wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:49 PM GMT

PDB ID	:	4V90
Title	:	THERMUS THERMOPHILUS RIBOSOME
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Deposited on	:	2014-02-22
Resolution	:	2.95 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

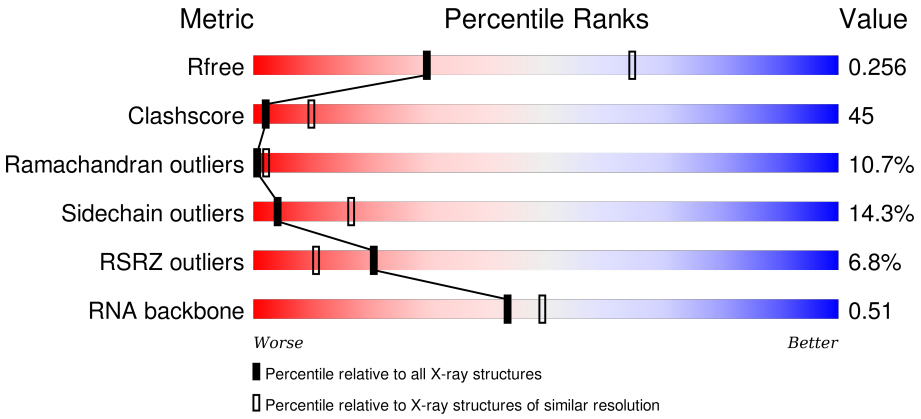
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)
RNA backbone	2183	1010 (3.36-2.56)

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 <=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	1519	3% 32% 48% 19%
2	AB	256	8% 21% 49% 18% 8%
3	AC	239	4% 23% 44% 18% 13%
4	AD	209	3% 45% 45% 9%

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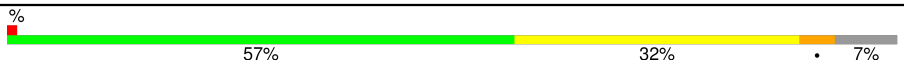
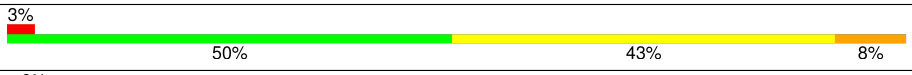
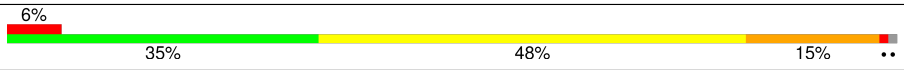
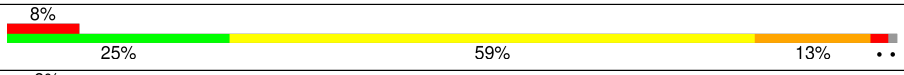
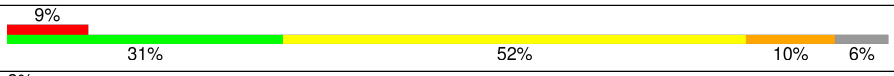
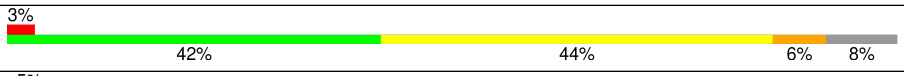
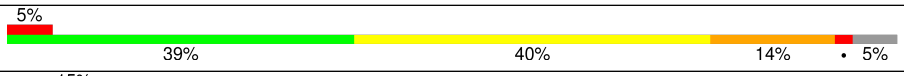
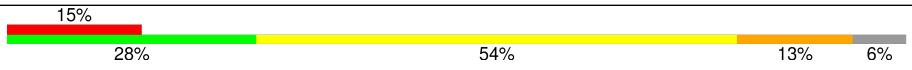
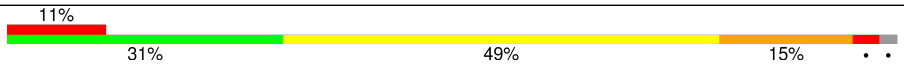
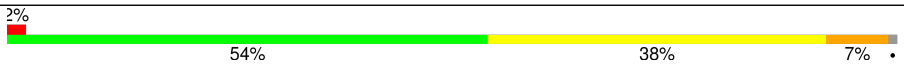
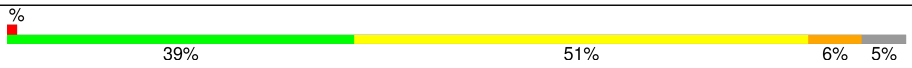
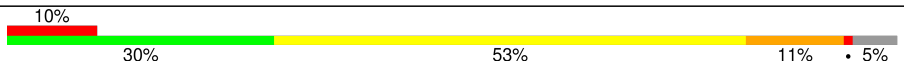
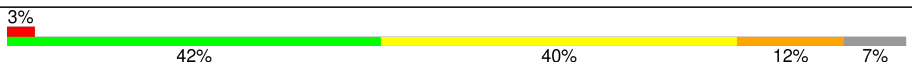
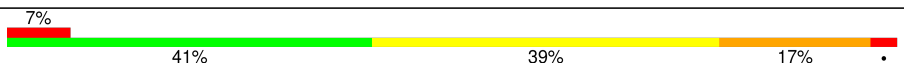
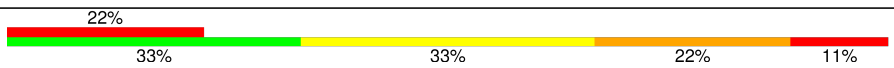
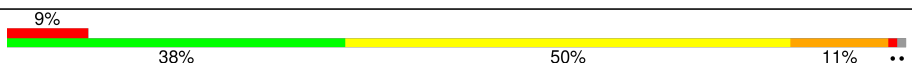
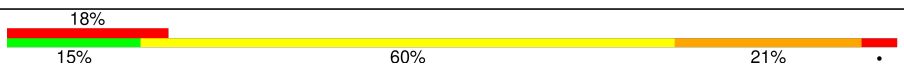
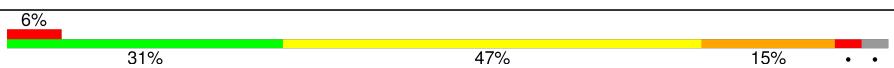
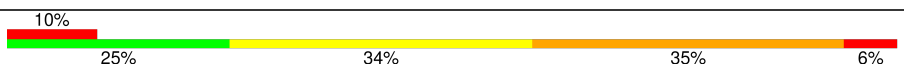
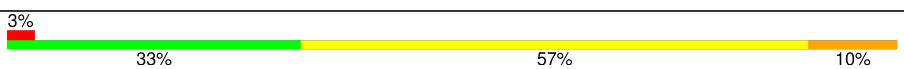
Mol	Chain	Length	Quality of chain
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	132	
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	76	
23	AX	9	
24	AY	691	
25	B0	84	
26	B1	97	
27	B2	71	
28	B3	60	
29	B4	71	

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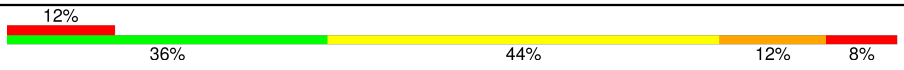
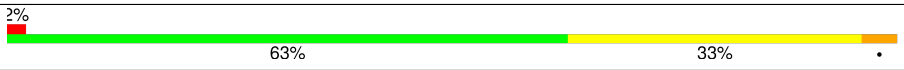
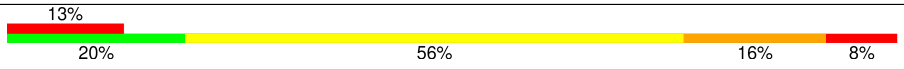
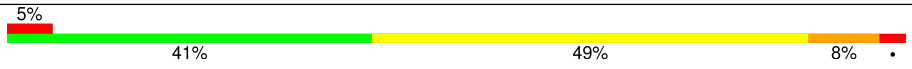
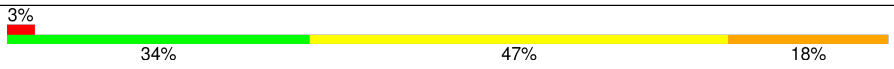
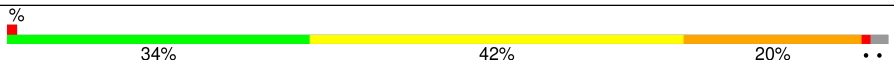
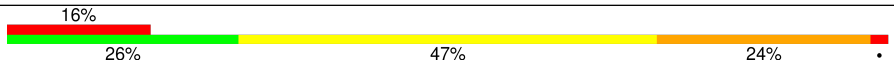
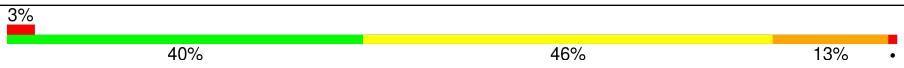
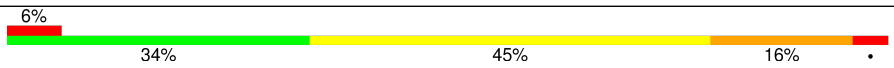
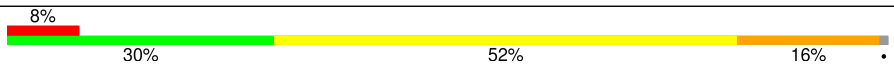
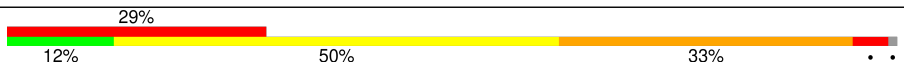
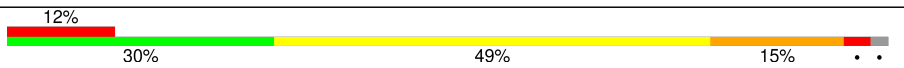
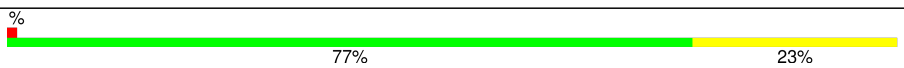
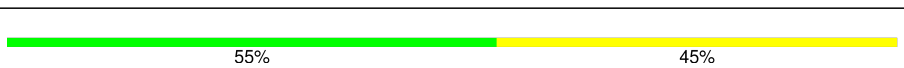
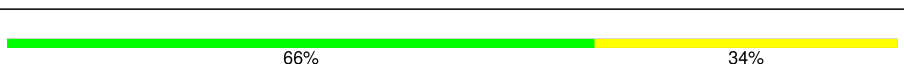
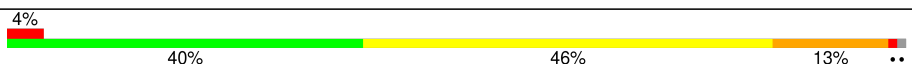
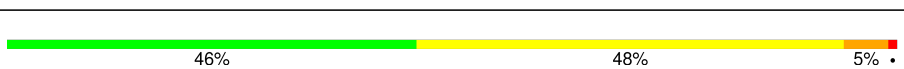
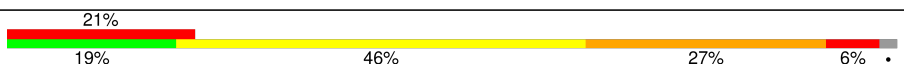
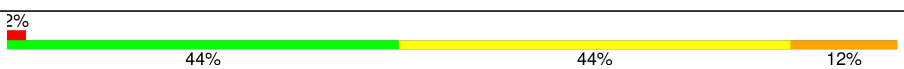
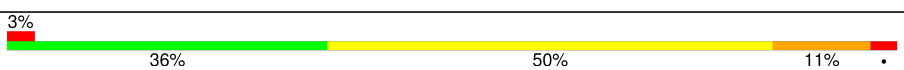
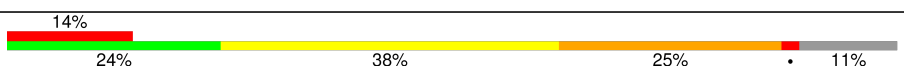
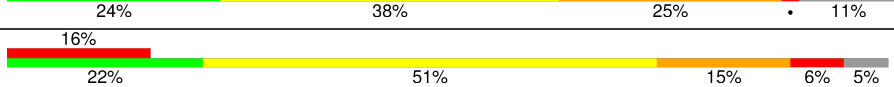
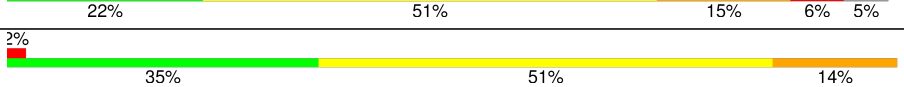
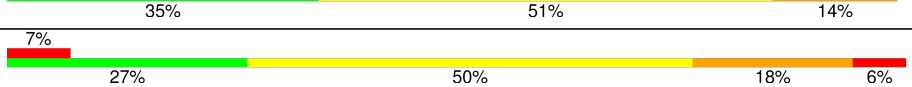
Mol	Chain	Length	Quality of chain
30	B5	59	
31	B6	53	
32	B7	48	
33	B8	64	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	228	
38	BD	275	
39	BE	206	
40	BF	210	
41	BG	181	
42	BH	180	
43	BJ	130	
44	BK	140	
45	BL	71	
46	BN	140	
47	BO	122	
48	BP	149	
49	BQ	141	
50	BR	117	
51	BS	111	
52	BT	146	
53	BU	117	
54	BV	101	

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Mol	Chain	Length	Quality of chain
55	BW	113	4% 52% 39% 8%
56	BX	95	2% 48% 45%
57	BY	109	21% 18% 40% 28% 6% 7%
58	BZ	205	12% 24% 50% 15% 10%

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
59	MG	AA	1604	-	-	-	X
59	MG	AA	1615	-	-	-	X
59	MG	AA	1616	-	-	-	X
59	MG	AA	1623	-	-	-	X
59	MG	AA	1625	-	-	-	X
59	MG	AA	1636	-	-	-	X
59	MG	AA	1638	-	-	-	X
59	MG	AA	1639	-	-	-	X
59	MG	AA	1645	-	-	-	X
59	MG	AA	1649	-	-	-	X
59	MG	AA	1665	-	-	-	X
59	MG	AA	1671	-	-	-	X
59	MG	AA	1677	-	-	-	X
59	MG	AA	1678	-	-	-	X
59	MG	AA	1684	-	-	-	X
59	MG	AA	1686	-	-	-	X
59	MG	AA	1690	-	-	-	X
59	MG	AA	1692	-	-	-	X
59	MG	AA	1700	-	-	-	X
59	MG	AA	1704	-	-	-	X
59	MG	AA	1715	-	-	-	X
59	MG	AA	1724	-	-	-	X
59	MG	AA	1729	-	-	-	X
59	MG	AA	1733	-	-	-	X
59	MG	AA	1741	-	-	-	X
59	MG	AA	1756	-	-	-	X
59	MG	AA	1760	-	-	-	X
59	MG	AA	1762	-	-	-	X
59	MG	AA	1777	-	-	-	X
59	MG	B0	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3004	-	-	-	X
59	MG	BA	3006	-	-	-	X
59	MG	BA	3007	-	-	-	X
59	MG	BA	3024	-	-	-	X
59	MG	BA	3039	-	-	-	X
59	MG	BA	3043	-	-	-	X
59	MG	BA	3044	-	-	-	X
59	MG	BA	3048	-	-	-	X
59	MG	BA	3051	-	-	-	X
59	MG	BA	3052	-	-	-	X
59	MG	BA	3053	-	-	-	X
59	MG	BA	3056	-	-	-	X
59	MG	BA	3071	-	-	-	X
59	MG	BA	3075	-	-	-	X
59	MG	BA	3077	-	-	-	X
59	MG	BA	3078	-	-	-	X
59	MG	BA	3082	-	-	-	X
59	MG	BA	3084	-	-	-	X
59	MG	BA	3087	-	-	-	X
59	MG	BA	3088	-	-	-	X
59	MG	BA	3091	-	-	-	X
59	MG	BA	3094	-	-	-	X
59	MG	BA	3097	-	-	-	X
59	MG	BA	3098	-	-	-	X
59	MG	BA	3104	-	-	-	X
59	MG	BA	3108	-	-	-	X
59	MG	BA	3109	-	-	-	X
59	MG	BA	3110	-	-	-	X
59	MG	BA	3111	-	-	-	X
59	MG	BA	3113	-	-	-	X
59	MG	BA	3116	-	-	-	X
59	MG	BA	3120	-	-	-	X
59	MG	BA	3125	-	-	-	X
59	MG	BA	3127	-	-	-	X
59	MG	BA	3129	-	-	-	X
59	MG	BA	3139	-	-	-	X
59	MG	BA	3145	-	-	-	X
59	MG	BA	3149	-	-	-	X
59	MG	BA	3153	-	-	-	X
59	MG	BA	3154	-	-	-	X
59	MG	BA	3169	-	-	-	X
59	MG	BA	3172	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3174	-	-	-	X
59	MG	BA	3176	-	-	-	X
59	MG	BA	3180	-	-	-	X
59	MG	BA	3181	-	-	-	X
59	MG	BA	3184	-	-	-	X
59	MG	BA	3189	-	-	-	X
59	MG	BA	3196	-	-	-	X
59	MG	BA	3199	-	-	-	X
59	MG	BA	3206	-	-	-	X
59	MG	BA	3207	-	-	-	X
59	MG	BA	3209	-	-	-	X
59	MG	BA	3210	-	-	-	X
59	MG	BA	3214	-	-	-	X
59	MG	BA	3228	-	-	-	X
59	MG	BA	3236	-	-	-	X
59	MG	BA	3248	-	-	-	X
59	MG	BA	3257	-	-	-	X
59	MG	BA	3258	-	-	-	X
59	MG	BA	3266	-	-	-	X
59	MG	BA	3271	-	-	-	X
59	MG	BA	3277	-	-	-	X
59	MG	BA	3279	-	-	-	X
59	MG	BA	3282	-	-	-	X
59	MG	BA	3295	-	-	-	X
59	MG	BA	3298	-	-	-	X
59	MG	BA	3310	-	-	-	X
59	MG	BA	3312	-	-	-	X
59	MG	BA	3313	-	-	-	X
59	MG	BA	3315	-	-	-	X
60	ZN	AD	301	-	-	-	X
61	GCP	AY	701	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 153829 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 RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1507	32391	14418	6002	10465	1506	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1030	C	-	INSERTION	GB 48256
AA	1034	G	-	INSERTION	GB 48256
AA	1245	A	-	INSERTION	GB 48256
AA	1246	C	-	INSERTION	GB 48256

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AB	235	1901	1213	342	341	5	0	0	1

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	207	1613	1016	315	281	1	0	0	1

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	88	Total	C	N	O	S	0	0	1
			692	440	128	122	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	291	530	75			

- Molecule 23 is a RNA chain called 5'-R(*UP*AP*AP*AP*AP*AP*UP*GP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	9	Total	C	N	O	P	0	0	0
			188	86	34	60	8			

- Molecule 24 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	687	Total	C	N	O	S	0	0	1
			5376	3412	922	1022	20			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0	0
			62476	27807	11683	20086	2900			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	2155	G	A	CONFLICT	GB 55771382

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 37 is a protein called RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	227	Total	C	N	O	S	0	0	0
			1735	1096	318	318	3			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	179	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	176	Total	C	N	O	S	0	0	1
			1345	853	253	237	2			

- Molecule 43 is a protein called CHAIN J.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BJ	130	Total	C	N	O	0	0	0
			654	393	130	131			

- Molecule 44 is a protein called CHAIN K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BK	140	Total	C	N	O	0	0	0
			701	420	140	141			

- Molecule 45 is a protein called CHAIN L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BL	71	Total	C	N	O	0	0	0
			356	213	71	72			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B5	1	Total	Mg	0	0
			1	1		
59	BU	1	Total	Mg	0	0
			1	1		
59	BA	320	Total	Mg	0	0
			320	320		

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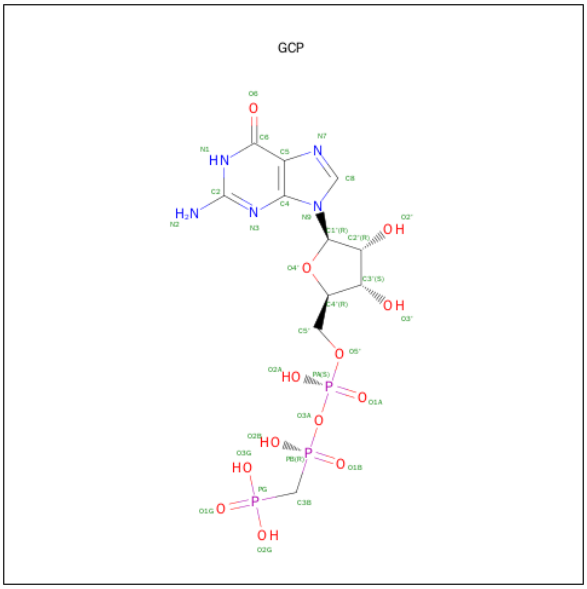
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AA	198	Total Mg 198 198	0	0
59	B0	1	Total Mg 1 1	0	0
59	AY	1	Total Mg 1 1	0	0
59	BC	1	Total Mg 1 1	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	B9	1	Total Zn 1 1	0	0
60	AD	1	Total Zn 1 1	0	0
60	AN	1	Total Zn 1 1	0	0

- Molecule 61 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AY	1	Total C N O P 32 11 5 13 3	0	0

- Molecule 62 is water.

