



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:10 PM GMT

PDB ID : 4V7W
Title : Structure of the Thermus thermophilus ribosome complexed with chloramphenicol.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-16
Resolution : 3.00 Å(reported)

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

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

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

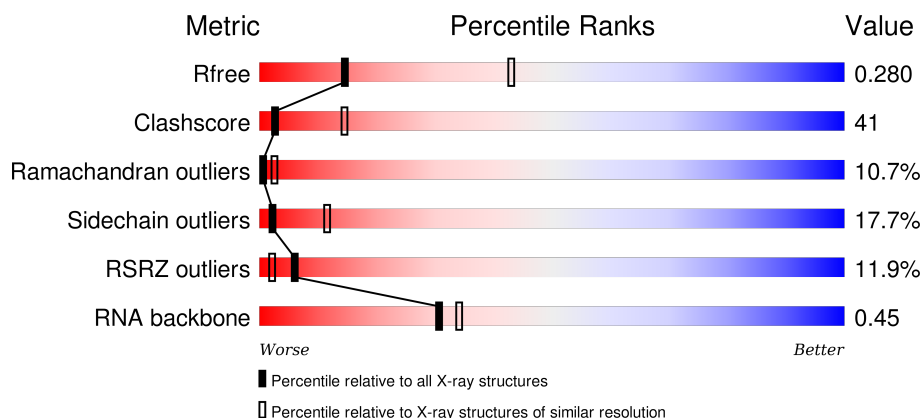
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>20%</div> <div>22% 61% 15% ..</div> </div>
1	CA	1522	<div> <div>17%</div> <div>22% 60% 16% .</div> </div>
2	AB	256	<div> <div>15%</div> <div>25% 53% 11% . 8%</div> </div>
2	CB	256	<div> <div>20%</div> <div>27% 50% 13% . 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	B0	85	
22	D0	85	
23	B1	98	
23	D1	98	
24	B2	72	
24	D2	72	
25	B3	60	
25	D3	60	
26	B4	71	
26	D4	71	
27	B5	60	
27	D5	60	

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Mol	Chain	Length	Quality of chain
28	B6	54	
28	D6	54	
29	B7	49	
29	D7	49	
30	B8	65	
30	D8	65	
31	BA	2787	
31	DA	2787	
32	BB	122	
32	DB	122	
33	BD	276	
33	DD	276	
34	BE	206	
34	DE	206	
35	BF	210	
35	DF	210	
36	BG	182	
36	DG	182	
37	BH	180	
37	DH	180	
38	BI	148	
38	DI	148	
39	BN	140	
39	DN	140	
40	BO	122	

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Mol	Chain	Length	Quality of chain
40	DO	122	
41	BP	150	
41	DP	150	
42	BQ	141	
42	DQ	141	
43	BR	118	
43	DR	118	
44	BS	112	
44	DS	112	
45	BT	146	
45	DT	146	
46	BU	118	
46	DU	118	
47	BV	101	
47	DV	101	
48	BW	113	
48	DW	113	
49	BX	96	
49	DX	96	
50	BY	110	
50	DY	110	
51	BZ	206	
51	DZ	206	

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
52	MG	AA	1607	-	-	-	X
52	MG	AA	1608	-	-	-	X
52	MG	AA	1614	-	-	-	X
52	MG	AA	1617	-	-	-	X
52	MG	AA	1623	-	-	-	X
52	MG	AA	1624	-	-	-	X
52	MG	AA	1625	-	-	-	X
52	MG	AA	1629	-	-	-	X
52	MG	AA	1631	-	-	-	X
52	MG	AA	1642	-	-	-	X
52	MG	AA	1651	-	-	-	X
52	MG	AA	1652	-	-	-	X
52	MG	BA	3001	-	-	-	X
52	MG	BA	3002	-	-	-	X
52	MG	BA	3006	-	-	-	X
52	MG	BA	3008	-	-	-	X
52	MG	BA	3009	-	-	-	X
52	MG	BA	3010	-	-	-	X
52	MG	BA	3012	-	-	-	X
52	MG	BA	3016	-	-	-	X
52	MG	BA	3020	-	-	-	X
52	MG	BA	3021	-	-	-	X
52	MG	BA	3023	-	-	-	X
52	MG	BA	3028	-	-	-	X
52	MG	BA	3032	-	-	-	X
52	MG	BA	3034	-	-	-	X
52	MG	BA	3037	-	-	-	X
52	MG	BA	3038	-	-	-	X
52	MG	BA	3039	-	-	-	X
52	MG	BA	3040	-	-	-	X
52	MG	BA	3041	-	-	-	X
52	MG	BA	3044	-	-	-	X
52	MG	BA	3046	-	-	-	X
52	MG	BA	3047	-	-	-	X
52	MG	BA	3049	-	-	-	X
52	MG	BA	3051	-	-	-	X
52	MG	BA	3052	-	-	-	X
52	MG	BA	3053	-	-	-	X
52	MG	BA	3055	-	-	-	X
52	MG	BA	3057	-	-	-	X
52	MG	BA	3058	-	-	-	X
52	MG	BA	3060	-	-	-	X
52	MG	BA	3061	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	BA	3063	-	-	-	X
52	MG	BA	3066	-	-	-	X
52	MG	BA	3070	-	-	-	X
52	MG	BA	3071	-	-	-	X
52	MG	BA	3072	-	-	-	X
52	MG	BA	3074	-	-	-	X
52	MG	BA	3075	-	-	-	X
52	MG	BA	3080	-	-	-	X
52	MG	BA	3088	-	-	-	X
52	MG	BA	3090	-	-	-	X
52	MG	BA	3092	-	-	-	X
52	MG	BA	3094	-	-	-	X
52	MG	BA	3095	-	-	-	X
52	MG	BA	3096	-	-	-	X
52	MG	BA	3100	-	-	-	X
52	MG	BA	3101	-	-	-	X
52	MG	BA	3109	-	-	-	X
52	MG	BA	3111	-	-	-	X
52	MG	BA	3112	-	-	-	X
52	MG	BA	3117	-	-	-	X
52	MG	BA	3119	-	-	-	X
52	MG	BA	3123	-	-	-	X
52	MG	BA	3124	-	-	-	X
52	MG	BA	3125	-	-	-	X
52	MG	BA	3127	-	-	-	X
52	MG	BA	3142	-	-	-	X
52	MG	BA	3144	-	-	-	X
52	MG	BA	3148	-	-	-	X
52	MG	BA	3150	-	-	-	X
52	MG	BA	3156	-	-	-	X
52	MG	BA	3162	-	-	-	X
52	MG	BA	3165	-	-	-	X
52	MG	BA	3167	-	-	-	X
52	MG	BA	3171	-	-	-	X
52	MG	BA	3174	-	-	-	X
52	MG	BA	3175	-	-	-	X
52	MG	BA	3179	-	-	-	X
52	MG	BA	3182	-	-	-	X
52	MG	BA	3191	-	-	-	X
52	MG	BA	3196	-	-	-	X
52	MG	BA	3200	-	-	-	X
52	MG	BA	3202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	BA	3213	-	-	-	X
52	MG	BA	3216	-	-	-	X
52	MG	BA	3224	-	-	-	X
52	MG	BA	3230	-	-	-	X
52	MG	BA	3236	-	-	-	X
52	MG	BA	3237	-	-	-	X
52	MG	BA	3242	-	-	-	X
52	MG	BA	3250	-	-	-	X
52	MG	BA	3261	-	-	-	X
52	MG	BA	3277	-	-	-	X
52	MG	BA	3280	-	-	-	X
52	MG	BA	3283	-	-	-	X
52	MG	BA	3284	-	-	-	X
52	MG	BA	3285	-	-	-	X
52	MG	BA	3287	-	-	-	X
52	MG	BA	3294	-	-	-	X
52	MG	BA	3298	-	-	-	X
52	MG	BA	3308	-	-	-	X
52	MG	BA	3313	-	-	-	X
52	MG	BA	3316	-	-	-	X
52	MG	BA	3319	-	-	-	X
52	MG	BA	3321	-	-	-	X
52	MG	BA	3323	-	-	-	X
52	MG	BA	3325	-	-	-	X
52	MG	BA	3326	-	-	-	X
52	MG	BA	3327	-	-	-	X
52	MG	BA	3343	-	-	-	X
52	MG	BA	3347	-	-	-	X
52	MG	BA	3350	-	-	-	X
52	MG	BA	3351	-	-	-	X
52	MG	BA	3355	-	-	-	X
52	MG	BA	3360	-	-	-	X
52	MG	BA	3361	-	-	-	X
52	MG	BD	301	-	-	-	X
52	MG	BF	301	-	-	-	X
52	MG	BQ	202	-	-	-	X
52	MG	CA	1607	-	-	-	X
52	MG	CA	1609	-	-	-	X
52	MG	CA	1610	-	-	-	X
52	MG	CA	1612	-	-	-	X
52	MG	CA	1613	-	-	-	X
52	MG	CA	1620	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	CA	1621	-	-	-	X
52	MG	CA	1625	-	-	-	X
52	MG	CA	1627	-	-	-	X
52	MG	CA	1637	-	-	-	X
52	MG	CA	1647	-	-	-	X
52	MG	CA	1648	-	-	-	X
52	MG	D1	101	-	-	-	X
52	MG	DA	3001	-	-	-	X
52	MG	DA	3002	-	-	-	X
52	MG	DA	3006	-	-	-	X
52	MG	DA	3008	-	-	-	X
52	MG	DA	3009	-	-	-	X
52	MG	DA	3010	-	-	-	X
52	MG	DA	3012	-	-	-	X
52	MG	DA	3016	-	-	-	X
52	MG	DA	3017	-	-	-	X
52	MG	DA	3018	-	-	-	X
52	MG	DA	3020	-	-	-	X
52	MG	DA	3023	-	-	-	X
52	MG	DA	3028	-	-	-	X
52	MG	DA	3030	-	-	-	X
52	MG	DA	3032	-	-	-	X
52	MG	DA	3034	-	-	-	X
52	MG	DA	3038	-	-	-	X
52	MG	DA	3039	-	-	-	X
52	MG	DA	3040	-	-	-	X
52	MG	DA	3041	-	-	-	X
52	MG	DA	3044	-	-	-	X
52	MG	DA	3046	-	-	-	X
52	MG	DA	3047	-	-	-	X
52	MG	DA	3049	-	-	-	X
52	MG	DA	3052	-	-	-	X
52	MG	DA	3053	-	-	-	X
52	MG	DA	3055	-	-	-	X
52	MG	DA	3056	-	-	-	X
52	MG	DA	3057	-	-	-	X
52	MG	DA	3058	-	-	-	X
52	MG	DA	3060	-	-	-	X
52	MG	DA	3061	-	-	-	X
52	MG	DA	3063	-	-	-	X
52	MG	DA	3070	-	-	-	X
52	MG	DA	3071	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	DA	3074	-	-	-	X
52	MG	DA	3075	-	-	-	X
52	MG	DA	3080	-	-	-	X
52	MG	DA	3089	-	-	-	X
52	MG	DA	3090	-	-	-	X
52	MG	DA	3091	-	-	-	X
52	MG	DA	3092	-	-	-	X
52	MG	DA	3093	-	-	-	X
52	MG	DA	3094	-	-	-	X
52	MG	DA	3097	-	-	-	X
52	MG	DA	3098	-	-	-	X
52	MG	DA	3099	-	-	-	X
52	MG	DA	3106	-	-	-	X
52	MG	DA	3108	-	-	-	X
52	MG	DA	3109	-	-	-	X
52	MG	DA	3115	-	-	-	X
52	MG	DA	3116	-	-	-	X
52	MG	DA	3118	-	-	-	X
52	MG	DA	3120	-	-	-	X
52	MG	DA	3121	-	-	-	X
52	MG	DA	3122	-	-	-	X
52	MG	DA	3123	-	-	-	X
52	MG	DA	3124	-	-	-	X
52	MG	DA	3135	-	-	-	X
52	MG	DA	3138	-	-	-	X
52	MG	DA	3140	-	-	-	X
52	MG	DA	3141	-	-	-	X
52	MG	DA	3145	-	-	-	X
52	MG	DA	3146	-	-	-	X
52	MG	DA	3148	-	-	-	X
52	MG	DA	3150	-	-	-	X
52	MG	DA	3156	-	-	-	X
52	MG	DA	3159	-	-	-	X
52	MG	DA	3165	-	-	-	X
52	MG	DA	3166	-	-	-	X
52	MG	DA	3168	-	-	-	X
52	MG	DA	3171	-	-	-	X
52	MG	DA	3178	-	-	-	X
52	MG	DA	3183	-	-	-	X
52	MG	DA	3184	-	-	-	X
52	MG	DA	3186	-	-	-	X
52	MG	DA	3188	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	DA	3210	-	-	-	X
52	MG	DA	3214	-	-	-	X
52	MG	DA	3216	-	-	-	X
52	MG	DA	3222	-	-	-	X
52	MG	DA	3223	-	-	-	X
52	MG	DA	3229	-	-	-	X
52	MG	DA	3234	-	-	-	X
52	MG	DA	3245	-	-	-	X
52	MG	DA	3248	-	-	-	X
52	MG	DA	3260	-	-	-	X
52	MG	DA	3267	-	-	-	X
52	MG	DA	3283	-	-	-	X
52	MG	DA	3285	-	-	-	X
52	MG	DA	3289	-	-	-	X
52	MG	DA	3290	-	-	-	X
52	MG	DA	3303	-	-	-	X
52	MG	DA	3312	-	-	-	X
52	MG	DA	3320	-	-	-	X
52	MG	DD	301	-	-	-	X
52	MG	DF	301	-	-	-	X
52	MG	DU	201	-	-	-	X
52	MG	DX	101	-	-	-	X
53	ZN	CD	301	-	-	X	-
54	K	DA	3333	-	-	-	X
55	CLM	BA	3370	-	-	-	X
55	CLM	DA	3334	-	-	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 277987 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- 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			
5	CE	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			
6	CF	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			
7	CG	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			
8	CH	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
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374
CI	58	ARG	HIS	CONFLICT	UNP P80374

- 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			
10	CJ	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			
11	CK	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			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	VAL	-	INSERTION	UNP Q5SHN3
AL	3	ALA	-	INSERTION	UNP Q5SHN3
AL	4	LEU	-	INSERTION	UNP Q5SHN3
CL	2	VAL	-	INSERTION	UNP Q5SHN3
CL	3	ALA	-	INSERTION	UNP Q5SHN3
CL	4	LEU	-	INSERTION	UNP Q5SHN3

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			
13	CM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	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			
15	CO	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			
16	CP	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			
17	CQ	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			
18	CR	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	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	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			
20	CT	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			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	B0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			
22	D0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	B1	89	Total	C	N	O	0	0	1
			693	435	140	118			
23	D1	89	Total	C	N	O	0	0	1
			693	435	140	118			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			
24	D2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
25	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	B4	32	Total	C	N	O	0	0	0
			157	93	32	32			
26	D4	32	Total	C	N	O	0	0	0
			157	93	32	32			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
28	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
29	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
30	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			
31	DA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 33 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
33	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 34 is a protein called 50S ribosomal protein L3.

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

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
36	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
37	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
38	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			
42	DQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			
45	DT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	BA	368	Total	Mg	0	0
			368	368		
52	CA	53	Total	Mg	0	0
			53	53		
52	DQ	1	Total	Mg	0	0
			1	1		
52	DF	1	Total	Mg	0	0
			1	1		
52	BE	1	Total	Mg	0	0
			1	1		
52	DU	1	Total	Mg	0	0
			1	1		
52	B1	1	Total	Mg	0	0
			1	1		
52	BP	2	Total	Mg	0	0
			2	2		
52	DR	1	Total	Mg	0	0
			1	1		
52	B5	2	Total	Mg	0	0
			2	2		
52	BB	7	Total	Mg	0	0
			7	7		
52	BF	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	AA	56	Total	Mg	0	0
			56	56		
52	BQ	2	Total	Mg	0	0
			2	2		
52	BU	1	Total	Mg	0	0
			1	1		
52	DD	1	Total	Mg	0	0
			1	1		
52	BR	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	DA	332	Total 332	Mg 332	0	0
52	DE	1	Total 1	Mg 1	0	0
52	D1	1	Total 1	Mg 1	0	0
52	DX	1	Total 1	Mg 1	0	0
52	DP	1	Total 1	Mg 1	0	0
52	D5	2	Total 2	Mg 2	0	0
52	BD	1	Total 1	Mg 1	0	0
52	DB	4	Total 4	Mg 4	0	0

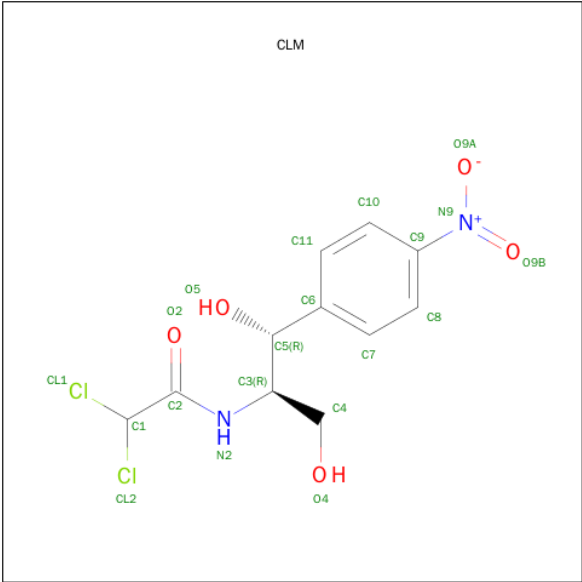
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	CN	1	Total 1	Zn 1	0	0
53	AD	1	Total 1	Zn 1	0	0
53	CD	1	Total 1	Zn 1	0	0
53	AN	1	Total 1	Zn 1	0	0

- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	1	Total 1	K 1	0	0
54	DA	1	Total 1	K 1	0	0

- Molecule 55 is CHLORAMPHENICOL (three-letter code: CLM) (formula: C₁₁H₁₂Cl₂N₂O₅).

