



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:41 PM GMT

PDB ID : 4V54
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with ribosome recycling factor (RRF).
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-16
Resolution : 3.30 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

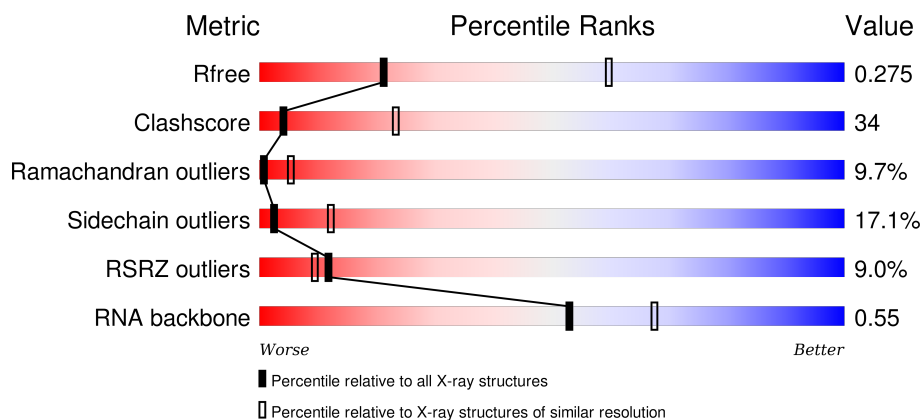
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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>2%</div> <div>27% 60% 13%</div> </div>
1	CA	1542	<div> <div>%</div> <div>26% 61% 12%</div> </div>
2	AC	232	<div> <div>3%</div> <div>30% 47% 11% 11%</div> </div>
2	CC	232	<div> <div>3%</div> <div>31% 45% 12% 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	

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Mol	Chain	Length	Quality of chain
53	B6	185	
53	D6	185	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	2057	-	-	-	X
54	MG	BB	3087	-	-	-	X
54	MG	DB	3030	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 286960 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a protein called ribosome recycling factor.

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

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

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

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

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	289	Total	O	0	0
			289	289		
56	AE	4	Total	O	0	0
			4	4		
56	AK	1	Total	O	0	0
			1	1		
56	AL	1	Total	O	0	0
			1	1		
56	AN	3	Total	O	0	0
			3	3		
56	AP	1	Total	O	0	0
			1	1		

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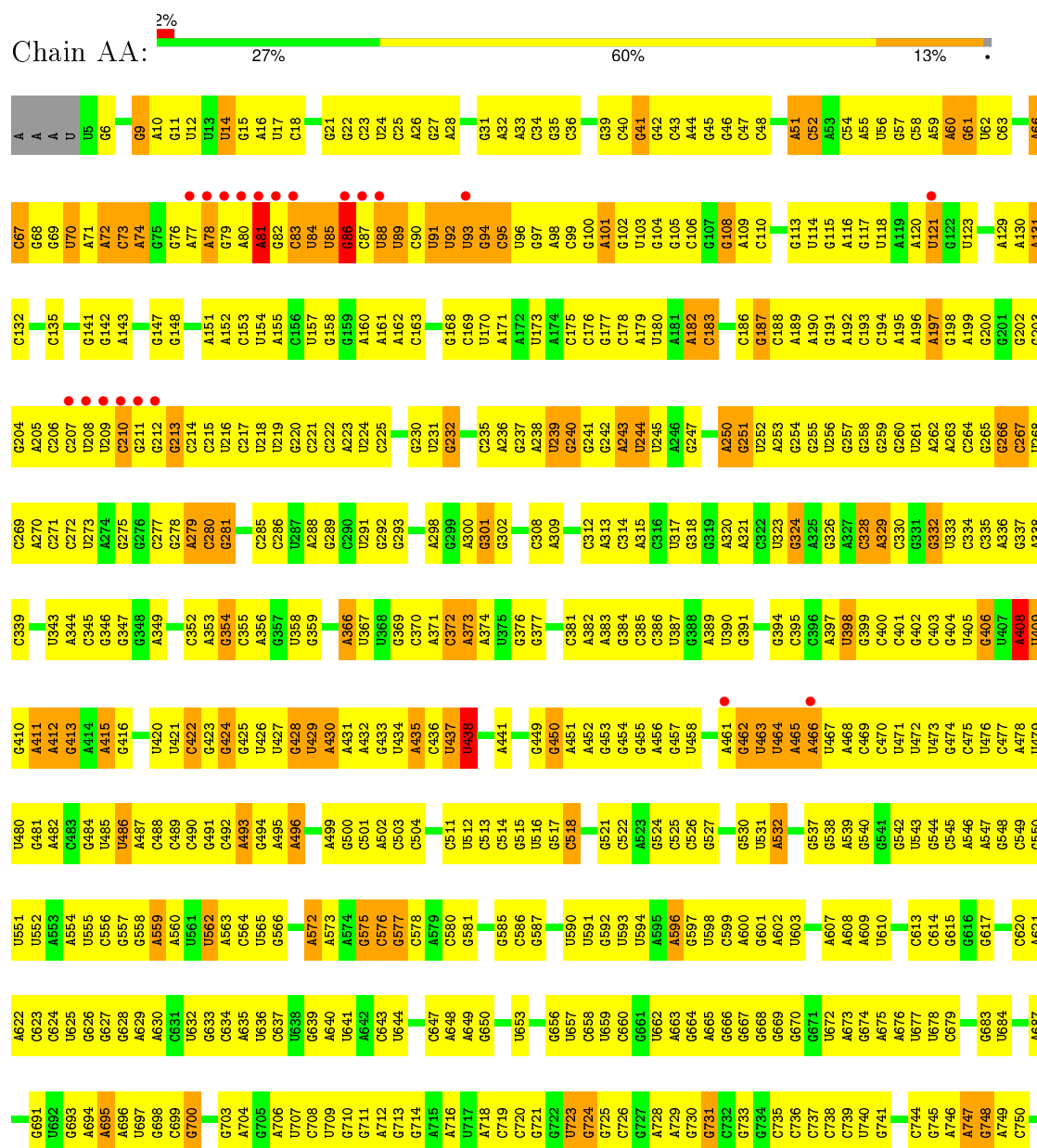
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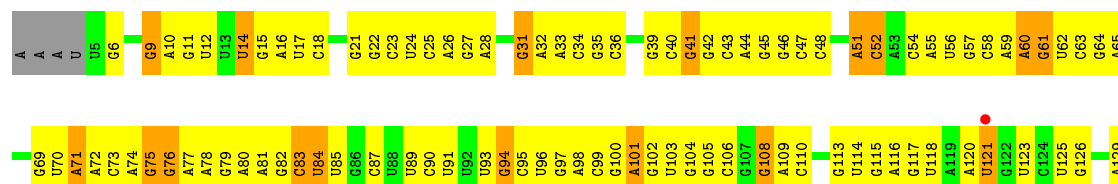
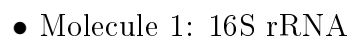
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AT	1	Total 1	O 1	0	0
56	BB	495	Total 495	O 495	0	0
56	BC	4	Total 4	O 4	0	0
56	BD	1	Total 1	O 1	0	0
56	BE	3	Total 3	O 3	0	0
56	B2	1	Total 1	O 1	0	0
56	BL	1	Total 1	O 1	0	0
56	BT	1	Total 1	O 1	0	0
56	CE	2	Total 2	O 2	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	1	Total 1	O 1	0	0
56	CN	4	Total 4	O 4	0	0
56	CT	1	Total 1	O 1	0	0
56	CA	300	Total 300	O 300	0	0
56	DB	505	Total 505	O 505	0	0
56	DC	4	Total 4	O 4	0	0
56	DD	1	Total 1	O 1	0	0
56	DE	2	Total 2	O 2	0	0

3 Residue-property plots

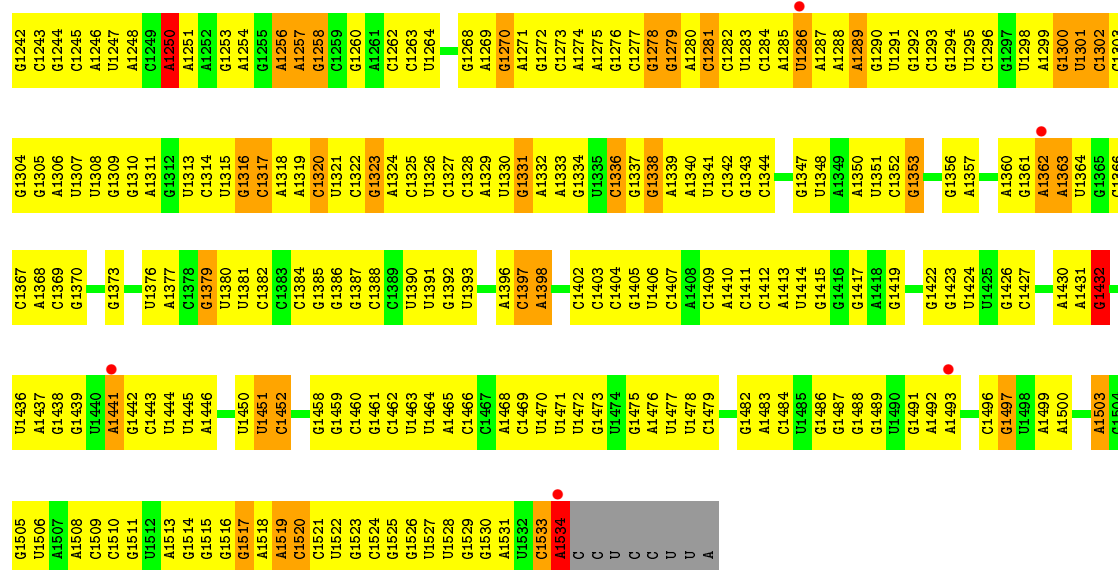
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA

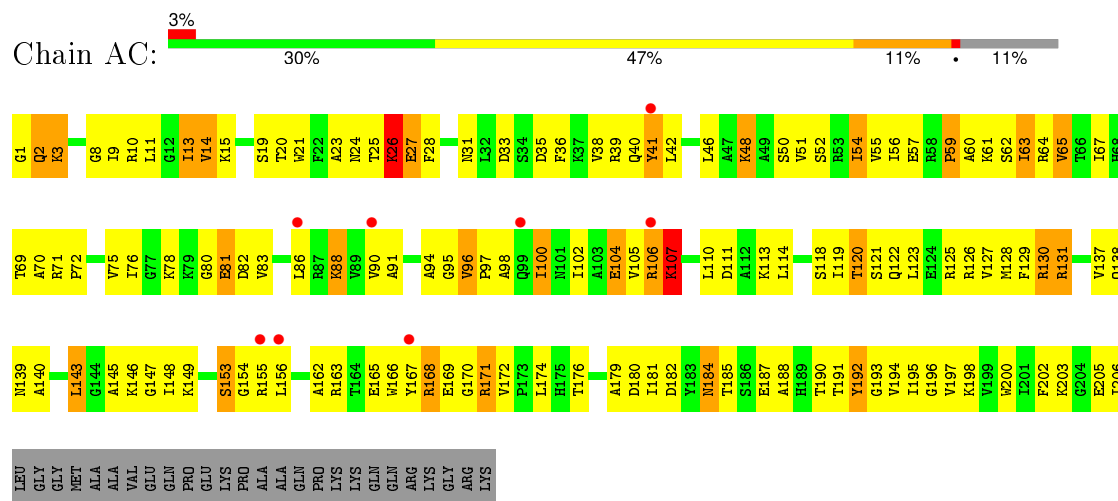




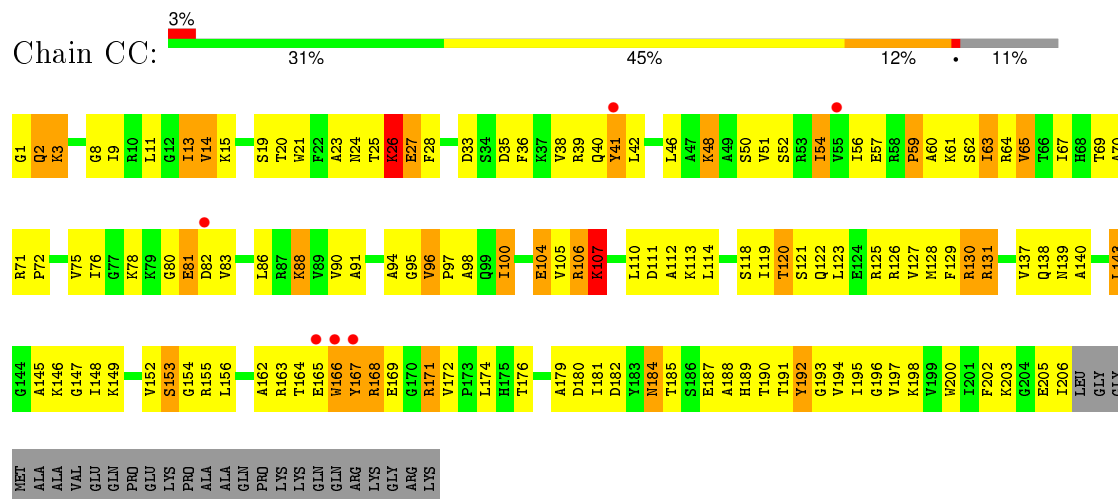
A1176	C1100	A1036	G976	A909	G830	A749	G683	G617	G548	U476	G406	A336	G266	G202	A130
G1177	A1101	C1037	A977	C910	A831	C750	U684	C620	C949	C477	U407	G337	C267	G203	A131
G1178	A1102	C1038	A978	G911	G832	C754	A687	A621	G950	C478	A408	A338	U268	G204	C132
A1180	C1103	G1039	C979	U911	G833	G755	G691	A622	U551	U479	U409	C339	A270	A205	
G1181	U1115	U1040	G981	C912	U834			G623	U552	U480	G410		C207	C206	C135
G1182	U1118	A1042	U982	A914	G836	G763	A694	C624	A554	A482	A412	U343	C271	U208	G141
U1183	C1119	G1043	A983	A915	U837	G764	A695	U625	U555	G483	G413	C345	C272	U209	G142
G1184	A1044	C984	G984	U916	G838	C765	A696	G627	C956	U486	A415	G346	A274	C210	A143
	C985	U1045	C985	A917	C839	G766	A697	U628	C957	U485	G416		G275	G211	G147
A1189	U1121	A1046	U986	A918	C840	A767	U697	G629	G958	U486		A349	G276	G212	G148
G1190	G1047	G1047	G987	A919	C841	A768	G698	A629	A559	A487		C352	C277	G213	
A1191	U1048	U1049	U988	U920	U842	C769	C699	A630	A560	C488	U420	A353	G278	C214	
	G1124			U921	U843	C770	G700	U631	U561	C489	U421	A353	A279	C215	A151
A1192	C1129	G1050	U991	G922	G844	A777	G703	U632	U562	C490	C422	C354	G280	U216	A152
G1193	A1130	C1051	A991	A923	A845	G778	A704	U633	A563	G491	G423	C355	C281	C217	C153
U1194	U1052	U1052	U992	C924	G846		G705	C634	C564	C492	G424	A356		U218	U154
C1195	G1131	G1053	G993	G925	G847		G706	A635	U565	A493	G425	G357	C285	U219	A155
A1196	C1132	C1054	A994	G926	C848		U707	U636	G566	G494	U426	U358	C286	G220	C156
A1197	G1133		C995	G927	G849		U708	C637		A495	U427	G359	U287	C221	U157
	U1134	G1057	A996	G928			C708	U638	A572	A496	G428		A288	C222	G158
C1200	U1135	G1058		G929	G852		U709	U639	A573	C489	U429	A363	C289	A223	A159
A1201	C1136	C1059	U997	C930	C853	A787	G710	A640	A574	C490	A430	A371	G290	U224	A160
U1202	C1137	U1060	C999	C931			G711	U641	G575	C501	A431	A372	U291	U225	A161
C1203	G1138	G1061	A1000	C931	C856		A712	A642	C576	A502	A432	A373	G292		A162
	G1139	U1062	C1001		C857		G713	C643	G577	C503	G433	A374		G230	C163
G1206	C1140		G1002	C934	C858	U793	G714	U644		C504	U434		A298	U231	
G1207	C1141	G1064	G1003	A935	G859	A794	A715		A579	C435	G232	C370	G299	G232	G168
	U1142	U1065	A1004	G939	U860	C795	A716	C647	G581	C511	A300	A371	A300	C233	C169
U1211	G1143	C1066	A1005	C940	G861	C796	U717	A648	G581	U512	C234	C372	G301	C234	U170
U1212	U1066		G1006	G941	C862	C797	A718	A649		C513	G302	A373	G302	C235	A171
A1213	A1145	G1068	U1007		U863	U798	C719	C650	G585	C514	A303	A374	A303	A236	A172
A1214	A1146	C1069	U1008	A946	A864		C720		C586	C515		U375		G237	U173
G1215	C1147	U1070	G1009	G947	A865	A802	G721	U653	G587	U516	A308	G376	C308	U239	A174
A1216	U1148	C1071	U1010	C948	C866	G803	G722			C517	G239	A377	A309	G240	C175
C1217	C1149	G1072	A1011	A949	G867	U804	U723	G656	U590	C518	A451	C381	G312	G241	G176
G1218	A1150	U1073	A1012	U950	C868	C805	G724	U657	U591		A452	A382	A313	G242	C178
A1219	A1151	G1074	G1013	G951	G869	C806	G725	C658	G592	U531	G453	A383	C314	A243	A179
G1220	A1152	U1075	A1014	U952	G869	A807	G726	U659	U593	C522	G454	G394	A315	U244	U180
G1221	G1153						G727	C660	U594	A523	G455	C385	C316	U245	A181
		U1078	A1016	U955	U875	C810	A728	G661	A595	G524	A456	C386	U317	A246	A182
A1222	A1157	G1079	U1017	U956	C876	C811	A729	U662	A596	C525	G457	U387	G318	G247	
C1223	C1158	A1080	G1018	U957	A878	G812	G730	A663	G597	C526	U458		G319		C183
U1224	U1159	A1081	A1019	A958		U813	G731	G664	U598	G527		C388			
A1225	G1160		G1020	A959	C882	A614	C732	A665	C599		A461	A389	A320	A280	C186
C1226	C1161	G1084	A1021	U960	C883	A815	G733	G666	A600	G530	G462	U390	A321	G251	G187
C1228	C1162	U1085	A1022	U961	U884	A816	G734	G667	G601	U531	U463	G391	C322	U252	C188
A1229	U1086	U1086	U1023	C962	G885	C817	C735	G668	A602	A532	U464	G394	U323	A253	A189
G1230	G1164		G1024	G963	G886	G818	C736	G669	U603		A465	C395	A325	G254	A190
G1231	U1165	G1089	U1025	A964		A819	C737	G670		G537	A466	C396	G326	G255	G191
U1232	G1166	U1090	U1026	U965	A892	U820	C738	G671	A607	G538		C397	G327	U256	A192
G1233	U1167	U1091	C1027	G966	C893	G821	C739	U672	A608	A539	U467	U398	A327	G257	C193
C1234	U1168	A1092	C1028	C967	G894	U822	U740	A673	A609	G540	A468	G399	A329	G258	C194
U1235	A1169	U1093	U1029	A968		C823	G741	G674	U610	G541	C469	U399	A329	G259	A195
A1236	U1094			A969		G824		A675	C611	G542	C470	C400	C330	G260	A196
C1237	A1171	U1095	U1031		A901	A825		A676	C612	U543	U471	C401	G331	U261	A197
A1238	C1172	C1086	G1032	C972	G902	A826	C744	G677	C613	G544	U472	G402	G332	A262	G198
U1239	U1173	C1097	G1033	G973	G903	U827	G745	U677	C614	G545	U473	C403	U333	A263	A199
U1240	G1174	C1098	U1034	A974	U904	U828	A746	G679	G615	A546	G474	G404	C334	C264	G200
G1241	G1175	G1099	A1035	A975	A906	G829	G748		G616	A547	C475	U405	C335	G265	G201