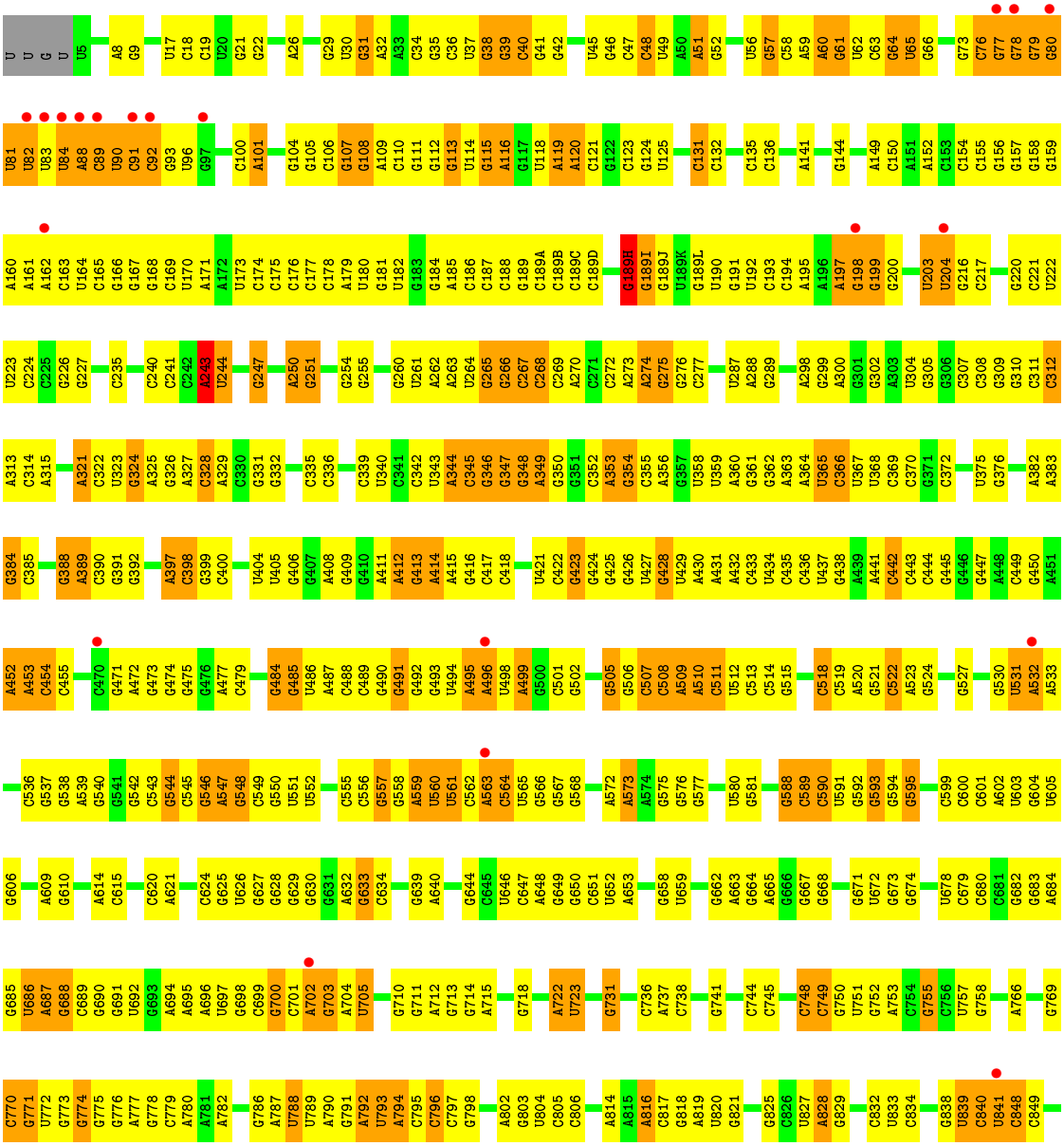
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	AY	2	Total O 2 2	0	0

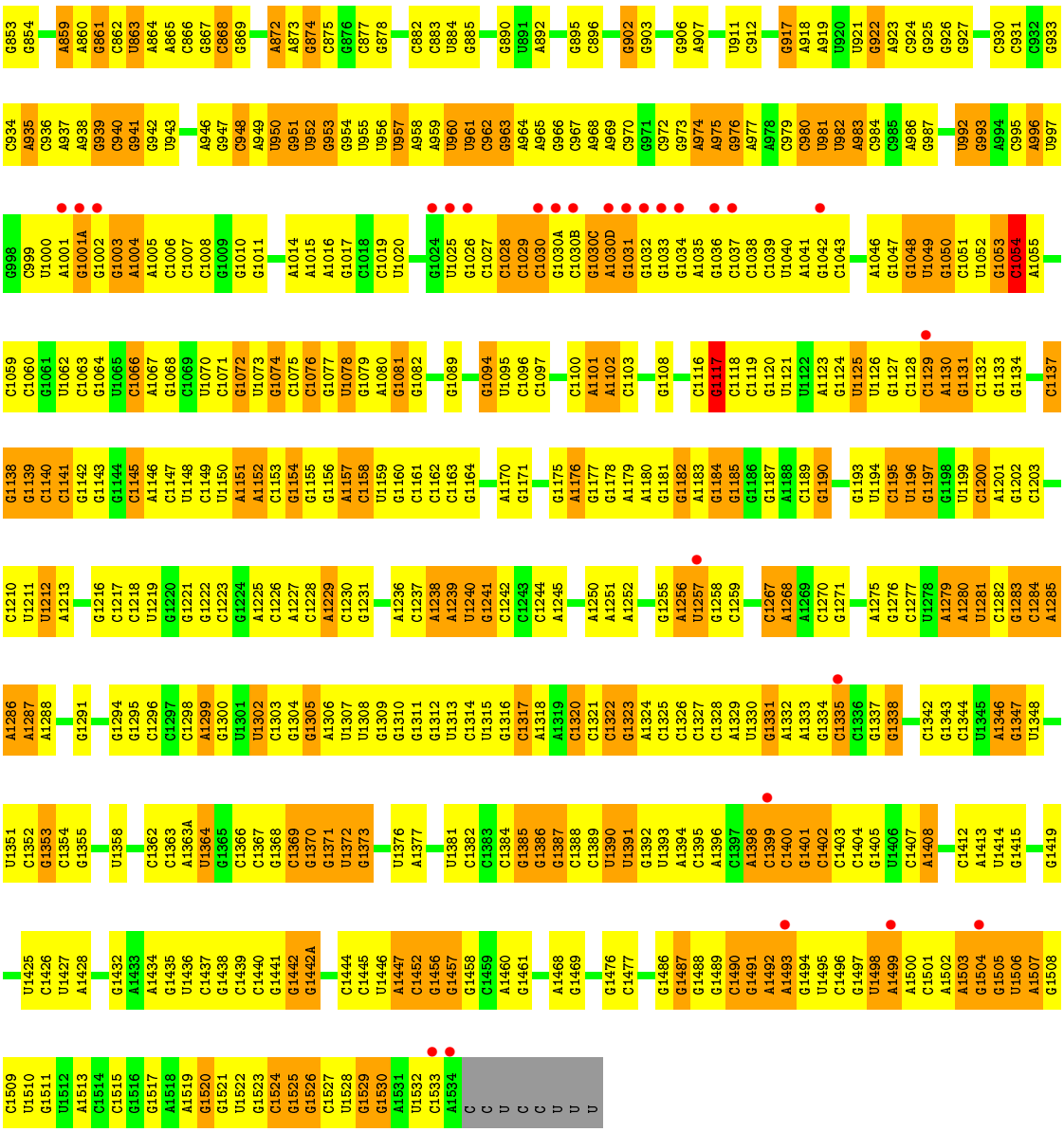
3 Residue-property plots (i)

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 (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 RIBOSOMAL RNA

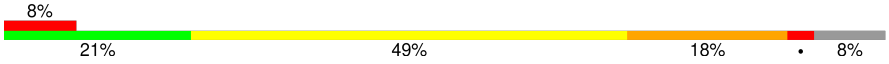
Chain AA:

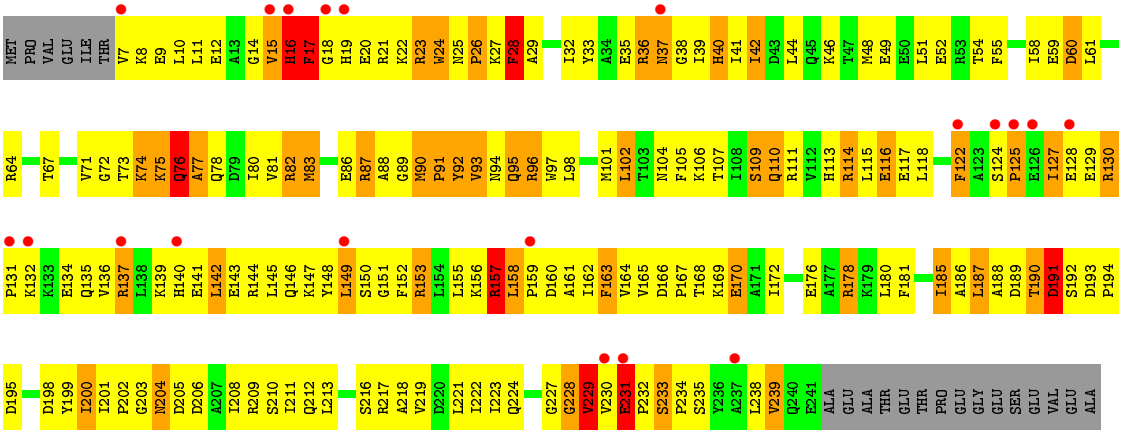




• Molecule 2: 30S RIBOSOMAL PROTEIN S2

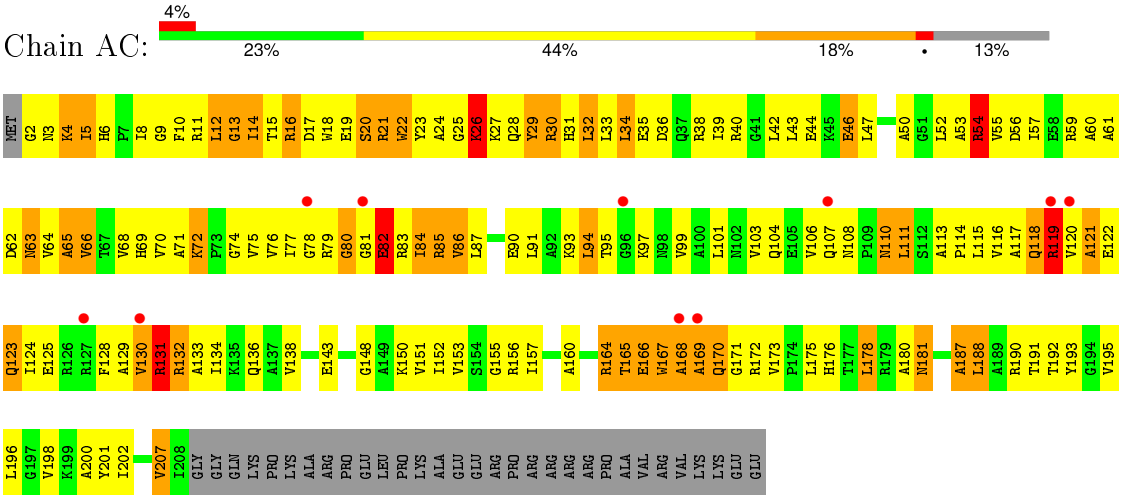
Chain AB:





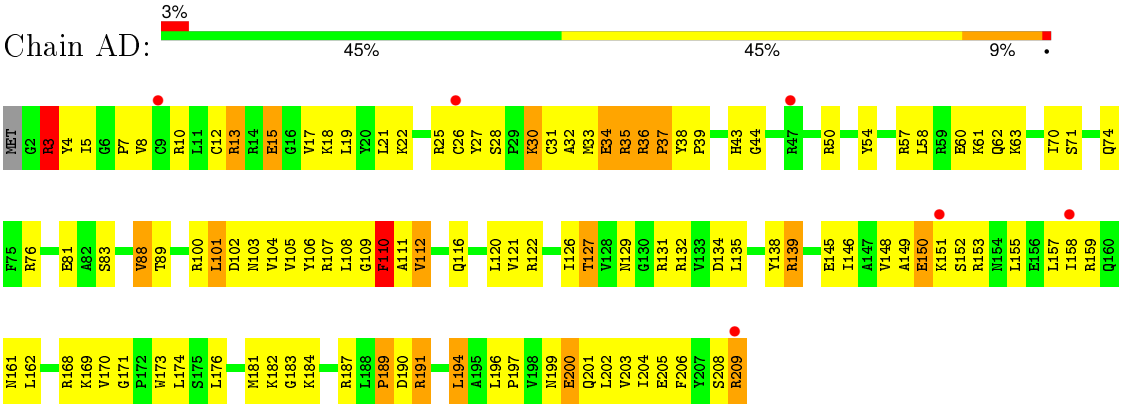
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



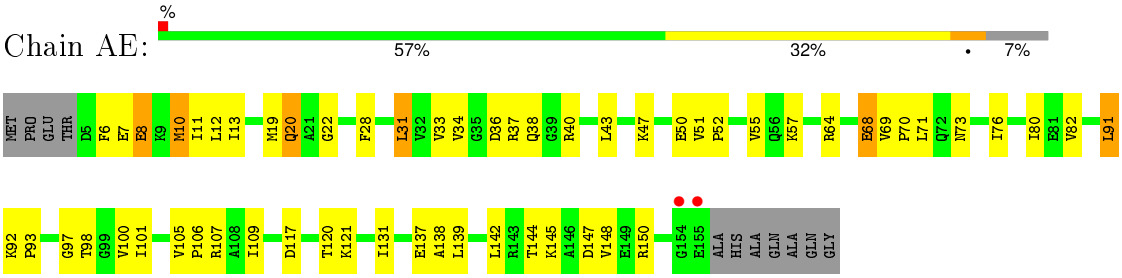
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



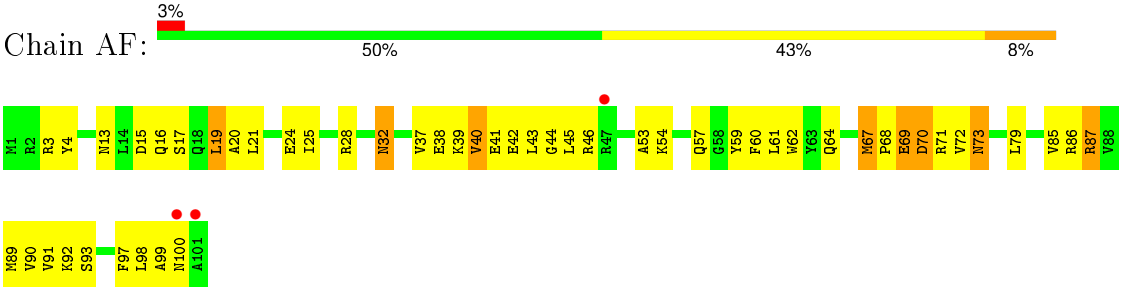
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



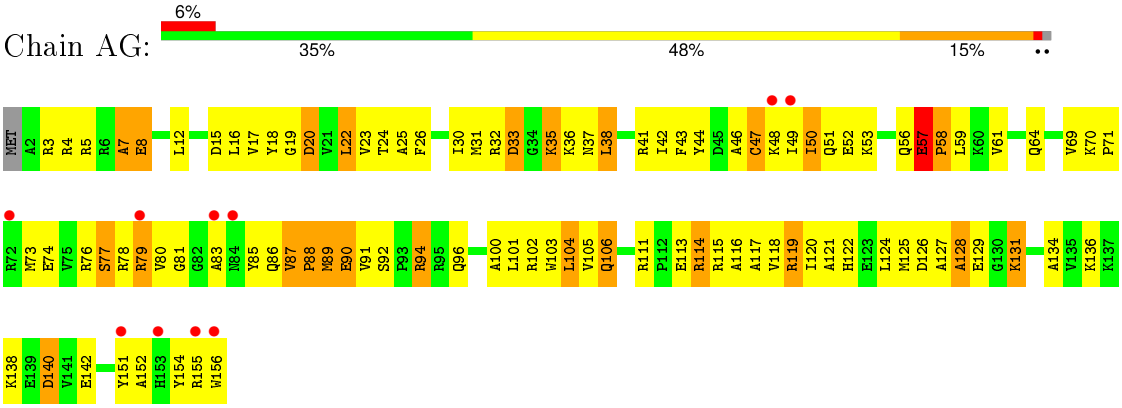
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



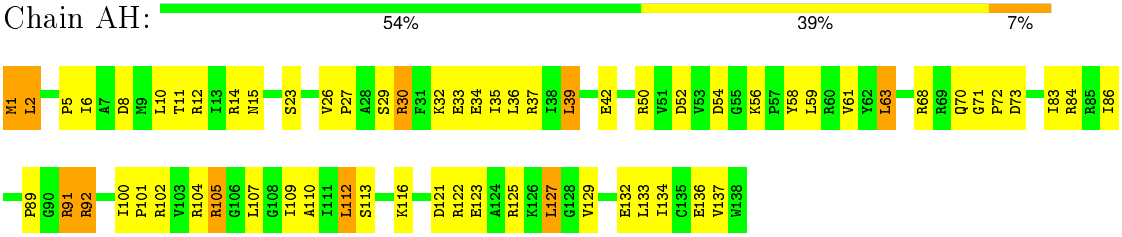
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



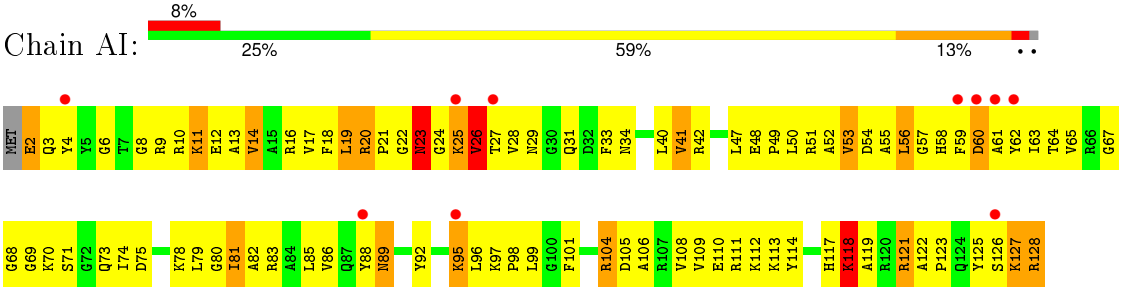
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



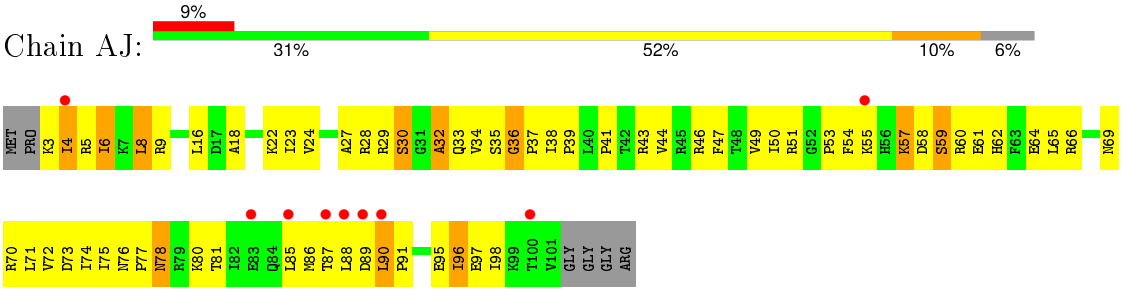
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



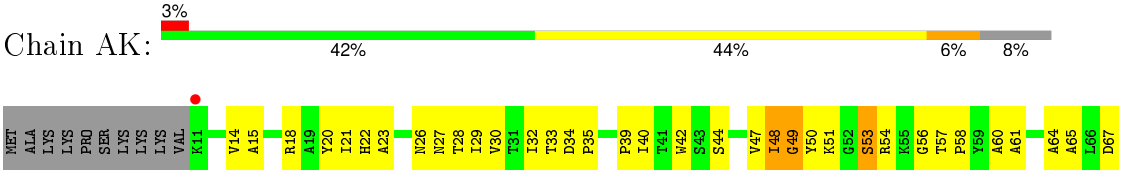
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

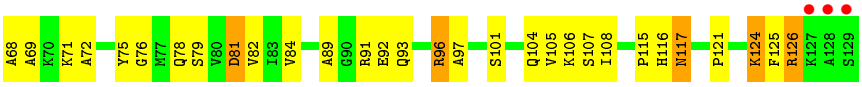
Chain AJ:



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

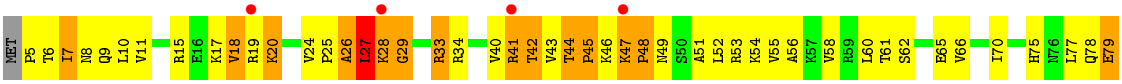
Chain AK:

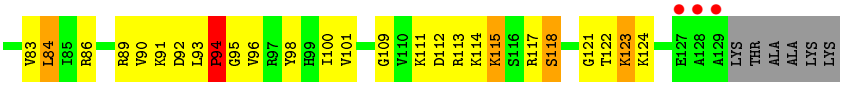




• Molecule 12: 30S RIBOSOMAL PROTEIN S12

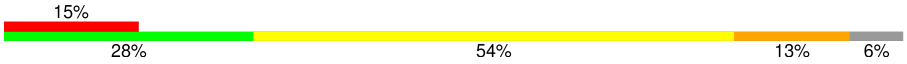
Chain AL:

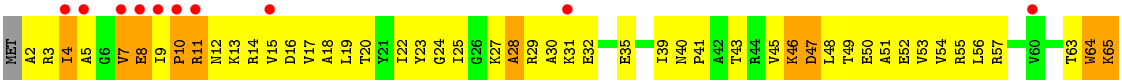


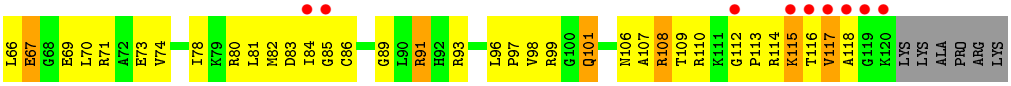


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:

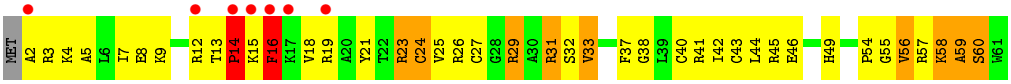






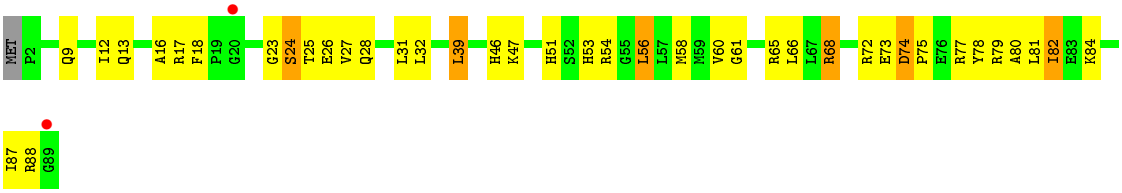
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



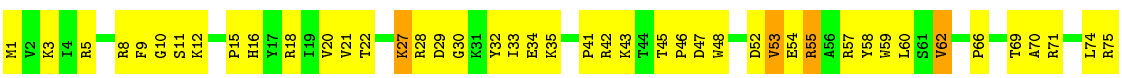
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

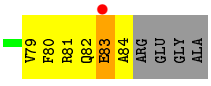
Chain AO:



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

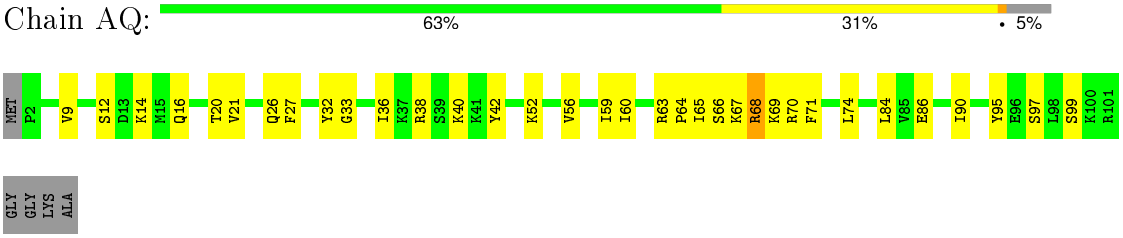
Chain AP:





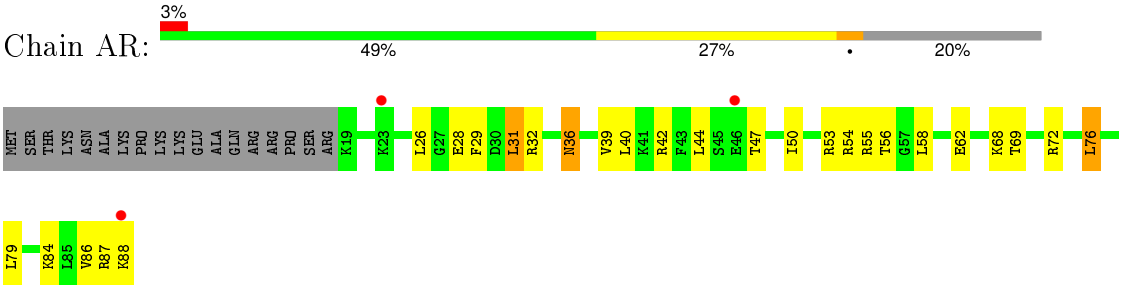
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



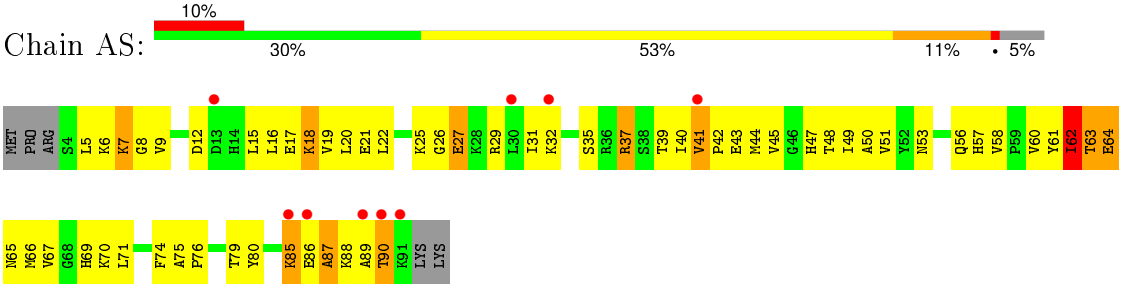
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



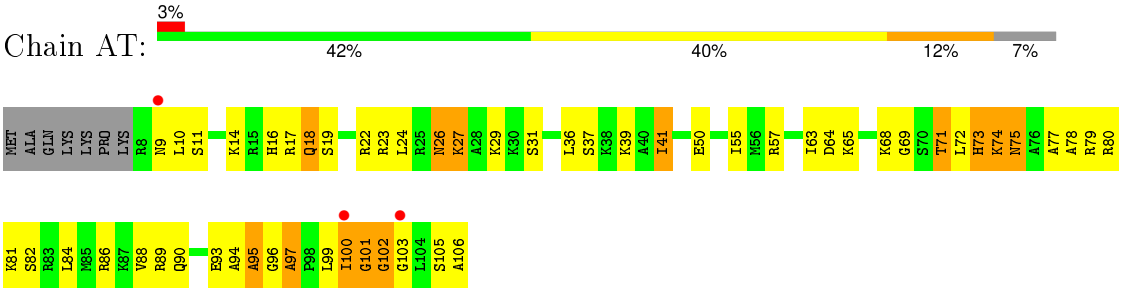
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



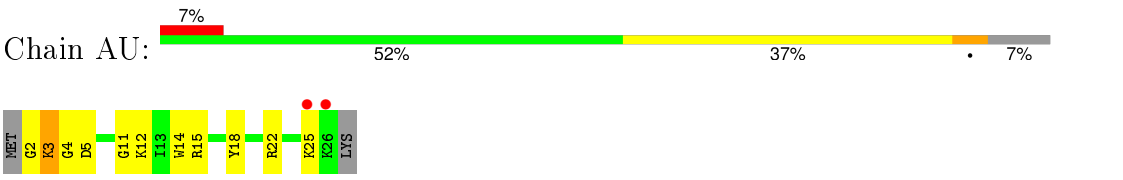
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



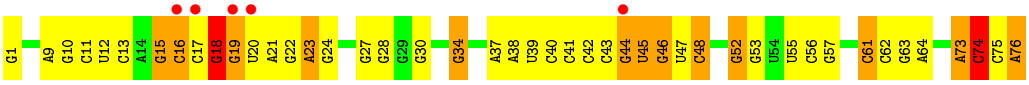
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



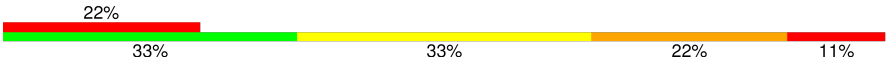
• Molecule 22: RNA (77-MER)

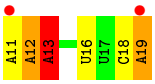
Chain AV:



• Molecule 23: 5'-R(*UP*AP*AP*AP*AP*AP*UP*GP*UP)-3'

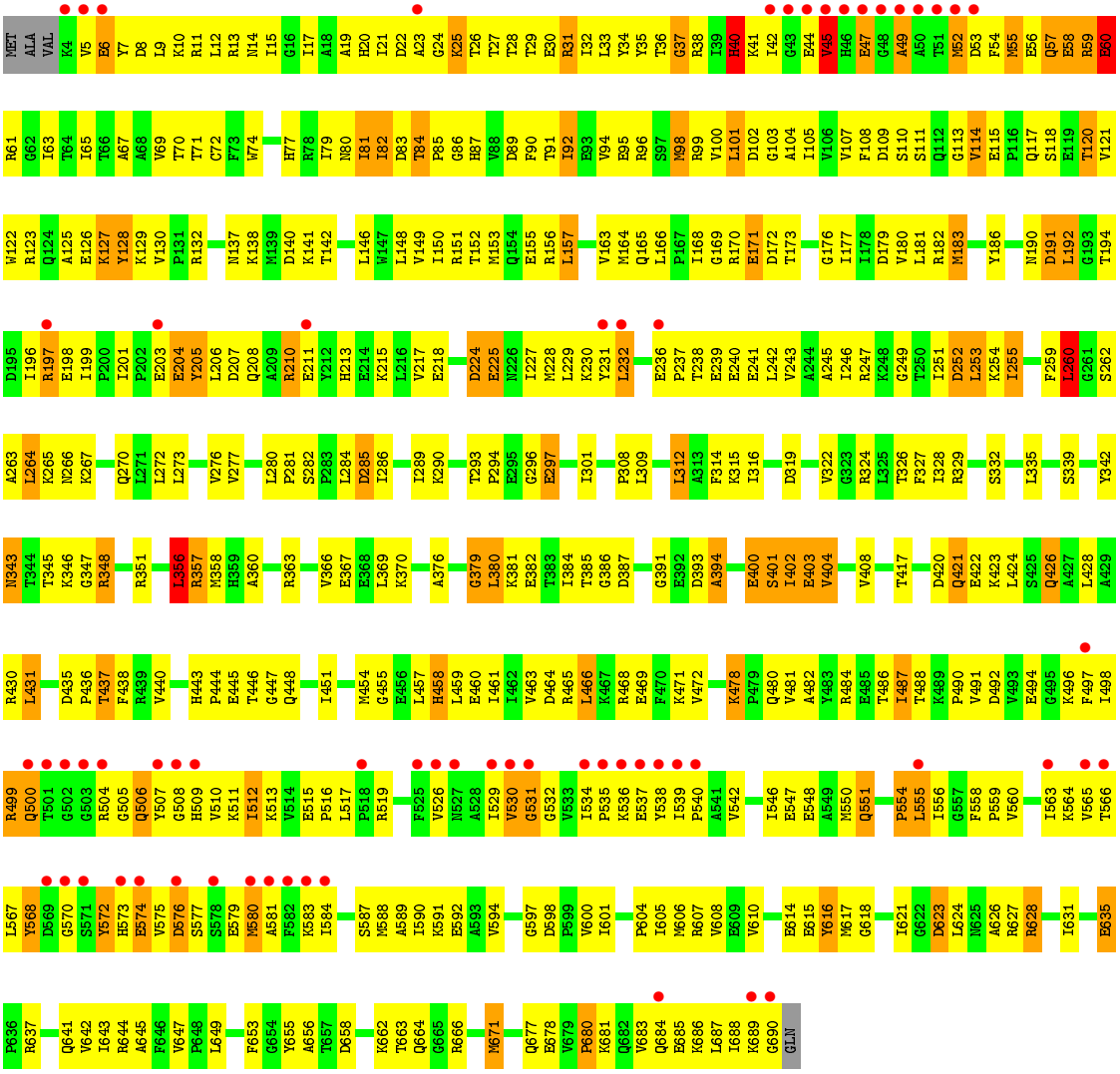
Chain AX:





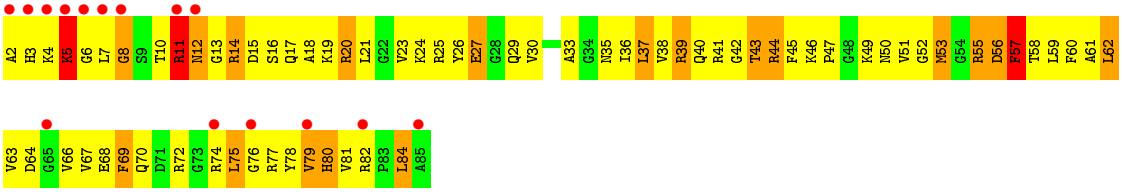
• Molecule 24: ELONGATION FACTOR G

Chain AY:



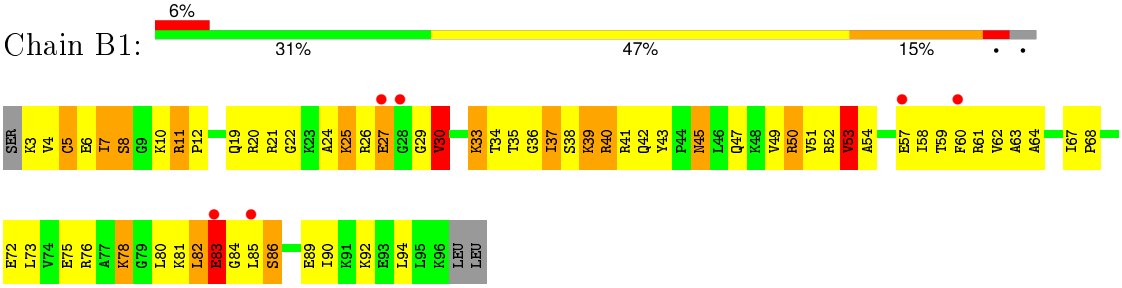
• Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



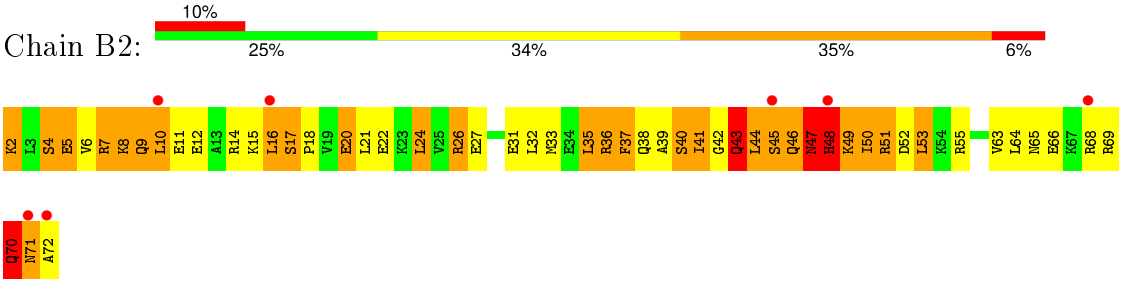
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain B1:



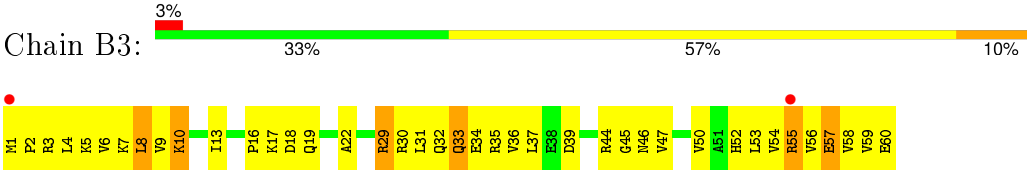
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain B2:



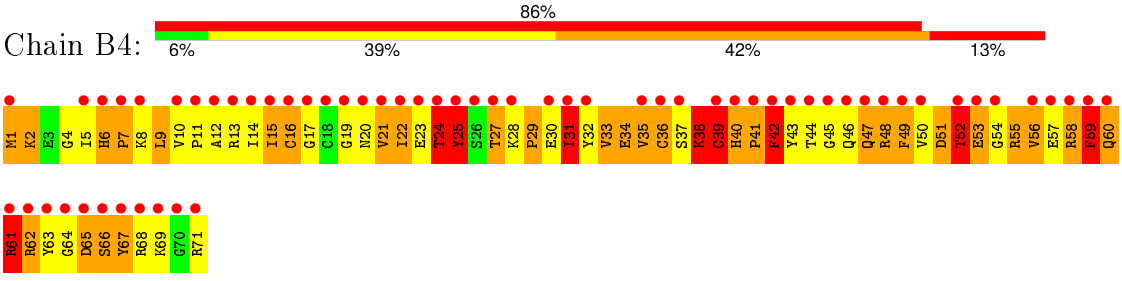
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:



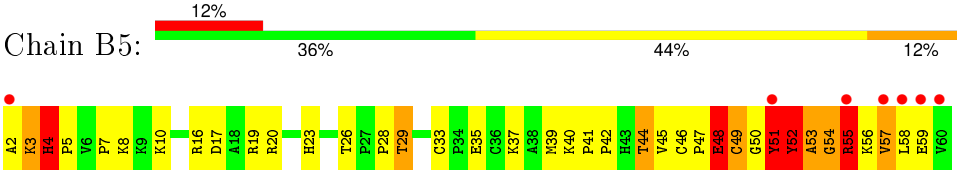
• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



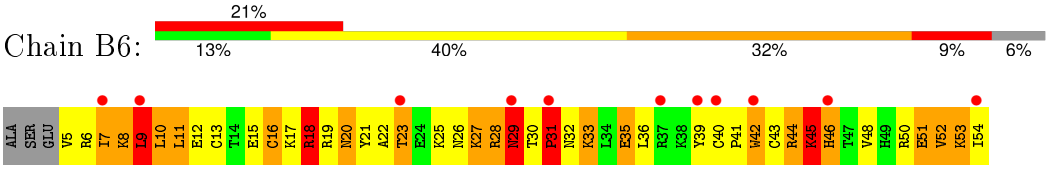
• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:



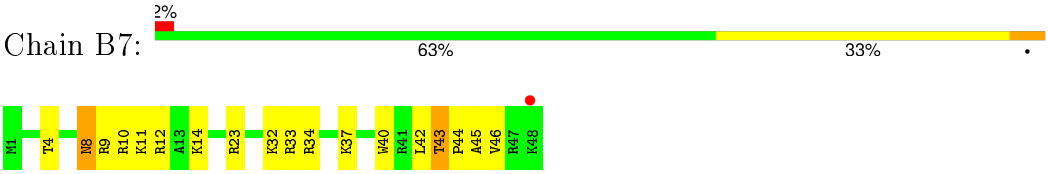
- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6:



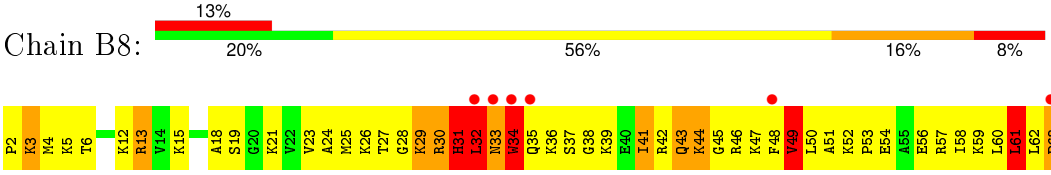
- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7:



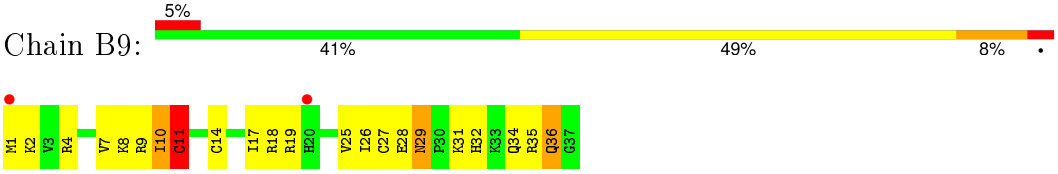
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8:



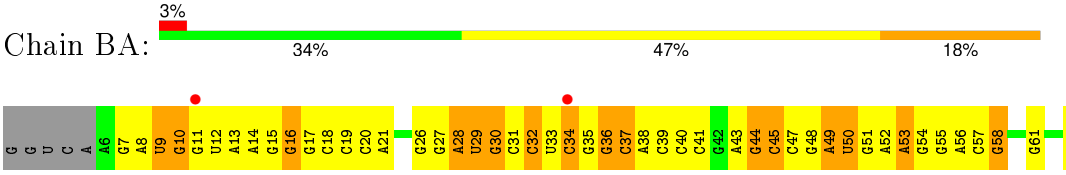
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

