



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:38 PM GMT

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

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

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

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

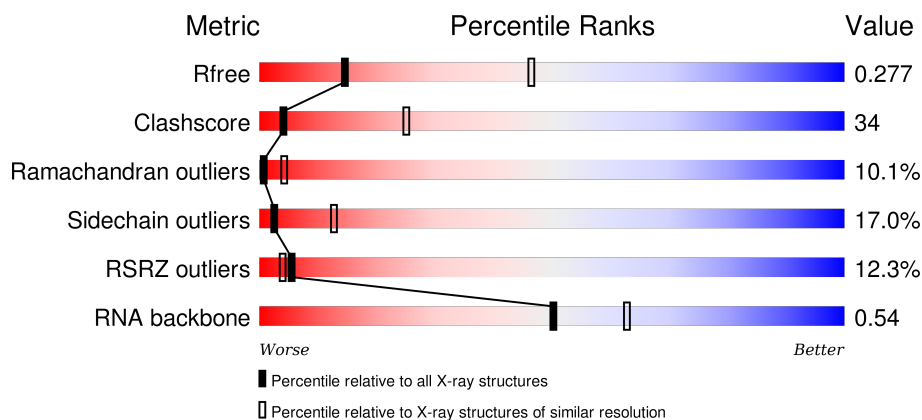
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)
RNA backbone	2183	1004 (3.72-2.72)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	<div> <div>28%</div> <div>60%</div> <div>12%</div> <div>.</div> </div>
1	CA	1542	<div> <div>28%</div> <div>60%</div> <div>11%</div> <div>.</div> </div>
2	AC	232	<div> <div>16%</div> <div>32%</div> <div>44%</div> <div>13%</div> <div>11%</div> </div>
2	CC	232	<div> <div>12%</div> <div>31%</div> <div>46%</div> <div>12%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	NMY	BB	3001	-	-	-	X
53	NMY	CA	1601	-	-	-	X
53	NMY	DB	3001	-	-	-	X
54	MG	AA	1620	-	-	-	X
54	MG	AA	1658	-	-	-	X
54	MG	BB	3082	-	-	-	X
54	MG	BB	3088	-	-	-	X
54	MG	CA	1638	-	-	-	X
54	MG	DB	3031	-	-	-	X
54	MG	DB	3060	-	-	-	X
54	MG	DB	3097	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284172 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

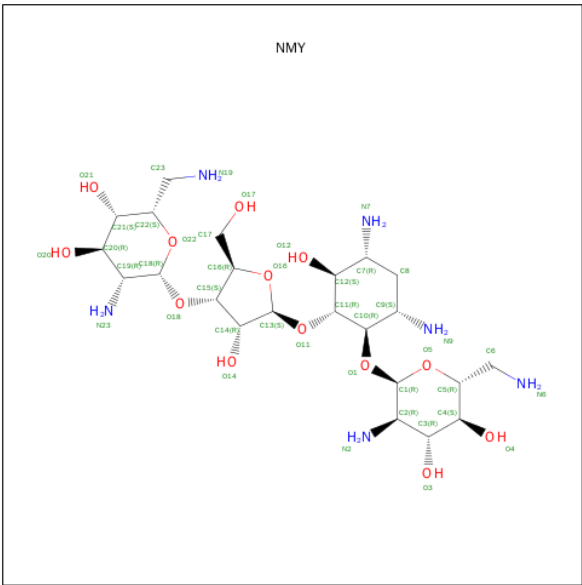
- Molecule 51 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 53 is NEOMYCIN (three-letter code: NMY) (formula: C₂₃H₄₆N₆O₁₃).



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

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

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

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

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

- Molecule 56 is water.

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

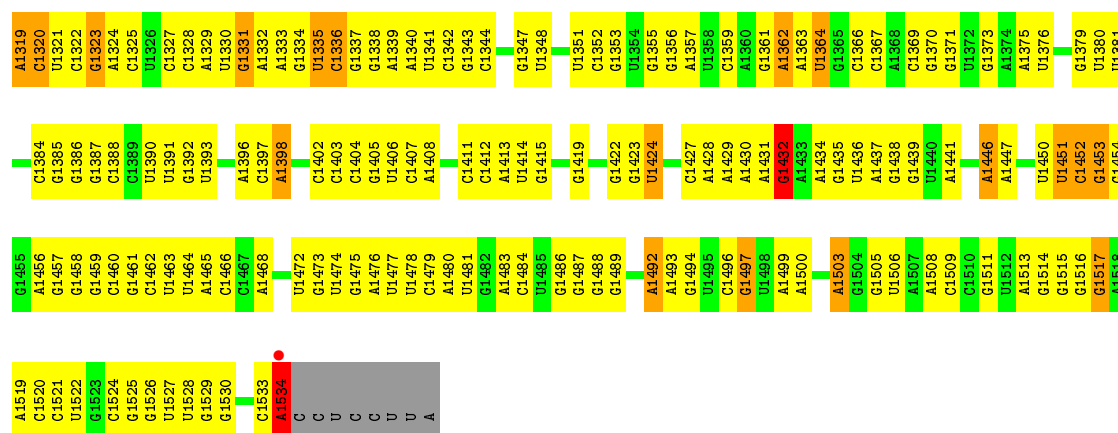
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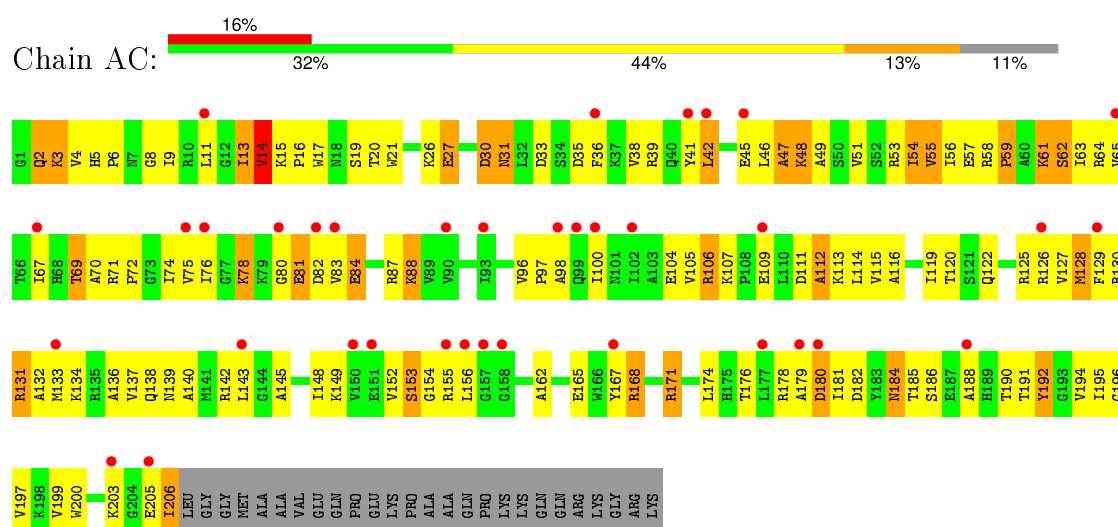
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DE	1	Total	O	0	0
			1	1		
56	DL	2	Total	O	0	0
			2	2		
56	DR	1	Total	O	0	0
			1	1		



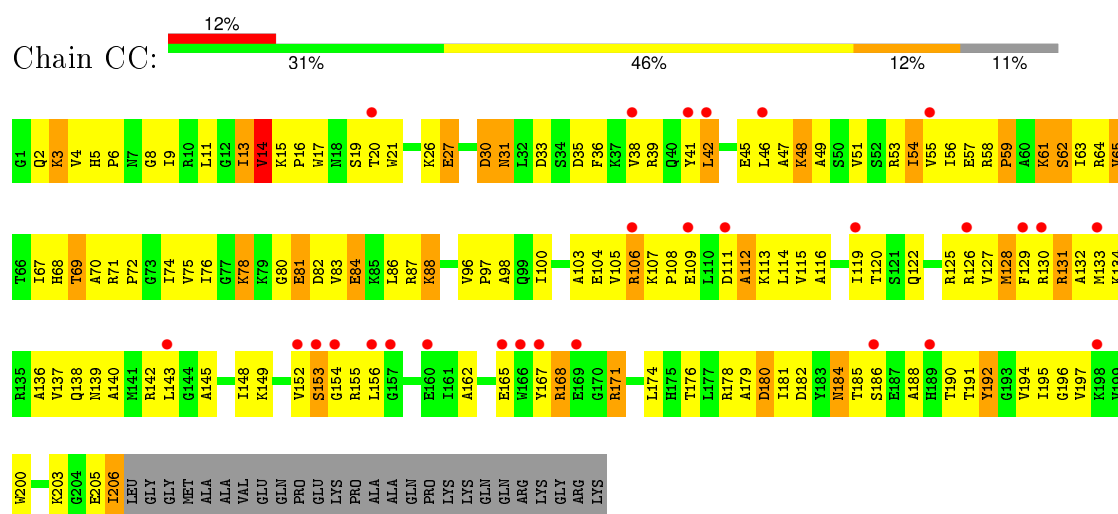
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A1252	G1191	A1191	C1119	G1050	U986	U916	G833	U762	G691	U619	C549	U485	G414	A274	G212
A1253	A1192	G1120	U1120	G1053	G987	U917	U834	U763	U692	C620	G550	U486	G415	G275	G213
G1255	G1193	G1121	U1121	C1054	G988	G917	U835	G764	G693	A621	U552	A487	G416	G276	G214
A1256	G1194	U1122	U1123	A1054	U991	A918	C840	G765	G694	C623	A553	C488	U420	G277	G215
G1260	A1195	G1195	U1124	U1056	U992	U920	C841	G766	A695	C624	A554	C490	U421	G278	U216
A1261	A1196	G1125	U1125	G1057	G993	U921	U842	A767	A696	C625	U555	G491	U422	A279	U216
C1262	G1197	U1126	U1126	U1057	A994	G922	U843	A768	U697	G626	U556	G492	G423	C280	U219
C1263	G1198	U1127	U1127	U1058	G995	A923	G844	A769	G698	G627	U557	G493	G424	G281	U220
G1270	G1199	U1128	U1128	U1059	A996	A934	A845	G770	G699	G628	G558	G494	G425	C284	G221
A1271	C1200	C1132	G1132	U1062	U997	G925	G846	C770	G700	U632	A559	A495	G426	C285	G222
A1272	U1201	C1063	G1063	C1063	C998	G926	G847	G775	U701	U633	A560	A496	G428	C286	A223
C1273	U1202	U1133	G1133	G1064	C999	G827	C848	G776	A702	G633	U561	A499	U429	U224	U224
A1274	C1203	C1136	U1136	U1065	A1000	G928	G849	A777	G703	C634	U562	A366	U430	G289	G226
G1206	G1207	C1137	U1137	C1066	C1001	G929	G850	A778	G704	A635	G566	A367	A431	G298	U229
C1208	G1208	G1138	U1138	A1067	G1002	G932	U855	C779	G705	U636	A572	C501	G432	G299	G230
C1209	G1209	G1139	U1139	G1068	G1003	G933	G858	A780	U707	U638	A573	C503	G433	A300	G231
G1278	G1278	C1140	U1140	C1069	A1004	G934	G859	A781	U708	G639	A574	C504	U434	G301	U232
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C1281	C1281	G1142	U1142	G1071	G1006	A935	A860	A783	U710	U641	G576	C506	U436	A306	C234
U1282	U1282	G1143	U1143	G1072	U1007	C936	G861	A784	U711	A642	C577	C507	U437	G307	G235
C1283	C1283	U1212	U1212	U1073	U1008	G939	G862	G785	G712	U643	G578	C508	U438	A236	G237
U1284	U1284	C1147	U1147	U1076	U1010	C940	A864	A792	G713	U644	C579	C509	U439	G308	U238
G1285	G1285	U1148	U1148	G1077	C1011	G941	A865	U793	G714	A648	A579	C510	C440	A309	G239
A1286	A1286	C1149	U1149	U1078	C1012	G942	G866	A794	A715	U649	C580	C511	G441	G310	G240
C1287	C1287	G1150	U1150	G1079	G1013	A946	G867	A795	A716	G650	G581	C512	G442	G311	U241
A1288	A1288	C1151	U1151	A1080	G947	C948	G868	C796	A717	C651	G582	C513	G443	G312	G242
A1289	A1289	A1152	U1152	A1081	G1015	A949	G869	C797	C719	U652	G583	C514	G444	G313	G243
G1290	G1290	C1158	U1158	G1084	U1017	U950	A872	U798	G720	U653	C584	C515	G445	G314	G244
U1291	U1291	U1159	U1159	U1085	U1018	U951	A873	A802	G721	G656	G585	C516	G446	A320	U245
C1292	C1292	G1160	U1160	U1086	A1019	U952	G874	G803	U723	U657	G586	C517	G447	G321	G246
G1293	G1293	C1161	U1161	G1087	G1020	G953	G875	U804	G724	C658	U590	C518	G448	G322	U247
C1294	C1294	C1162	U1162	G1088	A1021	U954	A878	C805	G725	U659	U591	C519	G449	G323	G248
U1295	U1295	A1163	U1163	U1089	U1022	U956	G879	C806	G726	C660	G592	C520	G450	G324	G249
C1296	C1296	G1164	U1164	U1091	A1022	U957	C880	A807	G727	G661	U593	C521	G451	G325	G250
G1297	G1297	U1165	U1165	U1092	U1025	U960	G881	C810	A728	U662	U594	C522	G452	A326	G251
A1298	A1298	C1166	U1166	G1094	G1026	U961	G882	C811	A729	A663	A595	C523	G453	G327	U252
C1300	C1300	U1167	U1167	U1095	C1027	U962	C883	C812	G730	C664	A596	C524	G454	G328	G253
U1301	U1301	G1168	U1168	C1096	C1028	G966	U884	G813	G731	A665	G597	C525	G455	G329	G254
C1302	C1302	A1169	U1169	C1097	U1029	G967	G885	U814	G732	G666	U598	C526	G456	G330	G255
G1303	G1303	U1170	U1170	U1098	U1030	U968	C886	U815	G733	G667	U599	C527	G457	A327	U256
C1304	C1304	A1171	U1171	C1099	C1031	A969	C887	A816	G734	U672	A600	C528	G458	G328	G257
G1305	G1305	C1172	U1172	U1100	G1032	C970	G894	A817	C735	A673	G601	C529	G459	A329	G258
A1306	A1306	U1173	U1173	A1101	G1033	G971	G895	C817	C736	G674	A602	C530	G460	G330	G259
U1307	U1307	G1174	U1174	C1096	G1034	C972	C896	G818	C737	G675	U603	C531	G461	G331	G260
C1308	C1308	U1175	U1175	C1103	A1035	G973	C897	A819	C738	A676	A607	C532	G462	G332	U261
G1309	G1309	A1176	U1176	G1104	A1036	A974	A901	U820	C739	U676	G608	C533	G463	U333	A262
C1310	C1310	U1177	U1177	U1105	G1039	A975	G902	G821	U740	U677	A608	C534	G464	G334	A263
A1311	A1311	G1178	U1178	G1106	U1040	G976	G903	U822	G741	U678	A609	C535	G465	G335	A264
G1312	G1312	C1179	U1179	C923	U1041	G977	U904	C924	G742	C979	U610	C536	G466	A336	G265
C1313	C1313	A1180	U1180	A978	G978	A978	U905	G824	A743	C680	C611	C537	G467	G337	G266
U1314	U1314	G1181	U1181	C979	U905	C980	A906	A825	C744	A681	C612	C538	G468	G338	G267
C1315	C1315	U1182	U1182	A906	A907	U981	A907	C826	G745	G682	C613	C539	G469	A339	U268
U1247	U1247	C1183	U1183	U982	A908	U982	A908	U827	A746	G683	C614	C540	U470	G345	G269
C1248	C1248	G1184	U1184	U983	A909	U983	A909	U828	G747	U684	G615	C541	G471	G346	A270
A1318	A1318	U1185	U1185	U1114	G1047	A983	C910	G929	A748	U686	G616	C542	G472	G347	G271
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• Molecule 2: 30S ribosomal protein S3

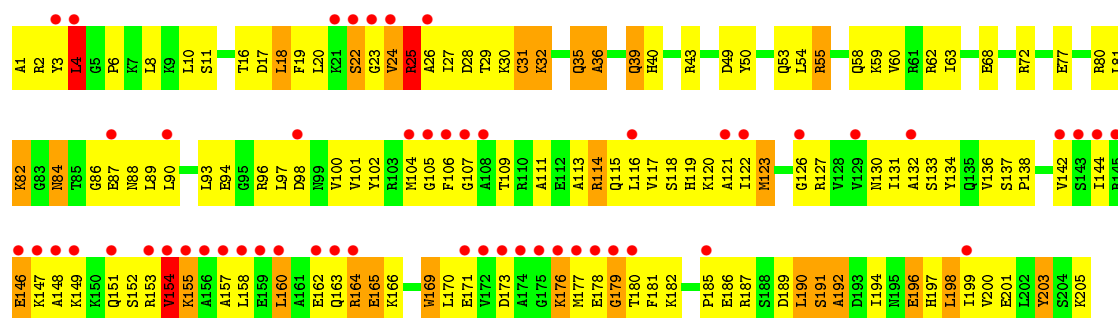


• Molecule 2: 30S ribosomal protein S3

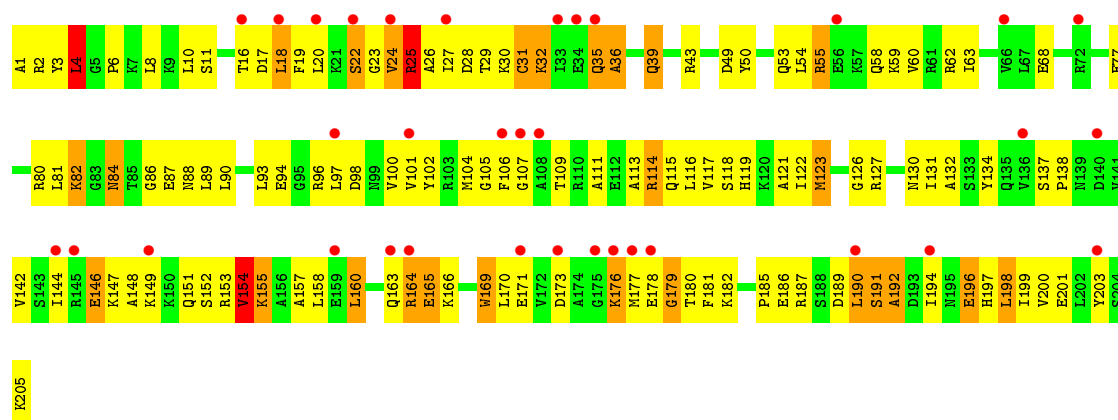


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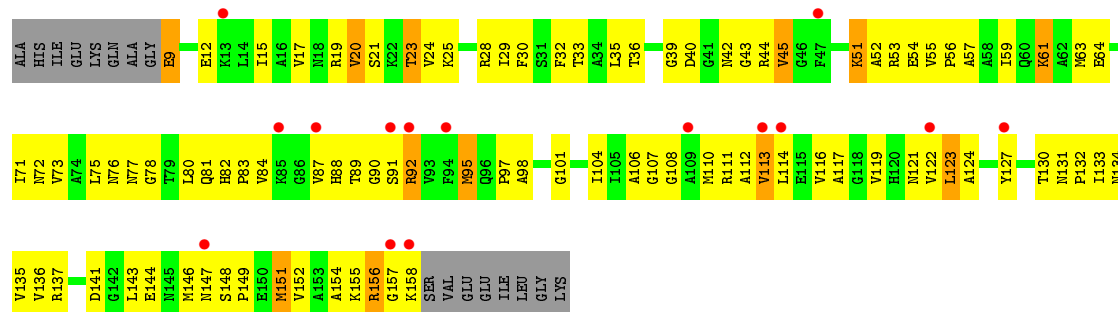




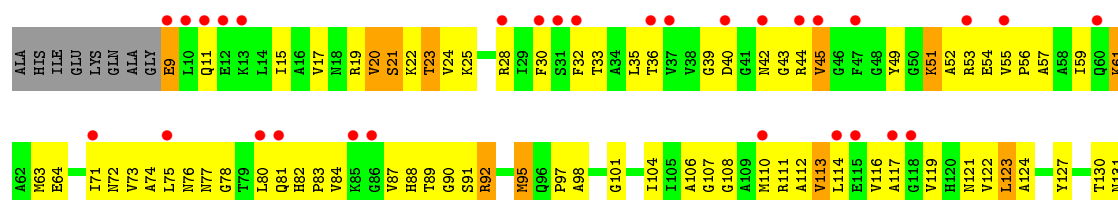
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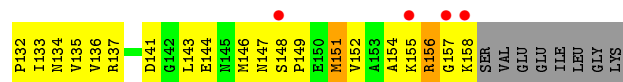