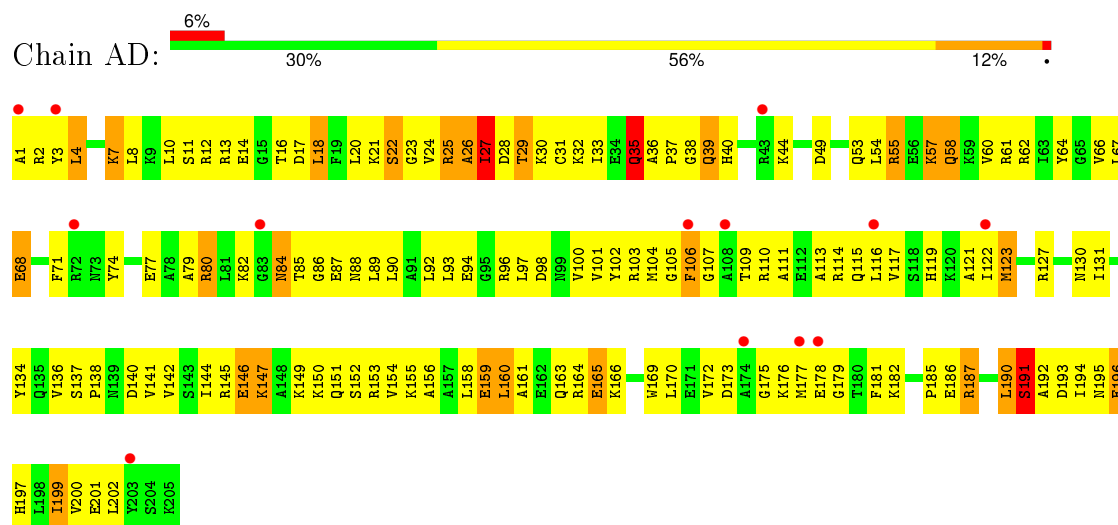
• Molecule 2: 30S ribosomal protein S3



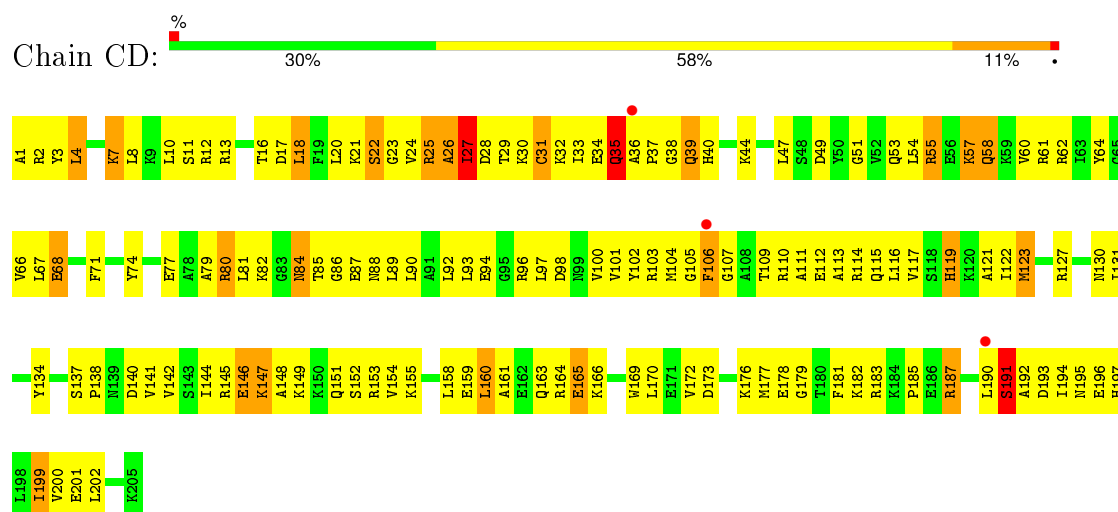
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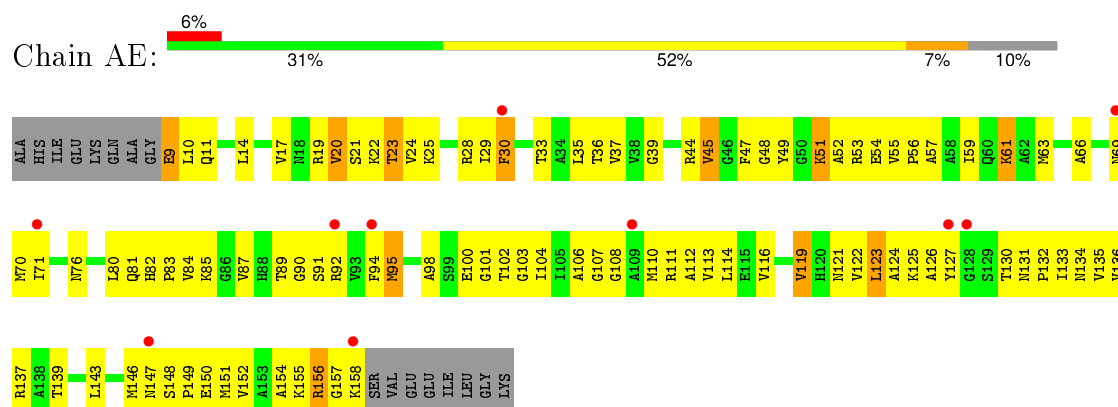
• Molecule 3: 30S ribosomal protein S4



• Molecule 3: 30S ribosomal protein S4

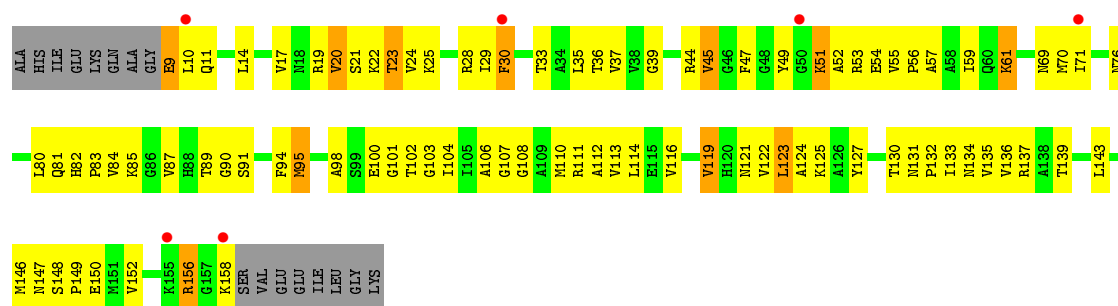


• Molecule 4: 30S ribosomal protein S5

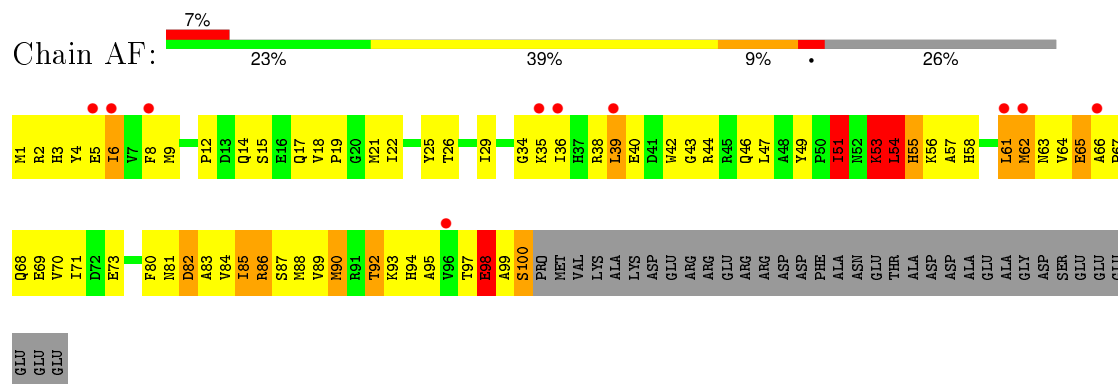


• Molecule 4: 30S ribosomal protein S5

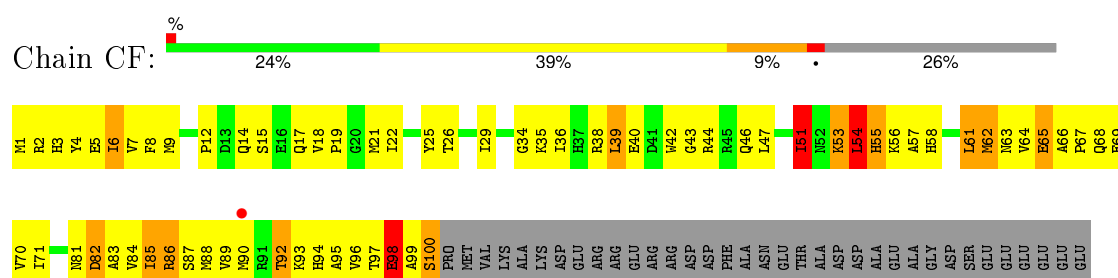




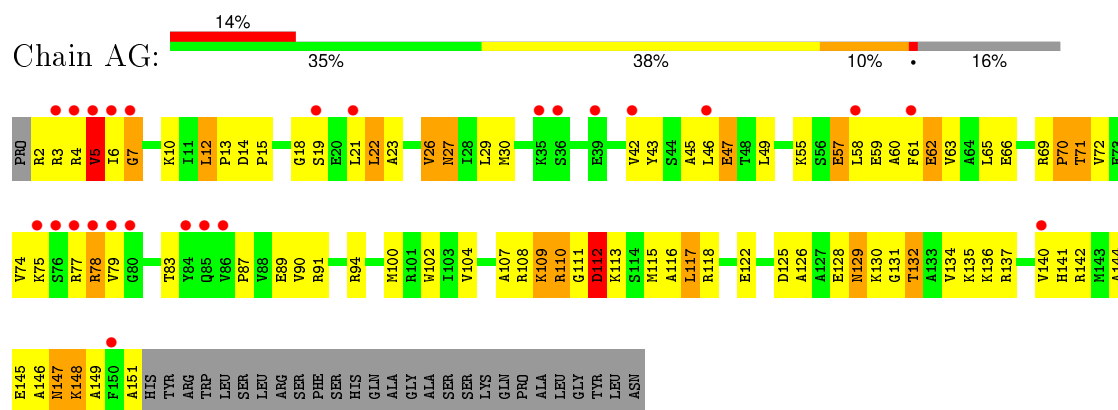
• Molecule 5: 30S ribosomal protein S6



• Molecule 5: 30S ribosomal protein S6

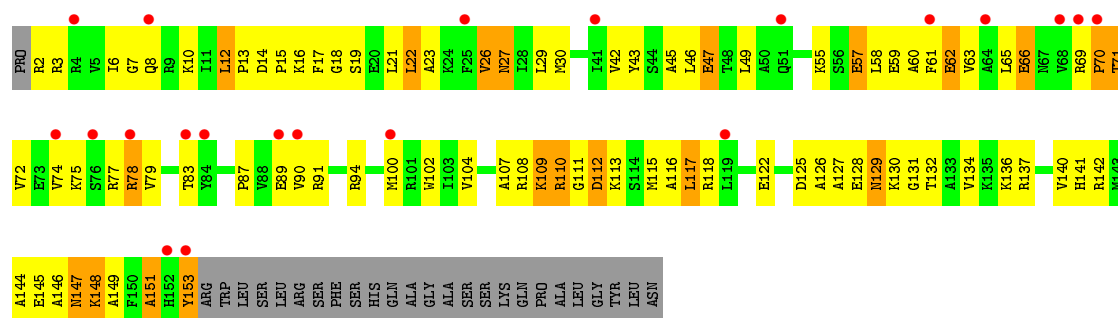


• Molecule 6: 30S ribosomal protein S7

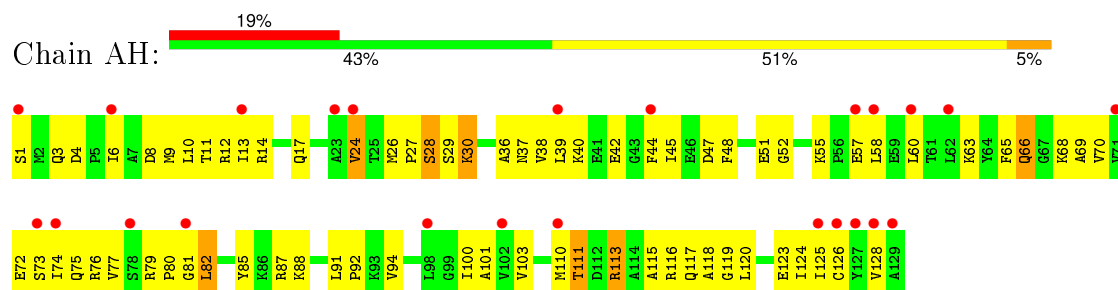


• Molecule 6: 30S ribosomal protein S7

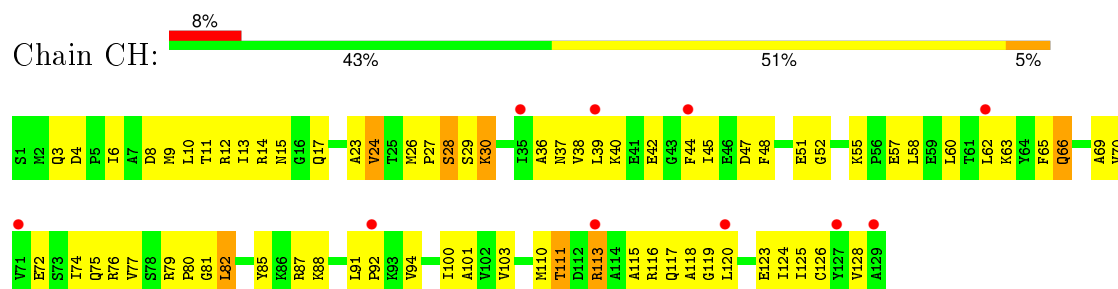




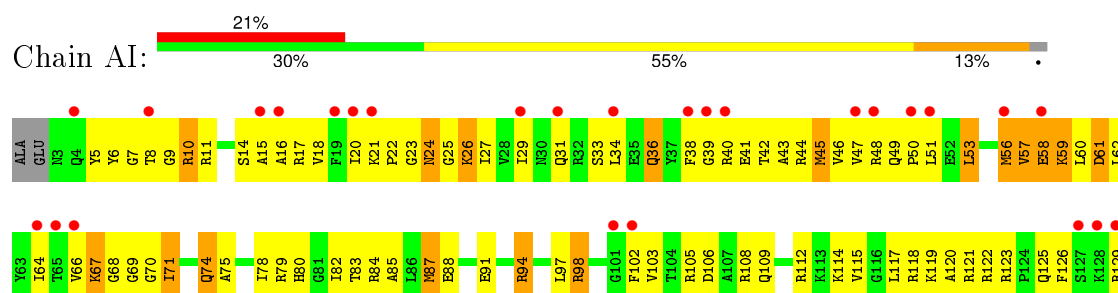
• Molecule 7: 30S ribosomal protein S8



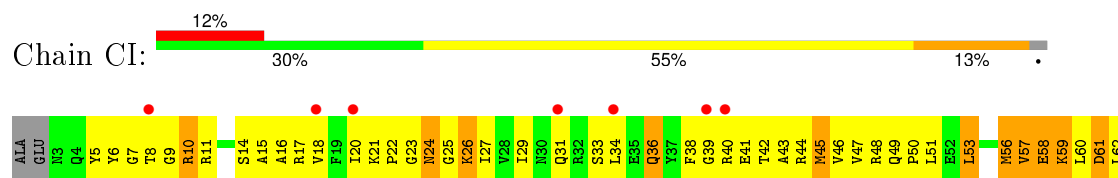
• Molecule 7: 30S ribosomal protein S8

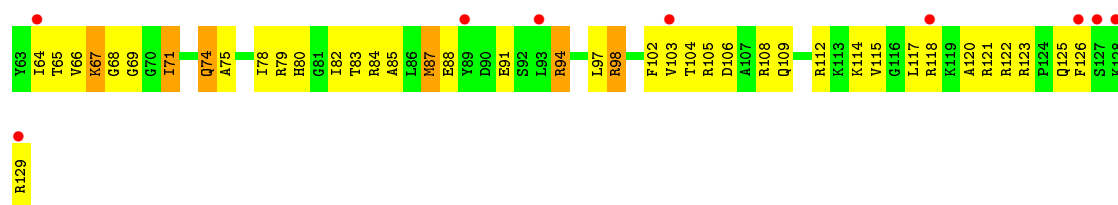


• Molecule 8: 30S ribosomal protein S9

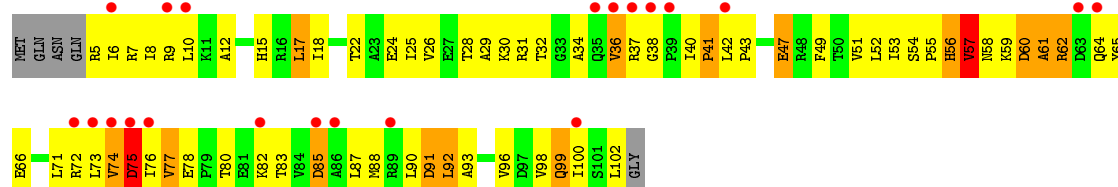


• Molecule 8: 30S ribosomal protein S9

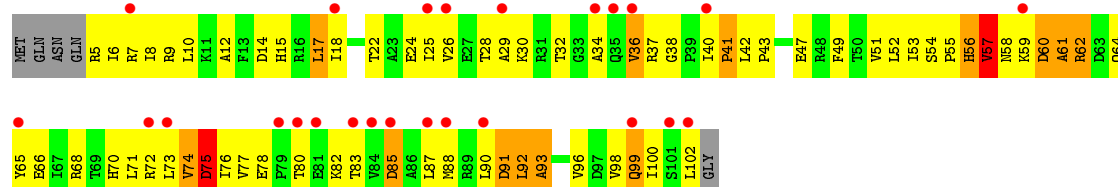




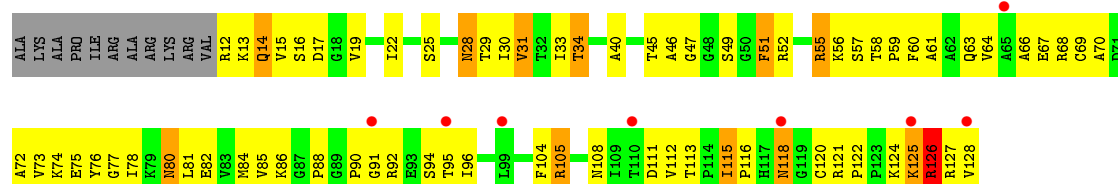
- Molecule 9: 30S ribosomal protein S10



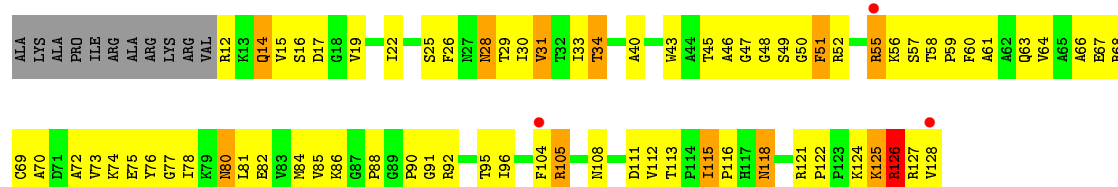
- Molecule 9: 30S ribosomal protein S10



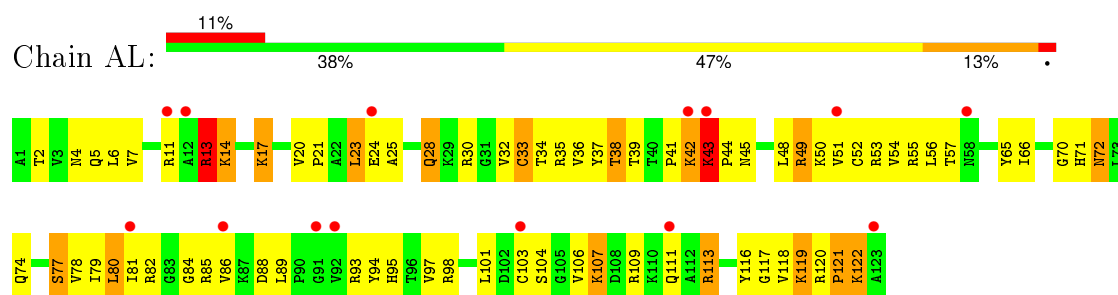
- Molecule 10: 30S ribosomal protein S11



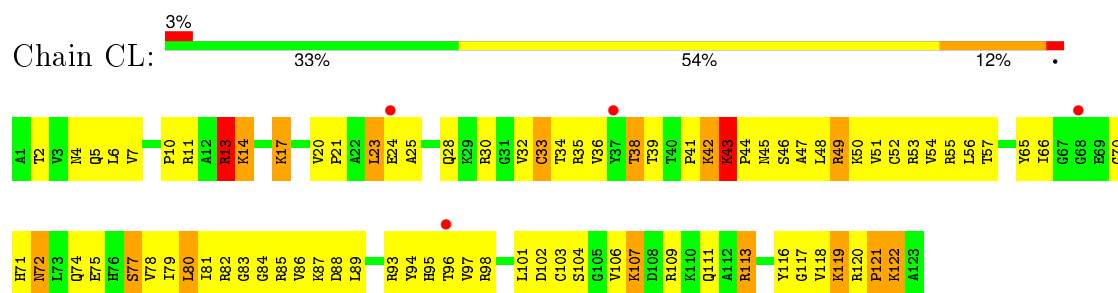
- Molecule 10: 30S ribosomal protein S11



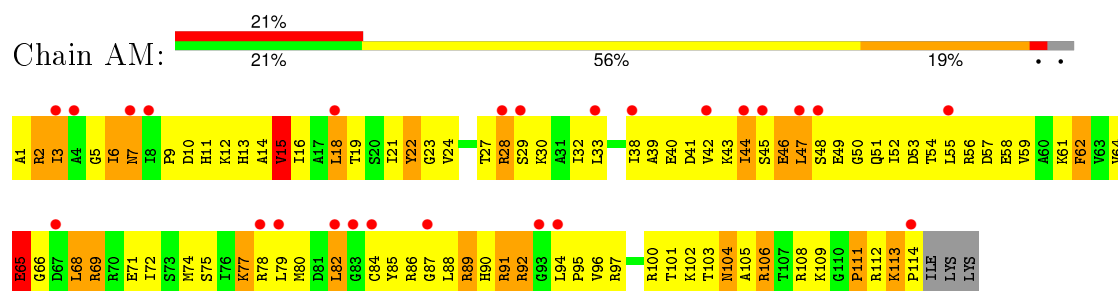
- Molecule 11: 30S ribosomal protein S12



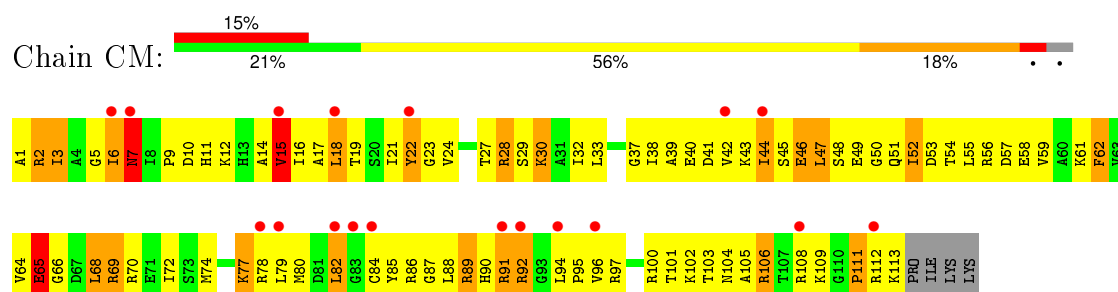
- Molecule 11: 30S ribosomal protein S12



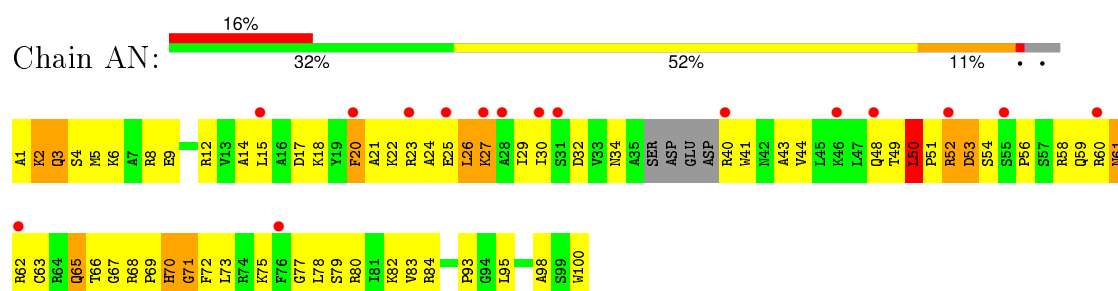
- Molecule 12: 30S ribosomal protein S13