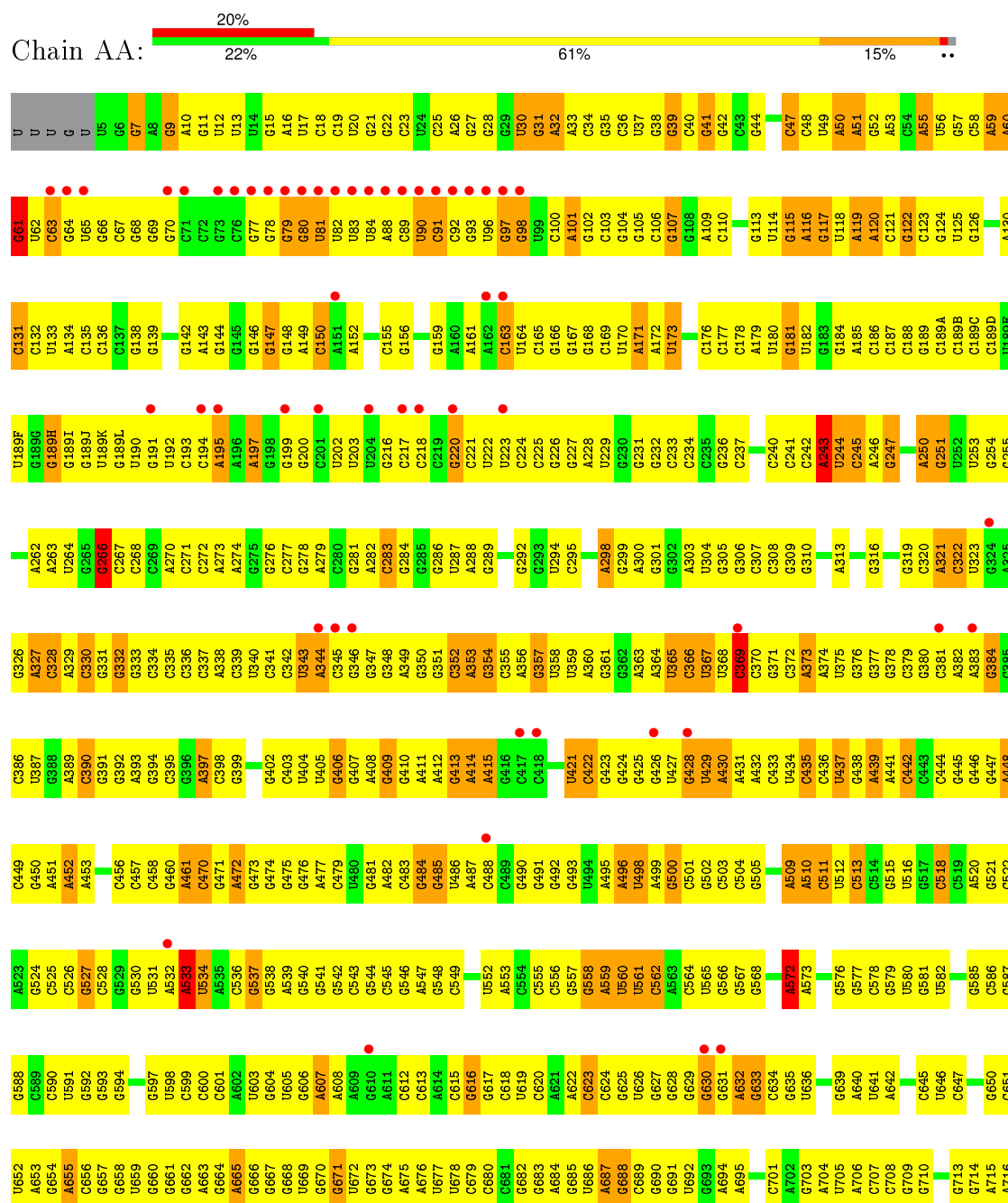


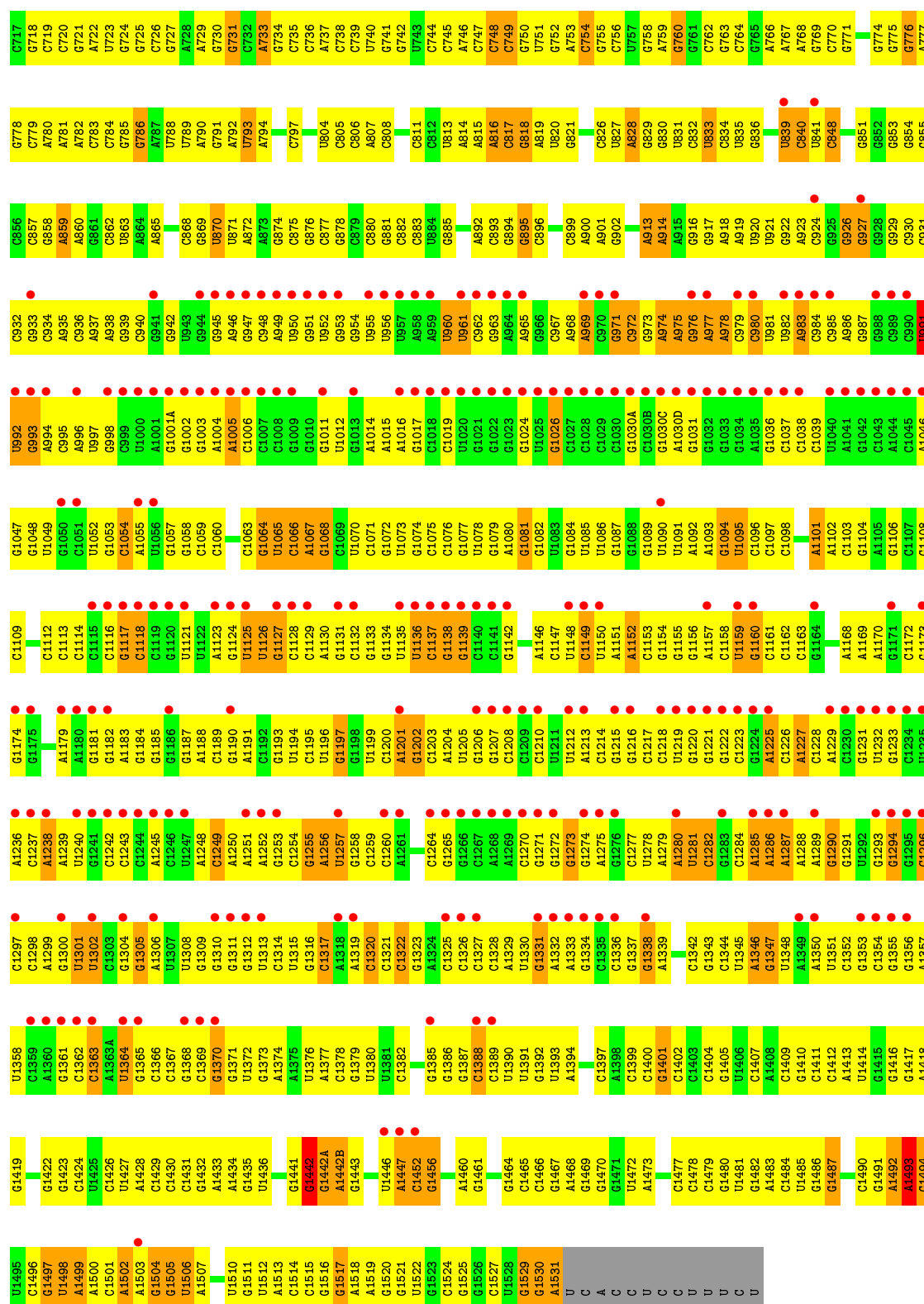
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	BA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
55	DA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

3 Residue-property plots

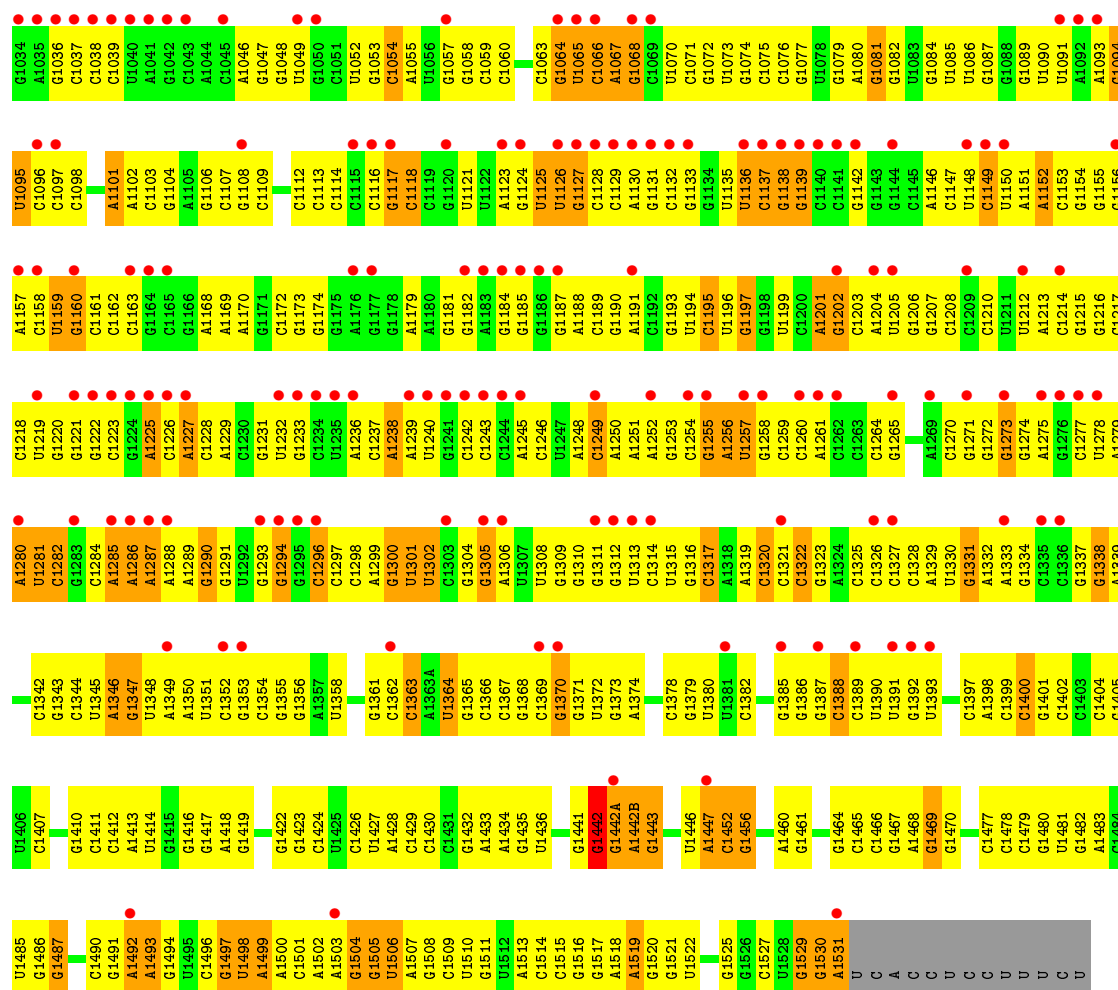
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA