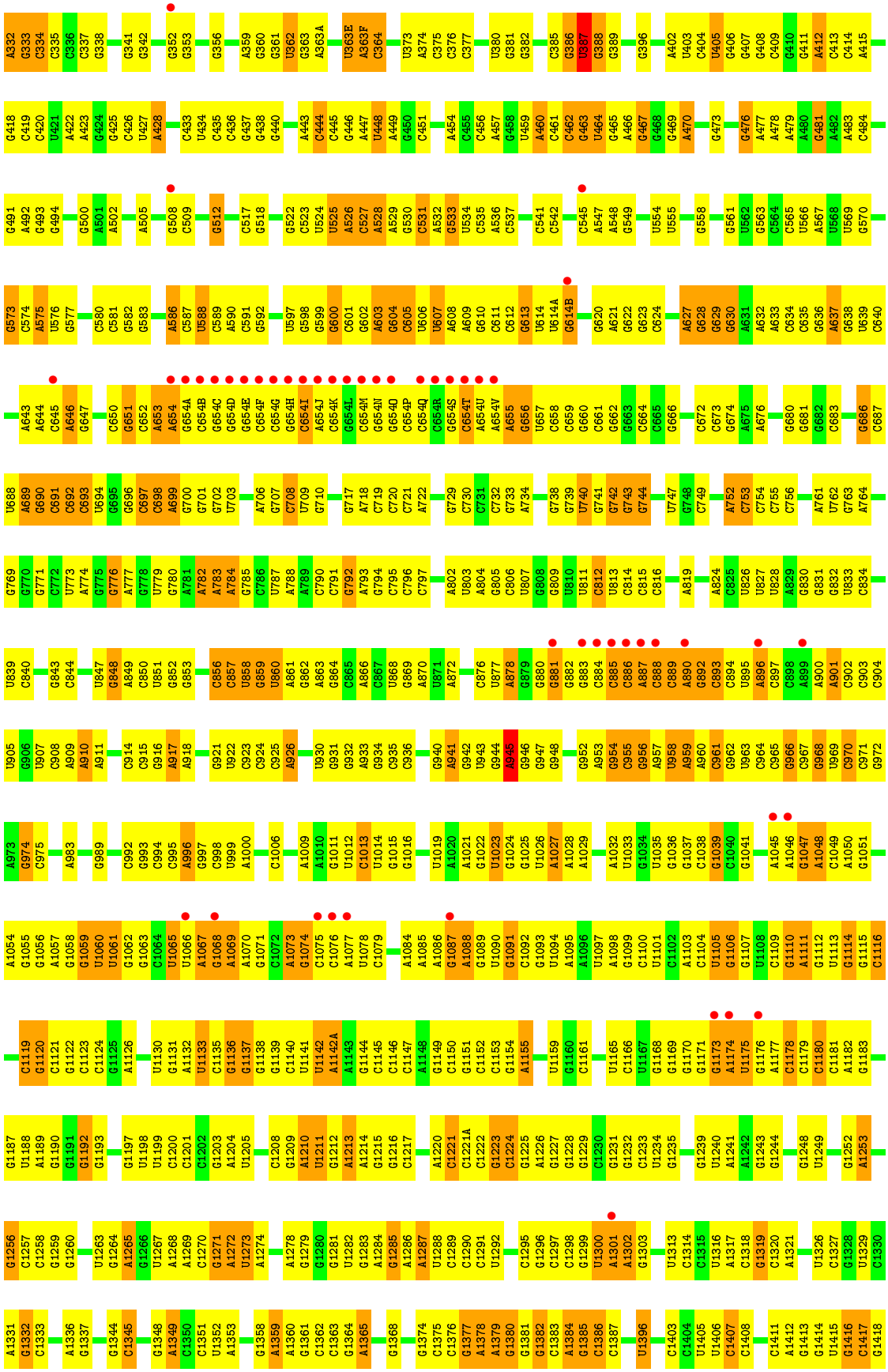
Chain B9:

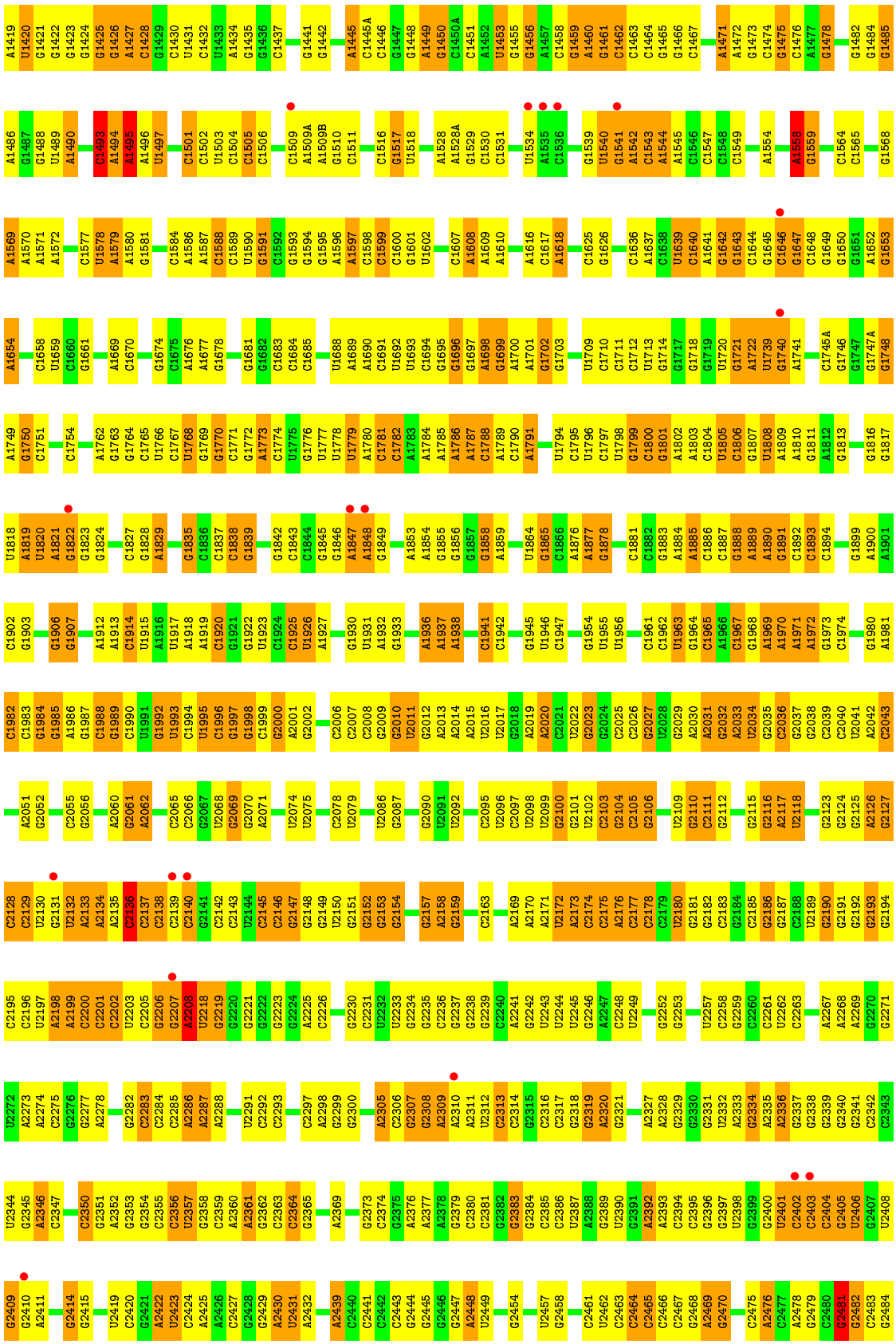


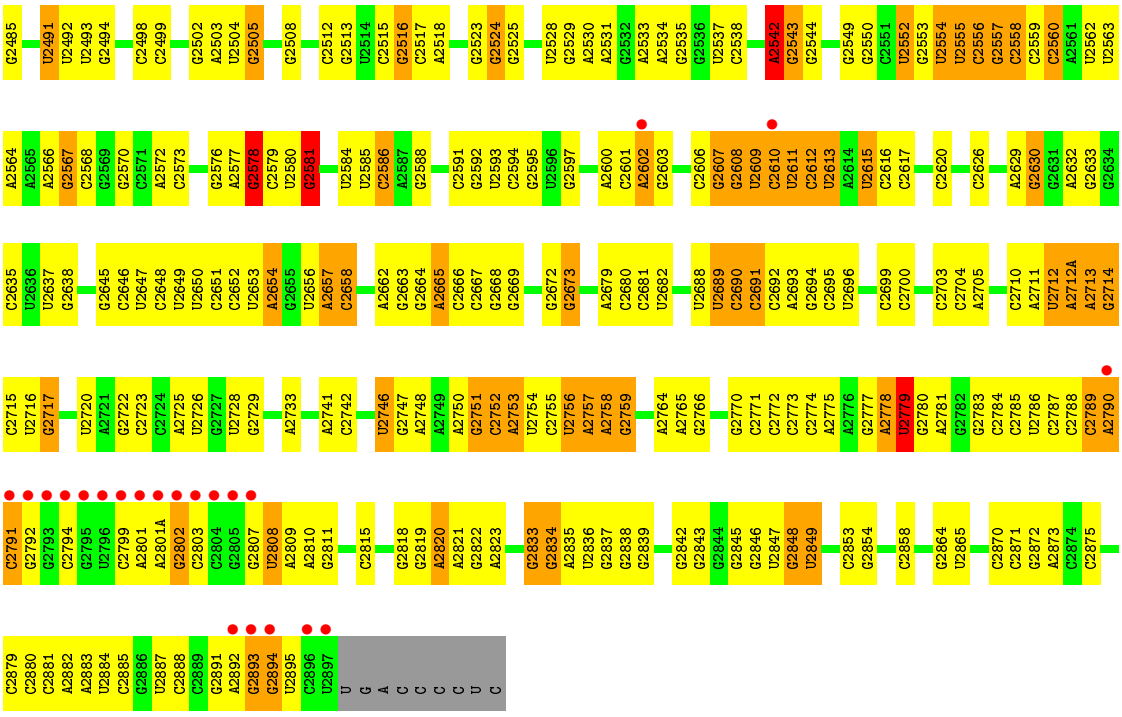
- Molecule 35: 23S RIBOSOMAL RNA

Chain BA:



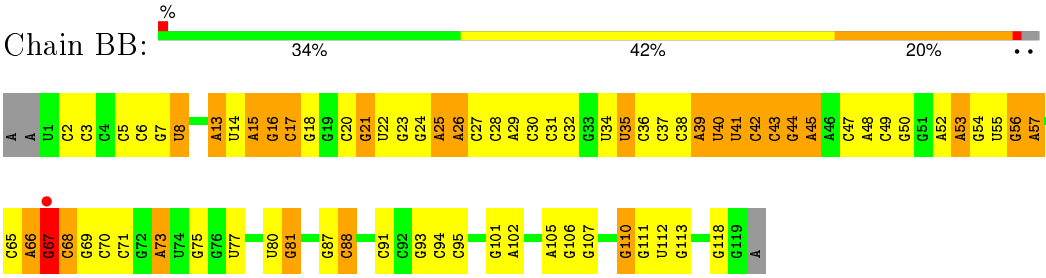






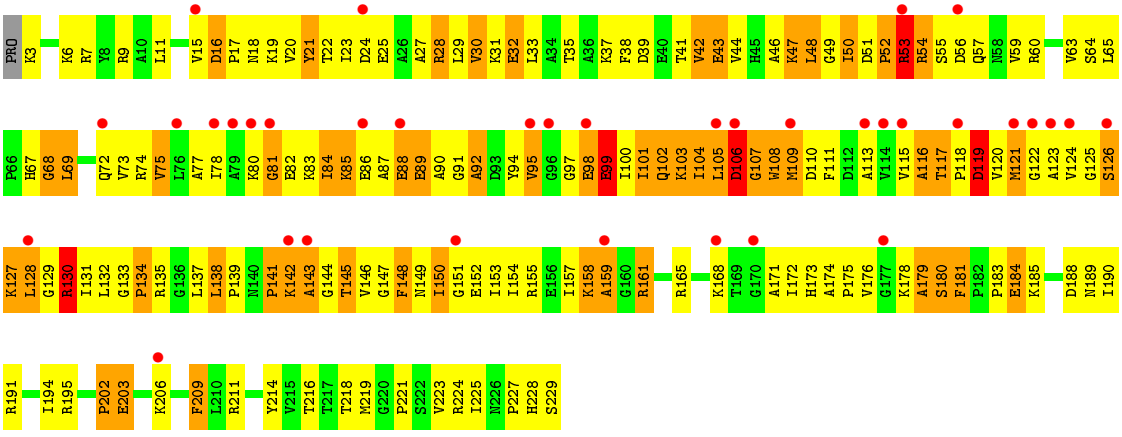
- Molecule 36: 5S RIBOSOMAL RNA

Chain BB:



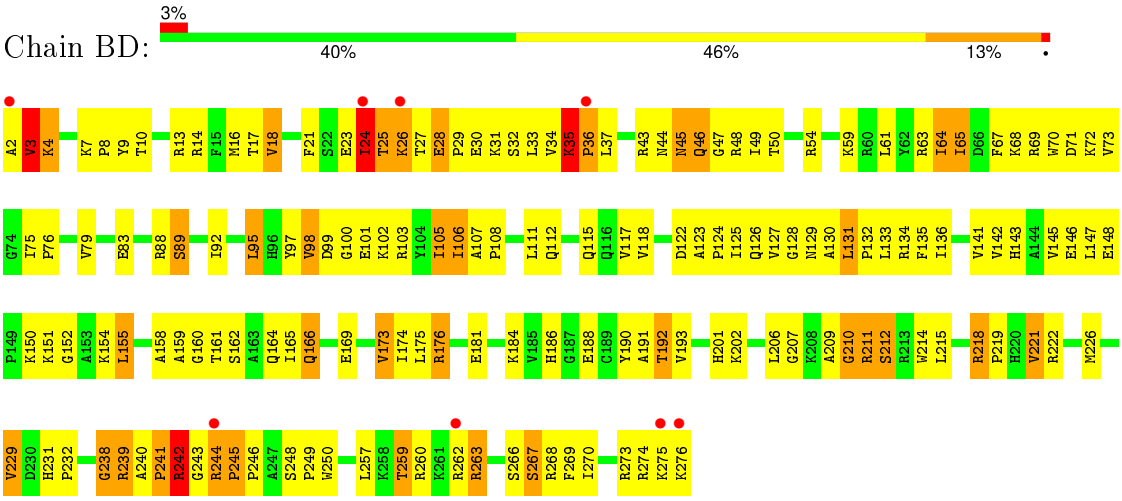
- Molecule 37: RIBOSOMAL PROTEIN L1

Chain BC:



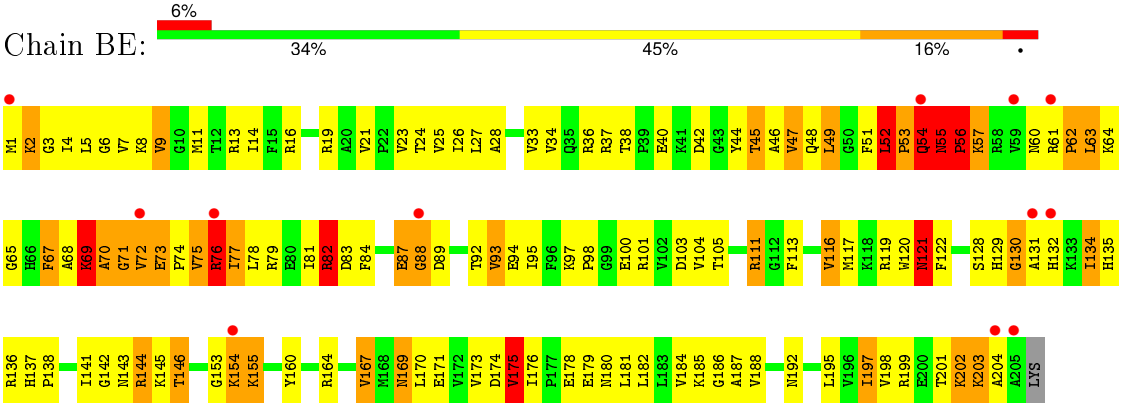
- Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain BD:



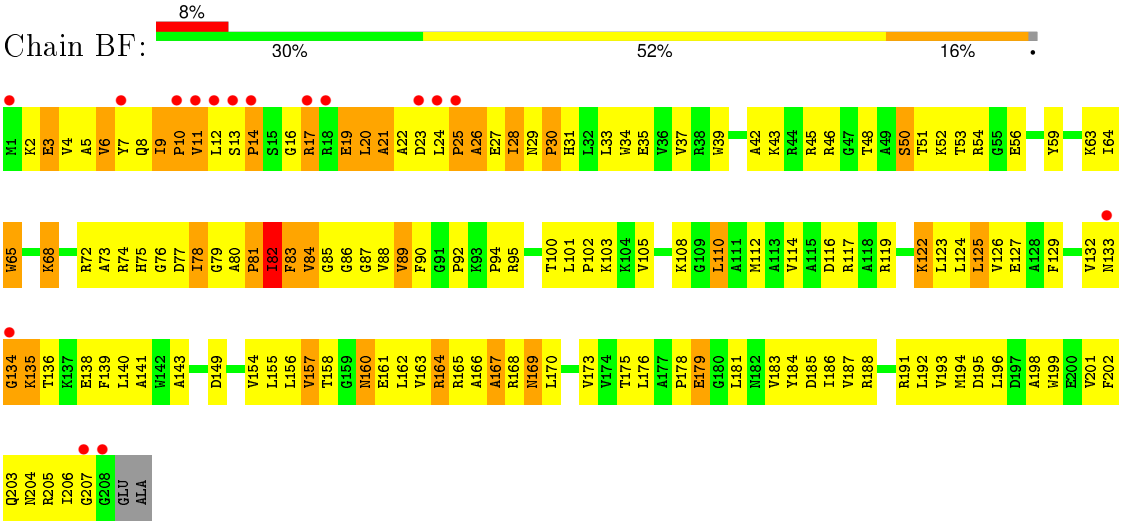
- Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:



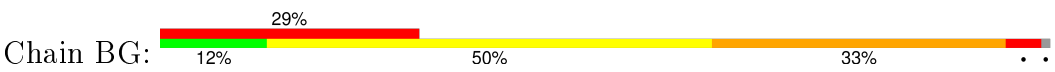
- Molecule 40: 50S RIBOSOMAL PROTEIN L4

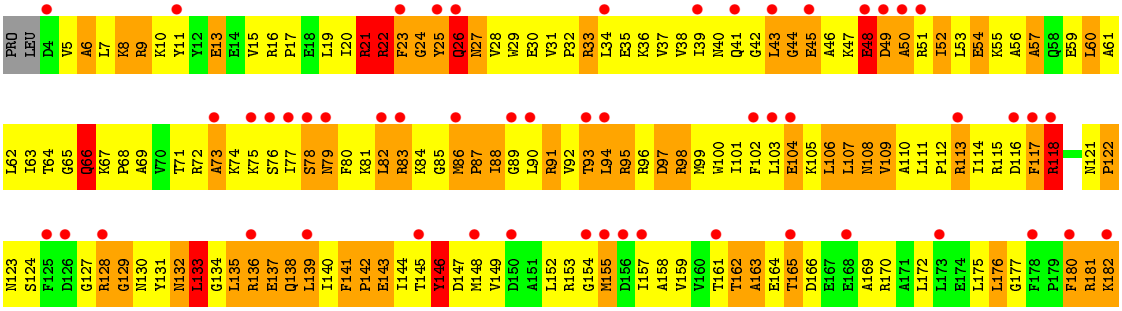
Chain BF:

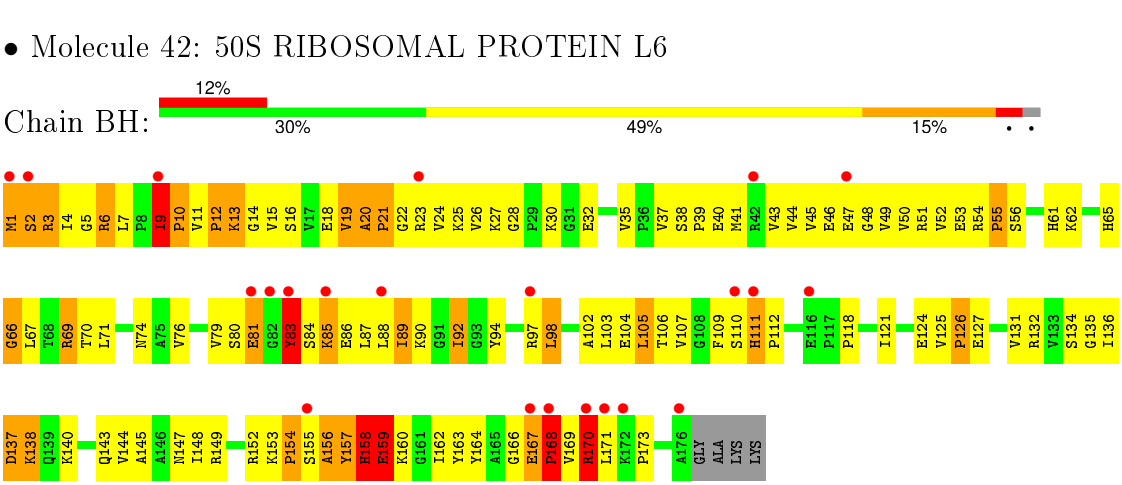


- Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain BG:





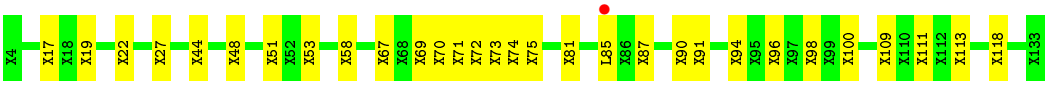


• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:

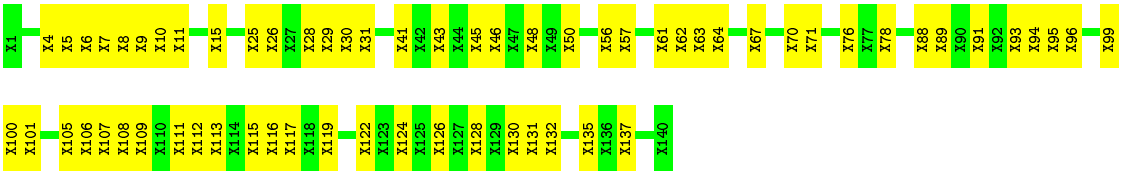
• Molecule 43: CHAIN J

Chain BJ:



• Molecule 44: CHAIN K

Chain BK:

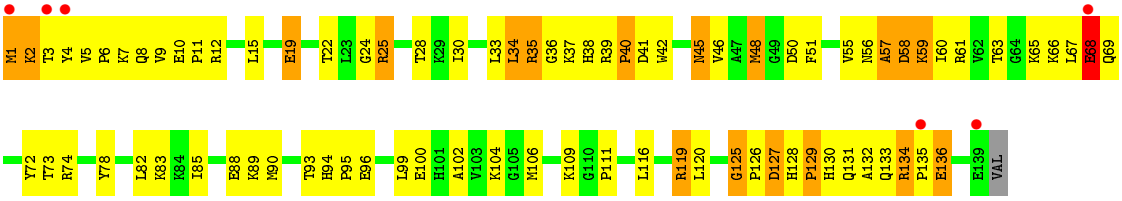


• Molecule 45: CHAIN L

Chain BL:

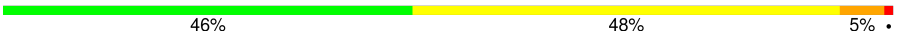
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

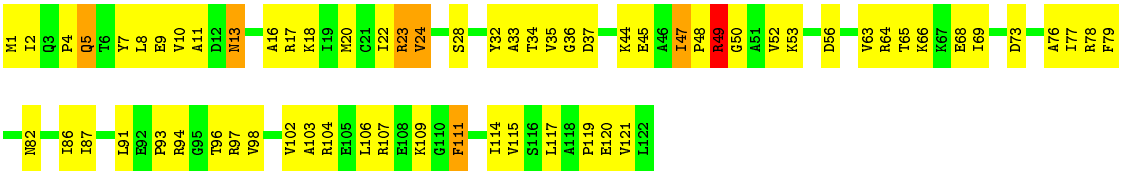
Chain BN:



• Molecule 47: 50S RIBOSOMAL PROTEIN L14

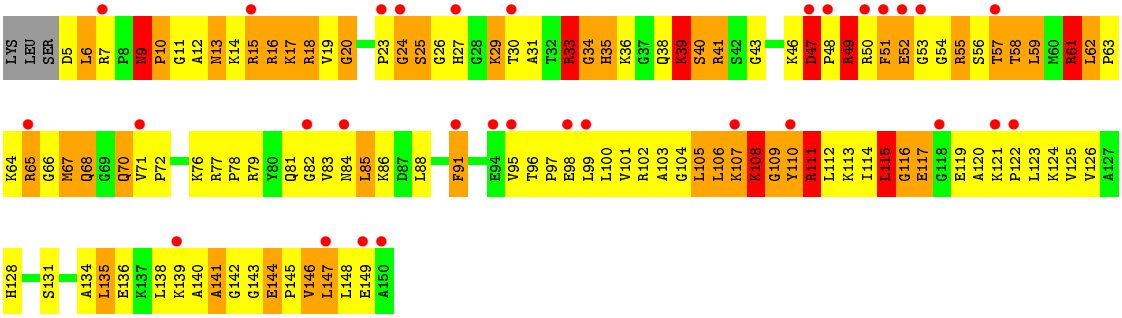
Chain BO:





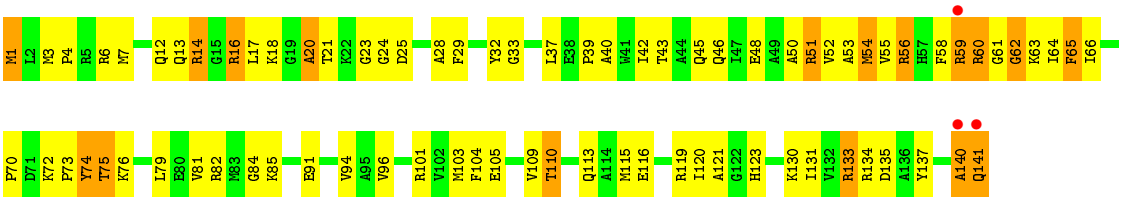
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP:



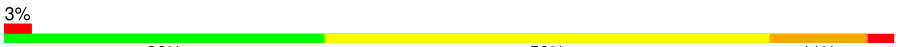
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

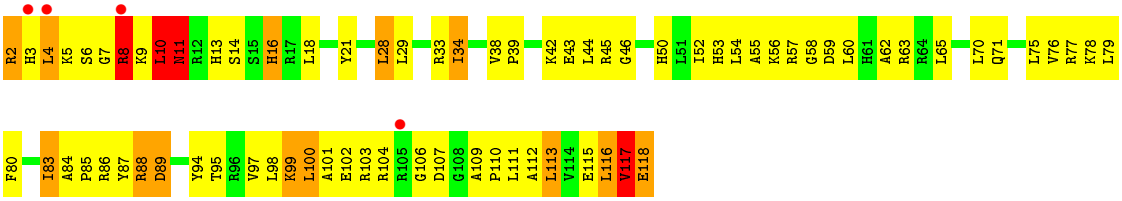
Chain BQ:



• Molecule 50: 50S RIBOSOMAL PROTEIN L17

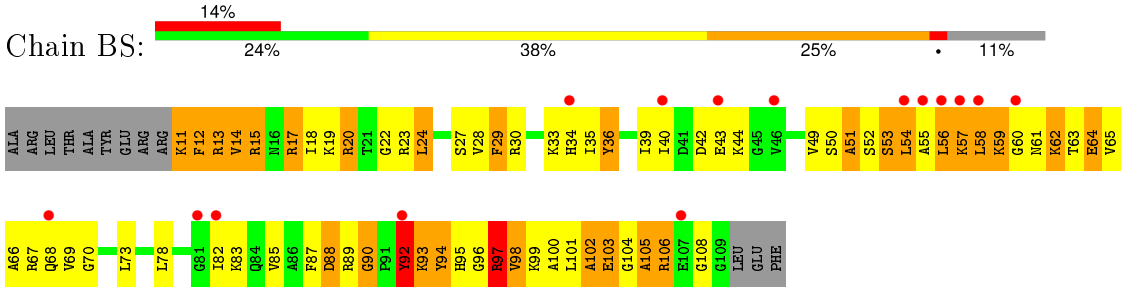
Chain BR:





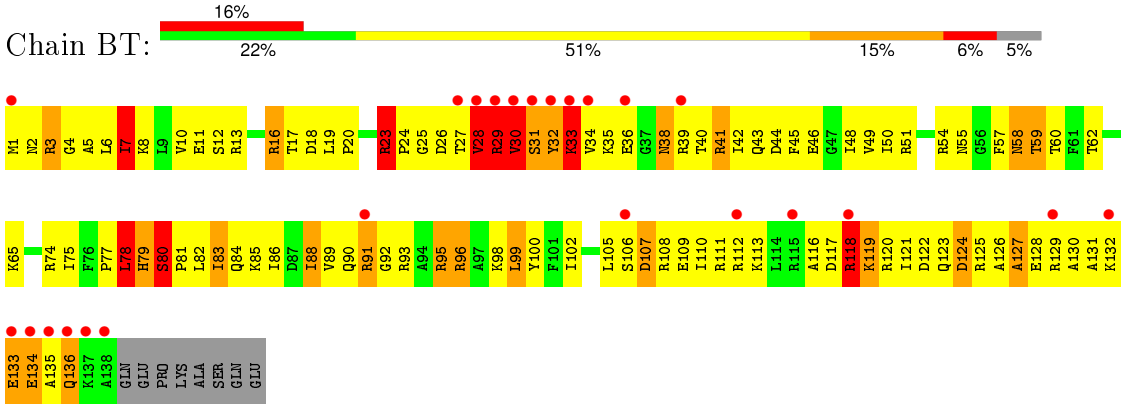
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



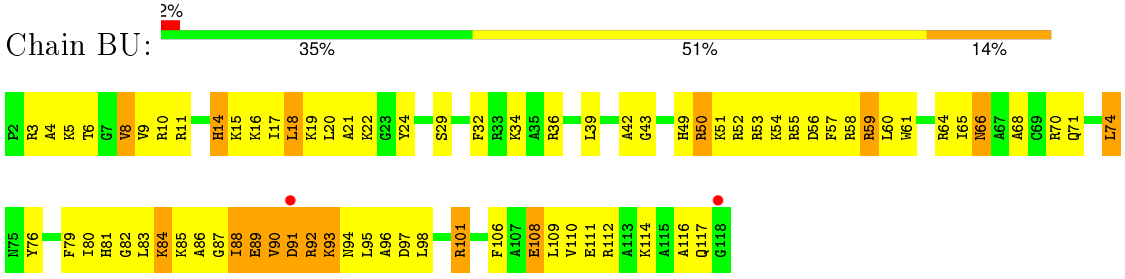
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT:



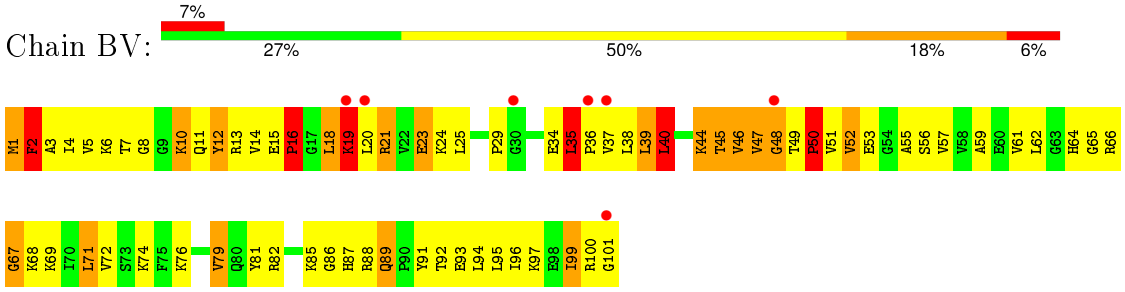
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



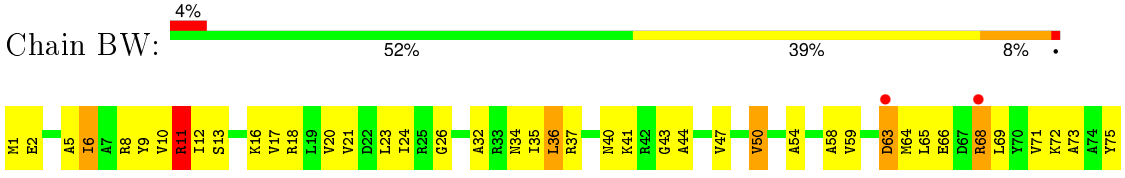
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

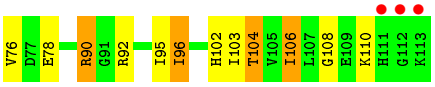
Chain BV:



• Molecule 55: 50S RIBOSOMAL PROTEIN L22

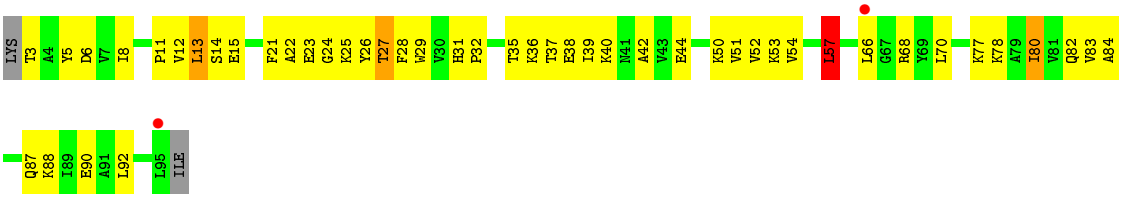
Chain BW:





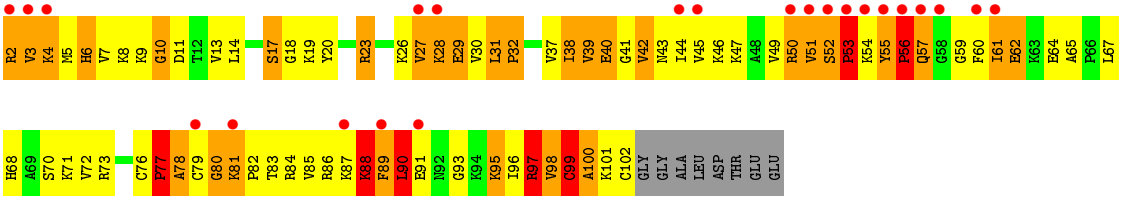
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



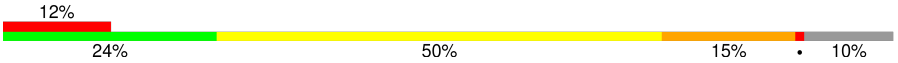
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

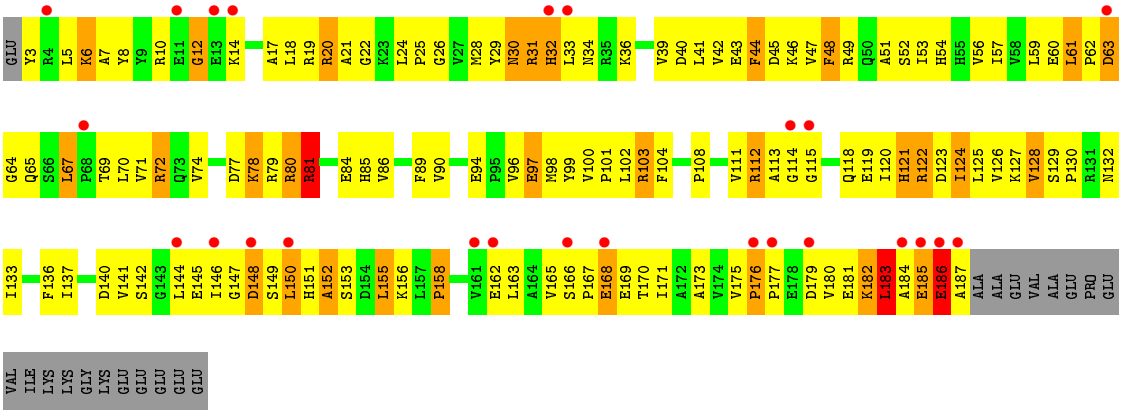
Chain BY:



• Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	202.90Å 242.63Å 309.32Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	49.75 – 2.95 49.75 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.75-2.95) 100.0 (49.75-2.95)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.244 0.226 , 0.256	Depositor DCC
R_{free} test set	30895 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 60.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 617901 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	153829	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GCP, 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	0.41	0/36258	0.70	5/56589 (0.0%)
2	AB	0.26	0/1936	0.46	0/2611
3	AC	0.36	0/1637	0.58	0/2207
4	AD	0.36	0/1733	0.61	0/2318
5	AE	0.46	0/1163	0.67	0/1566
6	AF	0.36	0/856	0.63	0/1154
7	AG	0.36	0/1276	0.62	0/1709
8	AH	0.39	0/1136	0.69	0/1527
9	AI	0.36	0/1029	0.69	0/1379
10	AJ	0.40	0/808	0.69	0/1087
11	AK	0.39	0/900	0.68	0/1213
12	AL	0.42	0/987	0.73	1/1322 (0.1%)
13	AM	0.32	0/948	0.60	0/1272
14	AN	0.41	0/501	0.77	0/664
15	AO	0.37	0/745	0.62	0/992
16	AP	0.40	0/717	0.71	0/965
17	AQ	0.40	0/837	0.69	0/1119
18	AR	0.38	0/579	0.60	0/768
19	AS	0.37	0/706	0.64	0/950
20	AT	0.39	0/765	0.76	0/1007
21	AU	0.43	0/213	0.62	0/279
22	AV	0.84	2/1809 (0.1%)	1.27	7/2819 (0.2%)
23	AX	1.26	2/210 (1.0%)	1.37	2/325 (0.6%)
24	AY	0.33	0/5477	0.61	3/7415 (0.0%)
25	B0	0.29	0/671	0.43	0/892
26	B1	0.37	0/739	0.58	0/983
27	B2	10.54	1/600 (0.2%)	0.42	0/793
28	B3	0.32	0/473	0.50	0/636
29	B4	0.29	0/594	0.45	0/795
30	B5	0.40	0/473	0.70	0/639
31	B6	0.48	0/440	0.80	0/586
32	B7	0.44	0/427	0.71	0/561

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	B8	0.56	0/516	0.87	1/681 (0.1%)
34	B9	0.45	0/310	0.72	0/407
35	BA	0.46	1/69972 (0.0%)	0.72	25/109230 (0.0%)
36	BB	0.37	0/2853	0.72	1/4451 (0.0%)
37	BC	0.32	0/1766	0.62	0/2380
38	BD	0.47	0/2195	0.82	1/2955 (0.0%)
39	BE	0.42	0/1597	0.71	0/2155
40	BF	0.39	0/1659	0.66	0/2246
41	BG	0.45	0/1483	0.80	1/1994 (0.1%)
42	BH	0.40	0/1371	0.67	0/1853
43	BJ	0.20	0/7	0.87	0/8
46	BN	0.46	0/1132	0.76	0/1527
47	BO	0.44	0/943	0.71	0/1269
48	BP	0.45	0/1131	0.86	4/1504 (0.3%)
49	BQ	0.41	0/1143	0.65	0/1527
50	BR	0.43	0/974	0.75	0/1302
51	BS	0.39	0/779	0.66	0/1038
52	BT	0.42	0/1156	0.66	0/1544
53	BU	0.48	0/975	0.70	0/1297
54	BV	0.40	0/790	0.72	0/1057
55	BW	0.42	0/907	0.71	0/1216
56	BX	0.47	0/740	0.69	1/995 (0.1%)
57	BY	0.52	0/789	0.87	0/1053
58	BZ	0.34	0/1500	0.63	0/2037
All	All	0.77	6/164331 (0.0%)	0.71	52/244868 (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	1
24	AY	0	1
35	BA	0	19
36	BB	0	2
All	All	0	23

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B2	72	ALA	C-OXT	258.07	6.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1453	U	O3'-P	-17.05	1.40	1.61
22	AV	37	A	N3-C4	7.56	1.39	1.34
22	AV	37	A	C6-N1	7.26	1.40	1.35
23	AX	11	A	N9-C4	5.43	1.41	1.37

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	BA	2208	A	P-O3'-C3'	9.92	131.60	119.70
22	AV	37	A	N1-C2-N3	-9.87	124.36	129.30
22	AV	74	C	O4'-C1'-N1	8.40	114.92	108.20
22	AV	37	A	N9-C4-C5	-7.54	102.79	105.80
22	AV	37	A	N1-C6-N6	6.87	122.72	118.60

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	189(H)	G	Sidechain
24	AY	499	ARG	Sidechain
35	BA	271(H)	G	Sidechain
35	BA	271(Q)	G	Sidechain
35	BA	271(Y)	U	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32391	0	16349	1995	0
2	AB	1901	0	1947	322	1
3	AC	1613	0	1677	223	28
4	AD	1703	0	1765	125	0
5	AE	1147	0	1207	56	0
6	AF	843	0	857	53	0
7	AG	1257	0	1296	138	0
8	AH	1116	0	1177	63	0
9	AI	1010	0	1037	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	114	0
11	AK	885	0	904	56	0
12	AL	971	0	1057	112	0
13	AM	938	0	995	124	0
14	AN	492	0	529	68	0
15	AO	734	0	771	49	0
16	AP	701	0	720	58	0
17	AQ	824	0	891	47	0
18	AR	574	0	644	26	0
19	AS	692	0	714	109	0
20	AT	763	0	861	71	11
21	AU	209	0	221	12	0
22	AV	1619	0	823	60	0
23	AX	188	0	98	7	0
24	AY	5376	0	5433	565	0
25	B0	662	0	688	160	0
26	B1	732	0	808	114	0
27	B2	598	0	651	125	11
28	B3	468	0	523	66	0
29	B4	581	0	577	214	0
30	B5	459	0	478	75	0
31	B6	433	0	461	128	0
32	B7	419	0	467	29	0
33	B8	508	0	576	112	0
34	B9	307	0	335	31	0
35	BA	62476	0	31499	3287	28
36	BB	2551	0	1295	107	0
37	BC	1735	0	1790	277	1
38	BD	2145	0	2234	255	0
39	BE	1564	0	1629	233	0
40	BF	1624	0	1677	220	0
41	BG	1459	0	1516	395	0
42	BH	1345	0	1430	187	0
43	BJ	654	0	156	22	0
44	BK	701	0	168	46	0
45	BL	356	0	86	20	0
46	BN	1105	0	1180	111	0
47	BO	933	0	996	67	0
48	BP	1114	0	1186	302	0
49	BQ	1122	0	1179	111	0
50	BR	960	0	1021	104	0
51	BS	771	0	832	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	BT	1142	0	1200	229	0
53	BU	958	0	1015	122	0
54	BV	779	0	852	147	0
55	BW	896	0	953	56	0
56	BX	726	0	778	47	0
57	BY	776	0	870	164	0
58	BZ	1468	0	1492	216	0
59	AA	198	0	0	0	0
59	AY	1	0	0	0	0
59	B0	1	0	0	0	0
59	B5	1	0	0	0	0
59	BA	320	0	0	0	0
59	BC	1	0	0	0	0
59	BU	1	0	0	0	0
60	AD	1	0	0	0	0
60	AN	1	0	0	0	0
60	B9	1	0	0	0	0
61	AY	32	0	14	11	0
62	AY	2	0	0	2	0
All	All	153829	0	105425	11647	40

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 45.