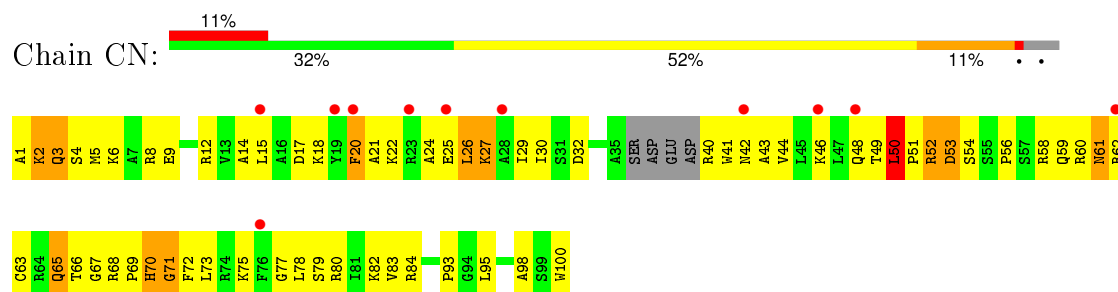
- Molecule 12: 30S ribosomal protein S13



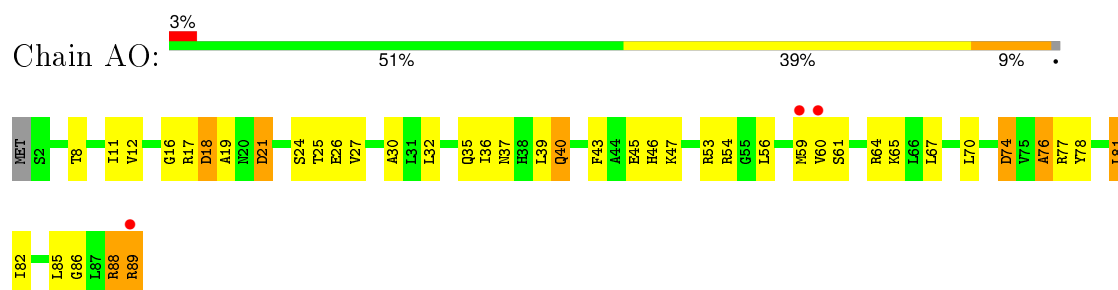
- Molecule 13: 30S ribosomal protein S14



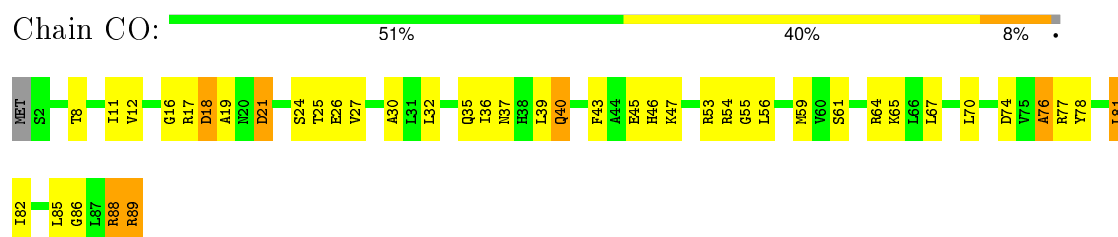
- Molecule 13: 30S ribosomal protein S14



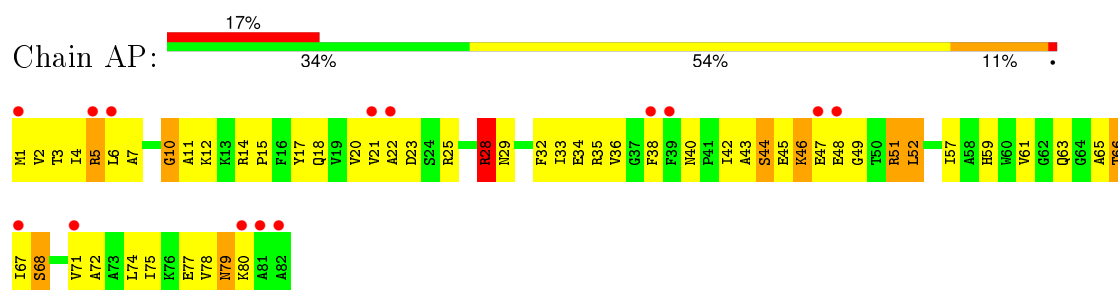
- Molecule 14: 30S ribosomal protein S15



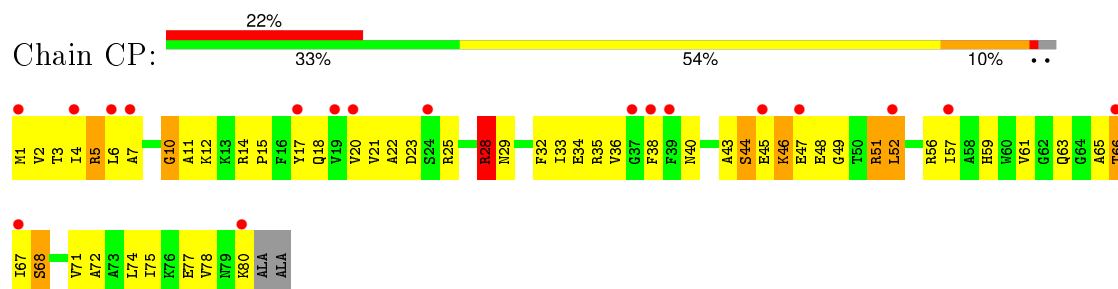
- Molecule 14: 30S ribosomal protein S15



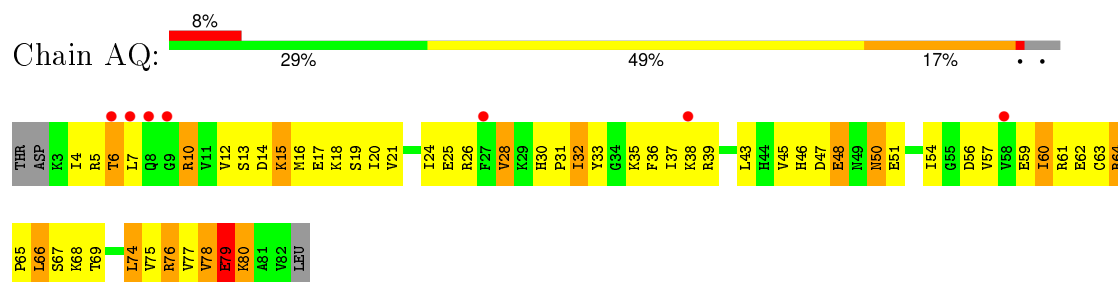
- Molecule 15: 30S ribosomal protein S16



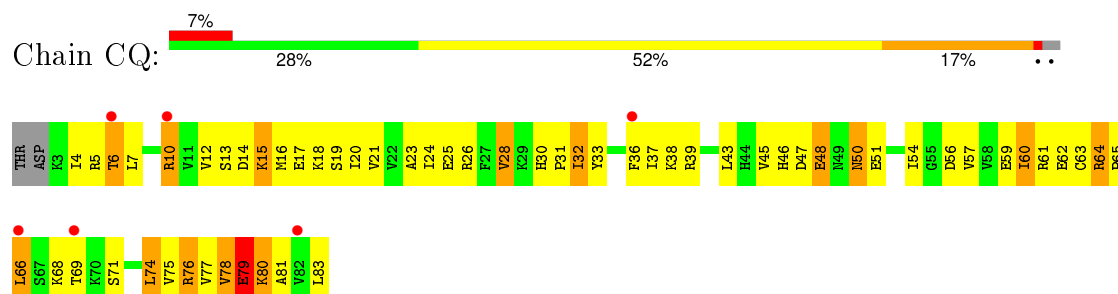
- Molecule 15: 30S ribosomal protein S16



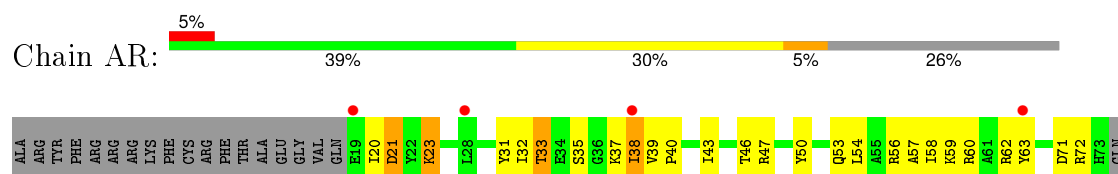
- Molecule 16: 30S ribosomal protein S17



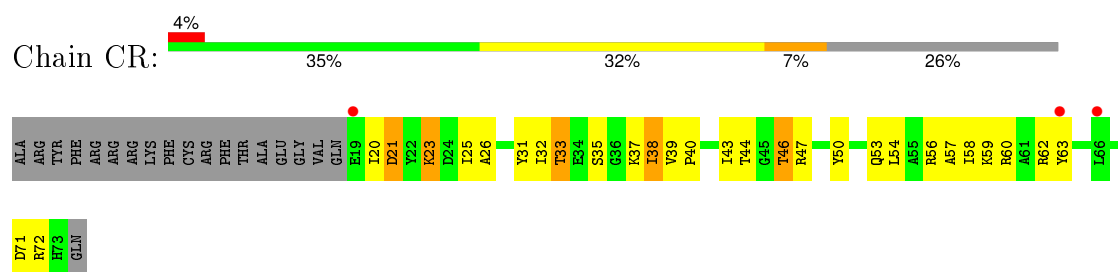
- Molecule 16: 30S ribosomal protein S17



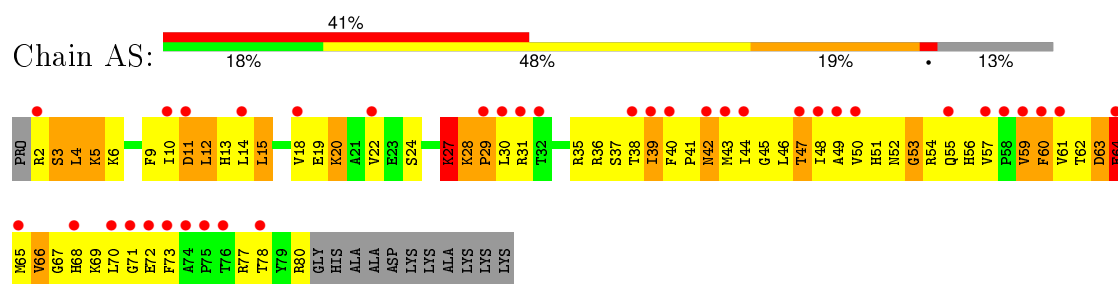
- Molecule 17: 30S ribosomal protein S18



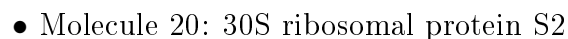
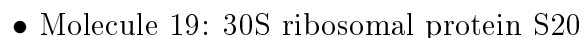
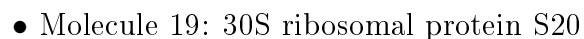
- Molecule 17: 30S ribosomal protein S18

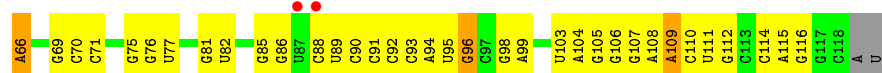


- Molecule 18: 30S ribosomal protein S19

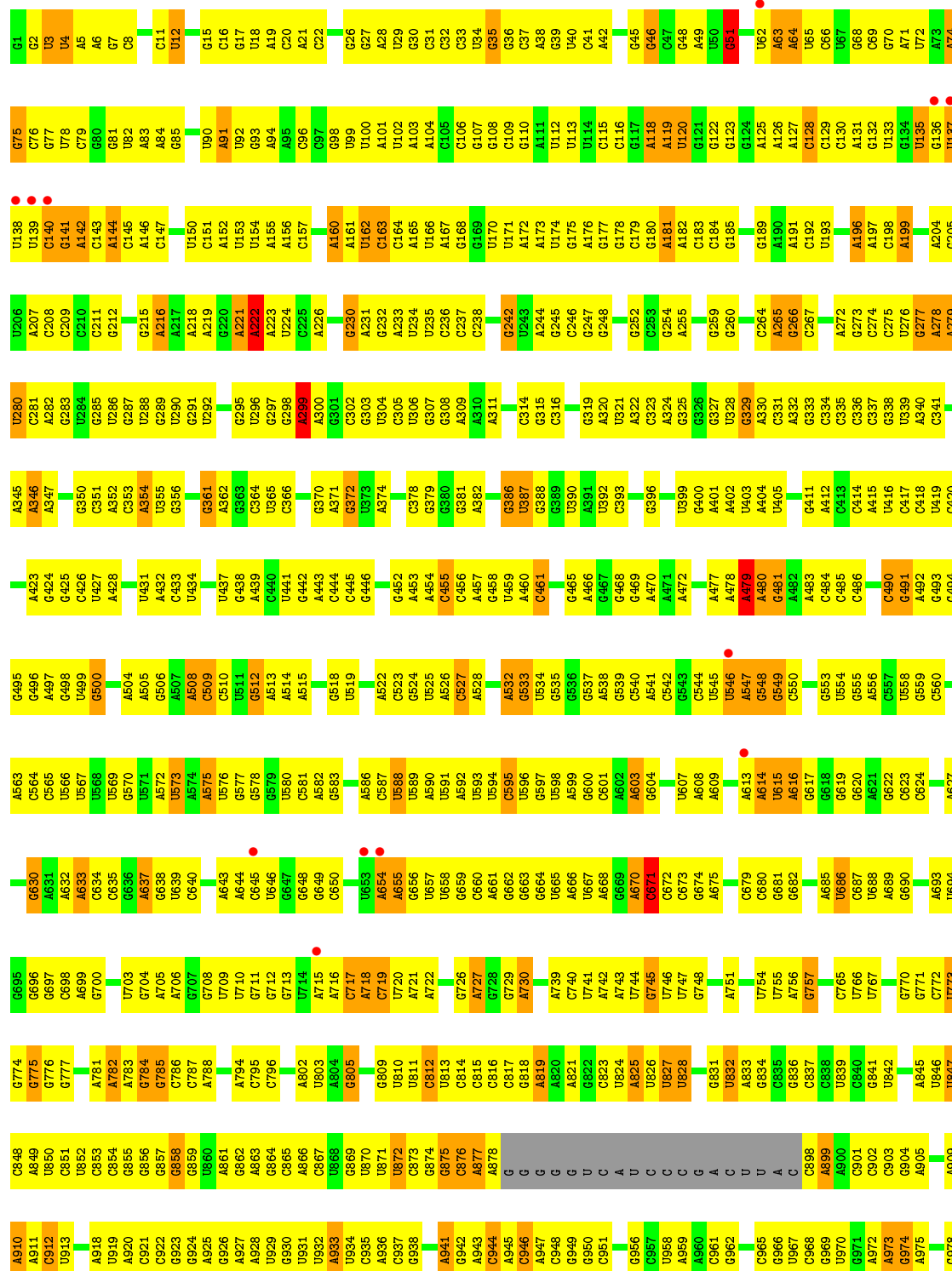


- Molecule 18: 30S ribosomal protein S19





• Molecule 23: 23S rRNA

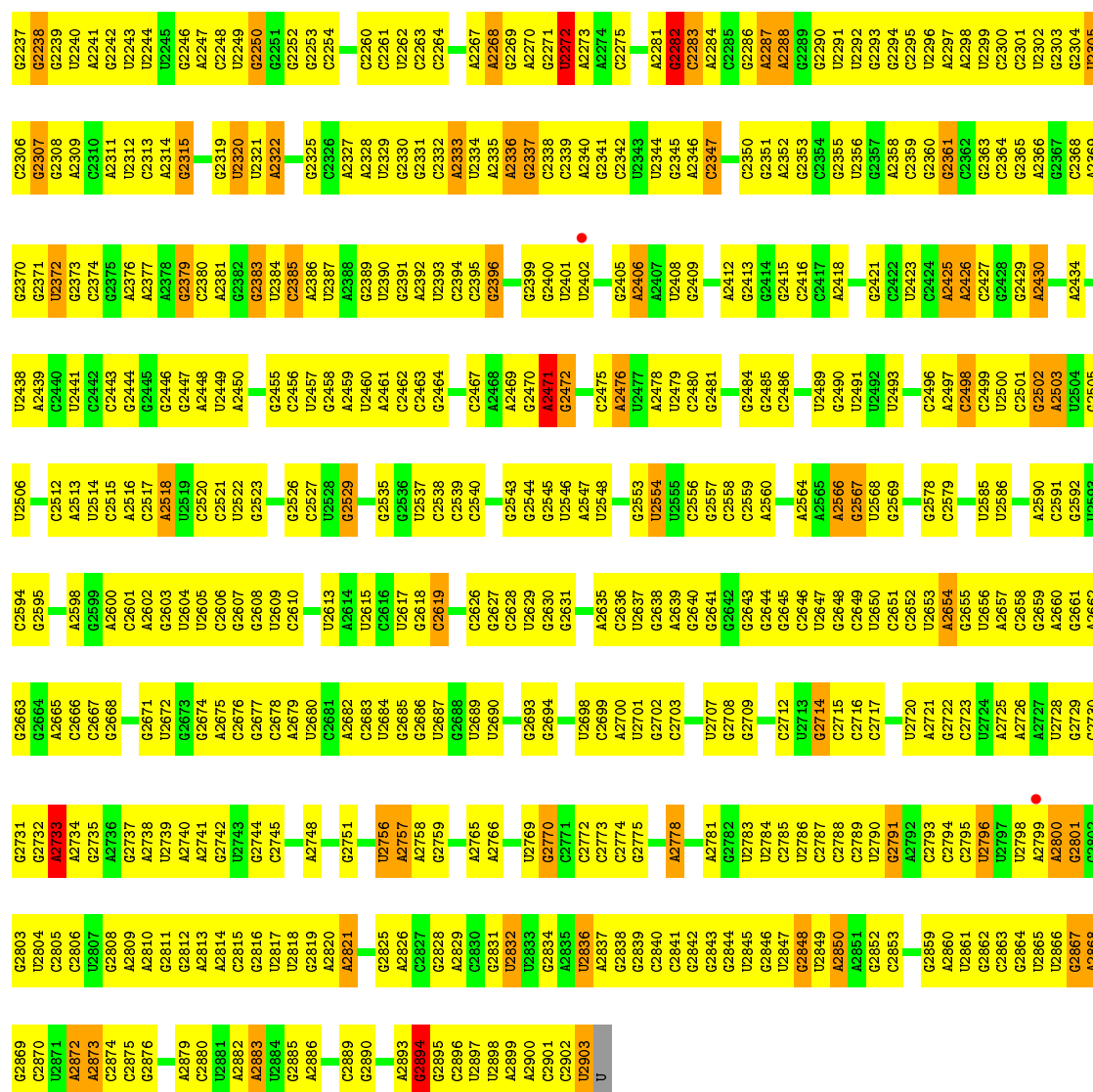


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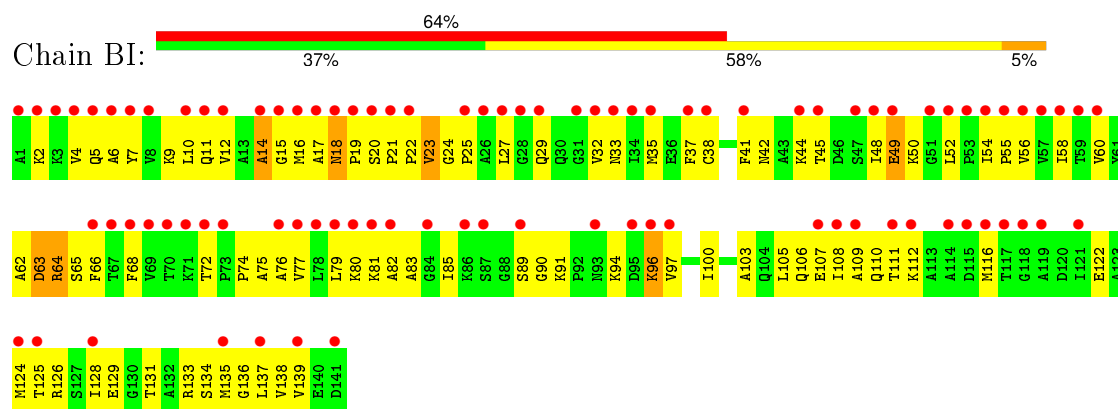


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	A972	A	U842	U842	G771	A693	C623	G559	G491	U419	A340	A279	U137	U137
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	A975		C848	C848	G775	G696	G630	C565	G495	A346	A282	G283	C208	G141
	G978		U849	U849	G776	G697	A631	U566	G496	A347	G284	U284	C209	A142
	A981		C850	C850	G777	C698	A632	U567	G497	U427	G285	G286	C210	C143
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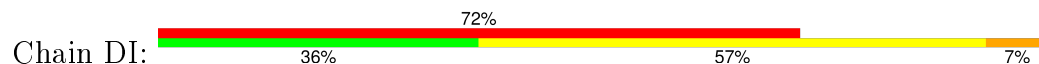


