



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 03:21 AM UTC

PDB ID : 4V5Y / pdb_00004v5y
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with paromomycin and ribosome recycling factor (RRF).
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 : 2007-06-19
Resolution : 4.45 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.48.1

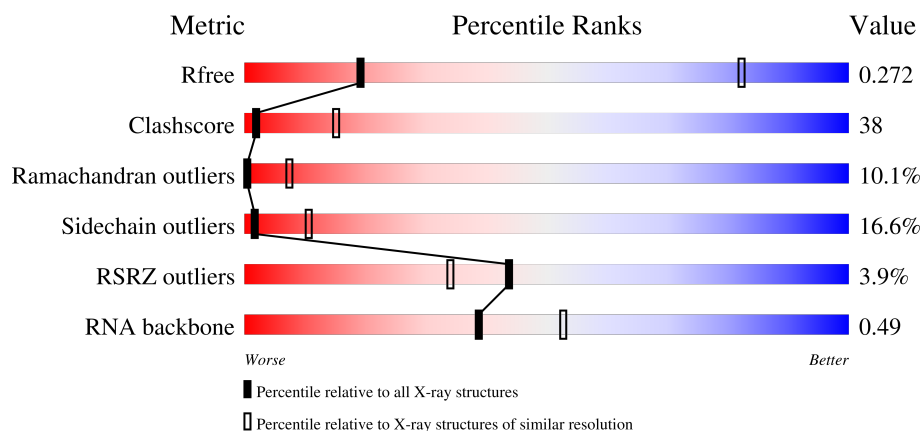
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.45 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}	164625	1042 (5.02-3.90)
Clashscore	180529	1098 (5.02-3.90)
Ramachandran outliers	177936	1001 (5.02-3.90)
Sidechain outliers	177891	1003 (5.04-3.88)
RSRZ outliers	164620	1038 (5.02-3.90)
RNA backbone	3690	1158 (5.90-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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	23% 64% 11% ..
1	CA	1542	24% 63% 11% ..
2	AC	232	3% 27% 49% 12% 11%

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Mol	Chain	Length	Quality of chain
2	CC	232	
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	

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Mol	Chain	Length	Quality of chain
15	AP	82	
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	

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Mol	Chain	Length	Quality of chain
27	DK	123	
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	

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Mol	Chain	Length	Quality of chain
40	BH	149	
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	

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Mol	Chain	Length	Quality of chain
52	DW	84	
53	B6	185	
53	D6	185	

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
54	MG	AA	1623	-	-	-	X
54	MG	CA	1629	-	-	-	X
54	MG	CE	201	-	-	-	X
54	MG	DB	3058	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 287128 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			

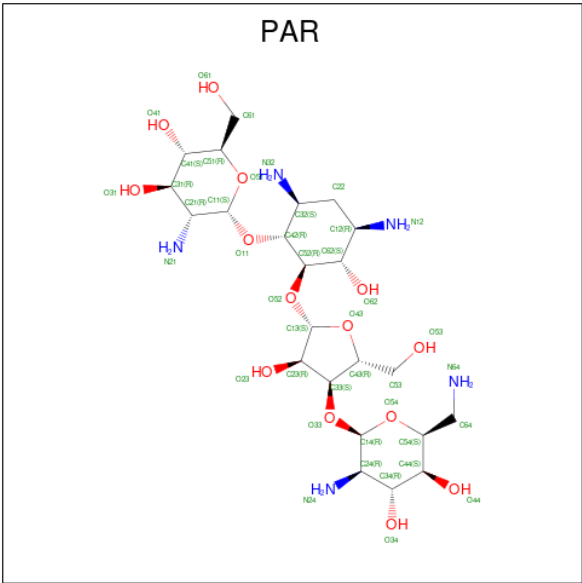
- Molecule 53 is a protein called 50S ribosomal protein RRF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
53	D6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	60	Total	Mg	0	0
			60	60		
54	BB	110	Total	Mg	0	0
			110	110		
54	CA	61	Total	Mg	0	0
			61	61		
54	CE	1	Total	Mg	0	0
			1	1		
54	DB	111	Total	Mg	0	0
			111	111		

- Molecule 55 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	AA	1	Total	C	N	O	0	0
			42	23	5	14		
55	BB	1	Total	C	N	O	0	0
			42	23	5	14		
55	CA	1	Total	C	N	O	0	0
			42	23	5	14		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	DB	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	291	Total	O	0	0
			291	291		
57	AL	3	Total	O	0	0
			3	3		
57	AN	4	Total	O	0	0
			4	4		
57	AT	2	Total	O	0	0
			2	2		
57	BB	495	Total	O	0	0
			495	495		
57	BC	6	Total	O	0	0
			6	6		
57	BD	1	Total	O	0	0
			1	1		
57	BE	2	Total	O	0	0
			2	2		
57	BL	1	Total	O	0	0
			1	1		
57	BT	1	Total	O	0	0
			1	1		
57	CA	296	Total	O	0	0
			296	296		
57	CE	3	Total	O	0	0
			3	3		
57	CL	4	Total	O	0	0
			4	4		
57	CN	4	Total	O	0	0
			4	4		

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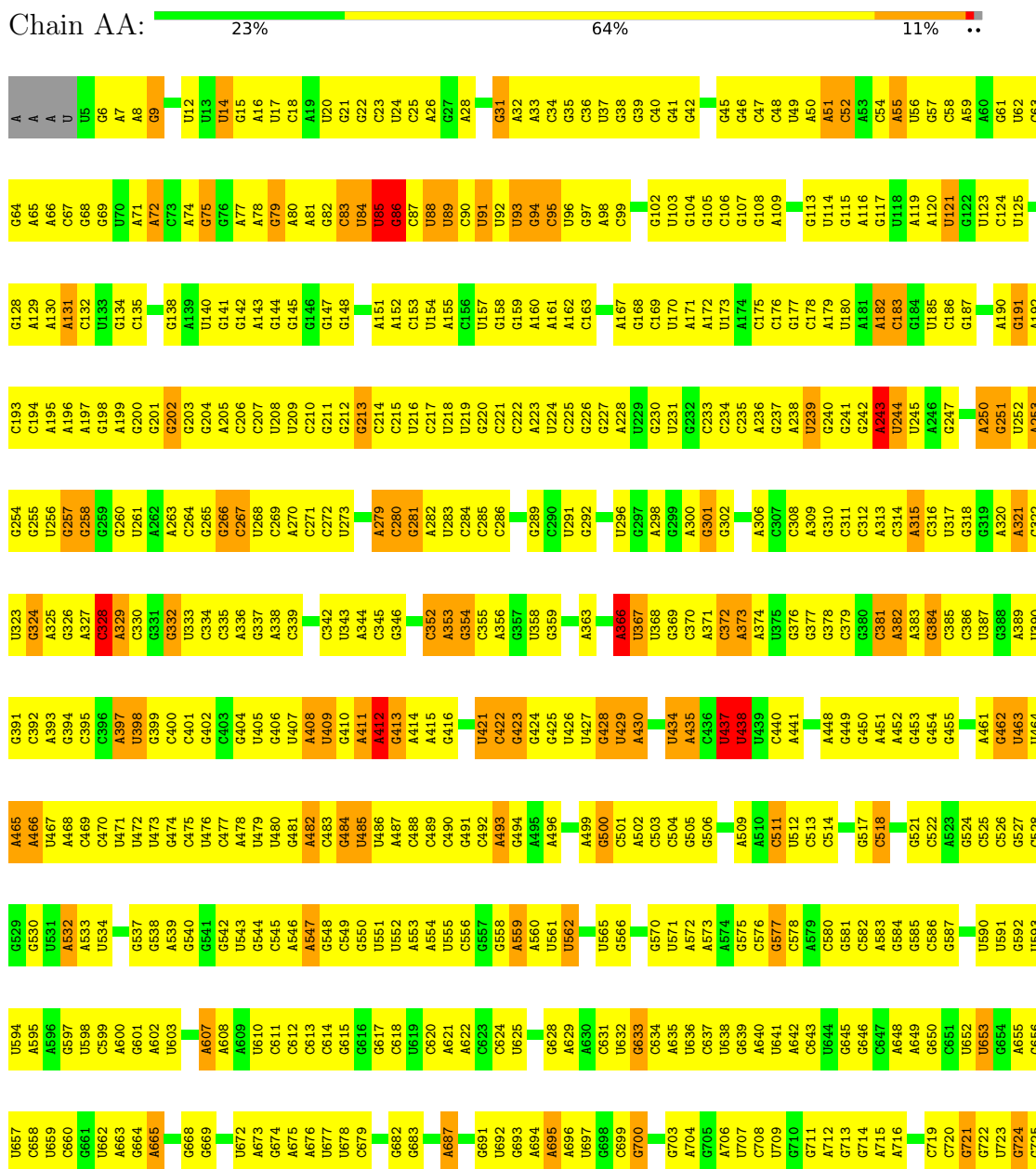
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CP	1	Total 1	O 1	0	0
57	CT	1	Total 1	O 1	0	0
57	DB	502	Total 502	O 502	0	0
57	DC	4	Total 4	O 4	0	0
57	DD	1	Total 1	O 1	0	0
57	DE	1	Total 1	O 1	0	0
57	DL	2	Total 2	O 2	0	0
57	DQ	1	Total 1	O 1	0	0
57	DR	1	Total 1	O 1	0	0

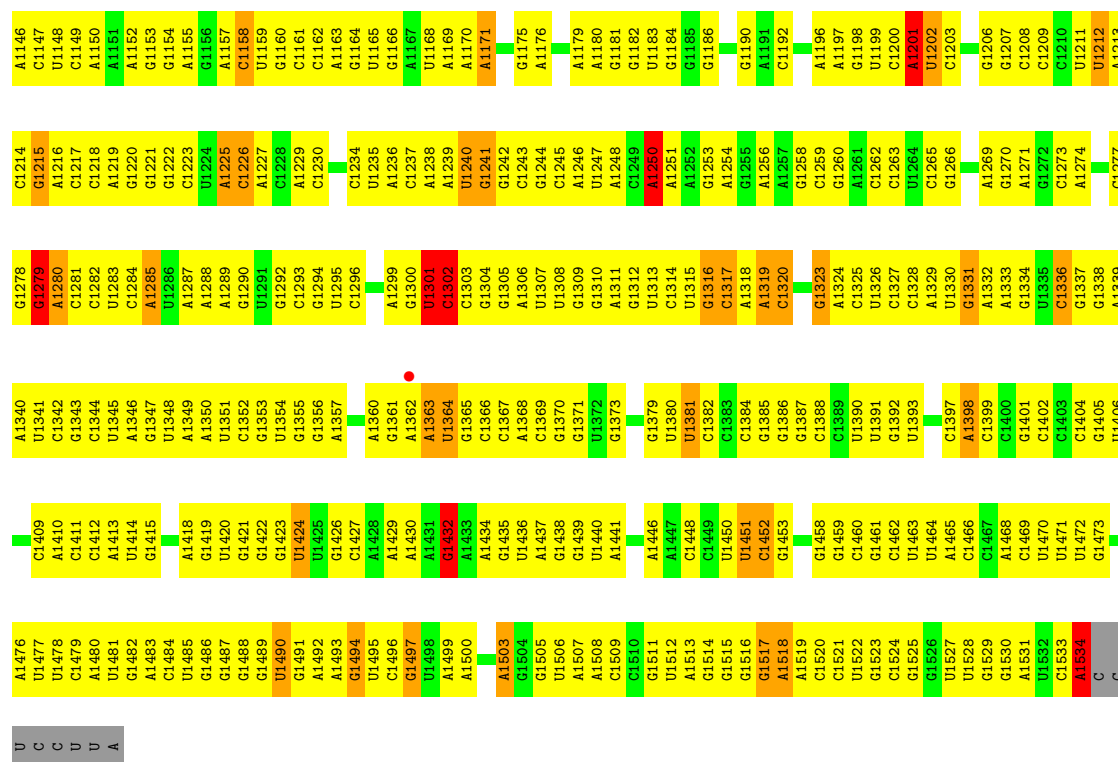
3 Residue-property plots

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

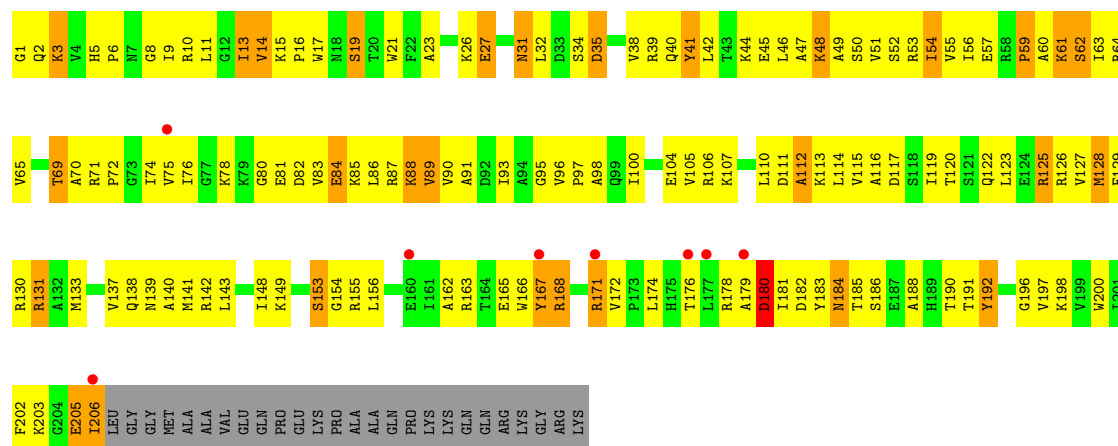
• Molecule 1: 16S rRNA



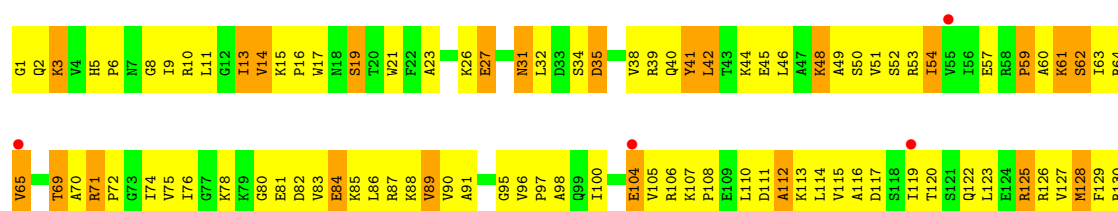
A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	C1109	A1110	A1111	A1112	A1113	A1114	A1115	A1118	C1119	C1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	C1128	G1131	C1132	G1133	C1136	C1137	G1138	G1139	C1140	C1141	G1142	G1143	A1144	A1145																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
A1016	A1019	G1020	A1021	A1022	G1023	G1024	G1025	G1026	G1027	G1028	A1029	U1030	C1031	A1034	G1035	A1036	C1037	C1038	A1039	A1040	A1041	A1042	G1043	A1044	C1045	A1046	G1047	A1048	U1049	G1053	C1054	A1055	U1056	G1057	G1058	C1059	U1060	G1061	U1062	C1063	G1064	U1065	C1066	A1067	G1068	C1069	U1070	C1071	G1072	U1073	U1076	G1077	U1078	G1079																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G951	U952	G953	G954	U955	U956	U957	A958	A959	U960	U961	G966	C967	A968	A969	C970	A971	C972	C973	A974	A975	G976	A977	A978	C979	C980	U981	U982	A983	C984	C985	U986	G987	U991	U992	G993	A994	A996	U997	C998	C999	A1000	C1001	G1002	G1003	C934	A935	C936	C939	C940	U946	G947	C948	A949	U950																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
C876	G877	A878	C879	C880	C881	C882	C883	U884	C885	C886	C887	C898	C899	A900	A901	G902	G903	U904	U905	A974	A975	G976	A977	A908	A909	C910	U911	C912	A913	A914	A915	G916	A918	A919	U920	U921	G922	A923	G925	G926	G927	C930	C931	C932	G933	C934	A935	C936	C939	C940	U946	G947	C948	A949	U950																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
C806	A807	C808	U809	C810	C811	C812	U813	A814	A815	A816	C817	C818	A819	U820	U821	U822	A825	C826	U827	U828	G829	G832	C833	U834	U835	C836	C841	U842	U843	U844	A845	C846	C847	C848	G849	C852	C853	U854	U855	C856	C857	C858	C859	C860	C861	C862	A865	C866	U867	C868	C869	A872	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207	C1208	C1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379	C1380	C1381	C1382	C1383	C1384	C1385	C1386	C1387	C1388	C1389	C1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	C1470	C1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741	C1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803	C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	C1944	C1945	C1946	C1947	C1948	C1949	C1950	C1951	C1952	C1953	C1954	C1955	C1956	C1957	C1958	C1959	C1960	C1961	C1962	C1963	C1964	C1965	C1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1975	C1976	C1977	C1978	C1979	C1980	C1981	C1982	C1983	C1984	C1985	C1986	C1987	C1988	C1989	C1990	C199

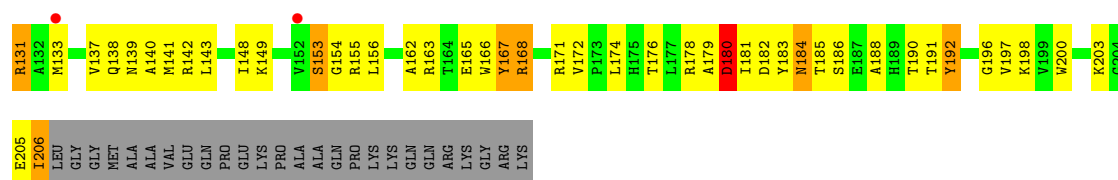


• Molecule 2: 30S ribosomal protein S3

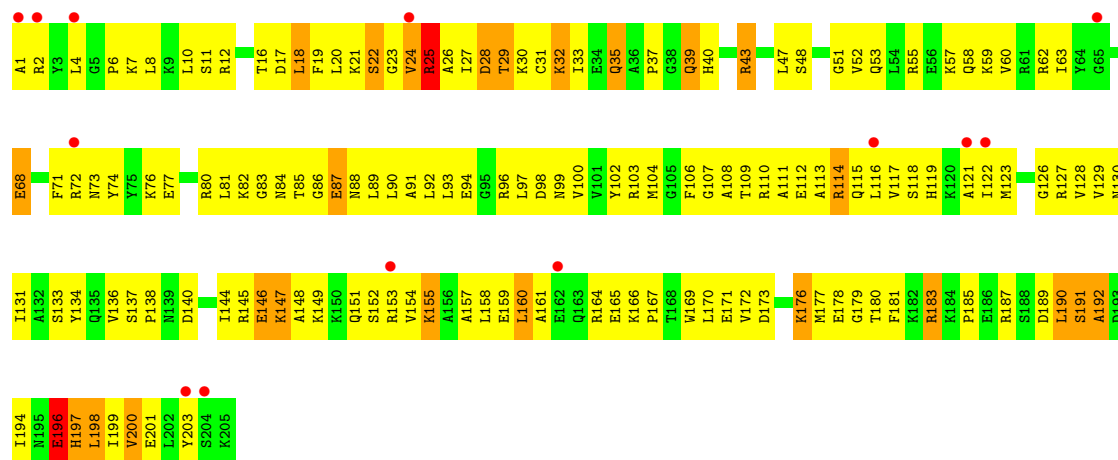


• Molecule 2: 30S ribosomal protein S3

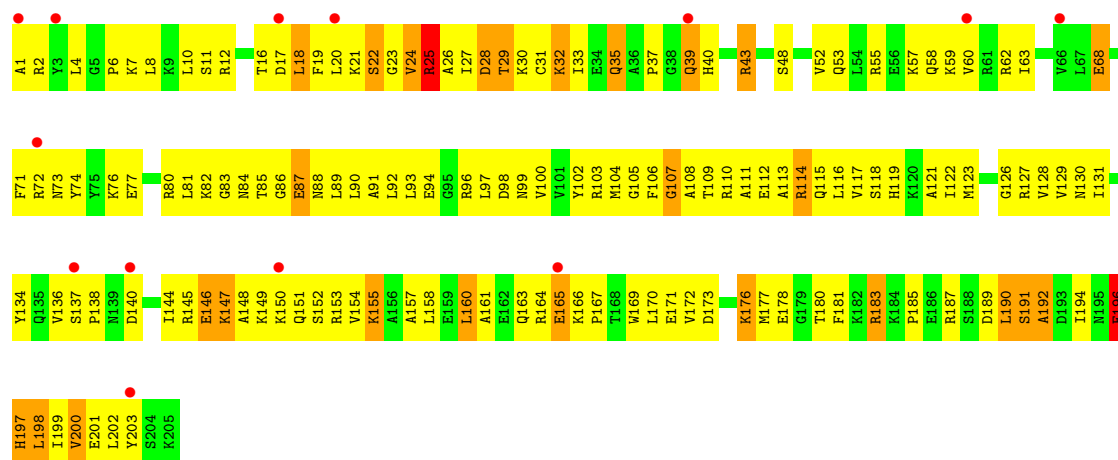




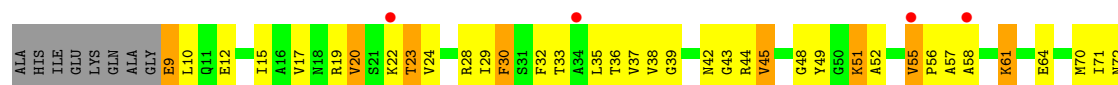
• Molecule 3: 30S ribosomal protein S4

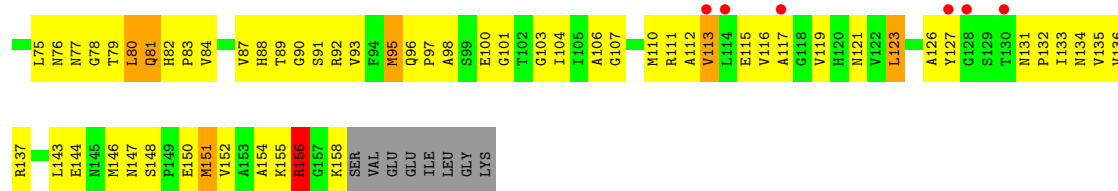


• Molecule 3: 30S ribosomal protein S4

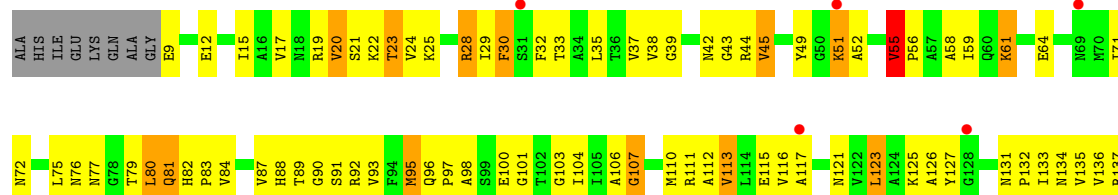


• Molecule 4: 30S ribosomal protein S5

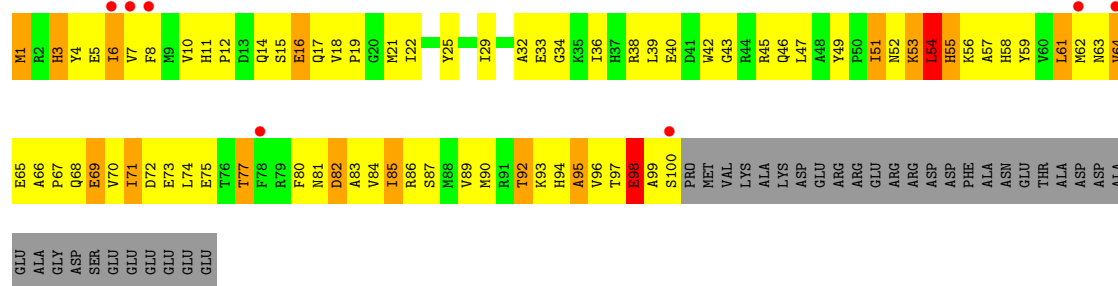
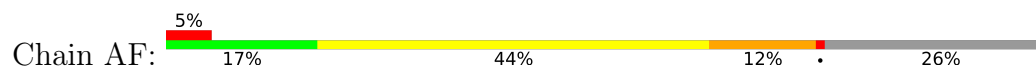




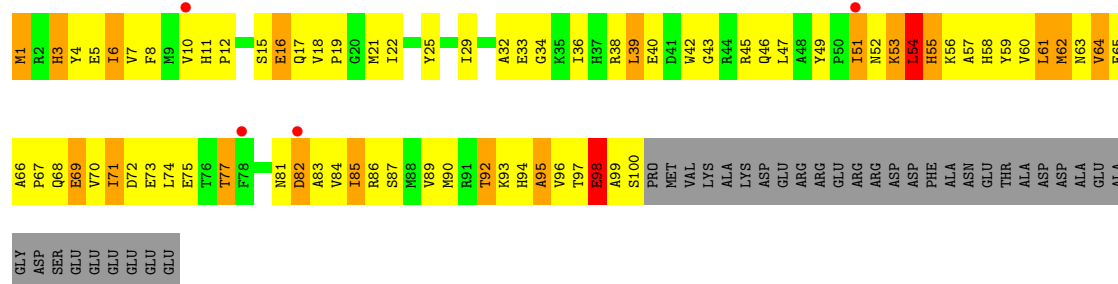
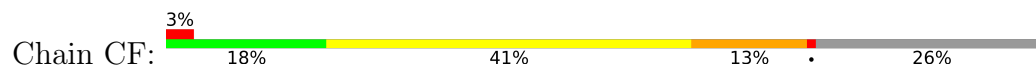
• Molecule 4: 30S ribosomal protein S5



