	0
54	MG	BB	3048	1/1	0.78	0.13	128,128,128,128	0
54	MG	CA	1642	1/1	0.78	0.09	94,94,94,94	0
54	MG	AA	1619	1/1	0.78	0.13	85,85,85,85	0
54	MG	AA	1620	1/1	0.79	0.18	130,130,130,130	0
54	MG	AA	1653	1/1	0.79	0.09	79,79,79,79	0
54	MG	CA	1616	1/1	0.79	0.09	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BB	3079	1/1	0.80	0.12	75,75,75,75	0
54	MG	BB	3043	1/1	0.80	0.08	170,170,170,170	0
54	MG	DB	3060	1/1	0.80	0.24	124,124,124,124	0
54	MG	DB	3031	1/1	0.81	0.24	32,32,32,32	0
54	MG	BB	3095	1/1	0.81	0.15	46,46,46,46	0
54	MG	DB	3097	1/1	0.81	0.21	33,33,33,33	0
54	MG	BB	3058	1/1	0.81	0.17	76,76,76,76	0
54	MG	BB	3039	1/1	0.83	0.07	131,131,131,131	0
54	MG	AA	1609	1/1	0.83	0.20	127,127,127,127	0
54	MG	BB	3029	1/1	0.84	0.22	32,32,32,32	0
54	MG	AA	1640	1/1	0.84	0.24	104,104,104,104	0
54	MG	CA	1615	1/1	0.84	0.07	41,41,41,41	0
54	MG	DB	3051	1/1	0.84	0.08	87,87,87,87	0
54	MG	BB	3082	1/1	0.85	0.33	59,59,59,59	0
54	MG	AA	1647	1/1	0.85	0.13	87,87,87,87	0
54	MG	BB	3020	1/1	0.85	0.09	45,45,45,45	0
54	MG	DB	3035	1/1	0.85	0.20	81,81,81,81	0
54	MG	DB	3017	1/1	0.86	0.08	6,6,6,6	0
54	MG	AA	1621	1/1	0.86	0.07	85,85,85,85	0
54	MG	BB	3052	1/1	0.86	0.09	59,59,59,59	0
54	MG	CA	1621	1/1	0.86	0.31	118,118,118,118	0
54	MG	AA	1627	1/1	0.86	0.10	15,15,15,15	1
54	MG	DB	3034	1/1	0.86	0.08	43,43,43,43	0
54	MG	AA	1657	1/1	0.86	0.09	69,69,69,69	0
54	MG	CE	201	1/1	0.87	0.08	97,97,97,97	0
54	MG	CA	1636	1/1	0.87	0.08	56,56,56,56	0
54	MG	BB	3055	1/1	0.87	0.06	58,58,58,58	0
54	MG	AA	1637	1/1	0.87	0.10	89,89,89,89	0
54	MG	DB	3005	1/1	0.87	0.20	30,30,30,30	0
54	MG	AA	1625	1/1	0.88	0.11	72,72,72,72	0
54	MG	CA	1643	1/1	0.88	0.10	43,43,43,43	0
54	MG	DB	3104	1/1	0.88	0.09	21,21,21,21	0
54	MG	AA	1641	1/1	0.88	0.11	56,56,56,56	0
53	NMY	AA	1601	42/42	0.88	0.29	71,71,71,71	0
54	MG	AA	1606	1/1	0.88	0.05	47,47,47,47	0
54	MG	CA	1623	1/1	0.88	0.03	131,131,131,131	0