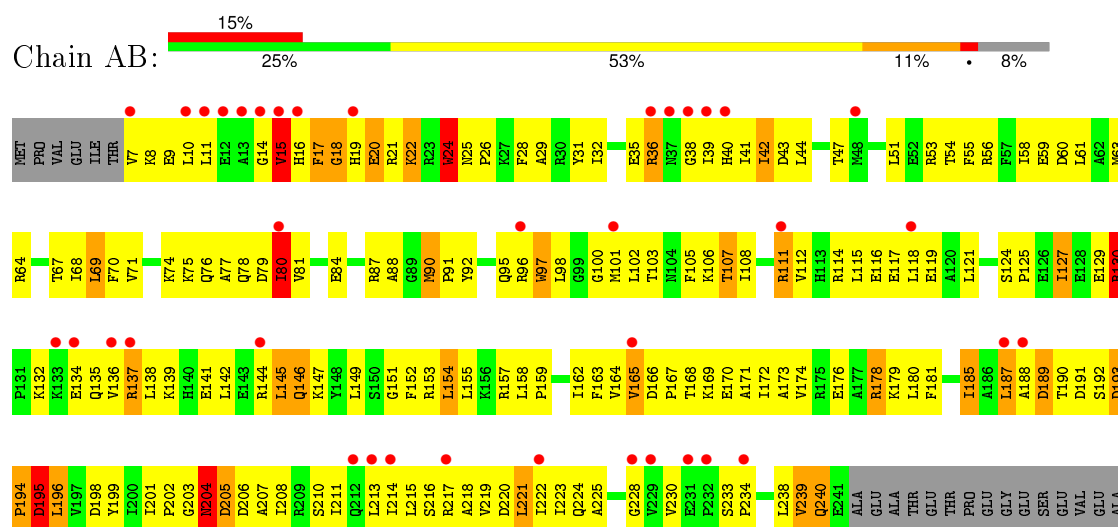






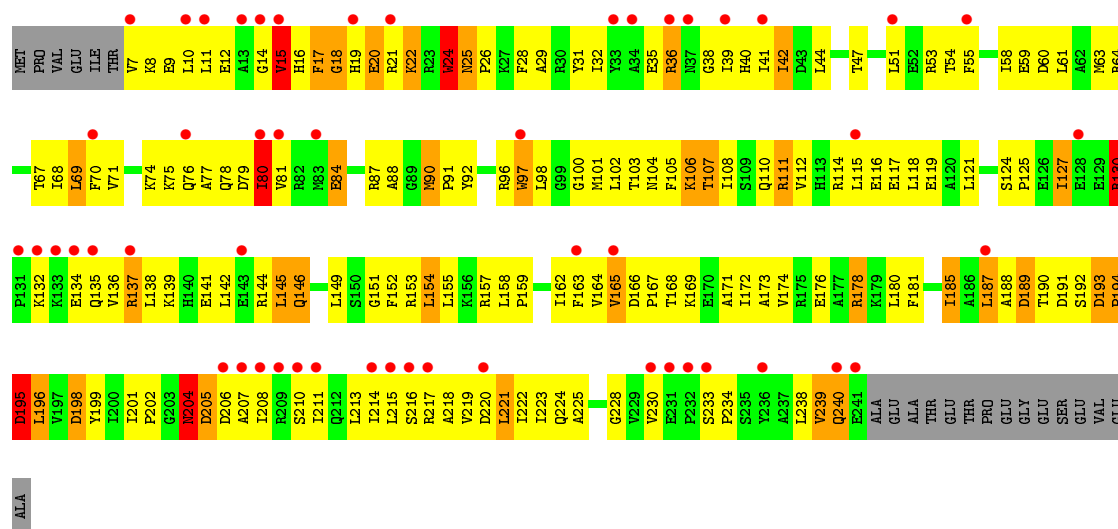


• Molecule 2: 30S ribosomal protein S2

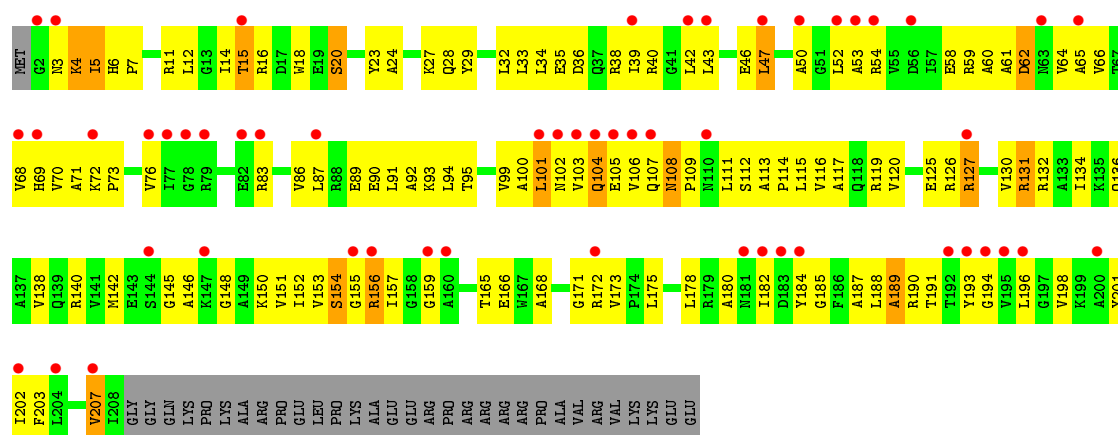


• Molecule 2: 30S ribosomal protein S2

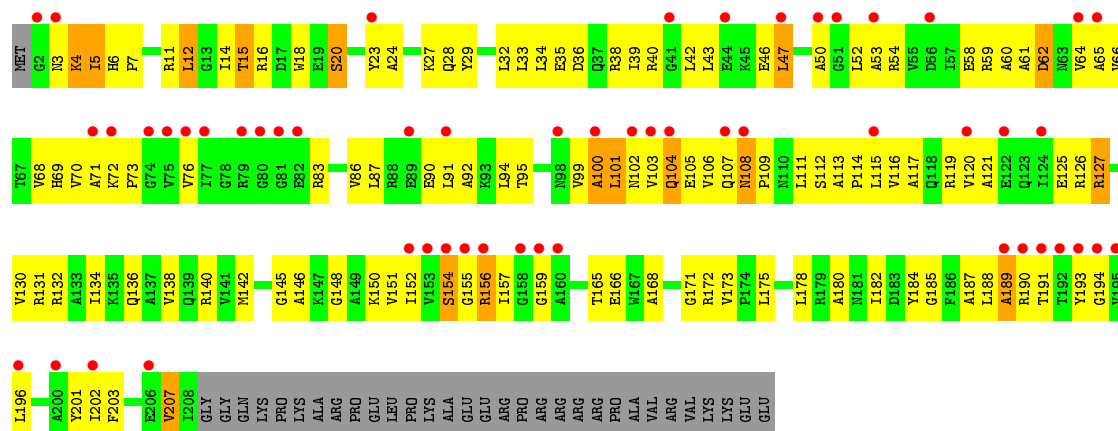




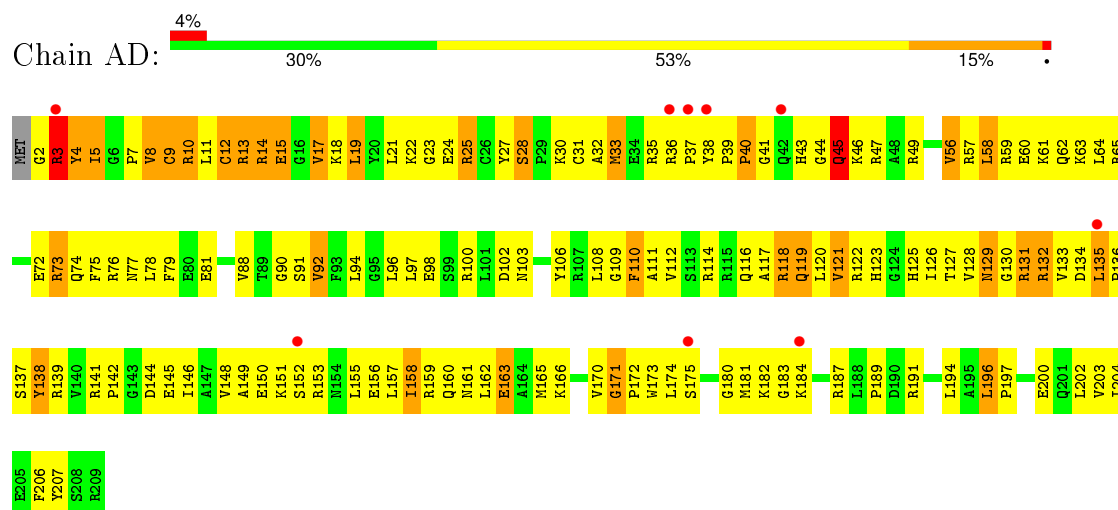
• Molecule 3: 30S ribosomal protein S3



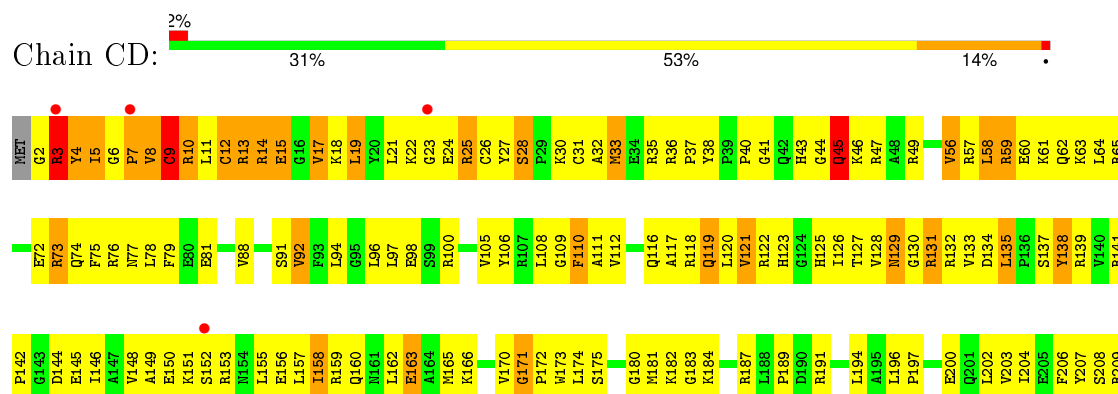
• Molecule 3: 30S ribosomal protein S3



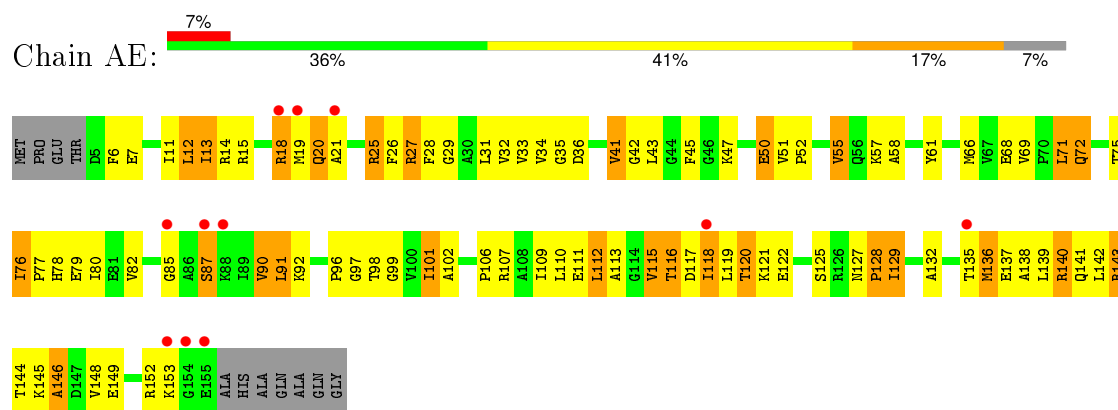
- Molecule 4: 30S ribosomal protein S4



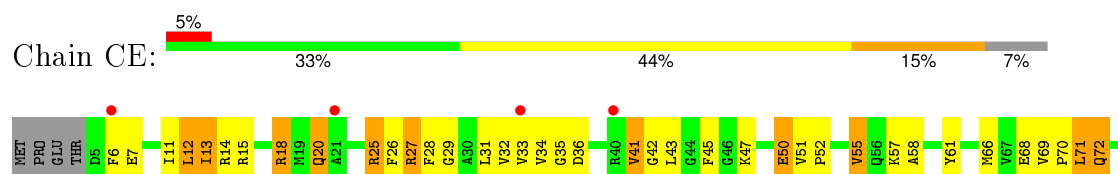
- Molecule 4: 30S ribosomal protein S4

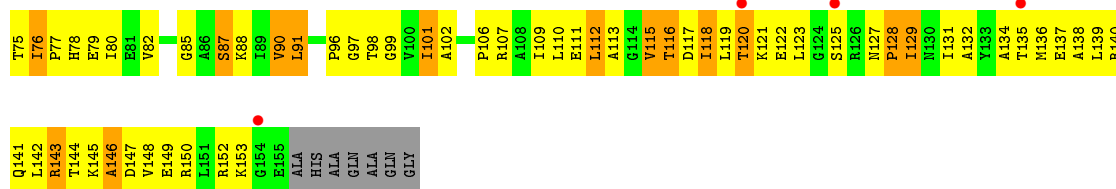


- Molecule 5: 30S ribosomal protein S5

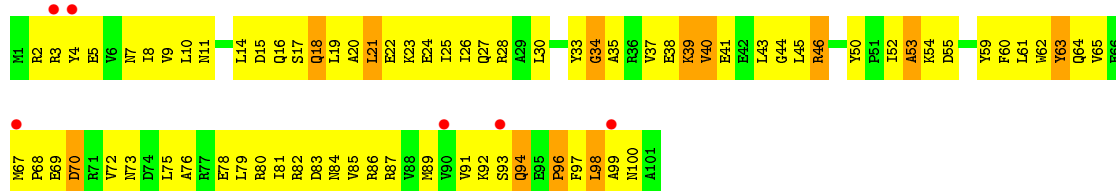


- Molecule 5: 30S ribosomal protein S5

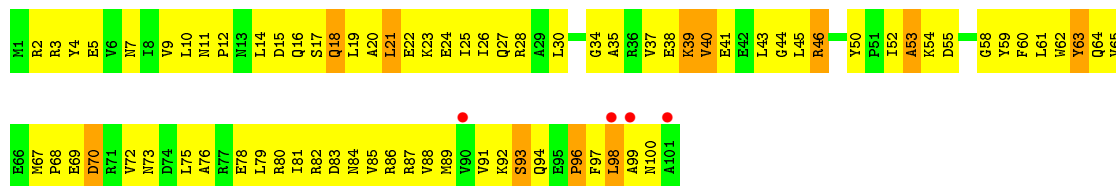




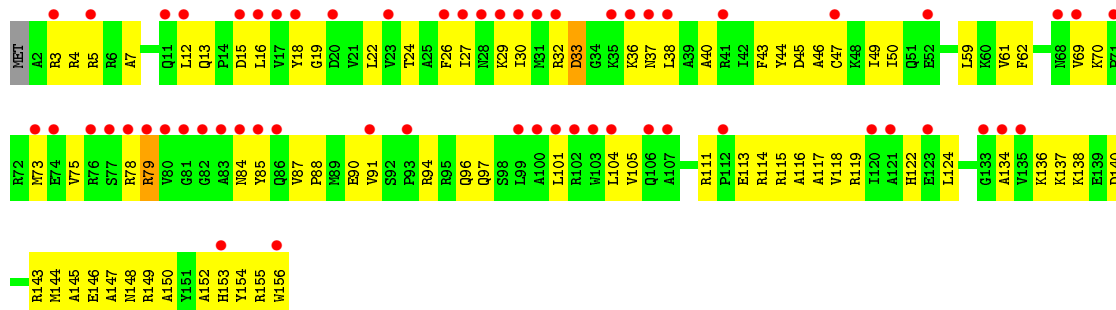
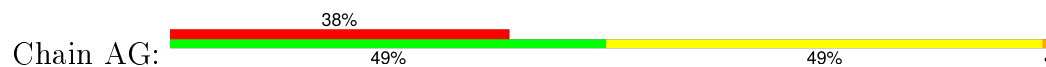
• Molecule 6: 30S ribosomal protein S6



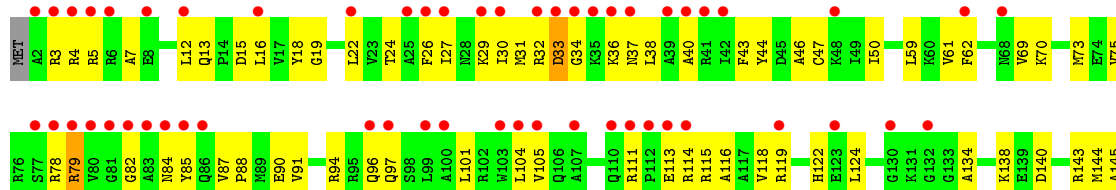
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

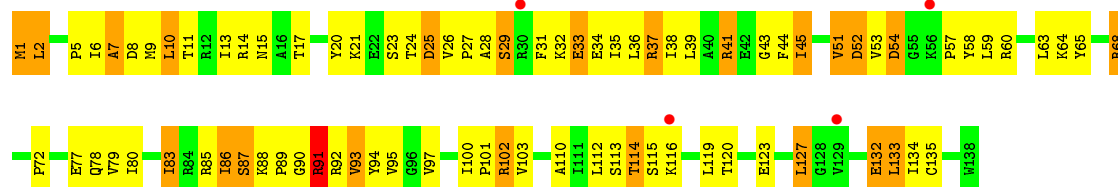
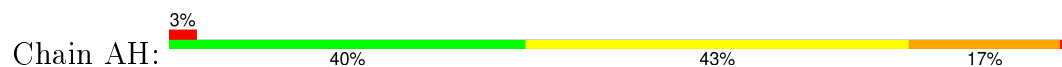


• Molecule 7: 30S ribosomal protein S7

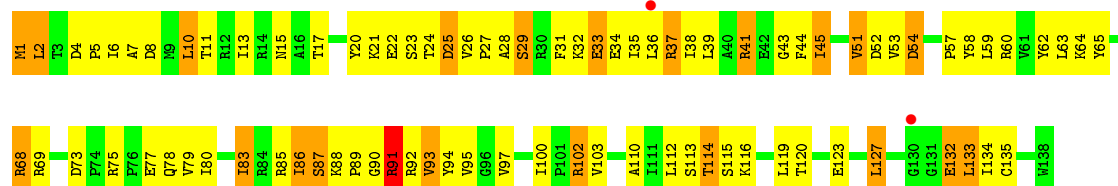




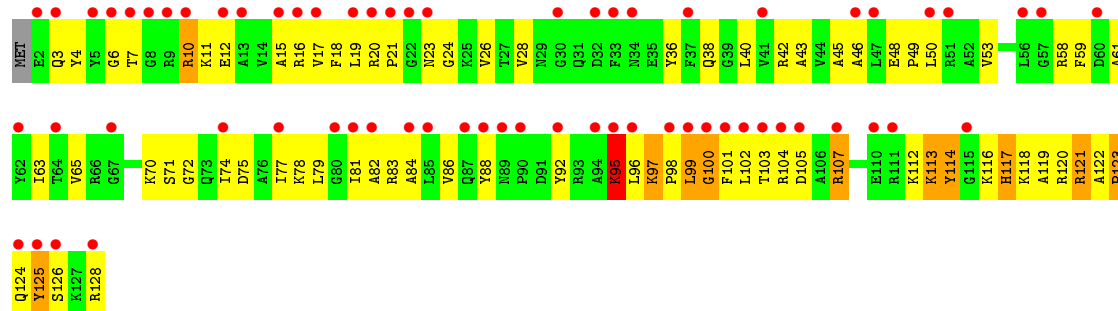
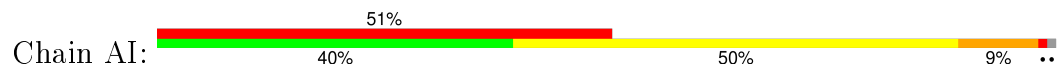
• Molecule 8: 30S ribosomal protein S8



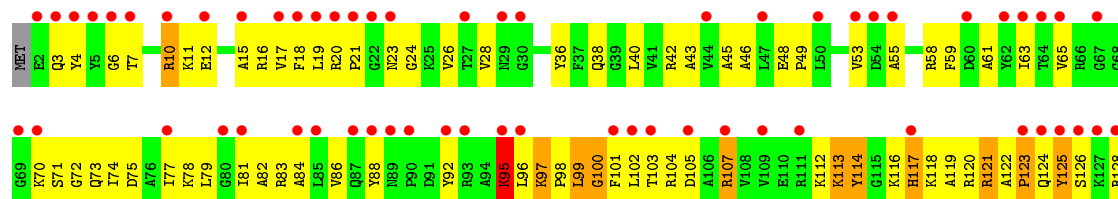
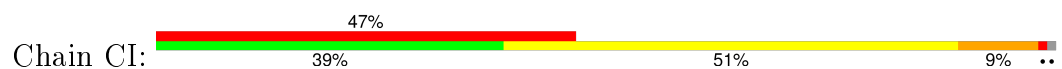
• Molecule 8: 30S ribosomal protein S8



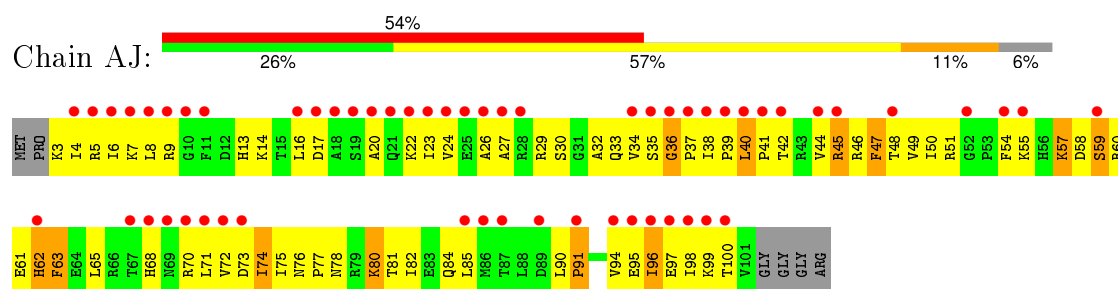
• Molecule 9: 30S ribosomal protein S9



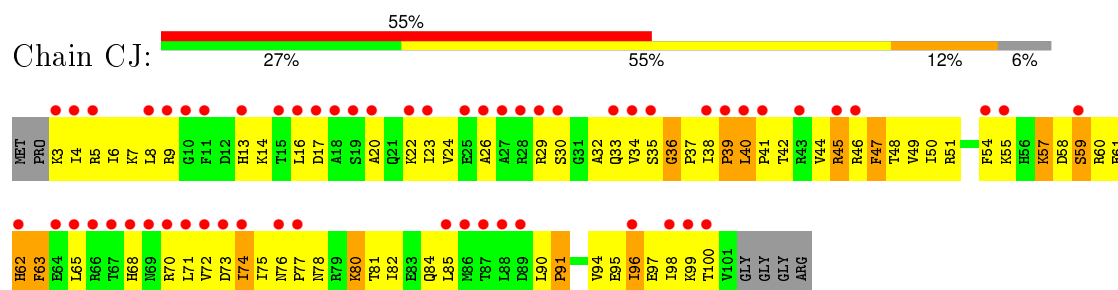
• Molecule 9: 30S ribosomal protein S9



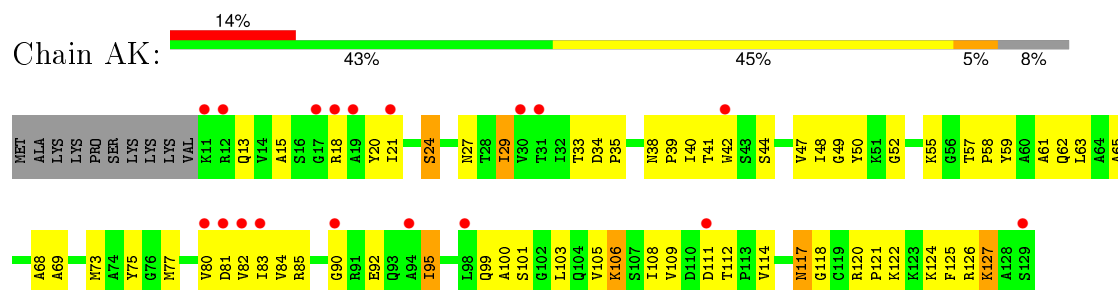
• Molecule 10: 30S ribosomal protein S10