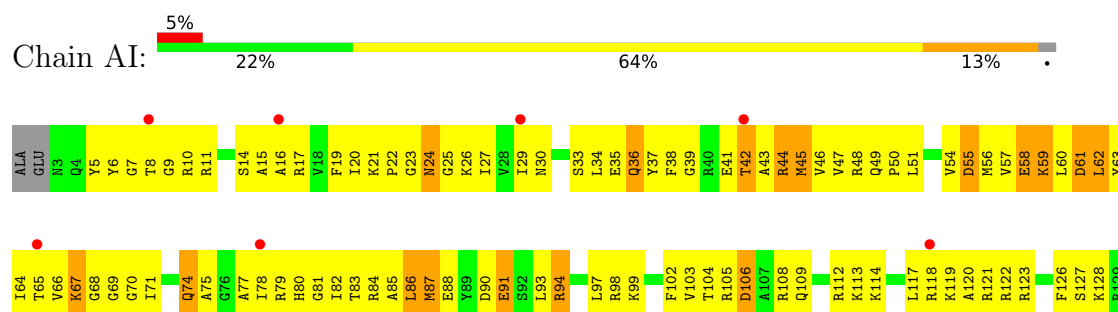
• Molecule 5: 30S ribosomal protein S6



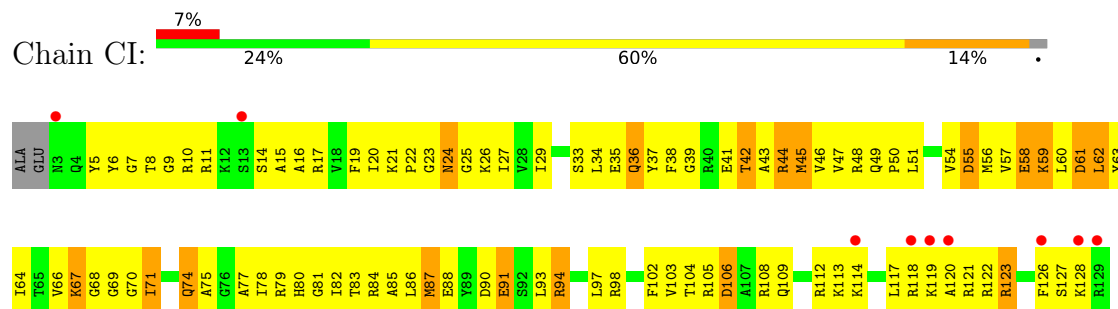
• Molecule 5: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S7



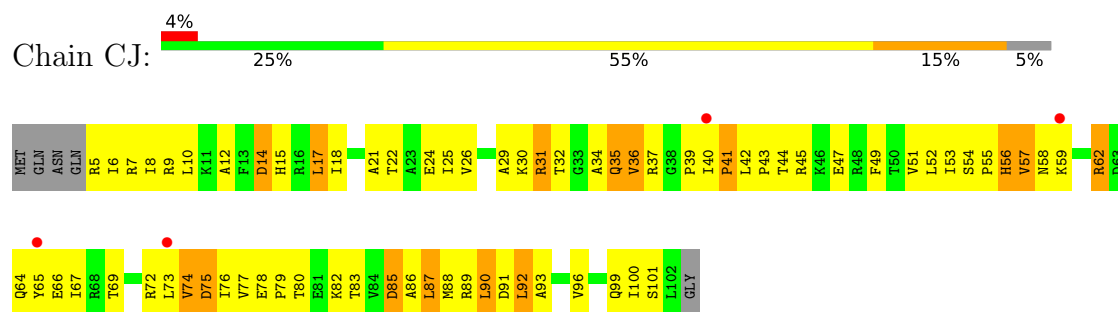
• Molecule 8: 30S ribosomal protein S9



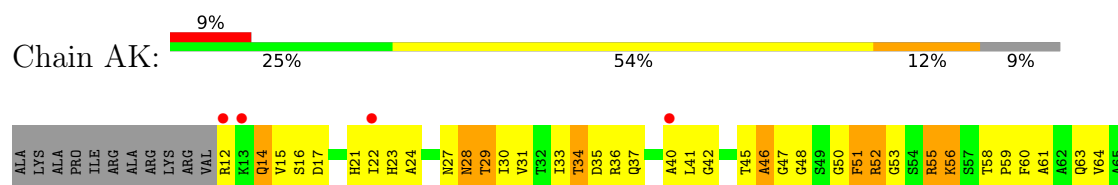
• Molecule 9: 30S ribosomal protein S10

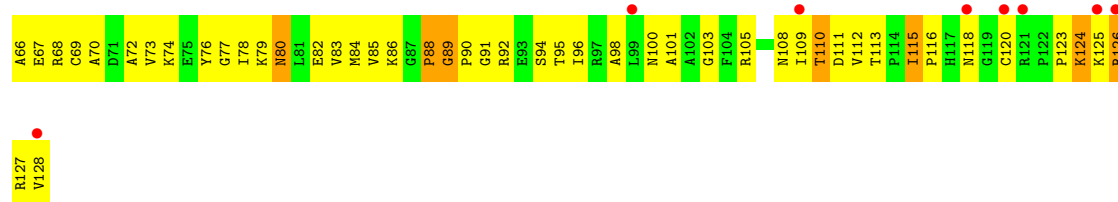


• Molecule 9: 30S ribosomal protein S10

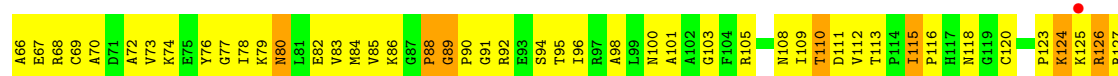


• Molecule 10: 30S ribosomal protein S11

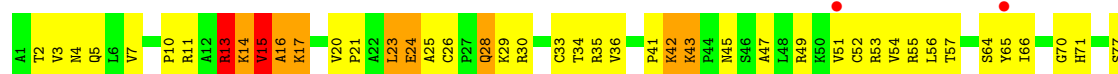




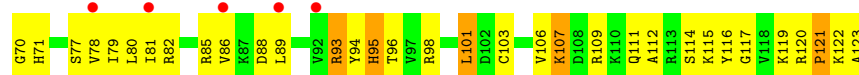
• Molecule 10: 30S ribosomal protein S11



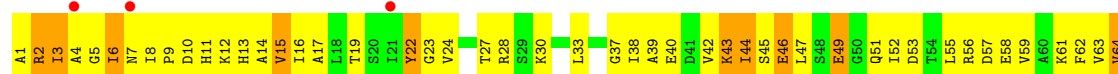
• Molecule 11: 30S ribosomal protein S12



• Molecule 11: 30S ribosomal protein S12

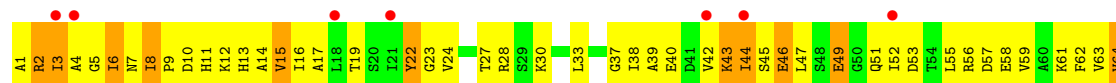


• Molecule 12: 30S ribosomal protein S13

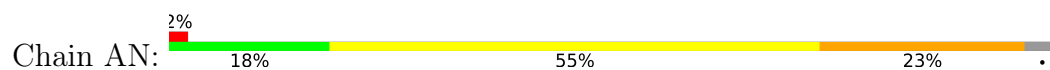




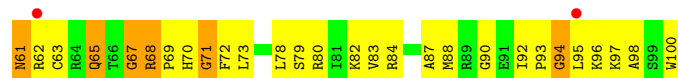
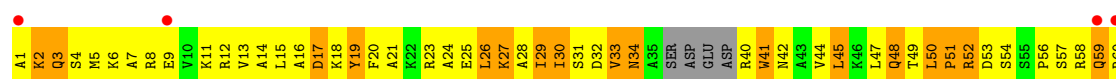
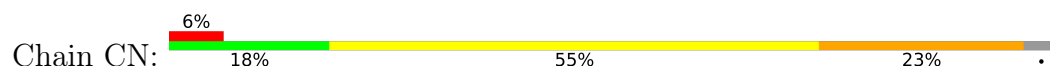
• Molecule 12: 30S ribosomal protein S13



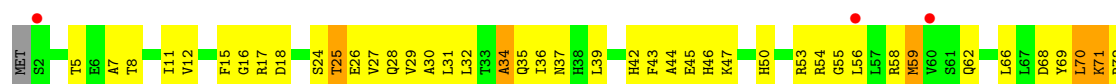
• Molecule 13: 30S ribosomal protein S14



• Molecule 13: 30S ribosomal protein S14

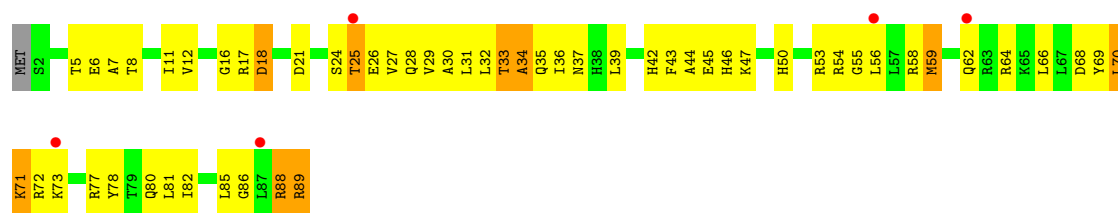


• Molecule 14: 30S ribosomal protein S15

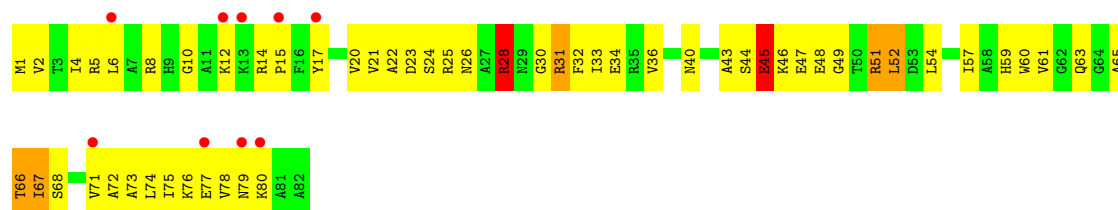


• Molecule 14: 30S ribosomal protein S15

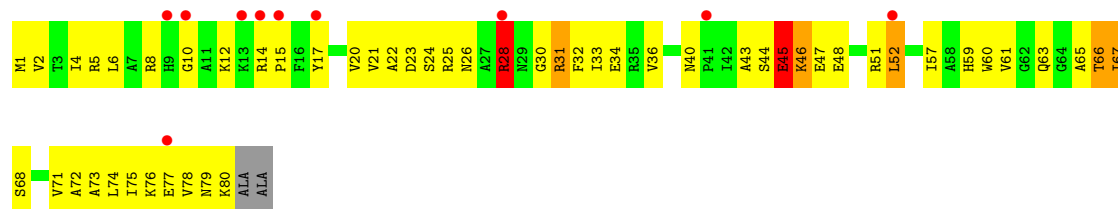




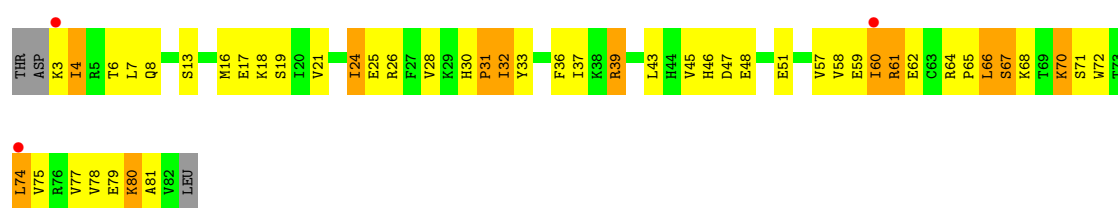
• Molecule 15: 30S ribosomal protein S16



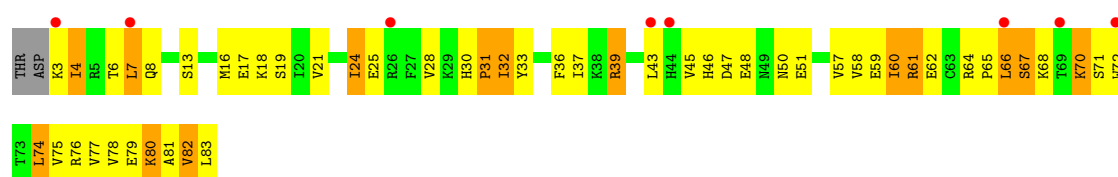
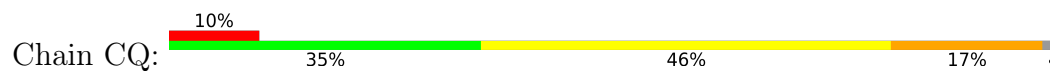
• Molecule 15: 30S ribosomal protein S16



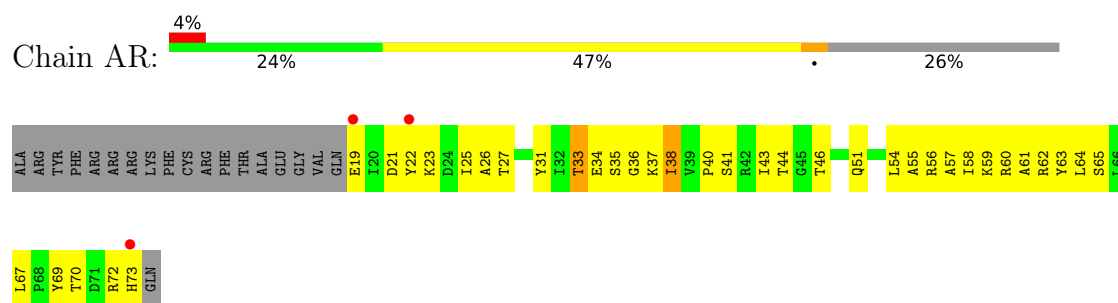
• Molecule 16: 30S ribosomal protein S17



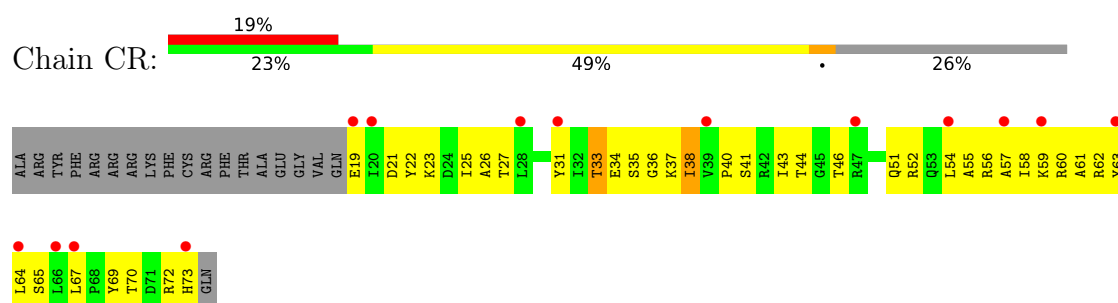
• Molecule 16: 30S ribosomal protein S17



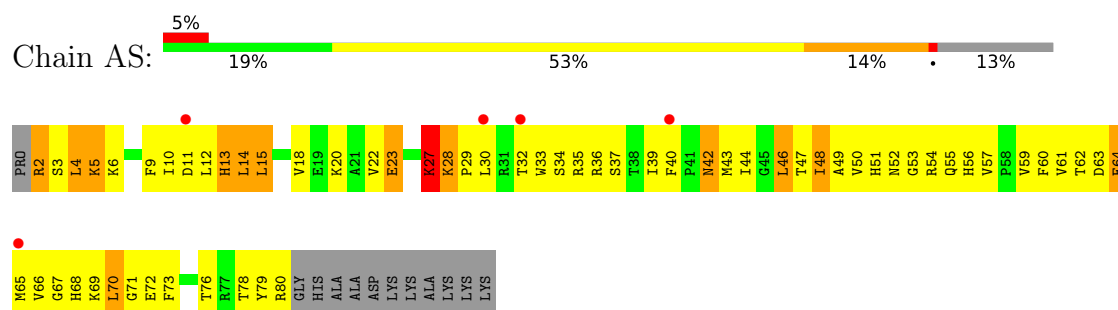
• Molecule 17: 30S ribosomal protein S18



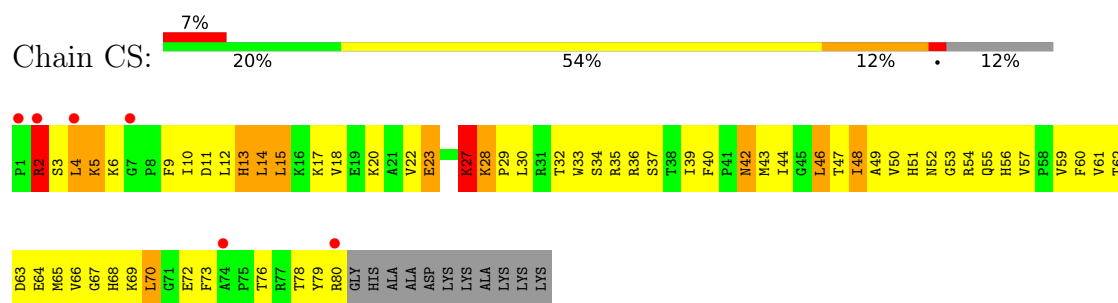
• Molecule 17: 30S ribosomal protein S18



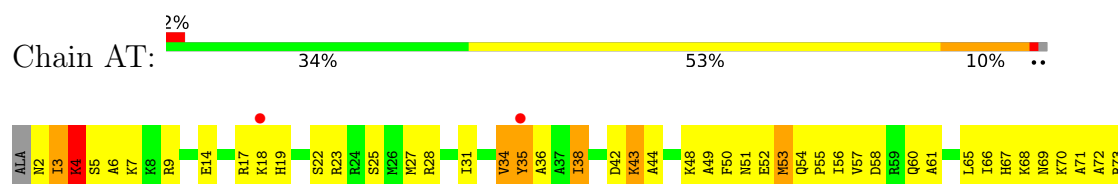
• Molecule 18: 30S ribosomal protein S19



• Molecule 18: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S20

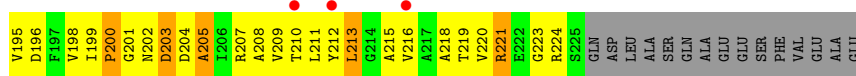
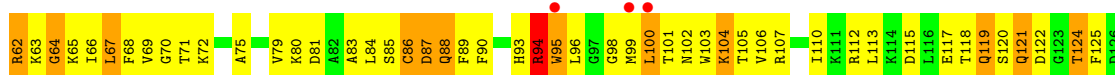




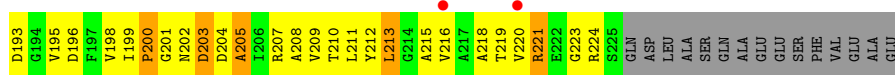
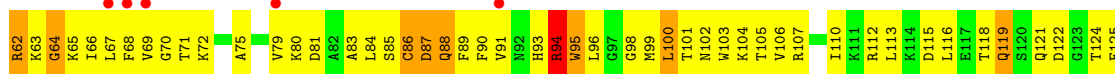
- Molecule 19: 30S ribosomal protein S20



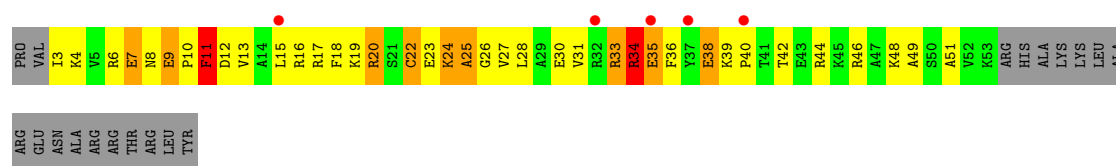
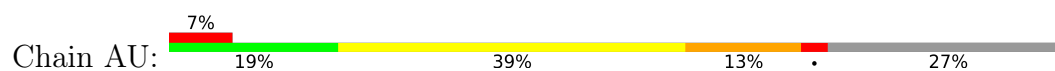
- Molecule 20: 30S ribosomal protein S2



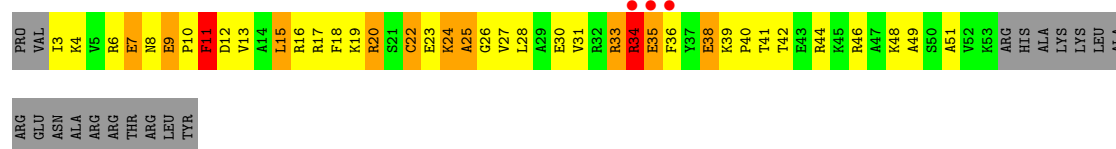
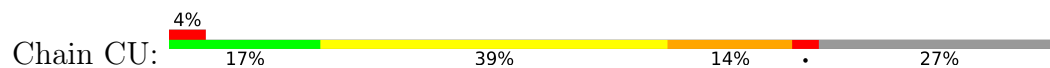
- Molecule 20: 30S ribosomal protein S2



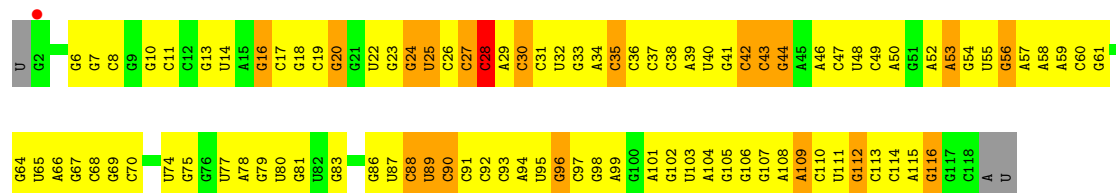
- Molecule 21: 30S ribosomal protein S21



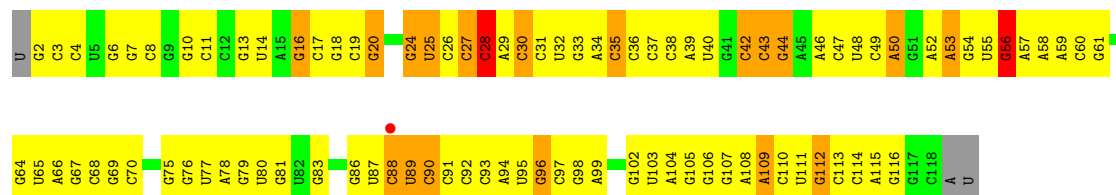
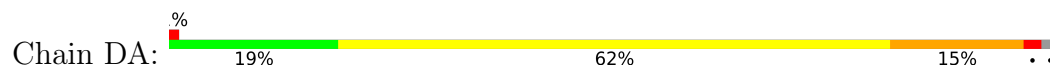
- Molecule 21: 30S ribosomal protein S21