54	MG	CA	1638	1/1	0.89	0.17	142,142,142,142	0
54	MG	AA	1624	1/1	0.89	0.32	32,32,32,32	1
54	MG	CA	1622	1/1	0.89	0.10	75,75,75,75	0
53	NMY	CA	1601	42/42	0.89	0.25	71,71,71,71	0
54	MG	AA	1661	1/1	0.89	0.11	79,79,79,79	0
54	MG	DB	3016	1/1	0.89	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BB	3019	1/1	0.89	0.10	45,45,45,45	0
54	MG	AA	1658	1/1	0.89	0.33	115,115,115,115	0
54	MG	DB	3058	1/1	0.89	0.05	43,43,43,43	0
54	MG	BB	3032	1/1	0.90	0.10	45,45,45,45	0
54	MG	DB	3038	1/1	0.90	0.15	17,17,17,17	0
54	MG	CA	1620	1/1	0.90	0.17	70,70,70,70	0
54	MG	AA	1628	1/1	0.90	0.14	57,57,57,57	0
54	MG	DB	3029	1/1	0.90	0.07	33,33,33,33	0
54	MG	AA	1617	1/1	0.90	0.07	45,45,45,45	0
54	MG	CA	1634	1/1	0.90	0.12	8,8,8,8	0
54	MG	BB	3018	1/1	0.90	0.07	43,43,43,43	0
54	MG	DB	3110	1/1	0.90	0.08	19,19,19,19	0
54	MG	BB	3081	1/1	0.90	0.21	52,52,52,52	0
54	MG	AA	1635	1/1	0.91	0.13	45,45,45,45	0
54	MG	AA	1654	1/1	0.91	0.13	51,51,51,51	0
54	MG	DB	3072	1/1	0.91	0.08	30,30,30,30	0
54	MG	DB	3107	1/1	0.91	0.10	27,27,27,27	0
54	MG	DB	3023	1/1	0.91	0.10	29,29,29,29	0
54	MG	BB	3094	1/1	0.91	0.22	93,93,93,93	0
54	MG	BB	3014	1/1	0.91	0.05	42,42,42,42	0
54	MG	BB	3096	1/1	0.91	0.12	42,42,42,42	0
54	MG	AA	1616	1/1	0.91	0.10	77,77,77,77	0
54	MG	BB	3091	1/1	0.91	0.09	75,75,75,75	0
54	MG	AA	1613	1/1	0.91	0.07	65,65,65,65	0
54	MG	AA	1651	1/1	0.91	0.06	109,109,109,109	0
54	MG	BB	3078	1/1	0.91	0.06	32,32,32,32	0
54	MG	DB	3030	1/1	0.91	0.13	74,74,74,74	0
54	MG	CA	1607	1/1	0.91	0.12	100,100,100,100	0
54	MG	AA	1630	1/1	0.92	0.07	35,35,35,35	0
54	MG	BB	3061	1/1	0.92	0.14	41,41,41,41	0
54	MG	AA	1648	1/1	0.92	0.48	94,94,94,94	0
54	MG	DB	3091	1/1	0.92	0.07	47,47,47,47	0
54	MG	AA	1642	1/1	0.92	0.07	59,59,59,59	0
54	MG	BB	3040	1/1	0.92	0.10	28,28,28,28	0
54	MG	CA	1627	1/1	0.92	0.08	29,29,29,29	1
54	MG	BB	3089	1/1	0.92	0.07	45,45,45,45	0
54	MG	BB	3111	1/1	0.92	0.14	81,81,81,81	0