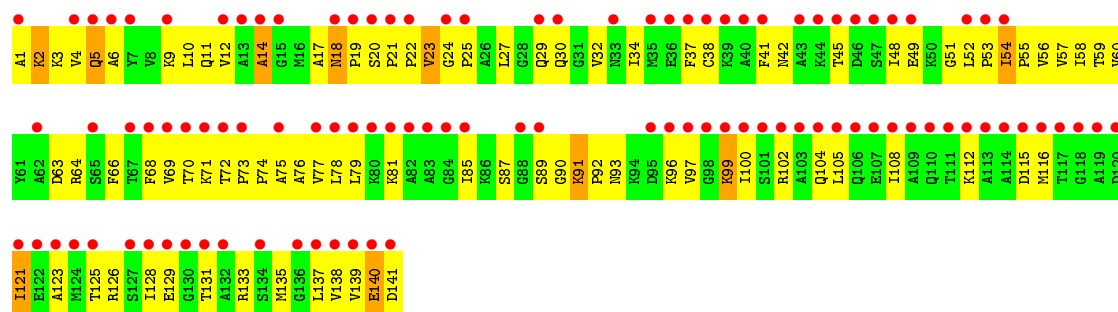


● Molecule 24: 50S ribosomal protein L11

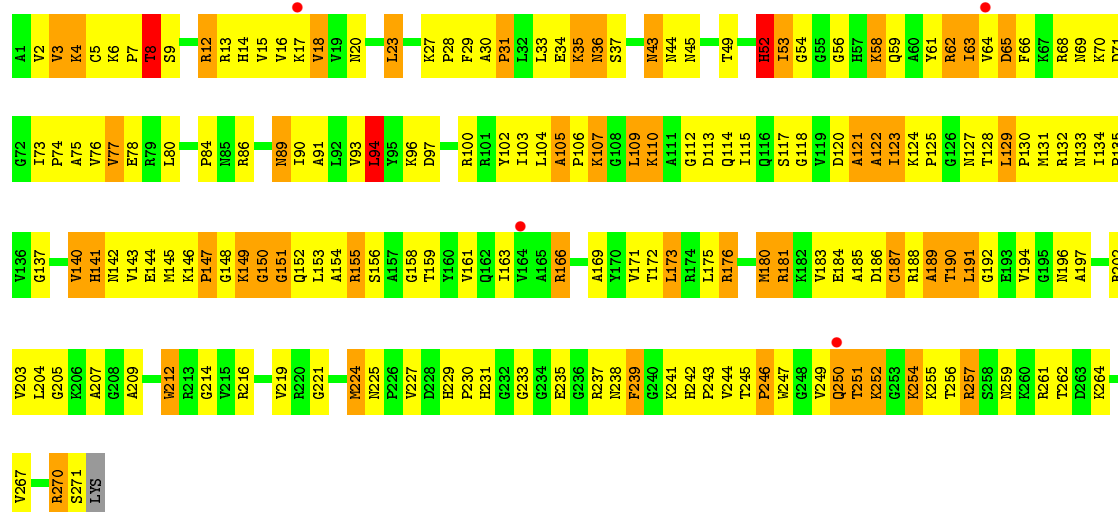


● Molecule 24: 50S ribosomal protein L11

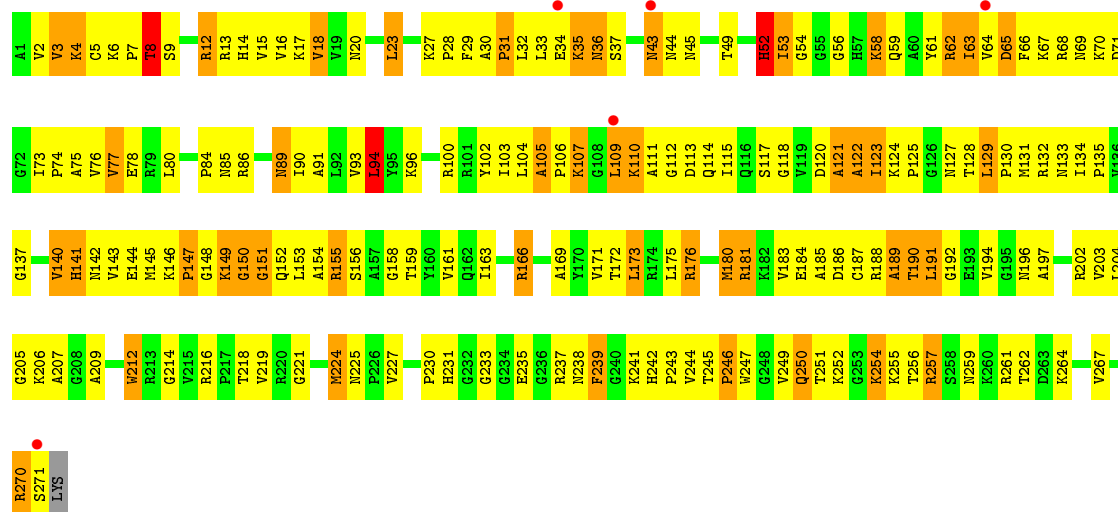




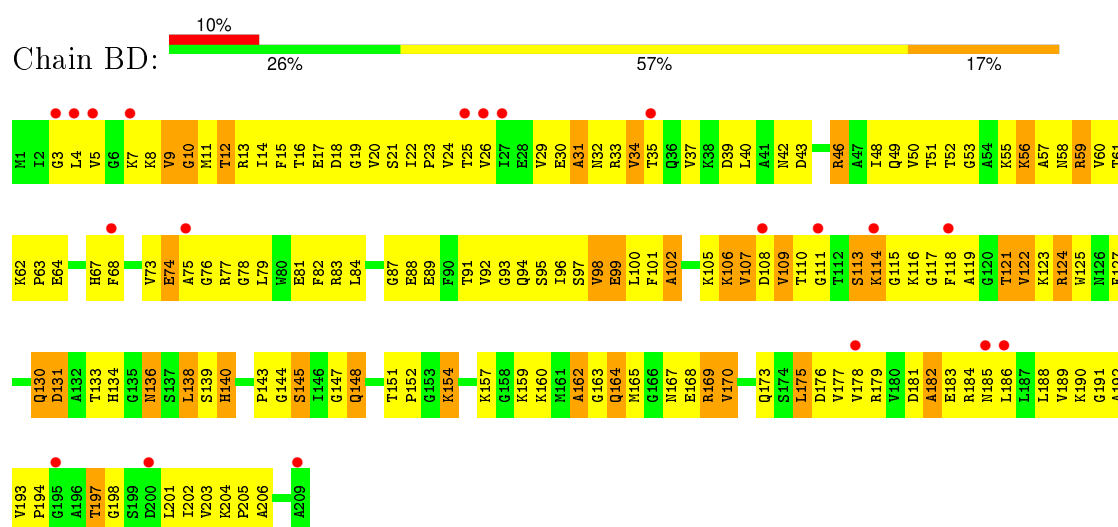
• Molecule 25: 50S ribosomal protein L2



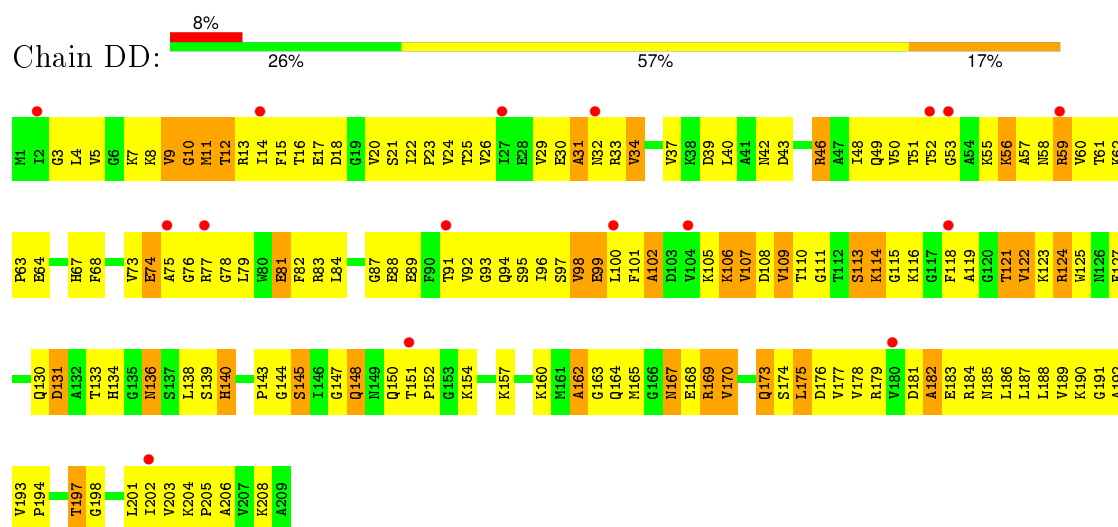
• Molecule 25: 50S ribosomal protein L2



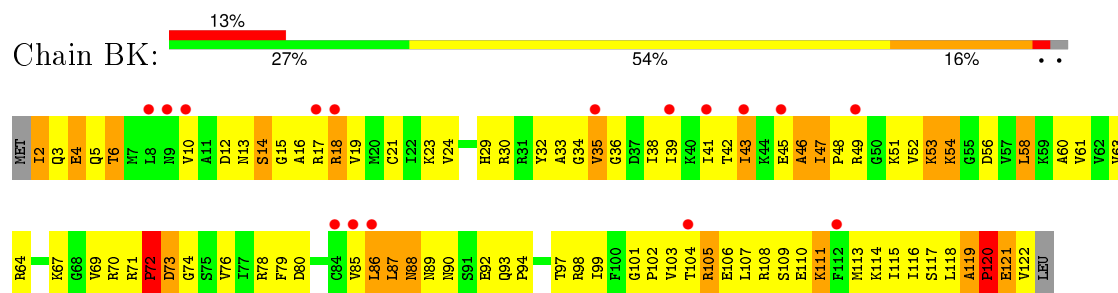
• Molecule 26: 50S ribosomal protein L3



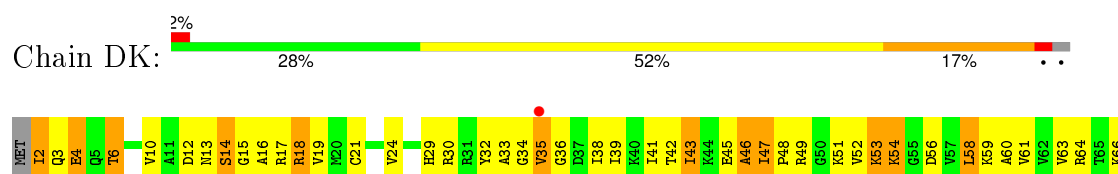
- Molecule 26: 50S ribosomal protein L3

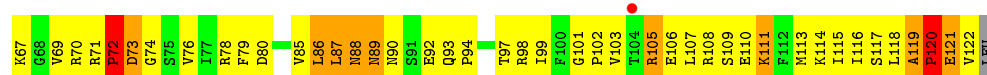


- Molecule 27: 50S ribosomal protein L14

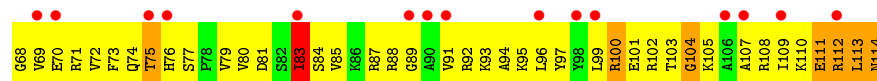
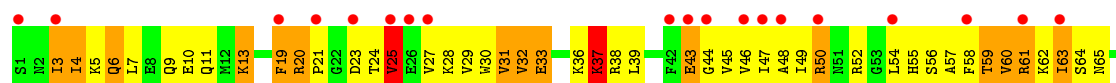


- Molecule 27: 50S ribosomal protein L14





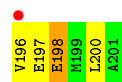
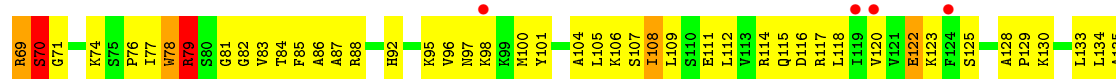
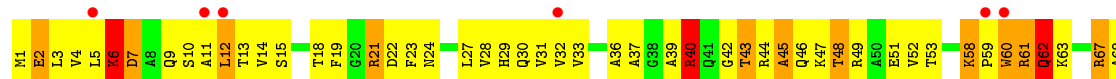
• Molecule 28: 50S ribosomal protein L19



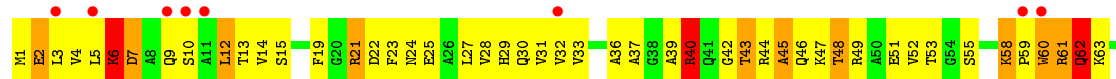
• Molecule 28: 50S ribosomal protein L19

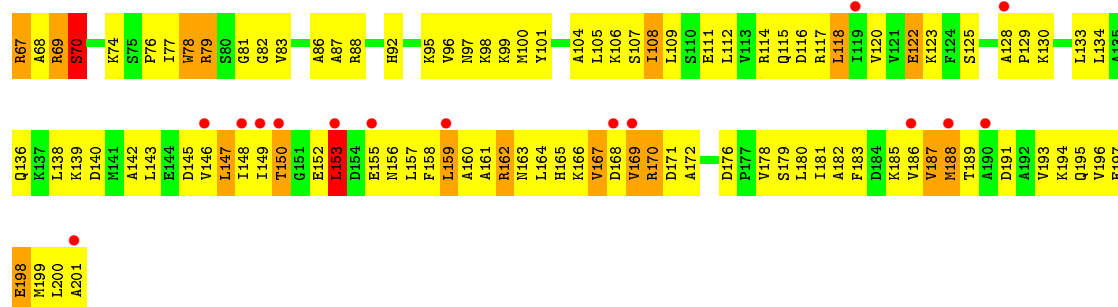


• Molecule 29: 50S ribosomal protein L4

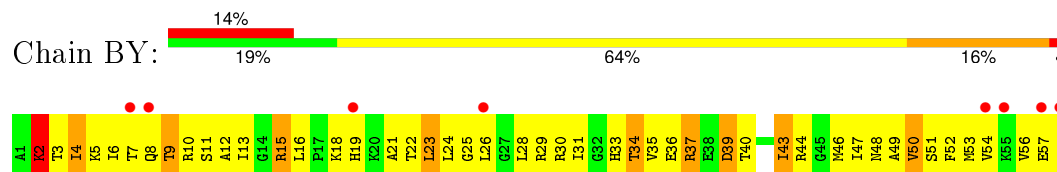


• Molecule 29: 50S ribosomal protein L4

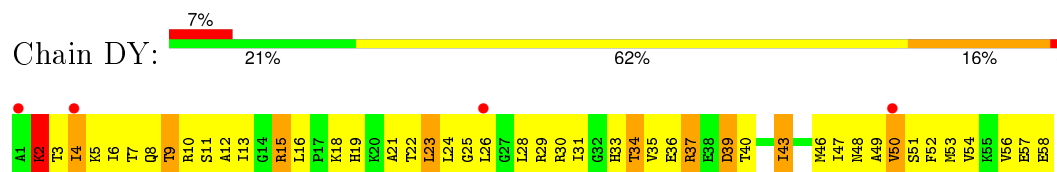




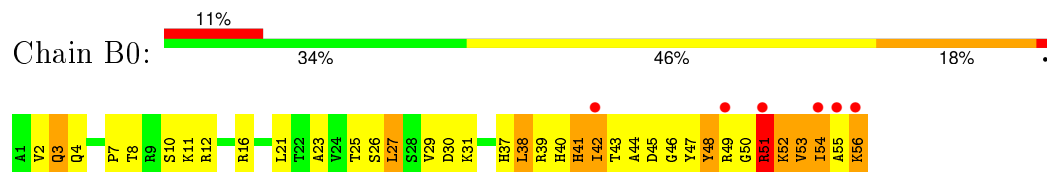
- Molecule 30: 50S ribosomal protein L30



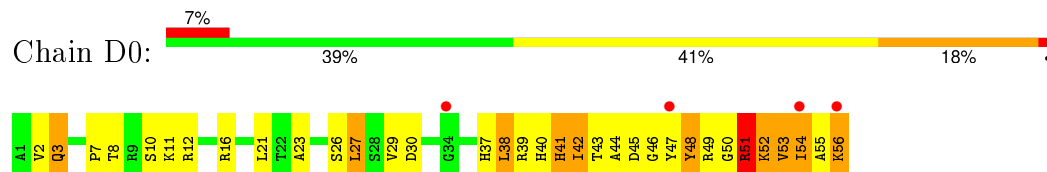
- Molecule 30: 50S ribosomal protein L30



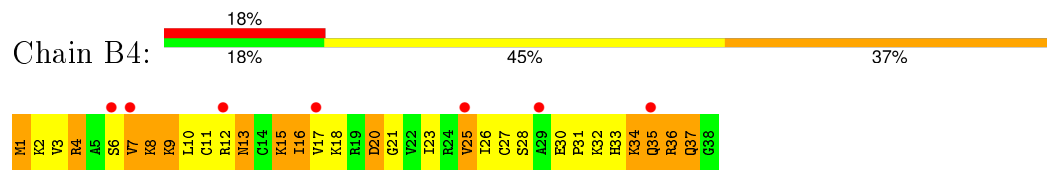
- Molecule 31: 50S ribosomal protein L32



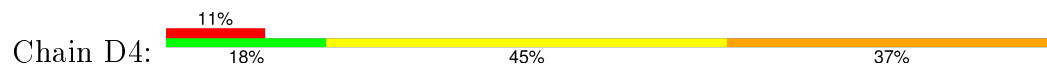
- Molecule 31: 50S ribosomal protein L32

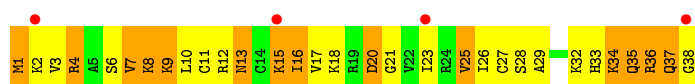


- Molecule 32: 50S ribosomal protein L36

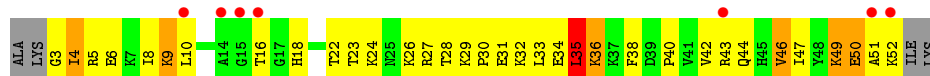


- Molecule 32: 50S ribosomal protein L36

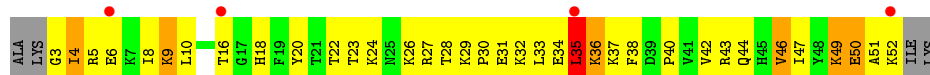




- Molecule 33: 50S ribosomal protein L33



- Molecule 33: 50S ribosomal protein L33



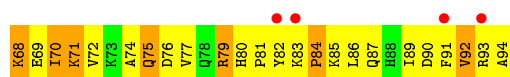
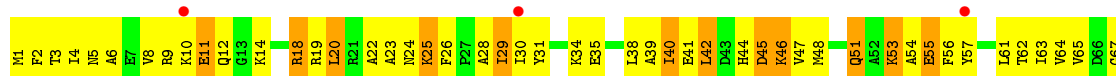
- Molecule 34: 50S ribosomal protein L35



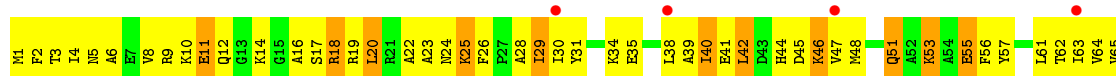
- Molecule 34: 50S ribosomal protein L35



- Molecule 35: 50S ribosomal protein L25

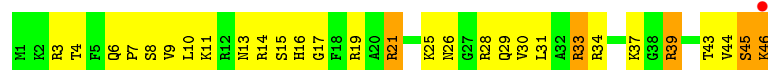


- Molecule 35: 50S ribosomal protein L25





- Molecule 36: 50S ribosomal protein L34



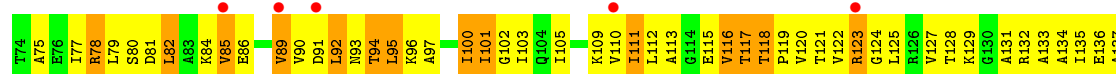
- Molecule 36: 50S ribosomal protein L34



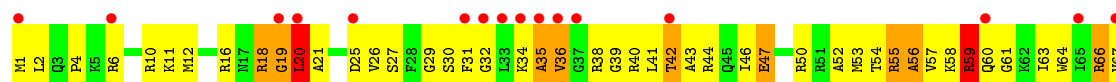
- Molecule 37: 50S ribosomal protein L15

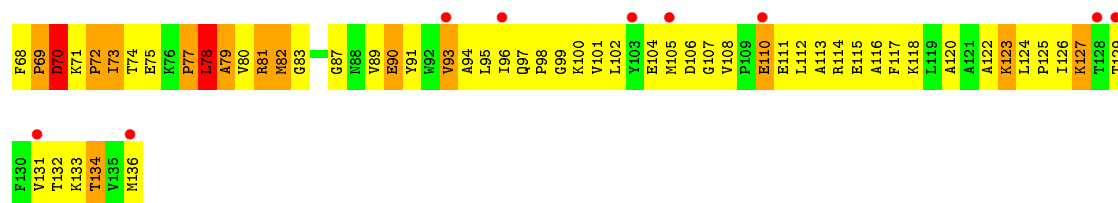


- Molecule 37: 50S ribosomal protein L15

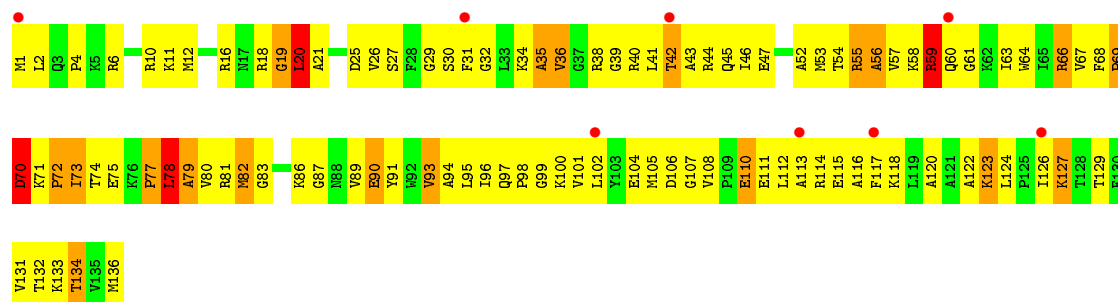


- Molecule 38: 50S ribosomal protein L16

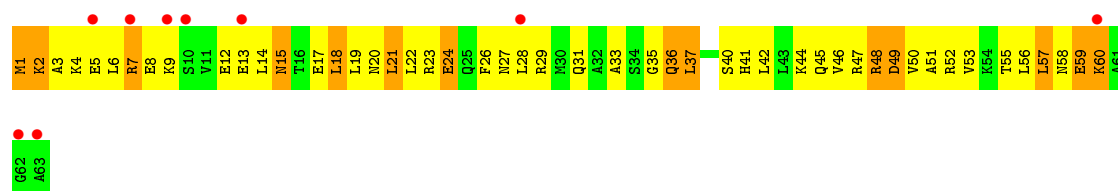




• Molecule 38: 50S ribosomal protein L16



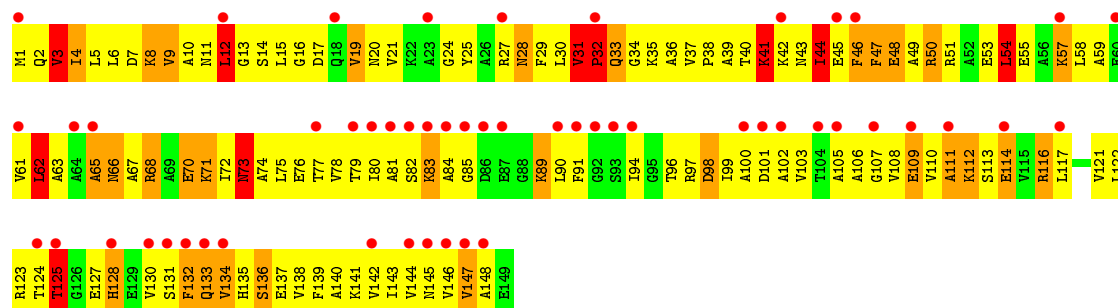
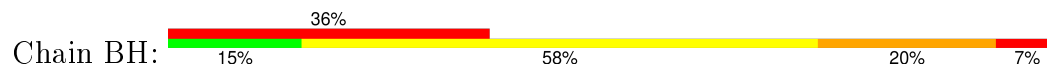
• Molecule 39: 50S ribosomal protein L29