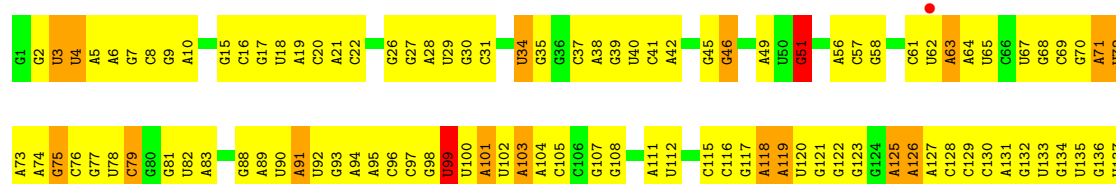
- Molecule 22: 5S rRNA



- Molecule 22: 5S rRNA



- Molecule 23: 23S rRNA



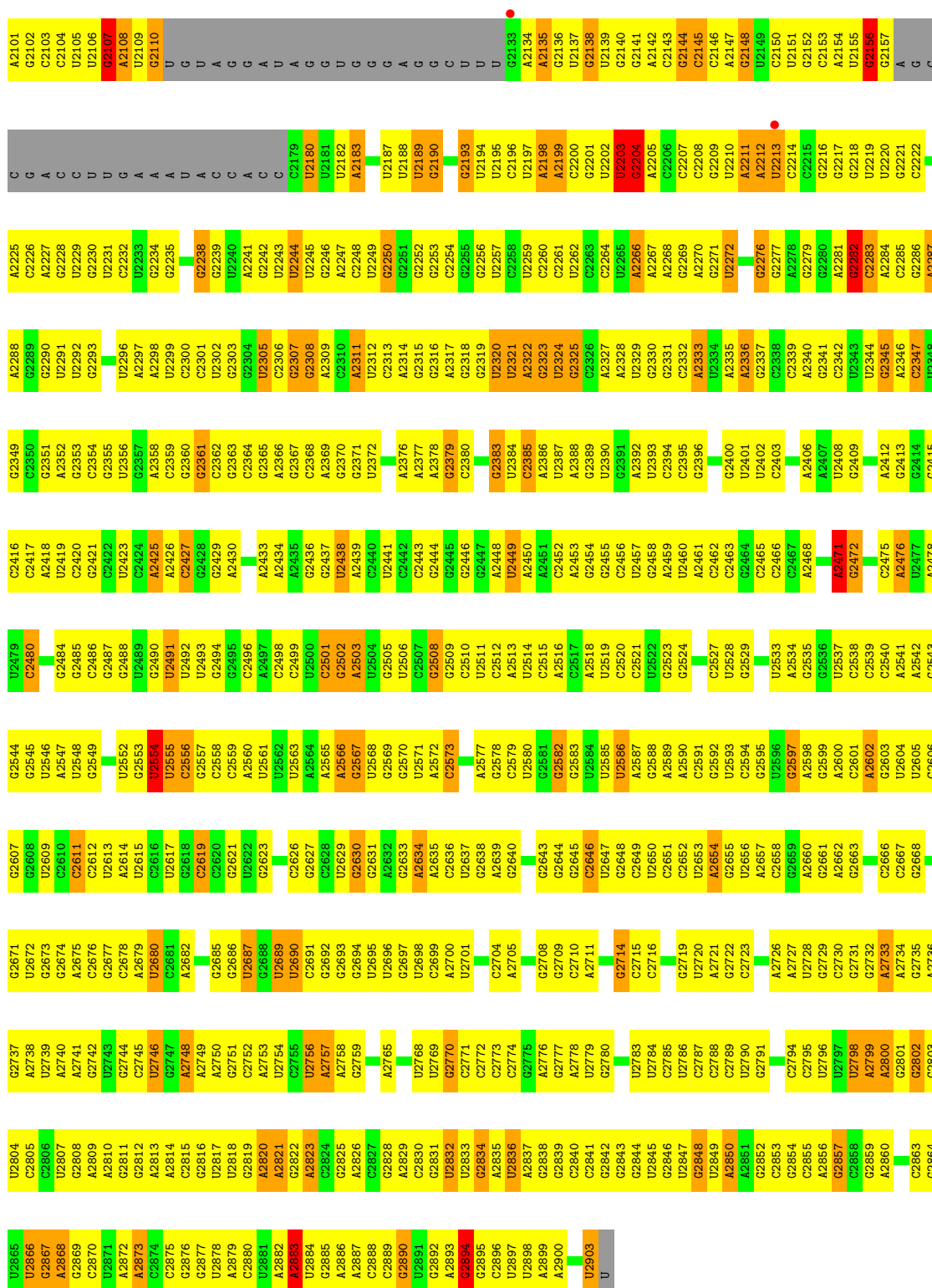
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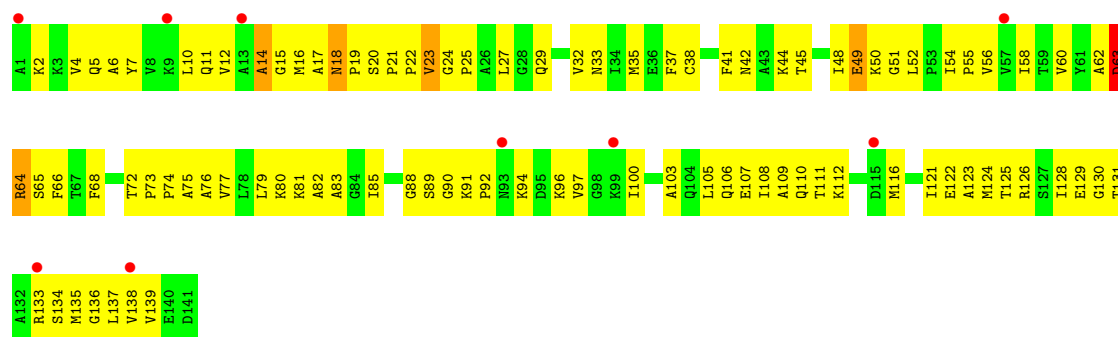


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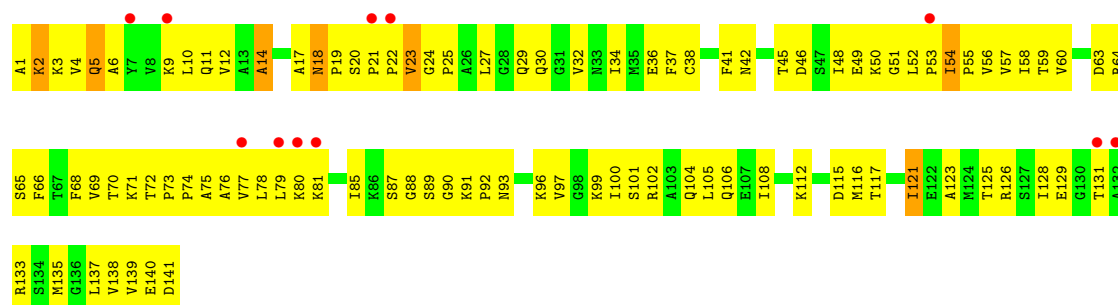
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A2029	G1891	G1828	C1761	A1700	U1559	C1493	A1431	G1369	U1236	C1167	C1167
C2029	C1892	A1829	A1762	A1701	U1560	A1495	G1432	A1304	A1237	G1168	
U2030	C1893	A1830	G1763	C1704	G1561	U1496	A1433	C1370	A1304	G1238	A1169
U1966	U1894	G1831	C1764	A1705	U1562		A1434	G1371	C1305	G1238	A1169
C1957	C1895	U1765	U1765	A1705	U1563	C1499	G1435	U1372	C1306	G1239	C1170
G2032	G1896	C1832	G1766	G1706	U1564	G1500	A1436	A1373	A1307	U1240	G1171
G1959	G1897	U1834	G1767	G1707	C1564	G1501	G1437	G1375	A1308	C1172	C1172
U2034	U1898	G1835	C1768	C1708	C1565	A1502	U1438	U1376	G1310	U1242	U1173
G2035	U1899	A1836	U1709	C1708	A1566	A1503	A1439	C1377		C1243	U1174
A2036	A1900	C1837	G1710	A1711	G1567	A1504	A1439	A1378	U1313	A1244	U1175
U2099	C1967	C1838	C1774		U1568	A1505	G1441	U1379		U1176	A1176
G2100									A1246	A1246	G1177



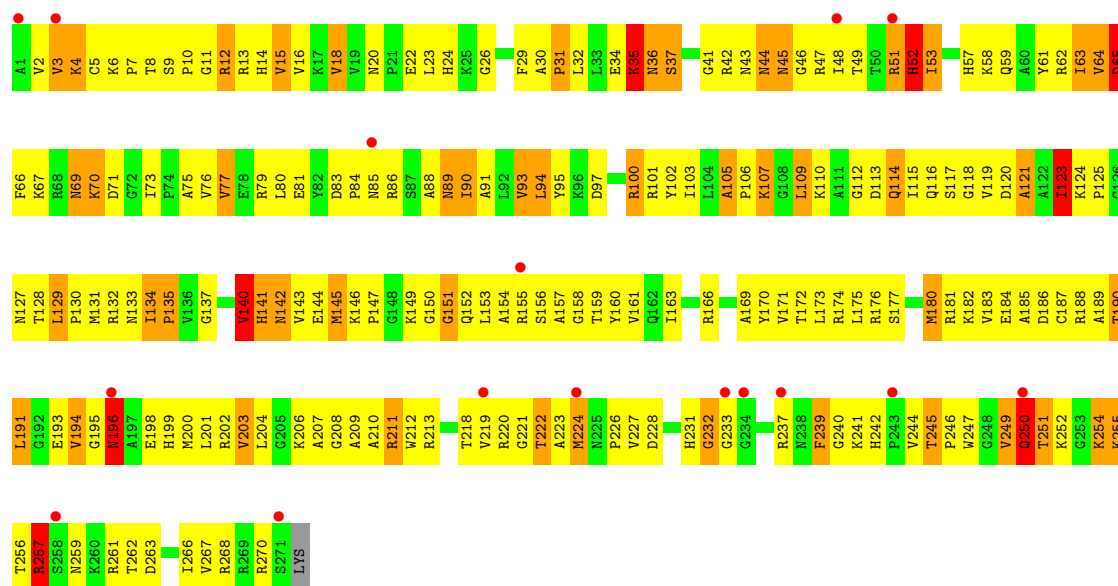
• Molecule 24: 50S ribosomal protein L11



• Molecule 24: 50S ribosomal protein L11

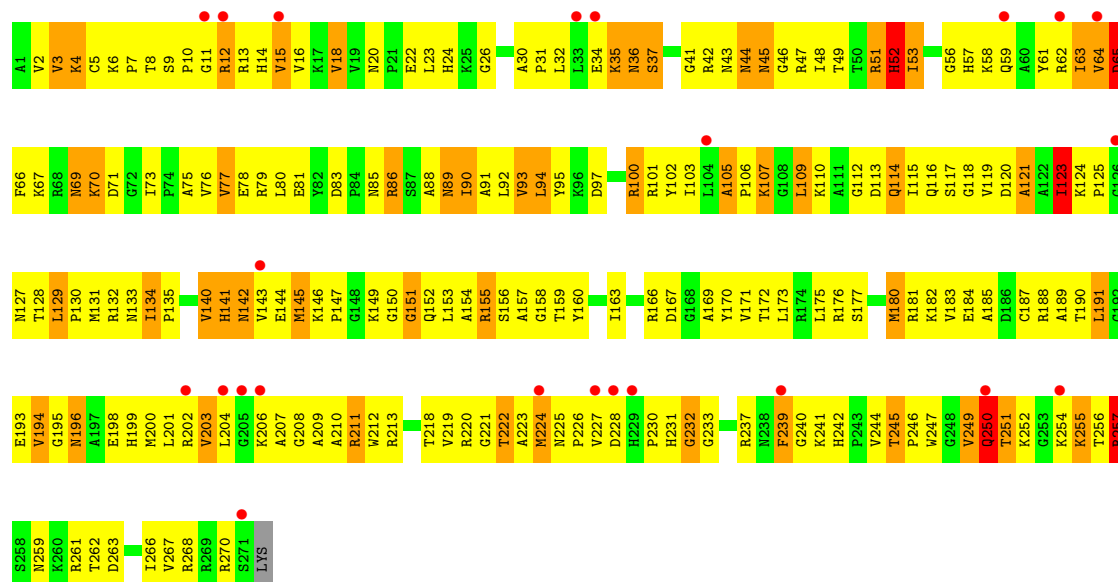


• Molecule 25: 50S ribosomal protein L2

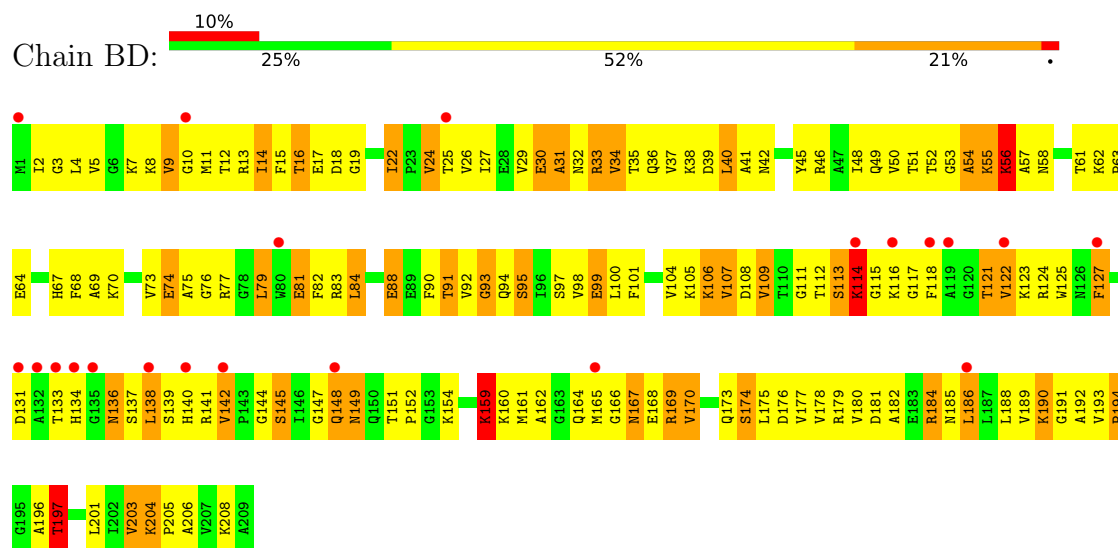


• Molecule 25: 50S ribosomal protein L2

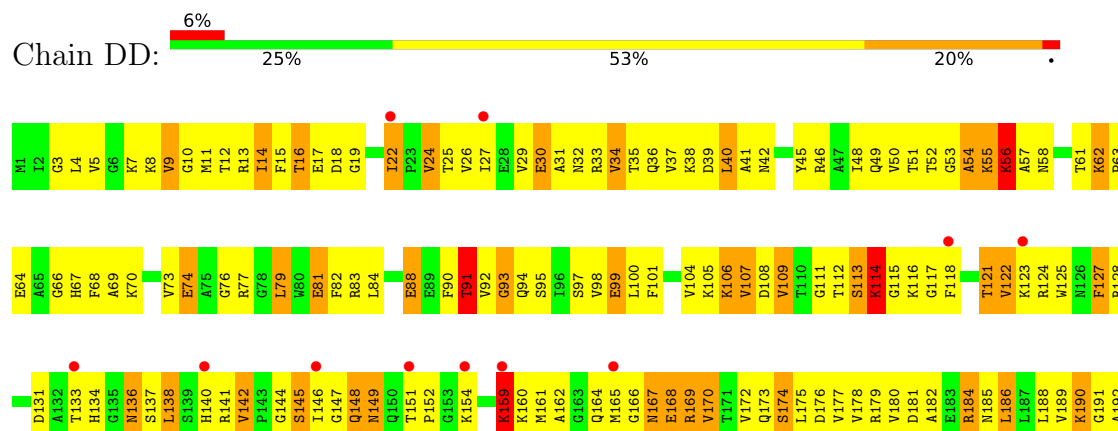


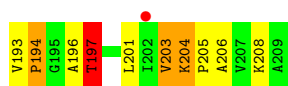


• Molecule 26: 50S ribosomal protein L3

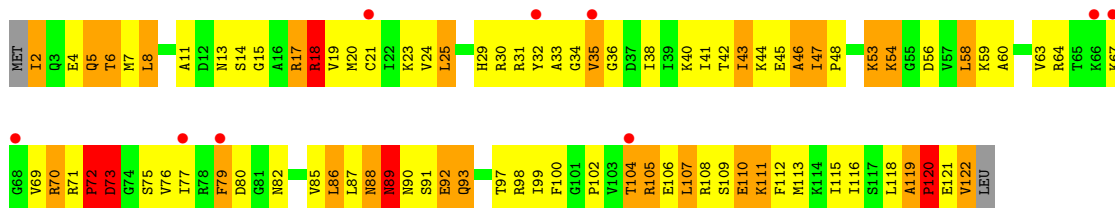


• Molecule 26: 50S ribosomal protein L3





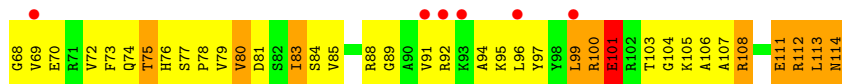
- Molecule 27: 50S ribosomal protein L14



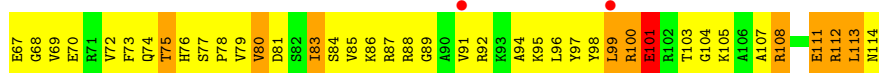
- Molecule 27: 50S ribosomal protein L14



- Molecule 28: 50S ribosomal protein L19

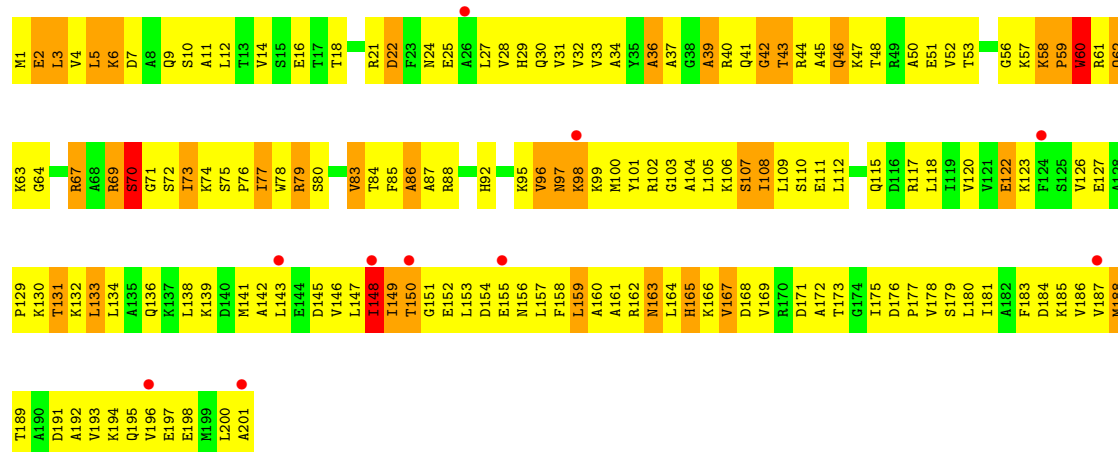


- Molecule 28: 50S ribosomal protein L19

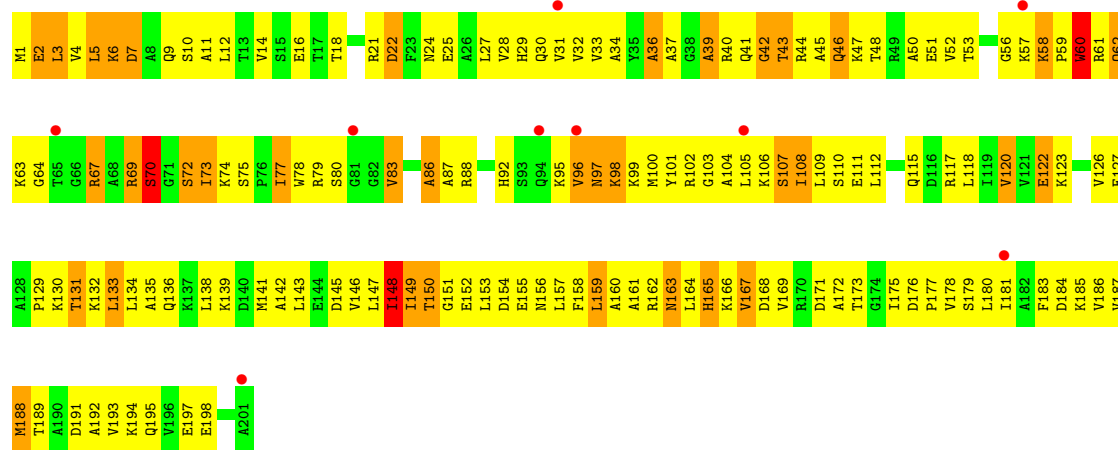


- Molecule 29: 50S ribosomal protein L4

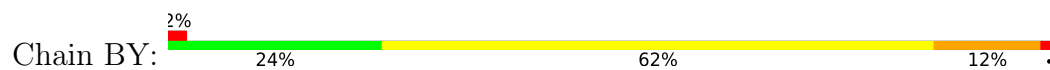




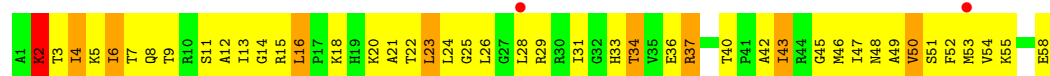
• Molecule 29: 50S ribosomal protein L4



• Molecule 30: 50S ribosomal protein L30

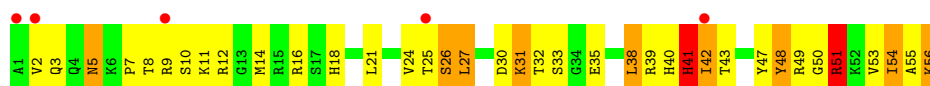


• Molecule 30: 50S ribosomal protein L30

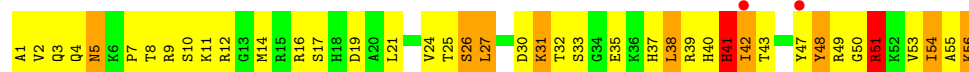


• Molecule 31: 50S ribosomal protein L32





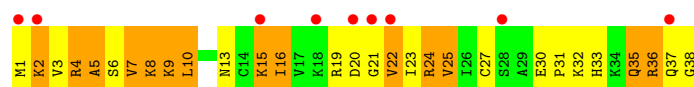
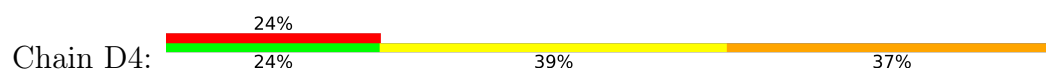
- Molecule 31: 50S ribosomal protein L32



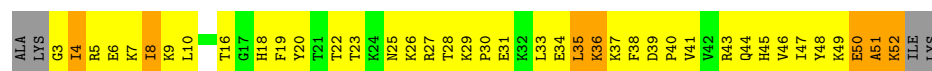
- Molecule 32: 50S ribosomal protein L36



- Molecule 32: 50S ribosomal protein L36



- Molecule 33: 50S ribosomal protein L33



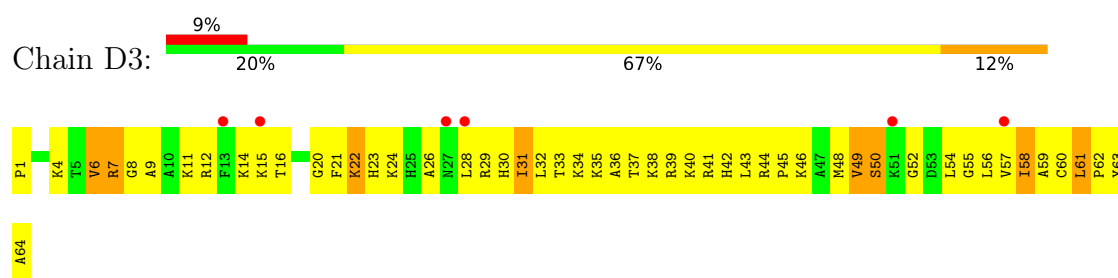
- Molecule 33: 50S ribosomal protein L33



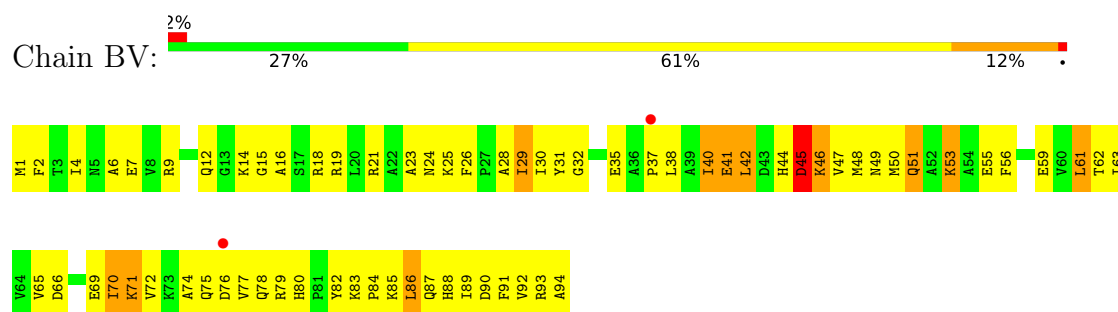
- Molecule 34: 50S ribosomal protein L35



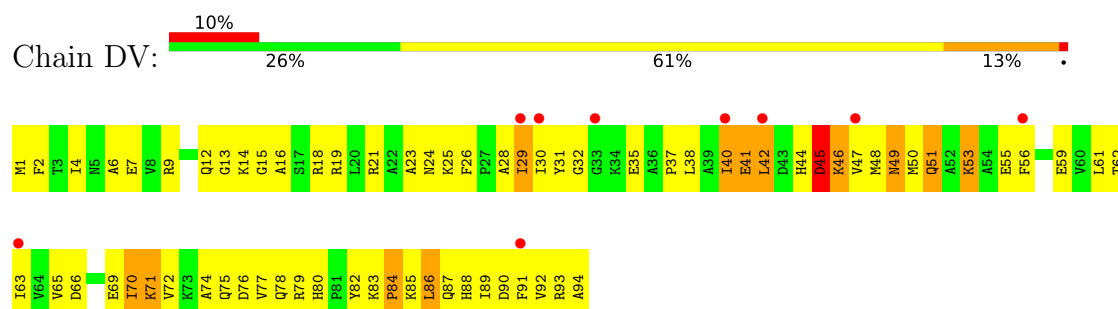
- Molecule 34: 50S ribosomal protein L35