54	MG	DB	3062	1/1	0.92	0.04	47,47,47,47	0
54	MG	DB	3086	1/1	0.92	0.11	18,18,18,18	0
54	MG	DB	3024	1/1	0.92	0.05	55,55,55,55	0
54	MG	DB	3078	1/1	0.92	0.13	46,46,46,46	0
54	MG	DB	3081	1/1	0.93	0.12	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1622	1/1	0.93	0.06	27,27,27,27	0
54	MG	CA	1641	1/1	0.93	0.09	63,63,63,63	0
54	MG	CA	1626	1/1	0.93	0.15	8,8,8,8	1
54	MG	DB	3014	1/1	0.93	0.14	48,48,48,48	0
54	MG	CA	1661	1/1	0.93	0.08	61,61,61,61	0
54	MG	AA	1652	1/1	0.93	0.06	73,73,73,73	0
54	MG	CA	1660	1/1	0.93	0.06	69,69,69,69	0
54	MG	BB	3023	1/1	0.93	0.22	41,41,41,41	0
54	MG	DB	3093	1/1	0.93	0.09	67,67,67,67	0
54	MG	AA	1612	1/1	0.93	0.06	37,37,37,37	0
54	MG	DB	3037	1/1	0.93	0.07	15,15,15,15	0
54	MG	BB	3010	1/1	0.93	0.08	82,82,82,82	0
54	MG	DB	3046	1/1	0.93	0.13	55,55,55,55	0
54	MG	AA	1632	1/1	0.93	0.14	37,37,37,37	0
54	MG	CN	201	1/1	0.93	0.07	48,48,48,48	0
54	MG	DB	3054	1/1	0.93	0.10	65,65,65,65	0
54	MG	CA	1648	1/1	0.93	0.11	55,55,55,55	0
54	MG	CA	1654	1/1	0.93	0.05	78,78,78,78	0
54	MG	CA	1652	1/1	0.93	0.17	77,77,77,77	0
54	MG	BB	3025	1/1	0.93	0.08	14,14,14,14	0
54	MG	BB	3073	1/1	0.93	0.10	67,67,67,67	0
54	MG	BB	3004	1/1	0.93	0.07	38,38,38,38	0
54	MG	DB	3098	1/1	0.93	0.15	36,36,36,36	0
54	MG	BB	3038	1/1	0.93	0.08	50,50,50,50	0
54	MG	BB	3030	1/1	0.93	0.09	36,36,36,36	0
54	MG	CA	1629	1/1	0.93	0.08	46,46,46,46	1
54	MG	CA	1610	1/1	0.93	0.04	79,79,79,79	0
54	MG	CA	1658	1/1	0.93	0.09	52,52,52,52	0
54	MG	BB	3005	1/1	0.94	0.04	39,39,39,39	0
54	MG	DB	3100	1/1	0.94	0.15	9,9,9,9	0
54	MG	BB	3092	1/1	0.94	0.10	32,32,32,32	0
54	MG	BB	3103	1/1	0.94	0.09	37,37,37,37	0
54	MG	BB	3065	1/1	0.94	0.08	24,24,24,24	0
54	MG	BB	3015	1/1	0.94	0.04	27,27,27,27	0
54	MG	BB	3035	1/1	0.94	0.08	32,32,32,32	0
54	MG	DB	3013	1/1	0.94	0.18	21,21,21,21	0
54	MG	BB	3110	1/1	0.94	0.07	30,30,30,30	0
54	MG	BB	3063	1/1	0.94	0.14	31,31,31,31	0
54	MG	DB	3065	1/1	0.94	0.07	16,16,16,16	0