• Molecule 4: 30S ribosomal protein S5

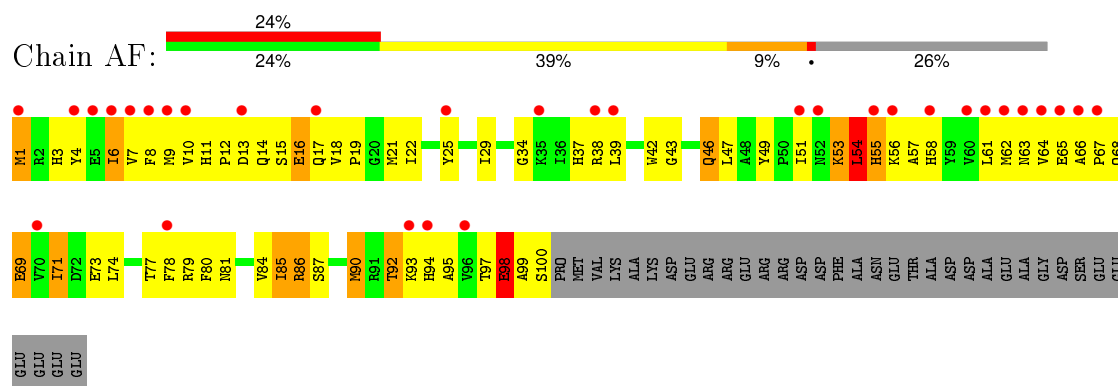


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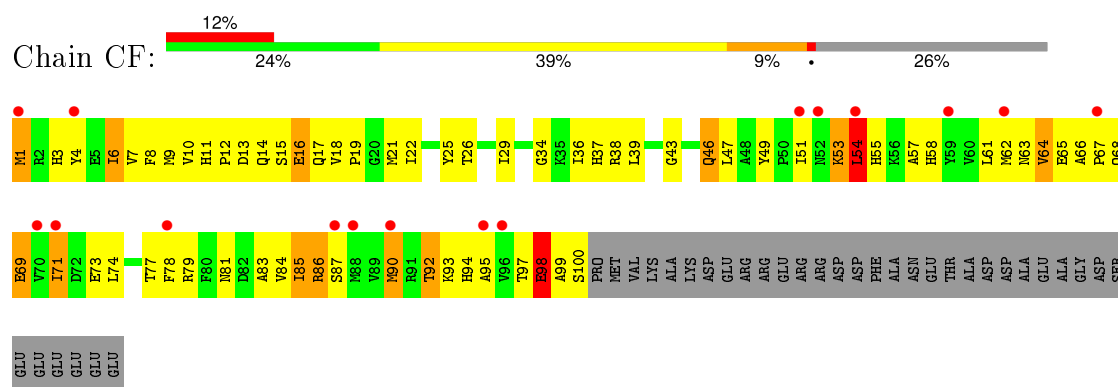




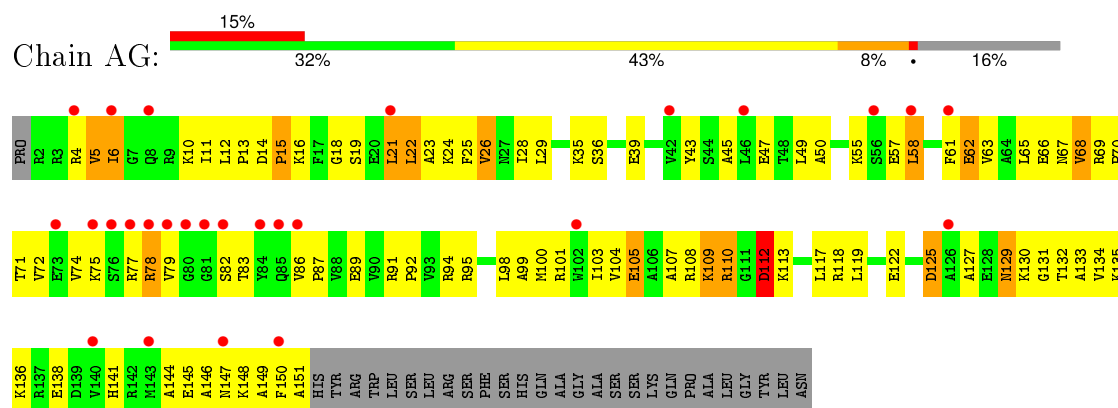
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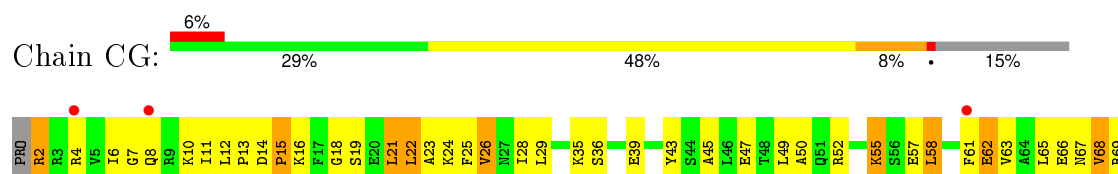
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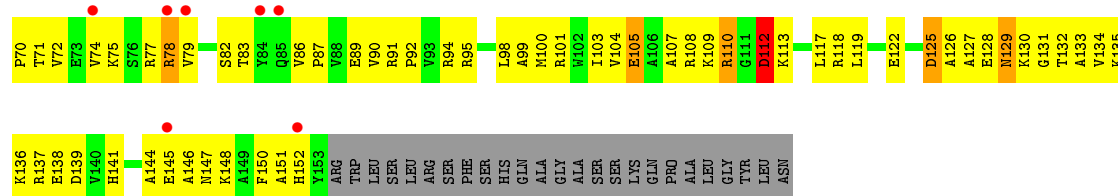


• Molecule 6: 30S ribosomal protein S7

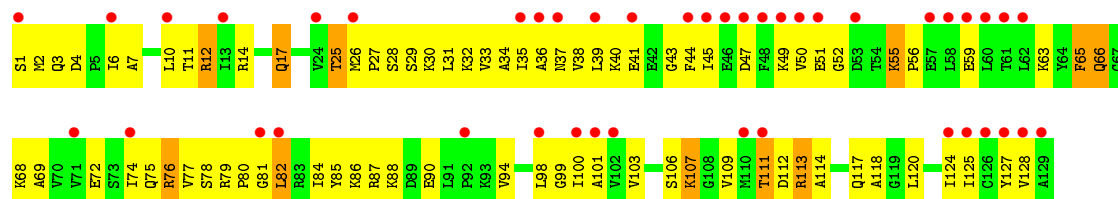


• Molecule 6: 30S ribosomal protein S7

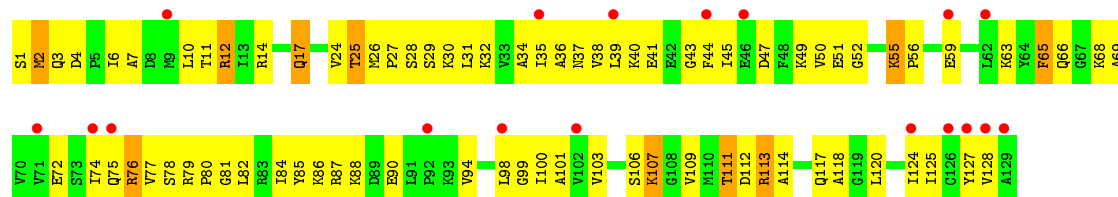




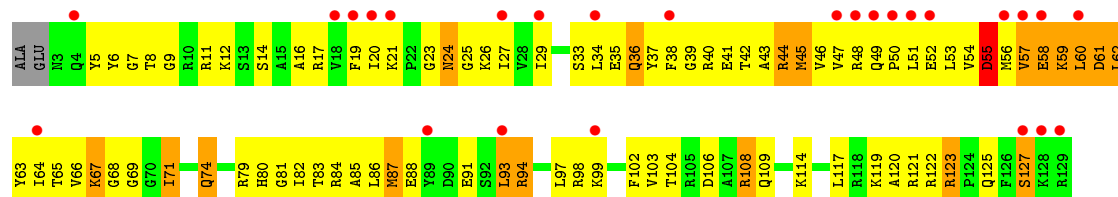
• Molecule 7: 30S ribosomal protein S8



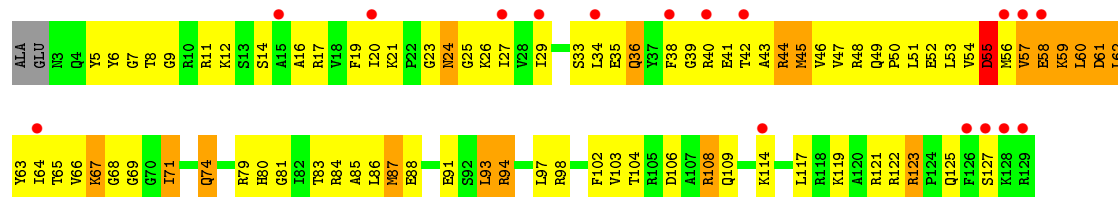
• Molecule 7: 30S ribosomal protein S8



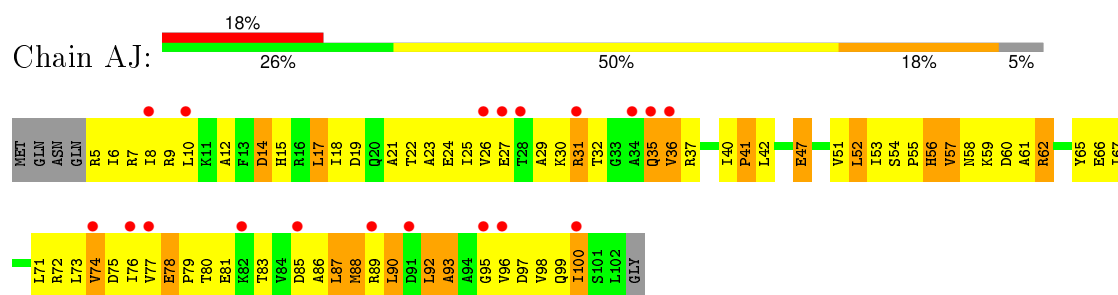
• Molecule 8: 30S ribosomal protein S9



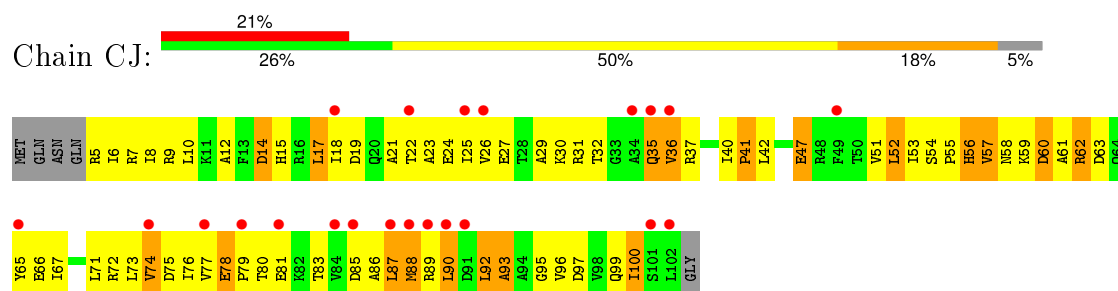
• Molecule 8: 30S ribosomal protein S9



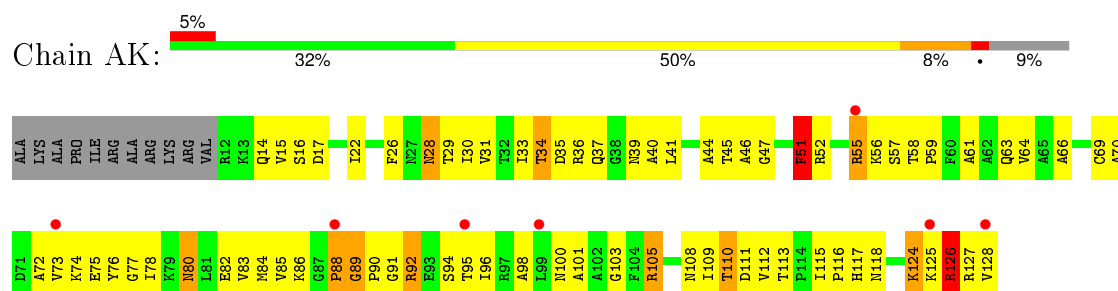
• Molecule 9: 30S ribosomal protein S10



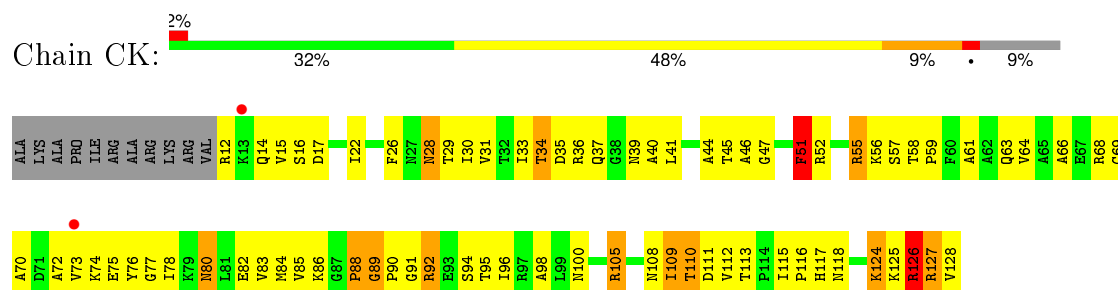
• Molecule 9: 30S ribosomal protein S10



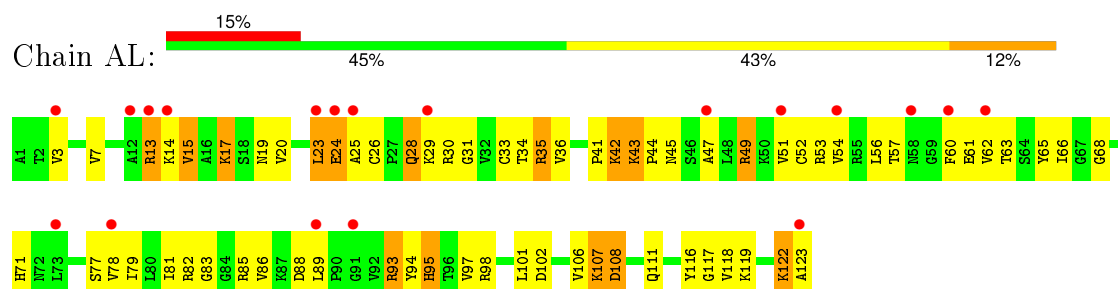
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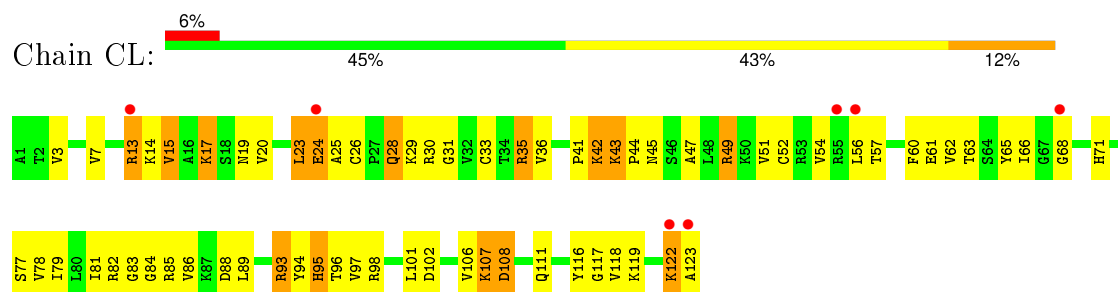
• Molecule 10: 30S ribosomal protein S11



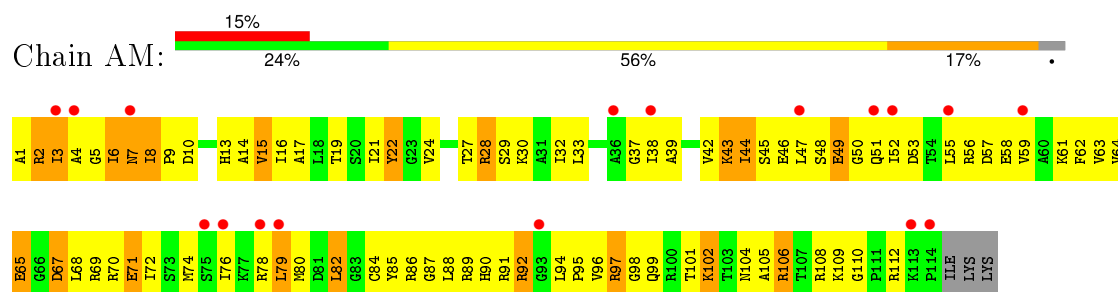
• Molecule 11: 30S ribosomal protein S12



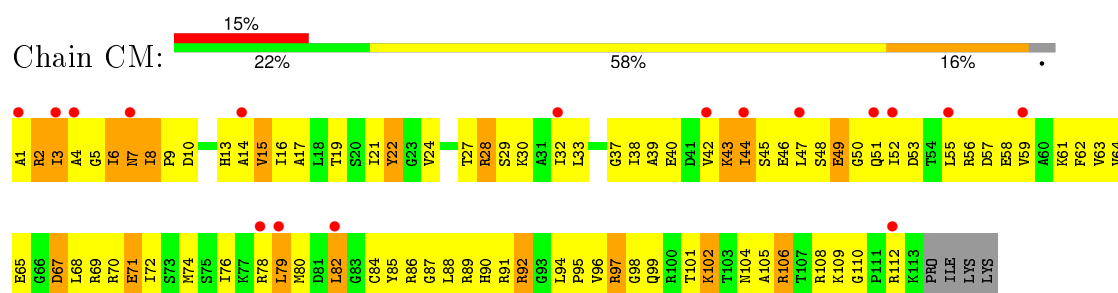
- Molecule 11: 30S ribosomal protein S12



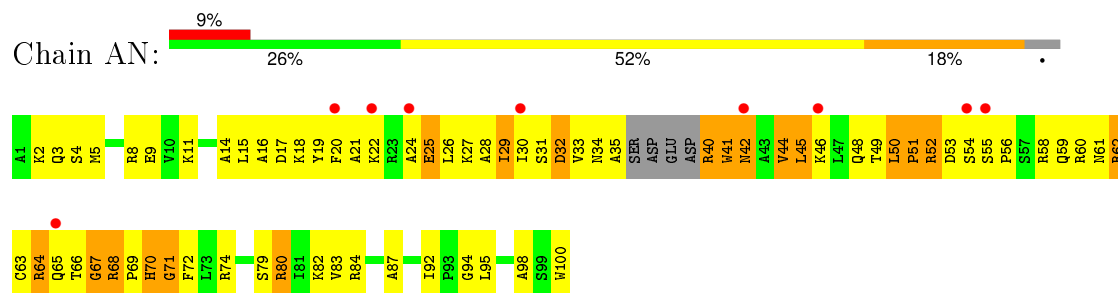
- Molecule 12: 30S ribosomal protein S13



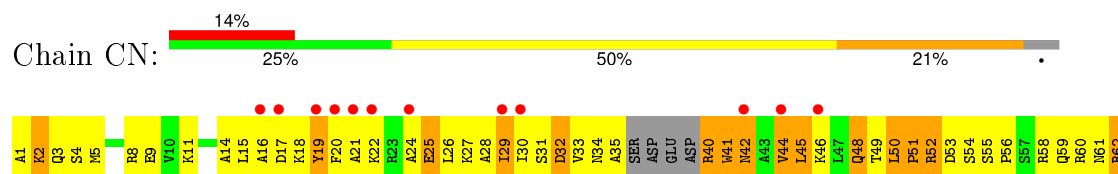
- Molecule 12: 30S ribosomal protein S13

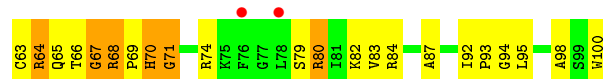


- Molecule 13: 30S ribosomal protein S14

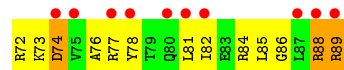
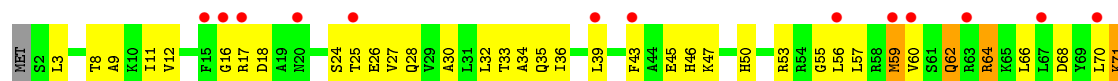
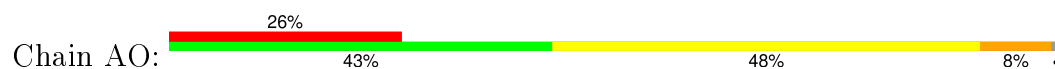


- Molecule 13: 30S ribosomal protein S14

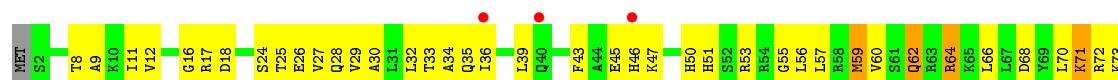
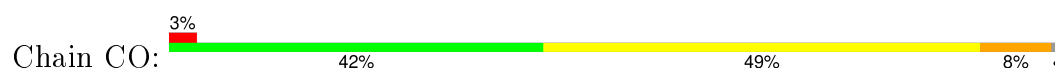