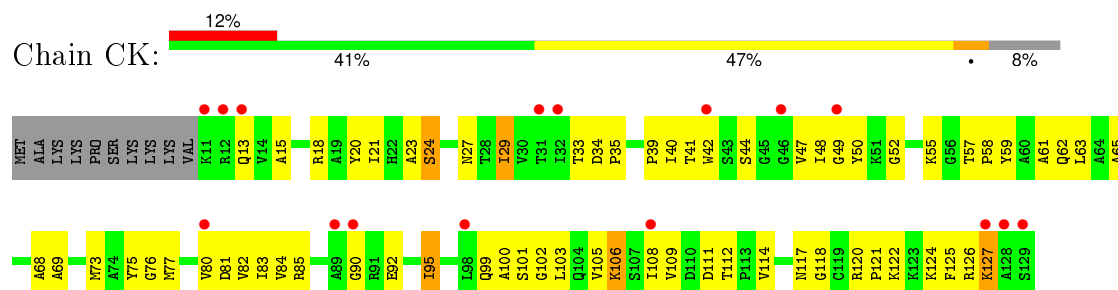
- Molecule 10: 30S ribosomal protein S10



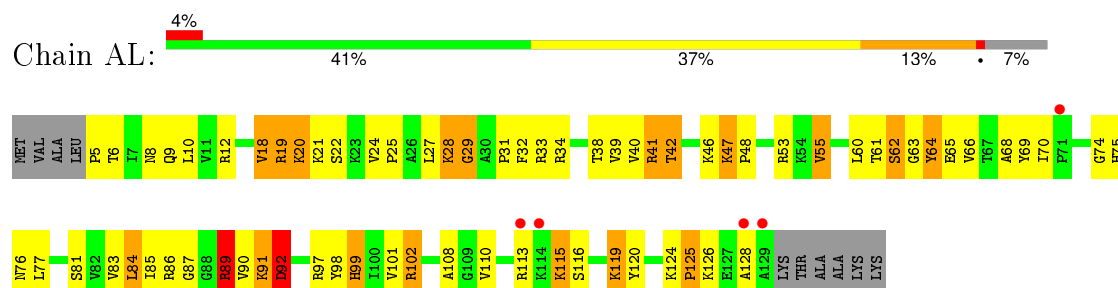
- Molecule 11: 30S ribosomal protein S11



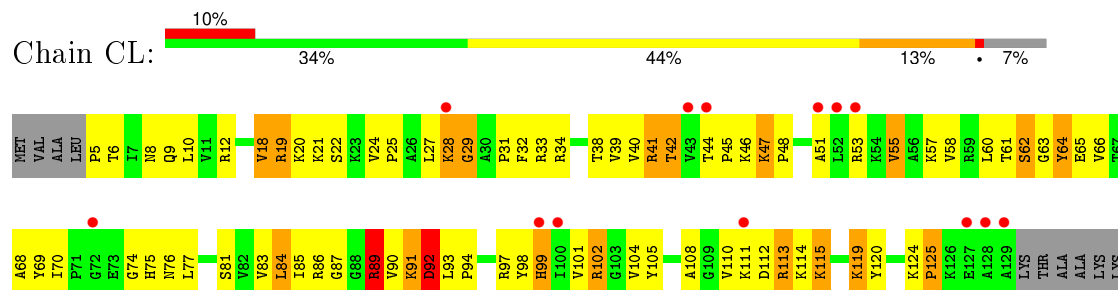
- Molecule 11: 30S ribosomal protein S11



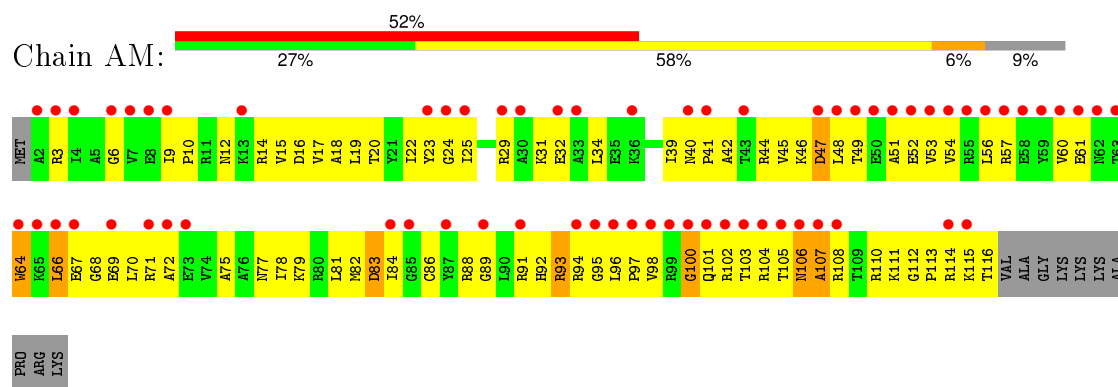
- Molecule 12: 30S ribosomal protein S12



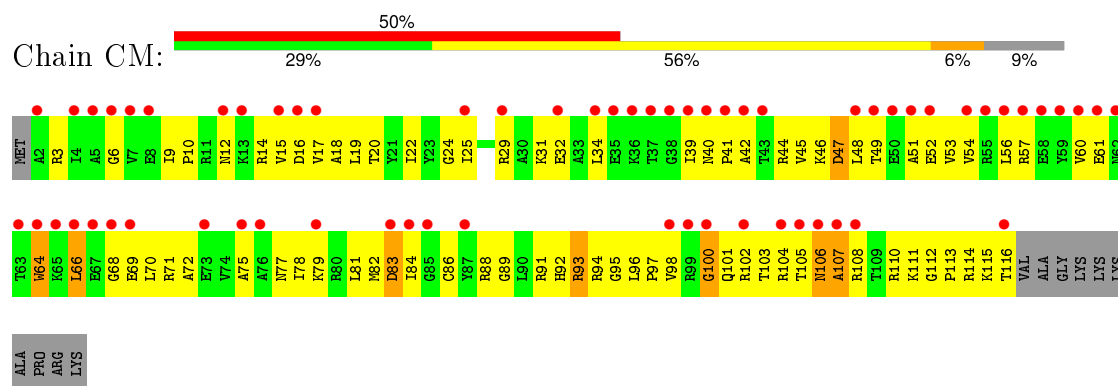
- Molecule 12: 30S ribosomal protein S12



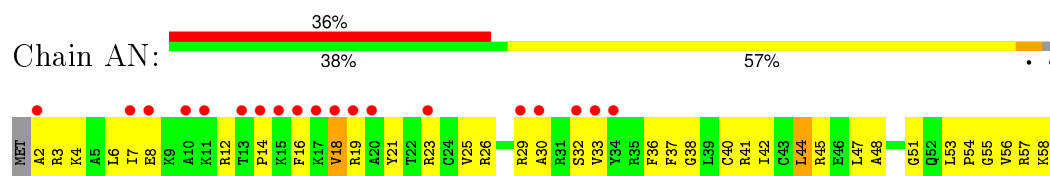
- Molecule 13: 30S ribosomal protein S13



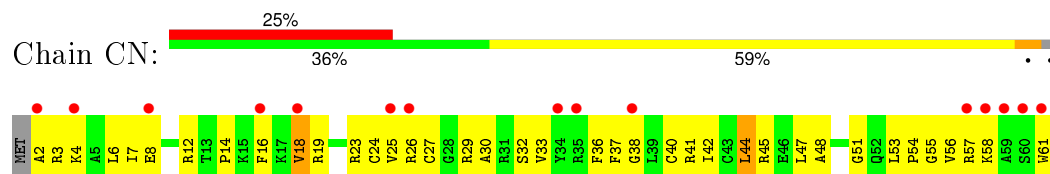
- Molecule 13: 30S ribosomal protein S13



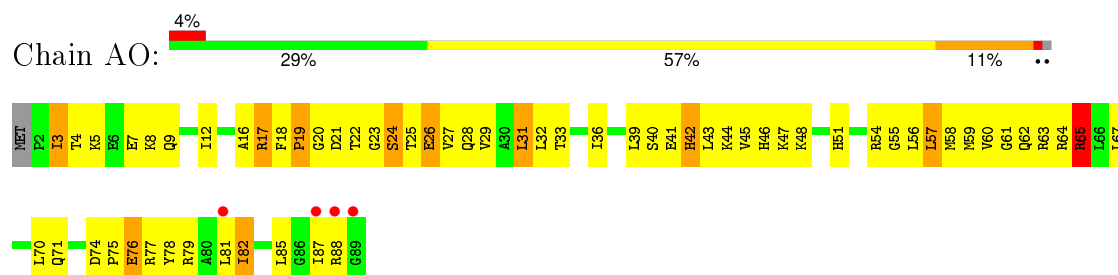
- Molecule 14: 30S ribosomal protein S14



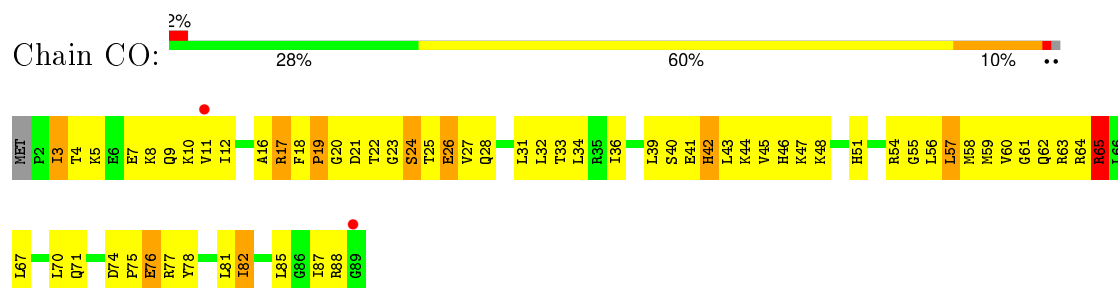
- Molecule 14: 30S ribosomal protein S14



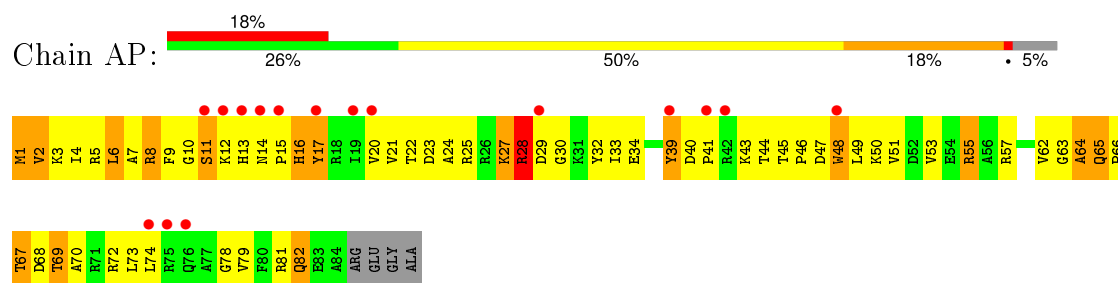
- Molecule 15: 30S ribosomal protein S15



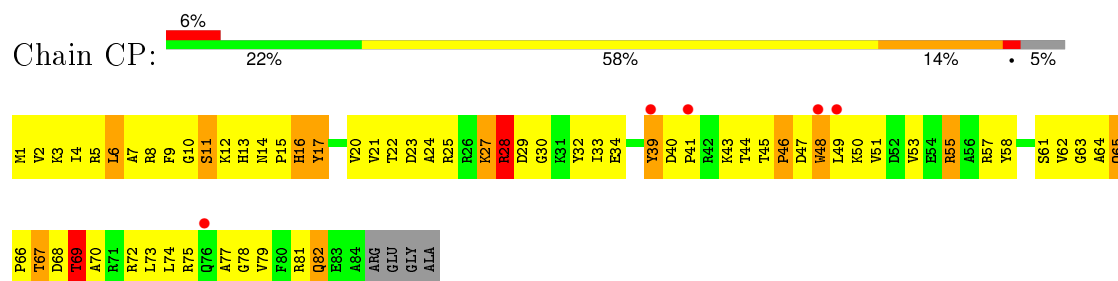
- Molecule 15: 30S ribosomal protein S15



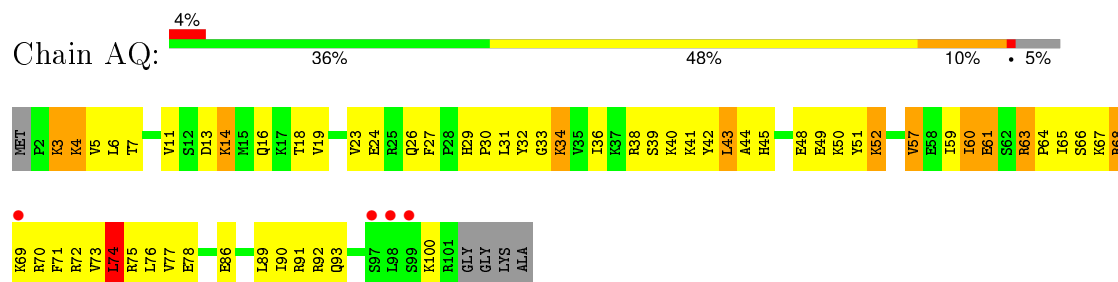
- Molecule 16: 30S ribosomal protein S16



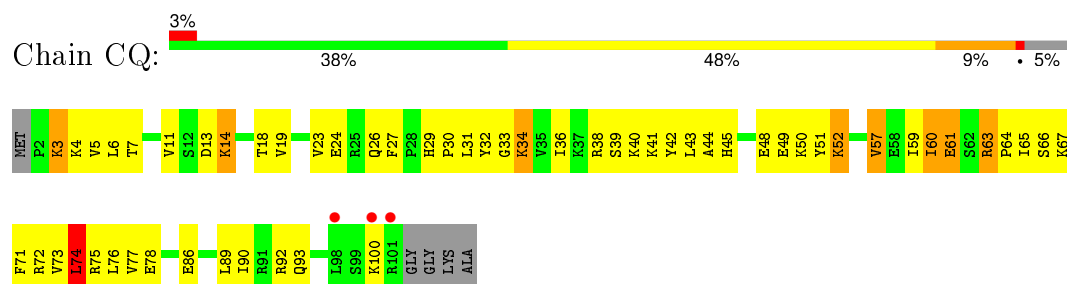
- Molecule 16: 30S ribosomal protein S16



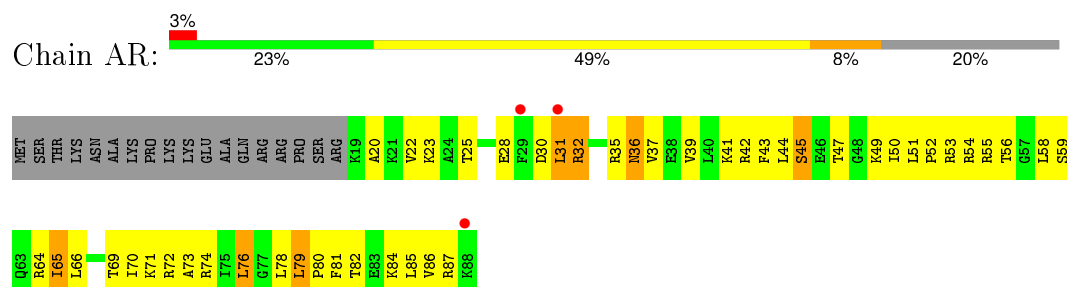
- Molecule 17: 30S ribosomal protein S17



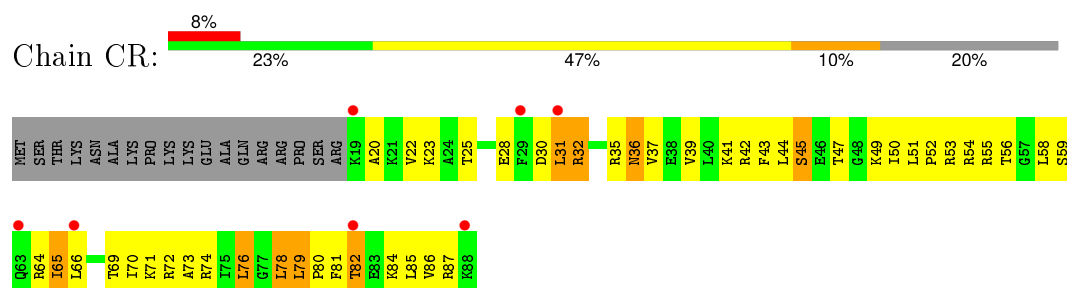
- Molecule 17: 30S ribosomal protein S17



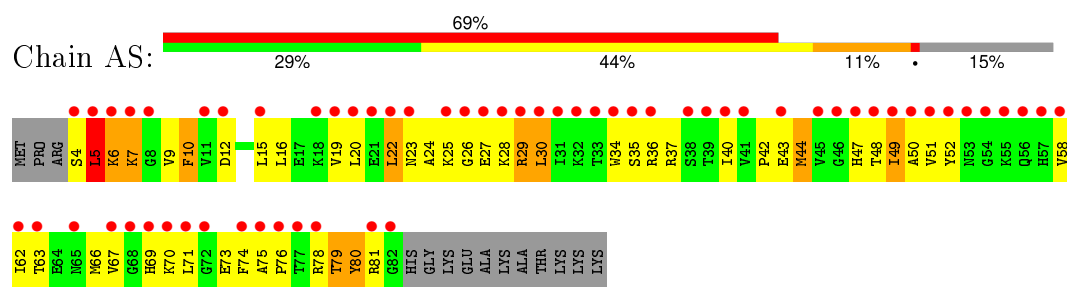
- Molecule 18: 30S ribosomal protein S18