54	MG	CA	1637	1/1	0.94	0.06	79,79,79,79	0
54	MG	AA	1634	1/1	0.94	0.04	52,52,52,52	0
54	MG	BB	3100	1/1	0.94	0.19	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DB	3087	1/1	0.94	0.19	25,25,25,25	0
54	MG	CA	1631	1/1	0.94	0.07	34,34,34,34	0
54	MG	BB	3054	1/1	0.94	0.05	46,46,46,46	0
54	MG	AA	1643	1/1	0.94	0.06	53,53,53,53	0
54	MG	DB	3027	1/1	0.94	0.07	36,36,36,36	0
54	MG	DB	3018	1/1	0.94	0.09	8,8,8,8	0
54	MG	DB	3010	1/1	0.94	0.07	5,5,5,5	0
54	MG	AA	1607	1/1	0.94	0.04	64,64,64,64	0
54	MG	BB	3066	1/1	0.94	0.06	44,44,44,44	0
54	MG	CA	1653	1/1	0.94	0.10	33,33,33,33	0
54	MG	BB	3076	1/1	0.94	0.14	60,60,60,60	0
54	MG	BB	3050	1/1	0.95	0.08	18,18,18,18	0
54	MG	BB	3102	1/1	0.95	0.10	28,28,28,28	0
54	MG	AA	1618	1/1	0.95	0.08	79,79,79,79	0
54	MG	CA	1630	1/1	0.95	0.08	40,40,40,40	0
54	MG	BB	3047	1/1	0.95	0.09	46,46,46,46	0
54	MG	BB	3045	1/1	0.95	0.09	67,67,67,67	0
54	MG	BB	3093	1/1	0.95	0.04	36,36,36,36	0
54	MG	BB	3090	1/1	0.95	0.07	49,49,49,49	0
55	ZN	D4	101	1/1	0.95	0.13	57,57,57,57	0
54	MG	DB	3025	1/1	0.95	0.09	44,44,44,44	0
54	MG	DB	3032	1/1	0.95	0.11	18,18,18,18	0
54	MG	CA	1632	1/1	0.95	0.15	47,47,47,47	0
54	MG	BB	3060	1/1	0.95	0.08	30,30,30,30	0
54	MG	DB	3057	1/1	0.95	0.07	5,5,5,5	0
54	MG	CA	1633	1/1	0.95	0.16	73,73,73,73	0
54	MG	BB	3021	1/1	0.95	0.06	22,22,22,22	0
54	MG	BB	3074	1/1	0.95	0.10	31,31,31,31	0
54	MG	DB	3015	1/1	0.95	0.07	22,22,22,22	0
54	MG	CA	1647	1/1	0.95	0.06	90,90,90,90	0
54	MG	CA	1611	1/1	0.95	0.06	60,60,60,60	0
54	MG	BB	3041	1/1	0.95	0.15	28,28,28,28	0
54	MG	DB	3056	1/1	0.95	0.07	12,12,12,12	0
54	MG	BB	3013	1/1	0.95	0.12	41,41,41,41	0
54	MG	BB	3080	1/1	0.95	0.09	37,37,37,37	0
54	MG	CA	1644	1/1	0.95	0.08	58,58,58,58	0
54	MG	BB	3051	1/1	0.95	0.05	41,41,41,41	0
54	MG	AA	1631	1/1	0.95	0.10	107,107,107,107	0
54	MG	DB	3111	1/1	0.95	0.14	28,28,28,28	0
54	MG	BB	3059	1/1	0.95	0.07	30,30,30,30	0