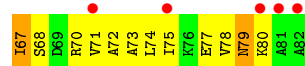
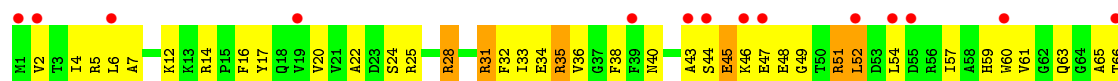
• Molecule 14: 30S ribosomal protein S15



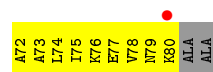
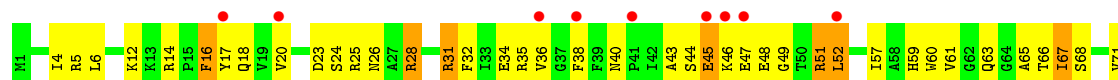
• Molecule 14: 30S ribosomal protein S15



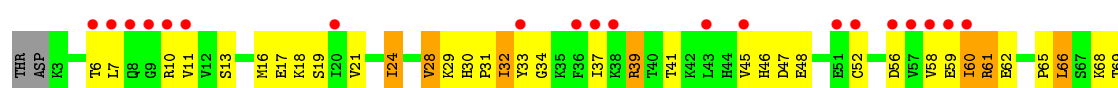
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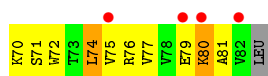


• Molecule 15: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S17

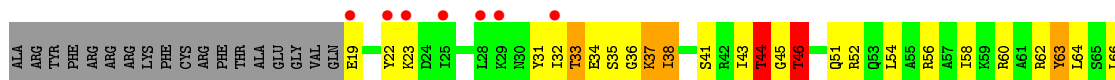




- Molecule 16: 30S ribosomal protein S17



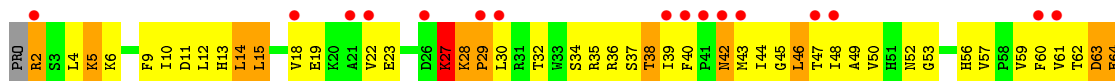
- Molecule 17: 30S ribosomal protein S18



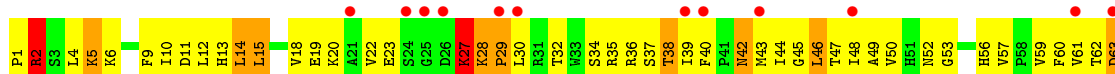
- Molecule 17: 30S ribosomal protein S18

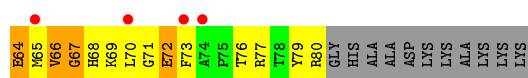


- Molecule 18: 30S ribosomal protein S19

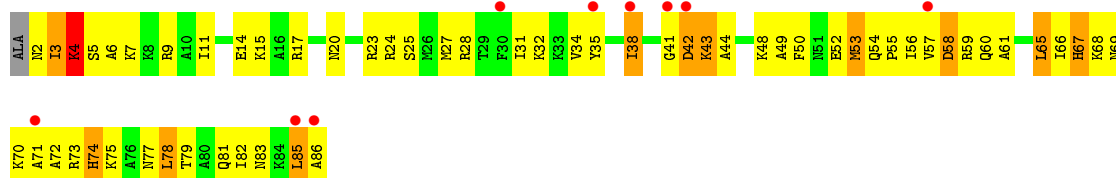


- Molecule 18: 30S ribosomal protein S19

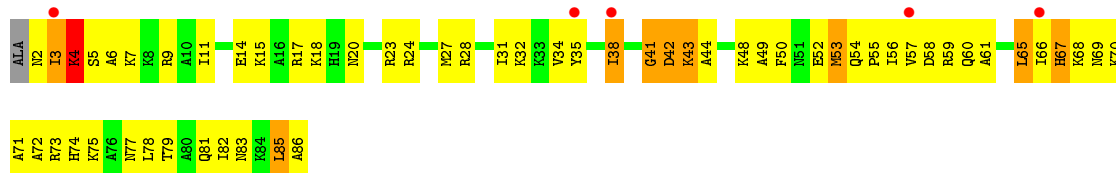




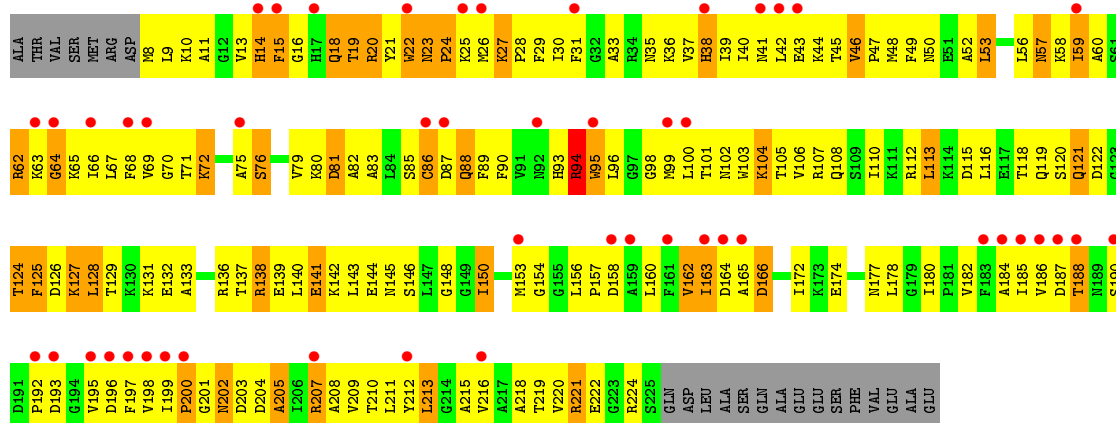
• Molecule 19: 30S ribosomal protein S20



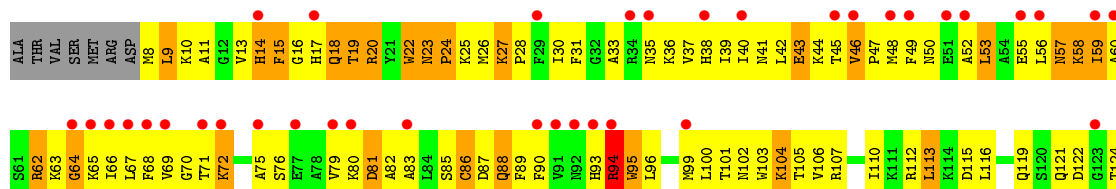
• Molecule 19: 30S ribosomal protein S20

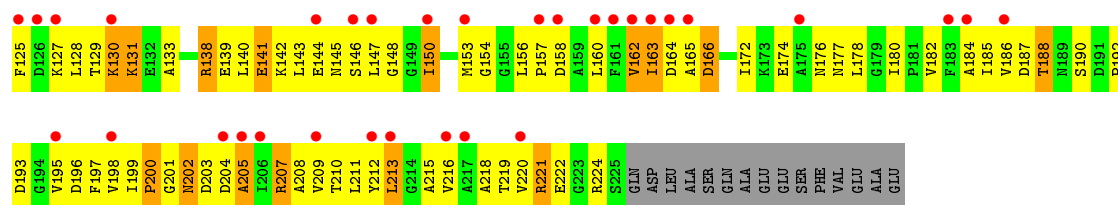


• Molecule 20: 30S ribosomal protein S2

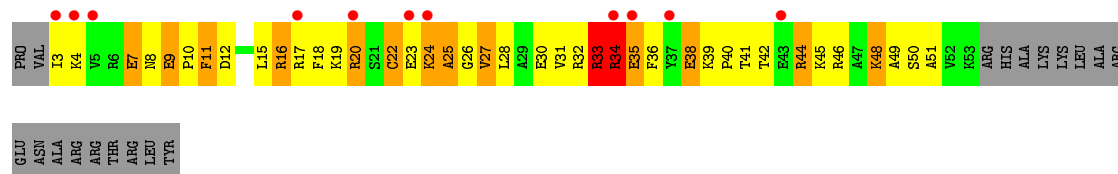


• Molecule 20: 30S ribosomal protein S2

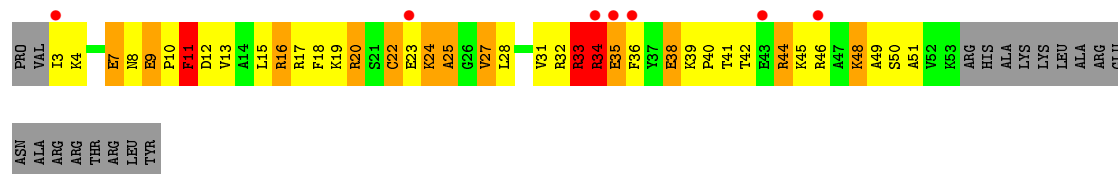
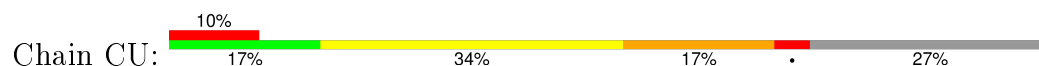




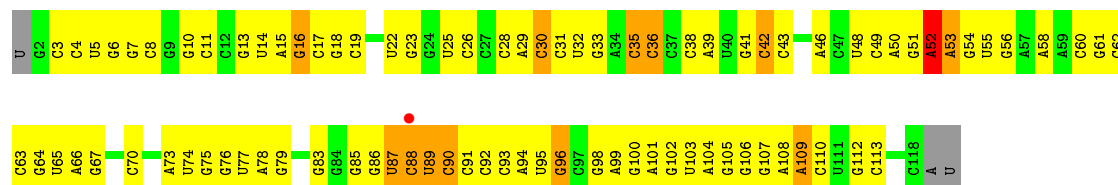
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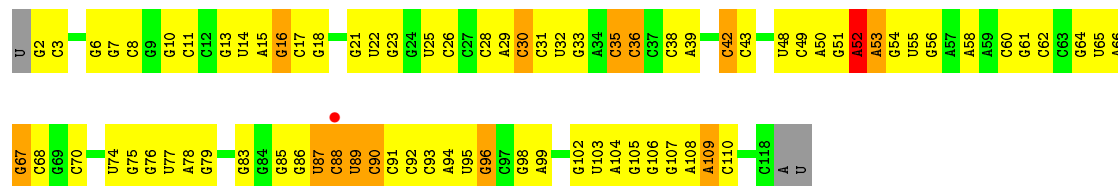
• Molecule 21: 30S ribosomal protein S21



• Molecule 22: 5S rRNA



• Molecule 22: 5S rRNA



• Molecule 23: 23S rRNA



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G1052	C987	U919	U850	G775	G700	A637	U570	U499	U427	C351	C281	C209	C143	C69	G2
A1054	A988	A920	C851	G776	U571	U638	G570	G500	A428	A352	A282	G214	C144	G70	U3
G1055	G989	C922	U852	G777	G704	C640	A572	A503	U431	A354	U284	G215	C145	A71	U4
G1056	G990	G923	C853	G778	A705	A504	U573	A504	A432	A355	G285	A216	C146	A72	A5
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C994	C994	A927	G785	G784	U576	U646	G577	C510	U436	G361	G289	G220	A152	G76	G9
C995	C995	G786	G859	G785	G577	G647	G577	C511	U437	A362	U290	A221	U153	G77	A10
A996	A996	G787	G860	G786	G577	G647	G577	C512	U438	A363	U291	A222	U154	G78	A11
G1062	G997	G930	A863	G787	U714	C650	U580	U511	G439	A364	G291	A223	U155	G79	U12
C1064	C998	U931	G864	A715	A716	G851	A581	U512	C440	G363	U296	G224	A156	G80	G15
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A1077	G1011	G942	A877	G808	A727	G662	U591	A531	C455	G372	U304	G245	U165	A91	G30
A1080	G1012	A943	A878	G812	G729	G663	U592	A532	C456	A373	U305	G246	U166	A92	G31
U1081	A1013	C944	G	C814	A730	G664	U593	A533	A457	U379	G306	G247	U167	A95	G32
U1082	A1014	A945	G	C815	A730	U665	U594	A534	A458	G379	G307	G248	U168	A96	G33
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U1086	U1018	G949	U	C819	C738	A668	U600	A538	C462	G389	G311	G252	U172	U102	G36
A1087	U1019	G950	C	C820	A739	G669	G600	A539	G463	U390	G312	G253	U173	A103	G37
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U1097	A1028	U958	A	C826	A745	A675	C611	A545	U469	A401	G318	G259	U179	U120	G44
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G1102	U1033	U967	C	C831	A752	G682	U616	A550	A474	G409	A330	G264	U184	A125	U50
A1103	G1034	C968	C898	U832	A753	U683	U617	A551	A475	G410	G331	G265	U185	A126	G51
C1104	U1035	G969	A899	A833	U754	U684	U618	A552	A476	G411	G332	G266	U186	A127	G52
U1105	G1036	U970	A900	G834	U755	U685	U619	A553	G481	A412	G333	G267	U187	C128	A53
G1106	G1037	G971	C901	C835	A756	U686	G620	A554	G482	A413	G334	G268	U188	C129	G54
U1107	U1038	A972	C902	C836	G757	U687	G621	A555	G483	C413	G335	G269	U189	C130	G55
C1108	G1039	U973	C903	C837	C758	U688	G622	A556	G484	C414	G336	G270	U190	A131	G56
U1109	A1040	G974	G904	C838	C759	U689	G623	A557	G485	C415	G337	G271	U191	G132	G57
G1110	G1041	A975	G905	C839	A764	A690	U624	A558	U486	A416	G338	G272	U192	U135	G58
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U1112	A1046	A979	A909	C841	U766	C691	U626	A560	G488	C418	U340	G274	U194	U137	U63
U1113	G1047	U980	A910	U842	U767	C692	G627	A561	G489	U419	G341	G275	U195	U138	A63
C1114	A1048	C981	A911	U843	U768	U694	U630	A562	G490	C420	G342	G276	U196	U139	A64
G1115	G1049	A982	U912	U844	U769	G695	U631	A563	G491	G421	A345	G277	U197	C140	U65
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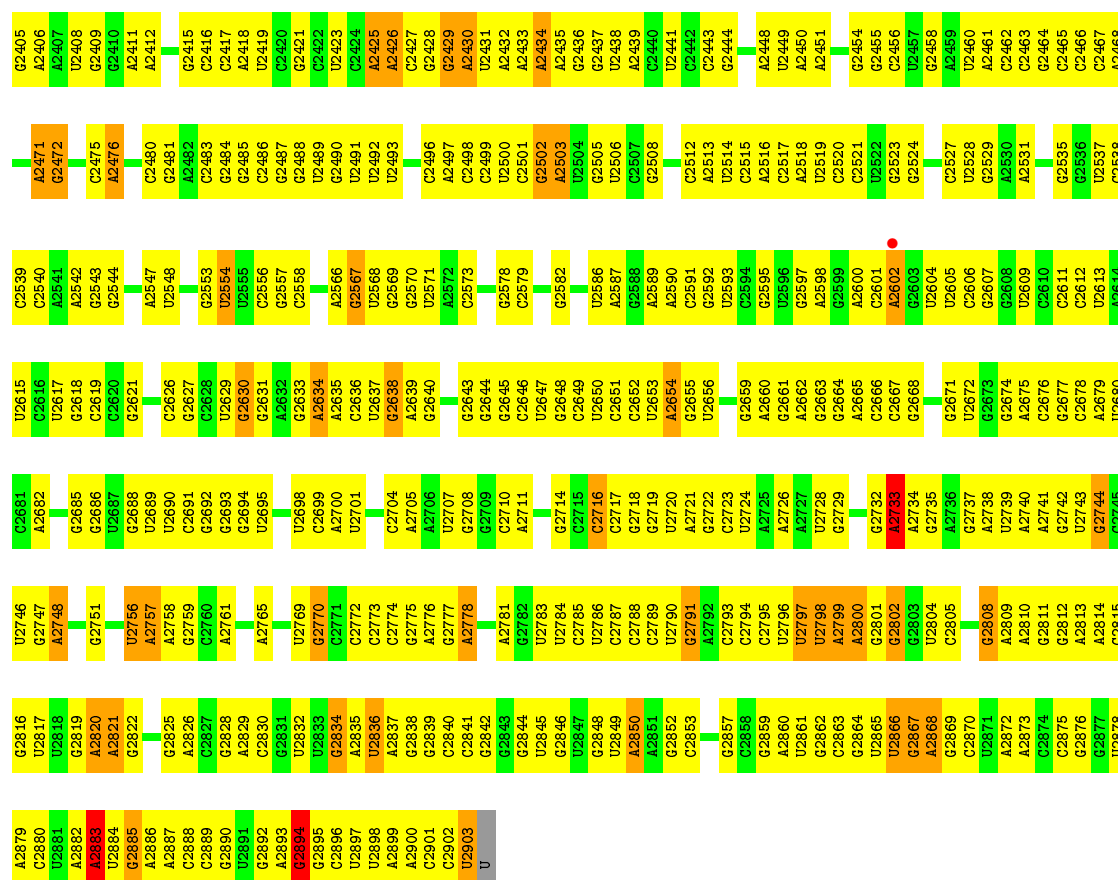
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C	U2100	A2033	A2033	U1820	U1745	A1677	U1534		C1399	A1322	G1250	C1170
C	U2101	U2034	U2034	A1821	U1746	G1677	C1535	G1464	G1251	C1323	G1251	G1171
C	G2102	G2035	G2035	G1822	C1748	A1678	G1536	G1465	G1252	G1324	C1252	C1172
C	C2103	A2037	A2037	U1823	A1749	U1680	G1537	U1466	U1400	U1325	A1253	U1173
C	C2104	G2038	G2038	G1824	G1750	A1598	U1538	A1469	G1401	U1326		
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C	U2109	A1966	A1966	G1897	G1756	G1684	C1541	G1470	U1405	G1257	G1257	U1176
C	U2110	U2041	U2041	U1898	A1757	C1685	U1542	G1471	U1406	U1258	G1177	C1177
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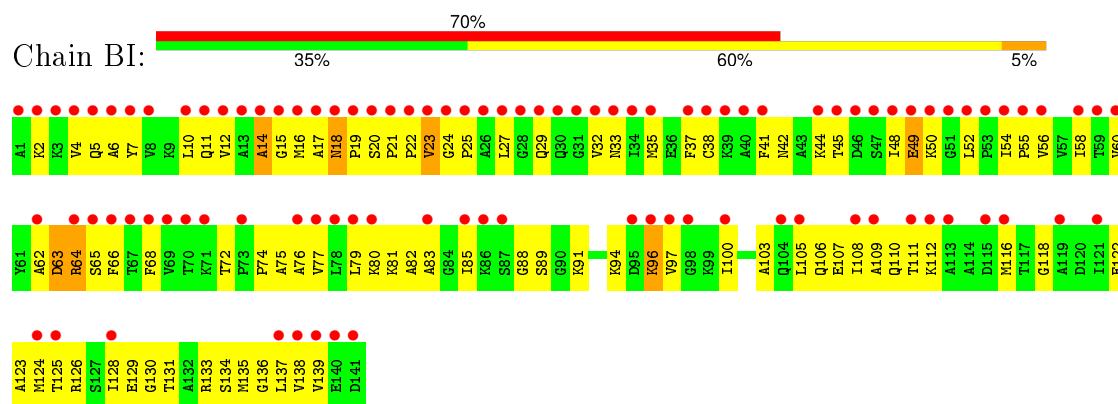




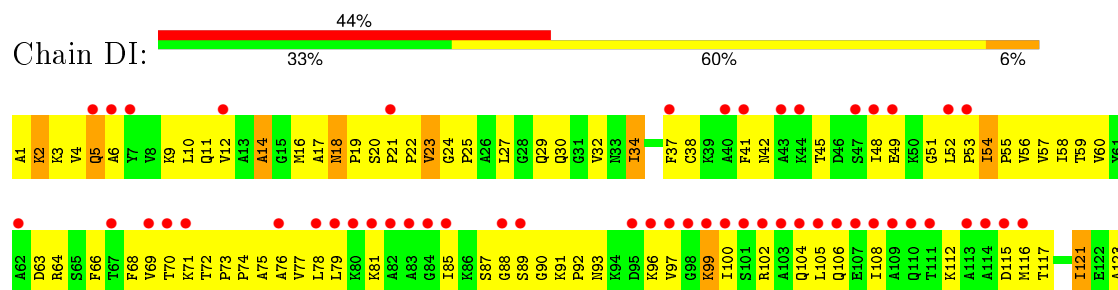
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PDB
PROTEIN DATA BANK