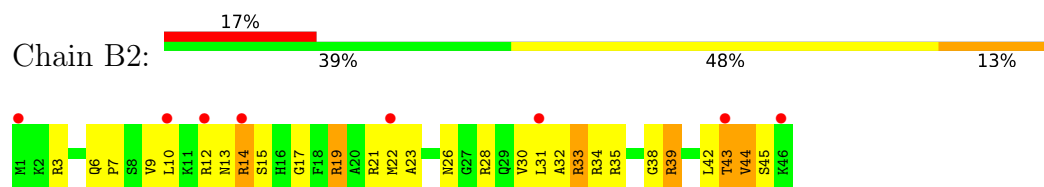
- Molecule 35: 50S ribosomal protein L25



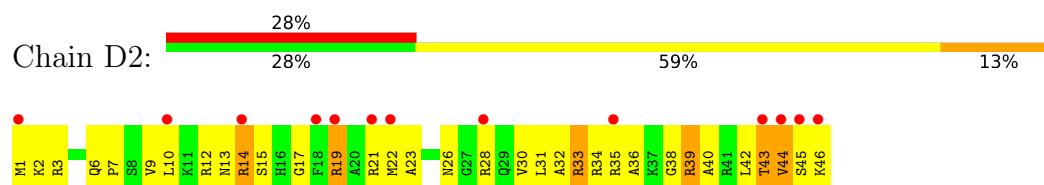
- Molecule 35: 50S ribosomal protein L25



- Molecule 36: 50S ribosomal protein L34

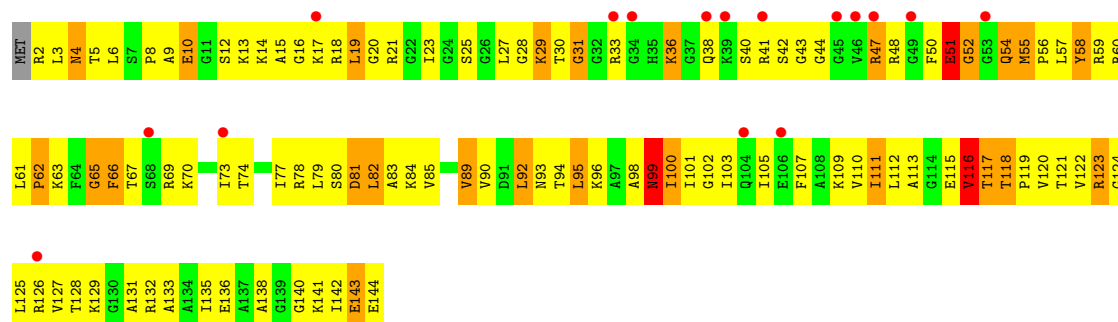


- Molecule 36: 50S ribosomal protein L34

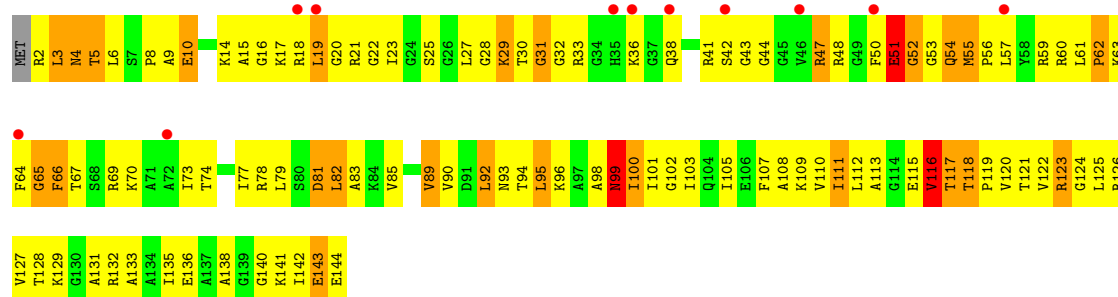


- Molecule 37: 50S ribosomal protein L15

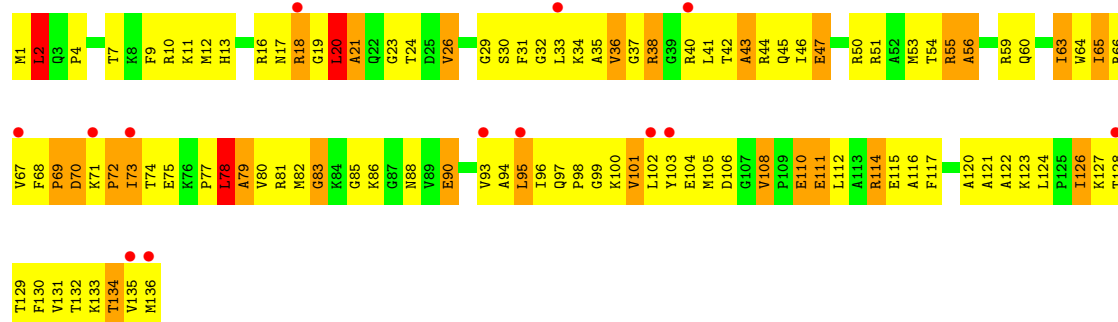




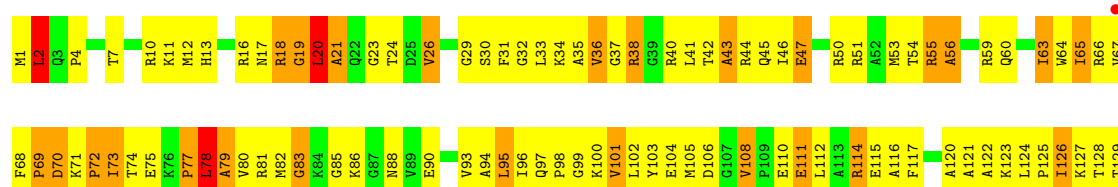
• Molecule 37: 50S ribosomal protein L15



• Molecule 38: 50S ribosomal protein L16

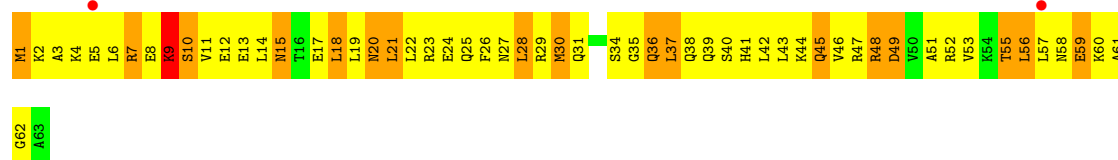
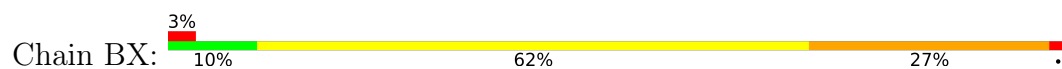


• Molecule 38: 50S ribosomal protein L16

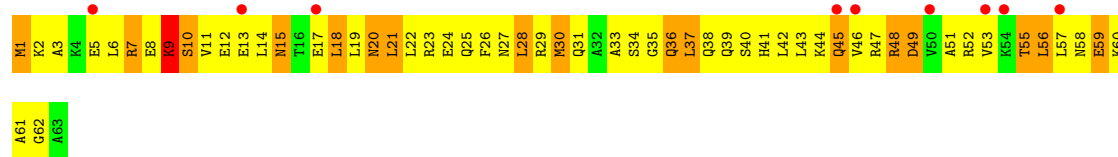
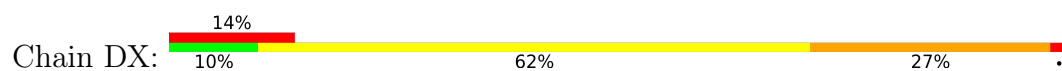


F130
V131
T132
K133
T134
V135
M136

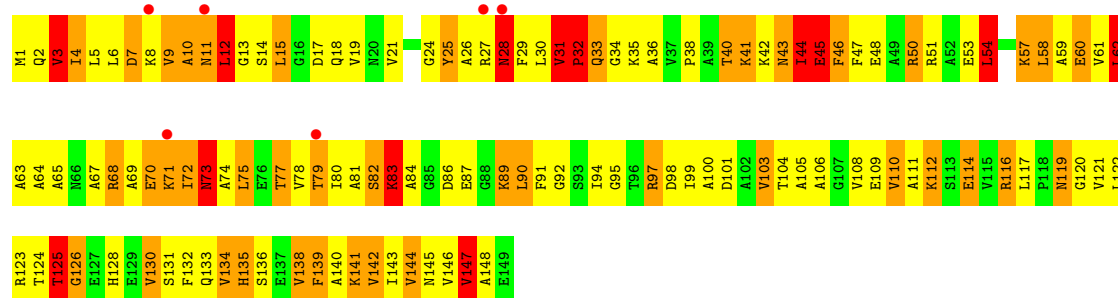
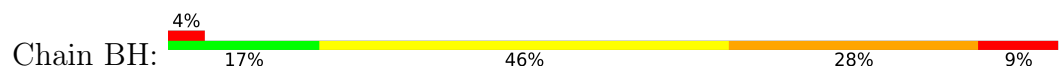
• Molecule 39: 50S ribosomal protein L29



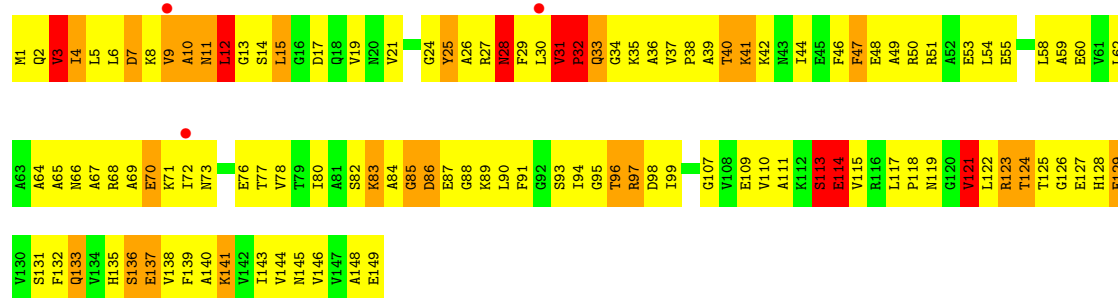
• Molecule 39: 50S ribosomal protein L29



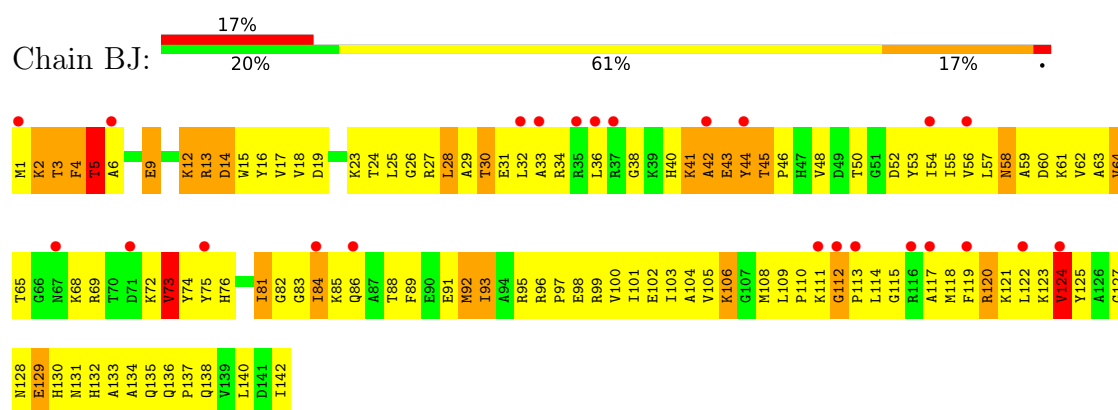
• Molecule 40: 50S ribosomal protein L9



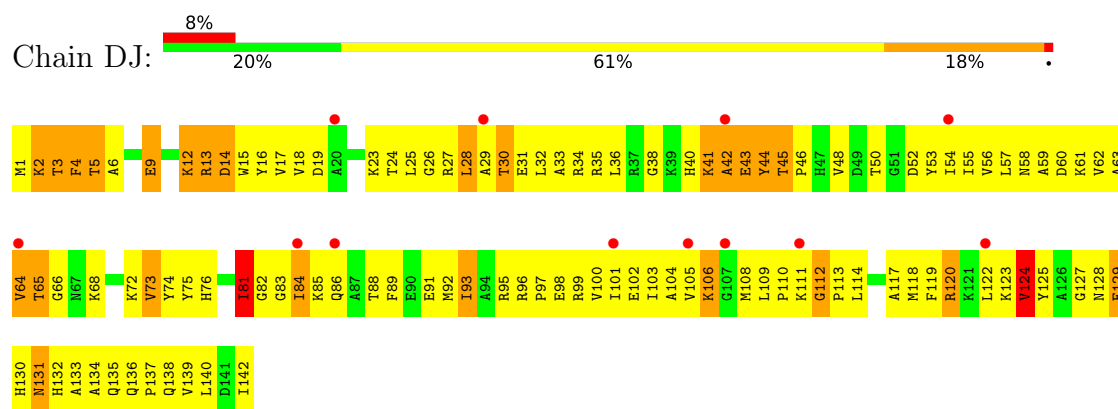
• Molecule 40: 50S ribosomal protein L9



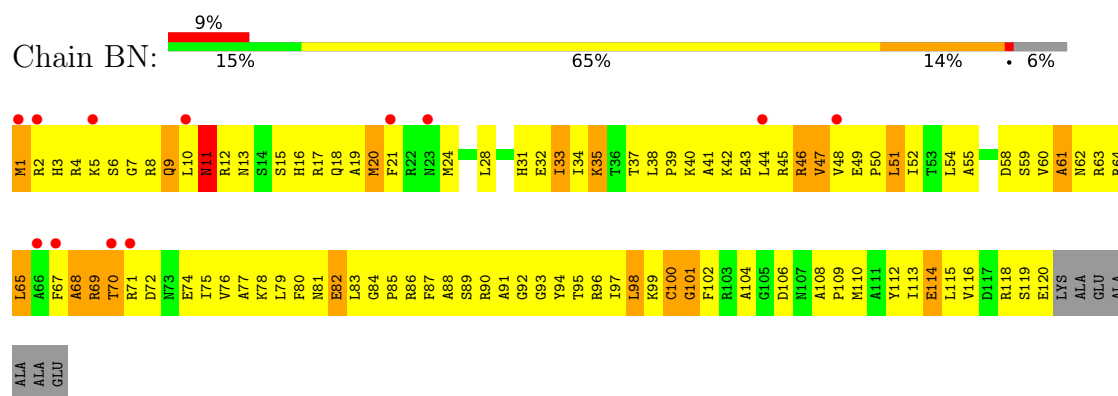
• Molecule 41: 50S ribosomal protein L13



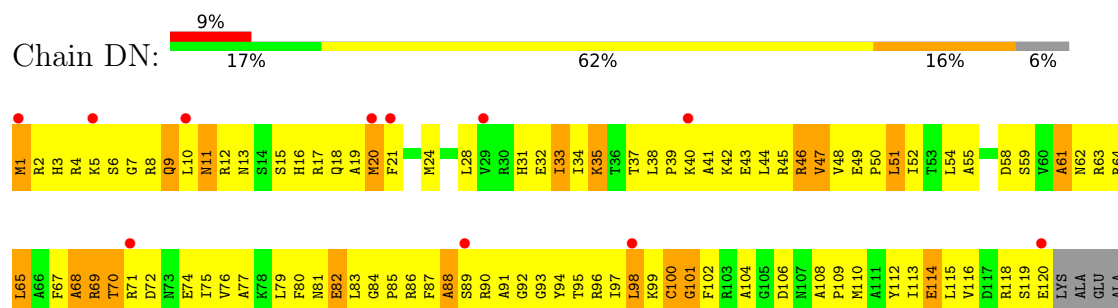
• Molecule 41: 50S ribosomal protein L13



• Molecule 42: 50S ribosomal protein L17



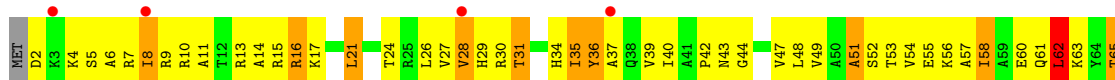
• Molecule 42: 50S ribosomal protein L17



ALA
ALA
GLU

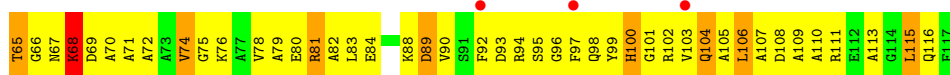
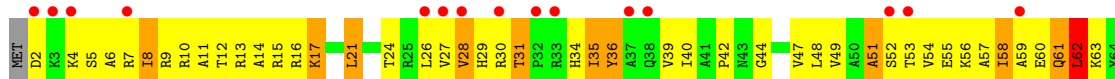
• Molecule 43: 50S ribosomal protein L18

Chain BO: 7% 23% 59% 15% ..



• Molecule 43: 50S ribosomal protein L18

Chain DO: 15% 22% 60% 15% ..



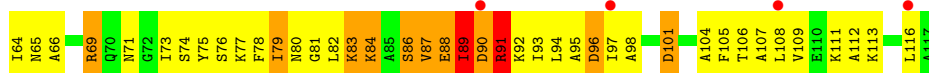
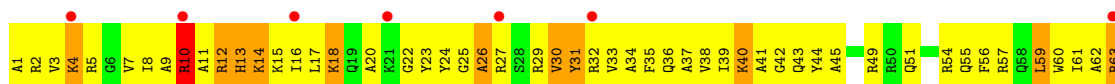
• Molecule 44: 50S ribosomal protein L20

Chain BQ: 9% 24% 55% 19% .



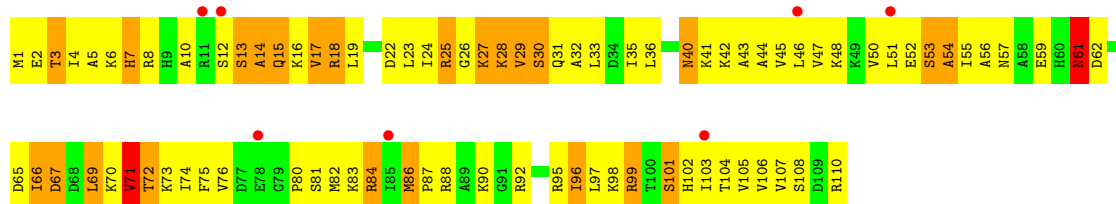
• Molecule 44: 50S ribosomal protein L20

Chain DQ: 9% 21% 59% 18% .

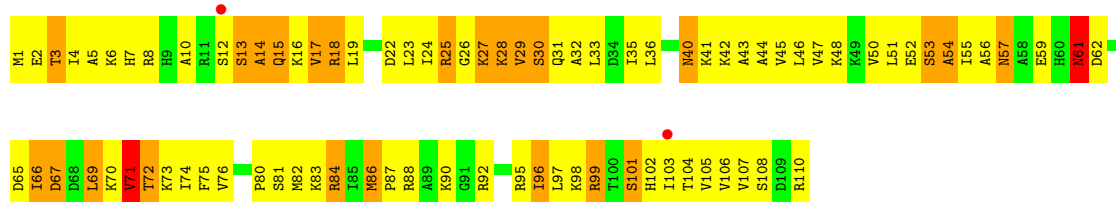


• Molecule 45: 50S ribosomal protein L22

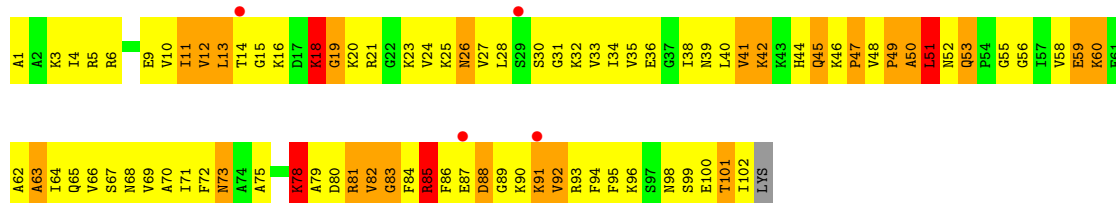
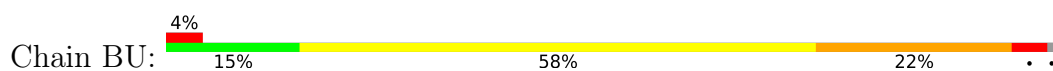
Chain BS: 6% 22% 55% 22% .



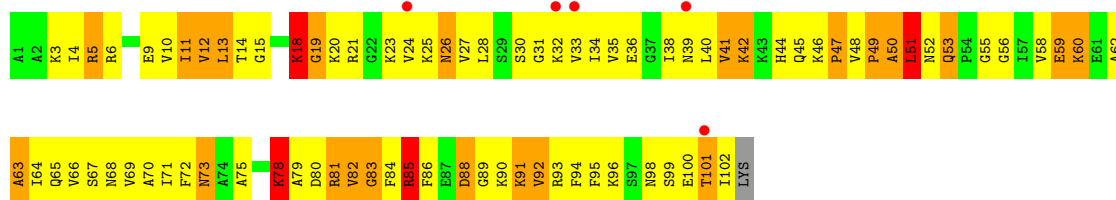
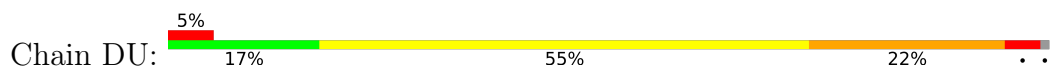
• Molecule 45: 50S ribosomal protein L22



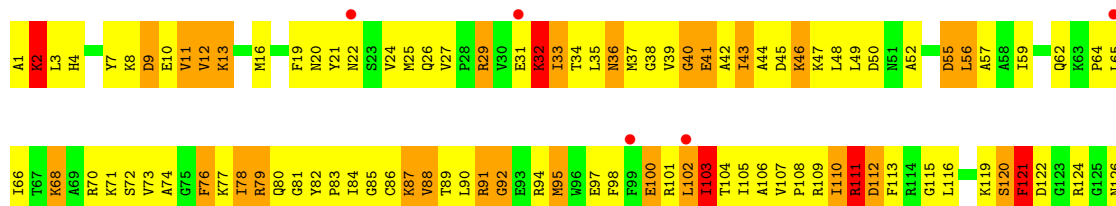
• Molecule 46: 50S ribosomal protein L24