• Molecule 39: 50S ribosomal protein L29



• Molecule 40: 50S ribosomal protein L9



- Chain DH:
-
- 32%
- 18%
- 56%
- 22%
- M1 Q2 V3 I4 L5 D7 K8 V9 A10 L11 L12 G13 S14 L15 G16 D17 Q18 V19 N20 V21 G24 Y25 A26 R27 N28 F29 L30 V31 P32 Q33 G34 K35 A36 V37 P38 A39 T40 K41 K42 K43 L44 E45 F46 F47 E48 A49 R50 E51 A52 E53 L54 E55 A56 K57 L58 A59 E60 V64 L62 A63 A64 V65 M66 A67 R68 A69 E70 K71 L72 M73 A74 L75 E76 T77 V78 T79 L80 A81 S82 K83 A84 G85 D86 E87 G88 K89 L90 I94 G95 T96 R97 D98 I99 A100 D101 A102 V103 T104 A105 V108 E109 F110 A111 K112 S113 E114 V115 R116 L117 P118 R119 G120 V121 L122 R123 T124 T125 G126 E127 H128 E129 V130 S131 F132 Q133 V134 H135 S136 E137 V138 F139 A140 K141 V142 L143 V144 M145 V146 E149

- Chain BJ:
-

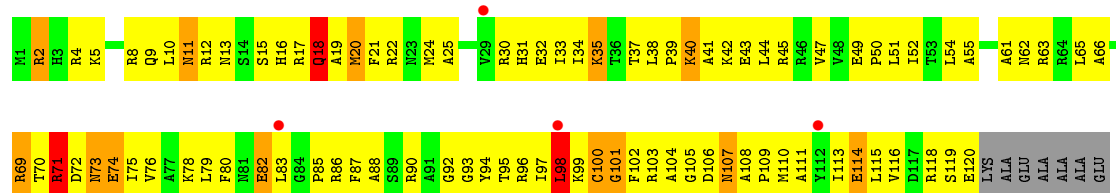
- Chain DJ:

Category	Percentage
Red Segment	9%
Green Segment	23%
Yellow Segment	59%

- Chain BN:
-
- 7% 21% 60% 11% 6%

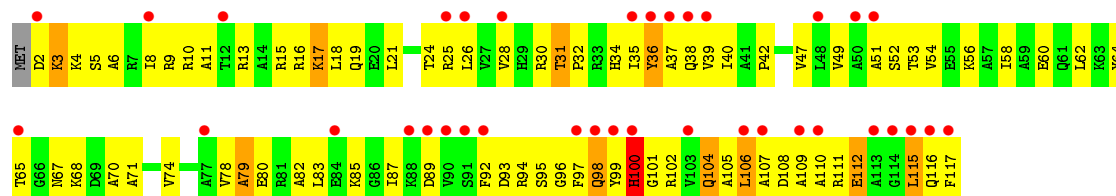
- Molecule 42: 50S ribosomal protein L17

Chain DN:  3% 23% 59% 10% 6%



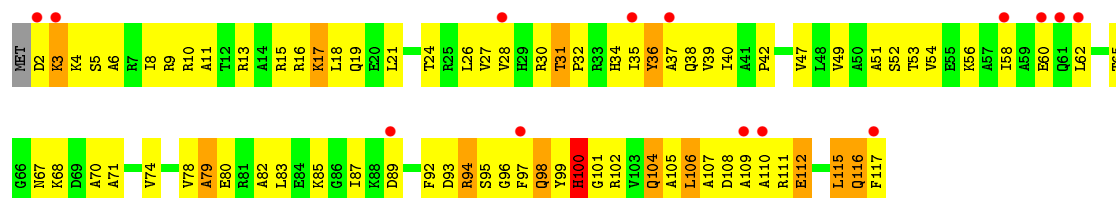
- Molecule 43: 50S ribosomal protein L18

Chain BO:  31% 32% 58% 9%




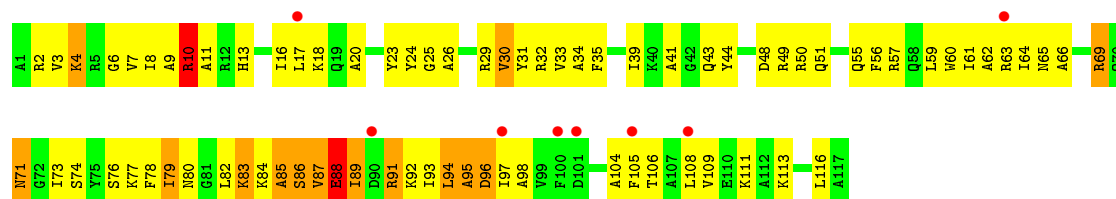
- Molecule 43: 50S ribosomal protein L18

Chain DO:  12% 32% 56% 10%



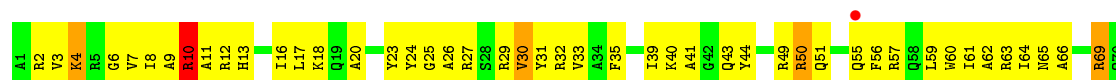
- Molecule 44: 50S ribosomal protein L20

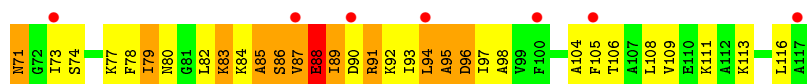
Chain BQ:  7% 34% 52% 12%



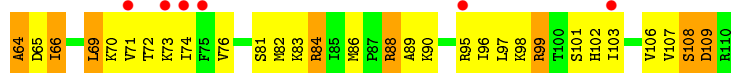
- Molecule 44: 50S ribosomal protein L20

Chain DQ:  7% 33% 52% 13%

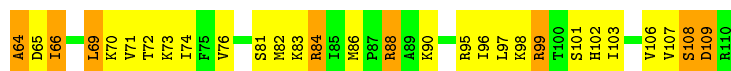
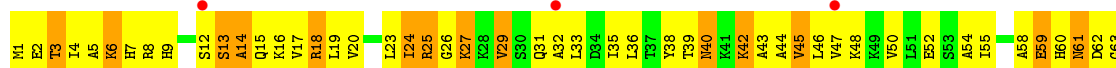




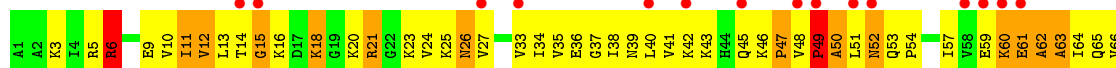
- Molecule 45: 50S ribosomal protein L22



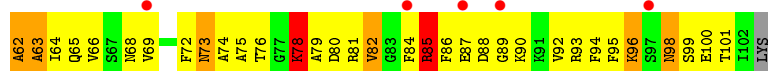
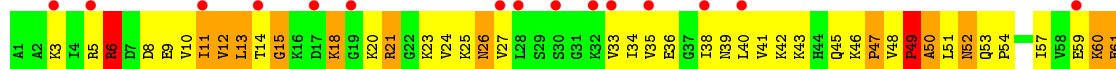
- Molecule 45: 50S ribosomal protein L22



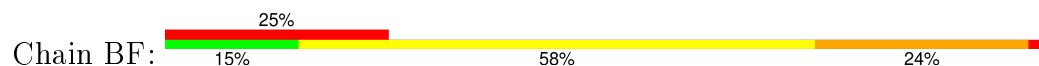
- Molecule 46: 50S ribosomal protein L24

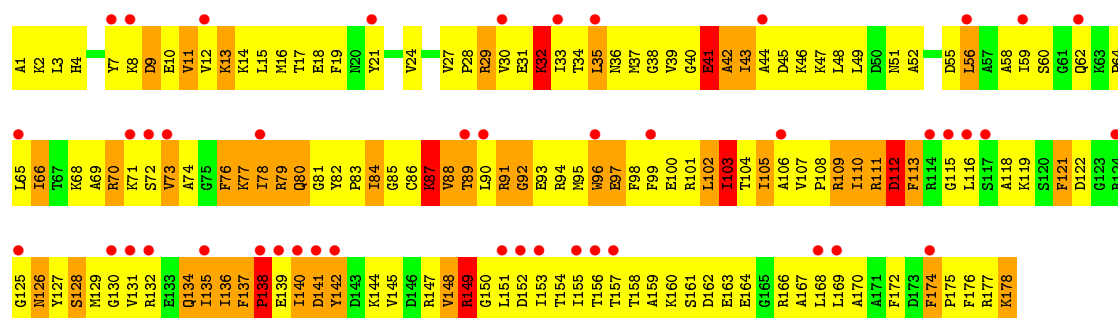


- Molecule 46: 50S ribosomal protein L24

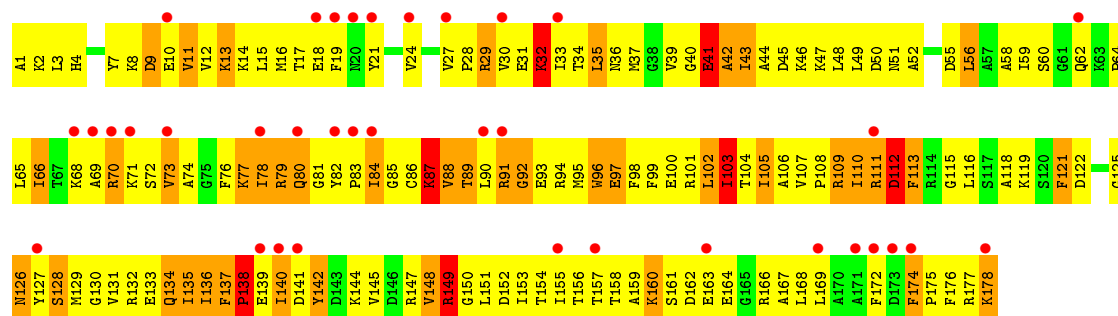
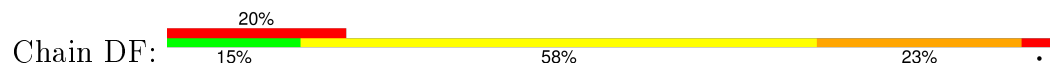


- Molecule 47: 50S ribosomal protein L5

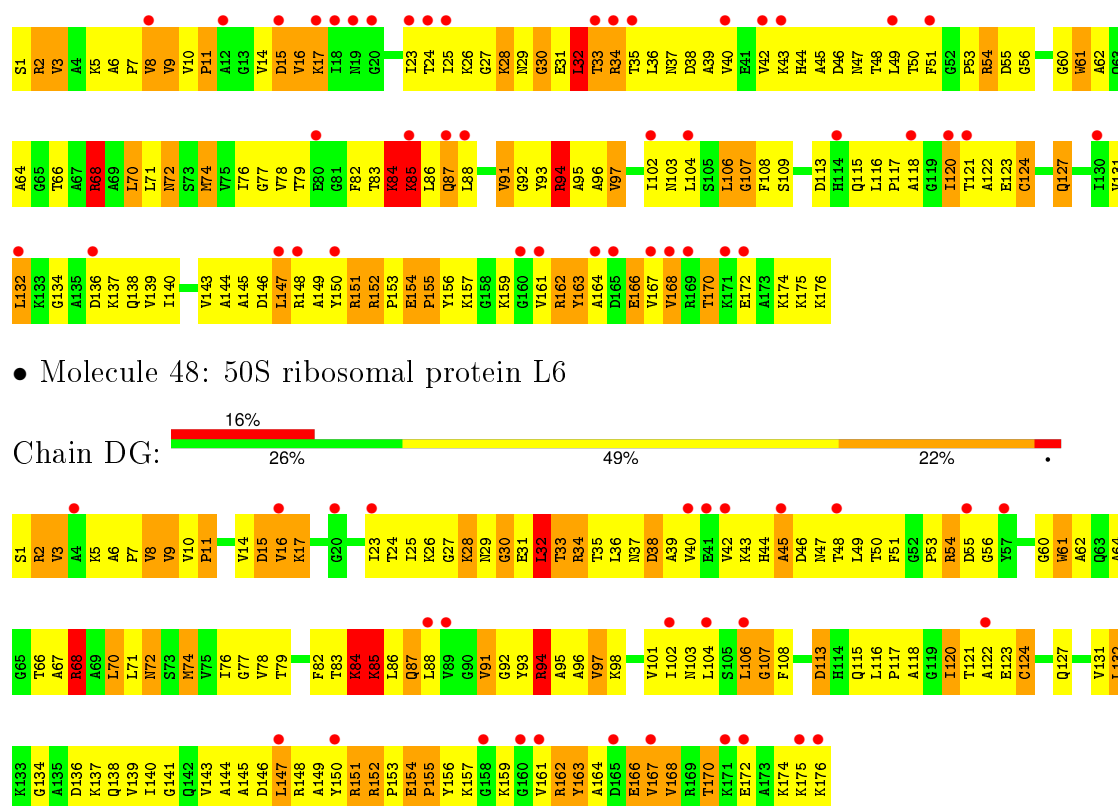




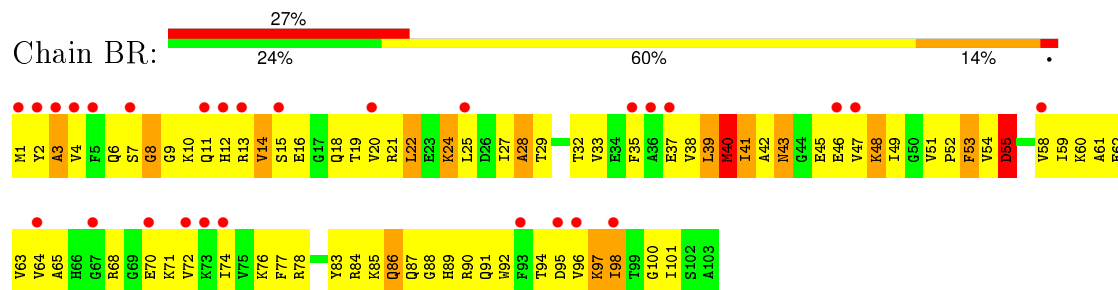
• Molecule 47: 50S ribosomal protein L5



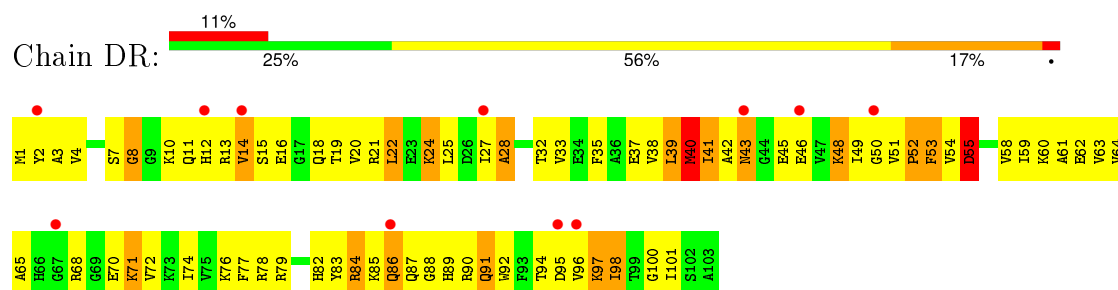
• Molecule 48: 50S ribosomal protein L6



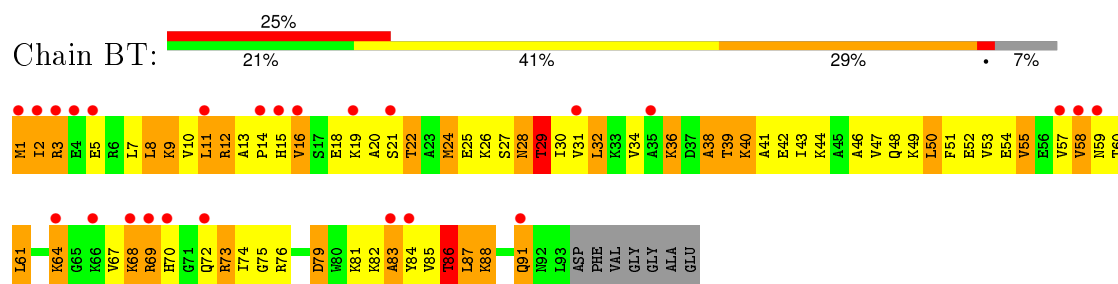
- Molecule 49: 50S ribosomal protein L21



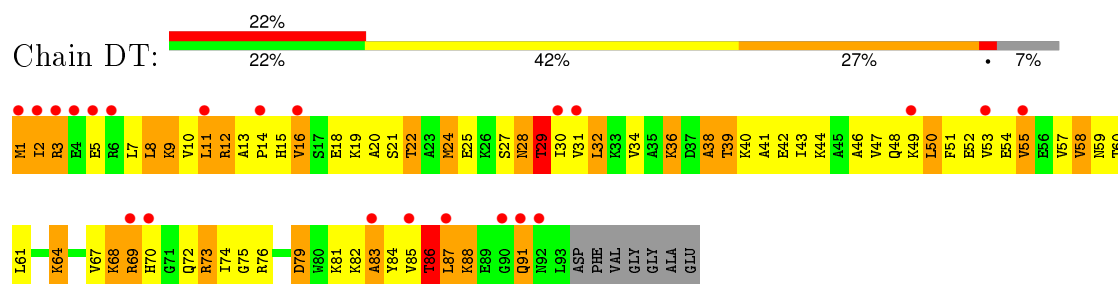
- Molecule 49: 50S ribosomal protein L21



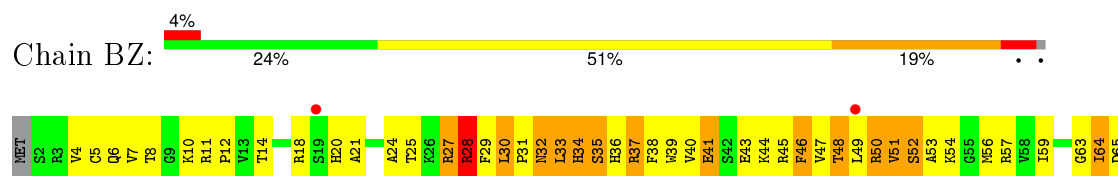
- Molecule 50: 50S ribosomal protein L23



- Molecule 50: 50S ribosomal protein L23

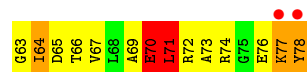
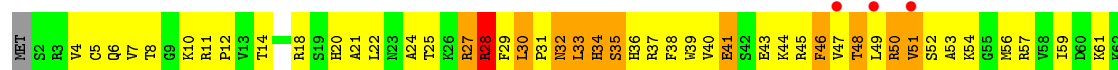


- Molecule 51: 50S ribosomal protein L28

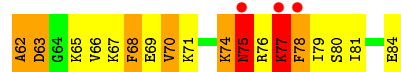
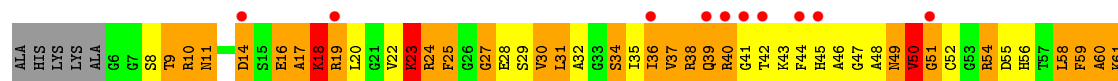
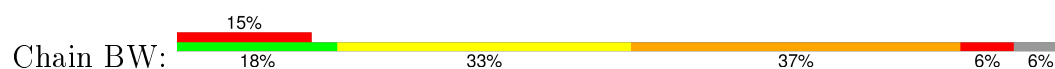




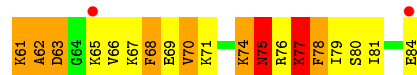
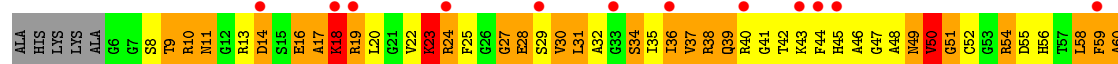
- Molecule 51: 50S ribosomal protein L28



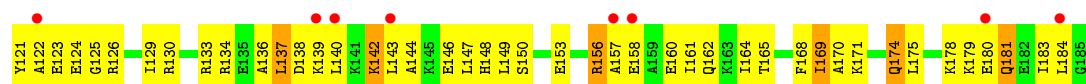
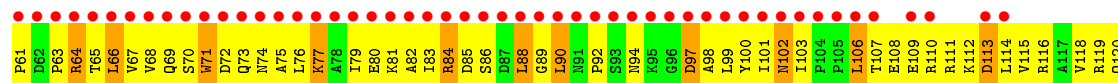
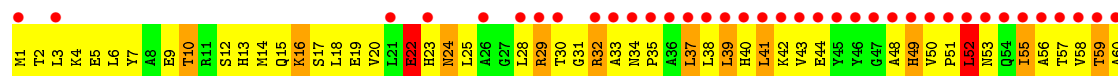
- Molecule 52: 50S ribosomal protein L27



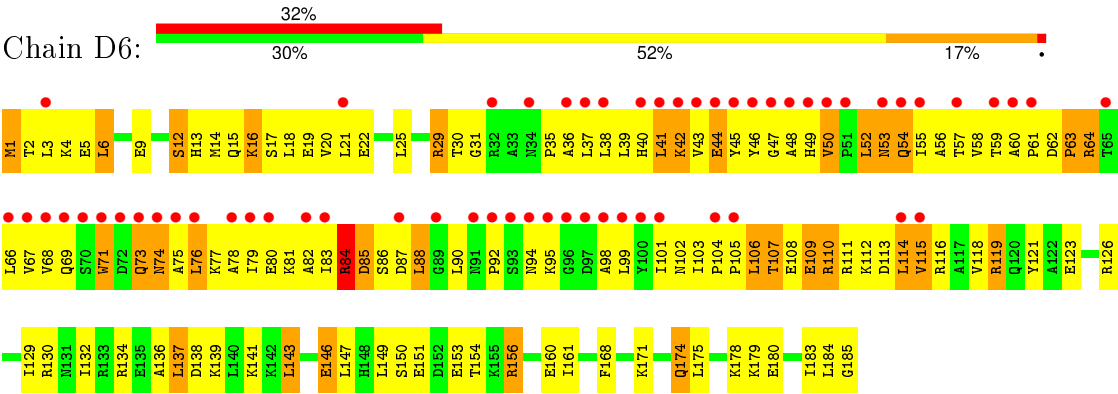
- Molecule 52: 50S ribosomal protein L27