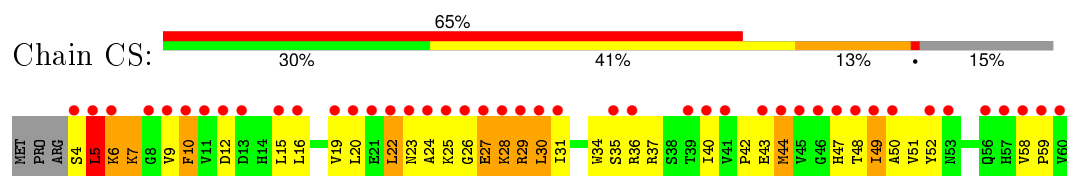
- Molecule 18: 30S ribosomal protein S18

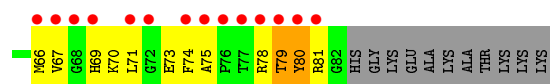


- Molecule 19: 30S ribosomal protein S19

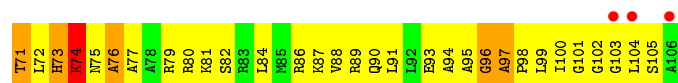


- Molecule 19: 30S ribosomal protein S19

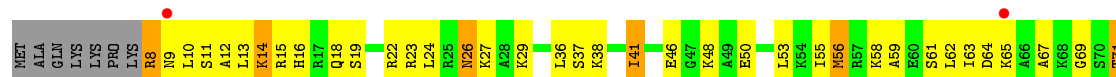




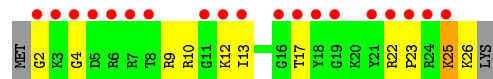
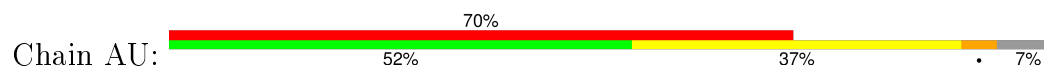
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



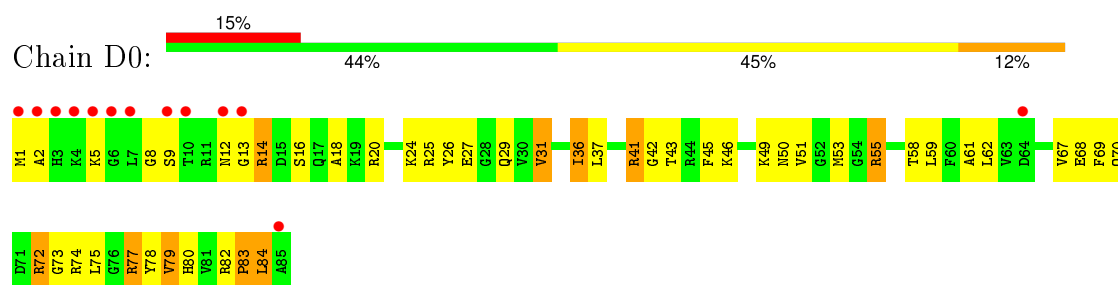
- Molecule 21: 30S ribosomal protein Thx



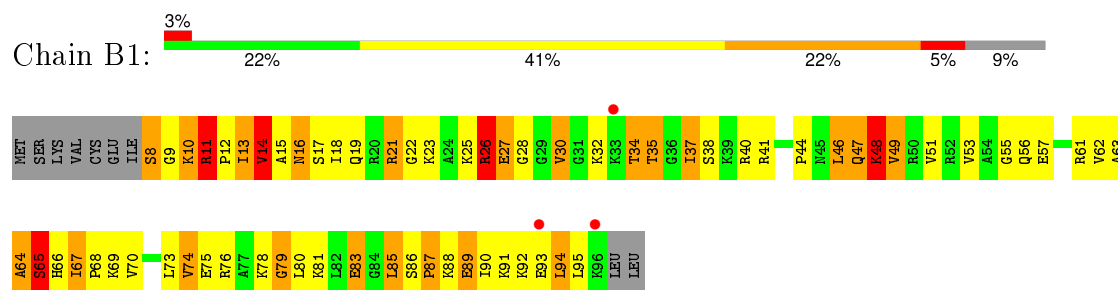
- Molecule 22: 50S ribosomal protein L27



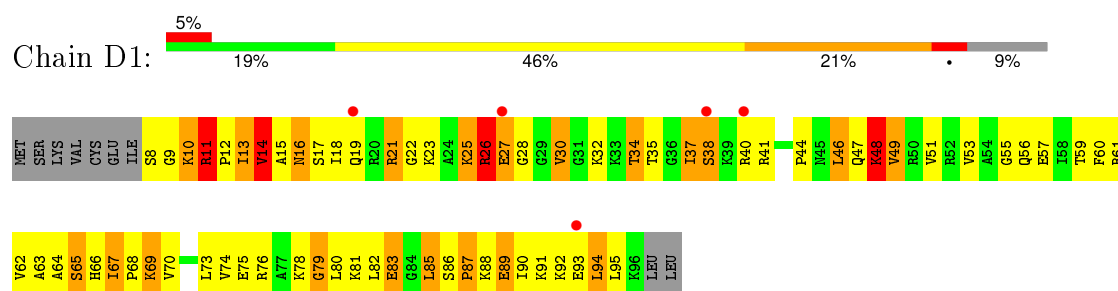
- Molecule 22: 50S ribosomal protein L27



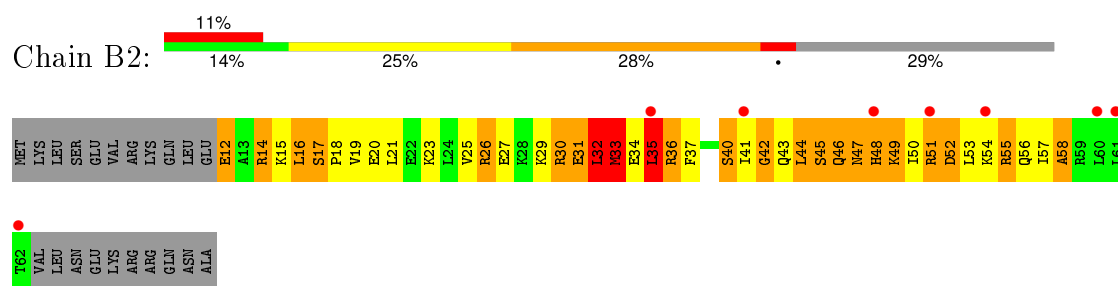
- Molecule 23: 50S ribosomal protein L28



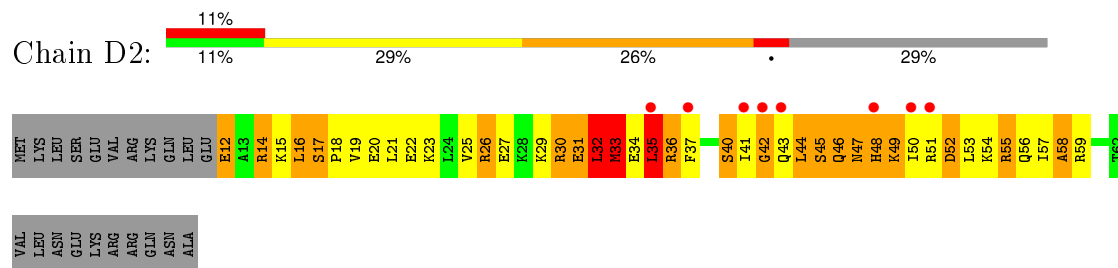
- Molecule 23: 50S ribosomal protein L28



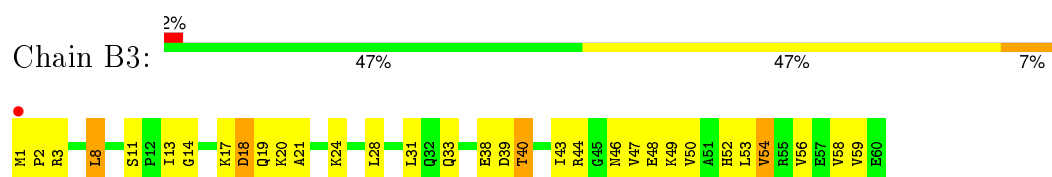
- Molecule 24: 50S ribosomal protein L29



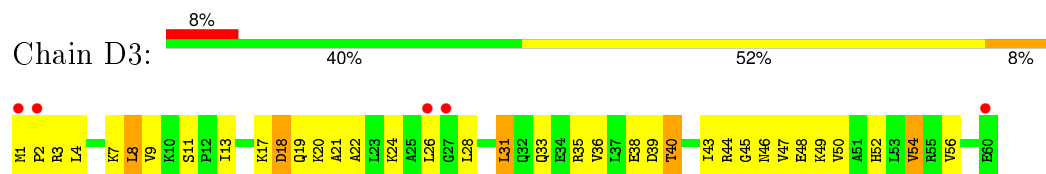
- Molecule 24: 50S ribosomal protein L29



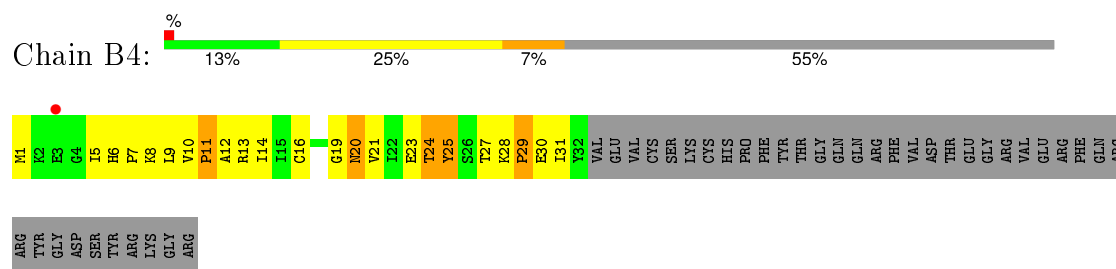
- Molecule 25: 50S ribosomal protein L30



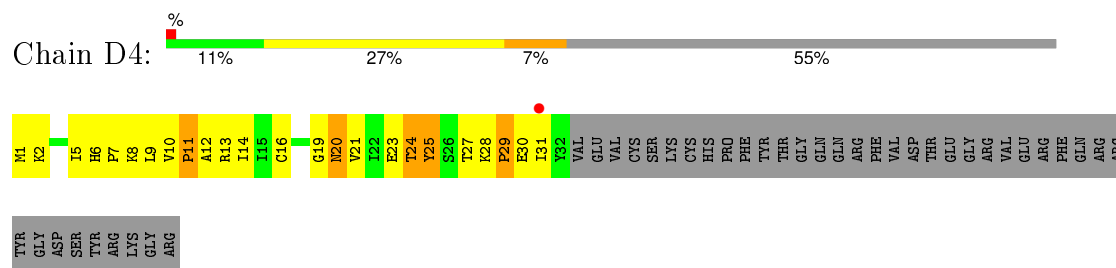
- Molecule 25: 50S ribosomal protein L30



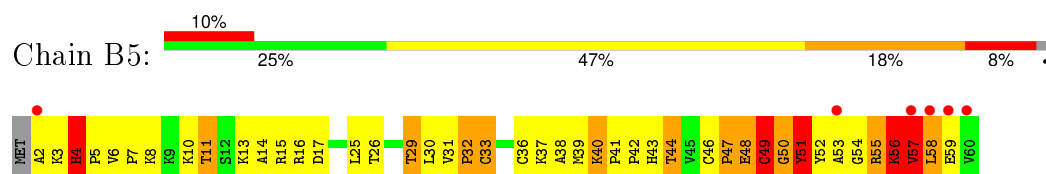
- Molecule 26: 50S ribosomal protein L31



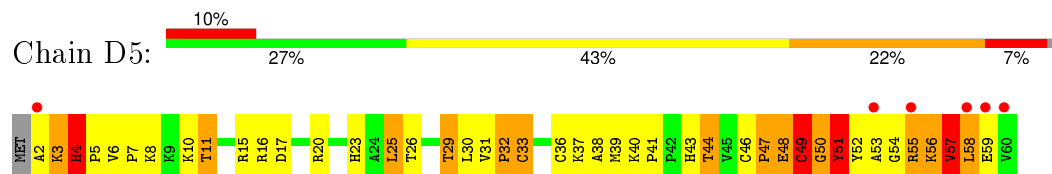
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

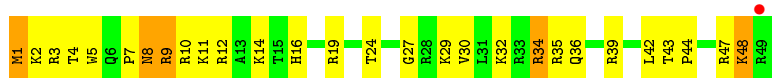
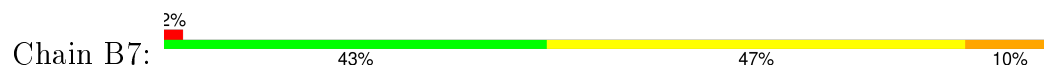




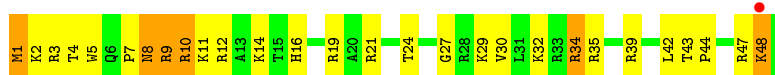
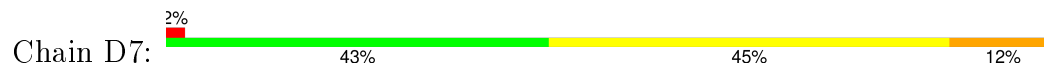
- Molecule 28: 50S ribosomal protein L33



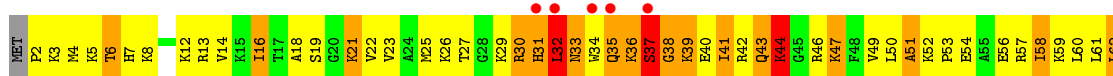
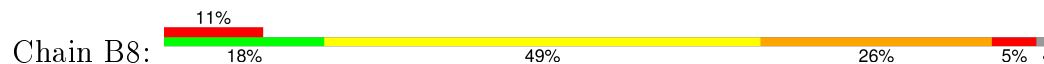
- Molecule 29: 50S ribosomal protein L34



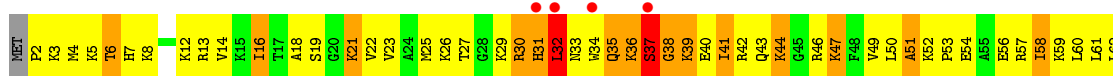
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