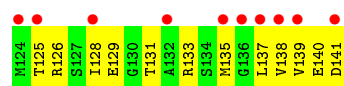


• Molecule 24: 50S ribosomal protein L11

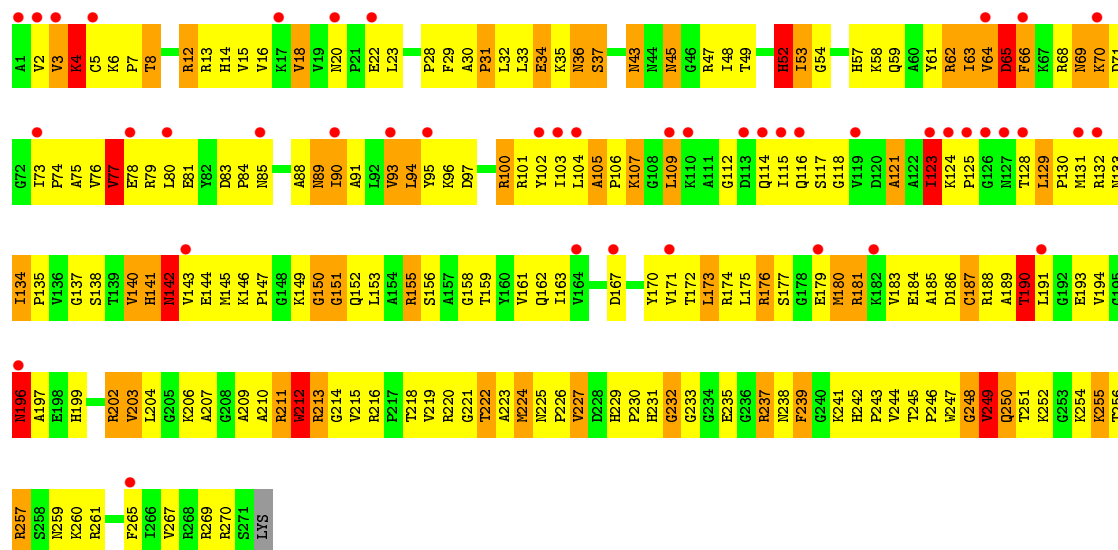


• Molecule 24: 50S ribosomal protein L11

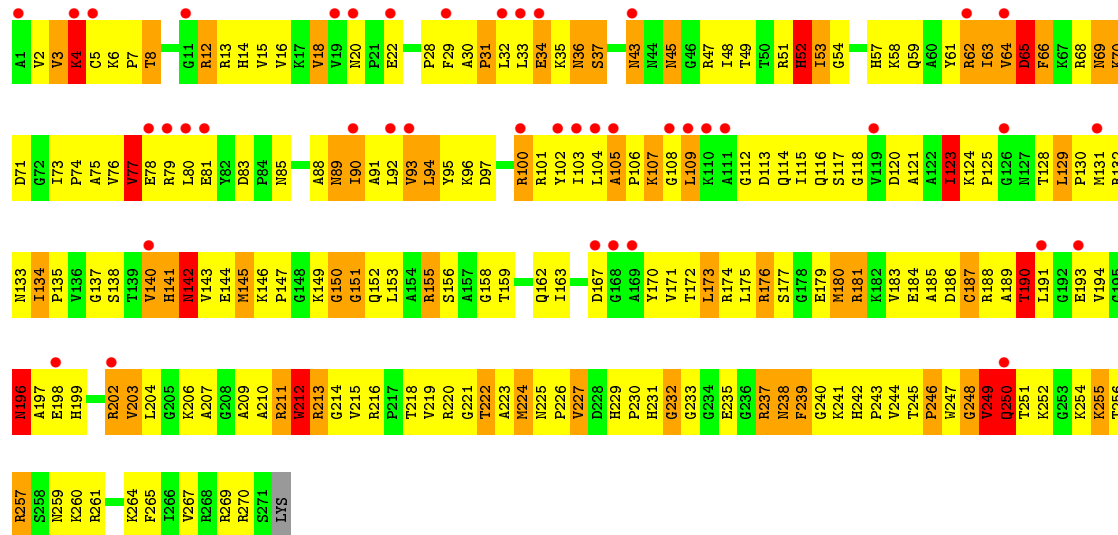




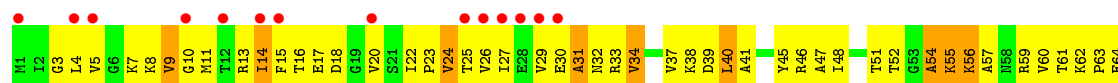
• Molecule 25: 50S ribosomal protein L2

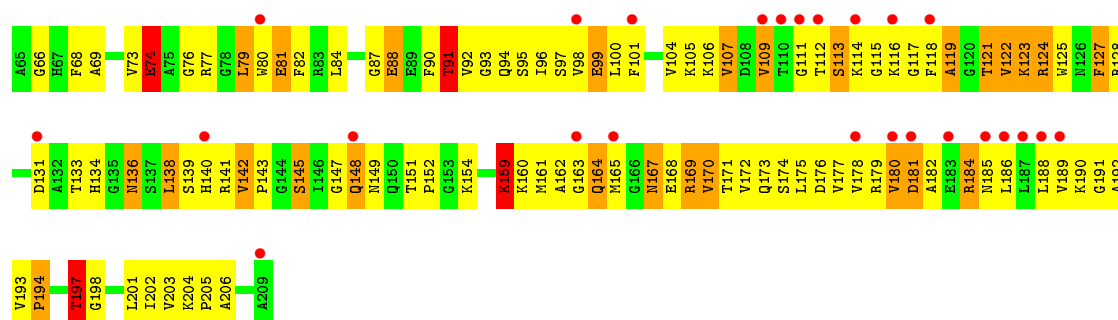


• Molecule 25: 50S ribosomal protein L2

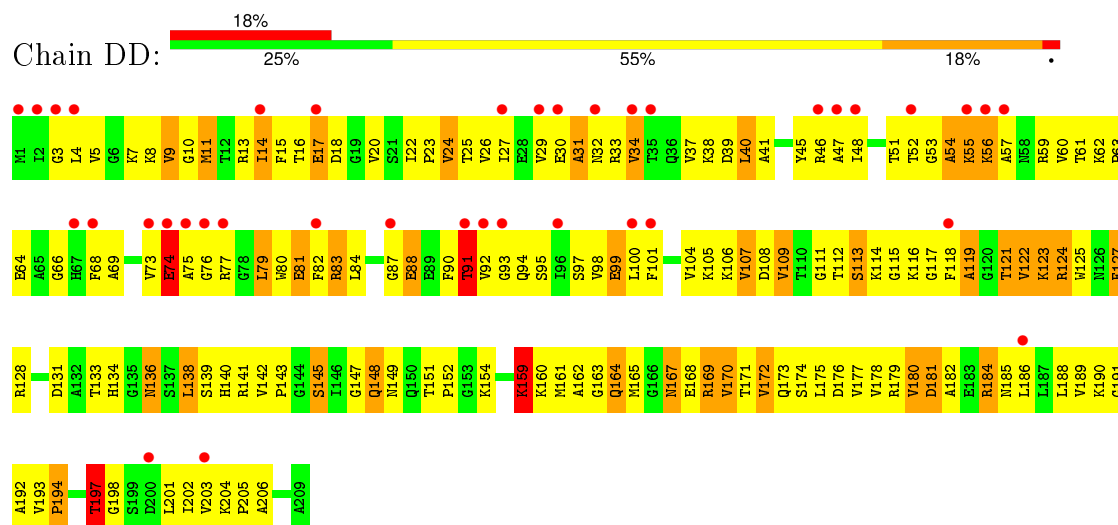


• Molecule 26: 50S ribosomal protein L3

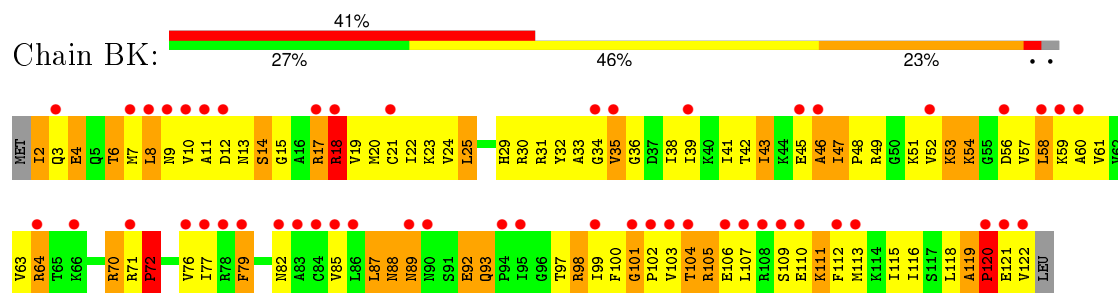




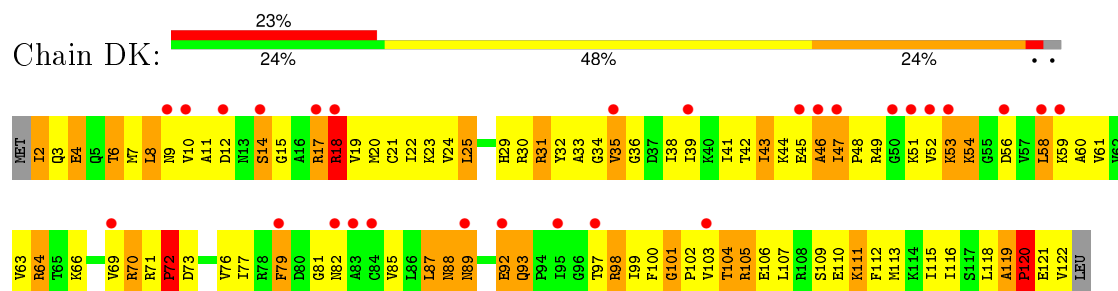
- Molecule 26: 50S ribosomal protein L3



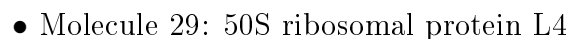
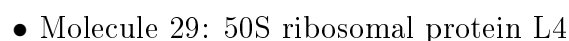
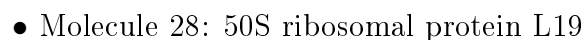
- Molecule 27: 50S ribosomal protein L14



- Molecule 27: 50S ribosomal protein L14

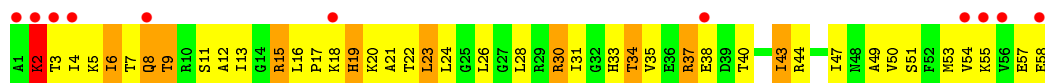


- Molecule 28: 50S ribosomal protein L19

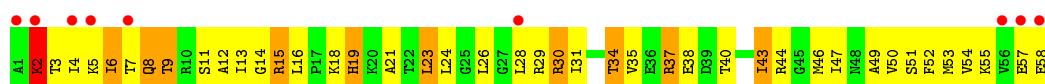




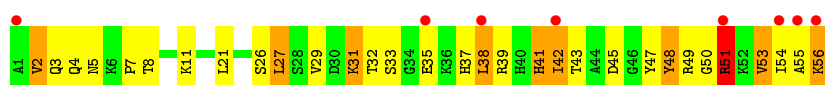
- Molecule 30: 50S ribosomal protein L30



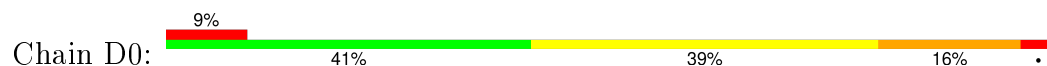
- Molecule 30: 50S ribosomal protein L30



- Molecule 31: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L32



- Molecule 32: 50S ribosomal protein L36



- Molecule 32: 50S ribosomal protein L36

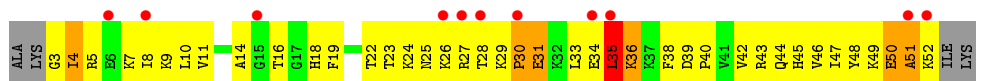


- Molecule 33: 50S ribosomal protein L33

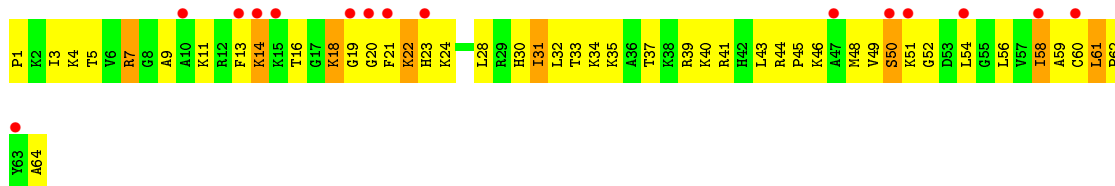




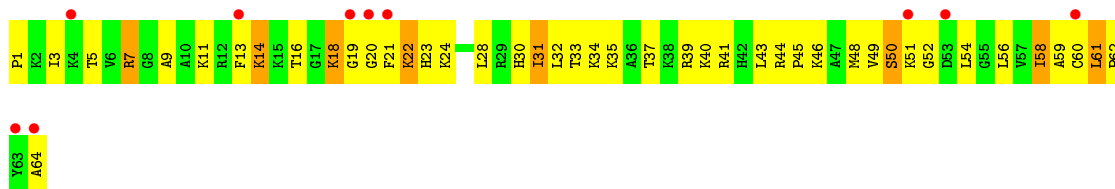
• Molecule 33: 50S ribosomal protein L33



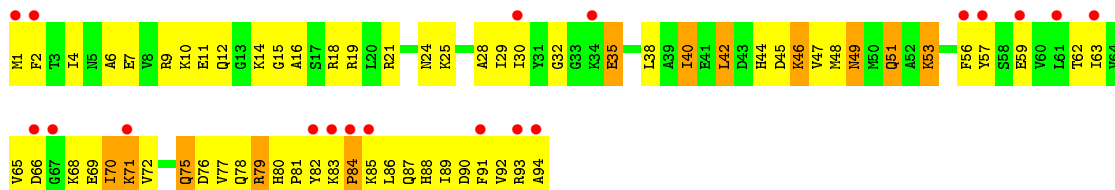
• Molecule 34: 50S ribosomal protein L35



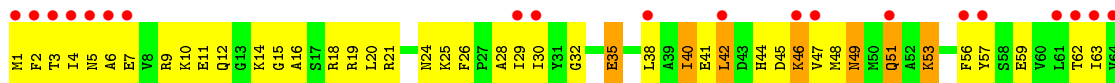
• Molecule 34: 50S ribosomal protein L35

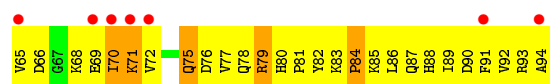


• Molecule 35: 50S ribosomal protein L25

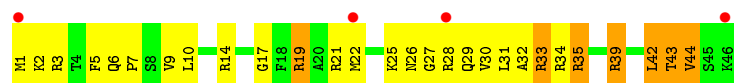


• Molecule 35: 50S ribosomal protein L25

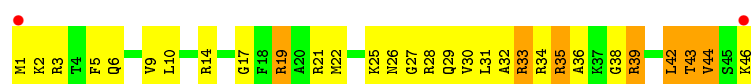




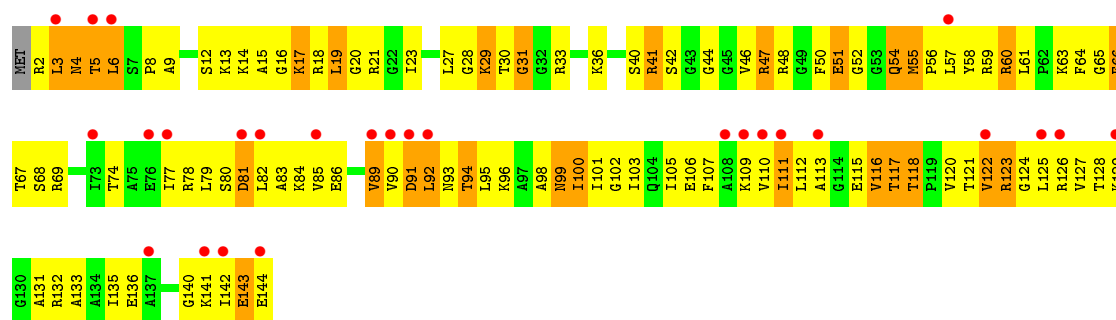
- Molecule 36: 50S ribosomal protein L34



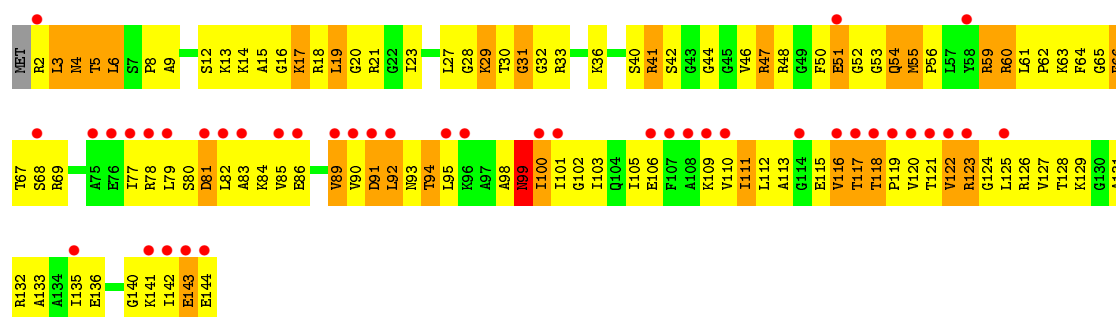
- Molecule 36: 50S ribosomal protein L34



- Molecule 37: 50S ribosomal protein L15

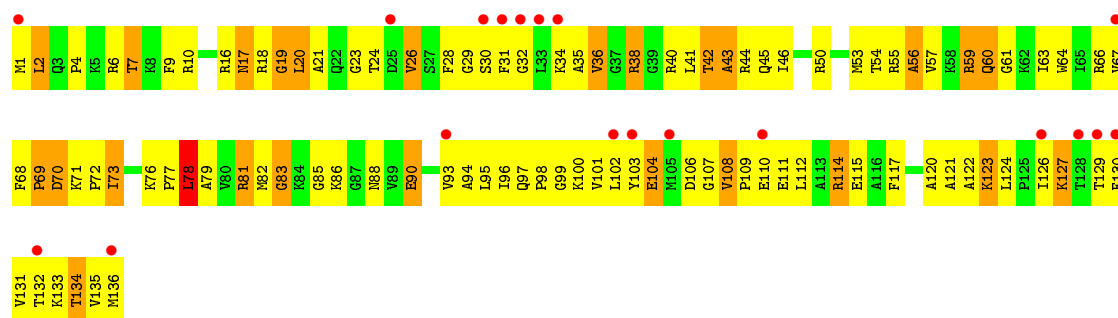


- Molecule 37: 50S ribosomal protein L15

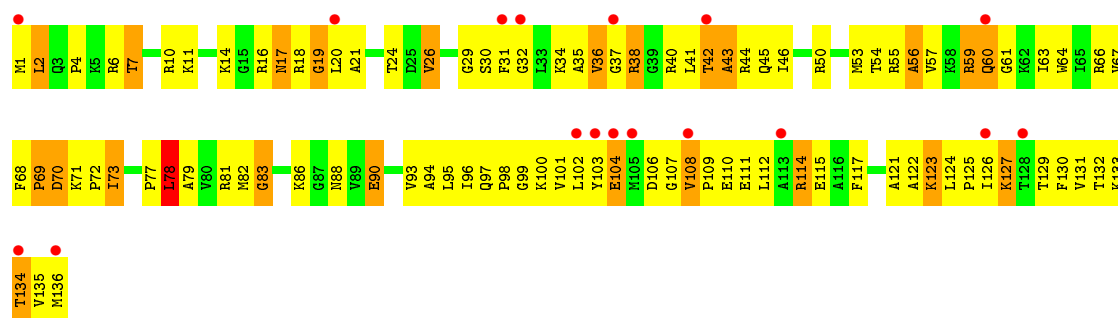


- Molecule 38: 50S ribosomal protein L16

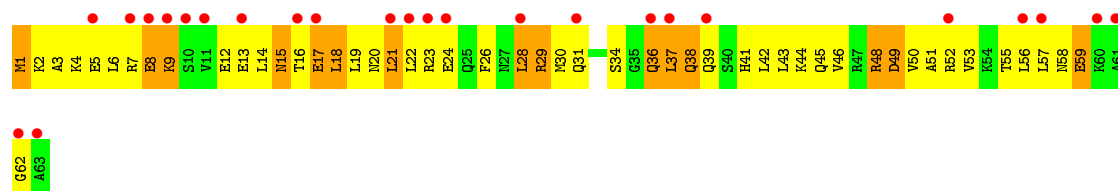




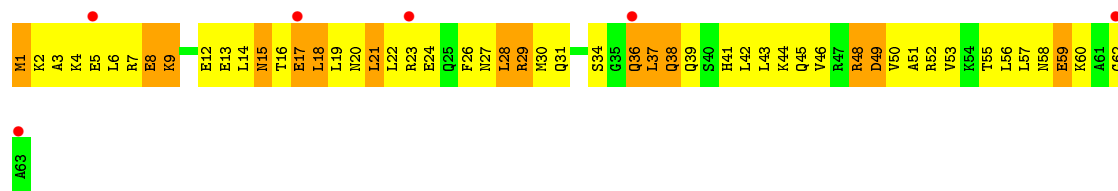
• Molecule 38: 50S ribosomal protein L16