The worst 5 of 11647 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)
30:B5:46:CYS:SG	30:B5:47:PRO:HD2	1.41	1.57
29:B4:12:ALA:H	29:B4:24:THR:CG2	1.16	1.56
9:AI:19:LEU:HA	9:AI:61:ALA:CB	1.39	1.53
52:BT:80:SER:HB3	52:BT:81:PRO:CD	1.40	1.51
9:AI:18:PHE:C	9:AI:61:ALA:HB1	1.27	1.50

The worst 5 of 40 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AT:100:ILE:CG1	27:B2:43:GLN:CD[2_554]	0.34	1.86
20:AT:100:ILE:CD1	27:B2:43:GLN:NE2[2_554]	0.69	1.51
3:AC:79:ARG:CD	35:BA:2139:C:C4[2_555]	0.83	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:79:ARG:CD	35:BA:2139:C:C5[2_555]	0.87	1.33
3:AC:79:ARG:CG	35:BA:2139:C:C6[2_555]	0.96	1.24

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	AB	233/256 (91%)	163 (70%)	44 (19%)	26 (11%)	0 2
3	AC	205/239 (86%)	145 (71%)	32 (16%)	28 (14%)	0 1
4	AD	206/209 (99%)	160 (78%)	35 (17%)	11 (5%)	2 12
5	AE	149/162 (92%)	134 (90%)	12 (8%)	3 (2%)	9 38
6	AF	99/101 (98%)	80 (81%)	13 (13%)	6 (6%)	2 9
7	AG	153/156 (98%)	113 (74%)	26 (17%)	14 (9%)	1 3
8	AH	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	26 67
9	AI	125/128 (98%)	93 (74%)	21 (17%)	11 (9%)	1 4
10	AJ	97/105 (92%)	73 (75%)	15 (16%)	9 (9%)	1 3
11	AK	117/129 (91%)	95 (81%)	19 (16%)	3 (3%)	7 30
12	AL	123/132 (93%)	101 (82%)	11 (9%)	11 (9%)	1 4
13	AM	117/126 (93%)	74 (63%)	32 (27%)	11 (9%)	1 3
14	AN	58/61 (95%)	44 (76%)	7 (12%)	7 (12%)	0 1
15	AO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	16 53
16	AP	82/88 (93%)	73 (89%)	7 (8%)	2 (2%)	7 33
17	AQ	98/105 (93%)	86 (88%)	10 (10%)	2 (2%)	9 38
18	AR	68/88 (77%)	58 (85%)	8 (12%)	2 (3%)	6 27
19	AS	86/93 (92%)	53 (62%)	21 (24%)	12 (14%)	0 1
20	AT	97/106 (92%)	79 (81%)	10 (10%)	8 (8%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	AU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1 4
24	AY	685/691 (99%)	537 (78%)	99 (14%)	49 (7%)	1 6
25	B0	82/84 (98%)	56 (68%)	19 (23%)	7 (8%)	1 4
26	B1	92/97 (95%)	73 (79%)	14 (15%)	5 (5%)	2 11
27	B2	69/71 (97%)	45 (65%)	11 (16%)	13 (19%)	0 0
28	B3	58/60 (97%)	50 (86%)	7 (12%)	1 (2%)	11 43
29	B4	69/71 (97%)	16 (23%)	17 (25%)	36 (52%)	0 0
30	B5	57/59 (97%)	45 (79%)	3 (5%)	9 (16%)	0 1
31	B6	48/53 (91%)	22 (46%)	11 (23%)	15 (31%)	0 0
32	B7	46/48 (96%)	43 (94%)	3 (6%)	0	100 100
33	B8	62/64 (97%)	42 (68%)	8 (13%)	12 (19%)	0 0
34	B9	35/37 (95%)	23 (66%)	9 (26%)	3 (9%)	1 4
37	BC	225/228 (99%)	121 (54%)	56 (25%)	48 (21%)	0 0
38	BD	273/275 (99%)	222 (81%)	33 (12%)	18 (7%)	1 7
39	BE	203/206 (98%)	145 (71%)	34 (17%)	24 (12%)	0 1
40	BF	206/210 (98%)	165 (80%)	19 (9%)	22 (11%)	0 2
41	BG	177/181 (98%)	78 (44%)	49 (28%)	50 (28%)	0 0
42	BH	174/180 (97%)	112 (64%)	31 (18%)	31 (18%)	0 0
43	BJ	1/130 (1%)	0	1 (100%)	0	100 100
46	BN	137/140 (98%)	110 (80%)	15 (11%)	12 (9%)	1 4
47	BO	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	7 31
48	BP	144/149 (97%)	84 (58%)	23 (16%)	37 (26%)	0 0
49	BQ	139/141 (99%)	115 (83%)	18 (13%)	6 (4%)	3 16
50	BR	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	1 6
51	BS	97/111 (87%)	52 (54%)	25 (26%)	20 (21%)	0 0
52	BT	136/146 (93%)	90 (66%)	25 (18%)	21 (15%)	0 1
53	BU	115/117 (98%)	87 (76%)	22 (19%)	6 (5%)	2 12
54	BV	99/101 (98%)	73 (74%)	11 (11%)	15 (15%)	0 1
55	BW	111/113 (98%)	93 (84%)	14 (13%)	4 (4%)	4 21
56	BX	91/95 (96%)	79 (87%)	11 (12%)	1 (1%)	17 56
57	BY	99/109 (91%)	54 (54%)	17 (17%)	28 (28%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
58	BZ	183/205 (89%)	131 (72%)	30 (16%)	22 (12%)	0 1
All	All	6506/6949 (94%)	4803 (74%)	1007 (16%)	696 (11%)	0 2

5 of 696 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	26	PRO
2	AB	37	ASN
2	AB	76	GLN
2	AB	77	ALA

5.3.2 Protein sidechains (i)

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	AB	202/220 (92%)	157 (78%)	45 (22%)	1 4
3	AC	160/188 (85%)	129 (81%)	31 (19%)	2 7
4	AD	180/181 (99%)	155 (86%)	25 (14%)	4 17
5	AE	115/123 (94%)	109 (95%)	6 (5%)	29 66
6	AF	90/90 (100%)	83 (92%)	7 (8%)	16 46
7	AG	126/127 (99%)	108 (86%)	18 (14%)	4 17
8	AH	119/119 (100%)	103 (87%)	16 (13%)	5 19
9	AI	98/99 (99%)	85 (87%)	13 (13%)	5 19
10	AJ	88/92 (96%)	82 (93%)	6 (7%)	20 54
11	AK	90/99 (91%)	84 (93%)	6 (7%)	20 55
12	AL	104/109 (95%)	90 (86%)	14 (14%)	5 18
13	AM	94/101 (93%)	84 (89%)	10 (11%)	8 29
14	AN	49/50 (98%)	43 (88%)	6 (12%)	6 23
15	AO	79/80 (99%)	71 (90%)	8 (10%)	9 32
16	AP	72/74 (97%)	68 (94%)	4 (6%)	26 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	61 88
18	AR	61/77 (79%)	55 (90%)	6 (10%)	10 34
19	AS	74/80 (92%)	68 (92%)	6 (8%)	15 44
20	AT	76/82 (93%)	68 (90%)	8 (10%)	8 30
21	AU	19/22 (86%)	18 (95%)	1 (5%)	28 65
24	AY	579/582 (100%)	516 (89%)	63 (11%)	8 28
25	B0	66/66 (100%)	45 (68%)	21 (32%)	0 1
26	B1	78/82 (95%)	60 (77%)	18 (23%)	1 4
27	B2	66/66 (100%)	42 (64%)	24 (36%)	0 1
28	B3	51/52 (98%)	44 (86%)	7 (14%)	4 18
29	B4	63/63 (100%)	48 (76%)	15 (24%)	1 3
30	B5	51/51 (100%)	42 (82%)	9 (18%)	2 10
31	B6	49/51 (96%)	37 (76%)	12 (24%)	1 3
32	B7	41/41 (100%)	39 (95%)	2 (5%)	31 68
33	B8	53/54 (98%)	42 (79%)	11 (21%)	1 6
34	B9	34/34 (100%)	31 (91%)	3 (9%)	12 40
37	BC	179/180 (99%)	160 (89%)	19 (11%)	8 29
38	BD	217/217 (100%)	185 (85%)	32 (15%)	4 15
39	BE	165/166 (99%)	133 (81%)	32 (19%)	2 7
40	BF	165/166 (99%)	146 (88%)	19 (12%)	7 26
41	BG	153/155 (99%)	123 (80%)	30 (20%)	1 7
42	BH	146/148 (99%)	131 (90%)	15 (10%)	9 31
43	BJ	1/1 (100%)	1 (100%)	0	100 100
46	BN	117/119 (98%)	103 (88%)	14 (12%)	6 24
47	BO	100/100 (100%)	93 (93%)	7 (7%)	19 53
48	BP	112/115 (97%)	84 (75%)	28 (25%)	1 3
49	BQ	111/111 (100%)	96 (86%)	15 (14%)	5 18
50	BR	100/100 (100%)	82 (82%)	18 (18%)	2 9
51	BS	77/87 (88%)	62 (80%)	15 (20%)	2 7
52	BT	120/127 (94%)	94 (78%)	26 (22%)	1 5
53	BU	92/93 (99%)	80 (87%)	12 (13%)	5 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	BV	82/82 (100%)	65 (79%)	17 (21%)	1 6
55	BW	91/92 (99%)	79 (87%)	12 (13%)	5 20
56	BX	74/77 (96%)	68 (92%)	6 (8%)	15 44
57	BY	84/90 (93%)	65 (77%)	19 (23%)	1 4
58	BZ	162/178 (91%)	138 (85%)	24 (15%)	4 15
All	All	5469/5656 (97%)	4686 (86%)	783 (14%)	4 17

5 of 783 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	B2	44	LEU
37	BC	138	LEU
55	BW	21	VAL
28	B3	8	LEU
31	B6	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
25	B0	17	GLN
37	BC	189	ASN
53	BU	94	ASN
25	B0	70	GLN
28	B3	46	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1519 (99%)	320 (21%)	51 (3%)
22	AV	75/76 (98%)	24 (32%)	2 (2%)
23	AX	8/9 (88%)	3 (37%)	0
35	BA	2897/2915 (99%)	665 (22%)	60 (2%)
36	BB	118/122 (96%)	26 (22%)	2 (1%)
All	All	4603/4641 (99%)	1038 (22%)	115 (2%)

5 of 1038 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	38	G
1	AA	39	G

5 of 115 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	AV	16	C
35	BA	627	A
35	BA	2439	A
35	BA	49	A
35	BA	331	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 527 ligands modelled in this entry, 526 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
61	GCP	AY	701	59	26,34,34	1.89	9 (34%)	34,54,54	2.04	9 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	GCP	AY	701	59	-	0/15/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GCP	C6-C5	-3.87	1.33	1.41
61	AY	701	GCP	PB-O2B	-3.31	1.48	1.56
61	AY	701	GCP	PG-O3G	-3.15	1.47	1.54
61	AY	701	GCP	C5-C4	-2.93	1.33	1.40
61	AY	701	GCP	PG-O2G	-2.68	1.48	1.54

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	AY	701	GCP	N3-C2-N1	-5.31	119.36	127.44
61	AY	701	GCP	C4'-O4'-C1'	-5.24	103.96	109.72
61	AY	701	GCP	PA-O3A-PB	-4.54	119.98	132.73
61	AY	701	GCP	O1G-PG-C3B	-3.12	104.02	111.13
61	AY	701	GCP	C5-C6-N1	-2.91	119.61	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	701	GCP	11	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	BA	3

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Mol	Chain	Number of breaks
1	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	496:A	O3'	498:U	P	3.07
1	BA	45:C	O3'	47:C	P	2.97
1	BA	1133:U	O3'	1135:C	P	2.48
1	BA	2203:U	O3'	2205:C	P	2.42

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, 95^{th} 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	1507/1519 (99%)	0.21	46 (3%) 52 33	24, 47, 125, 239	0
2	AB	235/256 (91%)	0.48	20 (8%) 13 6	34, 61, 112, 122	0
3	AC	207/239 (86%)	0.33	10 (4%) 34 20	30, 54, 84, 102	0
4	AD	208/209 (99%)	0.15	6 (2%) 55 35	36, 57, 80, 89	0
5	AE	151/162 (93%)	-0.08	2 (1%) 79 61	29, 40, 59, 81	0
6	AF	101/101 (100%)	0.24	3 (2%) 54 33	41, 68, 86, 99	0
7	AG	155/156 (99%)	0.48	10 (6%) 22 12	44, 67, 112, 126	0
8	AH	138/138 (100%)	-0.11	0 100 100	32, 45, 63, 74	0
9	AI	127/128 (99%)	0.42	10 (7%) 15 8	33, 61, 81, 90	0
10	AJ	99/105 (94%)	0.51	9 (9%) 11 6	38, 58, 100, 104	0
11	AK	119/129 (92%)	0.28	4 (3%) 49 30	26, 53, 76, 94	0
12	AL	125/132 (94%)	0.29	7 (5%) 28 15	27, 45, 64, 96	0
13	AM	119/126 (94%)	1.05	19 (15%) 3 1	46, 83, 107, 117	0
14	AN	60/61 (98%)	0.41	7 (11%) 6 3	35, 48, 83, 91	0
15	AO	88/89 (98%)	0.21	2 (2%) 64 43	33, 51, 75, 85	0
16	AP	84/88 (95%)	0.17	1 (1%) 81 63	37, 47, 70, 95	0
17	AQ	100/105 (95%)	-0.07	0 100 100	27, 44, 62, 65	0
18	AR	70/88 (79%)	0.28	3 (4%) 39 23	36, 57, 94, 95	0
19	AS	88/93 (94%)	0.85	9 (10%) 9 5	59, 82, 103, 109	0
20	AT	99/106 (93%)	0.13	3 (3%) 54 33	33, 45, 68, 73	0
21	AU	25/27 (92%)	1.03	2 (8%) 15 8	43, 59, 79, 81	0
22	AV	76/76 (100%)	0.42	5 (6%) 22 11	33, 74, 111, 145	0
23	AX	9/9 (100%)	1.12	2 (22%) 1 1	28, 51, 122, 134	0
24	AY	687/691 (99%)	0.55	64 (9%) 11 6	39, 67, 119, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	B0	84/84 (100%)	1.80	15 (17%) 2 1	43, 56, 121, 140	0
26	B1	94/97 (96%)	0.50	6 (6%) 23 12	26, 47, 76, 88	0
27	B2	71/71 (100%)	0.64	7 (9%) 9 5	41, 57, 88, 112	0
28	B3	60/60 (100%)	0.59	2 (3%) 50 31	35, 56, 75, 100	0
29	B4	71/71 (100%)	3.88	61 (85%) 0 0	129, 151, 159, 159	0
30	B5	59/59 (100%)	0.62	7 (11%) 6 3	20, 42, 109, 122	0
31	B6	50/53 (94%)	1.54	11 (22%) 1 1	41, 72, 91, 98	0
32	B7	48/48 (100%)	0.02	1 (2%) 67 46	18, 30, 60, 86	0
33	B8	64/64 (100%)	0.66	8 (12%) 5 2	32, 49, 70, 87	0
34	B9	37/37 (100%)	0.69	2 (5%) 29 17	40, 52, 62, 76	0
35	BA	2901/2915 (99%)	0.22	99 (3%) 49 30	18, 42, 116, 244	0
36	BB	119/122 (97%)	0.24	1 (0%) 87 73	42, 88, 115, 130	0
37	BC	227/228 (99%)	0.83	36 (15%) 3 1	25, 78, 124, 135	0
38	BD	275/275 (100%)	0.01	8 (2%) 55 35	18, 32, 58, 93	0
39	BE	205/206 (99%)	0.35	12 (5%) 26 14	23, 42, 78, 86	0
40	BF	208/210 (99%)	0.44	16 (7%) 16 8	17, 52, 104, 121	0
41	BG	179/181 (98%)	1.49	53 (29%) 1 0	94, 122, 138, 144	0
42	BH	176/180 (97%)	0.91	22 (12%) 5 2	52, 75, 97, 108	0
43	BJ	1/130 (0%)	2.84	1 (100%) 0 0	121, 121, 121, 121	0
44	BK	0/140	-	-	-	-
45	BL	0/71	-	-	-	-
46	BN	139/140 (99%)	0.14	6 (4%) 39 23	31, 45, 72, 93	0
47	BO	122/122 (100%)	-0.25	0 100 100	25, 39, 54, 63	0
48	BP	146/149 (97%)	1.26	31 (21%) 1 1	34, 67, 96, 118	0
49	BQ	141/141 (100%)	0.22	3 (2%) 67 46	33, 49, 75, 115	0
50	BR	117/117 (100%)	0.13	4 (3%) 49 30	23, 40, 59, 67	0
51	BS	99/111 (89%)	1.02	15 (15%) 3 1	68, 91, 113, 122	0
52	BT	138/146 (94%)	0.96	24 (17%) 2 1	32, 53, 122, 144	0
53	BU	117/117 (100%)	-0.04	2 (1%) 73 53	28, 42, 69, 85	0
54	BV	101/101 (100%)	0.42	7 (6%) 20 10	25, 62, 83, 87	0
55	BW	113/113 (100%)	0.15	5 (4%) 38 22	26, 38, 69, 104	0
56	BX	93/95 (97%)	-0.14	2 (2%) 65 44	30, 41, 58, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
57	BY	101/109 (92%)	1.31	23 (22%) 1 1	37, 61, 118, 127	0
58	BZ	185/205 (90%)	0.87	25 (13%) 4 2	25, 81, 96, 109	0
All	All	11218/11801 (95%)	0.40	759 (6%) 20 11	17, 52, 116, 244	0