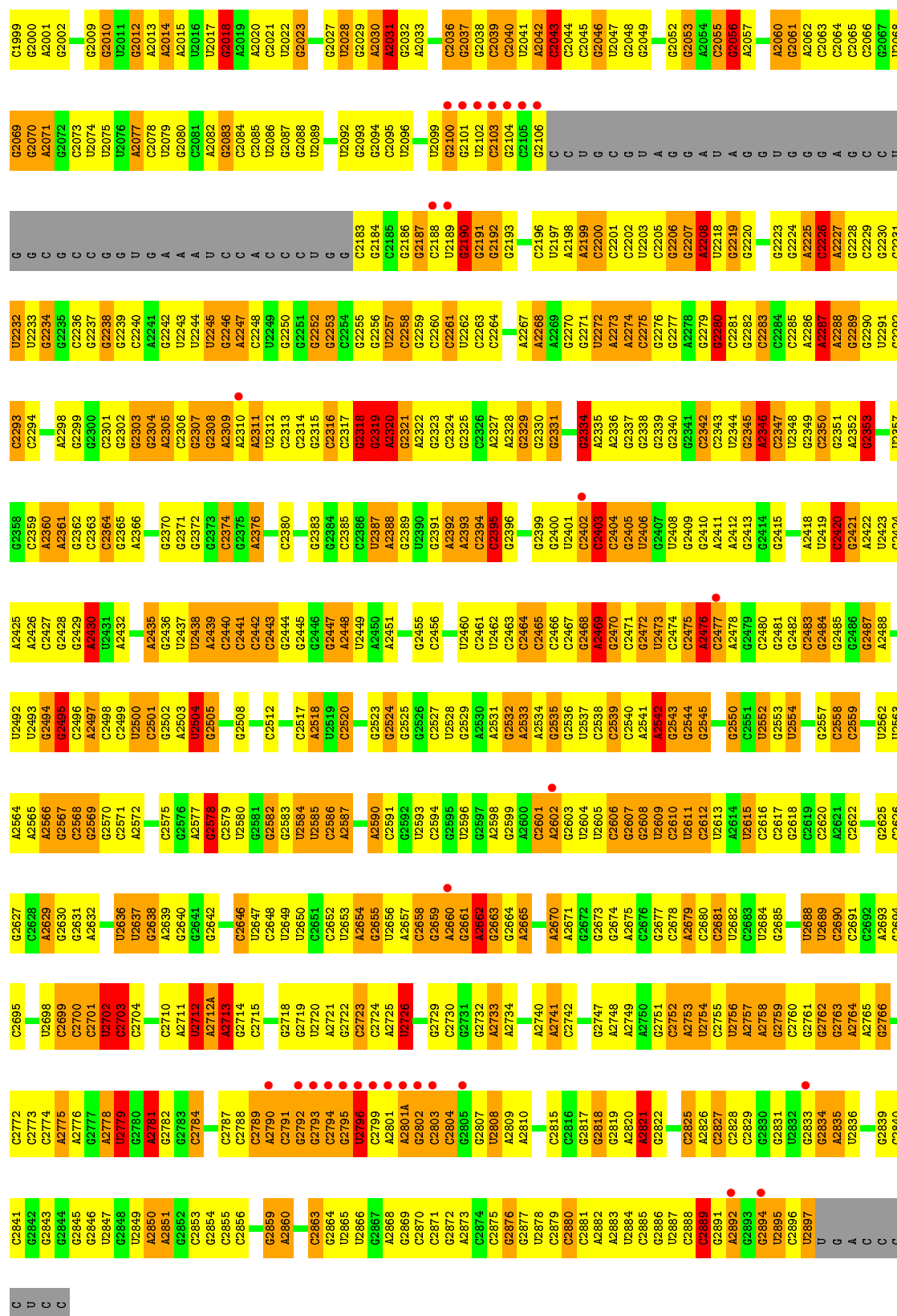


- Molecule 31: 23S ribosomal RNA





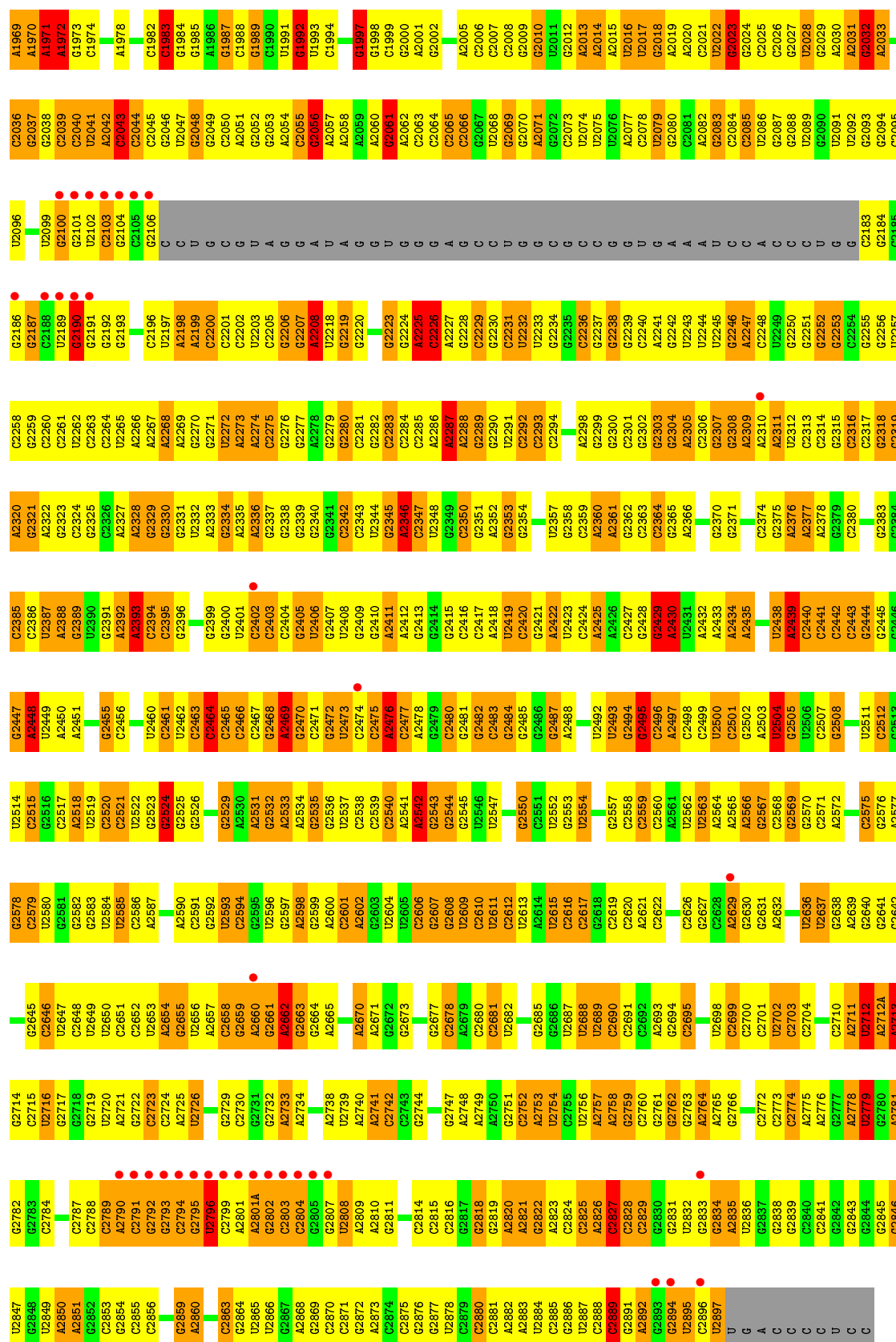
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G1930	G1857	A1788	G1703	A1837	A1571	A1487	G1436	A1301	G1235	U1166	A1045	A983
G1934	G1858	A1789	G1704	C1838	C1574	C1499	G1437	A1302	G1236	U1167	A1046	A984
G1935	G1862	A1790	G1705	U1839	G1575	G1500	A1438	G1303	G1237	G1168	A1047	C985
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G1939	G1865	G1793	G1712	G1642	U1579	C1503	G1441	G1309	G1239	G1171	A1050	A988
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A1938	G1867	U1796	G1714	C1644	G1581	C1505	G1443	A1241	A1242	A1173	C1052	A990
G1941	G1868	G1797	G1715	G1645	C1582	C1506	G1444	G1311	G1176	A1175	C1053	C991
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G1989	A1916	G1839	G1773	G1625	G1625	A1553	U1484	A1349	A1287	G1219	G1144	G1031
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C1994	C1781	C1781	C1781	C1631	C1631	G1559	U1489	U1357	U1293	G1224	G1157	G1037
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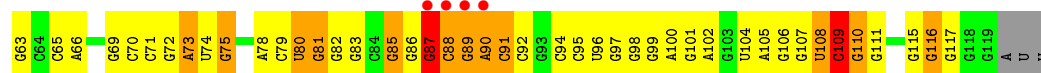
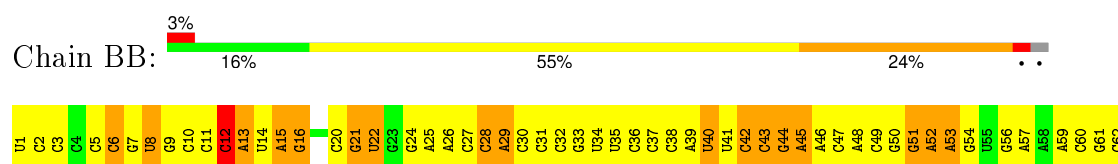


• Molecule 31: 23S ribosomal RNA

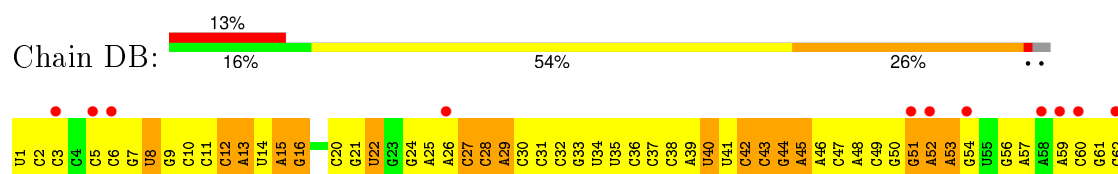
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C912	A841	G710	C584	C516	U373	C313	G271I	G212	G140	G68	C
U913	C842	G711	G585	C517	A374	A314	C271J	G213	A141	C69	A
C914	G843	G712	A586	G518	C375	G315	U271K	A213	A142	G70	A6
	U847		C587	U519	C376	C316	U271L	G214	C142A	A71	G7
A917	G848	G717	U888	G520	C377		G271M	G215	G143	U72	A8
A918	A782	A718	C589	G521	C378	C319	U271N	A216	G143A	A73	U9
C919	G719	C719	A590	G522	G379	A320	C271O	G217	G144	A74	G10
G920	U851	C720	G591	C523	U380	G321	C271P	A218	G145	G75	G11
G921		G721	G592	U524		A322	G271Q		G146	C76	U12
U922	G854	A722	G593	U525	U384	G323	G271R	A222	U147	A13	A13
C923	G855	G723	U594	A526	C385	A324	G271S		C148	A14	A14
C924	C856	U724	C595	A527	G386	G325	G271T	A225	A149	G79	
C925	A788	G725	U596	A528	U387	G326	C271U	G226	C150	G80	G17
A926	G726	G726	U597	A529	G388	G327		A227	C151	G82	C18
G927	U858	A727	G598	G530	G389	U328	G271X	A228	G152	G83	C19
U928	C859	G727	C531	C531	G389	G329	U271Y	A229	C153	A84	C20
G930	U860	G728	G599	A532	A394	A330	C271Z	U230	G154	G85	A21
U931	C861	G729	G601	A533	U395	A331	G271Z	C231	C154A	C86	C22
G932	G862	C731	G602	U534	C396	A332	G272B	G232	U157	C87	G23
A933	C863	G732	A603	C535	G397	G333	G272C	A233	U158		G24
G934	G864	G733	U667	A536	G398	C334	G272D		G171	U90	U25
C935	C865	G734	G605	C537		C335		C236	C172	A92	G26
C936	C867	A735	U606		A401	C336		C237	G173	G93	G27
U937	G869	G736	U607	C540	U405	C337	C272E	C238	C174	C94	A28
G938	C870	C737	C541	G541	G406	G338	U272H	U239	G175	G94A	U29
	A871	G738	C542	C542	A407	U339	G272I	G240	G176	G95	G30
U941	U870	C739	G610	C543		A340	G274	A241	G177	G96	G31
G942	A872	U740	C611	A547	C409	G341	G275	U243	G178	C97	G32
U943	G873	G741		A548	G410	C342	C279	U244	G179		U33
G944	A874	G742	U614	G549	G411	C343	C280	A244	G180	G100	C34
A945	C875	G743	G614A	G551	A412	G344	G281	G245	A181	G102	G35
G946	G876	G744	A614C	G552	C413	A345	A282	C246	A182	A103	G36
G947	U877	G745	G615	G553	C414			G247	C183	U104	C37
G948	A878	A746	G616	U557	A415	G348	U284	G248	C184	C105	A38
C949	G879	U747	G616	G558	C416	G349	C285	C249	U185	C106	C39
	U880		C618	G559	G417	U350	C286	G250	G186	C107	C40
G950	C881	A750	G619	C560	G418	G351	C287	A251	G187	U108	C41
C951	C882	A751	G620	C561	C419	G352	C288	G252	G188	G109	G42
G952	C883	A752	G621	G562	A423	G353		C253	G189	G110	A43
A953	C884	G753	G622	U562		G354	C291	G254	A190	G44	G44
G954	C885	C754	G623	G563	U427	G355	C292	A255	C192	C115	C45
C955	A819	G755	G624	U566	A428	G356	U293	A256	G117	G116	
	A820		G625	U567	G428	A357		A257	U193	G117	A49
U958	A824	G756	G626	A567	A429	U358	C296	G258	G194	A118	U50
A959	C825	U757	U626	U568	G430	A359	C297	G259	A195	A119	G51
A960	U826	C691	G627	U569	U431	G360	G298	G260	A196	U120	A52
C961	U827	A761	G629	G570	A432	G361	A299	G261	A197	A53	A53
	U828		G630	A571	C433	U362	A300	A262	C198	G123	G54
G964	U829	A764	A631	A572		G363	G301	G263	A199	G124	G55
C965	G830	G765	G573	G574	U441	A363A	C302	C264	U200	C128	A56
G966	G831	C766	C634	C575	G442	G363B	U303	A265	C201	C129	C57
C967	U698	G767	G635	A575	A443		G304	G266	U202	G58	G58
G968	C832	U767	G636	U576	C444		G305		G203	C130	
U969	U833	G768	G636	G577	C445	U363E	U306	A271A	A204	G131	G61
C970	G700	G769	A637	G578	C446	A363F	G307		G205	C132	C62
U971	G701	G770	G638	A578	U447	C365	G308	G271D	U206	G133	U63
C972	A705	G770	U639	U511	A447		G309		C133		
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G1904	G1831	C1767	C1685	G1623	A1554	G1485	G1420	A1353	G1226	G1163	C1040	G975A
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U1943	A1802	A1802	U1739	A1655	C1592	G1516	G1456	A1322	C1261	U1198		U1012
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C1967	A1900	C1827	G1763	G1681	A1616	C1550	G1480	C1416	G1284	C1222	G1157	G1036
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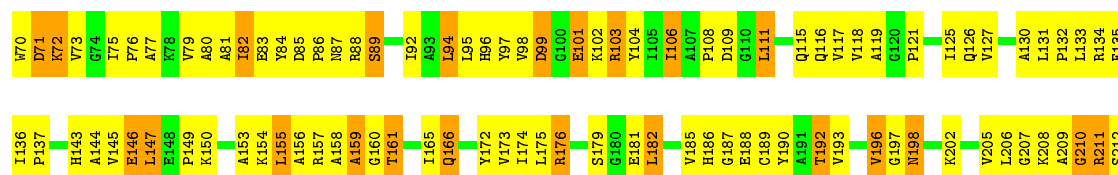
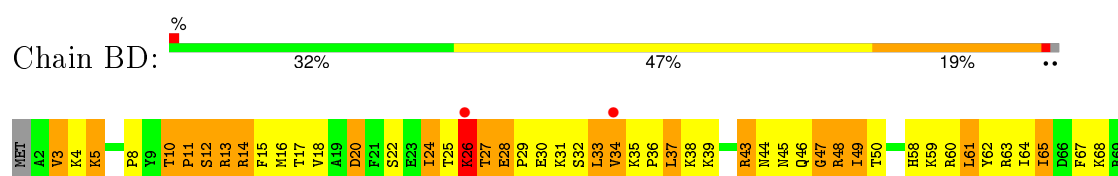




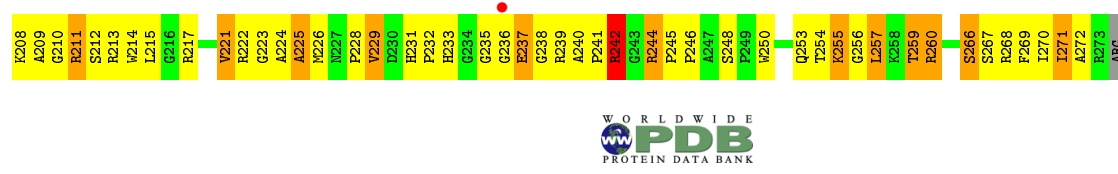
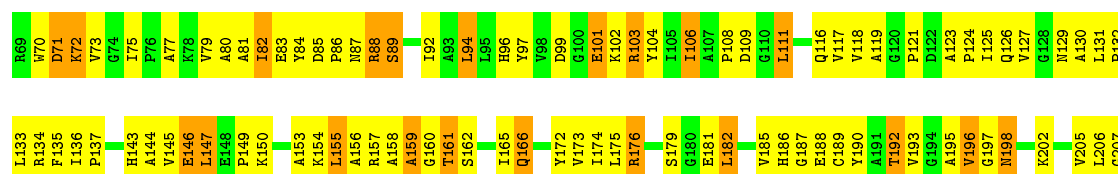
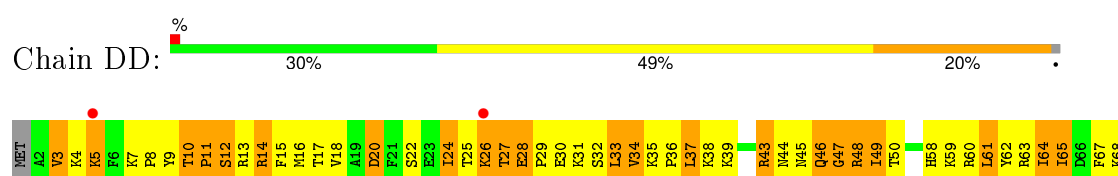
• Molecule 32: 5S ribosomal RNA