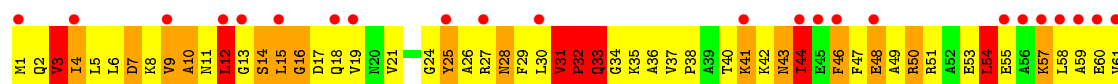
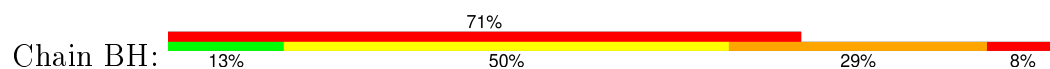
• Molecule 39: 50S ribosomal protein L29

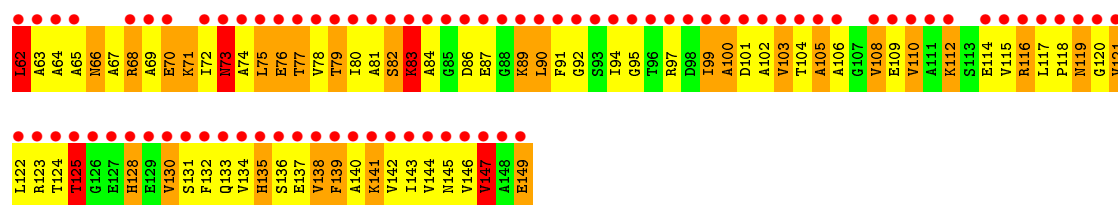


• Molecule 39: 50S ribosomal protein L29

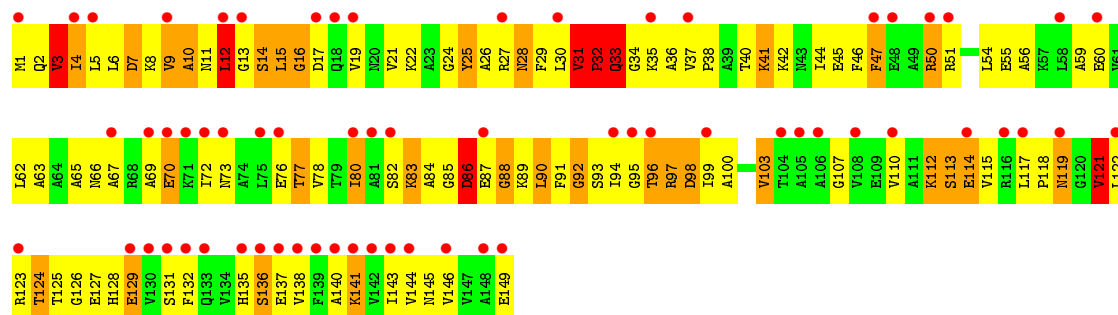


• Molecule 40: 50S ribosomal protein L9

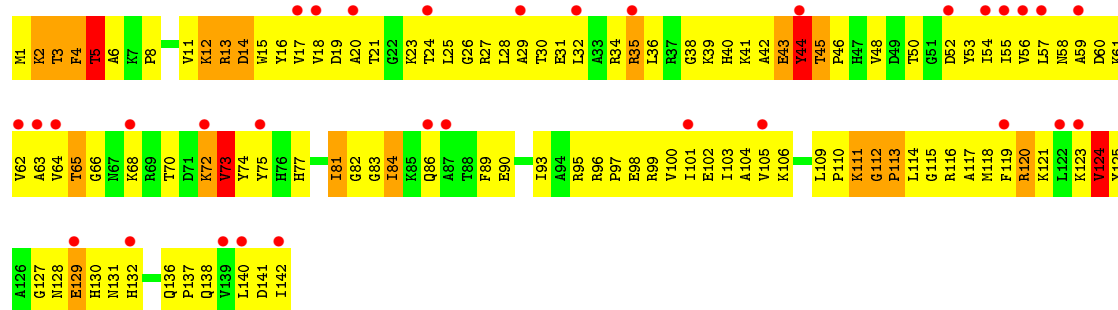




• Molecule 40: 50S ribosomal protein L9



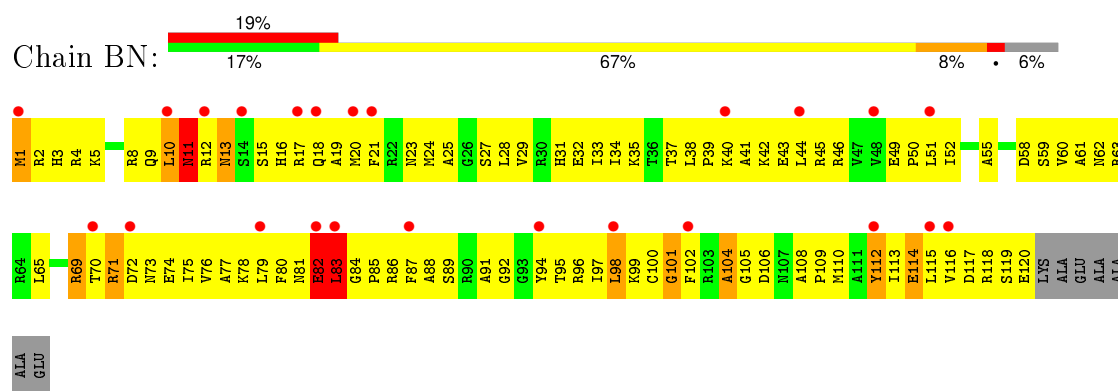
• Molecule 41: 50S ribosomal protein L13



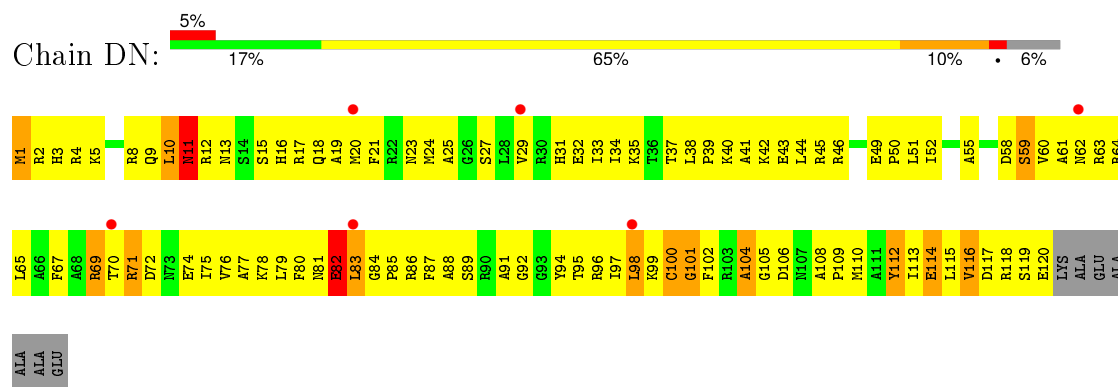
• Molecule 41: 50S ribosomal protein L13



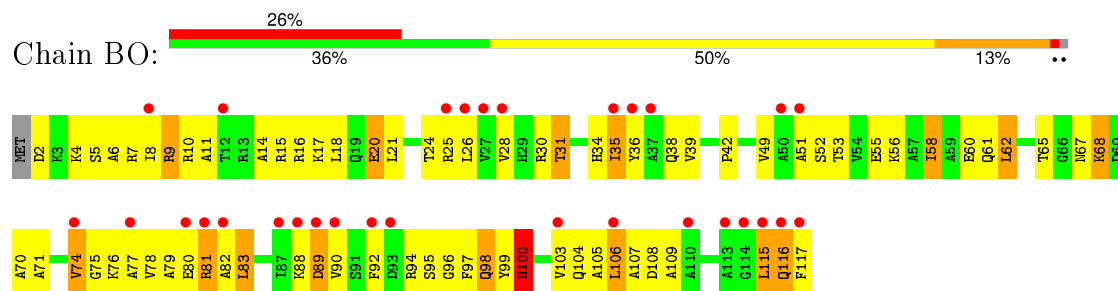
• Molecule 42: 50S ribosomal protein L17



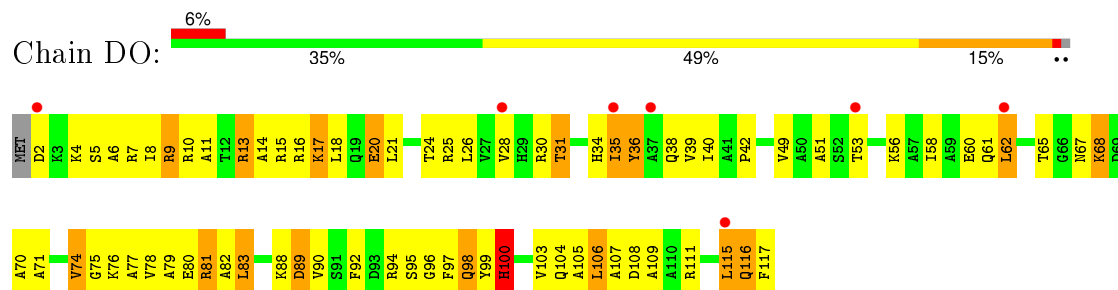
- Molecule 42: 50S ribosomal protein L17



- Molecule 43: 50S ribosomal protein L18

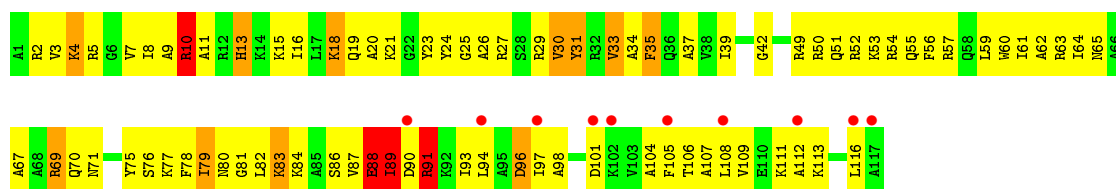


- Molecule 43: 50S ribosomal protein L18

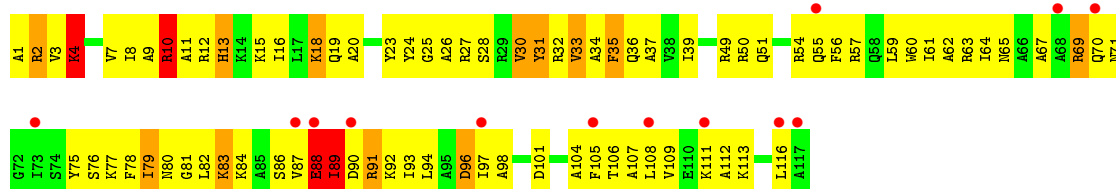
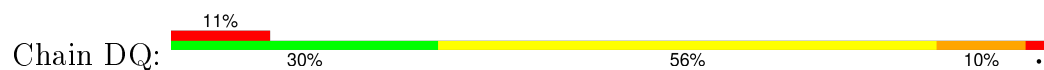


- Molecule 44: 50S ribosomal protein L20

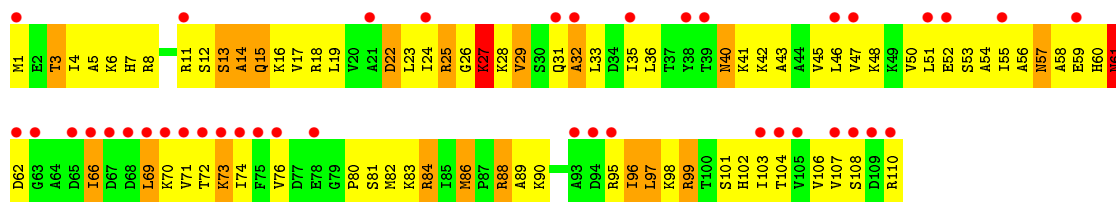




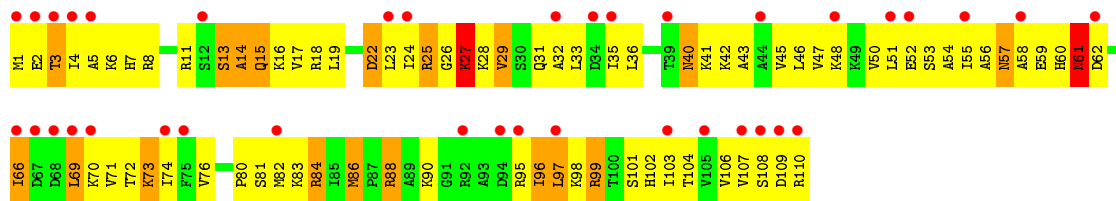
• Molecule 44: 50S ribosomal protein L20



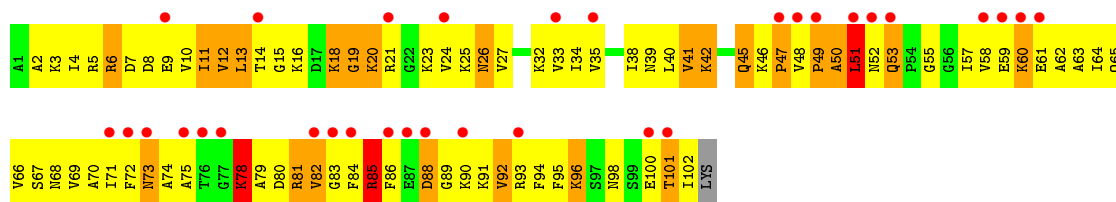
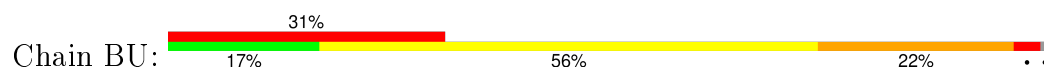
• Molecule 45: 50S ribosomal protein L22



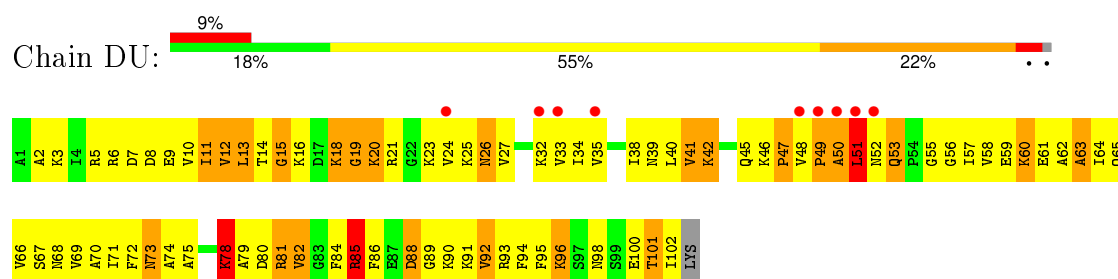
• Molecule 45: 50S ribosomal protein L22



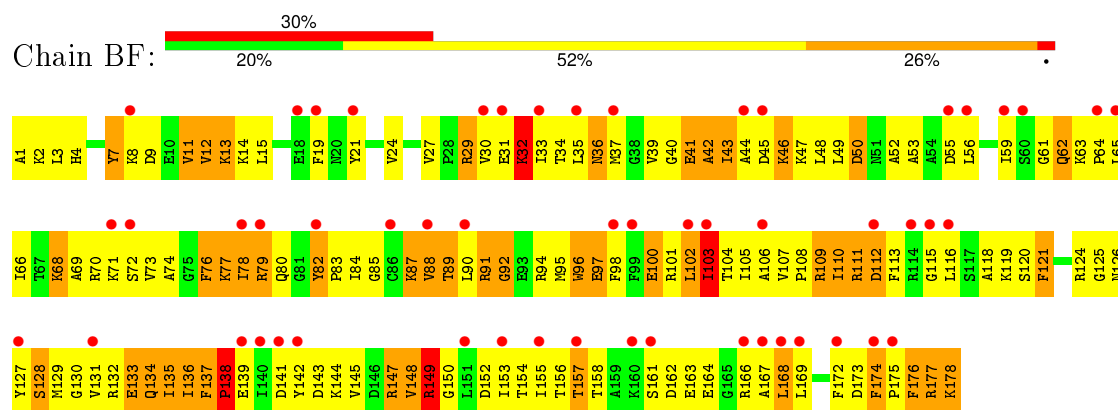
• Molecule 46: 50S ribosomal protein L24



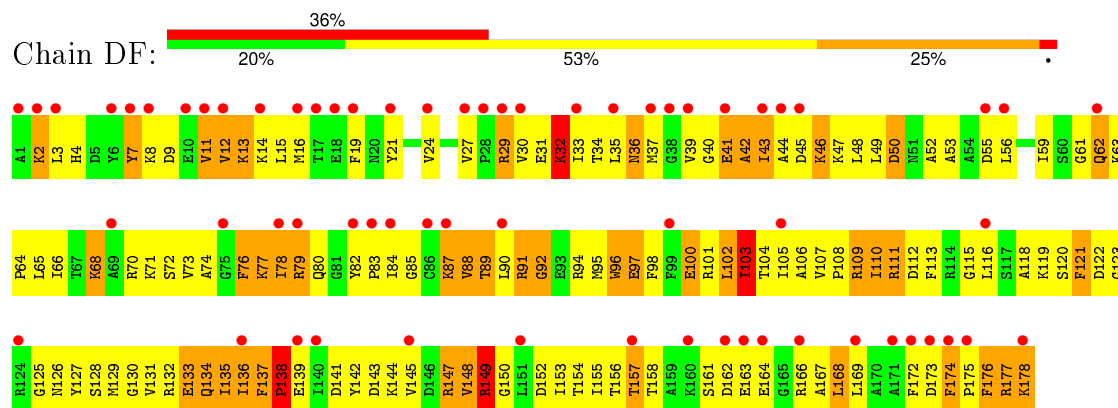
• Molecule 46: 50S ribosomal protein L24



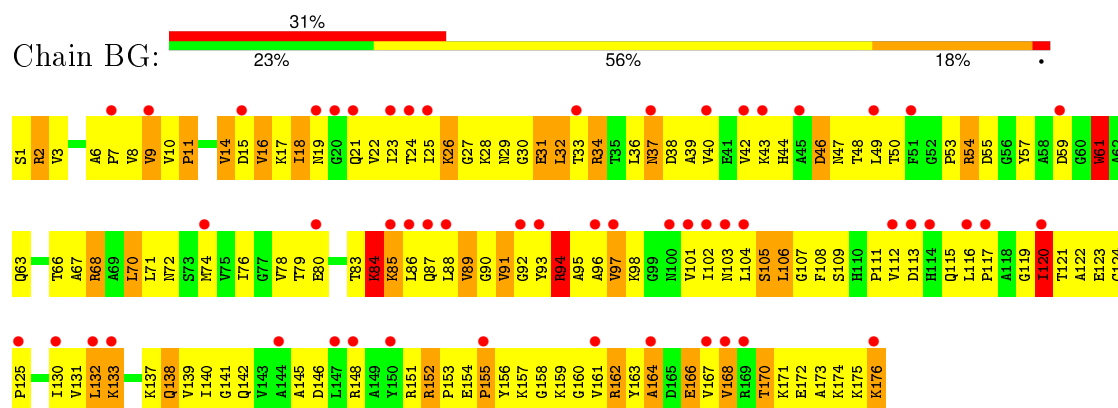
• Molecule 47: 50S ribosomal protein L5



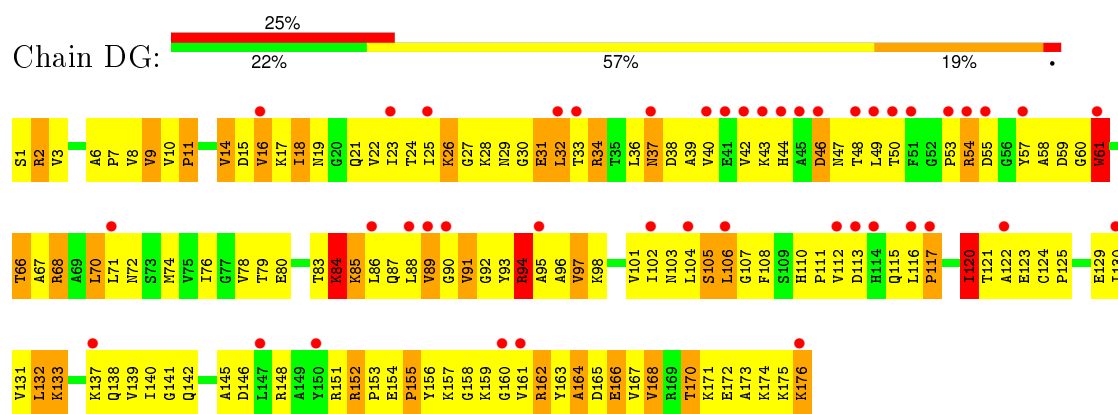
• Molecule 47: 50S ribosomal protein L5



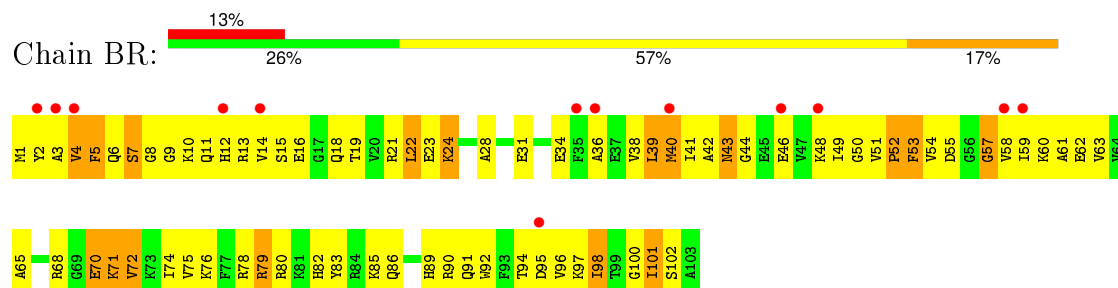
• Molecule 48: 50S ribosomal protein L6



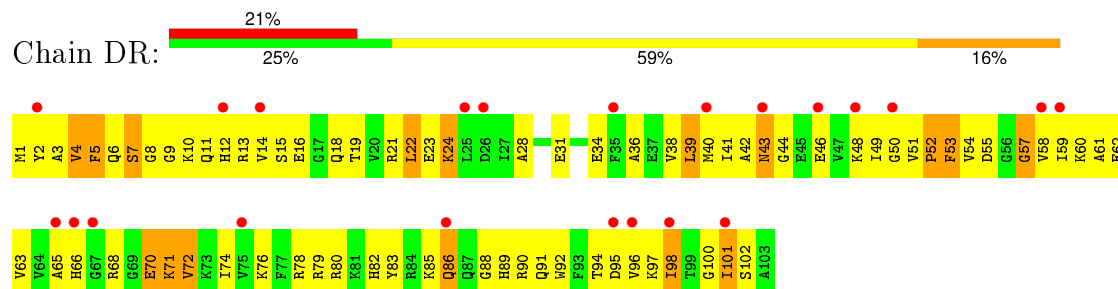
• Molecule 48: 50S ribosomal protein L6



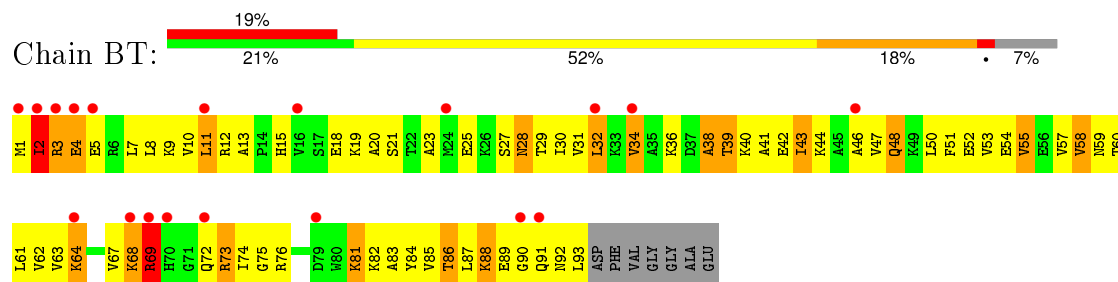
• Molecule 49: 50S ribosomal protein L21