- Molecule 53: ribosome recycling factor



- Molecule 53: ribosome recycling factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.90Å 378.20Å 736.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 82.86 – 3.32	Depositor EDS
% Data completeness (in resolution range)	85.8 (40.00-3.30) 87.2 (82.86-3.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.275 , 0.304 0.248 , 0.275	Depositor DCC
R_{free} test set	35383 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 57.9	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	2 of 738833 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	286960	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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

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	0.26	0/36762	0.75	11/57350 (0.0%)
1	CA	0.26	0/36762	0.75	18/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.45	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.43	0/2227
4	AE	0.23	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	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.46	0/1375
8	CI	0.24	0/1034	0.46	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	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.48	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	0.44	0/1043
13	CN	0.24	0/785	0.44	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	0.45	0/884
15	CP	0.25	0/648	0.45	0/870
16	AQ	0.23	0/657	0.47	0/881
16	CQ	0.24	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	0.23	0/671	0.40	0/888
19	CT	0.23	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	0.25	0/2803	0.74	1/4371 (0.0%)
22	DA	0.25	0/2803	0.74	1/4371 (0.0%)
23	BB	0.28	6/68314 (0.0%)	0.77	55/106569 (0.1%)
23	DB	0.28	8/68314 (0.0%)	0.78	51/106569 (0.0%)
24	BI	0.24	0/1046	0.47	0/1410
24	DI	0.25	0/1046	0.48	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	0.55	0/1258
27	DK	0.24	0/939	0.55	0/1258
28	BP	0.25	0/929	0.50	0/1242
28	DP	0.24	0/929	0.50	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	0.47	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	0.47	0/676
34	D3	0.24	0/513	0.47	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.26	0/380	0.48	0/498
36	D2	0.26	0/380	0.48	0/498
37	BL	0.23	0/1054	0.49	0/1403
37	DL	0.23	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	0.49	0/1460
39	BX	0.24	0/510	0.52	0/677
39	DX	0.24	0/510	0.52	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	0.51	0/1301
42	DN	0.24	0/973	0.51	0/1301
43	BO	0.23	0/902	0.49	0/1209
43	DO	0.23	0/902	0.49	0/1209
44	BQ	0.25	0/960	0.49	0/1278
44	DQ	0.25	0/960	0.49	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	0.47	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	0.48	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	0.55	0/994
50	DT	0.23	0/744	0.55	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	0.52	0/797
52	DW	0.28	0/603	0.52	0/797
53	B6	0.24	0/1497	0.48	0/2017
53	D6	0.23	0/1497	0.48	0/2017
All	All	0.26	14/309354 (0.0%)	0.70	137/462003 (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	14
1	CA	0	13
23	BB	0	29

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	DB	0	29
All	All	0	85

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-16.41	1.26	1.41
23	DB	1086	A	C5-C6	-16.29	1.26	1.41
23	DB	1088	A	C6-N1	-10.64	1.28	1.35
23	BB	1088	A	C6-N1	-10.54	1.28	1.35
23	DB	1060	U	C2-N3	7.91	1.43	1.37

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-29.30	75.55	110.70
23	BB	2204	G	O5'-P-OP2	-27.99	77.11	110.70
23	BB	2791	G	O5'-P-OP1	-27.68	77.49	110.70
23	DB	2791	G	O5'-P-OP2	-27.63	77.54	110.70
23	DB	2791	G	O5'-P-OP1	18.08	132.40	110.70

There are no chirality outliers.

5 of 85 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	437	U	Sidechain
1	AA	81	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	32831	0	16521	1151	0
2	AC	1624	0	1699	141	0
2	CC	1624	0	1699	138	0
3	AD	1643	0	1710	151	0
3	CD	1643	0	1710	155	0
4	AE	1105	0	1148	107	0
4	CE	1105	0	1148	102	0
5	AF	817	0	808	85	0
5	CF	817	0	808	82	0
6	AG	1174	0	1230	102	0
6	CG	1196	0	1246	91	0
7	AH	979	0	1034	62	0
7	CH	979	0	1034	62	0
8	AI	1022	0	1070	123	0
8	CI	1022	0	1070	126	0
9	AJ	786	0	828	76	0
9	CJ	786	0	828	76	0
10	AK	877	0	887	84	0
10	CK	877	0	887	73	0
11	AL	955	0	1019	85	0
11	CL	955	0	1019	92	0
12	AM	883	0	944	104	0
12	CM	876	0	937	109	0
13	AN	774	0	827	96	0
13	CN	774	0	827	95	0
14	AO	714	0	734	46	0
14	CO	714	0	734	51	0
15	AP	649	0	666	60	0
15	CP	638	0	656	60	0
16	AQ	648	0	691	64	0
16	CQ	657	0	702	65	0
17	AR	455	0	478	36	0
17	CR	455	0	478	37	0
18	AS	637	0	665	89	0
18	CS	644	0	675	91	0
19	AT	665	0	714	45	0
19	CT	665	0	714	44	0
20	AB	1704	0	1732	195	0
20	CB	1704	0	1732	198	0
21	AU	425	0	449	69	0
21	CU	425	0	449	68	0
22	BA	2507	0	1270	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	2507	0	1270	83	0
23	BB	60995	0	30679	2163	0
23	DB	60995	0	30677	2184	0
24	BI	1032	0	1088	112	0
24	DI	1032	0	1088	183	0
25	BC	2082	0	2157	232	0
25	DC	2082	0	2157	232	0
26	BD	1565	0	1616	186	0
26	DD	1565	0	1616	184	0
27	BK	930	0	1000	110	0
27	DK	930	0	1000	113	0
28	BP	917	0	965	136	0
28	DP	917	0	965	145	0
29	BE	1552	0	1619	188	0
29	DE	1552	0	1619	191	0
30	BY	449	0	491	52	0
30	DY	449	0	491	52	0
31	B0	444	0	461	39	0
31	D0	444	0	461	31	0
32	B4	302	0	340	50	0
32	D4	302	0	340	53	0
33	B1	409	0	440	51	0
33	D1	409	0	440	43	0
34	B3	504	0	574	54	0
34	D3	504	0	574	57	0
35	BV	753	0	780	86	0
35	DV	753	0	780	84	0
36	B2	377	0	418	34	0
36	D2	377	0	418	32	0
37	BL	1045	0	1117	138	0
37	DL	1045	0	1117	144	0
38	BM	1074	0	1157	120	0
38	DM	1074	0	1157	118	0
39	BX	509	0	543	56	0
39	DX	509	0	543	58	0
40	BH	1111	0	1148	220	0
40	DH	1111	0	1148	161	0
41	BJ	1129	0	1162	156	0
41	DJ	1129	0	1162	161	0
42	BN	960	0	1000	111	0
42	DN	960	0	1000	108	0
43	BO	892	0	923	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DO	892	0	923	81	0
44	BQ	947	0	1022	125	0
44	DQ	947	0	1022	136	0
45	BS	857	0	922	94	0
45	DS	857	0	922	93	0
46	BU	779	0	834	111	0
46	DU	779	0	834	111	0
47	BF	1420	0	1460	242	0
47	DF	1420	0	1460	233	0
48	BG	1323	0	1374	158	0
48	DG	1323	0	1374	159	0
49	BR	816	0	839	85	0
49	DR	816	0	839	96	0
50	BT	738	0	807	120	0
50	DT	738	0	807	115	0
51	BZ	625	0	652	63	0
51	DZ	625	0	652	61	0
52	BW	596	0	610	138	0
52	DW	596	0	610	152	0
53	B6	1478	0	1526	204	0
53	D6	1478	0	1526	177	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	61	0	0	0	0
54	CE	1	0	0	0	0
54	DB	111	0	0	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	289	0	0	1	0
56	AE	4	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AN	3	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	B2	1	0	0	0	0
56	BB	495	0	0	5	0
56	BC	4	0	0	0	0
56	BD	1	0	0	0	0
56	BE	3	0	0	0	0
56	BL	1	0	0	0	0
56	BT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CA	300	0	0	0	0
56	CE	2	0	0	0	0
56	CK	1	0	0	0	0
56	CL	1	0	0	0	0
56	CN	4	0	0	0	0
56	CT	1	0	0	0	0
56	DB	505	0	0	7	0
56	DC	4	0	0	1	0
56	DD	1	0	0	0	0
56	DE	2	0	0	0	0
All	All	286960	0	193714	16198	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 16198 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	1.39	1.17
13:CN:63:CYS:HB3	13:CN:67:GLY:H	1.09	1.16
13:AN:63:CYS:HB3	13:AN:67:GLY:H	1.05	1.15
10:AK:124:LYS:HA	21:AU:34:ARG:HB3	1.27	1.14
29:DE:21:ARG:HD2	29:DE:107:SER:HB3	1.30	1.13

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%)	152 (74%)	36 (18%)	16 (8%)	1	9
2	CC	204/232 (88%)	151 (74%)	37 (18%)	16 (8%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	151 (74%)	39 (19%)	13 (6%)	2	13
3	CD	203/205 (99%)	150 (74%)	41 (20%)	12 (6%)	2	15
4	AE	148/166 (89%)	125 (84%)	20 (14%)	3 (2%)	9	43
4	CE	148/166 (89%)	125 (84%)	20 (14%)	3 (2%)	9	43
5	AF	98/135 (73%)	71 (72%)	18 (18%)	9 (9%)	1	6
5	CF	98/135 (73%)	69 (70%)	21 (21%)	8 (8%)	1	8
6	AG	148/178 (83%)	114 (77%)	28 (19%)	6 (4%)	3	24
6	CG	150/178 (84%)	118 (79%)	25 (17%)	7 (5%)	3	20
7	AH	127/129 (98%)	106 (84%)	17 (13%)	4 (3%)	5	32
7	CH	127/129 (98%)	105 (83%)	18 (14%)	4 (3%)	5	32
8	AI	125/129 (97%)	92 (74%)	28 (22%)	5 (4%)	4	24
8	CI	125/129 (97%)	93 (74%)	28 (22%)	4 (3%)	5	31
9	AJ	96/103 (93%)	73 (76%)	13 (14%)	10 (10%)	1	4
9	CJ	96/103 (93%)	74 (77%)	12 (12%)	10 (10%)	1	4
10	AK	115/128 (90%)	85 (74%)	25 (22%)	5 (4%)	3	23
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	2	18
11	AL	121/123 (98%)	84 (69%)	28 (23%)	9 (7%)	1	10
11	CL	121/123 (98%)	86 (71%)	25 (21%)	10 (8%)	1	8
12	AM	112/117 (96%)	85 (76%)	16 (14%)	11 (10%)	1	5
12	CM	111/117 (95%)	83 (75%)	17 (15%)	11 (10%)	1	5
13	AN	92/100 (92%)	65 (71%)	19 (21%)	8 (9%)	1	7
13	CN	92/100 (92%)	66 (72%)	18 (20%)	8 (9%)	1	7
14	AO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	4	29
14	CO	86/89 (97%)	70 (81%)	14 (16%)	2 (2%)	8	39
15	AP	80/82 (98%)	62 (78%)	10 (12%)	8 (10%)	1	5
15	CP	78/82 (95%)	61 (78%)	11 (14%)	6 (8%)	1	9
16	AQ	78/83 (94%)	59 (76%)	15 (19%)	4 (5%)	2	19
16	CQ	79/83 (95%)	60 (76%)	15 (19%)	4 (5%)	2	19
17	AR	53/74 (72%)	48 (91%)	5 (9%)	0	100	100
17	CR	53/74 (72%)	48 (91%)	5 (9%)	0	100	100
18	AS	77/91 (85%)	59 (77%)	12 (16%)	6 (8%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CS	78/91 (86%)	61 (78%)	11 (14%)	6 (8%)	1	9
19	AT	83/86 (96%)	64 (77%)	15 (18%)	4 (5%)	3	20
19	CT	83/86 (96%)	65 (78%)	14 (17%)	4 (5%)	3	20
20	AB	216/240 (90%)	153 (71%)	48 (22%)	15 (7%)	1	11
20	CB	216/240 (90%)	150 (69%)	49 (23%)	17 (8%)	1	8
21	AU	49/70 (70%)	31 (63%)	10 (20%)	8 (16%)	0	1
21	CU	49/70 (70%)	31 (63%)	10 (20%)	8 (16%)	0	1
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	4	28
24	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	6	34
25	BC	269/272 (99%)	176 (65%)	61 (23%)	32 (12%)	0	3
25	DC	269/272 (99%)	177 (66%)	59 (22%)	33 (12%)	0	2
26	BD	207/209 (99%)	123 (59%)	56 (27%)	28 (14%)	0	2
26	DD	207/209 (99%)	122 (59%)	55 (27%)	30 (14%)	0	1
27	BK	119/123 (97%)	80 (67%)	25 (21%)	14 (12%)	0	3
27	DK	119/123 (97%)	81 (68%)	24 (20%)	14 (12%)	0	3
28	BP	112/114 (98%)	68 (61%)	29 (26%)	15 (13%)	0	2
28	DP	112/114 (98%)	69 (62%)	28 (25%)	15 (13%)	0	2
29	BE	199/201 (99%)	126 (63%)	54 (27%)	19 (10%)	1	6
29	DE	199/201 (99%)	127 (64%)	52 (26%)	20 (10%)	1	5
30	BY	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	4
30	DY	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	4
31	B0	54/56 (96%)	40 (74%)	5 (9%)	9 (17%)	0	1
31	D0	54/56 (96%)	40 (74%)	5 (9%)	9 (17%)	0	1
32	B4	36/38 (95%)	22 (61%)	5 (14%)	9 (25%)	0	0
32	D4	36/38 (95%)	22 (61%)	5 (14%)	9 (25%)	0	0
33	B1	48/54 (89%)	37 (77%)	6 (12%)	5 (10%)	1	4
33	D1	48/54 (89%)	36 (75%)	7 (15%)	5 (10%)	1	4
34	B3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	1	5
34	D3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	1	5
35	BV	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	5	30
35	DV	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	B2	44/46 (96%)	36 (82%)	7 (16%)	1 (2%)	8	39
36	D2	44/46 (96%)	35 (80%)	7 (16%)	2 (4%)	3	21
37	BL	141/144 (98%)	92 (65%)	31 (22%)	18 (13%)	0	2
37	DL	141/144 (98%)	94 (67%)	28 (20%)	19 (14%)	0	2
38	BM	134/136 (98%)	90 (67%)	24 (18%)	20 (15%)	0	1
38	DM	134/136 (98%)	90 (67%)	24 (18%)	20 (15%)	0	1
39	BX	61/63 (97%)	40 (66%)	17 (28%)	4 (7%)	1	12
39	DX	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	12
40	BH	147/149 (99%)	74 (50%)	50 (34%)	23 (16%)	0	1
40	DH	147/149 (99%)	92 (63%)	38 (26%)	17 (12%)	0	3
41	BJ	140/142 (99%)	96 (69%)	31 (22%)	13 (9%)	1	6
41	DJ	140/142 (99%)	95 (68%)	32 (23%)	13 (9%)	1	6
42	BN	118/127 (93%)	84 (71%)	25 (21%)	9 (8%)	1	9
42	DN	118/127 (93%)	82 (70%)	25 (21%)	11 (9%)	1	6
43	BO	114/117 (97%)	87 (76%)	21 (18%)	6 (5%)	2	17
43	DO	114/117 (97%)	86 (75%)	21 (18%)	7 (6%)	2	14
44	BQ	115/117 (98%)	81 (70%)	21 (18%)	13 (11%)	0	3
44	DQ	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	1	4
45	BS	108/110 (98%)	72 (67%)	21 (19%)	15 (14%)	0	2
45	DS	108/110 (98%)	73 (68%)	20 (18%)	15 (14%)	0	2
46	BU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
46	DU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
47	BF	176/178 (99%)	106 (60%)	36 (20%)	34 (19%)	0	1
47	DF	176/178 (99%)	106 (60%)	36 (20%)	34 (19%)	0	1
48	BG	174/176 (99%)	108 (62%)	41 (24%)	25 (14%)	0	1
48	DG	174/176 (99%)	109 (63%)	39 (22%)	26 (15%)	0	1
49	BR	101/103 (98%)	74 (73%)	16 (16%)	11 (11%)	0	4
49	DR	101/103 (98%)	73 (72%)	17 (17%)	11 (11%)	0	4
50	BT	91/100 (91%)	52 (57%)	23 (25%)	16 (18%)	0	1
50	DT	91/100 (91%)	52 (57%)	24 (26%)	15 (16%)	0	1
51	BZ	75/78 (96%)	50 (67%)	16 (21%)	9 (12%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DZ	75/78 (96%)	50 (67%)	17 (23%)	8 (11%)	0	4
52	BW	77/84 (92%)	32 (42%)	20 (26%)	25 (32%)	0	0
52	DW	77/84 (92%)	33 (43%)	18 (23%)	26 (34%)	0	0
53	B6	183/185 (99%)	140 (76%)	36 (20%)	7 (4%)	4	26
53	D6	183/185 (99%)	146 (80%)	28 (15%)	9 (5%)	3	19
All	All	11607/12284 (94%)	8146 (70%)	2335 (20%)	1126 (10%)	1	5

5 of 1126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	25	THR
2	AC	54	ILE
2	AC	100	ILE
2	AC	104	GLU

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%)	145 (85%)	25 (15%)	4	18
2	CC	170/189 (90%)	145 (85%)	25 (15%)	4	18
3	AD	172/172 (100%)	138 (80%)	34 (20%)	1	7
3	CD	172/172 (100%)	138 (80%)	34 (20%)	1	7
4	AE	113/125 (90%)	99 (88%)	14 (12%)	6	25
4	CE	113/125 (90%)	99 (88%)	14 (12%)	6	25
5	AF	87/116 (75%)	70 (80%)	17 (20%)	2	7
5	CF	87/116 (75%)	70 (80%)	17 (20%)	2	7
6	AG	123/146 (84%)	101 (82%)	22 (18%)	2	10
6	CG	125/146 (86%)	103 (82%)	22 (18%)	2	10
7	AH	104/104 (100%)	95 (91%)	9 (9%)	13	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	CH	104/104 (100%)	96 (92%)	8 (8%)	16	51
8	AI	105/106 (99%)	86 (82%)	19 (18%)	2	9
8	CI	105/106 (99%)	86 (82%)	19 (18%)	2	9
9	AJ	86/90 (96%)	75 (87%)	11 (13%)	5	23
9	CJ	86/90 (96%)	76 (88%)	10 (12%)	7	29
10	AK	90/98 (92%)	74 (82%)	16 (18%)	2	10
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2	10
11	AL	103/103 (100%)	87 (84%)	16 (16%)	3	16
11	CL	103/103 (100%)	87 (84%)	16 (16%)	3	16
12	AM	92/95 (97%)	71 (77%)	21 (23%)	1	4
12	CM	91/95 (96%)	69 (76%)	22 (24%)	1	3
13	AN	79/83 (95%)	71 (90%)	8 (10%)	9	35
13	CN	79/83 (95%)	71 (90%)	8 (10%)	9	35
14	AO	76/77 (99%)	70 (92%)	6 (8%)	15	49
14	CO	76/77 (99%)	70 (92%)	6 (8%)	15	49
15	AP	65/65 (100%)	57 (88%)	8 (12%)	6	25
15	CP	65/65 (100%)	56 (86%)	9 (14%)	4	20
16	AQ	74/77 (96%)	59 (80%)	15 (20%)	1	6
16	CQ	75/77 (97%)	60 (80%)	15 (20%)	1	6
17	AR	48/64 (75%)	43 (90%)	5 (10%)	9	34
17	CR	48/64 (75%)	43 (90%)	5 (10%)	9	34
18	AS	70/78 (90%)	53 (76%)	17 (24%)	1	3
18	CS	71/78 (91%)	55 (78%)	16 (22%)	1	4
19	AT	65/65 (100%)	54 (83%)	11 (17%)	2	12
19	CT	65/65 (100%)	54 (83%)	11 (17%)	2	12
20	AB	180/198 (91%)	145 (81%)	35 (19%)	2	7
20	CB	180/198 (91%)	144 (80%)	36 (20%)	1	6
21	AU	44/60 (73%)	28 (64%)	16 (36%)	0	1
21	CU	44/60 (73%)	27 (61%)	17 (39%)	0	0
24	BI	109/109 (100%)	107 (98%)	2 (2%)	66	85
24	DI	109/109 (100%)	103 (94%)	6 (6%)	27	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	BC	216/217 (100%)	186 (86%)	30 (14%)	4	20
25	DC	216/217 (100%)	187 (87%)	29 (13%)	5	21
26	BD	164/164 (100%)	146 (89%)	18 (11%)	8	31
26	DD	164/164 (100%)	148 (90%)	16 (10%)	10	37
27	BK	102/104 (98%)	84 (82%)	18 (18%)	2	10
27	DK	102/104 (98%)	84 (82%)	18 (18%)	2	10
28	BP	99/99 (100%)	78 (79%)	21 (21%)	1	5
28	DP	99/99 (100%)	78 (79%)	21 (21%)	1	5
29	BE	165/165 (100%)	136 (82%)	29 (18%)	2	10
29	DE	165/165 (100%)	137 (83%)	28 (17%)	2	12
30	BY	48/48 (100%)	41 (85%)	7 (15%)	4	18
30	DY	48/48 (100%)	41 (85%)	7 (15%)	4	18
31	B0	47/47 (100%)	37 (79%)	10 (21%)	1	5
31	D0	47/47 (100%)	37 (79%)	10 (21%)	1	5
32	B4	34/34 (100%)	26 (76%)	8 (24%)	1	4
32	D4	34/34 (100%)	26 (76%)	8 (24%)	1	4
33	B1	45/48 (94%)	39 (87%)	6 (13%)	5	21
33	D1	45/48 (94%)	39 (87%)	6 (13%)	5	21
34	B3	51/51 (100%)	47 (92%)	4 (8%)	16	50
34	D3	51/51 (100%)	47 (92%)	4 (8%)	16	50
35	BV	78/78 (100%)	59 (76%)	19 (24%)	1	3
35	DV	78/78 (100%)	59 (76%)	19 (24%)	1	3
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%)	92 (90%)	10 (10%)	10	37
37	DL	102/103 (99%)	92 (90%)	10 (10%)	10	37
38	BM	109/109 (100%)	90 (83%)	19 (17%)	2	11
38	DM	109/109 (100%)	90 (83%)	19 (17%)	2	11
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	5
39	DX	55/55 (100%)	43 (78%)	12 (22%)	1	5
40	BH	114/114 (100%)	79 (69%)	35 (31%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DH	114/114 (100%)	82 (72%)	32 (28%)	0	2
41	BJ	116/116 (100%)	96 (83%)	20 (17%)	2	12
41	DJ	116/116 (100%)	98 (84%)	18 (16%)	3	16
42	BN	100/103 (97%)	84 (84%)	16 (16%)	3	14
42	DN	100/103 (97%)	84 (84%)	16 (16%)	3	14
43	BO	86/87 (99%)	74 (86%)	12 (14%)	4	20
43	DO	86/87 (99%)	72 (84%)	14 (16%)	3	14
44	BQ	89/89 (100%)	78 (88%)	11 (12%)	6	25
44	DQ	89/89 (100%)	78 (88%)	11 (12%)	6	25
45	BS	93/93 (100%)	82 (88%)	11 (12%)	6	27
45	DS	93/93 (100%)	82 (88%)	11 (12%)	6	27
46	BU	83/84 (99%)	71 (86%)	12 (14%)	4	18
46	DU	83/84 (99%)	70 (84%)	13 (16%)	3	15
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1	4
47	DF	149/149 (100%)	115 (77%)	34 (23%)	1	4
48	BG	137/137 (100%)	106 (77%)	31 (23%)	1	4
48	DG	137/137 (100%)	105 (77%)	32 (23%)	1	4
49	BR	84/84 (100%)	71 (84%)	13 (16%)	3	16
49	DR	84/84 (100%)	71 (84%)	13 (16%)	3	16
50	BT	80/84 (95%)	59 (74%)	21 (26%)	0	2
50	DT	80/84 (95%)	59 (74%)	21 (26%)	0	2
51	BZ	67/68 (98%)	52 (78%)	15 (22%)	1	4
51	DZ	67/68 (98%)	52 (78%)	15 (22%)	1	4
52	BW	59/62 (95%)	42 (71%)	17 (29%)	0	1
52	DW	59/62 (95%)	43 (73%)	16 (27%)	0	2
53	B6	157/157 (100%)	126 (80%)	31 (20%)	1	7
53	D6	157/157 (100%)	121 (77%)	36 (23%)	1	4
All	All	9647/10014 (96%)	7996 (83%)	1651 (17%)	2	12