54	MG	AA	1629	1/1	0.95	0.05	70,70,70,70	0
54	MG	AA	1649	1/1	0.95	0.11	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DB	3011	1/1	0.95	0.07	7,7,7,7	0
54	MG	CA	1628	1/1	0.95	0.04	61,61,61,61	0
54	MG	DB	3105	1/1	0.95	0.10	40,40,40,40	0
54	MG	BB	3099	1/1	0.95	0.16	41,41,41,41	0
54	MG	DB	3055	1/1	0.95	0.09	42,42,42,42	0
55	ZN	B4	101	1/1	0.95	0.06	72,72,72,72	0
54	MG	BB	3083	1/1	0.95	0.12	5,5,5,5	0
54	MG	BB	3084	1/1	0.96	0.10	21,21,21,21	0
54	MG	BB	3064	1/1	0.96	0.06	26,26,26,26	0
54	MG	DB	3044	1/1	0.96	0.06	12,12,12,12	0
54	MG	AA	1655	1/1	0.96	0.04	38,38,38,38	0
54	MG	DB	3063	1/1	0.96	0.04	71,71,71,71	0
54	MG	DB	3048	1/1	0.96	0.17	23,23,23,23	0
54	MG	CA	1624	1/1	0.96	0.03	34,34,34,34	0
54	MG	AA	1602	1/1	0.96	0.05	29,29,29,29	0
54	MG	BB	3109	1/1	0.96	0.13	32,32,32,32	0
54	MG	BB	3037	1/1	0.96	0.07	42,42,42,42	0
54	MG	BB	3033	1/1	0.96	0.07	55,55,55,55	0
54	MG	CA	1639	1/1	0.96	0.08	14,14,14,14	0
54	MG	DB	3033	1/1	0.96	0.12	62,62,62,62	0
54	MG	DB	3008	1/1	0.96	0.11	16,16,16,16	0
54	MG	CA	1649	1/1	0.96	0.07	73,73,73,73	0
54	MG	BB	3085	1/1	0.96	0.15	44,44,44,44	0
54	MG	AA	1644	1/1	0.96	0.07	24,24,24,24	0
54	MG	DB	3094	1/1	0.96	0.15	21,21,21,21	0
54	MG	BB	3009	1/1	0.96	0.13	64,64,64,64	0
54	MG	BB	3087	1/1	0.96	0.23	41,41,41,41	0
54	MG	BB	3105	1/1	0.96	0.11	21,21,21,21	0
54	MG	DB	3101	1/1	0.96	0.09	5,5,5,5	0
54	MG	AA	1639	1/1	0.96	0.09	57,57,57,57	0
54	MG	AA	1633	1/1	0.96	0.10	51,51,51,51	0
54	MG	BB	3088	1/1	0.96	0.21	57,57,57,57	0
54	MG	BB	3070	1/1	0.96	0.08	15,15,15,15	0
54	MG	DB	3070	1/1	0.96	0.18	23,23,23,23	0
54	MG	DB	3085	1/1	0.96	0.17	25,25,25,25	0
54	MG	CA	1646	1/1	0.96	0.05	72,72,72,72	0
54	MG	DB	3108	1/1	0.96	0.07	21,21,21,21	0
54	MG	BB	3072	1/1	0.96	0.09	52,52,52,52	0
54	MG	BB	3068	1/1	0.96	0.10	55,55,55,55	0
54	MG	AA	1614	1/1	0.96	0.03	64,64,64,64	0
54	MG	CA	1651	1/1	0.96	0.06	40,40,40,40	0