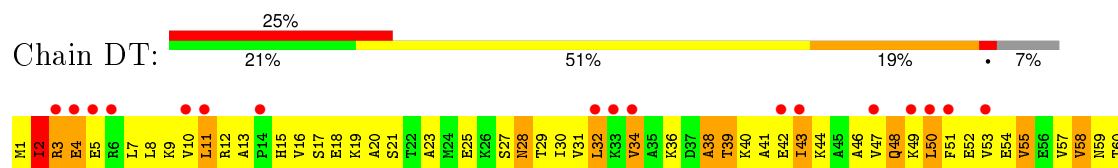
• Molecule 49: 50S ribosomal protein L21



• Molecule 50: 50S ribosomal protein L23

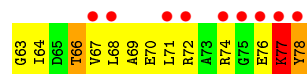
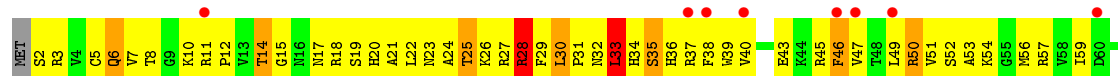


• Molecule 50: 50S ribosomal protein L23

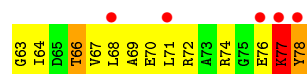
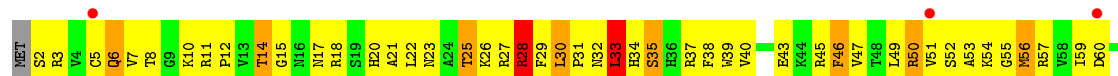




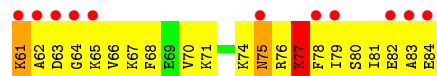
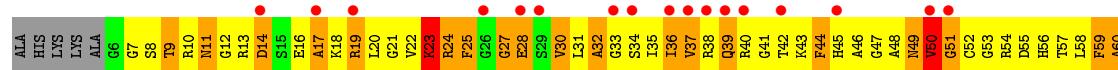
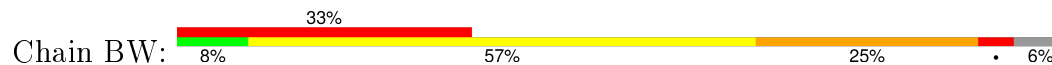
- Molecule 51: 50S ribosomal protein L28



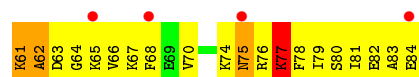
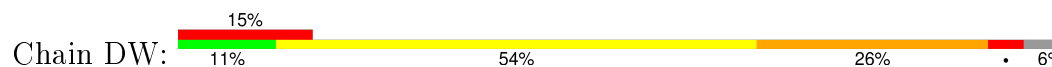
- Molecule 51: 50S ribosomal protein L28



- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.21 138.41 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.21) 66.7 (138.41-3.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.309 0.243 , 0.277	Depositor DCC
R_{free} test set	30050 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 62.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 626512 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	284172	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

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

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.25	1/36762 (0.0%)	0.75	12/57350 (0.0%)
1	CA	0.26	1/36762 (0.0%)	0.75	16/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.24	0/1118	0.46	0/1504
4	CE	0.23	0/1118	0.46	0/1504
5	AF	0.24	0/835	0.45	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.45	0/1326
7	CH	0.23	0/989	0.45	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.49	0/1077
10	AK	0.24	0/893	0.47	0/1205
10	CK	0.24	0/893	0.47	0/1205
11	AL	0.22	0/969	0.49	0/1300
11	CL	0.22	0/969	0.49	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.48	0/1043
13	CN	0.24	0/785	0.48	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.23	0/722	0.47	0/964
15	AP	0.25	0/659	0.46	0/884
15	CP	0.25	0/648	0.46	0/870
16	AQ	0.23	0/657	0.47	0/881
16	CQ	0.23	0/666	0.48	0/892

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 109 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

The worst 5 of 16001 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.38	1.21
40:DH:31:VAL:HB	40:DH:32:PRO:HD2	1.30	1.11
21:CU:36:PHE:HB3	21:CU:40:PRO:HD3	1.32	1.11
6:CG:2:ARG:HH11	6:CG:2:ARG:HB3	1.10	1.11
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.29	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	204/232 (88%)	155 (76%)	35 (17%)	14 (7%)	1	11
2	CC	204/232 (88%)	155 (76%)	36 (18%)	13 (6%)	2	13
3	AD	203/205 (99%)	154 (76%)	34 (17%)	15 (7%)	1	9
3	CD	203/205 (99%)	151 (74%)	37 (18%)	15 (7%)	1	9
4	AE	148/166 (89%)	120 (81%)	25 (17%)	3 (2%)	9	48
4	CE	148/166 (89%)	120 (81%)	24 (16%)	4 (3%)	6	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AF	98/135 (73%)	67 (68%)	26 (26%)	5 (5%)	2	20
5	CF	98/135 (73%)	65 (66%)	28 (29%)	5 (5%)	2	20
6	AG	148/178 (83%)	124 (84%)	18 (12%)	6 (4%)	3	27
6	CG	150/178 (84%)	127 (85%)	18 (12%)	5 (3%)	5	32
7	AH	127/129 (98%)	98 (77%)	25 (20%)	4 (3%)	5	34
7	CH	127/129 (98%)	97 (76%)	27 (21%)	3 (2%)	7	43
8	AI	125/129 (97%)	95 (76%)	20 (16%)	10 (8%)	1	7
8	CI	125/129 (97%)	97 (78%)	19 (15%)	9 (7%)	1	10
9	AJ	96/103 (93%)	73 (76%)	15 (16%)	8 (8%)	1	7
9	CJ	96/103 (93%)	74 (77%)	13 (14%)	9 (9%)	1	5
10	AK	115/128 (90%)	88 (76%)	22 (19%)	5 (4%)	3	25
10	CK	115/128 (90%)	85 (74%)	25 (22%)	5 (4%)	3	25
11	AL	121/123 (98%)	79 (65%)	33 (27%)	9 (7%)	1	9
11	CL	121/123 (98%)	80 (66%)	32 (26%)	9 (7%)	1	9
12	AM	112/117 (96%)	76 (68%)	27 (24%)	9 (8%)	1	7
12	CM	111/117 (95%)	77 (69%)	26 (23%)	8 (7%)	1	10
13	AN	92/100 (92%)	58 (63%)	24 (26%)	10 (11%)	0	3
13	CN	92/100 (92%)	58 (63%)	23 (25%)	11 (12%)	0	3
14	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	4	31
14	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	4	31
15	AP	80/82 (98%)	60 (75%)	14 (18%)	6 (8%)	1	9
15	CP	78/82 (95%)	58 (74%)	14 (18%)	6 (8%)	1	8
16	AQ	78/83 (94%)	58 (74%)	16 (20%)	4 (5%)	2	20
16	CQ	79/83 (95%)	59 (75%)	16 (20%)	4 (5%)	2	20
17	AR	53/74 (72%)	43 (81%)	8 (15%)	2 (4%)	4	28
17	CR	53/74 (72%)	43 (81%)	9 (17%)	1 (2%)	10	49
18	AS	77/91 (85%)	54 (70%)	17 (22%)	6 (8%)	1	8
18	CS	78/91 (86%)	54 (69%)	17 (22%)	7 (9%)	1	5
19	AT	83/86 (96%)	65 (78%)	12 (14%)	6 (7%)	1	10
19	CT	83/86 (96%)	66 (80%)	11 (13%)	6 (7%)	1	10
20	AB	216/240 (90%)	150 (69%)	44 (20%)	22 (10%)	1	4

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BM	134/136 (98%)	86 (64%)	31 (23%)	17 (13%)	0	2
38	DM	134/136 (98%)	86 (64%)	32 (24%)	16 (12%)	0	3
39	BX	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	1	7
39	DX	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	1	7
40	BH	147/149 (99%)	77 (52%)	41 (28%)	29 (20%)	0	0
40	DH	147/149 (99%)	85 (58%)	39 (26%)	23 (16%)	0	1
41	BJ	140/142 (99%)	88 (63%)	36 (26%)	16 (11%)	0	3
41	DJ	140/142 (99%)	89 (64%)	33 (24%)	18 (13%)	0	2
42	BN	118/127 (93%)	72 (61%)	34 (29%)	12 (10%)	1	4
42	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	1	4
43	BO	114/117 (97%)	84 (74%)	25 (22%)	5 (4%)	3	24
43	DO	114/117 (97%)	83 (73%)	25 (22%)	6 (5%)	2	19
44	BQ	115/117 (98%)	73 (64%)	34 (30%)	8 (7%)	1	10
44	DQ	115/117 (98%)	70 (61%)	38 (33%)	7 (6%)	2	15
45	BS	108/110 (98%)	69 (64%)	28 (26%)	11 (10%)	1	4
45	DS	108/110 (98%)	69 (64%)	29 (27%)	10 (9%)	1	5
46	BU	100/103 (97%)	53 (53%)	25 (25%)	22 (22%)	0	0
46	DU	100/103 (97%)	54 (54%)	23 (23%)	23 (23%)	0	0
47	BF	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0	1
47	DF	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0	1
48	BG	174/176 (99%)	100 (58%)	48 (28%)	26 (15%)	0	1
48	DG	174/176 (99%)	101 (58%)	48 (28%)	25 (14%)	0	1
49	BR	101/103 (98%)	65 (64%)	25 (25%)	11 (11%)	0	3
49	DR	101/103 (98%)	64 (63%)	28 (28%)	9 (9%)	1	5
50	BT	91/100 (91%)	50 (55%)	31 (34%)	10 (11%)	0	3
50	DT	91/100 (91%)	51 (56%)	30 (33%)	10 (11%)	0	3
51	BZ	75/78 (96%)	53 (71%)	18 (24%)	4 (5%)	2	19
51	DZ	75/78 (96%)	50 (67%)	21 (28%)	4 (5%)	2	19
52	BW	77/84 (92%)	29 (38%)	27 (35%)	21 (27%)	0	0
52	DW	77/84 (92%)	29 (38%)	26 (34%)	22 (29%)	0	0
All	All	11241/11914 (94%)	7579 (67%)	2528 (22%)	1134 (10%)	1	4

5 of 1134 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	137 (81%)	33 (19%)	2	9
2	CC	170/189 (90%)	137 (81%)	33 (19%)	2	9
3	AD	172/172 (100%)	148 (86%)	24 (14%)	4	20
3	CD	172/172 (100%)	148 (86%)	24 (14%)	4	20
4	AE	113/125 (90%)	95 (84%)	18 (16%)	3	15
4	CE	113/125 (90%)	95 (84%)	18 (16%)	3	15
5	AF	87/116 (75%)	71 (82%)	16 (18%)	2	11
5	CF	87/116 (75%)	70 (80%)	17 (20%)	2	9
6	AG	123/146 (84%)	104 (85%)	19 (15%)	3	16
6	CG	125/146 (86%)	103 (82%)	22 (18%)	2	12
7	AH	104/104 (100%)	95 (91%)	9 (9%)	13	45
7	CH	104/104 (100%)	94 (90%)	10 (10%)	10	39
8	AI	105/106 (99%)	88 (84%)	17 (16%)	3	14
8	CI	105/106 (99%)	87 (83%)	18 (17%)	2	13
9	AJ	86/90 (96%)	71 (83%)	15 (17%)	2	12
9	CJ	86/90 (96%)	71 (83%)	15 (17%)	2	12
10	AK	90/98 (92%)	76 (84%)	14 (16%)	3	15
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2	11
11	AL	103/103 (100%)	88 (85%)	15 (15%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	CL	103/103 (100%)	88 (85%)	15 (15%)	4	18
12	AM	92/95 (97%)	76 (83%)	16 (17%)	2	12
12	CM	91/95 (96%)	75 (82%)	16 (18%)	2	12
13	AN	79/83 (95%)	65 (82%)	14 (18%)	2	12
13	CN	79/83 (95%)	65 (82%)	14 (18%)	2	12
14	AO	76/77 (99%)	70 (92%)	6 (8%)	15	52
14	CO	76/77 (99%)	70 (92%)	6 (8%)	15	52
15	AP	65/65 (100%)	58 (89%)	7 (11%)	8	34
15	CP	65/65 (100%)	59 (91%)	6 (9%)	11	41
16	AQ	74/77 (96%)	65 (88%)	9 (12%)	6	27
16	CQ	75/77 (97%)	66 (88%)	9 (12%)	6	28
17	AR	48/64 (75%)	40 (83%)	8 (17%)	3	13
17	CR	48/64 (75%)	41 (85%)	7 (15%)	4	18
18	AS	70/78 (90%)	56 (80%)	14 (20%)	1	8
18	CS	71/78 (91%)	57 (80%)	14 (20%)	1	8
19	AT	65/65 (100%)	54 (83%)	11 (17%)	2	13
19	CT	65/65 (100%)	54 (83%)	11 (17%)	2	13
20	AB	180/198 (91%)	148 (82%)	32 (18%)	2	11
20	CB	180/198 (91%)	150 (83%)	30 (17%)	3	13
21	AU	44/60 (73%)	30 (68%)	14 (32%)	0	0
21	CU	44/60 (73%)	30 (68%)	14 (32%)	0	0
24	BI	109/109 (100%)	107 (98%)	2 (2%)	66	89
24	DI	109/109 (100%)	104 (95%)	5 (5%)	33	73
25	BC	216/217 (100%)	176 (82%)	40 (18%)	2	10
25	DC	216/217 (100%)	176 (82%)	40 (18%)	2	10
26	BD	164/164 (100%)	142 (87%)	22 (13%)	5	23
26	DD	164/164 (100%)	141 (86%)	23 (14%)	4	20
27	BK	102/104 (98%)	79 (78%)	23 (22%)	1	5
27	DK	102/104 (98%)	79 (78%)	23 (22%)	1	5
28	BP	99/99 (100%)	81 (82%)	18 (18%)	2	11
28	DP	99/99 (100%)	81 (82%)	18 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BE	165/165 (100%)	136 (82%)	29 (18%)	2	12
29	DE	165/165 (100%)	137 (83%)	28 (17%)	2	13
30	BY	48/48 (100%)	38 (79%)	10 (21%)	1	7
30	DY	48/48 (100%)	38 (79%)	10 (21%)	1	7
31	B0	47/47 (100%)	36 (77%)	11 (23%)	1	4
31	D0	47/47 (100%)	35 (74%)	12 (26%)	1	2
32	B4	34/34 (100%)	28 (82%)	6 (18%)	2	12
32	D4	34/34 (100%)	28 (82%)	6 (18%)	2	12
33	B1	45/48 (94%)	40 (89%)	5 (11%)	8	32
33	D1	45/48 (94%)	41 (91%)	4 (9%)	12	44
34	B3	51/51 (100%)	47 (92%)	4 (8%)	16	53
34	D3	51/51 (100%)	47 (92%)	4 (8%)	16	53
35	BV	78/78 (100%)	62 (80%)	16 (20%)	1	7
35	DV	78/78 (100%)	62 (80%)	16 (20%)	1	7
36	B2	38/38 (100%)	32 (84%)	6 (16%)	3	15
36	D2	38/38 (100%)	32 (84%)	6 (16%)	3	15
37	BL	102/103 (99%)	89 (87%)	13 (13%)	5	25
37	DL	102/103 (99%)	88 (86%)	14 (14%)	4	21
38	BM	109/109 (100%)	91 (84%)	18 (16%)	3	13
38	DM	109/109 (100%)	91 (84%)	18 (16%)	3	13
39	BX	55/55 (100%)	40 (73%)	15 (27%)	0	2
39	DX	55/55 (100%)	40 (73%)	15 (27%)	0	2
40	BH	114/114 (100%)	64 (56%)	50 (44%)	0	0
40	DH	114/114 (100%)	86 (75%)	28 (25%)	1	3
41	BJ	116/116 (100%)	101 (87%)	15 (13%)	5	24
41	DJ	116/116 (100%)	100 (86%)	16 (14%)	4	21
42	BN	100/103 (97%)	87 (87%)	13 (13%)	5	24
42	DN	100/103 (97%)	87 (87%)	13 (13%)	5	24
43	BO	86/87 (99%)	70 (81%)	16 (19%)	2	10
43	DO	86/87 (99%)	70 (81%)	16 (19%)	2	10
44	BQ	89/89 (100%)	74 (83%)	15 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	13
45	BS	93/93 (100%)	79 (85%)	14 (15%)	3	17
45	DS	93/93 (100%)	79 (85%)	14 (15%)	3	17
46	BU	83/84 (99%)	68 (82%)	15 (18%)	2	11
46	DU	83/84 (99%)	68 (82%)	15 (18%)	2	11
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1	4
47	DF	149/149 (100%)	115 (77%)	34 (23%)	1	5
48	BG	137/137 (100%)	113 (82%)	24 (18%)	2	12
48	DG	137/137 (100%)	113 (82%)	24 (18%)	2	12
49	BR	84/84 (100%)	73 (87%)	11 (13%)	5	24
49	DR	84/84 (100%)	73 (87%)	11 (13%)	5	24
50	BT	80/84 (95%)	66 (82%)	14 (18%)	2	12
50	DT	80/84 (95%)	65 (81%)	15 (19%)	2	10
51	BZ	67/68 (98%)	52 (78%)	15 (22%)	1	5
51	DZ	67/68 (98%)	52 (78%)	15 (22%)	1	5
52	BW	59/62 (95%)	45 (76%)	14 (24%)	1	4
52	DW	59/62 (95%)	45 (76%)	14 (24%)	1	4
All	All	9333/9700 (96%)	7746 (83%)	1587 (17%)	2	13

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

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

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

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

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Mol	Chain	Res	Type
52	BW	75	ASN

5.3.3 RNA ⓘ

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

5 of 1370 RNA backbone outliers are listed below:

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

5 of 73 RNA pucker outliers are listed below:

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

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
53	NMY	AA	1601	-	45,45,45	1.86	12 (26%)	58,67,67	1.20	6 (10%)
53	NMY	BB	3001	-	45,45,45	1.86	13 (28%)	58,67,67	1.15	6 (10%)
53	NMY	CA	1601	-	45,45,45	1.85	11 (24%)	58,67,67	1.28	7 (12%)
53	NMY	DB	3001	-	45,45,45	1.92	14 (31%)	58,67,67	1.18	6 (10%)

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

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

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	DB	3001	NMY	C6-C5	2.00	1.57	1.52
53	BB	3001	NMY	C14-C15	2.02	1.57	1.53
53	DB	3001	NMY	C18-C19	2.02	1.56	1.52
53	DB	3001	NMY	O18-C15	2.02	1.49	1.43
53	BB	3001	NMY	C6-C5	2.06	1.57	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	AA	1601	NMY	O11-C13-C14	2.01	111.93	107.75
53	CA	1601	NMY	O14-C14-C15	2.18	117.46	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
53	AA	1601	NMY	O14-C14-C15	2.21	117.53	111.16
53	CA	1601	NMY	O11-C13-C14	2.24	112.41	107.75
53	BB	3001	NMY	O11-C13-C14	2.29	112.50	107.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.61	12 (0%) 87 80	22, 76, 152, 180	0
1	CA	1530/1542 (99%)	-0.62	3 (0%) 95 94	12, 57, 136, 180	0
2	AC	206/232 (88%)	0.80	36 (17%) 2 1	16, 66, 135, 180	0
2	CC	206/232 (88%)	0.77	28 (13%) 4 3	14, 74, 124, 180	0
3	AD	205/205 (100%)	1.34	53 (25%) 1 1	8, 84, 155, 180	0
3	CD	205/205 (100%)	0.89	34 (16%) 2 2	15, 62, 135, 180	0
4	AE	150/166 (90%)	0.75	15 (10%) 9 6	7, 67, 122, 158	0
4	CE	150/166 (90%)	1.15	34 (22%) 1 1	10, 59, 122, 180	0
5	AF	100/135 (74%)	1.54	32 (32%) 1 1	32, 80, 148, 180	0
5	CF	100/135 (74%)	1.02	16 (16%) 3 2	23, 69, 138, 180	0
6	AG	150/178 (84%)	0.74	27 (18%) 2 1	39, 105, 151, 180	0
6	CG	152/178 (85%)	0.25	10 (6%) 22 13	32, 89, 152, 180	0
7	AH	129/129 (100%)	1.35	43 (33%) 0 1	29, 79, 133, 180	0
7	CH	129/129 (100%)	0.65	18 (13%) 4 3	7, 55, 120, 148	0
8	AI	127/129 (98%)	0.84	26 (20%) 1 1	37, 90, 164, 180	0
8	CI	127/129 (98%)	0.63	17 (13%) 4 3	32, 95, 162, 180	0
9	AJ	98/103 (95%)	1.01	19 (19%) 1 1	17, 85, 158, 180	0
9	CJ	98/103 (95%)	1.10	22 (22%) 1 1	22, 89, 150, 180	0
10	AK	117/128 (91%)	0.51	7 (5%) 25 15	17, 63, 128, 162	0
10	CK	117/128 (91%)	0.17	2 (1%) 73 62	10, 51, 116, 164	0
11	AL	123/123 (100%)	0.89	19 (15%) 3 2	19, 74, 135, 180	0
11	CL	123/123 (100%)	0.62	7 (5%) 27 17	6, 50, 127, 180	0
12	AM	114/117 (97%)	0.68	17 (14%) 3 2	52, 119, 180, 180	0
12	CM	113/117 (96%)	0.74	17 (15%) 3 2	53, 105, 167, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.60	9 (9%) 11 7	24, 79, 118, 152	0
13	CN	96/100 (96%)	0.64	14 (14%) 3 3	26, 82, 119, 139	0
14	AO	88/89 (98%)	1.25	23 (26%) 1 1	39, 76, 123, 180	0
14	CO	88/89 (98%)	0.38	3 (3%) 49 35	15, 55, 123, 154	0
15	AP	82/82 (100%)	1.53	19 (23%) 1 1	30, 87, 150, 180	0
15	CP	80/82 (97%)	0.61	10 (12%) 5 3	8, 56, 135, 180	0
16	AQ	80/83 (96%)	1.25	24 (30%) 1 1	49, 96, 155, 180	0
16	CQ	81/83 (97%)	0.60	8 (9%) 9 6	25, 66, 128, 180	0
17	AR	55/74 (74%)	1.03	10 (18%) 2 1	15, 74, 125, 165	0
17	CR	55/74 (74%)	0.70	7 (12%) 5 3	19, 63, 119, 170	0
18	AS	79/91 (86%)	1.00	20 (25%) 1 1	73, 121, 176, 180	0
18	CS	80/91 (87%)	1.02	16 (20%) 1 1	58, 109, 168, 180	0
19	AT	85/86 (98%)	0.48	9 (10%) 8 5	52, 104, 164, 180	0
19	CT	85/86 (98%)	0.07	5 (5%) 26 15	22, 62, 125, 179	0
20	AB	218/240 (90%)	0.94	49 (22%) 1 1	29, 99, 155, 180	0
20	CB	218/240 (90%)	1.33	69 (31%) 1 1	31, 102, 160, 180	0
21	AU	51/70 (72%)	1.08	11 (21%) 1 1	43, 92, 146, 180	0
21	CU	51/70 (72%)	0.76	7 (13%) 4 3	40, 85, 133, 166	0
22	BA	117/120 (97%)	-0.68	1 (0%) 85 79	49, 83, 138, 174	0
22	DA	117/120 (97%)	-0.57	1 (0%) 85 79	36, 75, 124, 180	0
23	BB	2841/2904 (97%)	-0.37	28 (0%) 84 77	16, 60, 154, 180	0
23	DB	2841/2904 (97%)	-0.40	11 (0%) 93 90	6, 47, 151, 180	0
24	BI	141/141 (100%)	3.73	98 (69%) 0 0	93, 176, 180, 180	0
24	DI	141/141 (100%)	2.02	62 (43%) 0 0	101, 177, 180, 180	0
25	BC	271/272 (99%)	0.96	44 (16%) 3 2	9, 50, 104, 180	0
25	DC	271/272 (99%)	0.88	42 (15%) 3 2	5, 35, 87, 135	0
26	BD	209/209 (100%)	0.95	39 (18%) 2 1	20, 76, 135, 180	0
26	DD	209/209 (100%)	1.05	38 (18%) 2 1	5, 50, 126, 180	0
27	BK	121/123 (98%)	1.97	51 (42%) 0 0	14, 72, 133, 180	0
27	DK	121/123 (98%)	1.30	28 (23%) 1 1	6, 43, 104, 164	0
28	BP	114/114 (100%)	2.01	54 (47%) 0 0	35, 86, 151, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.72	12 (10%) 8 5	6, 49, 113, 160	0
29	BE	201/201 (100%)	1.48	67 (33%) 0 1	10, 67, 144, 180	0
29	DE	201/201 (100%)	1.03	40 (19%) 1 1	5, 72, 137, 180	0
30	BY	58/58 (100%)	0.87	11 (18%) 2 1	34, 74, 139, 180	0
30	DY	58/58 (100%)	0.64	9 (15%) 3 2	21, 60, 141, 177	0
31	B0	56/56 (100%)	0.88	8 (14%) 4 3	15, 74, 151, 180	0
31	D0	56/56 (100%)	0.53	5 (8%) 12 7	9, 49, 124, 180	0
32	B4	38/38 (100%)	0.82	6 (15%) 3 2	35, 91, 145, 151	0
32	D4	38/38 (100%)	-0.11	0 100 100	18, 68, 129, 150	0
33	B1	50/54 (92%)	2.16	23 (46%) 0 0	52, 90, 134, 174	0
33	D1	50/54 (92%)	1.22	11 (22%) 1 1	14, 76, 127, 175	0
34	B3	64/64 (100%)	1.07	15 (23%) 1 1	26, 59, 87, 158	0
34	D3	64/64 (100%)	0.83	10 (15%) 3 2	9, 49, 112, 156	0
35	BV	94/94 (100%)	0.95	19 (20%) 1 1	29, 97, 155, 178	0
35	DV	94/94 (100%)	1.07	27 (28%) 1 1	21, 89, 153, 167	0
36	B2	46/46 (100%)	0.59	4 (8%) 13 8	14, 50, 83, 144	0
36	D2	46/46 (100%)	0.52	2 (4%) 39 26	5, 38, 76, 180	0
37	BL	143/144 (99%)	0.91	27 (18%) 2 1	25, 70, 133, 180	0
37	DL	143/144 (99%)	1.26	42 (29%) 1 1	9, 59, 117, 147	0
38	BM	136/136 (100%)	1.05	19 (13%) 4 3	21, 68, 136, 180	0
38	DM	136/136 (100%)	0.69	17 (12%) 5 3	13, 54, 118, 167	0
39	BX	63/63 (100%)	1.65	25 (39%) 0 0	21, 81, 149, 175	0
39	DX	63/63 (100%)	0.56	6 (9%) 10 7	38, 97, 156, 180	0
40	BH	149/149 (100%)	4.26	106 (71%) 0 0	31, 134, 180, 180	0
40	DH	149/149 (100%)	1.96	64 (42%) 0 0	32, 110, 160, 180	0
41	BJ	142/142 (100%)	1.10	32 (22%) 1 1	23, 82, 140, 169	0
41	DJ	142/142 (100%)	0.79	16 (11%) 7 5	17, 61, 126, 180	0
42	BN	120/127 (94%)	0.95	24 (20%) 1 1	24, 71, 139, 180	0
42	DN	120/127 (94%)	0.36	6 (5%) 32 21	7, 43, 91, 172	0
43	BO	116/117 (99%)	1.05	30 (25%) 1 1	35, 83, 145, 180	0
43	DO	116/117 (99%)	0.54	7 (6%) 25 15	19, 73, 135, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.31	10 (8%) 13 8	10, 66, 129, 167	0
44	DQ	117/117 (100%)	0.80	13 (11%) 7 5	8, 50, 104, 180	0
45	BS	110/110 (100%)	1.64	40 (36%) 0 1	6, 62, 123, 152	0
45	DS	110/110 (100%)	1.61	37 (33%) 0 1	12, 48, 129, 180	0
46	BU	102/103 (99%)	1.63	32 (31%) 1 1	21, 77, 140, 180	0
46	DU	102/103 (99%)	0.32	9 (8%) 12 8	22, 94, 154, 180	0
47	BF	178/178 (100%)	1.38	53 (29%) 1 1	56, 128, 177, 180	0
47	DF	178/178 (100%)	1.88	64 (35%) 0 1	30, 107, 168, 180	0
48	BG	176/176 (100%)	1.41	54 (30%) 1 1	49, 112, 163, 180	0
48	DG	176/176 (100%)	1.24	44 (25%) 1 1	35, 97, 161, 180	0
49	BR	103/103 (100%)	0.63	13 (12%) 5 3	25, 87, 151, 176	0
49	DR	103/103 (100%)	1.14	22 (21%) 1 1	23, 76, 139, 161	0
50	BT	93/100 (93%)	1.11	19 (20%) 1 1	22, 77, 159, 180	0
50	DT	93/100 (93%)	1.11	25 (26%) 1 1	24, 64, 156, 179	0
51	BZ	77/78 (98%)	0.98	17 (22%) 1 1	12, 51, 112, 143	0
51	DZ	77/78 (98%)	0.60	8 (10%) 8 5	9, 48, 94, 128	0
52	BW	79/84 (94%)	1.63	28 (35%) 0 1	18, 85, 141, 159	0
52	DW	79/84 (94%)	0.91	13 (16%) 2 2	20, 71, 134, 180	0
All	All	20417/21046 (97%)	0.40	2515 (12%) 5 4	5, 69, 156, 180	0