• Molecule 46: 50S ribosomal protein L24

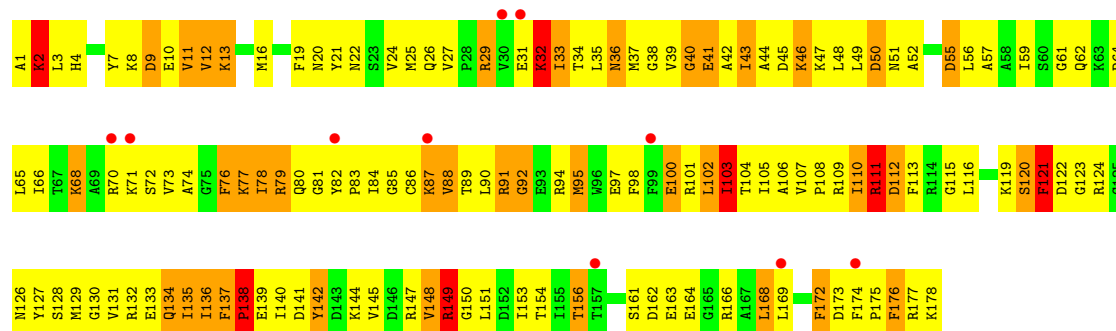


• Molecule 47: 50S ribosomal protein L5

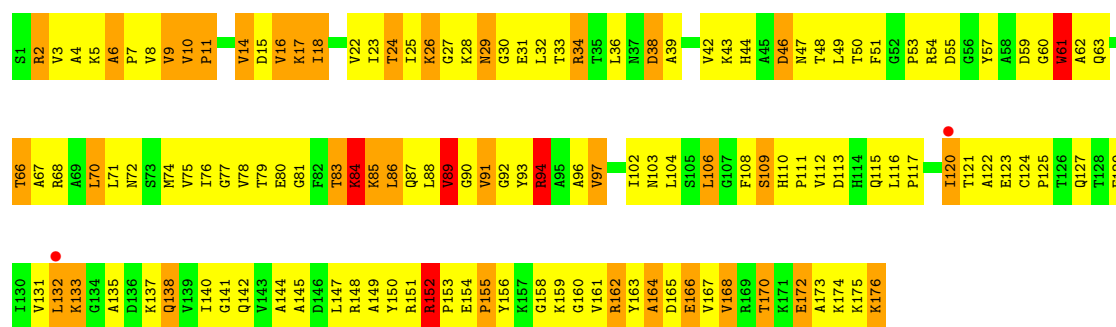




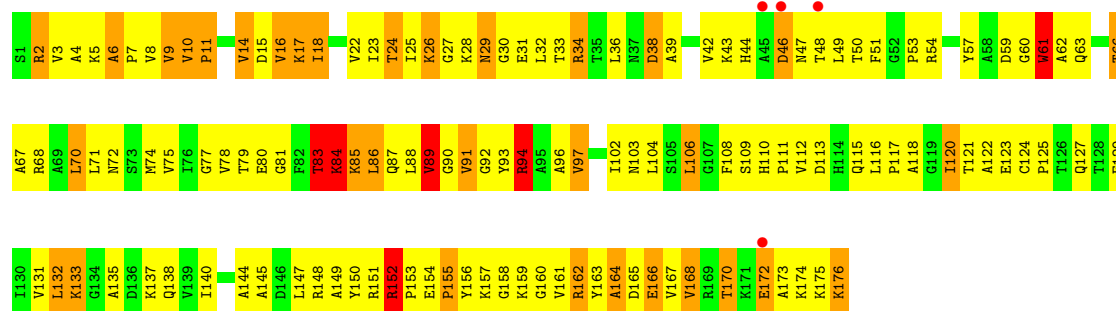
• Molecule 47: 50S ribosomal protein L5



• Molecule 48: 50S ribosomal protein L6

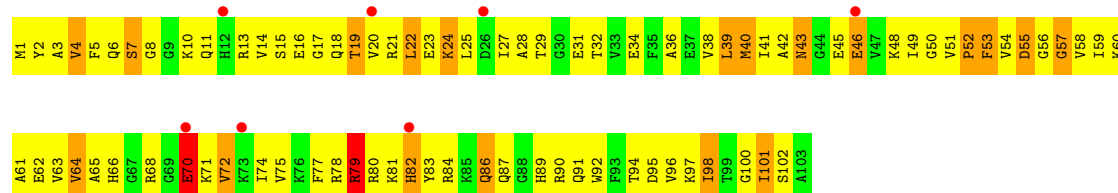


• Molecule 48: 50S ribosomal protein L6

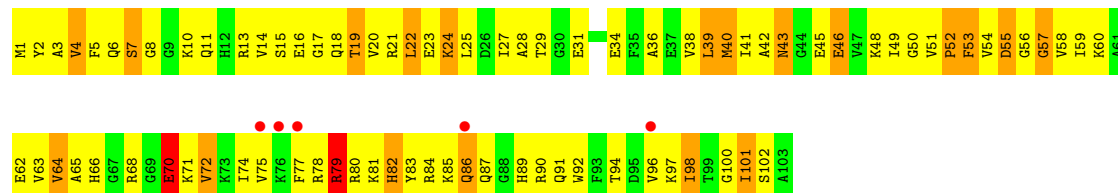


• Molecule 49: 50S ribosomal protein L21

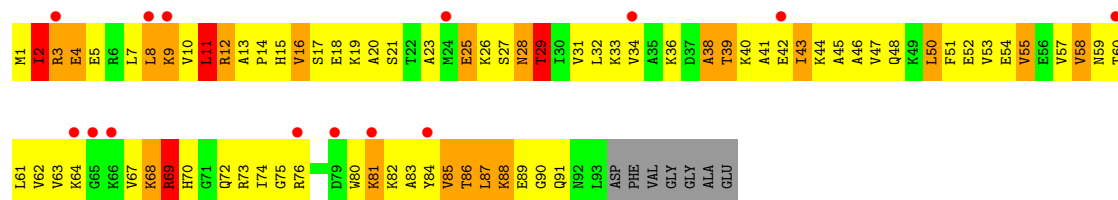
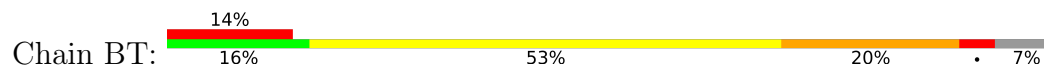




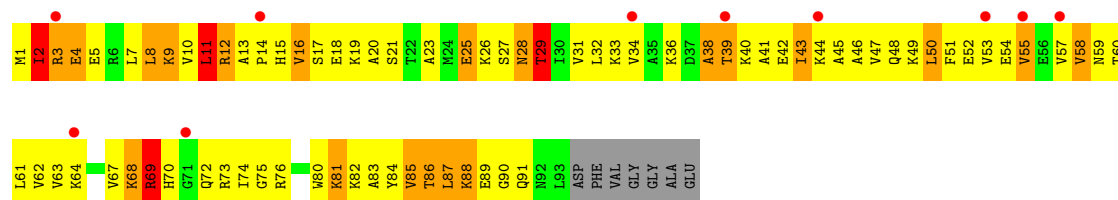
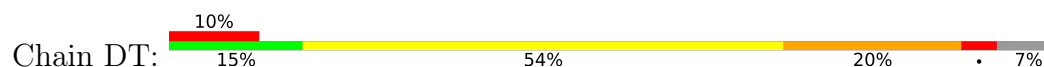
• Molecule 49: 50S ribosomal protein L21



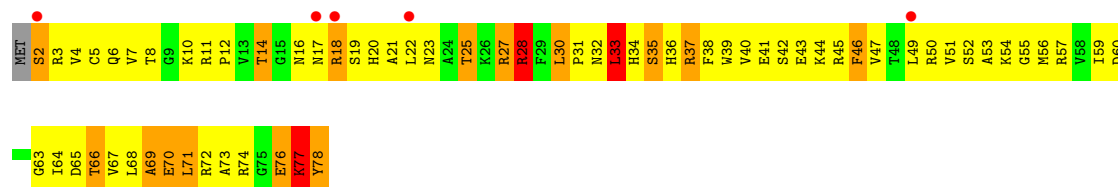
• Molecule 50: 50S ribosomal protein L23



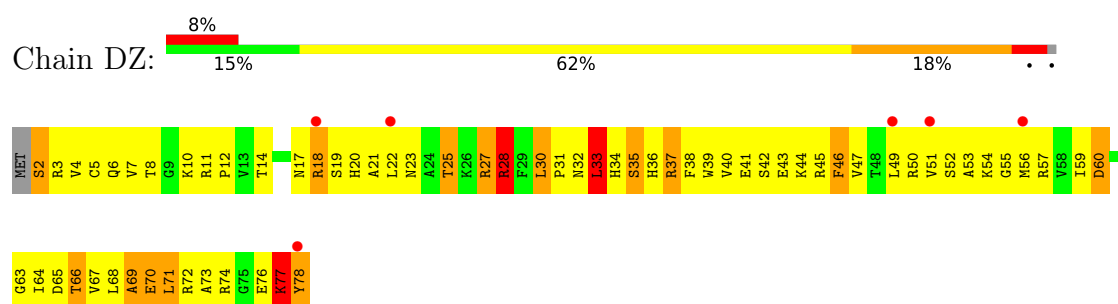
• Molecule 50: 50S ribosomal protein L23



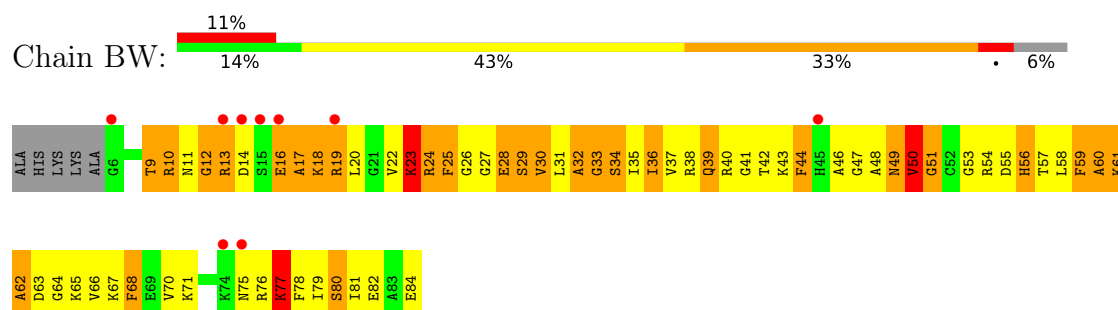
• Molecule 51: 50S ribosomal protein L28



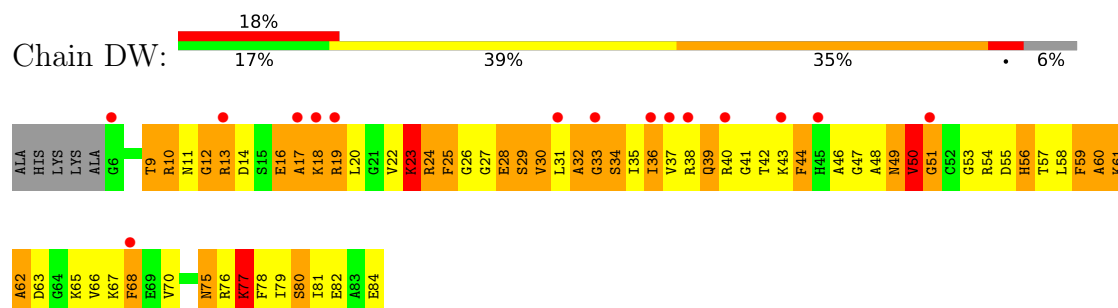
• Molecule 51: 50S ribosomal protein L28



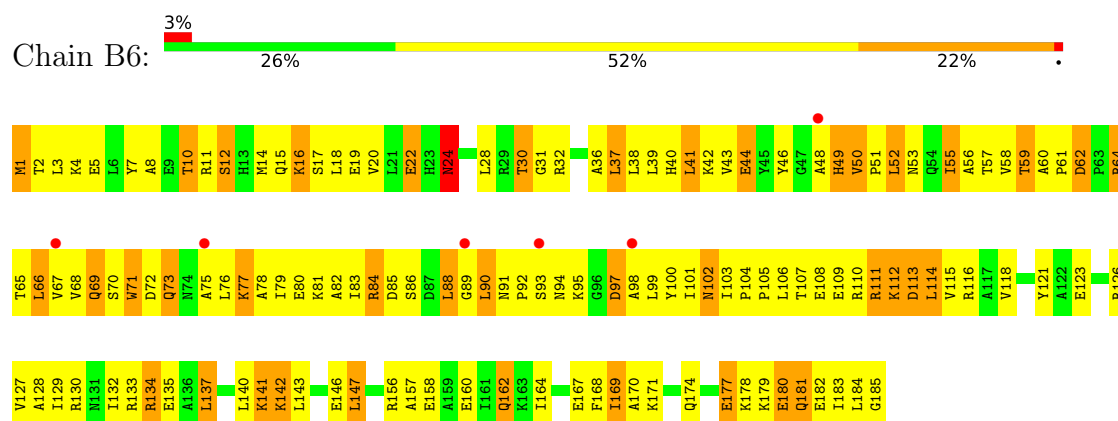
- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27

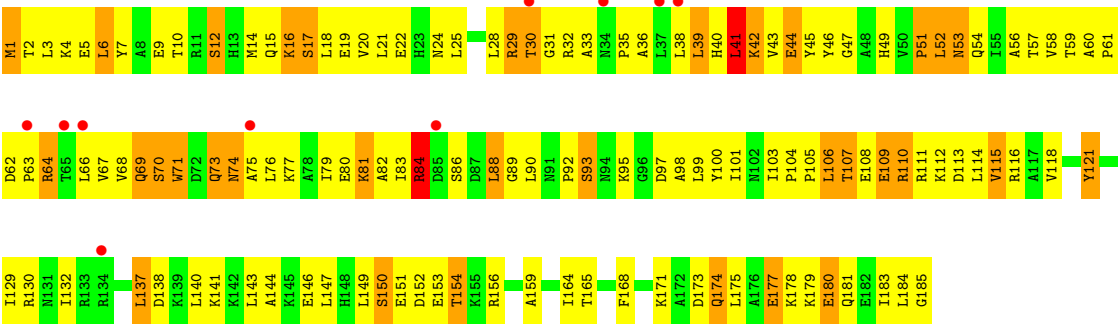


- Molecule 53: 50S ribosomal protein RRF



- Molecule 53: 50S ribosomal protein RRF





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.87Å 378.75Å 738.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.45 40.00 – 4.45	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.00-4.45) 95.5 (40.00-4.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 4.46Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.263 , 0.309 0.234 , 0.272	Depositor DCC
R_{free} test set	16978 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	150.5	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	287128	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 2.03% 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: MG, PAR, ZN

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	0.28	0/36762	0.65	33/57350 (0.1%)
1	CA	0.28	0/36762	0.66	35/57350 (0.1%)
2	AC	0.28	0/1651	0.69	0/2225
2	CC	0.28	0/1651	0.69	0/2225
3	AD	0.26	0/1665	0.70	1/2227 (0.0%)
3	CD	0.26	0/1665	0.70	1/2227 (0.0%)
4	AE	0.28	0/1118	0.75	0/1504
4	CE	0.29	0/1118	0.77	1/1504 (0.1%)
5	AF	0.29	0/835	0.70	0/1128
5	CF	0.29	0/835	0.69	0/1128
6	AG	0.28	0/1187	0.80	2/1591 (0.1%)
6	CG	0.28	0/1211	0.80	2/1624 (0.1%)
7	AH	0.27	0/989	0.72	0/1326
7	CH	0.27	0/989	0.71	0/1326
8	AI	0.27	0/1034	0.69	0/1375
8	CI	0.27	0/1034	0.70	0/1375
9	AJ	0.30	0/796	0.78	0/1077
9	CJ	0.30	0/796	0.78	0/1077
10	AK	0.30	0/893	0.77	0/1205
10	CK	0.30	0/893	0.77	0/1205
11	AL	0.26	0/969	0.74	0/1300
11	CL	0.26	0/969	0.76	1/1300 (0.1%)
12	AM	0.26	0/892	0.72	0/1193
12	CM	0.27	0/884	0.73	0/1181
13	AN	0.27	0/785	0.74	1/1043 (0.1%)
13	CN	0.27	0/785	0.74	1/1043 (0.1%)
14	AO	0.26	0/722	0.78	3/964 (0.3%)
14	CO	0.26	0/722	0.79	3/964 (0.3%)
15	AP	0.29	0/659	0.79	2/884 (0.2%)
15	CP	0.28	0/648	0.79	2/870 (0.2%)
16	AQ	0.27	0/657	0.72	0/881
16	CQ	0.27	0/666	0.71	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.28	0/462	0.71	0/621
17	CR	0.28	0/462	0.71	0/621
18	AS	0.28	0/652	0.68	0/877
18	CS	0.28	0/660	0.70	0/888
19	AT	0.28	0/671	0.71	0/888
19	CT	0.29	0/671	0.71	0/888
20	AB	0.30	0/1735	0.74	0/2338
20	CB	0.29	0/1735	0.74	0/2338
21	AU	0.29	0/430	0.82	0/570
21	CU	0.28	0/430	0.83	1/570 (0.2%)
22	BA	0.35	1/2803 (0.0%)	0.70	3/4371 (0.1%)
22	DA	0.36	2/2803 (0.1%)	0.71	4/4371 (0.1%)
23	BB	0.29	3/68314 (0.0%)	0.68	90/106569 (0.1%)
23	DB	0.29	2/68314 (0.0%)	0.68	97/106569 (0.1%)
24	BI	0.32	0/1046	0.82	1/1410 (0.1%)
24	DI	0.35	0/1046	0.85	0/1410
25	BC	0.28	0/2121	0.74	0/2852
25	DC	0.28	0/2121	0.74	0/2852
26	BD	0.28	0/1586	0.76	2/2134 (0.1%)
26	DD	0.28	0/1586	0.76	2/2134 (0.1%)
27	BK	0.29	0/939	0.86	2/1258 (0.2%)
27	DK	0.29	0/939	0.86	2/1258 (0.2%)
28	BP	0.28	0/929	0.79	2/1242 (0.2%)
28	DP	0.28	0/929	0.82	3/1242 (0.2%)
29	BE	0.27	0/1571	0.84	4/2113 (0.2%)
29	DE	0.27	0/1571	0.83	3/2113 (0.1%)
30	BY	0.29	0/453	0.79	0/605
30	DY	0.30	0/453	0.80	0/605
31	B0	0.26	0/450	0.75	1/599 (0.2%)
31	D0	0.26	0/450	0.75	1/599 (0.2%)
32	B4	0.27	0/303	0.75	1/397 (0.3%)
32	D4	0.27	0/303	0.74	1/397 (0.3%)
33	B1	0.29	0/416	0.74	0/554
33	D1	0.30	0/416	0.73	0/554
34	B3	0.28	0/513	0.73	0/676
34	D3	0.27	0/513	0.73	0/676
35	BV	0.26	0/766	0.71	0/1025
35	DV	0.26	0/766	0.72	0/1025
36	B2	0.28	0/380	0.83	0/498
36	D2	0.28	0/380	0.80	0/498
37	BL	0.27	0/1054	0.77	0/1403
37	DL	0.27	0/1054	0.76	0/1403
38	BM	0.29	0/1093	0.76	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.29	0/1093	0.76	0/1460
39	BX	0.25	0/510	0.86	2/677 (0.3%)
39	DX	0.25	0/510	0.85	2/677 (0.3%)
40	BH	0.30	0/1122	0.72	1/1515 (0.1%)
40	DH	0.29	0/1122	0.77	2/1515 (0.1%)
41	BJ	0.28	0/1152	0.75	1/1551 (0.1%)
41	DJ	0.28	0/1152	0.75	1/1551 (0.1%)
42	BN	0.27	0/973	0.84	1/1301 (0.1%)
42	DN	0.27	0/973	0.84	0/1301
43	BO	0.27	0/902	0.83	3/1209 (0.2%)
43	DO	0.27	0/902	0.83	2/1209 (0.2%)
44	BQ	0.28	0/960	0.87	2/1278 (0.2%)
44	DQ	0.28	0/960	0.86	3/1278 (0.2%)
45	BS	0.28	0/864	0.87	3/1156 (0.3%)
45	DS	0.28	0/864	0.88	3/1156 (0.3%)
46	BU	0.27	0/787	0.71	0/1051
46	DU	0.27	0/787	0.71	0/1051
47	BF	0.28	0/1444	0.86	3/1937 (0.2%)
47	DF	0.28	0/1444	0.86	3/1937 (0.2%)
48	BG	0.28	0/1343	0.73	4/1816 (0.2%)
48	DG	0.28	0/1343	0.73	4/1816 (0.2%)
49	BR	0.26	0/829	0.68	0/1107
49	DR	0.26	0/829	0.68	0/1107
50	BT	0.27	0/744	0.90	4/994 (0.4%)
50	DT	0.27	0/744	0.90	4/994 (0.4%)
51	BZ	0.27	0/635	0.86	1/848 (0.1%)
51	DZ	0.27	0/635	0.86	1/848 (0.1%)
52	BW	0.28	0/603	0.79	0/797
52	DW	0.28	0/603	0.79	0/797
53	B6	0.29	0/1497	0.80	3/2017 (0.1%)
53	D6	0.28	0/1497	0.77	2/2017 (0.1%)
All	All	0.29	8/309354 (0.0%)	0.70	363/462003 (0.1%)

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	14
1	CA	0	12
22	BA	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	DA	0	2
23	BB	0	50
23	DB	0	48
All	All	0	128

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	2276	G	O3'-P	-11.29	1.44	1.61
23	BB	2276	G	O3'-P	-8.28	1.48	1.61
23	BB	2318	G	O3'-P	7.75	1.72	1.61
23	BB	1086	A	C5-C6	-7.31	1.26	1.41
23	DB	1086	A	C5-C6	-7.26	1.26	1.41

The worst 5 of 363 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-10.99	75.02	108.00
23	DB	508	A	C4'-C3'-O3'	-10.70	96.95	113.00
23	BB	2204	G	O5'-P-OP2	-10.54	76.37	108.00
23	DB	2323	G	O3'-P-O5'	-10.37	88.44	104.00
23	BB	508	A	C4'-C3'-O3'	-10.21	97.68	113.00

There are no chirality outliers.

5 of 128 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

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	1252	0
1	CA	32831	0	16521	1247	0
2	AC	1624	0	1699	145	0
2	CC	1624	0	1699	146	0
3	AD	1643	0	1710	181	0
3	CD	1643	0	1710	175	0
4	AE	1105	0	1148	107	0
4	CE	1105	0	1148	110	0
5	AF	817	0	808	86	0
5	CF	817	0	808	82	0
6	AG	1174	0	1230	116	0
6	CG	1196	0	1246	100	0
7	AH	979	0	1034	102	0
7	CH	979	0	1034	98	0
8	AI	1022	0	1070	148	0
8	CI	1022	0	1070	143	0
9	AJ	786	0	828	80	0
9	CJ	786	0	828	86	0
10	AK	877	0	887	110	0
10	CK	877	0	887	103	0
11	AL	955	0	1019	85	0
11	CL	955	0	1019	87	0
12	AM	883	0	944	113	0
12	CM	876	0	937	115	0
13	AN	774	0	827	120	0
13	CN	774	0	827	124	0
14	AO	714	0	734	49	0
14	CO	714	0	734	53	0
15	AP	649	0	666	56	0
15	CP	638	0	656	56	0
16	AQ	648	0	691	59	0
16	CQ	657	0	702	64	0
17	AR	455	0	478	47	0
17	CR	455	0	478	51	0
18	AS	637	0	665	92	0
18	CS	644	0	675	93	0
19	AT	665	0	714	62	0
19	CT	665	0	714	58	0
20	AB	1704	0	1732	202	0
20	CB	1704	0	1732	217	0
21	AU	425	0	449	79	0
21	CU	425	0	449	71	0
22	BA	2507	0	1270	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	2507	0	1270	121	1
23	BB	60995	0	30679	2402	0
23	DB	60995	0	30677	2534	1
24	BI	1032	0	1088	125	0
24	DI	1032	0	1088	193	0
25	BC	2082	0	2157	276	0
25	DC	2082	0	2157	272	0
26	BD	1565	0	1616	206	0
26	DD	1565	0	1616	210	0
27	BK	930	0	1000	115	0
27	DK	930	0	1000	123	0
28	BP	917	0	965	105	0
28	DP	917	0	965	103	0
29	BE	1552	0	1619	220	0
29	DE	1552	0	1619	209	0
30	BY	449	0	491	51	0
30	DY	449	0	491	52	0
31	B0	444	0	461	59	0
31	D0	444	0	461	57	0
32	B4	302	0	340	35	0
32	D4	302	0	341	41	0
33	B1	409	0	440	48	0
33	D1	409	0	440	47	0
34	B3	504	0	574	56	0
34	D3	504	0	574	58	0
35	BV	753	0	780	95	0
35	DV	753	0	780	106	0
36	B2	377	0	418	38	0
36	D2	377	0	418	43	0
37	BL	1045	0	1117	168	0
37	DL	1045	0	1117	168	0
38	BM	1074	0	1157	128	0
38	DM	1074	0	1157	129	0
39	BX	509	0	543	77	0
39	DX	509	0	543	71	0
40	BH	1111	0	1148	215	0
40	DH	1111	0	1148	154	0
41	BJ	1129	0	1162	149	0
41	DJ	1129	0	1162	155	0
42	BN	960	0	1000	136	0
42	DN	960	0	1000	137	0
43	BO	892	0	923	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DO	892	0	923	124	0
44	BQ	947	0	1022	160	0
44	DQ	947	0	1022	169	0
45	BS	857	0	922	113	0
45	DS	857	0	922	116	0
46	BU	779	0	834	123	0
46	DU	779	0	834	123	0
47	BF	1420	0	1460	251	0
47	DF	1420	0	1460	259	0
48	BG	1323	0	1374	205	0
48	DG	1323	0	1374	204	0
49	BR	816	0	839	127	0
49	DR	816	0	839	131	0
50	BT	738	0	807	125	0
50	DT	738	0	807	118	0
51	BZ	625	0	652	80	0
51	DZ	625	0	652	76	0
52	BW	596	0	610	129	0
52	DW	596	0	610	136	0
53	B6	1478	0	1526	190	0
53	D6	1478	0	1526	179	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	61	0	0	0	0
54	CE	1	0	0	0	0
54	DB	111	0	0	0	0
55	AA	42	0	45	3	0
55	BB	42	0	45	0	0
55	CA	42	0	45	2	0
55	DB	42	0	45	1	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	291	0	0	5	0
57	AL	3	0	0	0	0
57	AN	4	0	0	0	0
57	AT	2	0	0	0	0
57	BB	495	0	0	8	0
57	BC	6	0	0	0	0
57	BD	1	0	0	0	0
57	BE	2	0	0	0	0
57	BL	1	0	0	0	0
57	BT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CA	296	0	0	1	0
57	CE	3	0	0	0	0
57	CL	4	0	0	0	0
57	CN	4	0	0	0	0
57	CP	1	0	0	0	0
57	CT	1	0	0	0	0
57	DB	502	0	0	15	0
57	DC	4	0	0	0	0
57	DD	1	0	0	0	0
57	DE	1	0	0	0	0
57	DL	2	0	0	0	0
57	DQ	1	0	0	0	0
57	DR	1	0	0	0	0
All	All	287128	0	193895	18118	1

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

The worst 5 of 18118 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	1.37	1.19
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.28	1.15
49:DR:60:LYS:H	49:DR:100:GLY:HA3	1.08	1.15
2:CC:126:ARG:HH22	2:CC:190:THR:HG23	1.09	1.14
2:AC:126:ARG:HH22	2:AC:190:THR:HG23	1.08	1.13

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:DA:53:A:OP1	23:DB:1592:C:O2'[1_655]	2.08	0.12