54	MG	BB	3056	1/1	0.96	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DB	3109	1/1	0.97	0.05	10,10,10,10	0
54	MG	DB	3068	1/1	0.97	0.07	19,19,19,19	0
54	MG	BB	3097	1/1	0.97	0.05	32,32,32,32	0
54	MG	CA	1602	1/1	0.97	0.05	6,6,6,6	0
54	MG	AA	1656	1/1	0.97	0.13	60,60,60,60	0
54	MG	DB	3007	1/1	0.97	0.07	12,12,12,12	0
54	MG	AA	1646	1/1	0.97	0.03	94,94,94,94	0
54	MG	DB	3088	1/1	0.97	0.10	48,48,48,48	0
54	MG	BB	3104	1/1	0.97	0.04	8,8,8,8	0
54	MG	BB	3012	1/1	0.97	0.17	25,25,25,25	0
54	MG	BB	3002	1/1	0.97	0.05	24,24,24,24	0
54	MG	BB	3086	1/1	0.97	0.14	66,66,66,66	0
54	MG	BB	3075	1/1	0.97	0.10	13,13,13,13	0
54	MG	DB	3066	1/1	0.97	0.06	29,29,29,29	0
54	MG	BB	3077	1/1	0.97	0.08	37,37,37,37	0
54	MG	AA	1659	1/1	0.97	0.05	112,112,112,112	0
54	MG	BB	3107	1/1	0.97	0.07	54,54,54,54	0
54	MG	BB	3022	1/1	0.97	0.10	22,22,22,22	0
54	MG	CA	1613	1/1	0.97	0.09	77,77,77,77	0
54	MG	CA	1603	1/1	0.97	0.12	30,30,30,30	0
54	MG	BB	3026	1/1	0.97	0.10	54,54,54,54	0
54	MG	DB	3095	1/1	0.97	0.05	39,39,39,39	0
54	MG	BB	3031	1/1	0.97	0.03	47,47,47,47	0
54	MG	DB	3052	1/1	0.97	0.20	32,32,32,32	0
54	MG	DB	3019	1/1	0.97	0.14	48,48,48,48	0
54	MG	AA	1605	1/1	0.97	0.15	48,48,48,48	0
54	MG	DB	3090	1/1	0.97	0.17	34,34,34,34	0
54	MG	DB	3026	1/1	0.97	0.13	15,15,15,15	0
54	MG	CA	1645	1/1	0.97	0.16	45,45,45,45	0
54	MG	DB	3043	1/1	0.97	0.09	15,15,15,15	0
54	MG	DB	3069	1/1	0.97	0.10	6,6,6,6	0
54	MG	AA	1610	1/1	0.97	0.10	10,10,10,10	0
54	MG	BB	3062	1/1	0.97	0.04	29,29,29,29	0
54	MG	BB	3036	1/1	0.97	0.07	36,36,36,36	0
54	MG	CA	1659	1/1	0.97	0.07	62,62,62,62	0
54	MG	DB	3079	1/1	0.97	0.09	43,43,43,43	0
54	MG	CA	1656	1/1	0.97	0.07	27,27,27,27	0
54	MG	DB	3041	1/1	0.97	0.14	15,15,15,15	0
54	MG	DB	3074	1/1	0.97	0.05	28,28,28,28	0
54	MG	BB	3108	1/1	0.98	0.11	25,25,25,25	0
54	MG	DB	3064	1/1	0.98	0.10	33,33,33,33	0
54	MG	DB	3003	1/1	0.98	0.08	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DB	3040	1/1	0.98	0.07	58,58,58,58	0