The worst 5 of 759 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BA	654(E)	G	16.8
24	AY	48	GLY	16.6
25	B0	3	HIS	15.4
39	BE	205	ALA	15.3
49	BQ	141	GLN	14.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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
59	MG	AA	1615	1/1	0.88	0.75	57.77	51,51,51,51	0
59	MG	AA	1684	1/1	0.82	0.85	50.95	61,61,61,61	0
59	MG	BA	3312	1/1	0.94	0.52	47.56	44,44,44,44	0
59	MG	AA	1636	1/1	0.77	0.51	43.25	60,60,60,60	0
59	MG	BA	3174	1/1	0.54	0.64	41.92	97,97,97,97	0
59	MG	BA	3044	1/1	0.97	0.40	38.40	21,21,21,21	0
59	MG	BA	3110	1/1	0.97	0.49	30.19	31,31,31,31	0
59	MG	BA	3007	1/1	0.93	0.45	26.36	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	BA	3071	1/1	0.94	0.37	23.13	22,22,22,22	0
59	MG	BA	3209	1/1	0.76	0.63	19.33	81,81,81,81	0
59	MG	AA	1623	1/1	0.98	0.53	19.05	33,33,33,33	0
59	MG	AA	1762	1/1	0.59	0.41	18.48	100,100,100,100	0
59	MG	BA	3048	1/1	0.91	0.39	18.34	28,28,28,28	0
59	MG	BA	3207	1/1	0.86	0.29	18.31	30,30,30,30	0
59	MG	BA	3310	1/1	0.91	0.29	17.77	20,20,20,20	0
59	MG	BA	3006	1/1	0.97	0.41	17.44	30,30,30,30	0
59	MG	BA	3094	1/1	0.98	0.32	17.34	25,25,25,25	0
59	MG	BA	3266	1/1	0.92	0.31	17.21	71,71,71,71	0
59	MG	BA	3180	1/1	0.95	0.34	17.18	47,47,47,47	0
59	MG	BA	3196	1/1	0.88	0.38	17.11	53,53,53,53	0
59	MG	BA	3077	1/1	0.94	0.35	16.55	31,31,31,31	0
59	MG	AA	1649	1/1	0.93	0.40	16.53	23,23,23,23	0
59	MG	BA	3024	1/1	0.88	0.28	16.43	44,44,44,44	0
59	MG	BA	3149	1/1	0.96	0.48	15.93	29,29,29,29	0
59	MG	BA	3277	1/1	0.94	0.45	15.87	57,57,57,57	0
59	MG	BA	3154	1/1	0.82	0.60	15.81	59,59,59,59	0
59	MG	AA	1741	1/1	0.73	0.46	15.50	58,58,58,58	0
59	MG	BA	3056	1/1	0.90	0.37	15.32	38,38,38,38	0
59	MG	BA	3120	1/1	0.95	0.38	14.85	43,43,43,43	0
59	MG	BA	3172	1/1	0.96	0.45	14.49	31,31,31,31	0
59	MG	AA	1760	1/1	0.64	0.67	13.97	70,70,70,70	0
59	MG	AA	1604	1/1	0.85	0.41	13.90	59,59,59,59	0
59	MG	BA	3279	1/1	0.59	0.44	13.82	63,63,63,63	0
59	MG	BA	3108	1/1	0.86	0.27	13.64	34,34,34,34	0
59	MG	BA	3295	1/1	0.80	0.30	13.45	32,32,32,32	0
59	MG	BA	3176	1/1	0.95	0.46	12.56	23,23,23,23	0
59	MG	BA	3111	1/1	0.93	0.32	12.45	30,30,30,30	0
59	MG	BA	3169	1/1	0.85	0.37	12.31	43,43,43,43	0
59	MG	BA	3084	1/1	0.93	0.54	12.27	38,38,38,38	0
59	MG	BA	3184	1/1	0.90	0.24	12.08	40,40,40,40	0
59	MG	AA	1665	1/1	0.94	0.42	12.03	28,28,28,28	0
59	MG	AA	1733	1/1	0.93	0.31	11.90	67,67,67,67	0
59	MG	AA	1677	1/1	0.64	0.37	11.79	77,77,77,77	0
59	MG	AA	1616	1/1	0.94	0.41	11.11	30,30,30,30	0
59	MG	AA	1671	1/1	0.96	0.65	11.05	43,43,43,43	0
59	MG	BA	3088	1/1	0.89	0.24	10.92	27,27,27,27	0
59	MG	BA	3004	1/1	0.97	0.38	10.78	24,24,24,24	0
59	MG	BA	3039	1/1	0.97	0.39	10.39	38,38,38,38	0
59	MG	AA	1645	1/1	0.92	0.26	10.31	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	B0	101	1/1	0.86	0.77	9.83	72,72,72,72	0
59	MG	BA	3087	1/1	0.84	0.34	9.31	41,41,41,41	0
59	MG	BA	3116	1/1	0.82	0.28	9.23	78,78,78,78	0
59	MG	BA	3109	1/1	0.98	0.44	9.05	20,20,20,20	0
59	MG	BA	3125	1/1	0.74	0.38	8.99	122,122,122,122	0
59	MG	BA	3315	1/1	0.79	0.35	8.77	52,52,52,52	0
59	MG	BA	3104	1/1	0.98	0.32	8.55	30,30,30,30	0
59	MG	BA	3113	1/1	0.97	0.52	8.36	32,32,32,32	0
59	MG	BA	3199	1/1	0.94	0.27	8.28	26,26,26,26	0
59	MG	AA	1756	1/1	0.84	0.39	8.27	54,54,54,54	0
59	MG	BA	3153	1/1	0.85	0.24	8.12	54,54,54,54	0
59	MG	BA	3139	1/1	0.93	0.29	8.08	35,35,35,35	0
59	MG	AA	1692	1/1	0.93	0.23	8.05	48,48,48,48	0
59	MG	BA	3097	1/1	0.89	0.41	7.52	37,37,37,37	0
59	MG	BA	3248	1/1	0.83	0.44	7.48	58,58,58,58	0
59	MG	BA	3214	1/1	0.80	0.31	7.46	39,39,39,39	0
59	MG	BA	3258	1/1	0.77	0.32	7.43	51,51,51,51	0
59	MG	BA	3051	1/1	0.94	0.37	7.40	31,31,31,31	0
59	MG	BA	3271	1/1	0.84	0.34	7.36	28,28,28,28	0
59	MG	AA	1777	1/1	0.49	0.31	7.32	40,40,40,40	0
59	MG	BA	3129	1/1	0.87	0.29	7.26	51,51,51,51	0
59	MG	BA	3282	1/1	0.56	0.30	7.05	67,67,67,67	0
59	MG	BA	3091	1/1	0.97	0.22	6.88	21,21,21,21	0
59	MG	BA	3053	1/1	0.91	0.33	6.77	24,24,24,24	0
59	MG	AA	1678	1/1	0.96	0.35	6.63	29,29,29,29	0
59	MG	AA	1690	1/1	0.95	0.47	6.61	35,35,35,35	0
59	MG	BA	3313	1/1	0.96	0.26	6.46	36,36,36,36	0
59	MG	AA	1724	1/1	0.74	0.42	6.40	48,48,48,48	0
59	MG	BA	3082	1/1	0.95	0.49	6.21	23,23,23,23	0
59	MG	BA	3236	1/1	0.81	0.24	6.19	52,52,52,52	0
59	MG	BA	3127	1/1	0.93	0.24	5.92	38,38,38,38	0
59	MG	AA	1700	1/1	0.91	0.32	5.76	27,27,27,27	0
59	MG	BA	3043	1/1	0.98	0.23	5.35	28,28,28,28	0
59	MG	AA	1639	1/1	0.66	0.30	5.26	55,55,55,55	0
59	MG	BA	3145	1/1	0.86	0.23	5.08	32,32,32,32	0
59	MG	AA	1729	1/1	0.86	0.47	4.91	45,45,45,45	0
59	MG	BA	3189	1/1	0.93	0.19	4.84	26,26,26,26	0
59	MG	AA	1625	1/1	0.96	0.36	4.84	17,17,17,17	0
59	MG	BA	3052	1/1	0.97	0.31	4.79	32,32,32,32	0
59	MG	BA	3228	1/1	0.90	0.32	4.55	23,23,23,23	0
59	MG	AA	1686	1/1	0.90	0.25	4.52	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	BA	3210	1/1	0.95	0.29	4.50	23,23,23,23	0
59	MG	AA	1704	1/1	0.92	0.37	4.47	25,25,25,25	0
59	MG	BA	3075	1/1	0.88	0.23	4.06	31,31,31,31	0
59	MG	BA	3257	1/1	0.94	0.22	3.73	43,43,43,43	0
59	MG	AA	1715	1/1	0.75	0.24	3.22	42,42,42,42	0
59	MG	BA	3078	1/1	0.92	0.20	3.08	26,26,26,26	0
60	ZN	AD	301	1/1	0.96	0.35	3.03	54,54,54,54	0
59	MG	BA	3181	1/1	0.87	0.18	2.87	32,32,32,32	0
59	MG	AA	1638	1/1	0.76	0.17	2.86	38,38,38,38	0
59	MG	BA	3206	1/1	0.83	0.23	2.80	65,65,65,65	0
59	MG	BA	3298	1/1	0.93	0.17	2.73	20,20,20,20	0
59	MG	BA	3098	1/1	0.91	0.23	2.07	25,25,25,25	0
59	MG	AA	1653	1/1	0.94	0.31	1.97	19,19,19,19	0
59	MG	AA	1780	1/1	0.40	0.18	1.93	54,54,54,54	0
59	MG	AA	1682	1/1	0.96	0.27	1.81	53,53,53,53	0
59	MG	BA	3244	1/1	0.92	0.21	1.80	41,41,41,41	0
59	MG	BA	3232	1/1	0.89	0.24	1.78	33,33,33,33	0
59	MG	AA	1701	1/1	0.81	0.17	1.75	30,30,30,30	0
59	MG	AA	1725	1/1	0.93	0.25	1.72	35,35,35,35	0
59	MG	BA	3150	1/1	0.98	0.15	1.66	15,15,15,15	0
59	MG	AA	1673	1/1	0.94	0.21	1.45	35,35,35,35	0
59	MG	AA	1732	1/1	0.87	0.25	0.78	20,20,20,20	0
59	MG	BA	3219	1/1	0.81	0.16	0.66	44,44,44,44	0
59	MG	AA	1719	1/1	0.93	0.16	0.58	32,32,32,32	0
59	MG	BA	3141	1/1	0.89	0.20	0.50	29,29,29,29	0
59	MG	BA	3243	1/1	0.86	0.23	0.41	32,32,32,32	0
59	MG	AA	1726	1/1	0.83	0.21	0.36	45,45,45,45	0
59	MG	BA	3289	1/1	0.89	0.21	0.33	51,51,51,51	0
59	MG	BA	3269	1/1	0.66	0.16	0.29	48,48,48,48	0
59	MG	AA	1711	1/1	0.77	0.19	0.26	34,34,34,34	0
59	MG	AA	1761	1/1	0.86	0.20	0.20	30,30,30,30	0
59	MG	BA	3171	1/1	0.97	0.23	0.17	19,19,19,19	0
59	MG	BA	3157	1/1	0.93	0.17	0.13	17,17,17,17	0
59	MG	AA	1722	1/1	0.82	0.23	0.12	32,32,32,32	0
59	MG	AA	1687	1/1	0.95	0.20	0.11	30,30,30,30	0
59	MG	BA	3142	1/1	0.70	0.20	0.08	48,48,48,48	0
59	MG	AA	1736	1/1	0.94	0.19	-0.11	29,29,29,29	0
59	MG	BA	3208	1/1	0.91	0.23	-0.16	34,34,34,34	0
59	MG	BA	3217	1/1	0.95	0.18	-0.23	35,35,35,35	0
61	GCP	AY	701	32/32	0.87	0.21	-0.26	41,53,61,63	0
59	MG	AA	1693	1/1	0.92	0.17	-0.28	30,30,30,30	0
59	MG	BA	3288	1/1	0.98	0.18	-0.31	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	AA	1668	1/1	0.85	0.17	-0.32	34,34,34,34	0
59	MG	AA	1738	1/1	0.90	0.17	-0.46	53,53,53,53	0
59	MG	AA	1751	1/1	0.90	0.14	-0.87	46,46,46,46	0
59	MG	AA	1749	1/1	0.88	0.13	-0.89	38,38,38,38	0
59	MG	BA	3151	1/1	0.95	0.13	-1.04	33,33,33,33	0
60	ZN	AN	101	1/1	1.00	0.13	-1.06	45,45,45,45	0
59	MG	BA	3050	1/1	0.94	0.15	-1.20	23,23,23,23	0
59	MG	BA	3319	1/1	0.96	0.11	-1.47	35,35,35,35	0
59	MG	BA	3001	1/1	0.96	0.11	-1.47	35,35,35,35	0
59	MG	BA	3229	1/1	0.96	0.13	-1.75	5,5,5,5	0
59	MG	AA	1734	1/1	0.87	0.12	-1.93	41,41,41,41	0
59	MG	AA	1778	1/1	0.97	0.12	-2.02	6,6,6,6	0
59	MG	AA	1657	1/1	0.92	0.10	-2.04	32,32,32,32	0
59	MG	AA	1721	1/1	0.93	0.12	-2.20	17,17,17,17	0
59	MG	BA	3221	1/1	0.90	0.10	-2.20	43,43,43,43	0
59	MG	AA	1783	1/1	0.88	0.13	-2.58	43,43,43,43	0
59	MG	AA	1747	1/1	0.86	0.08	-2.84	23,23,23,23	0
59	MG	BA	3308	1/1	0.95	0.12	-2.93	58,58,58,58	0
59	MG	BA	3140	1/1	0.82	0.13	-3.14	45,45,45,45	0
59	MG	AA	1785	1/1	0.96	0.08	-3.20	47,47,47,47	0
60	ZN	B9	101	1/1	1.00	0.06	-3.39	49,49,49,49	0
59	MG	AY	702	1/1	0.93	0.08	-3.97	23,23,23,23	0
59	MG	BA	3259	1/1	0.92	0.12	-4.47	39,39,39,39	0
59	MG	AA	1710	1/1	0.95	0.06	-4.82	35,35,35,35	0
59	MG	BA	3061	1/1	0.93	0.05	-5.03	37,37,37,37	0
59	MG	AA	1705	1/1	0.97	0.08	-5.87	23,23,23,23	0
59	MG	AA	1660	1/1	0.94	0.10	-6.03	19,19,19,19	0
59	MG	AA	1699	1/1	0.68	0.25	-	33,33,33,33	0
59	MG	AA	1679	1/1	0.98	0.55	-	32,32,32,32	0
59	MG	AA	1664	1/1	0.93	0.39	-	29,29,29,29	0
59	MG	BA	3300	1/1	0.93	0.17	-	65,65,65,65	0
59	MG	BA	3255	1/1	0.86	0.24	-	35,35,35,35	0
59	MG	AA	1789	1/1	0.81	0.28	-	61,61,61,61	0
59	MG	AA	1791	1/1	0.95	0.09	-	57,57,57,57	0
59	MG	BA	3020	1/1	0.84	0.22	-	63,63,63,63	0
59	MG	BA	3118	1/1	0.95	0.30	-	29,29,29,29	0
59	MG	BA	3156	1/1	0.96	0.19	-	25,25,25,25	0
59	MG	AA	1666	1/1	0.76	0.53	-	83,83,83,83	0
59	MG	AA	1610	1/1	0.95	0.66	-	46,46,46,46	0
59	MG	AA	1794	1/1	0.83	0.27	-	53,53,53,53	0
59	MG	BA	3197	1/1	0.79	0.56	-	58,58,58,58	0
59	MG	BA	3132	1/1	0.82	0.33	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	BA	3234	1/1	0.86	0.20	-	63,63,63,63	0
59	MG	BA	3065	1/1	0.98	0.29	-	21,21,21,21	0
59	MG	AA	1748	1/1	0.85	0.36	-	56,56,56,56	0
59	MG	BA	3280	1/1	0.79	0.24	-	87,87,87,87	0
59	MG	BA	3060	1/1	0.90	0.39	-	31,31,31,31	0
59	MG	AA	1753	1/1	0.66	0.53	-	89,89,89,89	0
59	MG	BA	3175	1/1	0.79	0.19	-	62,62,62,62	0
59	MG	AA	1667	1/1	0.97	0.35	-	33,33,33,33	0
59	MG	BA	3106	1/1	0.84	0.22	-	47,47,47,47	0
59	MG	AA	1634	1/1	0.81	0.22	-	43,43,43,43	0
59	MG	BA	3144	1/1	0.88	0.23	-	28,28,28,28	0
59	MG	AA	1768	1/1	0.87	0.45	-	34,34,34,34	0
59	MG	BA	3079	1/1	0.86	0.34	-	34,34,34,34	0
59	MG	BA	3057	1/1	0.95	0.29	-	29,29,29,29	0
59	MG	BA	3166	1/1	0.80	0.28	-	68,68,68,68	0
59	MG	AA	1689	1/1	0.83	0.40	-	79,79,79,79	0
59	MG	AA	1674	1/1	0.75	0.44	-	74,74,74,74	0
59	MG	BA	3018	1/1	0.89	0.56	-	43,43,43,43	0
59	MG	BA	3074	1/1	0.97	0.36	-	3,3,3,3	0
59	MG	BA	3230	1/1	0.67	0.35	-	40,40,40,40	0
59	MG	BA	3224	1/1	0.96	0.46	-	32,32,32,32	0
59	MG	BA	3296	1/1	0.90	0.38	-	38,38,38,38	0
59	MG	BA	3105	1/1	0.88	0.20	-	69,69,69,69	0
59	MG	BA	3009	1/1	0.77	0.72	-	77,77,77,77	0
59	MG	AA	1770	1/1	0.96	0.29	-	41,41,41,41	0
59	MG	AA	1694	1/1	0.93	0.13	-	19,19,19,19	0
59	MG	BA	3303	1/1	0.92	0.09	-	42,42,42,42	0
59	MG	BA	3100	1/1	0.94	0.10	-	24,24,24,24	0
59	MG	AA	1707	1/1	0.81	0.22	-	60,60,60,60	0
59	MG	BA	3168	1/1	0.80	0.11	-	58,58,58,58	0
59	MG	BA	3183	1/1	0.95	0.14	-	58,58,58,58	0
59	MG	AA	1683	1/1	0.92	0.23	-	25,25,25,25	0
59	MG	AA	1765	1/1	0.91	0.56	-	63,63,63,63	0
59	MG	AA	1788	1/1	0.84	0.33	-	73,73,73,73	0
59	MG	BA	3225	1/1	0.76	0.14	-	44,44,44,44	0
59	MG	AA	1781	1/1	0.33	0.27	-	54,54,54,54	0
59	MG	BA	3242	1/1	0.73	0.44	-	78,78,78,78	0
59	MG	BA	3085	1/1	0.74	0.21	-	25,25,25,25	0
59	MG	BA	3249	1/1	0.96	0.31	-	22,22,22,22	0
59	MG	AA	1740	1/1	0.44	0.75	-	79,79,79,79	0
59	MG	AA	1739	1/1	0.91	0.42	-	28,28,28,28	0
59	MG	BA	3016	1/1	0.72	0.63	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	AA	1755	1/1	0.74	0.35	-	60,60,60,60	0
59	MG	BA	3028	1/1	0.65	0.40	-	60,60,60,60	0
59	MG	AA	1618	1/1	0.97	0.38	-	47,47,47,47	0
59	MG	BA	3267	1/1	0.77	0.34	-	62,62,62,62	0
59	MG	AA	1603	1/1	0.94	0.41	-	38,38,38,38	0
59	MG	AA	1757	1/1	0.87	0.30	-	57,57,57,57	0
59	MG	BA	3121	1/1	0.92	0.34	-	33,33,33,33	0
59	MG	AA	1659	1/1	0.97	0.39	-	34,34,34,34	0
59	MG	AA	1787	1/1	0.86	0.27	-	55,55,55,55	0
59	MG	BA	3128	1/1	0.74	0.26	-	38,38,38,38	0
59	MG	BA	3134	1/1	0.87	0.31	-	65,65,65,65	0
59	MG	BA	3069	1/1	0.97	0.33	-	18,18,18,18	0
59	MG	BA	3081	1/1	0.98	0.28	-	23,23,23,23	0
59	MG	BA	3095	1/1	0.81	0.38	-	47,47,47,47	0
59	MG	BA	3239	1/1	0.76	0.27	-	87,87,87,87	0
59	MG	BA	3102	1/1	0.96	0.23	-	30,30,30,30	0
59	MG	AA	1626	1/1	0.92	0.42	-	59,59,59,59	0
59	MG	BA	3307	1/1	0.94	0.16	-	40,40,40,40	0
59	MG	BA	3059	1/1	0.94	0.45	-	45,45,45,45	0
59	MG	AA	1779	1/1	0.63	0.53	-	81,81,81,81	0
59	MG	AA	1709	1/1	0.66	0.19	-	41,41,41,41	0
59	MG	BA	3314	1/1	0.91	0.10	-	49,49,49,49	0
59	MG	BA	3198	1/1	0.88	0.17	-	63,63,63,63	0
59	MG	BA	3201	1/1	0.77	0.41	-	64,64,64,64	0
59	MG	BA	3114	1/1	0.93	0.21	-	29,29,29,29	0
59	MG	AA	1769	1/1	0.91	0.36	-	33,33,33,33	0
59	MG	AA	1743	1/1	0.71	0.39	-	38,38,38,38	0
59	MG	BA	3291	1/1	0.92	0.32	-	27,27,27,27	0
59	MG	BA	3170	1/1	0.93	0.52	-	41,41,41,41	0
59	MG	AA	1776	1/1	0.96	0.29	-	25,25,25,25	0
59	MG	AA	1606	1/1	0.76	0.53	-	60,60,60,60	0
59	MG	AA	1730	1/1	0.96	0.13	-	62,62,62,62	0
59	MG	AA	1773	1/1	0.59	0.56	-	60,60,60,60	0
59	MG	BA	3013	1/1	0.93	0.49	-	37,37,37,37	0
59	MG	BA	3220	1/1	0.93	0.19	-	56,56,56,56	0
59	MG	AA	1635	1/1	0.72	0.22	-	65,65,65,65	0
59	MG	BA	3143	1/1	0.86	0.21	-	57,57,57,57	0
59	MG	BA	3241	1/1	0.90	0.19	-	65,65,65,65	0
59	MG	BA	3317	1/1	0.98	0.28	-	29,29,29,29	0