• Molecule 33: 50S ribosomal protein L2

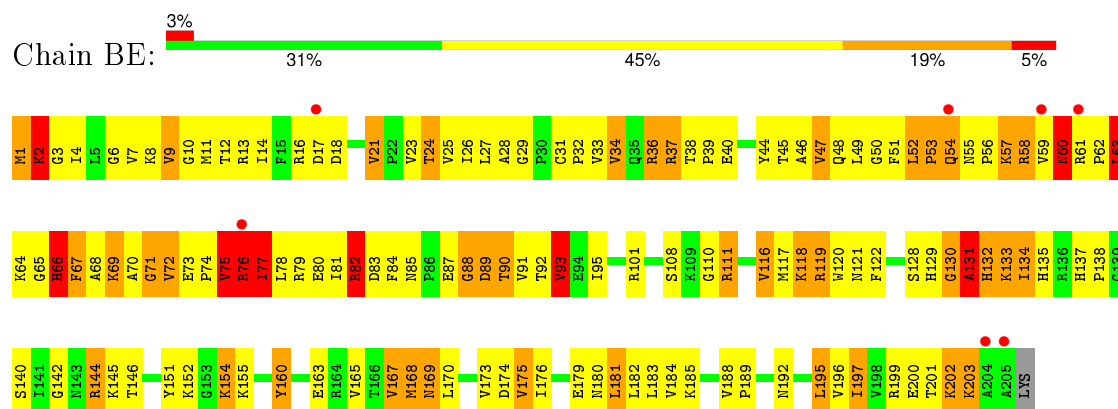


• Molecule 33: 50S ribosomal protein L2

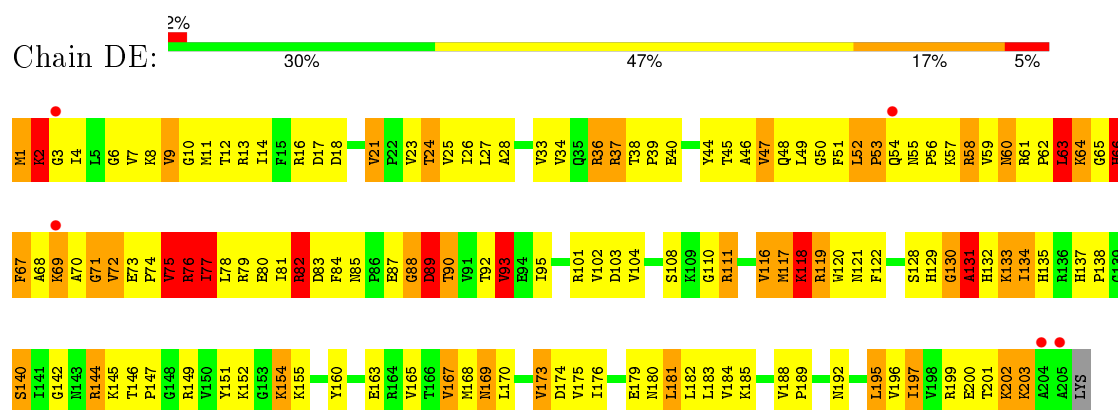


LYS
LYS

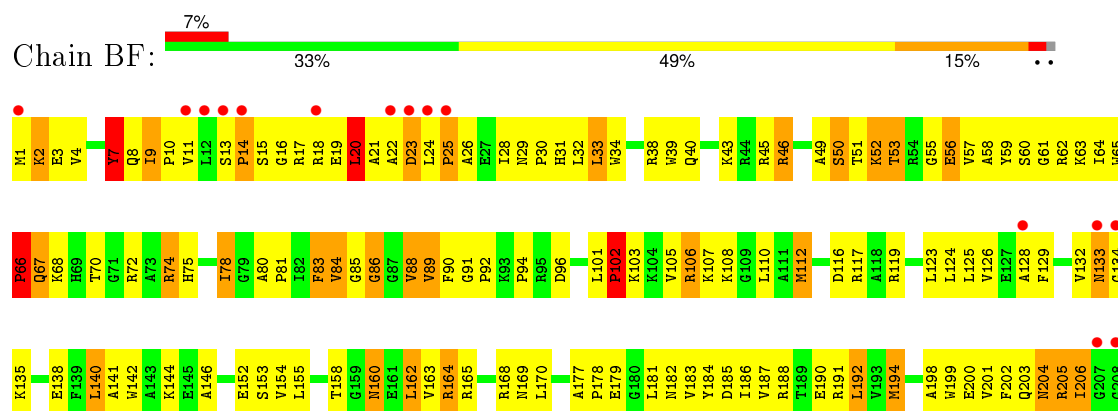
- Molecule 34: 50S ribosomal protein L3



- Molecule 34: 50S ribosomal protein L3

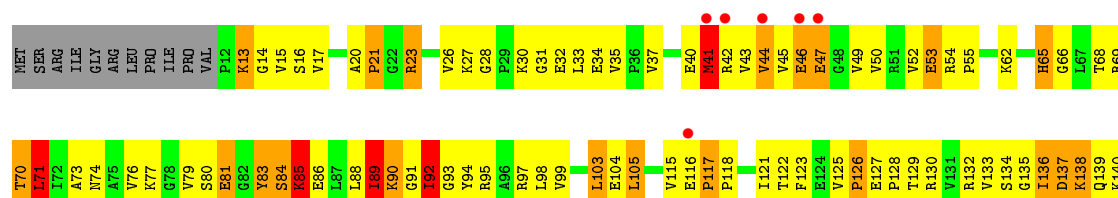


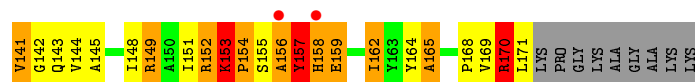
- Molecule 35: 50S ribosomal protein L4

GLU
ALA

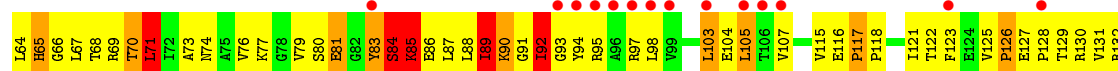
- Molecule 35: 50S ribosomal protein L4



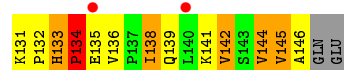
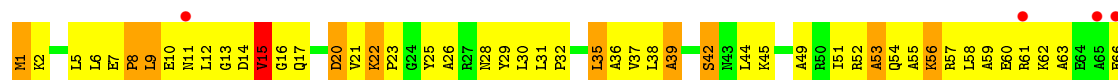




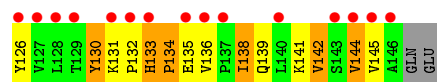
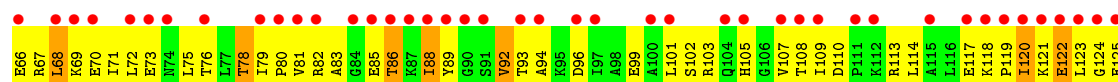
• Molecule 37: 50S ribosomal protein L6



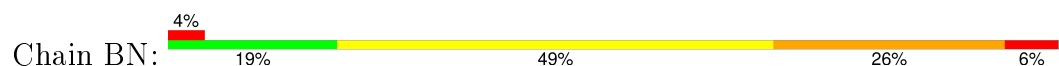
• Molecule 38: 50S ribosomal protein L9

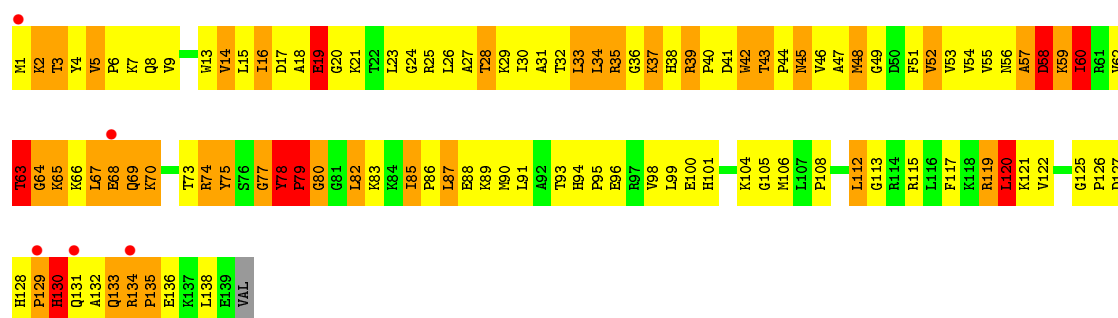


• Molecule 38: 50S ribosomal protein L9

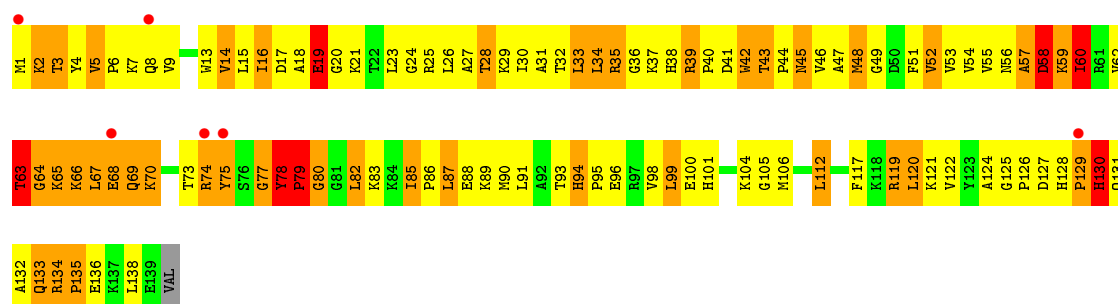
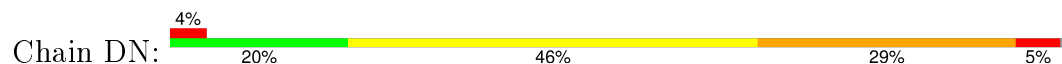


• Molecule 39: 50S ribosomal protein L13

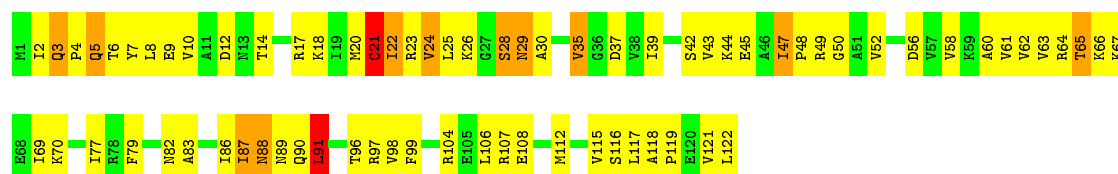




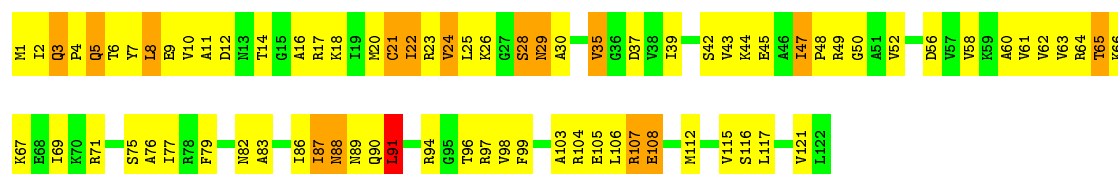
• Molecule 39: 50S ribosomal protein L13



• Molecule 40: 50S ribosomal protein L14

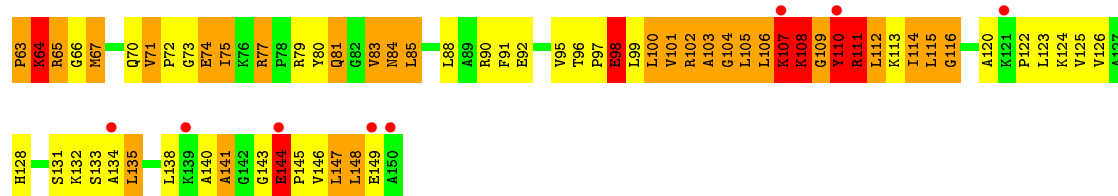


• Molecule 40: 50S ribosomal protein L14

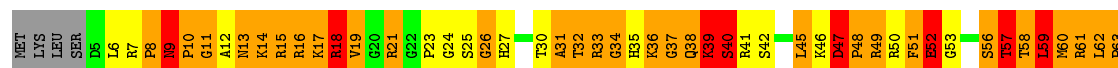
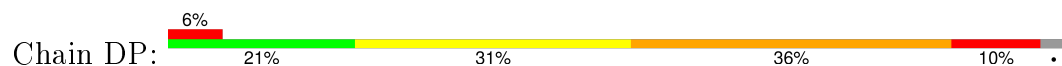


• Molecule 41: 50S ribosomal protein L15

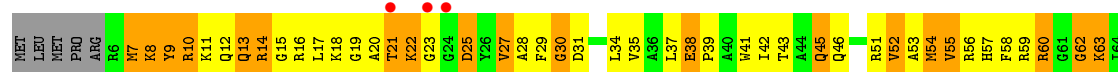




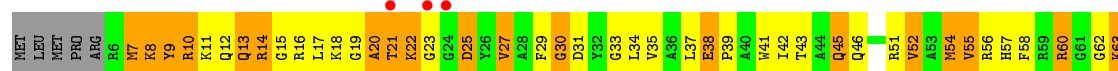
- Molecule 41: 50S ribosomal protein L15



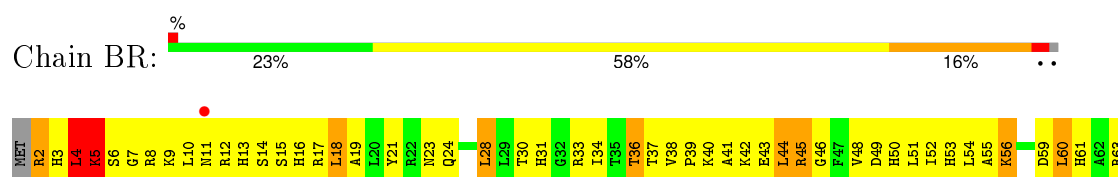
- Molecule 42: 50S ribosomal protein L16



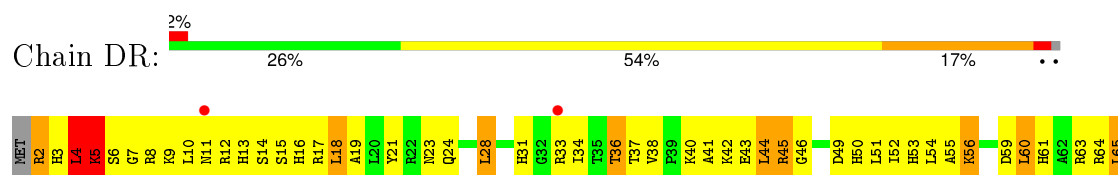
- Molecule 42: 50S ribosomal protein L16



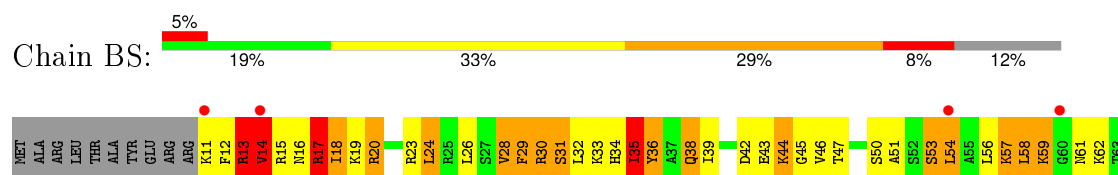
- Molecule 43: 50S ribosomal protein L17



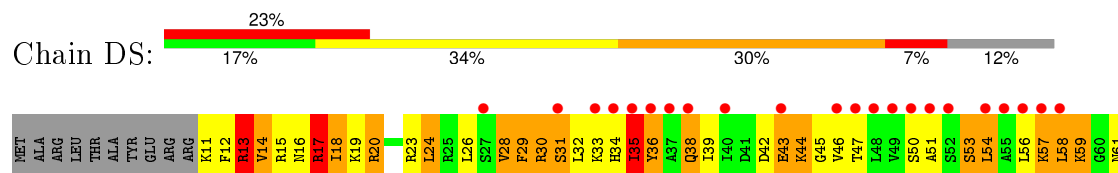
• Molecule 43: 50S ribosomal protein L17



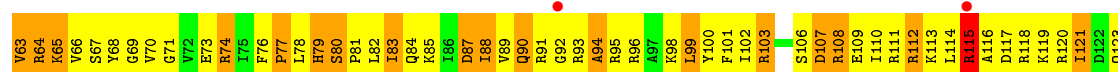
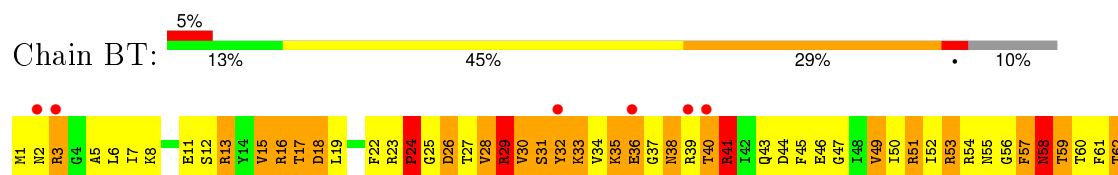
• Molecule 44: 50S ribosomal protein L18

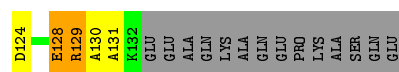


• Molecule 44: 50S ribosomal protein L18

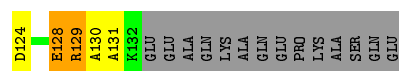
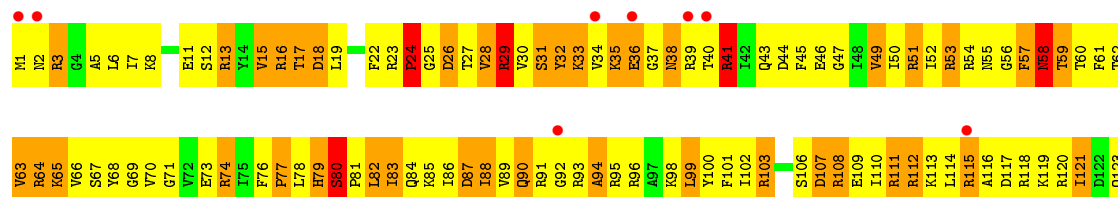
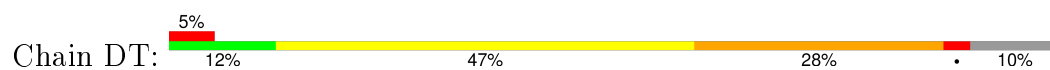


• Molecule 45: 50S ribosomal protein L19

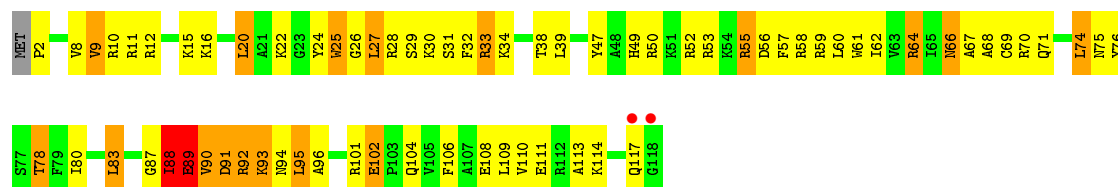




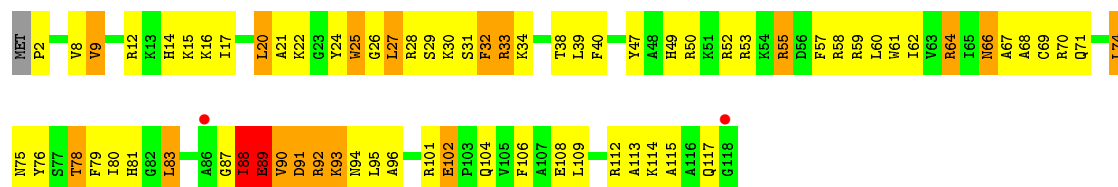
- Molecule 45: 50S ribosomal protein L19