54	MG	CA	1618	1/1	0.98	0.04	8,8,8,8	0
54	MG	DB	3106	1/1	0.98	0.12	39,39,39,39	0
54	MG	DB	3092	1/1	0.98	0.17	46,46,46,46	0
54	MG	CA	1625	1/1	0.98	0.06	34,34,34,34	0
54	MG	DB	3080	1/1	0.98	0.16	39,39,39,39	0
54	MG	DB	3004	1/1	0.98	0.09	14,14,14,14	0
54	MG	DB	3083	1/1	0.98	0.08	24,24,24,24	0
54	MG	BB	3028	1/1	0.98	0.08	32,32,32,32	0
54	MG	BB	3027	1/1	0.98	0.08	34,34,34,34	0
54	MG	DB	3009	1/1	0.98	0.08	19,19,19,19	0
54	MG	DB	3036	1/1	0.98	0.05	40,40,40,40	0
54	MG	DB	3039	1/1	0.98	0.13	19,19,19,19	0
54	MG	BB	3007	1/1	0.98	0.09	5,5,5,5	0
54	MG	BB	3053	1/1	0.98	0.08	25,25,25,25	0
54	MG	DB	3049	1/1	0.98	0.10	46,46,46,46	0
54	MG	BB	3017	1/1	0.98	0.10	28,28,28,28	0
54	MG	CA	1605	1/1	0.98	0.04	16,16,16,16	0
54	MG	DB	3045	1/1	0.98	0.03	22,22,22,22	0
54	MG	DB	3047	1/1	0.98	0.04	24,24,24,24	0
54	MG	AA	1645	1/1	0.98	0.10	60,60,60,60	0
54	MG	DB	3042	1/1	0.98	0.06	7,7,7,7	0
54	MG	DB	3112	1/1	0.98	0.15	37,37,37,37	0
54	MG	DB	3073	1/1	0.98	0.07	33,33,33,33	0
54	MG	DB	3102	1/1	0.98	0.14	14,14,14,14	0
54	MG	DB	3076	1/1	0.98	0.06	26,26,26,26	0
54	MG	AA	1608	1/1	0.98	0.06	54,54,54,54	0
54	MG	CA	1655	1/1	0.98	0.07	69,69,69,69	0
54	MG	DB	3099	1/1	0.98	0.15	29,29,29,29	0
54	MG	CA	1640	1/1	0.98	0.12	57,57,57,57	0
54	MG	AA	1611	1/1	0.98	0.04	28,28,28,28	0
54	MG	DB	3022	1/1	0.98	0.09	5,5,5,5	0
54	MG	DB	3050	1/1	0.98	0.14	32,32,32,32	0
54	MG	DB	3103	1/1	0.98	0.10	16,16,16,16	0
54	MG	DB	3028	1/1	0.98	0.10	8,8,8,8	0
54	MG	CA	1614	1/1	0.98	0.06	58,58,58,58	0
54	MG	DB	3002	1/1	0.98	0.10	5,5,5,5	0
54	MG	DB	3071	1/1	0.98	0.09	61,61,61,61	0
54	MG	BB	3046	1/1	0.98	0.08	46,46,46,46	0
54	MG	DB	3089	1/1	0.98	0.14	10,10,10,10	0
54	MG	BB	3069	1/1	0.98	0.11	32,32,32,32	0
54	MG	DB	3006	1/1	0.98	0.07	20,20,20,20	0

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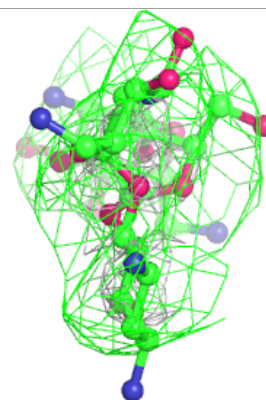
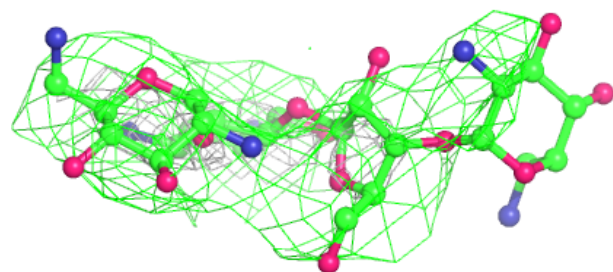