5 of 1651 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	BT	12	ARG

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Mol	Chain	Res	Type
6	CG	75	LYS
48	DG	37	ASN
51	BZ	41	GLU
2	CC	120	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 342 such sidechains are listed below:

Mol	Chain	Res	Type
49	BR	43	ASN
5	CF	46	GLN
47	DF	51	ASN
50	BT	92	ASN
53	B6	102	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	248 (16%)	28 (1%)
1	CA	1529/1542 (99%)	239 (15%)	25 (1%)
22	BA	116/120 (96%)	18 (15%)	0
22	DA	116/120 (96%)	19 (16%)	0
23	BB	2837/2904 (97%)	448 (15%)	20 (0%)
23	DB	2837/2904 (97%)	432 (15%)	19 (0%)
All	All	8964/9132 (98%)	1404 (15%)	92 (1%)

5 of 1404 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	15	G
1	AA	31	G
1	AA	32	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2213	U
1	CA	243	A
23	DB	2213	U

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Mol	Chain	Res	Type
23	BB	2282	G
23	BB	2873	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 345 ligands modelled in this entry, 345 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	-0.08	27 (1%) 71 65	20, 68, 149, 180	0
1	CA	1530/1542 (99%)	-0.18	10 (0%) 89 86	10, 51, 126, 180	0
2	AC	206/232 (88%)	0.49	8 (3%) 43 36	24, 58, 114, 180	0
2	CC	206/232 (88%)	0.40	6 (2%) 55 49	28, 67, 117, 175	0
3	AD	205/205 (100%)	0.55	13 (6%) 23 19	22, 77, 137, 154	0
3	CD	205/205 (100%)	0.22	3 (1%) 76 71	15, 53, 129, 160	0
4	AE	150/166 (90%)	0.44	10 (6%) 21 17	16, 62, 116, 154	0
4	CE	150/166 (90%)	0.43	6 (4%) 42 34	20, 50, 105, 159	0
5	AF	100/135 (74%)	0.62	10 (10%) 9 8	33, 73, 126, 163	0
5	CF	100/135 (74%)	0.28	1 (1%) 84 80	20, 63, 115, 146	0
6	AG	150/178 (84%)	0.80	25 (16%) 2 2	40, 87, 140, 168	0
6	CG	152/178 (85%)	0.78	21 (13%) 4 3	21, 80, 132, 169	0
7	AH	129/129 (100%)	0.94	24 (18%) 2 1	34, 71, 116, 137	0
7	CH	129/129 (100%)	0.50	10 (7%) 16 13	18, 50, 96, 131	0
8	AI	127/129 (98%)	1.05	27 (21%) 1 1	23, 81, 151, 180	0
8	CI	127/129 (98%)	0.76	16 (12%) 5 4	26, 82, 135, 180	0
9	AJ	98/103 (95%)	1.18	21 (21%) 1 1	21, 74, 134, 180	0
9	CJ	98/103 (95%)	1.36	25 (25%) 1 1	34, 83, 136, 163	0
10	AK	117/128 (91%)	0.42	8 (6%) 20 17	19, 57, 100, 155	0
10	CK	117/128 (91%)	0.23	3 (2%) 59 53	18, 48, 100, 142	0
11	AL	123/123 (100%)	0.97	14 (11%) 7 5	29, 68, 124, 169	0
11	CL	123/123 (100%)	0.49	4 (3%) 50 43	10, 44, 107, 159	0
12	AM	114/117 (97%)	1.15	25 (21%) 1 1	48, 105, 157, 171	0
12	CM	113/117 (96%)	0.91	18 (15%) 3 2	44, 98, 149, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.98	16 (16%)	2 2	31, 77, 136, 171	0
13	CN	96/100 (96%)	0.87	11 (11%)	6 5	31, 78, 137, 161	0
14	AO	88/89 (98%)	0.38	3 (3%)	49 42	33, 67, 119, 173	0
14	CO	88/89 (98%)	0.08	0 100	100	18, 53, 105, 133	0
15	AP	82/82 (100%)	1.21	14 (17%)	2 2	38, 78, 140, 157	0
15	CP	80/82 (97%)	1.34	18 (22%)	1 1	16, 44, 124, 180	0
16	AQ	80/83 (96%)	0.82	7 (8%)	12 10	47, 86, 139, 155	0
16	CQ	81/83 (97%)	0.67	6 (7%)	17 14	25, 56, 117, 151	0
17	AR	55/74 (74%)	0.82	4 (7%)	18 15	27, 66, 125, 149	0
17	CR	55/74 (74%)	0.61	3 (5%)	29 23	24, 51, 105, 154	0
18	AS	79/91 (86%)	2.05	37 (46%)	0 0	61, 116, 158, 179	0
18	CS	80/91 (87%)	2.03	37 (46%)	0 0	54, 107, 165, 177	0
19	AT	85/86 (98%)	1.28	21 (24%)	1 1	52, 92, 133, 180	0
19	CT	85/86 (98%)	0.81	10 (11%)	6 5	24, 52, 103, 156	0
20	AB	218/240 (90%)	0.87	38 (17%)	2 2	29, 88, 139, 180	0
20	CB	218/240 (90%)	0.79	36 (16%)	2 2	40, 92, 143, 161	0
21	AU	51/70 (72%)	1.02	10 (19%)	1 1	36, 90, 150, 153	0
21	CU	51/70 (72%)	1.01	10 (19%)	1 1	26, 74, 136, 174	0
22	BA	117/120 (97%)	-0.24	3 (2%)	59 53	46, 80, 115, 168	0
22	DA	117/120 (97%)	-0.08	4 (3%)	49 42	35, 69, 110, 178	0
23	BB	2841/2904 (97%)	-0.02	52 (1%)	71 65	16, 56, 145, 180	0
23	DB	2841/2904 (97%)	-0.05	37 (1%)	79 74	7, 45, 142, 180	0
24	BI	141/141 (100%)	3.01	90 (63%)	0 0	62, 152, 180, 180	0
24	DI	141/141 (100%)	3.57	102 (72%)	0 0	85, 155, 180, 180	0
25	BC	271/272 (99%)	0.46	4 (1%)	76 71	9, 45, 87, 170	0
25	DC	271/272 (99%)	0.40	5 (1%)	71 65	5, 37, 75, 125	0
26	BD	209/209 (100%)	0.66	20 (9%)	10 9	22, 66, 124, 167	0
26	DD	209/209 (100%)	0.53	16 (7%)	16 13	10, 44, 112, 139	0
27	BK	121/123 (98%)	0.88	16 (13%)	4 3	16, 67, 120, 154	0
27	DK	121/123 (98%)	0.38	2 (1%)	73 67	8, 39, 93, 152	0
28	BP	114/114 (100%)	1.22	34 (29%)	1 1	27, 77, 122, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.46	5 (4%) 38 31	5, 42, 104, 160	0
29	BE	201/201 (100%)	0.68	21 (10%) 8 7	16, 67, 132, 148	0
29	DE	201/201 (100%)	0.60	23 (11%) 7 5	5, 65, 124, 156	0
30	BY	58/58 (100%)	0.82	8 (13%) 4 3	42, 73, 129, 143	0
30	DY	58/58 (100%)	0.61	4 (6%) 20 16	9, 58, 127, 150	0
31	B0	56/56 (100%)	0.65	6 (10%) 8 6	33, 71, 126, 141	0
31	D0	56/56 (100%)	0.57	4 (7%) 19 15	11, 45, 122, 170	0
32	B4	38/38 (100%)	1.09	7 (18%) 2 1	23, 75, 134, 149	0
32	D4	38/38 (100%)	0.86	4 (10%) 8 7	29, 54, 106, 125	0
33	B1	50/54 (92%)	1.02	7 (14%) 4 3	43, 79, 117, 132	0
33	D1	50/54 (92%)	0.86	4 (8%) 15 12	34, 66, 111, 135	0
34	B3	64/64 (100%)	0.77	11 (17%) 2 2	31, 51, 91, 115	0
34	D3	64/64 (100%)	0.51	1 (1%) 74 69	20, 40, 75, 110	0
35	BV	94/94 (100%)	0.76	7 (7%) 17 14	32, 90, 135, 169	0
35	DV	94/94 (100%)	0.55	7 (7%) 17 14	28, 74, 131, 167	0
36	B2	46/46 (100%)	0.56	1 (2%) 65 59	13, 40, 87, 121	0
36	D2	46/46 (100%)	0.31	0 100 100	11, 32, 67, 131	0
37	BL	143/144 (99%)	0.62	8 (5%) 28 22	13, 64, 117, 161	0
37	DL	143/144 (99%)	0.44	6 (4%) 40 33	13, 54, 108, 133	0
38	BM	136/136 (100%)	0.93	25 (18%) 2 1	24, 68, 124, 174	0
38	DM	136/136 (100%)	0.61	8 (5%) 26 20	13, 46, 109, 131	0
39	BX	63/63 (100%)	0.78	9 (14%) 4 3	20, 86, 141, 171	0
39	DX	63/63 (100%)	0.52	5 (7%) 15 12	38, 84, 134, 172	0
40	BH	149/149 (100%)	1.79	53 (35%) 0 1	37, 121, 160, 180	0
40	DH	149/149 (100%)	1.47	47 (31%) 1 1	20, 108, 147, 180	0
41	BJ	142/142 (100%)	0.80	14 (9%) 9 8	25, 73, 126, 137	0
41	DJ	142/142 (100%)	0.72	13 (9%) 11 9	19, 55, 104, 167	0
42	BN	120/127 (94%)	0.48	9 (7%) 17 14	20, 65, 117, 173	0
42	DN	120/127 (94%)	0.45	4 (3%) 50 43	8, 40, 80, 125	0
43	BO	116/117 (99%)	1.46	36 (31%) 1 1	27, 82, 128, 179	0
43	DO	116/117 (99%)	0.91	14 (12%) 6 4	19, 68, 119, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.57	8 (6%) 20 17	5, 64, 111, 163	0
44	DQ	117/117 (100%)	0.46	8 (6%) 20 17	14, 48, 96, 180	0
45	BS	110/110 (100%)	0.66	10 (9%) 11 9	15, 58, 112, 161	0
45	DS	110/110 (100%)	0.60	3 (2%) 58 51	8, 42, 101, 132	0
46	BU	102/103 (99%)	1.13	20 (19%) 1 1	26, 75, 130, 171	0
46	DU	102/103 (99%)	1.04	20 (19%) 1 1	27, 83, 143, 180	0
47	BF	178/178 (100%)	1.35	45 (25%) 1 1	42, 113, 160, 180	0
47	DF	178/178 (100%)	1.11	36 (20%) 1 1	38, 97, 155, 180	0
48	BG	176/176 (100%)	1.18	43 (24%) 1 1	51, 103, 141, 162	0
48	DG	176/176 (100%)	0.91	28 (15%) 3 2	34, 91, 142, 169	0
49	BR	103/103 (100%)	1.48	28 (27%) 1 1	27, 86, 128, 157	0
49	DR	103/103 (100%)	0.75	11 (10%) 8 6	18, 76, 122, 148	0
50	BT	93/100 (93%)	1.29	25 (26%) 1 1	31, 70, 134, 164	0
50	DT	93/100 (93%)	1.30	22 (23%) 1 1	21, 66, 136, 173	0
51	BZ	77/78 (98%)	0.72	3 (3%) 43 36	22, 50, 93, 129	0
51	DZ	77/78 (98%)	0.41	5 (6%) 22 18	17, 46, 95, 130	0
52	BW	79/84 (94%)	1.09	13 (16%) 2 2	29, 81, 126, 153	0
52	DW	79/84 (94%)	1.19	14 (17%) 2 1	20, 59, 119, 135	0
53	B6	185/185 (100%)	2.79	96 (51%) 0 0	33, 116, 167, 180	0
53	D6	185/185 (100%)	1.71	60 (32%) 1 1	19, 88, 157, 180	0
All	All	20787/21416 (97%)	0.48	1870 (8%) 12 9	5, 63, 142, 180	0

The worst 5 of 1870 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	AP	81	ALA	13.5
53	D6	72	ASP	11.9
24	BI	1	ALA	11.5
24	DI	85	ILE	11.1
24	DI	99	LYS	10.9