59	MG	AA	1643	1/1	0.80	0.23	-	38,38,38,38	0
59	MG	AA	1764	1/1	0.79	0.27	-	61,61,61,61	0
59	MG	BA	3273	1/1	0.88	0.65	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	BA	3131	1/1	0.97	0.43	-	33,33,33,33	0
59	MG	BA	3305	1/1	0.80	0.10	-	52,52,52,52	0
59	MG	BA	3163	1/1	0.84	0.30	-	55,55,55,55	0
59	MG	AA	1716	1/1	0.65	0.37	-	71,71,71,71	0
59	MG	AA	1629	1/1	0.96	0.28	-	44,44,44,44	0
59	MG	BA	3179	1/1	0.37	0.43	-	87,87,87,87	0
59	MG	BA	3250	1/1	0.84	0.24	-	53,53,53,53	0
59	MG	AA	1797	1/1	0.80	0.19	-	58,58,58,58	0
59	MG	AA	1767	1/1	0.88	0.29	-	60,60,60,60	0
59	MG	BA	3293	1/1	0.89	0.50	-	76,76,76,76	0
59	MG	BA	3160	1/1	0.79	0.17	-	55,55,55,55	0
59	MG	BA	3063	1/1	0.97	0.15	-	22,22,22,22	0
59	MG	AA	1763	1/1	0.82	0.30	-	51,51,51,51	0
59	MG	BA	3284	1/1	0.72	0.42	-	61,61,61,61	0
59	MG	BA	3202	1/1	0.90	0.40	-	43,43,43,43	0
59	MG	AA	1612	1/1	0.96	0.46	-	47,47,47,47	0
59	MG	BA	3200	1/1	0.92	0.31	-	71,71,71,71	0
59	MG	AA	1670	1/1	0.92	0.21	-	57,57,57,57	0
59	MG	BA	3032	1/1	0.69	0.25	-	73,73,73,73	0
59	MG	BA	3205	1/1	0.95	0.12	-	35,35,35,35	0
59	MG	BA	3062	1/1	0.97	0.15	-	13,13,13,13	0
59	MG	BA	3286	1/1	0.93	0.34	-	42,42,42,42	0
59	MG	BA	3212	1/1	0.88	0.28	-	46,46,46,46	0
59	MG	AA	1784	1/1	0.88	0.17	-	37,37,37,37	0
59	MG	BA	3178	1/1	0.98	0.27	-	43,43,43,43	0
59	MG	BA	3086	1/1	0.95	0.26	-	46,46,46,46	0
59	MG	AA	1646	1/1	0.92	0.38	-	34,34,34,34	0
59	MG	BA	3316	1/1	0.95	0.38	-	34,34,34,34	0
59	MG	BA	3047	1/1	0.96	0.37	-	42,42,42,42	0
59	MG	AA	1611	1/1	0.80	0.34	-	75,75,75,75	0
59	MG	BA	3015	1/1	0.89	0.53	-	63,63,63,63	0
59	MG	AA	1742	1/1	0.91	0.22	-	45,45,45,45	0
59	MG	BA	3030	1/1	0.58	1.26	-	86,86,86,86	0
59	MG	AA	1752	1/1	0.90	0.22	-	59,59,59,59	0
59	MG	BA	3222	1/1	0.96	0.30	-	44,44,44,44	0
59	MG	BA	3019	1/1	0.55	0.72	-	77,77,77,77	0
59	MG	BA	3213	1/1	0.90	0.36	-	31,31,31,31	0
59	MG	B5	101	1/1	0.88	0.27	-	47,47,47,47	0
59	MG	BA	3027	1/1	0.88	0.30	-	71,71,71,71	0
59	MG	AA	1708	1/1	0.90	0.26	-	57,57,57,57	0
59	MG	BA	3099	1/1	0.97	0.21	-	19,19,19,19	0
59	MG	AA	1631	1/1	0.94	0.20	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	BA	3182	1/1	0.89	0.27	-	73,73,73,73	0
59	MG	BA	3042	1/1	0.80	0.37	-	45,45,45,45	0
59	MG	BA	3115	1/1	0.92	0.30	-	52,52,52,52	0
59	MG	BA	3049	1/1	0.92	0.46	-	47,47,47,47	0
59	MG	BA	3215	1/1	0.39	0.60	-	81,81,81,81	0
59	MG	AA	1627	1/1	0.86	0.23	-	74,74,74,74	0
59	MG	BA	3185	1/1	0.91	0.43	-	36,36,36,36	0
59	MG	BA	3309	1/1	0.96	0.17	-	50,50,50,50	0
59	MG	AA	1642	1/1	0.86	0.26	-	61,61,61,61	0
59	MG	AA	1662	1/1	0.90	0.33	-	34,34,34,34	0
59	MG	BA	3055	1/1	0.83	0.16	-	33,33,33,33	0
59	MG	BA	3287	1/1	0.92	0.17	-	41,41,41,41	0
59	MG	AA	1644	1/1	0.69	0.20	-	60,60,60,60	0
59	MG	AA	1614	1/1	0.96	0.40	-	26,26,26,26	0
59	MG	AA	1669	1/1	0.86	0.20	-	40,40,40,40	0
59	MG	BA	3223	1/1	0.95	0.34	-	32,32,32,32	0
59	MG	AA	1798	1/1	0.87	0.07	-	39,39,39,39	0
59	MG	BA	3247	1/1	0.37	0.36	-	49,49,49,49	0
59	MG	AA	1720	1/1	0.95	0.47	-	37,37,37,37	0
59	MG	AA	1602	1/1	0.88	0.48	-	42,42,42,42	0
59	MG	AA	1782	1/1	0.96	0.09	-	39,39,39,39	0
59	MG	BC	301	1/1	0.66	0.21	-	115,115,115,115	0
59	MG	AA	1605	1/1	0.94	0.42	-	40,40,40,40	0
59	MG	AA	1619	1/1	0.96	0.36	-	37,37,37,37	0
59	MG	BA	3068	1/1	0.91	0.19	-	33,33,33,33	0
59	MG	AA	1632	1/1	0.64	0.25	-	56,56,56,56	0
59	MG	BA	3194	1/1	0.38	0.35	-	74,74,74,74	0
59	MG	BA	3133	1/1	0.87	0.31	-	39,39,39,39	0
59	MG	BA	3211	1/1	0.90	0.65	-	58,58,58,58	0
59	MG	BA	3107	1/1	0.83	0.30	-	44,44,44,44	0
59	MG	BA	3096	1/1	0.97	0.20	-	23,23,23,23	0
59	MG	BA	3136	1/1	0.64	0.30	-	90,90,90,90	0
59	MG	BA	3036	1/1	0.83	0.28	-	47,47,47,47	0
59	MG	BA	3276	1/1	0.77	0.51	-	46,46,46,46	0
59	MG	AA	1654	1/1	0.92	0.26	-	24,24,24,24	0
59	MG	BA	3292	1/1	0.80	0.36	-	64,64,64,64	0
59	MG	BA	3072	1/1	0.84	0.63	-	70,70,70,70	0
59	MG	BA	3187	1/1	0.81	0.89	-	68,68,68,68	0
59	MG	BA	3256	1/1	0.95	0.44	-	52,52,52,52	0
59	MG	AA	1723	1/1	0.96	0.14	-	10,10,10,10	0
59	MG	BA	3245	1/1	0.95	0.23	-	25,25,25,25	0
59	MG	AA	1655	1/1	0.94	0.40	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	AA	1651	1/1	0.88	0.20	-	68,68,68,68	0
59	MG	BA	3148	1/1	0.80	0.29	-	53,53,53,53	0
59	MG	AA	1607	1/1	0.74	0.34	-	97,97,97,97	0
59	MG	AA	1681	1/1	0.96	0.45	-	34,34,34,34	0
59	MG	BA	3191	1/1	0.89	0.38	-	72,72,72,72	0
59	MG	BA	3119	1/1	0.98	0.26	-	24,24,24,24	0
59	MG	BA	3002	1/1	0.98	0.13	-	39,39,39,39	0
59	MG	AA	1717	1/1	0.94	0.43	-	41,41,41,41	0
59	MG	BA	3083	1/1	0.97	0.42	-	23,23,23,23	0
59	MG	AA	1637	1/1	0.68	0.58	-	65,65,65,65	0
59	MG	AA	1790	1/1	0.77	0.25	-	57,57,57,57	0
59	MG	BA	3124	1/1	0.99	0.27	-	15,15,15,15	0
59	MG	BA	3251	1/1	0.83	0.28	-	44,44,44,44	0
59	MG	BA	3192	1/1	0.92	0.36	-	51,51,51,51	0
59	MG	BA	3123	1/1	0.98	0.49	-	32,32,32,32	0
59	MG	BA	3301	1/1	0.91	0.41	-	45,45,45,45	0
59	MG	AA	1696	1/1	0.88	0.35	-	35,35,35,35	0
59	MG	BA	3195	1/1	0.93	0.25	-	32,32,32,32	0
59	MG	BA	3005	1/1	0.97	0.48	-	16,16,16,16	0
59	MG	AA	1795	1/1	0.96	0.15	-	46,46,46,46	0
59	MG	BA	3265	1/1	0.71	0.55	-	65,65,65,65	0
59	MG	AA	1672	1/1	0.93	0.18	-	42,42,42,42	0
59	MG	BA	3126	1/1	0.84	0.42	-	55,55,55,55	0
59	MG	BA	3158	1/1	0.95	0.30	-	27,27,27,27	0
59	MG	AA	1758	1/1	0.77	0.39	-	75,75,75,75	0
59	MG	AA	1745	1/1	0.80	0.44	-	66,66,66,66	0
59	MG	AA	1621	1/1	0.80	0.40	-	68,68,68,68	0
59	MG	BA	3270	1/1	0.83	0.34	-	70,70,70,70	0
59	MG	AA	1766	1/1	0.76	0.29	-	58,58,58,58	0
59	MG	AA	1744	1/1	0.80	0.21	-	90,90,90,90	0
59	MG	BA	3089	1/1	0.92	0.24	-	18,18,18,18	0
59	MG	BA	3029	1/1	0.87	0.33	-	73,73,73,73	0
59	MG	BA	3173	1/1	0.95	0.27	-	20,20,20,20	0
59	MG	AA	1695	1/1	0.78	0.34	-	50,50,50,50	0
59	MG	AA	1656	1/1	0.87	0.15	-	46,46,46,46	0
59	MG	BA	3025	1/1	0.74	0.32	-	42,42,42,42	0
59	MG	BA	3067	1/1	0.79	0.28	-	71,71,71,71	0
59	MG	AA	1775	1/1	0.91	0.13	-	45,45,45,45	0
59	MG	BA	3235	1/1	0.96	0.20	-	29,29,29,29	0
59	MG	AA	1714	1/1	0.69	0.53	-	44,44,44,44	0
59	MG	BA	3254	1/1	0.91	0.27	-	18,18,18,18	0
59	MG	BA	3281	1/1	0.41	0.46	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	AA	1727	1/1	0.90	0.14	-	55,55,55,55	0
59	MG	BA	3146	1/1	0.89	0.23	-	29,29,29,29	0
59	MG	BA	3092	1/1	0.96	0.59	-	37,37,37,37	0
59	MG	BA	3041	1/1	0.82	0.21	-	75,75,75,75	0
59	MG	BA	3268	1/1	0.59	0.35	-	85,85,85,85	0
59	MG	AA	1617	1/1	0.96	0.49	-	49,49,49,49	0
59	MG	BA	3193	1/1	0.81	0.53	-	64,64,64,64	0
59	MG	BA	3022	1/1	0.91	0.55	-	65,65,65,65	0
59	MG	BA	3152	1/1	0.94	0.41	-	64,64,64,64	0
59	MG	BA	3285	1/1	0.91	0.28	-	40,40,40,40	0
59	MG	AA	1728	1/1	0.77	0.32	-	47,47,47,47	0
59	MG	BA	3026	1/1	0.77	0.36	-	67,67,67,67	0
59	MG	AA	1620	1/1	0.85	0.44	-	75,75,75,75	0
59	MG	BA	3101	1/1	0.97	0.35	-	29,29,29,29	0
59	MG	BA	3080	1/1	0.98	0.41	-	38,38,38,38	0
59	MG	AA	1698	1/1	0.85	0.31	-	58,58,58,58	0
59	MG	AA	1786	1/1	0.88	0.15	-	35,35,35,35	0
59	MG	AA	1624	1/1	0.85	0.84	-	61,61,61,61	0
59	MG	BA	3130	1/1	0.92	0.55	-	56,56,56,56	0
59	MG	BA	3038	1/1	0.93	0.31	-	40,40,40,40	0
59	MG	BA	3311	1/1	0.96	0.35	-	22,22,22,22	0
59	MG	BA	3240	1/1	0.69	0.33	-	60,60,60,60	0
59	MG	BA	3216	1/1	0.91	0.20	-	54,54,54,54	0
59	MG	BA	3064	1/1	0.77	0.12	-	62,62,62,62	0
59	MG	BA	3012	1/1	0.64	0.44	-	79,79,79,79	0
59	MG	AA	1754	1/1	0.57	0.40	-	75,75,75,75	0
59	MG	AA	1796	1/1	0.79	0.28	-	44,44,44,44	0
59	MG	BA	3204	1/1	0.42	0.40	-	60,60,60,60	0
59	MG	BA	3031	1/1	0.92	0.35	-	35,35,35,35	0
59	MG	AA	1691	1/1	0.84	0.11	-	65,65,65,65	0
59	MG	BA	3070	1/1	0.98	0.45	-	25,25,25,25	0
59	MG	BA	3093	1/1	0.91	0.42	-	69,69,69,69	0
59	MG	AA	1650	1/1	0.76	0.26	-	36,36,36,36	0
59	MG	AA	1772	1/1	0.88	0.58	-	79,79,79,79	0
59	MG	BA	3299	1/1	0.86	0.41	-	53,53,53,53	0
59	MG	BA	3165	1/1	0.99	0.45	-	29,29,29,29	0
59	MG	AA	1647	1/1	0.75	0.46	-	79,79,79,79	0
59	MG	BA	3306	1/1	0.94	0.23	-	39,39,39,39	0
59	MG	AA	1706	1/1	0.95	0.16	-	43,43,43,43	0
59	MG	BA	3040	1/1	0.79	0.41	-	71,71,71,71	0
59	MG	AA	1759	1/1	0.97	0.33	-	37,37,37,37	0
59	MG	BA	3138	1/1	0.88	0.47	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	BA	3177	1/1	0.95	0.40	-	31,31,31,31	0
59	MG	BA	3090	1/1	0.89	0.32	-	56,56,56,56	0
59	MG	BA	3304	1/1	0.67	0.39	-	32,32,32,32	0
59	MG	BA	3003	1/1	0.96	0.35	-	20,20,20,20	0
59	MG	AA	1712	1/1	0.43	0.23	-	66,66,66,66	0
59	MG	AA	1750	1/1	0.93	0.30	-	42,42,42,42	0
59	MG	BA	3190	1/1	0.67	0.38	-	81,81,81,81	0
59	MG	AA	1735	1/1	0.89	0.41	-	62,62,62,62	0
59	MG	BA	3218	1/1	0.77	0.23	-	58,58,58,58	0
59	MG	BA	3264	1/1	0.76	0.56	-	77,77,77,77	0
59	MG	BA	3278	1/1	0.96	0.24	-	91,91,91,91	0
59	MG	AA	1702	1/1	0.97	0.53	-	44,44,44,44	0
59	MG	BA	3263	1/1	0.63	0.33	-	63,63,63,63	0
59	MG	AA	1688	1/1	0.94	0.25	-	30,30,30,30	0
59	MG	BA	3011	1/1	0.94	0.27	-	46,46,46,46	0
59	MG	BA	3237	1/1	0.84	0.20	-	94,94,94,94	0
59	MG	AA	1622	1/1	0.91	0.47	-	49,49,49,49	0
59	MG	AA	1731	1/1	0.87	0.09	-	48,48,48,48	0
59	MG	AA	1703	1/1	0.72	0.42	-	81,81,81,81	0
59	MG	BA	3260	1/1	0.80	0.46	-	72,72,72,72	0
59	MG	BA	3017	1/1	0.96	0.33	-	37,37,37,37	0
59	MG	BA	3283	1/1	0.81	0.21	-	73,73,73,73	0
59	MG	BA	3147	1/1	0.72	0.55	-	119,119,119,119	0
59	MG	BA	3238	1/1	0.86	0.28	-	42,42,42,42	0
59	MG	BA	3272	1/1	0.94	0.43	-	52,52,52,52	0
59	MG	AA	1676	1/1	0.82	0.24	-	62,62,62,62	0
59	MG	BA	3066	1/1	0.97	0.16	-	27,27,27,27	0
59	MG	AA	1675	1/1	0.95	0.27	-	45,45,45,45	0
59	MG	BA	3274	1/1	0.88	0.18	-	79,79,79,79	0
59	MG	BA	3294	1/1	0.94	0.20	-	42,42,42,42	0
59	MG	AA	1648	1/1	0.91	0.35	-	29,29,29,29	0
59	MG	BU	201	1/1	0.92	0.14	-	28,28,28,28	0
59	MG	BA	3164	1/1	0.88	0.24	-	49,49,49,49	0
59	MG	AA	1601	1/1	0.81	0.23	-	97,97,97,97	0
59	MG	BA	3046	1/1	0.89	0.28	-	27,27,27,27	0
59	MG	AA	1718	1/1	0.95	0.50	-	35,35,35,35	0
59	MG	AA	1663	1/1	0.85	0.47	-	37,37,37,37	0
59	MG	BA	3290	1/1	0.94	0.42	-	43,43,43,43	0
59	MG	AA	1640	1/1	0.79	0.26	-	74,74,74,74	0
59	MG	BA	3227	1/1	0.92	0.28	-	27,27,27,27	0
59	MG	AA	1641	1/1	0.97	0.17	-	17,17,17,17	0
59	MG	AA	1713	1/1	0.92	0.16	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	BA	3045	1/1	0.81	0.69	-	54,54,54,54	0
59	MG	AA	1658	1/1	0.89	0.19	-	25,25,25,25	0
59	MG	BA	3162	1/1	0.89	0.27	-	45,45,45,45	0
59	MG	BA	3203	1/1	0.94	0.27	-	30,30,30,30	0
59	MG	AA	1737	1/1	0.86	0.18	-	61,61,61,61	0
59	MG	BA	3117	1/1	0.90	0.19	-	26,26,26,26	0
59	MG	BA	3159	1/1	0.97	0.20	-	36,36,36,36	0
59	MG	BA	3035	1/1	0.97	0.51	-	31,31,31,31	0
59	MG	AA	1628	1/1	0.53	0.42	-	64,64,64,64	0
59	MG	BA	3233	1/1	0.86	0.20	-	42,42,42,42	0
59	MG	BA	3252	1/1	0.39	0.60	-	50,50,50,50	0
59	MG	BA	3135	1/1	0.95	0.25	-	58,58,58,58	0
59	MG	BA	3023	1/1	0.90	0.12	-	87,87,87,87	0
59	MG	BA	3302	1/1	0.89	0.39	-	52,52,52,52	0
59	MG	AA	1661	1/1	0.86	0.29	-	40,40,40,40	0
59	MG	AA	1680	1/1	0.96	0.19	-	37,37,37,37	0
59	MG	BA	3137	1/1	0.86	0.16	-	49,49,49,49	0
59	MG	BA	3320	1/1	0.98	0.13	-	39,39,39,39	0
59	MG	BA	3155	1/1	0.72	0.29	-	60,60,60,60	0
59	MG	BA	3188	1/1	0.93	0.41	-	34,34,34,34	0
59	MG	AA	1613	1/1	0.91	0.18	-	65,65,65,65	0
59	MG	BA	3253	1/1	0.84	0.40	-	98,98,98,98	0
59	MG	BA	3167	1/1	0.86	0.17	-	61,61,61,61	0
59	MG	BA	3037	1/1	0.90	0.40	-	49,49,49,49	0
59	MG	AA	1630	1/1	0.88	0.53	-	56,56,56,56	0
59	MG	BA	3262	1/1	0.90	0.15	-	68,68,68,68	0
59	MG	BA	3054	1/1	0.87	0.28	-	31,31,31,31	0
59	MG	BA	3010	1/1	0.98	0.41	-	33,33,33,33	0
59	MG	AA	1792	1/1	0.81	0.12	-	37,37,37,37	0
59	MG	BA	3103	1/1	0.97	0.20	-	35,35,35,35	0
59	MG	AA	1685	1/1	0.92	0.42	-	40,40,40,40	0
59	MG	BA	3246	1/1	0.94	0.31	-	34,34,34,34	0
59	MG	AA	1608	1/1	0.87	0.37	-	48,48,48,48	0
59	MG	BA	3226	1/1	0.82	0.34	-	56,56,56,56	0
59	MG	BA	3014	1/1	0.96	0.34	-	53,53,53,53	0
59	MG	BA	3008	1/1	0.96	0.46	-	45,45,45,45	0
59	MG	BA	3034	1/1	0.96	0.25	-	36,36,36,36	0
59	MG	BA	3231	1/1	0.97	0.34	-	13,13,13,13	0
59	MG	AA	1697	1/1	0.80	0.12	-	61,61,61,61	0
59	MG	BA	3112	1/1	0.85	0.71	-	51,51,51,51	0
59	MG	BA	3275	1/1	0.65	0.38	-	52,52,52,52	0
59	MG	AA	1746	1/1	0.90	0.39	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
59	MG	BA	3261	1/1	0.83	0.14	-	67,67,67,67	0
59	MG	AA	1771	1/1	0.75	0.23	-	40,40,40,40	0
59	MG	BA	3033	1/1	0.98	0.21	-	41,41,41,41	0
59	MG	AA	1609	1/1	0.95	0.42	-	40,40,40,40	0
59	MG	BA	3297	1/1	0.92	0.18	-	39,39,39,39	0
59	MG	AA	1793	1/1	0.86	0.23	-	50,50,50,50	0
59	MG	BA	3076	1/1	0.98	0.29	-	18,18,18,18	0
59	MG	BA	3058	1/1	0.97	0.31	-	31,31,31,31	0
59	MG	AA	1774	1/1	0.91	0.62	-	51,51,51,51	0
59	MG	BA	3021	1/1	0.96	0.32	-	37,37,37,37	0
59	MG	BA	3318	1/1	0.99	0.08	-	46,46,46,46	0
59	MG	AA	1652	1/1	0.94	0.44	-	41,41,41,41	0
59	MG	BA	3122	1/1	0.89	0.17	-	26,26,26,26	0
59	MG	BA	3186	1/1	0.86	0.14	-	50,50,50,50	0
59	MG	AA	1633	1/1	0.95	0.54	-	52,52,52,52	0
59	MG	BA	3161	1/1	0.95	0.42	-	30,30,30,30	0
59	MG	BA	3073	1/1	0.88	0.33	-	83,83,83,83	0

6.5 Other polymers

There are no such residues in this entry.