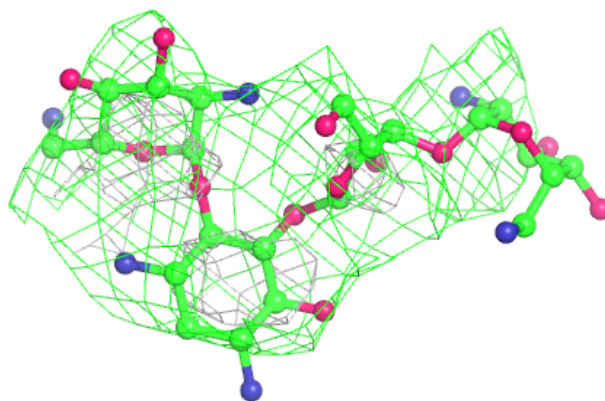
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1608	1/1	0.98	0.06	40,40,40,40	0
54	MG	BB	3106	1/1	0.99	0.14	33,33,33,33	0
54	MG	CA	1650	1/1	0.99	0.09	12,12,12,12	0
54	MG	BB	3016	1/1	0.99	0.07	18,18,18,18	0
54	MG	DB	3012	1/1	0.99	0.20	37,37,37,37	0
54	MG	BB	3024	1/1	0.99	0.13	7,7,7,7	0
54	MG	AA	1604	1/1	0.99	0.15	36,36,36,36	0
54	MG	DB	3075	1/1	0.99	0.12	7,7,7,7	0
54	MG	BB	3049	1/1	0.99	0.03	14,14,14,14	0
54	MG	DB	3082	1/1	0.99	0.07	6,6,6,6	0
54	MG	DB	3020	1/1	0.99	0.04	5,5,5,5	0
54	MG	BB	3057	1/1	0.99	0.05	20,20,20,20	0
54	MG	DB	3021	1/1	0.99	0.15	9,9,9,9	0
54	MG	CA	1604	1/1	0.99	0.08	52,52,52,52	0
54	MG	CA	1606	1/1	0.99	0.09	19,19,19,19	0
54	MG	CA	1617	1/1	0.99	0.07	9,9,9,9	0
54	MG	BB	3006	1/1	0.99	0.14	5,5,5,5	0
54	MG	BB	3042	1/1	0.99	0.08	8,8,8,8	0
54	MG	BB	3071	1/1	0.99	0.12	29,29,29,29	0
54	MG	BB	3003	1/1	0.99	0.07	24,24,24,24	0
54	MG	BB	3067	1/1	0.99	0.07	34,34,34,34	0
54	MG	DB	3077	1/1	0.99	0.12	47,47,47,47	0
54	MG	BB	3008	1/1	1.00	0.09	64,64,64,64	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.

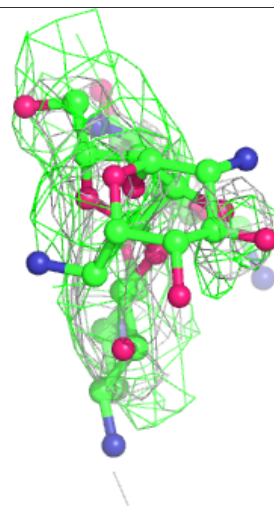
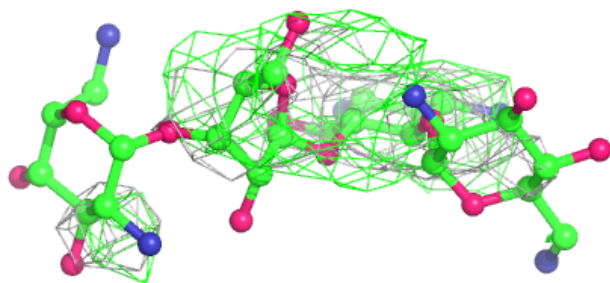
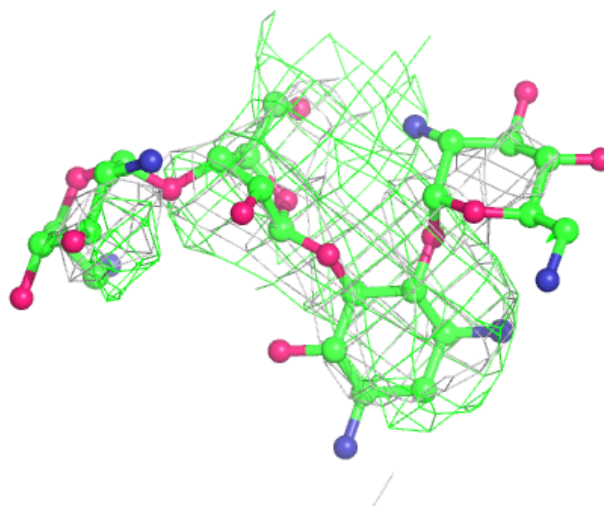
Electron density around NMY BB 3001:

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



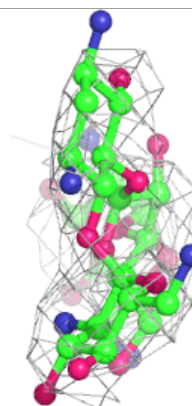
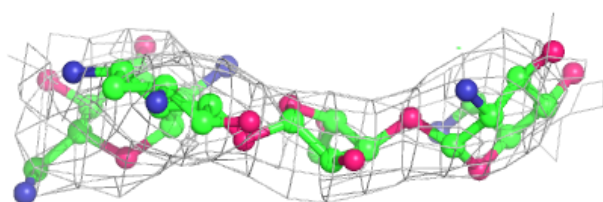
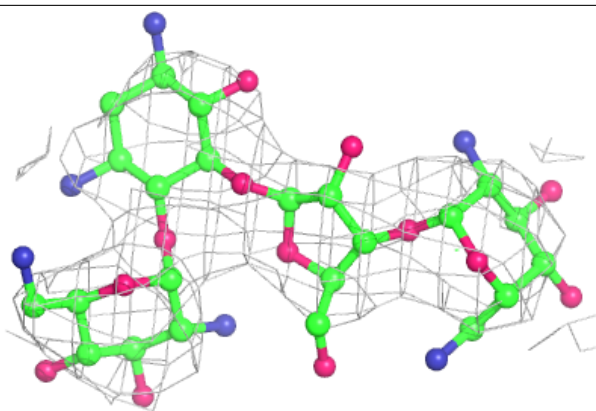
Electron density around NMY DB 3001:

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

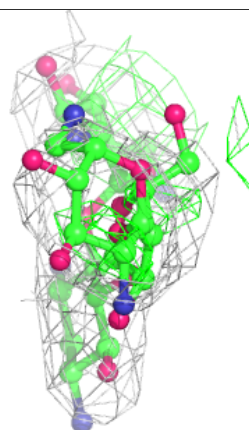
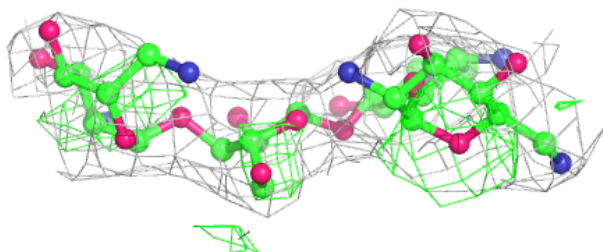
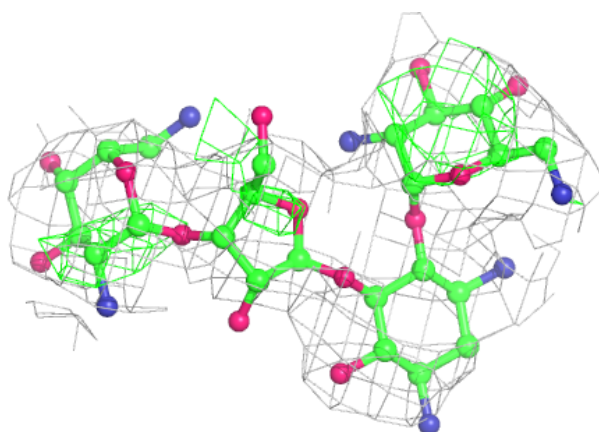


Electron density around NMY AA 1601:

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

**Electron density around NMY CA 1601:**

$2mF_o - DF_c$ (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.