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%)	150 (74%)	41 (20%)	13 (6%)	1	13
2	CC	204/232 (88%)	154 (76%)	36 (18%)	14 (7%)	1	12
3	AD	203/205 (99%)	151 (74%)	41 (20%)	11 (5%)	1	16
3	CD	203/205 (99%)	150 (74%)	41 (20%)	12 (6%)	1	14
4	AE	148/166 (89%)	113 (76%)	32 (22%)	3 (2%)	6	32
4	CE	148/166 (89%)	116 (78%)	28 (19%)	4 (3%)	4	26
5	AF	98/135 (73%)	66 (67%)	25 (26%)	7 (7%)	1	12
5	CF	98/135 (73%)	67 (68%)	24 (24%)	7 (7%)	1	12
6	AG	148/178 (83%)	121 (82%)	23 (16%)	4 (3%)	4	26
6	CG	150/178 (84%)	123 (82%)	23 (15%)	4 (3%)	4	26
7	AH	127/129 (98%)	96 (76%)	27 (21%)	4 (3%)	3	22
7	CH	127/129 (98%)	96 (76%)	28 (22%)	3 (2%)	5	28
8	AI	125/129 (97%)	96 (77%)	23 (18%)	6 (5%)	2	17
8	CI	125/129 (97%)	96 (77%)	22 (18%)	7 (6%)	1	15
9	AJ	96/103 (93%)	72 (75%)	16 (17%)	8 (8%)	0	10
9	CJ	96/103 (93%)	71 (74%)	17 (18%)	8 (8%)	0	10
10	AK	115/128 (90%)	86 (75%)	22 (19%)	7 (6%)	1	14
10	CK	115/128 (90%)	85 (74%)	23 (20%)	7 (6%)	1	14
11	AL	121/123 (98%)	76 (63%)	34 (28%)	11 (9%)	0	9
11	CL	121/123 (98%)	74 (61%)	36 (30%)	11 (9%)	0	9
12	AM	112/117 (96%)	77 (69%)	28 (25%)	7 (6%)	1	14
12	CM	111/117 (95%)	79 (71%)	25 (22%)	7 (6%)	1	14
13	AN	92/100 (92%)	58 (63%)	21 (23%)	13 (14%)	0	3
13	CN	92/100 (92%)	59 (64%)	21 (23%)	12 (13%)	0	4
14	AO	86/89 (97%)	66 (77%)	17 (20%)	3 (4%)	3	21
14	CO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	21
15	AP	80/82 (98%)	58 (72%)	18 (22%)	4 (5%)	1	16
15	CP	78/82 (95%)	56 (72%)	17 (22%)	5 (6%)	1	13
16	AQ	78/83 (94%)	58 (74%)	16 (20%)	4 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	CQ	79/83 (95%)	59 (75%)	15 (19%)	5 (6%)	1	14
17	AR	53/74 (72%)	45 (85%)	8 (15%)	0	100	100
17	CR	53/74 (72%)	44 (83%)	9 (17%)	0	100	100
18	AS	77/91 (85%)	52 (68%)	24 (31%)	1 (1%)	10	42
18	CS	78/91 (86%)	53 (68%)	23 (30%)	2 (3%)	4	26
19	AT	83/86 (96%)	67 (81%)	13 (16%)	3 (4%)	3	20
19	CT	83/86 (96%)	67 (81%)	13 (16%)	3 (4%)	3	20
20	AB	216/240 (90%)	159 (74%)	36 (17%)	21 (10%)	0	8
20	CB	216/240 (90%)	156 (72%)	37 (17%)	23 (11%)	0	6
21	AU	49/70 (70%)	27 (55%)	14 (29%)	8 (16%)	0	3
21	CU	49/70 (70%)	26 (53%)	14 (29%)	9 (18%)	0	2
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	3	20
24	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	3	23
25	BC	269/272 (99%)	164 (61%)	63 (23%)	42 (16%)	0	3
25	DC	269/272 (99%)	161 (60%)	68 (25%)	40 (15%)	0	3
26	BD	207/209 (99%)	118 (57%)	55 (27%)	34 (16%)	0	3
26	DD	207/209 (99%)	115 (56%)	59 (28%)	33 (16%)	0	3
27	BK	119/123 (97%)	72 (60%)	30 (25%)	17 (14%)	0	3
27	DK	119/123 (97%)	71 (60%)	30 (25%)	18 (15%)	0	3
28	BP	112/114 (98%)	62 (55%)	37 (33%)	13 (12%)	0	5
28	DP	112/114 (98%)	63 (56%)	35 (31%)	14 (12%)	0	4
29	BE	199/201 (99%)	124 (62%)	56 (28%)	19 (10%)	0	8
29	DE	199/201 (99%)	121 (61%)	58 (29%)	20 (10%)	0	7
30	BY	56/58 (97%)	36 (64%)	15 (27%)	5 (9%)	0	9
30	DY	56/58 (97%)	37 (66%)	14 (25%)	5 (9%)	0	9
31	B0	54/56 (96%)	35 (65%)	13 (24%)	6 (11%)	0	6
31	D0	54/56 (96%)	36 (67%)	11 (20%)	7 (13%)	0	4
32	B4	36/38 (95%)	18 (50%)	11 (31%)	7 (19%)	0	2
32	D4	36/38 (95%)	18 (50%)	11 (31%)	7 (19%)	0	2
33	B1	48/54 (89%)	36 (75%)	7 (15%)	5 (10%)	0	7
33	D1	48/54 (89%)	36 (75%)	7 (15%)	5 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	B3	62/64 (97%)	40 (64%)	16 (26%)	6 (10%)	0	8
34	D3	62/64 (97%)	41 (66%)	14 (23%)	7 (11%)	0	6
35	BV	92/94 (98%)	70 (76%)	16 (17%)	6 (6%)	1	13
35	DV	92/94 (98%)	69 (75%)	18 (20%)	5 (5%)	1	16
36	B2	44/46 (96%)	26 (59%)	15 (34%)	3 (7%)	1	12
36	D2	44/46 (96%)	26 (59%)	15 (34%)	3 (7%)	1	12
37	BL	141/144 (98%)	76 (54%)	42 (30%)	23 (16%)	0	3
37	DL	141/144 (98%)	76 (54%)	40 (28%)	25 (18%)	0	2
38	BM	134/136 (98%)	88 (66%)	31 (23%)	15 (11%)	0	6
38	DM	134/136 (98%)	89 (66%)	29 (22%)	16 (12%)	0	5
39	BX	61/63 (97%)	36 (59%)	18 (30%)	7 (12%)	0	5
39	DX	61/63 (97%)	37 (61%)	17 (28%)	7 (12%)	0	5
40	BH	147/149 (99%)	71 (48%)	49 (33%)	27 (18%)	0	2
40	DH	147/149 (99%)	96 (65%)	28 (19%)	23 (16%)	0	3
41	BJ	140/142 (99%)	89 (64%)	34 (24%)	17 (12%)	0	5
41	DJ	140/142 (99%)	88 (63%)	36 (26%)	16 (11%)	0	6
42	BN	118/127 (93%)	73 (62%)	34 (29%)	11 (9%)	0	9
42	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	0	7
43	BO	114/117 (97%)	80 (70%)	25 (22%)	9 (8%)	1	10
43	DO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	10
44	BQ	115/117 (98%)	70 (61%)	34 (30%)	11 (10%)	0	8
44	DQ	115/117 (98%)	69 (60%)	35 (30%)	11 (10%)	0	8
45	BS	108/110 (98%)	72 (67%)	22 (20%)	14 (13%)	0	4
45	DS	108/110 (98%)	70 (65%)	24 (22%)	14 (13%)	0	4
46	BU	100/103 (97%)	52 (52%)	28 (28%)	20 (20%)	0	1
46	DU	100/103 (97%)	50 (50%)	29 (29%)	21 (21%)	0	1
47	BF	176/178 (99%)	106 (60%)	43 (24%)	27 (15%)	0	3
47	DF	176/178 (99%)	107 (61%)	42 (24%)	27 (15%)	0	3
48	BG	174/176 (99%)	100 (58%)	49 (28%)	25 (14%)	0	3
48	DG	174/176 (99%)	99 (57%)	49 (28%)	26 (15%)	0	3
49	BR	101/103 (98%)	67 (66%)	21 (21%)	13 (13%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	DR	101/103 (98%)	68 (67%)	20 (20%)	13 (13%)	0	4
50	BT	91/100 (91%)	51 (56%)	26 (29%)	14 (15%)	0	3
50	DT	91/100 (91%)	50 (55%)	27 (30%)	14 (15%)	0	3
51	BZ	75/78 (96%)	51 (68%)	18 (24%)	6 (8%)	1	10
51	DZ	75/78 (96%)	51 (68%)	18 (24%)	6 (8%)	1	10
52	BW	77/84 (92%)	31 (40%)	21 (27%)	25 (32%)	0	0
52	DW	77/84 (92%)	31 (40%)	21 (27%)	25 (32%)	0	0
53	B6	183/185 (99%)	151 (82%)	25 (14%)	7 (4%)	2	19
53	D6	183/185 (99%)	132 (72%)	40 (22%)	11 (6%)	1	14
All	All	11607/12284 (94%)	7747 (67%)	2693 (23%)	1167 (10%)	0	7

5 of 1167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	54	ILE
2	AC	205	GLU
6	AG	6	ILE
8	AI	8	THR
9	AJ	36	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	142 (84%)	28 (16%)	2	11
2	CC	170/189 (90%)	141 (83%)	29 (17%)	1	10
3	AD	172/172 (100%)	148 (86%)	24 (14%)	3	14
3	CD	172/172 (100%)	148 (86%)	24 (14%)	3	14
4	AE	113/125 (90%)	95 (84%)	18 (16%)	2	12
4	CE	113/125 (90%)	94 (83%)	19 (17%)	1	10
5	AF	87/116 (75%)	70 (80%)	17 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CF	87/116 (75%)	69 (79%)	18 (21%)	1	6
6	AG	123/146 (84%)	107 (87%)	16 (13%)	3	15
6	CG	125/146 (86%)	109 (87%)	16 (13%)	3	15
7	AH	104/104 (100%)	96 (92%)	8 (8%)	10	30
7	CH	104/104 (100%)	95 (91%)	9 (9%)	8	26
8	AI	105/106 (99%)	89 (85%)	16 (15%)	2	12
8	CI	105/106 (99%)	89 (85%)	16 (15%)	2	12
9	AJ	86/90 (96%)	75 (87%)	11 (13%)	3	15
9	CJ	86/90 (96%)	75 (87%)	11 (13%)	3	15
10	AK	90/98 (92%)	77 (86%)	13 (14%)	2	13
10	CK	90/98 (92%)	77 (86%)	13 (14%)	2	13
11	AL	103/103 (100%)	93 (90%)	10 (10%)	6	22
11	CL	103/103 (100%)	92 (89%)	11 (11%)	5	20
12	AM	92/95 (97%)	80 (87%)	12 (13%)	3	15
12	CM	91/95 (96%)	79 (87%)	12 (13%)	3	15
13	AN	79/83 (95%)	66 (84%)	13 (16%)	2	11
13	CN	79/83 (95%)	66 (84%)	13 (16%)	2	11
14	AO	76/77 (99%)	67 (88%)	9 (12%)	4	17
14	CO	76/77 (99%)	66 (87%)	10 (13%)	3	15
15	AP	65/65 (100%)	59 (91%)	6 (9%)	7	24
15	CP	65/65 (100%)	59 (91%)	6 (9%)	7	24
16	AQ	74/77 (96%)	62 (84%)	12 (16%)	2	11
16	CQ	75/77 (97%)	63 (84%)	12 (16%)	2	11
17	AR	48/64 (75%)	45 (94%)	3 (6%)	15	36
17	CR	48/64 (75%)	45 (94%)	3 (6%)	15	36
18	AS	70/78 (90%)	54 (77%)	16 (23%)	0	4
18	CS	71/78 (91%)	54 (76%)	17 (24%)	0	4
19	AT	65/65 (100%)	55 (85%)	10 (15%)	2	12
19	CT	65/65 (100%)	55 (85%)	10 (15%)	2	12
20	AB	180/198 (91%)	148 (82%)	32 (18%)	1	9
20	CB	180/198 (91%)	150 (83%)	30 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AU	44/60 (73%)	34 (77%)	10 (23%)	0	5
21	CU	44/60 (73%)	34 (77%)	10 (23%)	0	5
24	BI	109/109 (100%)	108 (99%)	1 (1%)	75	83
24	DI	109/109 (100%)	105 (96%)	4 (4%)	29	51
25	BC	216/217 (100%)	180 (83%)	36 (17%)	2	10
25	DC	216/217 (100%)	180 (83%)	36 (17%)	2	10
26	BD	164/164 (100%)	138 (84%)	26 (16%)	2	12
26	DD	164/164 (100%)	137 (84%)	27 (16%)	2	11
27	BK	102/104 (98%)	77 (76%)	25 (24%)	0	3
27	DK	102/104 (98%)	77 (76%)	25 (24%)	0	3
28	BP	99/99 (100%)	81 (82%)	18 (18%)	1	8
28	DP	99/99 (100%)	81 (82%)	18 (18%)	1	8
29	BE	165/165 (100%)	136 (82%)	29 (18%)	1	9
29	DE	165/165 (100%)	136 (82%)	29 (18%)	1	9
30	BY	48/48 (100%)	40 (83%)	8 (17%)	2	10
30	DY	48/48 (100%)	40 (83%)	8 (17%)	2	10
31	B0	47/47 (100%)	39 (83%)	8 (17%)	1	10
31	D0	47/47 (100%)	39 (83%)	8 (17%)	1	10
32	B4	34/34 (100%)	25 (74%)	9 (26%)	0	3
32	D4	34/34 (100%)	25 (74%)	9 (26%)	0	3
33	B1	45/48 (94%)	40 (89%)	5 (11%)	5	18
33	D1	45/48 (94%)	41 (91%)	4 (9%)	8	25
34	B3	51/51 (100%)	48 (94%)	3 (6%)	16	38
34	D3	51/51 (100%)	48 (94%)	3 (6%)	16	38
35	BV	78/78 (100%)	63 (81%)	15 (19%)	1	7
35	DV	78/78 (100%)	62 (80%)	16 (20%)	1	6
36	B2	38/38 (100%)	33 (87%)	5 (13%)	3	15
36	D2	38/38 (100%)	33 (87%)	5 (13%)	3	15
37	BL	102/103 (99%)	88 (86%)	14 (14%)	3	15
37	DL	102/103 (99%)	88 (86%)	14 (14%)	3	15
38	BM	109/109 (100%)	83 (76%)	26 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DM	109/109 (100%)	84 (77%)	25 (23%)	0	4
39	BX	55/55 (100%)	40 (73%)	15 (27%)	0	3
39	DX	55/55 (100%)	40 (73%)	15 (27%)	0	3
40	BH	114/114 (100%)	68 (60%)	46 (40%)	0	0
40	DH	114/114 (100%)	91 (80%)	23 (20%)	1	6
41	BJ	116/116 (100%)	99 (85%)	17 (15%)	2	13
41	DJ	116/116 (100%)	99 (85%)	17 (15%)	2	13
42	BN	100/103 (97%)	86 (86%)	14 (14%)	3	14
42	DN	100/103 (97%)	86 (86%)	14 (14%)	3	14
43	BO	86/87 (99%)	70 (81%)	16 (19%)	1	8
43	DO	86/87 (99%)	72 (84%)	14 (16%)	2	11
44	BQ	89/89 (100%)	71 (80%)	18 (20%)	1	6
44	DQ	89/89 (100%)	73 (82%)	16 (18%)	1	8
45	BS	93/93 (100%)	78 (84%)	15 (16%)	2	11
45	DS	93/93 (100%)	78 (84%)	15 (16%)	2	11
46	BU	83/84 (99%)	68 (82%)	15 (18%)	1	9
46	DU	83/84 (99%)	68 (82%)	15 (18%)	1	9
47	BF	149/149 (100%)	117 (78%)	32 (22%)	1	5
47	DF	149/149 (100%)	120 (80%)	29 (20%)	1	7
48	BG	137/137 (100%)	114 (83%)	23 (17%)	1	10
48	DG	137/137 (100%)	114 (83%)	23 (17%)	1	10
49	BR	84/84 (100%)	72 (86%)	12 (14%)	2	14
49	DR	84/84 (100%)	72 (86%)	12 (14%)	2	14
50	BT	80/84 (95%)	66 (82%)	14 (18%)	1	9
50	DT	80/84 (95%)	66 (82%)	14 (18%)	1	9
51	BZ	67/68 (98%)	52 (78%)	15 (22%)	1	5
51	DZ	67/68 (98%)	54 (81%)	13 (19%)	1	7
52	BW	59/62 (95%)	46 (78%)	13 (22%)	1	5
52	DW	59/62 (95%)	45 (76%)	14 (24%)	0	4
53	B6	157/157 (100%)	119 (76%)	38 (24%)	0	4
53	D6	157/157 (100%)	122 (78%)	35 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9647/10014 (96%)	8043 (83%)	1604 (17%)	2 10

5 of 1604 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	CH	88	LYS
26	DD	30	GLU
53	D6	150	SER
9	CJ	87	LEU
7	CH	76	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 385 such sidechains are listed below:

Mol	Chain	Res	Type
9	CJ	15	HIS
26	DD	136	ASN
10	CK	118	ASN
20	CB	14	HIS
29	DE	9	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	246 (16%)	16 (1%)
1	CA	1529/1542 (99%)	244 (15%)	16 (1%)
22	BA	116/120 (96%)	18 (15%)	0
22	DA	116/120 (96%)	18 (15%)	0
23	BB	2837/2904 (97%)	448 (15%)	14 (0%)
23	DB	2837/2904 (97%)	450 (15%)	16 (0%)
All	All	8964/9132 (98%)	1424 (15%)	62 (0%)

5 of 1424 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	31	G
1	AA	32	A

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2832	U
23	DB	1509	A
1	CA	366	A
23	DB	1419	A
23	DB	2756	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
55	PAR	BB	3111	-	44,45,45	1.80	10 (22%)	63,67,67	1.13	5 (7%)
55	PAR	DB	3112	-	44,45,45	1.84	11 (25%)	63,67,67	1.18	5 (7%)
55	PAR	AA	1661	-	44,45,45	1.71	9 (20%)	63,67,67	1.14	5 (7%)
55	PAR	CA	1662	-	44,45,45	1.81	10 (22%)	63,67,67	1.16	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PAR	BB	3111	-	-	4/18/94/94	0/4/4/4
55	PAR	DB	3112	-	-	3/18/94/94	0/4/4/4
55	PAR	AA	1661	-	-	6/18/94/94	0/4/4/4
55	PAR	CA	1662	-	-	4/18/94/94	0/4/4/4

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	CA	1662	PAR	C31-C21	4.73	1.59	1.53
55	BB	3111	PAR	C31-C21	4.71	1.59	1.53
55	DB	3112	PAR	C31-C21	4.66	1.59	1.53
55	CA	1662	PAR	O54-C14	4.61	1.53	1.41
55	BB	3111	PAR	O54-C14	4.49	1.53	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DB	3112	PAR	O33-C14-C24	3.93	114.50	108.08
55	BB	3111	PAR	O33-C14-C24	3.76	114.23	108.08
55	DB	3112	PAR	O52-C13-O43	3.59	115.04	111.37
55	CA	1662	PAR	O33-C14-C24	3.53	113.85	108.08
55	AA	1661	PAR	O33-C14-C24	3.22	113.35	108.08

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

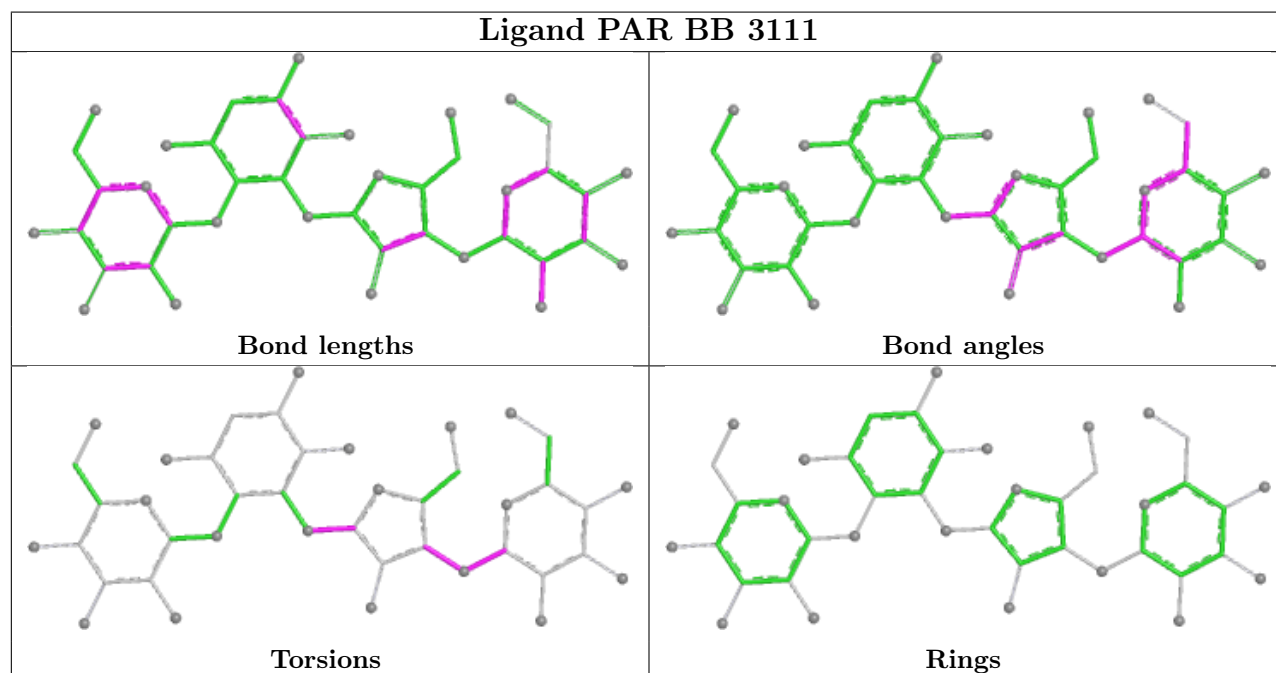
Mol	Chain	Res	Type	Atoms
55	AA	1661	PAR	C23-C13-O52-C52
55	BB	3111	PAR	C24-C14-O33-C33
55	CA	1662	PAR	C23-C13-O52-C52
55	CA	1662	PAR	O43-C13-O52-C52
55	DB	3112	PAR	C24-C14-O33-C33

There are no ring outliers.