The worst 5 of 2515 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
40	BH	84	ALA	20.3
40	BH	85	GLY	18.6
40	BH	142	VAL	14.4
40	BH	130	VAL	14.4
15	AP	81	ALA	13.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
53	NMY	DB	3001	42/42	0.68	0.53	15.96	88,88,88,88	42
54	MG	AA	1658	1/1	0.89	0.33	13.51	115,115,115,115	0
54	MG	BB	3082	1/1	0.85	0.33	10.04	59,59,59,59	0
53	NMY	BB	3001	42/42	0.59	0.49	7.85	100,100,100,100	42
54	MG	AA	1620	1/1	0.79	0.18	7.22	130,130,130,130	0
54	MG	CA	1638	1/1	0.88	0.17	4.33	142,142,142,142	0
53	NMY	CA	1601	42/42	0.89	0.25	3.82	71,71,71,71	0
54	MG	BB	3088	1/1	0.96	0.21	3.12	57,57,57,57	0
54	MG	DB	3060	1/1	0.80	0.24	3.07	124,124,124,124	0
54	MG	DB	3031	1/1	0.81	0.24	3.03	32,32,32,32	0
54	MG	DB	3097	1/1	0.81	0.21	2.61	33,33,33,33	0
53	NMY	AA	1601	42/42	0.88	0.29	1.82	71,71,71,71	0
54	MG	BB	3087	1/1	0.96	0.23	1.75	41,41,41,41	0
54	MG	AA	1636	1/1	0.70	0.12	1.37	88,88,88,88	0
54	MG	DB	3052	1/1	0.97	0.20	1.07	32,32,32,32	0
54	MG	CA	1633	1/1	0.96	0.16	0.67	73,73,73,73	0
54	MG	CA	1645	1/1	0.97	0.16	0.65	45,45,45,45	0
54	MG	CA	1632	1/1	0.95	0.15	0.56	47,47,47,47	0
54	MG	DB	3090	1/1	0.97	0.17	0.36	34,34,34,34	0
54	MG	BB	3041	1/1	0.95	0.15	-0.34	28,28,28,28	0
54	MG	CA	1653	1/1	0.94	0.10	-0.46	33,33,33,33	0
54	MG	DB	3111	1/1	0.95	0.14	-0.52	28,28,28,28	0
54	MG	BB	3099	1/1	0.95	0.16	-0.62	41,41,41,41	0
54	MG	AA	1637	1/1	0.87	0.10	-0.66	89,89,89,89	0
55	ZN	D4	101	1/1	0.95	0.13	-0.84	57,57,57,57	0
54	MG	DB	3070	1/1	0.96	0.18	-0.86	23,23,23,23	0
54	MG	BB	3012	1/1	0.97	0.17	-0.89	25,25,25,25	0
54	MG	DB	3091	1/1	0.92	0.07	-0.97	47,47,47,47	0
54	MG	DB	3085	1/1	0.96	0.17	-1.04	25,25,25,25	0
54	MG	DB	3100	1/1	0.94	0.15	-1.05	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1654	1/1	0.91	0.13	-1.05	51,51,51,51	0
54	MG	DB	3048	1/1	0.96	0.17	-1.10	23,23,23,23	0
54	MG	CN	201	1/1	0.93	0.07	-1.24	48,48,48,48	0
54	MG	CA	1636	1/1	0.87	0.08	-1.28	56,56,56,56	0
54	MG	AA	1621	1/1	0.86	0.07	-1.32	85,85,85,85	0
54	MG	CA	1639	1/1	0.96	0.08	-1.42	14,14,14,14	0
54	MG	DB	3015	1/1	0.95	0.07	-1.45	22,22,22,22	0
54	MG	DB	3075	1/1	0.99	0.12	-1.45	7,7,7,7	0
54	MG	AA	1631	1/1	0.95	0.10	-1.46	107,107,107,107	0
54	MG	DB	3080	1/1	0.98	0.16	-1.53	39,39,39,39	0
54	MG	CA	1613	1/1	0.97	0.09	-1.53	77,77,77,77	0
54	MG	CA	1615	1/1	0.83	0.07	-1.60	41,41,41,41	0
54	MG	AA	1645	1/1	0.98	0.10	-1.63	60,60,60,60	0
54	MG	BB	3109	1/1	0.96	0.13	-1.66	32,32,32,32	0
54	MG	CA	1640	1/1	0.98	0.12	-1.68	57,57,57,57	0
54	MG	BB	3086	1/1	0.97	0.14	-1.75	66,66,66,66	0
55	ZN	B4	101	1/1	0.95	0.06	-1.81	72,72,72,72	0
54	MG	BB	3095	1/1	0.81	0.15	-1.85	46,46,46,46	0
54	MG	BB	3005	1/1	0.94	0.04	-1.93	39,39,39,39	0
54	MG	AA	1608	1/1	0.98	0.06	-1.94	54,54,54,54	0
54	MG	BB	3022	1/1	0.97	0.10	-2.01	22,22,22,22	0
54	MG	AA	1639	1/1	0.96	0.09	-2.04	57,57,57,57	0
54	MG	AA	1604	1/1	0.98	0.15	-2.06	36,36,36,36	0
54	MG	BB	3006	1/1	0.99	0.14	-2.07	5,5,5,5	0
54	MG	BB	3013	1/1	0.95	0.12	-2.09	41,41,41,41	0
54	MG	BB	3038	1/1	0.93	0.08	-2.10	50,50,50,50	0
54	MG	BB	3063	1/1	0.94	0.14	-2.14	31,31,31,31	0
54	MG	AA	1614	1/1	0.96	0.03	-2.20	64,64,64,64	0
54	MG	DB	3004	1/1	0.98	0.09	-2.28	14,14,14,14	0
54	MG	BB	3030	1/1	0.94	0.09	-2.29	36,36,36,36	0
54	MG	DB	3089	1/1	0.98	0.14	-2.44	10,10,10,10	0
54	MG	AA	1611	1/1	0.98	0.04	-2.58	28,28,28,28	0
54	MG	DB	3008	1/1	0.96	0.11	-2.80	16,16,16,16	0
54	MG	AA	1652	1/1	0.93	0.06	-2.81	73,73,73,73	0
54	MG	BB	3089	1/1	0.92	0.07	-2.82	45,45,45,45	0
54	MG	CA	1606	1/1	0.99	0.09	-2.90	19,19,19,19	0
54	MG	CA	1643	1/1	0.88	0.10	-2.95	43,43,43,43	0
54	MG	BB	3074	1/1	0.95	0.10	-3.00	31,31,31,31	0
54	MG	BB	3024	1/1	0.99	0.13	-3.09	7,7,7,7	0
54	MG	AA	1630	1/1	0.92	0.07	-3.12	35,35,35,35	0
54	MG	CA	1624	1/1	0.96	0.03	-3.14	34,34,34,34	0
54	MG	BB	3084	1/1	0.96	0.10	-3.28	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3028	1/1	0.98	0.10	-3.40	8,8,8,8	0
54	MG	DB	3086	1/1	0.92	0.11	-3.43	18,18,18,18	0
54	MG	AA	1643	1/1	0.94	0.06	-3.59	53,53,53,53	0
54	MG	AA	1634	1/1	0.94	0.04	-3.63	52,52,52,52	0
54	MG	DB	3093	1/1	0.93	0.09	-3.80	67,67,67,67	0
54	MG	BB	3078	1/1	0.91	0.06	-3.81	32,32,32,32	0
54	MG	AA	1610	1/1	0.97	0.10	-3.95	10,10,10,10	0
54	MG	DB	3079	1/1	0.97	0.09	-3.97	43,43,43,43	0
54	MG	CA	1656	1/1	0.97	0.07	-3.99	27,27,27,27	0
54	MG	BB	3091	1/1	0.91	0.09	-4.06	75,75,75,75	0
54	MG	BB	3066	1/1	0.94	0.06	-4.06	44,44,44,44	0
54	MG	DB	3056	1/1	0.95	0.07	-4.07	12,12,12,12	0
54	MG	DB	3104	1/1	0.88	0.09	-4.11	21,21,21,21	0
54	MG	AA	1602	1/1	0.96	0.05	-4.15	29,29,29,29	0
54	MG	CA	1617	1/1	0.99	0.07	-4.15	9,9,9,9	0
54	MG	DB	3011	1/1	0.95	0.07	-4.24	7,7,7,7	0
54	MG	BB	3050	1/1	0.95	0.08	-4.33	18,18,18,18	0
54	MG	DB	3088	1/1	0.97	0.10	-4.39	48,48,48,48	0
54	MG	BB	3017	1/1	0.98	0.10	-4.69	28,28,28,28	0
54	MG	BB	3080	1/1	0.95	0.09	-4.74	37,37,37,37	0
54	MG	BB	3060	1/1	0.96	0.08	-4.76	30,30,30,30	0
54	MG	BB	3003	1/1	0.99	0.07	-4.90	24,24,24,24	0
54	MG	DB	3109	1/1	0.97	0.05	-5.04	10,10,10,10	0
54	MG	BB	3014	1/1	0.91	0.05	-5.12	42,42,42,42	0
54	MG	DB	3077	1/1	0.99	0.12	-5.14	47,47,47,47	0
54	MG	CA	1644	1/1	0.95	0.08	-5.18	58,58,58,58	0
54	MG	AA	1644	1/1	0.96	0.07	-5.20	24,24,24,24	0
54	MG	BB	3049	1/1	0.99	0.03	-5.23	14,14,14,14	0
54	MG	BB	3033	1/1	0.96	0.07	-5.63	55,55,55,55	0
54	MG	CA	1605	1/1	0.98	0.04	-5.64	16,16,16,16	0
54	MG	DB	3003	1/1	0.98	0.08	-5.65	9,9,9,9	0
54	MG	BB	3062	1/1	0.97	0.04	-5.72	29,29,29,29	0
54	MG	DB	3037	1/1	0.93	0.07	-5.85	15,15,15,15	0
54	MG	BB	3057	1/1	0.99	0.05	-5.97	20,20,20,20	0
54	MG	DB	3036	1/1	0.98	0.05	-6.03	40,40,40,40	0
54	MG	BB	3053	1/1	0.98	0.08	-6.31	25,25,25,25	0
54	MG	DB	3069	1/1	0.97	0.10	-6.35	6,6,6,6	0
54	MG	DB	3081	1/1	0.93	0.12	-6.37	18,18,18,18	0
54	MG	DB	3045	1/1	0.98	0.03	-6.41	22,22,22,22	0
54	MG	CA	1618	1/1	0.98	0.04	-6.41	8,8,8,8	0
54	MG	DB	3073	1/1	0.98	0.07	-6.42	33,33,33,33	0
54	MG	BB	3020	1/1	0.85	0.09	-6.45	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3051	1/1	0.95	0.05	-6.52	41,41,41,41	0
54	MG	BB	3104	1/1	0.97	0.04	-6.61	8,8,8,8	0
54	MG	BB	3070	1/1	0.96	0.08	-6.87	15,15,15,15	0
54	MG	DB	3010	1/1	0.94	0.07	-7.01	5,5,5,5	0
54	MG	DB	3057	1/1	0.95	0.08	-7.11	5,5,5,5	0
54	MG	BB	3002	1/1	0.97	0.05	-7.24	24,24,24,24	0
54	MG	CA	1655	1/1	0.98	0.07	-7.27	69,69,69,69	0
54	MG	DB	3042	1/1	0.98	0.06	-7.29	7,7,7,7	0
54	MG	BB	3036	1/1	0.97	0.07	-7.33	36,36,36,36	0
54	MG	CA	1602	1/1	0.97	0.05	-7.60	6,6,6,6	0
54	MG	BB	3067	1/1	0.99	0.07	-7.68	34,34,34,34	0
54	MG	AA	1655	1/1	0.96	0.04	-7.88	38,38,38,38	0
54	MG	DB	3071	1/1	0.98	0.09	-8.83	61,61,61,61	0
54	MG	DB	3002	1/1	0.98	0.10	-8.85	5,5,5,5	0
54	MG	DB	3007	1/1	0.97	0.07	-9.12	12,12,12,12	0
54	MG	DB	3020	1/1	0.99	0.04	-10.23	5,5,5,5	0
54	MG	AA	1653	1/1	0.79	0.09	-	79,79,79,79	0
54	MG	AA	1656	1/1	0.97	0.13	-	60,60,60,60	0
54	MG	DB	3023	1/1	0.91	0.10	-	29,29,29,29	0
54	MG	BB	3007	1/1	0.98	0.09	-	5,5,5,5	0
54	MG	AA	1606	1/1	0.88	0.05	-	47,47,47,47	0
54	MG	AA	1633	1/1	0.96	0.10	-	51,51,51,51	0
54	MG	AA	1651	1/1	0.92	0.06	-	109,109,109,109	0
54	MG	CA	1627	1/1	0.92	0.08	-	29,29,29,29	1
54	MG	BB	3018	1/1	0.90	0.07	-	43,43,43,43	0
54	MG	BB	3026	1/1	0.97	0.10	-	54,54,54,54	0
54	MG	DB	3068	1/1	0.97	0.07	-	19,19,19,19	0
54	MG	DB	3040	1/1	0.98	0.07	-	58,58,58,58	0
54	MG	DB	3030	1/1	0.91	0.13	-	74,74,74,74	0
54	MG	AA	1661	1/1	0.89	0.11	-	79,79,79,79	0
54	MG	DB	3072	1/1	0.91	0.08	-	30,30,30,30	0
54	MG	CA	1622	1/1	0.90	0.10	-	75,75,75,75	0
54	MG	BB	3108	1/1	0.98	0.11	-	25,25,25,25	0
54	MG	CA	1607	1/1	0.90	0.12	-	100,100,100,100	0
54	MG	DB	3083	1/1	0.98	0.08	-	24,24,24,24	0
54	MG	BB	3032	1/1	0.89	0.10	-	45,45,45,45	0
54	MG	CA	1658	1/1	0.93	0.09	-	52,52,52,52	0
54	MG	BB	3110	1/1	0.94	0.07	-	30,30,30,30	0
54	MG	DB	3053	1/1	0.70	0.09	-	102,102,102,102	0
54	MG	AA	1646	1/1	0.97	0.03	-	94,94,94,94	0
54	MG	BB	3023	1/1	0.93	0.22	-	41,41,41,41	0
54	MG	BB	3043	1/1	0.80	0.08	-	170,170,170,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1650	1/1	0.74	0.06	-	114,114,114,114	0
54	MG	BB	3097	1/1	0.97	0.05	-	32,32,32,32	0
54	MG	BB	3081	1/1	0.90	0.21	-	52,52,52,52	0
54	MG	AA	1627	1/1	0.86	0.10	-	15,15,15,15	1
54	MG	DB	3027	1/1	0.94	0.07	-	36,36,36,36	0
54	MG	DB	3108	1/1	0.96	0.07	-	21,21,21,21	0
54	MG	BB	3090	1/1	0.95	0.07	-	49,49,49,49	0
54	MG	CA	1611	1/1	0.95	0.06	-	60,60,60,60	0
54	MG	BB	3015	1/1	0.94	0.04	-	27,27,27,27	0
54	MG	AA	1616	1/1	0.91	0.10	-	77,77,77,77	0
54	MG	DB	3016	1/1	0.89	0.11	-	49,49,49,49	0
54	MG	BB	3010	1/1	0.93	0.08	-	82,82,82,82	0
54	MG	DB	3009	1/1	0.98	0.08	-	19,19,19,19	0
54	MG	BB	3059	1/1	0.95	0.07	-	30,30,30,30	0
54	MG	DB	3103	1/1	0.98	0.10	-	16,16,16,16	0
54	MG	CA	1642	1/1	0.78	0.09	-	94,94,94,94	0
54	MG	BB	3076	1/1	0.94	0.14	-	60,60,60,60	0
54	MG	AA	1649	1/1	0.95	0.11	-	19,19,19,19	0
54	MG	CA	1623	1/1	0.88	0.03	-	131,131,131,131	0
54	MG	DB	3105	1/1	0.95	0.10	-	40,40,40,40	0
54	MG	AA	1609	1/1	0.83	0.20	-	127,127,127,127	0
54	MG	BB	3107	1/1	0.97	0.07	-	54,54,54,54	0
54	MG	DB	3084	1/1	0.74	0.20	-	92,92,92,92	0
54	MG	BB	3092	1/1	0.94	0.10	-	32,32,32,32	0
54	MG	BB	3040	1/1	0.92	0.10	-	28,28,28,28	0
54	MG	BB	3058	1/1	0.81	0.17	-	76,76,76,76	0
54	MG	AA	1618	1/1	0.95	0.08	-	79,79,79,79	0
54	MG	DB	3005	1/1	0.87	0.20	-	30,30,30,30	0
54	MG	BB	3039	1/1	0.83	0.07	-	131,131,131,131	0
54	MG	CA	1654	1/1	0.93	0.05	-	78,78,78,78	0
54	MG	BB	3011	1/1	0.65	0.12	-	66,66,66,66	0
54	MG	DB	3065	1/1	0.94	0.07	-	16,16,16,16	0
54	MG	AA	1640	1/1	0.84	0.24	-	104,104,104,104	0
54	MG	AA	1626	1/1	0.55	0.19	-	64,64,64,64	1
54	MG	DB	3032	1/1	0.95	0.11	-	18,18,18,18	0
54	MG	DB	3078	1/1	0.92	0.13	-	46,46,46,46	0
54	MG	DB	3067	1/1	0.11	0.13	-	178,178,178,178	0
54	MG	BB	3004	1/1	0.93	0.07	-	38,38,38,38	0
54	MG	BB	3054	1/1	0.94	0.05	-	46,46,46,46	0
54	MG	DB	3098	1/1	0.93	0.15	-	36,36,36,36	0
54	MG	CA	1634	1/1	0.91	0.12	-	8,8,8,8	0
54	MG	BB	3009	1/1	0.96	0.12	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1607	1/1	0.94	0.04	-	64,64,64,64	0
54	MG	CA	1610	1/1	0.93	0.04	-	79,79,79,79	0
54	MG	DB	3017	1/1	0.86	0.08	-	6,6,6,6	0
54	MG	BB	3073	1/1	0.93	0.10	-	67,67,67,67	0
54	MG	AA	1647	1/1	0.85	0.13	-	87,87,87,87	0
54	MG	CA	1659	1/1	0.97	0.07	-	62,62,62,62	0
54	MG	AA	1622	1/1	0.93	0.06	-	27,27,27,27	0
54	MG	CA	1641	1/1	0.93	0.09	-	63,63,63,63	0
54	MG	CA	1646	1/1	0.96	0.05	-	72,72,72,72	0
54	MG	AA	1624	1/1	0.89	0.32	-	32,32,32,32	1
54	MG	DB	3014	1/1	0.93	0.14	-	48,48,48,48	0
54	MG	AA	1617	1/1	0.90	0.07	-	45,45,45,45	0
54	MG	BB	3079	1/1	0.80	0.12	-	75,75,75,75	0
54	MG	DB	3063	1/1	0.96	0.04	-	71,71,71,71	0
54	MG	DB	3101	1/1	0.96	0.09	-	5,5,5,5	0
54	MG	CA	1660	1/1	0.93	0.06	-	69,69,69,69	0
54	MG	DB	3034	1/1	0.86	0.08	-	43,43,43,43	0
54	MG	BB	3102	1/1	0.95	0.10	-	28,28,28,28	0
54	MG	CE	201	1/1	0.87	0.08	-	97,97,97,97	0
54	MG	AA	1629	1/1	0.95	0.05	-	70,70,70,70	0
54	MG	AA	1605	1/1	0.97	0.15	-	48,48,48,48	0
54	MG	AA	1615	1/1	0.46	0.08	-	110,110,110,110	0
54	MG	DB	3026	1/1	0.97	0.13	-	15,15,15,15	0
54	MG	CA	1649	1/1	0.96	0.07	-	73,73,73,73	0
54	MG	AA	1657	1/1	0.86	0.08	-	69,69,69,69	0
54	MG	BB	3045	1/1	0.95	0.09	-	67,67,67,67	0
54	MG	DB	3106	1/1	0.98	0.12	-	39,39,39,39	0
54	MG	CA	1625	1/1	0.98	0.06	-	34,34,34,34	0
54	MG	DB	3087	1/1	0.94	0.19	-	25,25,25,25	0
54	MG	DB	3021	1/1	0.99	0.15	-	9,9,9,9	0
54	MG	BB	3027	1/1	0.98	0.08	-	34,34,34,34	0
54	MG	AA	1628	1/1	0.90	0.14	-	57,57,57,57	0
54	MG	DB	3039	1/1	0.98	0.13	-	19,19,19,19	0
54	MG	BB	3083	1/1	0.95	0.12	-	5,5,5,5	0
54	MG	BB	3048	1/1	0.78	0.13	-	128,128,128,128	0
54	MG	DB	3049	1/1	0.98	0.10	-	46,46,46,46	0
54	MG	AA	1632	1/1	0.93	0.14	-	37,37,37,37	0
54	MG	CA	1635	1/1	0.68	0.09	-	96,96,96,96	0
54	MG	DB	3012	1/1	0.99	0.20	-	37,37,37,37	0
54	MG	DB	3013	1/1	0.94	0.18	-	21,21,21,21	0
54	MG	DB	3033	1/1	0.96	0.12	-	62,62,62,62	0
54	MG	CA	1648	1/1	0.93	0.11	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3034	1/1	0.73	0.23	-	136,136,136,136	0
54	MG	AA	1642	1/1	0.92	0.07	-	59,59,59,59	0
54	MG	DB	3076	1/1	0.98	0.06	-	26,26,26,26	0
54	MG	BB	3064	1/1	0.96	0.06	-	26,26,26,26	0
54	MG	BB	3072	1/1	0.96	0.09	-	52,52,52,52	0
54	MG	DB	3102	1/1	0.98	0.14	-	14,14,14,14	0
54	MG	CA	1647	1/1	0.95	0.06	-	90,90,90,90	0
54	MG	DB	3025	1/1	0.95	0.09	-	44,44,44,44	0
54	MG	BB	3016	1/1	0.99	0.07	-	18,18,18,18	0
54	MG	CA	1621	1/1	0.86	0.32	-	118,118,118,118	0
54	MG	BB	3069	1/1	0.98	0.11	-	32,32,32,32	0
54	MG	CA	1652	1/1	0.92	0.17	-	77,77,77,77	0
54	MG	AA	1641	1/1	0.88	0.11	-	56,56,56,56	0
54	MG	BB	3046	1/1	0.98	0.08	-	46,46,46,46	0
54	MG	CA	1650	1/1	0.99	0.09	-	12,12,12,12	0
54	MG	CA	1626	1/1	0.93	0.15	-	8,8,8,8	1
54	MG	DB	3006	1/1	0.98	0.07	-	20,20,20,20	0
54	MG	BB	3101	1/1	0.54	0.12	-	138,138,138,138	0
54	MG	DB	3038	1/1	0.90	0.15	-	17,17,17,17	0
54	MG	BB	3105	1/1	0.96	0.11	-	21,21,21,21	0
54	MG	DB	3051	1/1	0.84	0.08	-	87,87,87,87	0
54	MG	DB	3061	1/1	0.48	0.08	-	115,115,115,115	0
54	MG	BB	3035	1/1	0.94	0.08	-	32,32,32,32	0
54	MG	DB	3092	1/1	0.98	0.17	-	46,46,46,46	0
54	MG	CA	1637	1/1	0.94	0.06	-	79,79,79,79	0
54	MG	DB	3099	1/1	0.98	0.15	-	29,29,29,29	0
54	MG	AA	1623	1/1	0.68	0.28	-	129,129,129,129	0
54	MG	BB	3028	1/1	0.98	0.08	-	32,32,32,32	0
54	MG	DB	3107	1/1	0.91	0.10	-	27,27,27,27	0
54	MG	AA	1612	1/1	0.93	0.06	-	37,37,37,37	0
54	MG	CA	1629	1/1	0.93	0.08	-	46,46,46,46	1
54	MG	BB	3052	1/1	0.86	0.09	-	59,59,59,59	0
54	MG	DB	3035	1/1	0.85	0.20	-	81,81,81,81	0
54	MG	DB	3110	1/1	0.90	0.08	-	19,19,19,19	0
54	MG	CA	1612	1/1	0.76	0.10	-	84,84,84,84	0
54	MG	DB	3082	1/1	0.99	0.07	-	6,6,6,6	0
54	MG	CA	1657	1/1	0.70	0.15	-	91,91,91,91	0
54	MG	BB	3094	1/1	0.91	0.22	-	93,93,93,93	0
54	MG	BB	3096	1/1	0.91	0.12	-	42,42,42,42	0
54	MG	BB	3075	1/1	0.97	0.10	-	13,13,13,13	0
54	MG	BB	3019	1/1	0.89	0.10	-	45,45,45,45	0
54	MG	BB	3077	1/1	0.97	0.08	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1608	1/1	0.98	0.06	-	40,40,40,40	0
54	MG	AA	1603	1/1	0.41	0.15	-	133,133,133,133	0
54	MG	BB	3025	1/1	0.93	0.08	-	14,14,14,14	0
54	MG	CA	1603	1/1	0.97	0.12	-	30,30,30,30	0
54	MG	BB	3098	1/1	0.67	0.12	-	80,80,80,80	0
54	MG	DB	3095	1/1	0.97	0.05	-	39,39,39,39	0
54	MG	CA	1630	1/1	0.95	0.08	-	40,40,40,40	0
54	MG	DB	3022	1/1	0.98	0.09	-	5,5,5,5	0
54	MG	BB	3044	1/1	0.77	0.12	-	108,108,108,108	0
54	MG	AA	1625	1/1	0.88	0.11	-	72,72,72,72	0
54	MG	CA	1614	1/1	0.98	0.06	-	58,58,58,58	0
54	MG	BB	3068	1/1	0.97	0.10	-	55,55,55,55	0
54	MG	BB	3093	1/1	0.95	0.04	-	36,36,36,36	0
54	MG	CA	1651	1/1	0.96	0.06	-	40,40,40,40	0
54	MG	BB	3042	1/1	0.99	0.08	-	8,8,8,8	0
54	MG	CA	1609	1/1	0.76	0.13	-	121,121,121,121	0
54	MG	DB	3044	1/1	0.96	0.06	-	12,12,12,12	0
54	MG	AA	1619	1/1	0.78	0.13	-	85,85,85,85	0
54	MG	DB	3074	1/1	0.97	0.05	-	28,28,28,28	0
54	MG	DB	3064	1/1	0.98	0.10	-	33,33,33,33	0
54	MG	BB	3061	1/1	0.92	0.14	-	41,41,41,41	0
54	MG	DB	3055	1/1	0.95	0.09	-	42,42,42,42	0
54	MG	BB	3111	1/1	0.92	0.14	-	81,81,81,81	0
54	MG	DB	3024	1/1	0.92	0.05	-	55,55,55,55	0
54	MG	BB	3106	1/1	0.99	0.14	-	33,33,33,33	0
54	MG	BB	3065	1/1	0.94	0.08	-	24,24,24,24	0
54	MG	AA	1660	1/1	0.24	0.36	-	163,163,163,163	0
54	MG	CA	1620	1/1	0.90	0.17	-	70,70,70,70	0
54	MG	CA	1661	1/1	0.93	0.08	-	61,61,61,61	0
54	MG	BB	3031	1/1	0.97	0.03	-	47,47,47,47	0
54	MG	BB	3085	1/1	0.96	0.15	-	44,44,44,44	0
54	MG	DB	3054	1/1	0.93	0.10	-	65,65,65,65	0
54	MG	AA	1635	1/1	0.91	0.13	-	45,45,45,45	0
54	MG	BB	3103	1/1	0.94	0.09	-	37,37,37,37	0
54	MG	AA	1648	1/1	0.92	0.49	-	94,94,94,94	0
54	MG	DB	3029	1/1	0.90	0.07	-	33,33,33,33	0
54	MG	CA	1604	1/1	0.99	0.08	-	52,52,52,52	0
54	MG	BB	3047	1/1	0.95	0.09	-	46,46,46,46	0
54	MG	DB	3094	1/1	0.96	0.15	-	21,21,21,21	0
54	MG	AA	1659	1/1	0.97	0.05	-	112,112,112,112	0
54	MG	BB	3100	1/1	0.94	0.19	-	68,68,68,68	0
54	MG	BB	3071	1/1	0.99	0.12	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3047	1/1	0.98	0.04	-	24,24,24,24	0
54	MG	CA	1619	1/1	0.72	0.09	-	59,59,59,59	0
54	MG	AA	1613	1/1	0.91	0.07	-	65,65,65,65	0
54	MG	DB	3112	1/1	0.98	0.15	-	37,37,37,37	0
54	MG	CA	1631	1/1	0.94	0.07	-	34,34,34,34	0
54	MG	DB	3059	1/1	0.77	1.45	-	180,180,180,180	0
54	MG	BB	3037	1/1	0.96	0.07	-	42,42,42,42	0
54	MG	BB	3055	1/1	0.87	0.06	-	58,58,58,58	0
54	MG	DB	3019	1/1	0.97	0.14	-	48,48,48,48	0
54	MG	AA	1638	1/1	0.56	0.36	-	147,147,147,147	0
54	MG	DB	3062	1/1	0.92	0.04	-	47,47,47,47	0
54	MG	DB	3018	1/1	0.94	0.09	-	8,8,8,8	0
54	MG	DB	3066	1/1	0.97	0.06	-	29,29,29,29	0
54	MG	DB	3050	1/1	0.98	0.14	-	32,32,32,32	0
54	MG	DB	3043	1/1	0.97	0.09	-	15,15,15,15	0
54	MG	CA	1628	1/1	0.95	0.04	-	61,61,61,61	0
54	MG	BB	3021	1/1	0.95	0.06	-	22,22,22,22	0
54	MG	DB	3046	1/1	0.93	0.13	-	55,55,55,55	0
54	MG	DB	3096	1/1	0.72	0.11	-	127,127,127,127	0
54	MG	BB	3029	1/1	0.84	0.22	-	32,32,32,32	0
54	MG	BB	3008	1/1	1.00	0.09	-	64,64,64,64	0
54	MG	CA	1616	1/1	0.79	0.09	-	167,167,167,167	0
54	MG	DB	3058	1/1	0.89	0.05	-	43,43,43,43	0
54	MG	DB	3041	1/1	0.97	0.14	-	15,15,15,15	0
54	MG	BB	3056	1/1	0.96	0.13	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.