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
54	MG	AA	2057	1/1	0.89	0.61	31.00	93,93,93,93	0
54	MG	DB	3030	1/1	0.69	0.35	8.99	47,47,47,47	0
54	MG	BB	3087	1/1	0.87	0.25	3.53	100,100,100,100	0
54	MG	BB	3081	1/1	0.62	0.23	1.62	35,35,35,35	0
54	MG	DB	3089	1/1	0.97	0.21	1.62	50,50,50,50	0
54	MG	DB	3077	1/1	0.93	0.17	0.65	51,51,51,51	0
54	MG	BB	3040	1/1	0.94	0.19	0.47	60,60,60,60	0
54	MG	BB	3086	1/1	0.97	0.20	0.44	45,45,45,45	0
54	MG	DB	3020	1/1	0.95	0.20	0.15	14,14,14,14	0
54	MG	AA	2053	1/1	0.79	0.17	0.07	46,46,46,46	0
54	MG	DB	3084	1/1	0.96	0.20	-0.39	34,34,34,34	0
54	MG	DB	3099	1/1	0.93	0.18	-0.44	15,15,15,15	0
54	MG	DB	3096	1/1	0.95	0.16	-0.55	30,30,30,30	0
54	MG	DB	3051	1/1	0.94	0.17	-0.64	25,25,25,25	0
54	MG	CA	1654	1/1	0.78	0.15	-0.70	52,52,52,52	0
54	MG	DB	3059	1/1	0.39	0.15	-0.75	65,65,65,65	1
54	MG	DB	3027	1/1	0.98	0.19	-0.90	27,27,27,27	0
54	MG	DB	3111	1/1	0.97	0.19	-0.98	51,51,51,51	0
54	MG	BB	3062	1/1	0.91	0.18	-1.05	41,41,41,41	0
54	MG	CA	1632	1/1	0.96	0.18	-1.23	41,41,41,41	0
54	MG	DB	3012	1/1	0.94	0.18	-1.24	23,23,23,23	0
54	MG	DB	3034	1/1	0.83	0.19	-1.26	82,82,82,82	0
54	MG	AA	2015	1/1	0.94	0.13	-1.34	86,86,86,86	0
54	MG	BB	3090	1/1	0.76	0.18	-1.35	78,78,78,78	0
54	MG	CA	1614	1/1	0.95	0.12	-1.36	58,58,58,58	0
54	MG	BB	3099	1/1	0.87	0.12	-1.42	51,51,51,51	0
54	MG	BB	3110	1/1	0.90	0.14	-1.50	56,56,56,56	0
55	ZN	B4	101	1/1	0.70	0.09	-1.63	55,55,55,55	0
54	MG	CA	1616	1/1	0.89	0.09	-1.70	42,42,42,42	0
54	MG	DB	3078	1/1	0.96	0.11	-1.76	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	AA	2036	1/1	0.98	0.10	-1.78	65,65,65,65	0
54	MG	DB	3003	1/1	0.89	0.16	-1.79	29,29,29,29	0
54	MG	DB	3006	1/1	0.93	0.15	-1.86	26,26,26,26	0
54	MG	BB	3021	1/1	0.96	0.12	-1.86	43,43,43,43	0
54	MG	CA	1636	1/1	0.93	0.12	-1.91	63,63,63,63	0
54	MG	BB	3085	1/1	0.92	0.16	-1.91	56,56,56,56	0
54	MG	AA	2013	1/1	0.94	0.10	-1.92	85,85,85,85	0
54	MG	DB	3100	1/1	0.84	0.11	-1.94	17,17,17,17	0
54	MG	AA	2020	1/1	0.93	0.09	-1.95	84,84,84,84	0
54	MG	CA	1617	1/1	0.95	0.12	-2.05	21,21,21,21	0
55	ZN	D4	101	1/1	0.97	0.07	-2.08	55,55,55,55	0
54	MG	DB	3047	1/1	0.99	0.15	-2.21	13,13,13,13	0
54	MG	DB	3068	1/1	0.87	0.16	-2.30	8,8,8,8	0
54	MG	CA	1638	1/1	0.89	0.12	-2.30	90,90,90,90	0
54	MG	AA	2035	1/1	0.88	0.10	-2.31	102,102,102,102	0
54	MG	CA	1633	1/1	0.78	0.13	-2.37	42,42,42,42	0
54	MG	AA	2003	1/1	0.98	0.13	-2.60	31,31,31,31	0
54	MG	CA	1612	1/1	0.96	0.08	-2.62	46,46,46,46	0
54	MG	BB	3037	1/1	0.68	0.10	-2.63	23,23,23,23	0
54	MG	BB	3032	1/1	0.89	0.12	-2.63	34,34,34,34	0
54	MG	BB	3029	1/1	0.93	0.11	-2.79	28,28,28,28	0
54	MG	BB	3096	1/1	0.94	0.07	-2.93	37,37,37,37	0
54	MG	CA	1656	1/1	0.93	0.10	-2.95	22,22,22,22	0
54	MG	CA	1644	1/1	0.89	0.11	-3.01	52,52,52,52	0
54	MG	CA	1643	1/1	0.90	0.08	-3.03	20,20,20,20	0
54	MG	AA	2038	1/1	0.93	0.11	-3.07	63,63,63,63	0
54	MG	BB	3098	1/1	0.98	0.13	-3.17	30,30,30,30	0
54	MG	BB	3075	1/1	0.96	0.14	-3.20	37,37,37,37	0
54	MG	AA	2009	1/1	0.97	0.12	-3.31	21,21,21,21	0
54	MG	CA	1646	1/1	0.96	0.11	-3.35	46,46,46,46	0
54	MG	AA	2042	1/1	0.78	0.12	-3.35	32,32,32,32	0
54	MG	AA	2010	1/1	0.95	0.07	-3.39	36,36,36,36	0
54	MG	CA	1601	1/1	0.94	0.11	-3.44	9,9,9,9	0
54	MG	DB	3035	1/1	0.98	0.10	-3.46	57,57,57,57	0
54	MG	BB	3074	1/1	0.96	0.14	-3.50	21,21,21,21	0
54	MG	DB	3025	1/1	0.88	0.13	-3.50	28,28,28,28	0
54	MG	CA	1640	1/1	0.95	0.11	-3.52	43,43,43,43	0
54	MG	DB	3069	1/1	0.97	0.13	-3.53	21,21,21,21	0
54	MG	DB	3072	1/1	0.96	0.10	-3.54	23,23,23,23	0
54	MG	CA	1605	1/1	0.94	0.13	-3.54	38,38,38,38	0
54	MG	BB	3088	1/1	0.96	0.09	-3.68	75,75,75,75	0
54	MG	DB	3090	1/1	0.91	0.07	-3.69	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3007	1/1	0.99	0.08	-3.70	30,30,30,30	0
54	MG	BB	3001	1/1	0.96	0.08	-3.73	35,35,35,35	0
54	MG	BB	3002	1/1	0.93	0.11	-3.77	12,12,12,12	0
54	MG	AA	2033	1/1	0.97	0.07	-3.78	40,40,40,40	0
54	MG	DB	3085	1/1	0.82	0.12	-3.85	5,5,5,5	0
54	MG	DB	3009	1/1	0.99	0.15	-3.92	17,17,17,17	0
54	MG	AA	2030	1/1	0.84	0.08	-3.93	102,102,102,102	0
54	MG	BB	3013	1/1	0.95	0.09	-3.95	36,36,36,36	0
54	MG	BB	3012	1/1	0.98	0.09	-4.00	32,32,32,32	0
54	MG	AA	2044	1/1	0.89	0.09	-4.17	47,47,47,47	0
54	MG	BB	3019	1/1	0.94	0.07	-4.32	37,37,37,37	0
54	MG	AA	2043	1/1	0.71	0.11	-4.33	42,42,42,42	0
54	MG	AA	2001	1/1	0.98	0.07	-4.47	29,29,29,29	0
54	MG	AA	2007	1/1	0.97	0.08	-4.60	42,42,42,42	0
54	MG	BB	3094	1/1	0.83	0.09	-4.84	21,21,21,21	0
54	MG	DB	3092	1/1	0.94	0.11	-4.92	65,65,65,65	0
54	MG	DB	3055	1/1	0.90	0.12	-4.97	17,17,17,17	0
54	MG	DB	3056	1/1	0.92	0.10	-4.99	11,11,11,11	0
54	MG	DB	3010	1/1	0.97	0.10	-5.10	19,19,19,19	0
54	MG	DB	3014	1/1	0.97	0.07	-5.24	21,21,21,21	0
54	MG	BB	3083	1/1	0.97	0.11	-5.30	30,30,30,30	0
54	MG	BB	3011	1/1	0.96	0.09	-5.31	30,30,30,30	0
54	MG	CA	1618	1/1	0.97	0.07	-5.31	18,18,18,18	0
54	MG	DB	3108	1/1	0.92	0.11	-5.47	11,11,11,11	0
54	MG	CA	1655	1/1	0.97	0.09	-5.51	28,28,28,28	0
54	MG	BB	3052	1/1	0.89	0.09	-5.58	25,25,25,25	0
54	MG	BB	3069	1/1	0.94	0.07	-5.62	17,17,17,17	0
54	MG	BB	3048	1/1	0.95	0.08	-5.76	30,30,30,30	0
54	MG	BB	3035	1/1	0.95	0.10	-5.77	41,41,41,41	0
54	MG	BB	3061	1/1	0.87	0.07	-5.83	38,38,38,38	0
54	MG	DB	3074	1/1	0.83	0.08	-5.84	30,30,30,30	0
54	MG	BB	3108	1/1	0.93	0.11	-5.96	37,37,37,37	0
54	MG	DB	3070	1/1	0.94	0.12	-6.12	26,26,26,26	0
54	MG	DB	3019	1/1	0.96	0.07	-6.29	21,21,21,21	0
54	MG	BB	3005	1/1	0.92	0.10	-6.36	24,24,24,24	0
54	MG	CA	1645	1/1	0.97	0.09	-6.65	45,45,45,45	0
54	MG	AA	2029	1/1	0.94	0.08	-6.75	40,40,40,40	0
54	MG	DB	3044	1/1	0.97	0.06	-6.80	12,12,12,12	0
54	MG	DB	3103	1/1	0.97	0.09	-6.89	26,26,26,26	0
54	MG	BB	3023	1/1	0.97	0.07	-7.11	23,23,23,23	0
54	MG	DB	3087	1/1	0.98	0.11	-7.34	54,54,54,54	0
54	MG	BB	3103	1/1	0.96	0.09	-7.47	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3079	1/1	0.92	0.08	-7.65	34,34,34,34	0
54	MG	DB	3001	1/1	0.98	0.11	-7.65	9,9,9,9	0
54	MG	DB	3026	1/1	0.93	0.15	-7.88	41,41,41,41	0
54	MG	BB	3056	1/1	0.90	0.07	-9.01	31,31,31,31	0
54	MG	DB	3002	1/1	0.98	0.06	-9.46	11,11,11,11	0
54	MG	BB	3079	1/1	0.82	0.12	-10.61	63,63,63,63	0
54	MG	DB	3098	1/1	0.98	0.11	-11.19	29,29,29,29	0
54	MG	AA	2054	1/1	0.96	0.05	-12.76	49,49,49,49	0
54	MG	BB	3065	1/1	0.95	0.06	-12.82	40,40,40,40	0
54	MG	DB	3080	1/1	0.93	0.15	-13.21	29,29,29,29	0
54	MG	DB	3062	1/1	0.93	0.08	-	41,41,41,41	0
54	MG	DB	3013	1/1	0.84	0.22	-	47,47,47,47	0
54	MG	CA	1647	1/1	0.95	0.09	-	102,102,102,102	0
54	MG	BB	3045	1/1	0.94	0.05	-	41,41,41,41	0
54	MG	CE	201	1/1	0.91	0.20	-	102,102,102,102	0
54	MG	BB	3080	1/1	0.94	0.09	-	57,57,57,57	0
54	MG	CA	1606	1/1	0.94	0.09	-	59,59,59,59	0
54	MG	AA	2051	1/1	0.92	0.11	-	80,80,80,80	0
54	MG	CA	1653	1/1	0.97	0.04	-	55,55,55,55	0
54	MG	DB	3028	1/1	0.95	0.14	-	29,29,29,29	0
54	MG	CA	1652	1/1	0.86	0.09	-	54,54,54,54	0
54	MG	DB	3057	1/1	0.89	0.09	-	40,40,40,40	0
54	MG	CA	1648	1/1	0.84	0.15	-	47,47,47,47	0
54	MG	CA	1625	1/1	0.97	0.10	-	19,19,19,19	0
54	MG	DB	3091	1/1	0.94	0.12	-	29,29,29,29	0
54	MG	BB	3009	1/1	0.88	0.14	-	87,87,87,87	0
54	MG	BB	3039	1/1	0.91	0.15	-	43,43,43,43	0
54	MG	BB	3076	1/1	0.91	0.07	-	43,43,43,43	0
54	MG	CA	1634	1/1	0.72	0.11	-	32,32,32,32	0
54	MG	AA	2008	1/1	0.84	0.16	-	94,94,94,94	0
54	MG	CA	1642	1/1	0.96	0.04	-	63,63,63,63	0
54	MG	BB	3020	1/1	0.97	0.12	-	20,20,20,20	0
54	MG	BB	3068	1/1	0.90	0.12	-	43,43,43,43	0
54	MG	BB	3022	1/1	0.96	0.05	-	44,44,44,44	0
54	MG	DB	3032	1/1	0.89	0.12	-	33,33,33,33	0
54	MG	CA	1613	1/1	0.96	0.07	-	39,39,39,39	0
54	MG	BB	3063	1/1	0.91	0.14	-	52,52,52,52	0
54	MG	BB	3036	1/1	0.97	0.08	-	39,39,39,39	0
54	MG	DB	3086	1/1	0.97	0.19	-	26,26,26,26	0
54	MG	CA	1635	1/1	0.83	0.07	-	55,55,55,55	0
54	MG	AA	2056	1/1	0.91	0.32	-	46,46,46,46	0
54	MG	DB	3052	1/1	0.55	0.34	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1661	1/1	0.92	0.06	-	49,49,49,49	0
54	MG	CA	1650	1/1	0.96	0.16	-	41,41,41,41	0
54	MG	CA	1615	1/1	0.77	0.14	-	121,121,121,121	0
54	MG	AA	2024	1/1	0.94	0.08	-	61,61,61,61	0
54	MG	DB	3066	1/1	0.65	0.28	-	63,63,63,63	1
54	MG	AA	2052	1/1	0.94	0.07	-	50,50,50,50	0
54	MG	AA	2055	1/1	0.94	0.11	-	54,54,54,54	0
54	MG	CA	1626	1/1	0.94	0.30	-	42,42,42,42	1
54	MG	BB	3078	1/1	0.92	0.10	-	47,47,47,47	0
54	MG	CA	1631	1/1	0.97	0.09	-	38,38,38,38	0
54	MG	DB	3094	1/1	0.95	0.09	-	39,39,39,39	0
54	MG	DB	3037	1/1	0.93	0.16	-	45,45,45,45	0
54	MG	AA	2060	1/1	0.91	0.05	-	75,75,75,75	0
54	MG	AA	2022	1/1	0.79	0.29	-	77,77,77,77	0
54	MG	DB	3036	1/1	0.99	0.12	-	25,25,25,25	0
54	MG	BB	3047	1/1	0.84	0.11	-	70,70,70,70	0
54	MG	DB	3083	1/1	0.87	0.14	-	72,72,72,72	0
54	MG	BB	3097	1/1	0.66	0.13	-	101,101,101,101	0
54	MG	BB	3010	1/1	0.61	0.15	-	70,70,70,70	0
54	MG	DB	3008	1/1	0.96	0.14	-	33,33,33,33	0
54	MG	CA	1657	1/1	0.91	0.12	-	62,62,62,62	0
54	MG	CA	1619	1/1	0.80	0.10	-	51,51,51,51	0
54	MG	DB	3110	1/1	0.84	0.26	-	40,40,40,40	0
54	MG	BB	3007	1/1	0.91	0.11	-	74,74,74,74	0
54	MG	BB	3028	1/1	0.86	0.17	-	46,46,46,46	0
54	MG	AA	2017	1/1	0.95	0.29	-	75,75,75,75	0
54	MG	BB	3071	1/1	0.96	0.08	-	25,25,25,25	0
54	MG	DB	3054	1/1	0.92	0.08	-	25,25,25,25	0
54	MG	CA	1610	1/1	0.93	0.07	-	56,56,56,56	0
54	MG	DB	3021	1/1	0.98	0.12	-	21,21,21,21	0
54	MG	BB	3070	1/1	0.90	0.10	-	35,35,35,35	0
54	MG	DB	3050	1/1	0.91	0.05	-	70,70,70,70	0
54	MG	CA	1623	1/1	0.75	0.18	-	101,101,101,101	0
54	MG	BB	3030	1/1	0.93	0.07	-	40,40,40,40	0
54	MG	AA	2059	1/1	0.52	2.00	-	127,127,127,127	0
54	MG	BB	3102	1/1	0.86	0.09	-	38,38,38,38	0
54	MG	AA	2034	1/1	0.94	0.11	-	40,40,40,40	0
54	MG	BB	3105	1/1	0.97	0.16	-	65,65,65,65	0
54	MG	AA	2004	1/1	0.97	0.19	-	36,36,36,36	0
54	MG	DB	3041	1/1	0.98	0.13	-	36,36,36,36	0
54	MG	BB	3026	1/1	0.95	0.08	-	28,28,28,28	0
54	MG	CA	1628	1/1	0.91	0.11	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3092	1/1	0.94	0.05	-	51,51,51,51	0
54	MG	BB	3016	1/1	0.89	0.18	-	34,34,34,34	0
54	MG	AA	2040	1/1	0.96	0.10	-	56,56,56,56	0
54	MG	CA	1639	1/1	0.99	0.12	-	24,24,24,24	0
54	MG	DB	3023	1/1	0.95	0.09	-	33,33,33,33	0
54	MG	BB	3084	1/1	0.93	0.14	-	38,38,38,38	0
54	MG	CA	1611	1/1	0.88	0.11	-	81,81,81,81	0
54	MG	AA	2031	1/1	0.92	0.09	-	51,51,51,51	0
54	MG	CA	1660	1/1	0.88	0.08	-	96,96,96,96	0
54	MG	BB	3093	1/1	0.21	0.64	-	38,38,38,38	1
54	MG	CA	1603	1/1	0.95	0.10	-	29,29,29,29	0
54	MG	BB	3064	1/1	0.96	0.10	-	31,31,31,31	0
54	MG	BB	3073	1/1	0.80	0.17	-	70,70,70,70	0
54	MG	BB	3008	1/1	0.72	0.24	-	93,93,93,93	0
54	MG	AA	2027	1/1	0.91	0.21	-	62,62,62,62	0
54	MG	AA	2058	1/1	0.92	0.06	-	88,88,88,88	0
54	MG	DB	3101	1/1	0.97	0.16	-	5,5,5,5	0
54	MG	BB	3050	1/1	0.95	0.11	-	28,28,28,28	0
54	MG	AA	2002	1/1	0.83	0.14	-	85,85,85,85	0
54	MG	AA	2021	1/1	0.94	0.08	-	52,52,52,52	0
54	MG	DB	3106	1/1	0.94	0.10	-	9,9,9,9	0
54	MG	DB	3015	1/1	0.75	0.11	-	60,60,60,60	0
54	MG	CA	1620	1/1	0.92	0.06	-	58,58,58,58	0
54	MG	BB	3058	1/1	0.97	0.14	-	33,33,33,33	0
54	MG	BB	3066	1/1	0.97	0.07	-	21,21,21,21	0
54	MG	DB	3049	1/1	0.95	0.11	-	26,26,26,26	0
54	MG	AA	2045	1/1	0.85	0.07	-	63,63,63,63	0
54	MG	DB	3104	1/1	0.94	0.09	-	28,28,28,28	0
54	MG	BB	3067	1/1	0.96	0.09	-	45,45,45,45	0
54	MG	CA	1622	1/1	0.79	0.08	-	46,46,46,46	0
54	MG	AA	2006	1/1	0.90	0.06	-	71,71,71,71	0
54	MG	DB	3063	1/1	0.85	0.15	-	28,28,28,28	0
54	MG	DB	3053	1/1	0.96	0.09	-	28,28,28,28	0
54	MG	DB	3038	1/1	0.97	0.15	-	26,26,26,26	0
54	MG	BB	3027	1/1	0.94	0.14	-	34,34,34,34	0
54	MG	CA	1621	1/1	0.92	0.41	-	110,110,110,110	0
54	MG	DB	3011	1/1	0.94	0.17	-	16,16,16,16	0
54	MG	CA	1607	1/1	0.96	0.06	-	37,37,37,37	0
54	MG	DB	3017	1/1	0.91	0.13	-	18,18,18,18	0
54	MG	AA	2023	1/1	0.71	0.30	-	32,32,32,32	1
54	MG	CA	1637	1/1	0.90	0.10	-	53,53,53,53	0
54	MG	BB	3033	1/1	0.89	0.19	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3024	1/1	0.93	0.10	-	47,47,47,47	0
54	MG	BB	3006	1/1	0.94	0.09	-	28,28,28,28	0
54	MG	DB	3016	1/1	0.94	0.09	-	28,28,28,28	0
54	MG	DB	3061	1/1	0.95	0.05	-	51,51,51,51	0
54	MG	CA	1608	1/1	0.82	0.11	-	106,106,106,106	0
54	MG	CA	1629	1/1	0.92	0.07	-	20,20,20,20	1
54	MG	DB	3107	1/1	0.96	0.06	-	34,34,34,34	0
54	MG	BB	3014	1/1	0.85	0.14	-	58,58,58,58	0
54	MG	BB	3049	1/1	0.73	0.14	-	26,26,26,26	0
54	MG	BB	3051	1/1	0.84	0.11	-	35,35,35,35	0
54	MG	AA	2050	1/1	0.84	0.11	-	101,101,101,101	0
54	MG	AA	2018	1/1	0.84	0.07	-	78,78,78,78	0
54	MG	DB	3042	1/1	0.96	0.11	-	45,45,45,45	0
54	MG	CA	1602	1/1	0.98	0.20	-	34,34,34,34	0
54	MG	DB	3082	1/1	0.93	0.10	-	21,21,21,21	0
54	MG	AA	2005	1/1	0.95	0.07	-	36,36,36,36	0
54	MG	DB	3039	1/1	0.94	0.07	-	34,34,34,34	0
54	MG	BB	3004	1/1	0.95	0.09	-	52,52,52,52	0
54	MG	DB	3060	1/1	0.48	0.10	-	89,89,89,89	0
54	MG	BB	3091	1/1	0.97	0.11	-	31,31,31,31	0
54	MG	BB	3109	1/1	0.96	0.09	-	42,42,42,42	0
54	MG	BB	3042	1/1	0.63	0.10	-	123,123,123,123	0
54	MG	BB	3046	1/1	0.70	0.17	-	69,69,69,69	0
54	MG	DB	3031	1/1	0.97	0.09	-	17,17,17,17	0
54	MG	AA	2011	1/1	0.93	0.08	-	45,45,45,45	0
54	MG	AA	2012	1/1	0.84	0.06	-	63,63,63,63	0
54	MG	CA	1649	1/1	0.98	0.07	-	80,80,80,80	0
54	MG	CA	1630	1/1	0.96	0.10	-	39,39,39,39	0
54	MG	DB	3071	1/1	0.96	0.13	-	57,57,57,57	0
54	MG	AA	2046	1/1	0.89	0.09	-	46,46,46,46	0
54	MG	AA	2037	1/1	0.69	1.62	-	139,139,139,139	0
54	MG	BB	3015	1/1	0.92	0.10	-	40,40,40,40	0
54	MG	BB	3041	1/1	0.97	0.10	-	22,22,22,22	0
54	MG	AA	2014	1/1	0.69	0.13	-	101,101,101,101	0
54	MG	DB	3073	1/1	0.92	0.10	-	29,29,29,29	0
54	MG	CA	1641	1/1	0.77	0.22	-	61,61,61,61	0
54	MG	BB	3072	1/1	0.94	0.10	-	44,44,44,44	0
54	MG	DB	3048	1/1	0.87	0.11	-	41,41,41,41	0
54	MG	BB	3095	1/1	0.94	0.07	-	25,25,25,25	0
54	MG	DB	3018	1/1	0.91	0.12	-	23,23,23,23	0
54	MG	BB	3101	1/1	0.94	0.10	-	22,22,22,22	0
54	MG	CA	1659	1/1	0.92	0.11	-	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	2019	1/1	0.85	0.13	-	120,120,120,120	0
54	MG	AA	2028	1/1	0.90	0.10	-	66,66,66,66	0
54	MG	DB	3065	1/1	0.96	0.09	-	12,12,12,12	0
54	MG	BB	3104	1/1	0.88	0.14	-	20,20,20,20	0
54	MG	BB	3043	1/1	0.97	0.16	-	53,53,53,53	0
54	MG	BB	3018	1/1	0.94	0.14	-	45,45,45,45	0
54	MG	DB	3046	1/1	0.96	0.06	-	22,22,22,22	0
54	MG	DB	3058	1/1	0.71	2.00	-	145,145,145,145	0
54	MG	DB	3029	1/1	0.89	0.15	-	67,67,67,67	0
54	MG	BB	3077	1/1	0.88	0.07	-	36,36,36,36	0
54	MG	DB	3105	1/1	0.98	0.08	-	32,32,32,32	0
54	MG	DB	3095	1/1	0.91	0.38	-	19,19,19,19	1
54	MG	DB	3109	1/1	0.93	0.09	-	35,35,35,35	0
54	MG	CA	1627	1/1	0.86	0.37	-	5,5,5,5	1
54	MG	BB	3053	1/1	0.86	0.07	-	61,61,61,61	0
54	MG	AA	2026	1/1	0.75	0.15	-	5,5,5,5	1
54	MG	DB	3076	1/1	0.99	0.07	-	17,17,17,17	0
54	MG	DB	3088	1/1	0.94	0.12	-	28,28,28,28	0
54	MG	BB	3106	1/1	0.94	0.10	-	36,36,36,36	0
54	MG	CA	1604	1/1	0.99	0.10	-	36,36,36,36	0
54	MG	AA	2039	1/1	0.52	0.37	-	108,108,108,108	0
54	MG	BB	3038	1/1	0.89	0.10	-	98,98,98,98	0
54	MG	AA	2016	1/1	0.94	0.10	-	50,50,50,50	0
54	MG	DB	3081	1/1	0.99	0.11	-	17,17,17,17	0
54	MG	AA	2025	1/1	0.42	0.72	-	54,54,54,54	1
54	MG	CA	1624	1/1	0.92	0.10	-	22,22,22,22	0
54	MG	DB	3040	1/1	0.98	0.10	-	9,9,9,9	0
54	MG	BB	3059	1/1	0.91	0.11	-	32,32,32,32	0
54	MG	DB	3093	1/1	0.96	0.12	-	6,6,6,6	0
54	MG	DB	3097	1/1	0.88	0.13	-	32,32,32,32	0
54	MG	BB	3031	1/1	0.85	0.11	-	46,46,46,46	0
54	MG	BB	3107	1/1	0.96	0.08	-	31,31,31,31	0
54	MG	DB	3024	1/1	0.93	0.13	-	30,30,30,30	0
54	MG	BB	3060	1/1	0.99	0.10	-	47,47,47,47	0
54	MG	DB	3075	1/1	0.99	0.06	-	33,33,33,33	0
54	MG	BB	3003	1/1	0.92	0.11	-	47,47,47,47	0
54	MG	BB	3054	1/1	0.86	0.10	-	57,57,57,57	0
54	MG	CA	1651	1/1	0.96	0.07	-	50,50,50,50	0
54	MG	BB	3055	1/1	0.95	0.18	-	41,41,41,41	0
54	MG	DB	3064	1/1	0.78	0.15	-	37,37,37,37	0
54	MG	DB	3102	1/1	0.93	0.13	-	15,15,15,15	0
54	MG	AA	2032	1/1	0.85	0.43	-	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	BB	3089	1/1	0.93	0.08	-	38,38,38,38	0
54	MG	DB	3004	1/1	0.95	0.15	-	17,17,17,17	0
54	MG	DB	3022	1/1	0.76	0.17	-	32,32,32,32	0
54	MG	BB	3034	1/1	0.91	0.13	-	35,35,35,35	0
54	MG	DB	3043	1/1	0.98	0.10	-	8,8,8,8	0
54	MG	BB	3100	1/1	0.50	0.58	-	75,75,75,75	1
54	MG	DB	3067	1/1	0.97	0.09	-	18,18,18,18	0
54	MG	BB	3057	1/1	0.93	0.27	-	37,37,37,37	0
54	MG	CA	1658	1/1	0.91	0.19	-	33,33,33,33	0
54	MG	DB	3045	1/1	0.88	0.08	-	61,61,61,61	0
54	MG	BB	3017	1/1	0.84	0.15	-	59,59,59,59	0
54	MG	AA	2041	1/1	0.94	0.04	-	40,40,40,40	0
54	MG	DB	3033	1/1	0.89	0.12	-	20,20,20,20	0
54	MG	BB	3082	1/1	0.96	0.15	-	38,38,38,38	0
54	MG	AA	2048	1/1	0.96	0.11	-	27,27,27,27	0
54	MG	AA	2049	1/1	0.85	0.08	-	90,90,90,90	0
54	MG	DB	3005	1/1	0.96	0.05	-	56,56,56,56	0
54	MG	BB	3044	1/1	0.87	0.14	-	70,70,70,70	0
54	MG	BB	3025	1/1	0.92	0.13	-	49,49,49,49	0
54	MG	AA	2047	1/1	0.86	0.48	-	126,126,126,126	0
54	MG	CA	1609	1/1	0.95	0.11	-	56,56,56,56	0

6.5 Other polymers

There are no such residues in this entry.