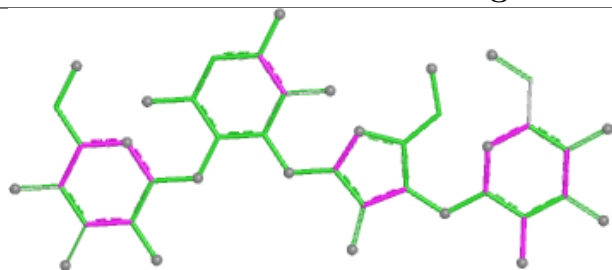
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	DB	3112	PAR	1	0
55	AA	1661	PAR	3	0
55	CA	1662	PAR	2	0

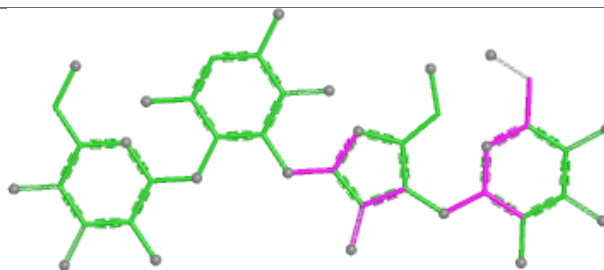
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



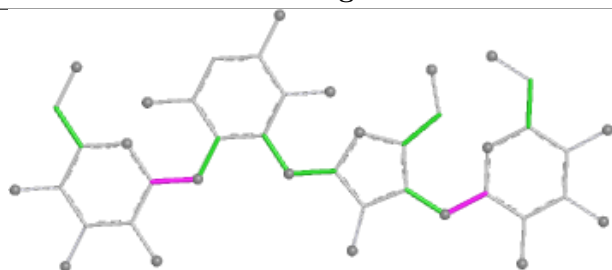
Ligand PAR DB 3112



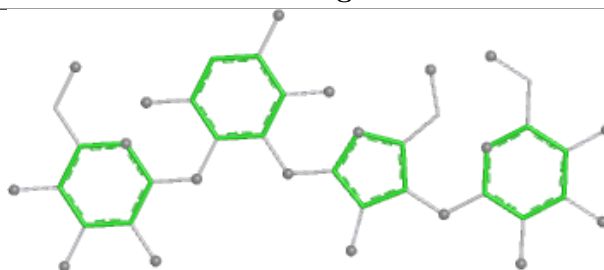
Bond lengths



Bond angles

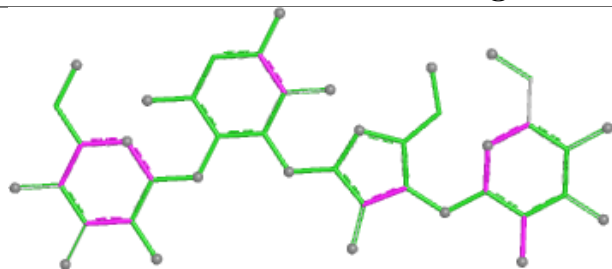


Torsions

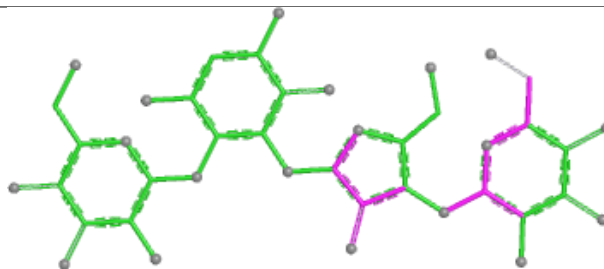


Rings

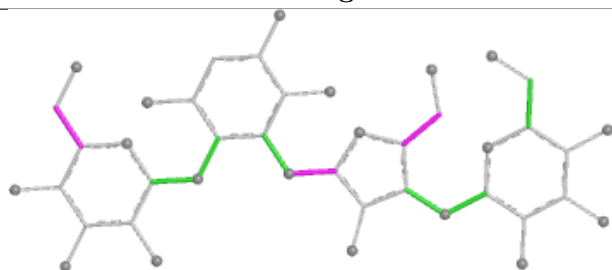
Ligand PAR AA 1661



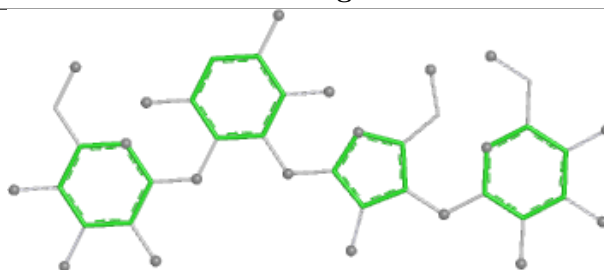
Bond lengths



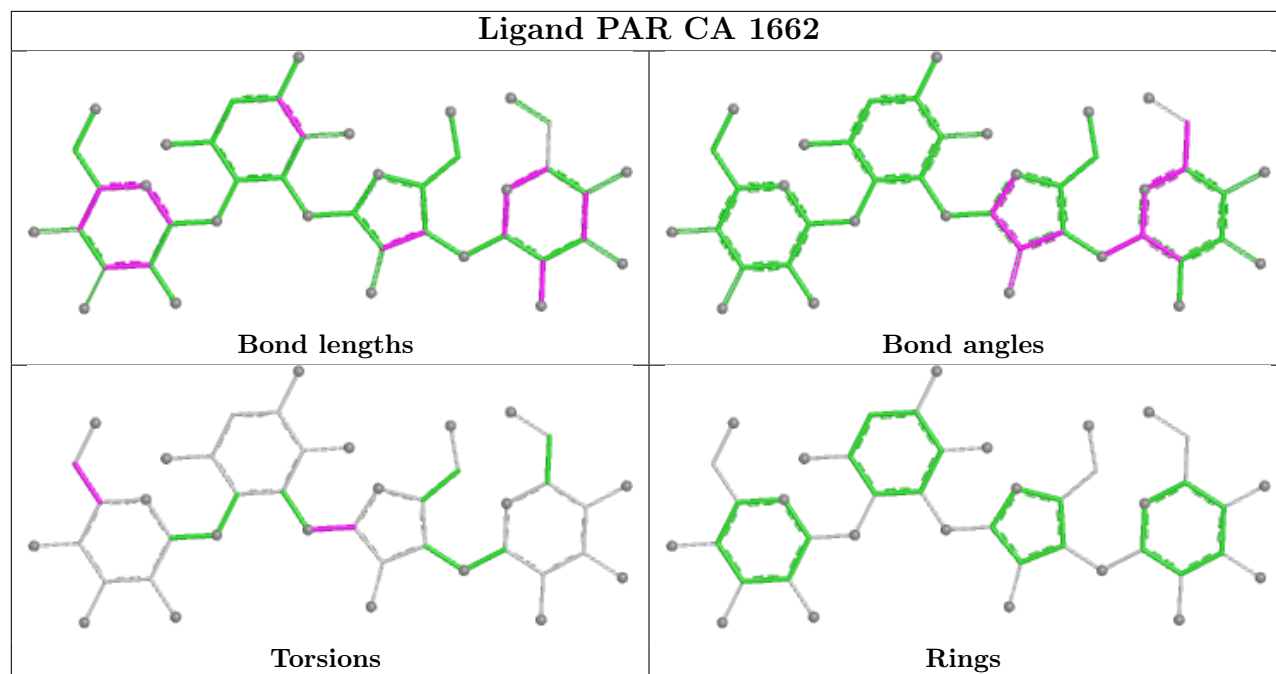
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.29	0 100 100	8, 88, 162, 180	0
1	CA	1530/1542 (99%)	-0.42	1 (0%) 92 88	5, 54, 146, 180	0
2	AC	206/232 (88%)	0.14	8 (3%) 44 34	9, 89, 158, 180	0
2	CC	206/232 (88%)	0.05	6 (2%) 54 40	9, 83, 141, 180	0
3	AD	205/205 (100%)	0.40	13 (6%) 27 24	5, 97, 172, 180	0
3	CD	205/205 (100%)	0.20	13 (6%) 27 24	5, 59, 151, 180	0
4	AE	150/166 (90%)	0.25	10 (6%) 25 22	5, 85, 159, 180	0
4	CE	150/166 (90%)	0.15	7 (4%) 37 31	5, 52, 137, 180	0
5	AF	100/135 (74%)	0.26	7 (7%) 24 21	8, 73, 146, 172	0
5	CF	100/135 (74%)	0.24	4 (4%) 43 34	5, 84, 153, 180	0
6	AG	150/178 (84%)	0.19	5 (3%) 49 38	10, 110, 170, 180	0
6	CG	152/178 (85%)	0.26	9 (5%) 29 25	28, 93, 162, 180	0
7	AH	129/129 (100%)	0.29	10 (7%) 20 19	15, 85, 159, 180	0
7	CH	129/129 (100%)	0.46	15 (11%) 11 12	5, 50, 128, 175	0
8	AI	127/129 (98%)	0.38	7 (5%) 32 26	5, 98, 163, 180	0
8	CI	127/129 (98%)	0.33	9 (7%) 23 21	5, 102, 180, 180	0
9	AJ	98/103 (95%)	0.13	2 (2%) 64 49	5, 105, 174, 180	0
9	CJ	98/103 (95%)	0.34	4 (4%) 42 33	10, 93, 158, 180	0
10	AK	117/128 (91%)	0.37	12 (10%) 13 14	9, 67, 129, 146	0
10	CK	117/128 (91%)	0.20	3 (2%) 57 43	5, 63, 134, 180	0
11	AL	123/123 (100%)	0.49	6 (4%) 36 29	19, 84, 158, 180	0
11	CL	123/123 (100%)	0.26	6 (4%) 36 29	5, 54, 113, 180	0
12	AM	114/117 (97%)	0.24	6 (5%) 33 27	55, 122, 180, 180	0
12	CM	113/117 (96%)	0.43	9 (7%) 20 18	31, 114, 180, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.24	2 (2%) 63 48	5, 108, 170, 180	0
13	CN	96/100 (96%)	0.45	6 (6%) 27 24	6, 99, 162, 180	0
14	AO	88/89 (98%)	0.02	3 (3%) 48 36	7, 86, 156, 180	0
14	CO	88/89 (98%)	0.31	5 (5%) 30 26	5, 60, 132, 175	0
15	AP	82/82 (100%)	0.34	9 (10%) 12 13	35, 106, 173, 180	0
15	CP	80/82 (97%)	0.59	10 (12%) 9 11	5, 47, 142, 180	0
16	AQ	80/83 (96%)	0.20	3 (3%) 44 34	48, 104, 180, 180	0
16	CQ	81/83 (97%)	0.26	8 (9%) 14 14	5, 53, 140, 173	0
17	AR	55/74 (74%)	0.26	3 (5%) 32 26	5, 65, 143, 180	0
17	CR	55/74 (74%)	1.05	14 (25%) 2 4	13, 68, 130, 180	0
18	AS	79/91 (86%)	0.59	5 (6%) 27 24	55, 129, 180, 180	0
18	CS	80/91 (87%)	0.37	6 (7%) 22 20	46, 108, 180, 180	0
19	AT	85/86 (98%)	0.27	2 (2%) 59 45	44, 105, 154, 180	0
19	CT	85/86 (98%)	0.58	12 (14%) 7 9	5, 56, 117, 161	0
20	AB	218/240 (90%)	0.20	13 (5%) 29 24	7, 105, 171, 180	0
20	CB	218/240 (90%)	0.31	15 (6%) 24 22	23, 111, 172, 180	0
21	AU	51/70 (72%)	0.61	5 (9%) 14 15	23, 104, 180, 180	0
21	CU	51/70 (72%)	0.38	3 (5%) 29 25	24, 96, 173, 180	0
22	BA	117/120 (97%)	-0.36	1 (0%) 81 67	37, 82, 145, 178	0
22	DA	117/120 (97%)	-0.20	1 (0%) 81 67	18, 84, 143, 180	0
23	BB	2841/2904 (97%)	-0.38	1 (0%) 100 100	6, 58, 150, 180	0
23	DB	2841/2904 (97%)	-0.41	5 (0%) 92 85	5, 38, 149, 180	0
24	BI	141/141 (100%)	0.69	9 (6%) 27 24	63, 161, 180, 180	0
24	DI	141/141 (100%)	0.63	11 (7%) 20 19	65, 157, 180, 180	0
25	BC	271/272 (99%)	0.21	16 (5%) 29 25	5, 48, 108, 166	0
25	DC	271/272 (99%)	0.42	23 (8%) 18 17	5, 30, 102, 180	0
26	BD	209/209 (100%)	0.51	21 (10%) 14 14	5, 79, 148, 180	0
26	DD	209/209 (100%)	0.46	12 (5%) 30 26	5, 51, 123, 180	0
27	BK	121/123 (98%)	0.53	9 (7%) 22 20	5, 74, 149, 180	0
27	DK	121/123 (98%)	0.14	5 (4%) 42 33	5, 33, 106, 180	0
28	BP	114/114 (100%)	0.38	7 (6%) 28 24	18, 89, 153, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.19	4 (3%) 47 36	5, 48, 124, 180	0
29	BE	201/201 (100%)	0.31	10 (4%) 35 29	5, 67, 146, 180	0
29	DE	201/201 (100%)	0.33	9 (4%) 39 31	5, 67, 142, 177	0
30	BY	58/58 (100%)	0.24	1 (1%) 69 53	18, 82, 151, 171	0
30	DY	58/58 (100%)	0.39	2 (3%) 48 36	5, 68, 126, 162	0
31	B0	56/56 (100%)	0.31	5 (8%) 17 16	5, 73, 153, 164	0
31	D0	56/56 (100%)	0.11	2 (3%) 46 35	5, 56, 147, 180	0
32	B4	38/38 (100%)	1.10	5 (13%) 8 10	45, 115, 169, 180	0
32	D4	38/38 (100%)	1.06	9 (23%) 2 5	36, 110, 169, 180	0
33	B1	50/54 (92%)	-0.03	0 100 100	22, 95, 157, 180	0
33	D1	50/54 (92%)	0.06	0 100 100	19, 73, 122, 161	0
34	B3	64/64 (100%)	0.56	7 (10%) 12 13	20, 63, 125, 145	0
34	D3	64/64 (100%)	0.73	6 (9%) 15 15	5, 35, 88, 129	0
35	BV	94/94 (100%)	0.04	2 (2%) 63 48	24, 96, 156, 180	0
35	DV	94/94 (100%)	0.48	9 (9%) 15 15	11, 93, 151, 180	0
36	B2	46/46 (100%)	0.98	8 (17%) 5 7	5, 75, 137, 180	0
36	D2	46/46 (100%)	1.18	13 (28%) 1 4	5, 44, 101, 180	0
37	BL	143/144 (99%)	0.71	16 (11%) 11 13	5, 71, 133, 180	0
37	DL	143/144 (99%)	0.37	11 (7%) 21 19	5, 51, 116, 180	0
38	BM	136/136 (100%)	0.50	13 (9%) 15 15	9, 70, 149, 180	0
38	DM	136/136 (100%)	0.24	1 (0%) 84 71	5, 50, 131, 176	0
39	BX	63/63 (100%)	0.32	2 (3%) 50 38	7, 84, 165, 180	0
39	DX	63/63 (100%)	0.76	9 (14%) 7 9	47, 108, 173, 180	0
40	BH	149/149 (100%)	0.27	6 (4%) 43 34	5, 130, 180, 180	0
40	DH	149/149 (100%)	0.12	3 (2%) 64 49	12, 97, 172, 180	0
41	BJ	142/142 (100%)	0.66	24 (16%) 5 7	6, 81, 147, 180	0
41	DJ	142/142 (100%)	0.40	12 (8%) 18 17	5, 58, 135, 180	0
42	BN	120/127 (94%)	0.43	12 (10%) 14 14	5, 68, 139, 178	0
42	DN	120/127 (94%)	0.47	11 (9%) 16 15	5, 38, 101, 180	0
43	BO	116/117 (99%)	0.43	8 (6%) 24 22	21, 91, 147, 180	0
43	DO	116/117 (99%)	0.93	18 (15%) 6 8	8, 86, 164, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.41	10 (8%) 18 17	5, 66, 135, 176	0
44	DQ	117/117 (100%)	0.69	11 (9%) 15 15	5, 48, 134, 180	0
45	BS	110/110 (100%)	0.34	7 (6%) 27 24	6, 58, 139, 180	0
45	DS	110/110 (100%)	0.16	2 (1%) 67 52	5, 50, 121, 180	0
46	BU	102/103 (99%)	0.34	4 (3%) 44 34	5, 89, 144, 180	0
46	DU	102/103 (99%)	0.15	5 (4%) 36 29	24, 99, 159, 180	0
47	BF	178/178 (100%)	0.26	12 (6%) 25 22	36, 111, 174, 180	0
47	DF	178/178 (100%)	0.18	10 (5%) 31 26	8, 103, 177, 180	0
48	BG	176/176 (100%)	0.08	2 (1%) 77 63	9, 114, 179, 180	0
48	DG	176/176 (100%)	0.14	4 (2%) 61 46	15, 91, 167, 180	0
49	BR	103/103 (100%)	0.54	7 (6%) 25 22	16, 93, 157, 180	0
49	DR	103/103 (100%)	0.34	5 (4%) 36 29	5, 88, 145, 180	0
50	BT	93/100 (93%)	0.79	14 (15%) 6 9	5, 88, 180, 180	0
50	DT	93/100 (93%)	0.75	10 (10%) 12 13	7, 90, 180, 180	0
51	BZ	77/78 (98%)	0.26	5 (6%) 26 24	5, 52, 127, 154	0
51	DZ	77/78 (98%)	0.63	6 (7%) 20 19	5, 43, 95, 135	0
52	BW	79/84 (94%)	0.64	9 (11%) 11 12	10, 85, 145, 179	0
52	DW	79/84 (94%)	0.83	15 (18%) 4 6	5, 66, 152, 180	0
53	B6	185/185 (100%)	0.27	6 (3%) 50 38	5, 125, 180, 180	0
53	D6	185/185 (100%)	0.24	10 (5%) 32 26	5, 90, 180, 180	0
All	All	20787/21416 (97%)	0.04	809 (3%) 44 34	5, 70, 162, 180	0

The worst 5 of 809 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	DO	28	VAL	8.7
6	CG	4	ARG	8.2
17	CR	31	TYR	7.5
15	CP	9	HIS	7.3
43	DO	3	LYS	7.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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	AA	1623	1/1	-0.82	0.47	33,33,33,33	1
54	MG	DB	3060	1/1	0.20	0.13	160,160,160,160	0
54	MG	CA	1629	1/1	0.31	0.42	96,96,96,96	1
54	MG	AA	1659	1/1	0.31	0.18	127,127,127,127	0
54	MG	AA	1639	1/1	0.51	0.26	126,126,126,126	0
54	MG	CA	1626	1/1	0.56	0.15	23,23,23,23	1
54	MG	AA	1657	1/1	0.57	0.15	155,155,155,155	0
54	MG	CE	201	1/1	0.60	0.96	145,145,145,145	0
54	MG	CA	1623	1/1	0.70	0.19	180,180,180,180	0
54	MG	AA	1622	1/1	0.71	0.17	111,111,111,111	0
54	MG	DB	3083	1/1	0.71	0.12	72,72,72,72	0
54	MG	BB	3003	1/1	0.74	0.06	60,60,60,60	0
54	MG	AA	1647	1/1	0.76	0.20	180,180,180,180	0
54	MG	DB	3058	1/1	0.77	0.84	157,157,157,157	0
54	MG	AA	1608	1/1	0.78	0.11	136,136,136,136	0
54	MG	CA	1614	1/1	0.78	0.08	85,85,85,85	0
54	MG	DB	3045	1/1	0.78	0.09	108,108,108,108	0
54	MG	CA	1657	1/1	0.79	0.18	97,97,97,97	0
54	MG	AA	1615	1/1	0.79	0.18	171,171,171,171	0
54	MG	DB	3052	1/1	0.80	0.08	166,166,166,166	0
54	MG	AA	1619	1/1	0.81	0.58	180,180,180,180	0
54	MG	CA	1627	1/1	0.82	0.12	35,35,35,35	1
54	MG	BB	3108	1/1	0.82	0.14	88,88,88,88	0
54	MG	AA	1637	1/1	0.82	0.53	146,146,146,146	0
54	MG	CA	1646	1/1	0.83	0.25	78,78,78,78	0
55	PAR	AA	1661	42/42	0.83	0.13	62,62,62,62	0
54	MG	CA	1608	1/1	0.84	0.15	178,178,178,178	0
54	MG	BB	3091	1/1	0.84	0.11	81,81,81,81	0
54	MG	AA	1602	1/1	0.84	0.12	105,105,105,105	0
54	MG	AA	1625	1/1	0.85	0.69	144,144,144,144	1
54	MG	DB	3059	1/1	0.85	0.14	152,152,152,152	0
54	MG	AA	1626	1/1	0.85	0.24	28,28,28,28	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3082	1/1	0.85	0.32	22,22,22,22	0
54	MG	CA	1649	1/1	0.85	0.19	134,134,134,134	0
54	MG	CA	1615	1/1	0.86	0.16	180,180,180,180	0
54	MG	AA	1632	1/1	0.86	0.13	80,80,80,80	0
55	PAR	DB	3112	42/42	0.86	0.42	55,55,55,55	42
54	MG	CA	1621	1/1	0.87	0.27	67,67,67,67	0
54	MG	CA	1654	1/1	0.87	0.07	72,72,72,72	0
54	MG	AA	1617	1/1	0.87	0.07	138,138,138,138	0
54	MG	AA	1610	1/1	0.88	0.17	82,82,82,82	0
55	PAR	BB	3111	42/42	0.88	0.65	100,100,100,100	42
54	MG	AA	1633	1/1	0.88	0.13	56,56,56,56	0
54	MG	BB	3033	1/1	0.89	0.06	125,125,125,125	0
54	MG	DB	3110	1/1	0.89	0.16	44,44,44,44	0
54	MG	CA	1660	1/1	0.89	0.24	58,58,58,58	0
54	MG	CA	1628	1/1	0.89	0.09	82,82,82,82	0
54	MG	BB	3013	1/1	0.89	0.08	86,86,86,86	0
54	MG	BB	3038	1/1	0.90	0.07	157,157,157,157	0
54	MG	CA	1616	1/1	0.90	0.10	94,94,94,94	0
54	MG	BB	3080	1/1	0.90	0.16	131,131,131,131	0
54	MG	BB	3097	1/1	0.90	0.08	95,95,95,95	0
54	MG	AA	1655	1/1	0.91	0.10	83,83,83,83	0
55	PAR	CA	1662	42/42	0.91	0.14	45,45,45,45	0
54	MG	AA	1614	1/1	0.91	0.10	131,131,131,131	0
54	MG	CA	1652	1/1	0.92	0.09	58,58,58,58	0
54	MG	CA	1658	1/1	0.92	0.14	70,70,70,70	0
54	MG	DB	3050	1/1	0.92	0.13	118,118,118,118	0
54	MG	CA	1609	1/1	0.92	0.11	81,81,81,81	0
54	MG	DB	3100	1/1	0.92	0.08	22,22,22,22	0
54	MG	AA	1650	1/1	0.93	0.05	116,116,116,116	0
54	MG	AA	1644	1/1	0.93	0.12	69,69,69,69	0
54	MG	CA	1637	1/1	0.93	0.07	116,116,116,116	0
54	MG	BB	3011	1/1	0.94	0.11	68,68,68,68	0
54	MG	CA	1636	1/1	0.94	0.17	90,90,90,90	0
54	MG	BB	3055	1/1	0.94	0.22	78,78,78,78	0
54	MG	BB	3100	1/1	0.94	0.05	109,109,109,109	0
54	MG	BB	3064	1/1	0.94	0.08	78,78,78,78	0
54	MG	BB	3078	1/1	0.94	0.15	92,92,92,92	0
54	MG	AA	1660	1/1	0.94	0.05	75,75,75,75	0
54	MG	AA	1658	1/1	0.94	0.05	97,97,97,97	0
56	ZN	D4	101	1/1	0.94	0.20	96,96,96,96	0
54	MG	BB	3019	1/1	0.95	0.07	56,56,56,56	0
54	MG	DB	3013	1/1	0.95	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3068	1/1	0.95	0.06	102,102,102,102	0
54	MG	BB	3004	1/1	0.95	0.18	44,44,44,44	0
54	MG	AA	1635	1/1	0.95	0.07	120,120,120,120	0
54	MG	CA	1633	1/1	0.95	0.10	106,106,106,106	0
54	MG	CA	1606	1/1	0.95	0.04	103,103,103,103	0
54	MG	AA	1613	1/1	0.95	0.07	82,82,82,82	0
54	MG	BB	3057	1/1	0.96	0.15	65,65,65,65	0
54	MG	BB	3093	1/1	0.96	0.10	98,98,98,98	0
54	MG	AA	1612	1/1	0.96	0.06	96,96,96,96	0
54	MG	CA	1625	1/1	0.96	0.09	46,46,46,46	0
54	MG	AA	1656	1/1	0.96	0.09	50,50,50,50	0
54	MG	BB	3073	1/1	0.96	0.10	70,70,70,70	0
54	MG	BB	3077	1/1	0.96	0.07	64,64,64,64	0
54	MG	BB	3010	1/1	0.96	0.06	38,38,38,38	0
54	MG	AA	1627	1/1	0.96	0.08	46,46,46,46	0
54	MG	DB	3022	1/1	0.96	0.07	85,85,85,85	0
54	MG	BB	3012	1/1	0.96	0.06	71,71,71,71	0
54	MG	BB	3090	1/1	0.96	0.06	115,115,115,115	0
54	MG	BB	3027	1/1	0.97	0.06	83,83,83,83	0
54	MG	BB	3028	1/1	0.97	0.13	95,95,95,95	0
54	MG	DB	3008	1/1	0.97	0.07	11,11,11,11	0
54	MG	DB	3011	1/1	0.97	0.05	22,22,22,22	0
54	MG	AA	1620	1/1	0.97	0.04	95,95,95,95	0
54	MG	AA	1651	1/1	0.97	0.16	55,55,55,55	0
54	MG	DB	3035	1/1	0.97	0.07	52,52,52,52	0
54	MG	DB	3037	1/1	0.97	0.05	45,45,45,45	0
54	MG	BB	3042	1/1	0.97	0.05	100,100,100,100	0
54	MG	BB	3043	1/1	0.97	0.04	97,97,97,97	0
54	MG	BB	3099	1/1	0.97	0.07	40,40,40,40	0
54	MG	DB	3054	1/1	0.97	0.06	69,69,69,69	0
54	MG	CA	1630	1/1	0.97	0.11	65,65,65,65	0
54	MG	AA	1652	1/1	0.97	0.14	126,126,126,126	0
54	MG	CA	1634	1/1	0.97	0.09	30,30,30,30	0
54	MG	DB	3061	1/1	0.97	0.05	95,95,95,95	0
54	MG	DB	3066	1/1	0.97	0.11	123,123,123,123	0
54	MG	DB	3072	1/1	0.97	0.07	48,48,48,48	0
54	MG	BB	3007	1/1	0.97	0.08	103,103,103,103	0
54	MG	DB	3086	1/1	0.97	0.11	25,25,25,25	0
54	MG	AA	1640	1/1	0.97	0.10	77,77,77,77	0
54	MG	AA	1630	1/1	0.97	0.08	118,118,118,118	0
54	MG	BB	3072	1/1	0.97	0.07	64,64,64,64	0
54	MG	AA	1645	1/1	0.97	0.06	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1646	1/1	0.97	0.05	98,98,98,98	0
54	MG	AA	1624	1/1	0.97	0.12	76,76,76,76	0
54	MG	CA	1619	1/1	0.97	0.06	78,78,78,78	0
54	MG	DB	3015	1/1	0.98	0.07	39,39,39,39	0
54	MG	BB	3047	1/1	0.98	0.04	92,92,92,92	0
54	MG	DB	3026	1/1	0.98	0.05	54,54,54,54	0
54	MG	DB	3028	1/1	0.98	0.09	33,33,33,33	0
54	MG	DB	3029	1/1	0.98	0.04	70,70,70,70	0
54	MG	DB	3030	1/1	0.98	0.10	30,30,30,30	0
54	MG	CA	1635	1/1	0.98	0.03	105,105,105,105	0
54	MG	BB	3051	1/1	0.98	0.14	75,75,75,75	0
54	MG	BB	3017	1/1	0.98	0.05	46,46,46,46	0
54	MG	CA	1640	1/1	0.98	0.09	35,35,35,35	0
54	MG	CA	1642	1/1	0.98	0.04	85,85,85,85	0
54	MG	DB	3053	1/1	0.98	0.14	65,65,65,65	0
54	MG	CA	1645	1/1	0.98	0.06	82,82,82,82	0
54	MG	AA	1606	1/1	0.98	0.04	73,73,73,73	0
54	MG	CA	1620	1/1	0.98	0.17	104,104,104,104	0
54	MG	BB	3009	1/1	0.98	0.04	76,76,76,76	0
54	MG	CA	1653	1/1	0.98	0.03	43,43,43,43	0
54	MG	DB	3064	1/1	0.98	0.06	23,23,23,23	0
54	MG	AA	1629	1/1	0.98	0.04	44,44,44,44	0
54	MG	BB	3070	1/1	0.98	0.07	40,40,40,40	0
54	MG	DB	3082	1/1	0.98	0.07	37,37,37,37	0
54	MG	AA	1634	1/1	0.98	0.03	79,79,79,79	0
54	MG	DB	3085	1/1	0.98	0.09	49,49,49,49	0
54	MG	CA	1659	1/1	0.98	0.04	70,70,70,70	0
54	MG	DB	3094	1/1	0.98	0.06	81,81,81,81	0
54	MG	DB	3095	1/1	0.98	0.07	62,62,62,62	0
54	MG	AA	1649	1/1	0.98	0.06	93,93,93,93	0
54	MG	CA	1661	1/1	0.98	0.06	40,40,40,40	0
54	MG	CA	1601	1/1	0.98	0.06	9,9,9,9	0
54	MG	BB	3075	1/1	0.98	0.05	55,55,55,55	0
54	MG	AA	1607	1/1	0.98	0.02	35,35,35,35	0
54	MG	BB	3016	1/1	0.98	0.06	94,94,94,94	0
56	ZN	B4	101	1/1	0.98	0.15	68,68,68,68	0
54	MG	DB	3014	1/1	0.98	0.10	39,39,39,39	0
54	MG	CA	1644	1/1	0.99	0.04	69,69,69,69	0
54	MG	BB	3088	1/1	0.99	0.07	11,11,11,11	0
54	MG	BB	3036	1/1	0.99	0.12	68,68,68,68	0
54	MG	CA	1647	1/1	0.99	0.03	58,58,58,58	0
54	MG	BB	3037	1/1	0.99	0.06	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1651	1/1	0.99	0.07	37,37,37,37	0
54	MG	BB	3092	1/1	0.99	0.03	60,60,60,60	0
54	MG	AA	1605	1/1	0.99	0.03	54,54,54,54	0
54	MG	BB	3094	1/1	0.99	0.05	55,55,55,55	0
54	MG	BB	3095	1/1	0.99	0.04	65,65,65,65	0
54	MG	BB	3096	1/1	0.99	0.04	69,69,69,69	0
54	MG	BB	3040	1/1	0.99	0.05	47,47,47,47	0
54	MG	AA	1642	1/1	0.99	0.03	63,63,63,63	0
54	MG	AA	1643	1/1	0.99	0.10	118,118,118,118	0
54	MG	BB	3101	1/1	0.99	0.06	64,64,64,64	0
54	MG	DB	3004	1/1	0.99	0.10	40,40,40,40	0
54	MG	DB	3005	1/1	0.99	0.03	52,52,52,52	0
54	MG	BB	3102	1/1	0.99	0.04	76,76,76,76	0
54	MG	BB	3104	1/1	0.99	0.04	43,43,43,43	0
54	MG	BB	3106	1/1	0.99	0.03	45,45,45,45	0
54	MG	BB	3045	1/1	0.99	0.05	32,32,32,32	0
54	MG	BB	3109	1/1	0.99	0.04	49,49,49,49	0
54	MG	DB	3017	1/1	0.99	0.06	23,23,23,23	0
54	MG	BB	3046	1/1	0.99	0.04	64,64,64,64	0
54	MG	DB	3025	1/1	0.99	0.04	18,18,18,18	0
54	MG	AA	1631	1/1	0.99	0.03	61,61,61,61	0
54	MG	DB	3027	1/1	0.99	0.06	11,11,11,11	0
54	MG	BB	3049	1/1	0.99	0.07	25,25,25,25	0
54	MG	AA	1611	1/1	0.99	0.03	75,75,75,75	0
54	MG	CA	1610	1/1	0.99	0.04	65,65,65,65	0
54	MG	DB	3034	1/1	0.99	0.04	52,52,52,52	0
54	MG	CA	1611	1/1	0.99	0.05	114,114,114,114	0
54	MG	DB	3036	1/1	0.99	0.11	51,51,51,51	0
54	MG	CA	1612	1/1	0.99	0.04	97,97,97,97	0
54	MG	DB	3039	1/1	0.99	0.02	34,34,34,34	0
54	MG	BB	3053	1/1	0.99	0.03	38,38,38,38	0
54	MG	DB	3046	1/1	0.99	0.07	38,38,38,38	0
54	MG	BB	3054	1/1	0.99	0.07	55,55,55,55	0
54	MG	DB	3051	1/1	0.99	0.10	20,20,20,20	0
54	MG	BB	3014	1/1	0.99	0.11	46,46,46,46	0
54	MG	CA	1618	1/1	0.99	0.09	23,23,23,23	0
54	MG	BB	3056	1/1	0.99	0.04	61,61,61,61	0
54	MG	AA	1618	1/1	0.99	0.05	105,105,105,105	0
54	MG	BB	3059	1/1	0.99	0.06	39,39,39,39	0
54	MG	AA	1601	1/1	0.99	0.13	10,10,10,10	0
54	MG	CA	1624	1/1	0.99	0.10	48,48,48,48	0
54	MG	AA	1603	1/1	0.99	0.03	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3065	1/1	0.99	0.07	68,68,68,68	0
54	MG	BB	3024	1/1	0.99	0.04	76,76,76,76	0
54	MG	DB	3071	1/1	0.99	0.03	41,41,41,41	0
54	MG	BB	3071	1/1	0.99	0.07	63,63,63,63	0
54	MG	DB	3076	1/1	0.99	0.05	27,27,27,27	0
54	MG	DB	3078	1/1	0.99	0.03	31,31,31,31	0
54	MG	DB	3079	1/1	0.99	0.06	30,30,30,30	0
54	MG	DB	3080	1/1	0.99	0.07	13,13,13,13	0
54	MG	BB	3026	1/1	0.99	0.02	44,44,44,44	0
54	MG	AA	1628	1/1	0.99	0.09	49,49,49,49	0
54	MG	AA	1604	1/1	0.99	0.03	37,37,37,37	0
54	MG	CA	1631	1/1	0.99	0.06	55,55,55,55	0
54	MG	DB	3087	1/1	0.99	0.13	67,67,67,67	0
54	MG	DB	3089	1/1	0.99	0.14	75,75,75,75	0
54	MG	DB	3090	1/1	0.99	0.13	35,35,35,35	0
54	MG	DB	3092	1/1	0.99	0.09	60,60,60,60	0
54	MG	DB	3093	1/1	0.99	0.06	9,9,9,9	0
54	MG	CA	1632	1/1	0.99	0.04	34,34,34,34	0
54	MG	BB	3030	1/1	0.99	0.06	83,83,83,83	0
54	MG	DB	3098	1/1	0.99	0.04	69,69,69,69	0
54	MG	BB	3031	1/1	0.99	0.10	44,44,44,44	0
54	MG	DB	3103	1/1	0.99	0.04	37,37,37,37	0
54	MG	DB	3108	1/1	0.99	0.06	13,13,13,13	0
54	MG	BB	3079	1/1	0.99	0.04	43,43,43,43	0
54	MG	DB	3111	1/1	0.99	0.13	68,68,68,68	0
54	MG	BB	3008	1/1	0.99	0.06	81,81,81,81	0
54	MG	BB	3081	1/1	0.99	0.06	31,31,31,31	0
54	MG	CA	1638	1/1	0.99	0.02	56,56,56,56	0
54	MG	BB	3035	1/1	0.99	0.09	60,60,60,60	0
54	MG	CA	1641	1/1	0.99	0.04	76,76,76,76	0
54	MG	BB	3087	1/1	0.99	0.07	102,102,102,102	0
54	MG	BB	3029	1/1	1.00	0.02	12,12,12,12	0
54	MG	DB	3001	1/1	1.00	0.04	5,5,5,5	0
54	MG	DB	3002	1/1	1.00	0.03	14,14,14,14	0
54	MG	DB	3003	1/1	1.00	0.03	5,5,5,5	0
54	MG	BB	3060	1/1	1.00	0.03	43,43,43,43	0
54	MG	BB	3110	1/1	1.00	0.05	41,41,41,41	0
54	MG	DB	3006	1/1	1.00	0.04	15,15,15,15	0
54	MG	DB	3007	1/1	1.00	0.03	27,27,27,27	0
54	MG	BB	3061	1/1	1.00	0.02	46,46,46,46	0
54	MG	DB	3009	1/1	1.00	0.02	22,22,22,22	0
54	MG	DB	3010	1/1	1.00	0.06	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1602	1/1	1.00	0.08	16,16,16,16	0
54	MG	DB	3012	1/1	1.00	0.04	8,8,8,8	0
54	MG	CA	1603	1/1	1.00	0.02	37,37,37,37	0
54	MG	CA	1604	1/1	1.00	0.09	11,11,11,11	0
54	MG	CA	1605	1/1	1.00	0.03	5,5,5,5	0
54	MG	DB	3016	1/1	1.00	0.07	5,5,5,5	0
54	MG	BB	3062	1/1	1.00	0.04	5,5,5,5	0
54	MG	DB	3018	1/1	1.00	0.06	17,17,17,17	0
54	MG	DB	3019	1/1	1.00	0.04	8,8,8,8	0
54	MG	DB	3020	1/1	1.00	0.06	5,5,5,5	0
54	MG	DB	3021	1/1	1.00	0.02	18,18,18,18	0
54	MG	CA	1607	1/1	1.00	0.08	20,20,20,20	0
54	MG	DB	3023	1/1	1.00	0.06	35,35,35,35	0
54	MG	DB	3024	1/1	1.00	0.03	47,47,47,47	0
54	MG	BB	3063	1/1	1.00	0.04	5,5,5,5	0
54	MG	AA	1641	1/1	1.00	0.02	32,32,32,32	0
54	MG	BB	3065	1/1	1.00	0.03	30,30,30,30	0
54	MG	BB	3066	1/1	1.00	0.02	34,34,34,34	0
54	MG	BB	3067	1/1	1.00	0.05	25,25,25,25	0
54	MG	CA	1613	1/1	1.00	0.01	24,24,24,24	0
54	MG	DB	3031	1/1	1.00	0.08	29,29,29,29	0
54	MG	DB	3032	1/1	1.00	0.07	21,21,21,21	0
54	MG	DB	3033	1/1	1.00	0.04	20,20,20,20	0
54	MG	AA	1648	1/1	1.00	0.04	5,5,5,5	0
54	MG	BB	3069	1/1	1.00	0.04	5,5,5,5	0
54	MG	BB	3032	1/1	1.00	0.03	31,31,31,31	0
54	MG	CA	1617	1/1	1.00	0.06	12,12,12,12	0
54	MG	DB	3038	1/1	1.00	0.01	23,23,23,23	0
54	MG	AA	1636	1/1	1.00	0.07	38,38,38,38	0
54	MG	DB	3040	1/1	1.00	0.04	5,5,5,5	0
54	MG	DB	3041	1/1	1.00	0.07	9,9,9,9	0
54	MG	DB	3042	1/1	1.00	0.03	36,36,36,36	0
54	MG	DB	3043	1/1	1.00	0.04	7,7,7,7	0
54	MG	DB	3044	1/1	1.00	0.03	16,16,16,16	0
54	MG	BB	3034	1/1	1.00	0.07	41,41,41,41	0
54	MG	AA	1621	1/1	1.00	0.12	27,27,27,27	0
54	MG	DB	3047	1/1	1.00	0.06	31,31,31,31	0
54	MG	DB	3048	1/1	1.00	0.07	8,8,8,8	0
54	MG	DB	3049	1/1	1.00	0.05	11,11,11,11	0
54	MG	BB	3074	1/1	1.00	0.05	7,7,7,7	0
54	MG	CA	1622	1/1	1.00	0.04	38,38,38,38	0
54	MG	AA	1638	1/1	1.00	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3076	1/1	1.00	0.02	48,48,48,48	0
54	MG	BB	3001	1/1	1.00	0.03	14,14,14,14	0
54	MG	DB	3055	1/1	1.00	0.03	26,26,26,26	0
54	MG	DB	3056	1/1	1.00	0.09	16,16,16,16	0
54	MG	DB	3057	1/1	1.00	0.01	17,17,17,17	0
54	MG	BB	3015	1/1	1.00	0.02	9,9,9,9	0
54	MG	BB	3039	1/1	1.00	0.04	12,12,12,12	0
54	MG	BB	3002	1/1	1.00	0.03	18,18,18,18	0
54	MG	BB	3041	1/1	1.00	0.05	15,15,15,15	0
54	MG	DB	3062	1/1	1.00	0.04	44,44,44,44	0
54	MG	DB	3063	1/1	1.00	0.03	23,23,23,23	0
54	MG	AA	1609	1/1	1.00	0.01	11,11,11,11	0
54	MG	BB	3083	1/1	1.00	0.04	51,51,51,51	0
54	MG	BB	3084	1/1	1.00	0.06	60,60,60,60	0
54	MG	DB	3067	1/1	1.00	0.04	13,13,13,13	0
54	MG	DB	3068	1/1	1.00	0.10	16,16,16,16	0
54	MG	DB	3069	1/1	1.00	0.11	5,5,5,5	0
54	MG	DB	3070	1/1	1.00	0.06	28,28,28,28	0
54	MG	BB	3085	1/1	1.00	0.04	76,76,76,76	0
54	MG	BB	3086	1/1	1.00	0.04	5,5,5,5	0
54	MG	DB	3073	1/1	1.00	0.03	25,25,25,25	0
54	MG	DB	3074	1/1	1.00	0.07	17,17,17,17	0
54	MG	DB	3075	1/1	1.00	0.05	10,10,10,10	0
54	MG	BB	3018	1/1	1.00	0.06	32,32,32,32	0
54	MG	DB	3077	1/1	1.00	0.04	17,17,17,17	0
54	MG	BB	3044	1/1	1.00	0.03	29,29,29,29	0
54	MG	BB	3089	1/1	1.00	0.03	30,30,30,30	0
54	MG	AA	1653	1/1	1.00	0.04	51,51,51,51	0
54	MG	DB	3081	1/1	1.00	0.02	20,20,20,20	0
54	MG	CA	1639	1/1	1.00	0.04	5,5,5,5	0
54	MG	BB	3020	1/1	1.00	0.08	23,23,23,23	0
54	MG	DB	3084	1/1	1.00	0.06	14,14,14,14	0
54	MG	BB	3021	1/1	1.00	0.03	62,62,62,62	0
54	MG	BB	3048	1/1	1.00	0.07	8,8,8,8	0
54	MG	CA	1643	1/1	1.00	0.02	11,11,11,11	0
54	MG	DB	3088	1/1	1.00	0.02	31,31,31,31	0
54	MG	BB	3022	1/1	1.00	0.02	34,34,34,34	0
54	MG	BB	3050	1/1	1.00	0.07	16,16,16,16	0
54	MG	DB	3091	1/1	1.00	0.07	11,11,11,11	0
54	MG	BB	3023	1/1	1.00	0.03	6,6,6,6	0
54	MG	BB	3052	1/1	1.00	0.02	59,59,59,59	0
54	MG	CA	1648	1/1	1.00	0.05	17,17,17,17	0

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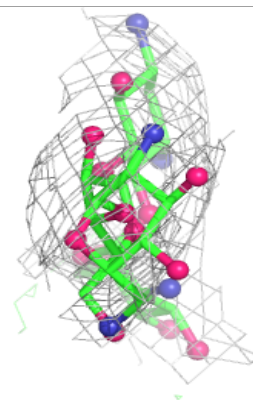
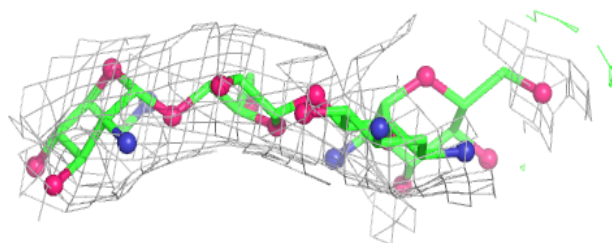
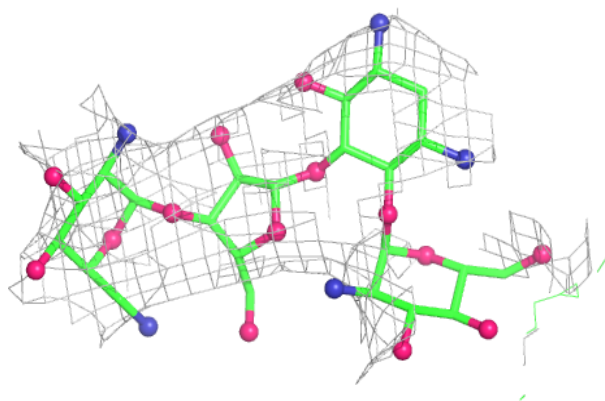
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3098	1/1	1.00	0.02	10,10,10,10	0
54	MG	DB	3096	1/1	1.00	0.11	37,37,37,37	0
54	MG	DB	3097	1/1	1.00	0.04	32,32,32,32	0
54	MG	CA	1650	1/1	1.00	0.02	5,5,5,5	0
54	MG	DB	3099	1/1	1.00	0.10	21,21,21,21	0
54	MG	BB	3005	1/1	1.00	0.07	9,9,9,9	0
54	MG	DB	3101	1/1	1.00	0.10	7,7,7,7	0
54	MG	DB	3102	1/1	1.00	0.03	20,20,20,20	0
54	MG	BB	3025	1/1	1.00	0.02	22,22,22,22	0
54	MG	DB	3104	1/1	1.00	0.05	21,21,21,21	0
54	MG	DB	3105	1/1	1.00	0.02	24,24,24,24	0
54	MG	DB	3106	1/1	1.00	0.03	17,17,17,17	0
54	MG	DB	3107	1/1	1.00	0.03	51,51,51,51	0
54	MG	BB	3006	1/1	1.00	0.03	37,37,37,37	0
54	MG	DB	3109	1/1	1.00	0.06	27,27,27,27	0
54	MG	AA	1654	1/1	1.00	0.02	52,52,52,52	0
54	MG	CA	1655	1/1	1.00	0.02	22,22,22,22	0
54	MG	CA	1656	1/1	1.00	0.04	7,7,7,7	0
54	MG	BB	3103	1/1	1.00	0.08	20,20,20,20	0
54	MG	AA	1616	1/1	1.00	0.02	15,15,15,15	0
54	MG	BB	3105	1/1	1.00	0.03	21,21,21,21	0
54	MG	BB	3058	1/1	1.00	0.03	17,17,17,17	0
54	MG	BB	3107	1/1	1.00	0.03	13,13,13,13	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.

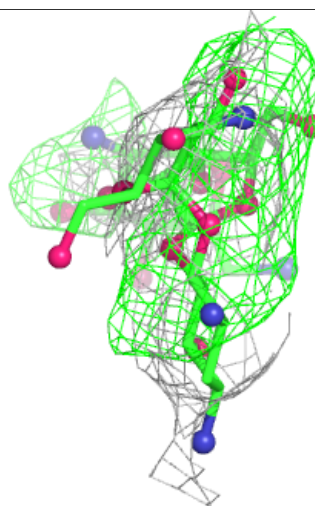
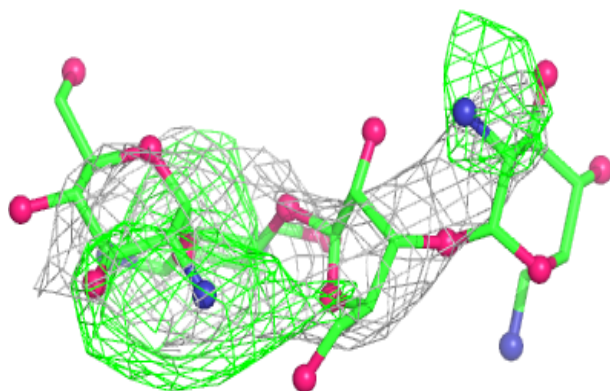
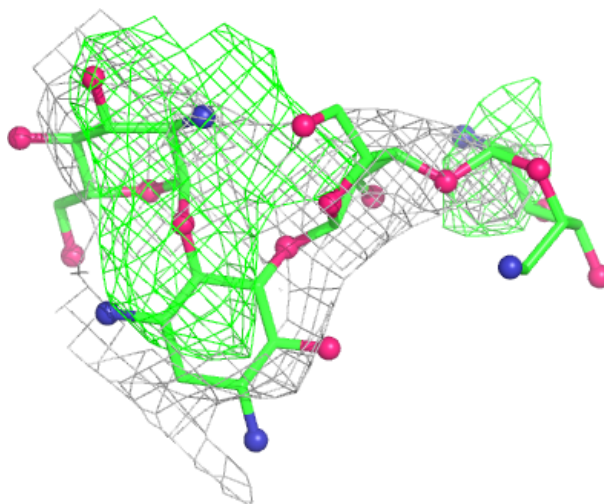
Electron density around PAR AA 1661:

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



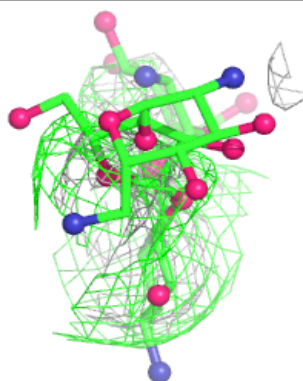
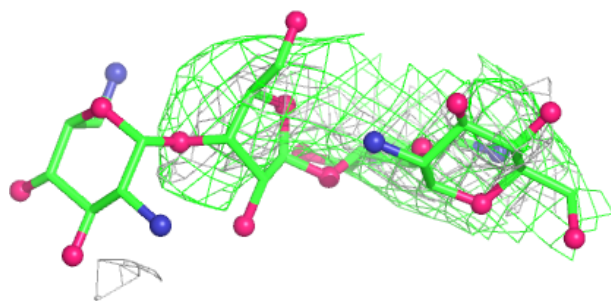
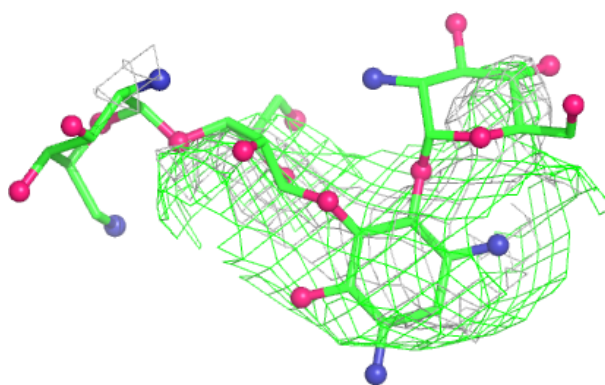
Electron density around PAR DB 3112:

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

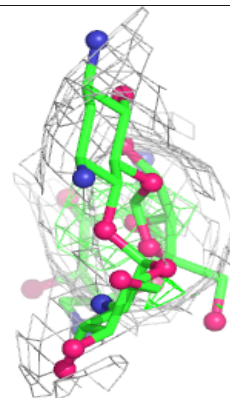
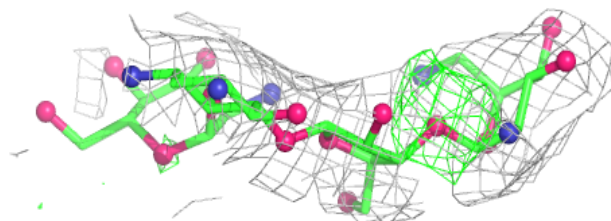
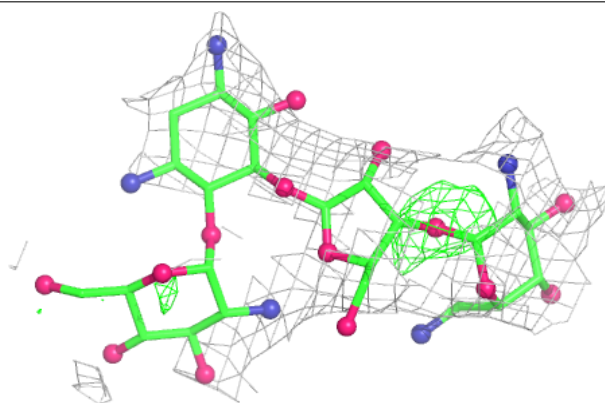


Electron density around PAR BB 3111:

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

**Electron density around PAR CA 1662:**

$2mF_o-DF_c$ (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.