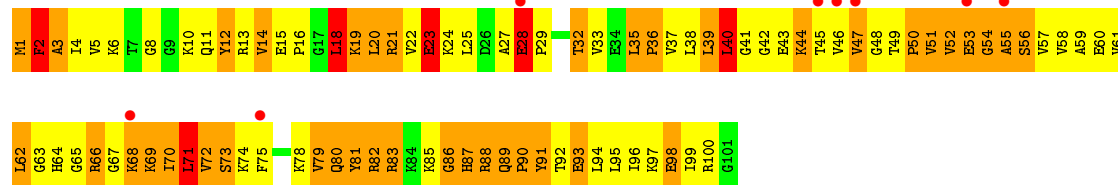
- Molecule 46: 50S ribosomal protein L20



- Molecule 46: 50S ribosomal protein L20

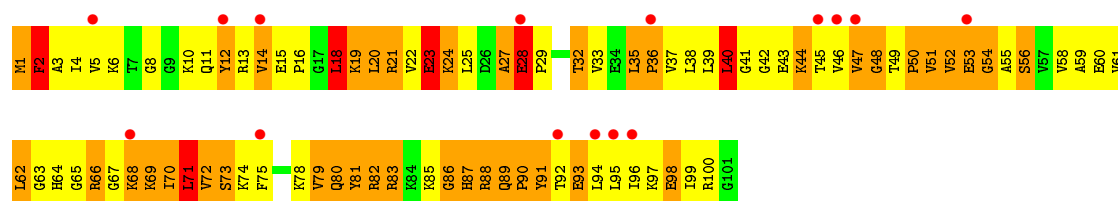


- Molecule 47: 50S ribosomal protein L21

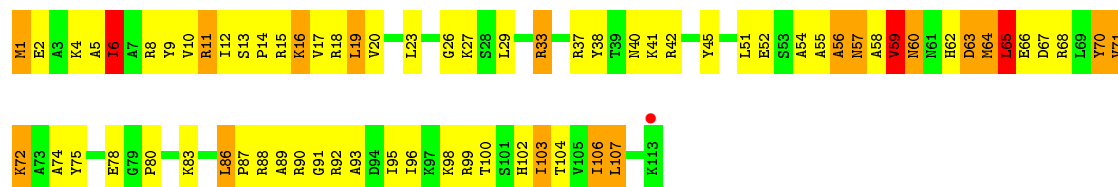


- Molecule 47: 50S ribosomal protein L21

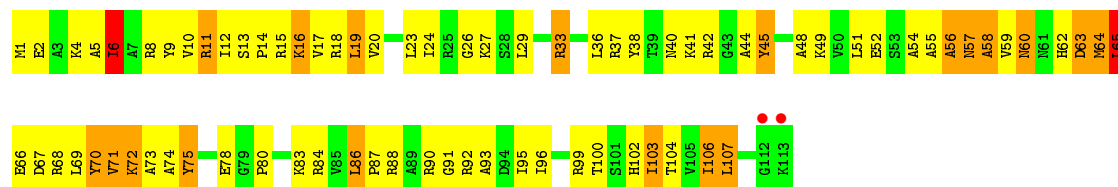




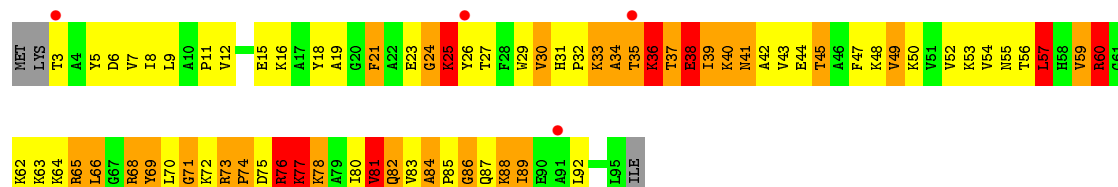
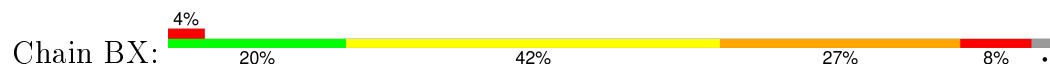
• Molecule 48: 50S ribosomal protein L22



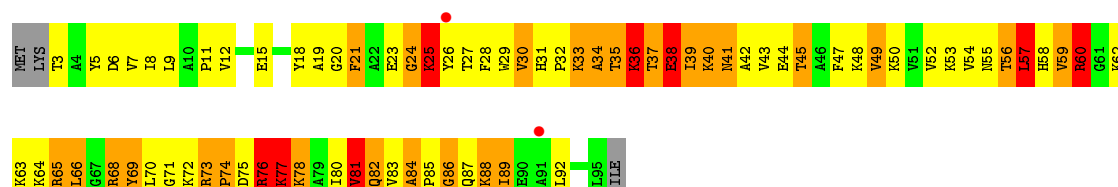
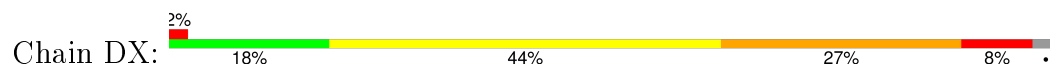
• Molecule 48: 50S ribosomal protein L22



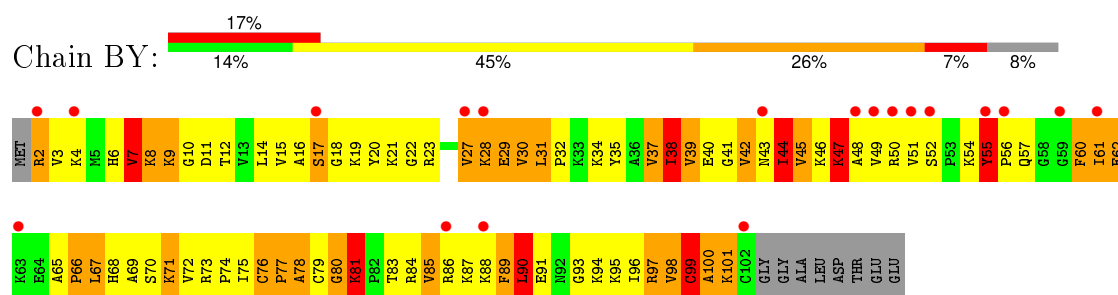
• Molecule 49: 50S ribosomal protein L23



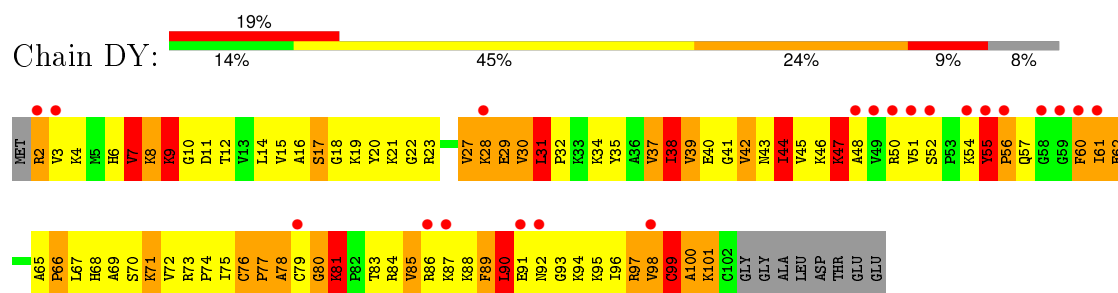
• Molecule 49: 50S ribosomal protein L23



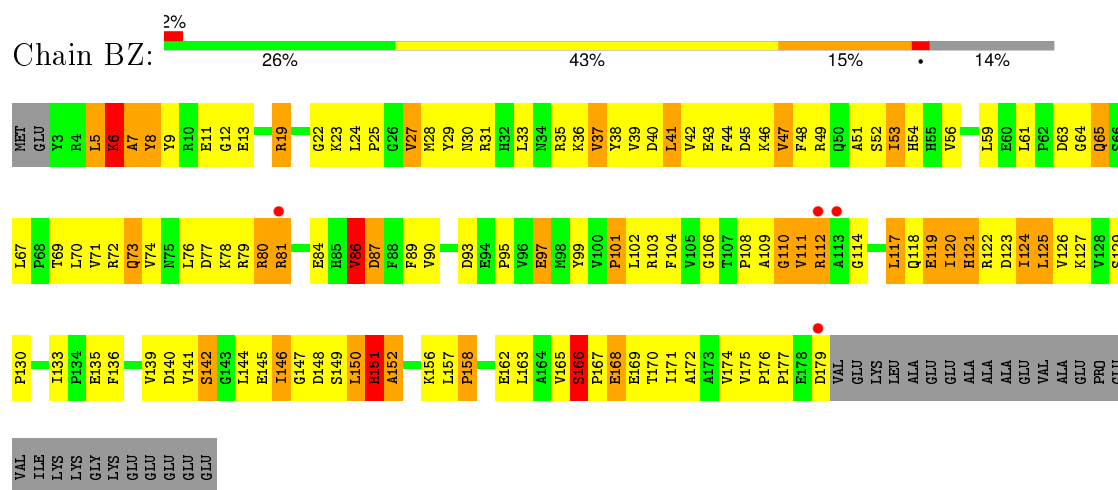
• Molecule 50: 50S ribosomal protein L24



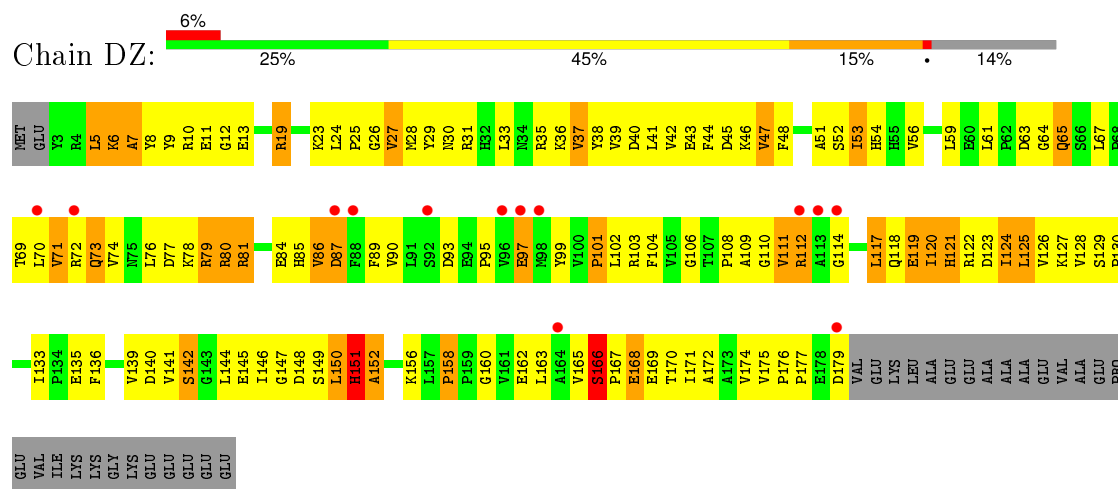
- Molecule 50: 50S ribosomal protein L24



- Molecule 51: 50S ribosomal protein L25



- Molecule 51: 50S ribosomal protein L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.18Å 448.40Å 621.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.00 49.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.57-3.00) 98.6 (49.57-3.00)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.01Å)	Xtriage
Refinement program	Phenix	Depositor
R, R_{free}	0.244 , 0.281 0.249 , 0.280	Depositor DCC
R_{free} test set	57196 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 86.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1140008 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	277987	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.54	0/36190	0.92	37/56486 (0.1%)
1	CA	0.53	0/36190	0.93	55/56486 (0.1%)
2	AB	0.29	0/1936	0.51	0/2611
2	CB	0.29	0/1936	0.50	0/2611
3	AC	0.27	0/1637	0.44	0/2207
3	CC	0.26	0/1637	0.44	0/2207
4	AD	0.36	0/1733	0.54	0/2318
4	CD	0.38	1/1733 (0.1%)	0.55	0/2318
5	AE	0.38	0/1163	0.58	0/1566
5	CE	0.37	0/1163	0.59	0/1566
6	AF	0.38	0/856	0.58	0/1154
6	CF	0.36	0/856	0.58	0/1154
7	AG	0.25	0/1276	0.44	0/1709
7	CG	0.25	0/1276	0.44	0/1709
8	AH	0.34	0/1136	0.56	0/1527
8	CH	0.34	0/1136	0.55	0/1527
9	AI	0.25	0/1028	0.44	0/1375
9	CI	0.25	0/1028	0.44	0/1375
10	AJ	0.27	0/808	0.48	0/1087
10	CJ	0.26	0/808	0.49	0/1087
11	AK	0.33	0/900	0.55	0/1213
11	CK	0.35	0/900	0.54	0/1213
12	AL	0.42	0/987	0.65	0/1322
12	CL	0.42	0/987	0.65	0/1322
13	AM	0.26	0/928	0.47	0/1238
13	CM	0.26	0/928	0.46	0/1238
14	AN	0.26	0/501	0.42	0/664
14	CN	0.26	0/501	0.42	0/664
15	AO	0.36	0/745	0.59	0/992
15	CO	0.35	0/745	0.58	0/992
16	AP	0.34	0/717	0.59	0/965
16	CP	0.35	0/717	0.60	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.36	0/837	0.58	0/1119
17	CQ	0.37	0/837	0.59	0/1119
18	AR	0.35	0/579	0.58	0/768
18	CR	0.36	0/579	0.57	0/768
19	AS	0.26	0/643	0.43	0/867
19	CS	0.26	0/643	0.44	0/867
20	AT	0.36	0/765	0.57	0/1007
20	CT	0.35	0/765	0.56	0/1007
21	AU	0.26	0/213	0.43	0/279
21	CU	0.26	0/213	0.43	0/279
22	B0	0.53	0/658	0.70	0/878
22	D0	0.49	0/658	0.70	0/878
23	B1	0.78	0/700	0.99	2/931 (0.2%)
23	D1	0.67	0/700	0.95	1/931 (0.1%)
24	B2	0.66	0/423	0.94	0/560
24	D2	0.55	0/423	0.89	0/560
25	B3	0.61	0/473	0.69	0/636
25	D3	0.49	0/473	0.67	0/636
26	B4	0.30	0/156	0.68	0/215
26	D4	0.30	0/156	0.65	0/215
27	B5	0.84	1/473 (0.2%)	1.02	2/639 (0.3%)
27	D5	0.77	0/473	0.97	1/639 (0.2%)
28	B6	0.89	0/387	1.07	0/517
28	D6	0.71	0/387	1.01	0/517
29	B7	0.64	0/427	0.79	0/563
29	D7	0.67	0/427	0.76	0/563
30	B8	0.72	0/516	1.09	2/681 (0.3%)
30	D8	0.64	0/516	1.04	0/681
31	BA	1.06	84/65745 (0.1%)	1.42	971/102639 (0.9%)
31	DA	0.85	35/65745 (0.1%)	1.41	1008/102639 (1.0%)
32	BB	0.83	0/2853	1.18	23/4451 (0.5%)
32	DB	0.66	0/2853	1.13	19/4451 (0.4%)
33	BD	0.63	0/2155	0.85	2/2907 (0.1%)
33	DD	0.59	0/2155	0.83	1/2907 (0.0%)
34	BE	0.63	0/1597	0.82	0/2155
34	DE	0.56	0/1597	0.81	0/2155
35	BF	0.60	0/1659	0.76	0/2246
35	DF	0.52	1/1659 (0.1%)	0.74	0/2246
36	BG	0.34	0/1498	0.55	0/2013
36	DG	0.30	0/1498	0.54	0/2013
37	BH	0.60	0/1246	0.74	0/1684
37	DH	0.44	0/1246	0.69	0/1684
38	BI	0.38	0/1147	0.61	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.40	0/1147	0.61	0/1553
39	BN	0.71	0/1132	0.93	2/1527 (0.1%)
39	DN	0.59	0/1132	0.87	1/1527 (0.1%)
40	BO	0.59	1/943 (0.1%)	0.73	0/1269
40	DO	0.52	0/943	0.73	1/1269 (0.1%)
41	BP	0.69	0/1131	1.03	8/1504 (0.5%)
41	DP	0.60	0/1131	0.98	6/1504 (0.4%)
42	BQ	0.70	0/1100	0.85	1/1470 (0.1%)
42	DQ	0.60	0/1100	0.83	0/1470
43	BR	0.63	0/974	0.82	1/1302 (0.1%)
43	DR	0.56	0/974	0.80	1/1302 (0.1%)
44	BS	0.50	0/779	0.77	0/1038
44	DS	0.43	0/779	0.73	0/1038
45	BT	0.59	0/1114	0.85	2/1488 (0.1%)
45	DT	0.52	0/1114	0.83	1/1488 (0.1%)
46	BU	0.69	0/975	0.76	0/1297
46	DU	0.56	0/975	0.72	0/1297
47	BV	0.72	0/789	0.95	1/1054 (0.1%)
47	DV	0.58	0/789	0.89	1/1054 (0.1%)
48	BW	0.68	0/907	0.84	2/1216 (0.2%)
48	DW	0.58	0/907	0.81	2/1216 (0.2%)
49	BX	0.70	0/740	0.96	2/995 (0.2%)
49	DX	0.63	0/740	0.94	2/995 (0.2%)
50	BY	0.70	1/789 (0.1%)	0.91	0/1053
50	DY	0.60	0/789	0.87	1/1053 (0.1%)
51	BZ	0.47	0/1436	0.67	2/1951 (0.1%)
51	DZ	0.41	0/1436	0.66	1/1951 (0.1%)
All	All	0.75	124/301000 (0.0%)	1.13	2162/449812 (0.5%)

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
23	B1	0	1
23	D1	0	1
24	B2	0	1
24	D2	0	1
27	B5	0	1
27	D5	0	1
28	B6	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	BA	19	0
31	DA	19	0
33	BD	0	3
33	DD	0	3
34	BE	0	2
34	DE	0	2
37	BH	0	1
37	DH	0	1
41	BP	0	5
41	DP	0	4
42	BQ	0	1
42	DQ	0	1
43	BR	0	2
43	DR	0	2
44	BS	0	1
44	DS	0	1
45	BT	0	2
45	DT	0	2
46	BU	0	1
47	BV	0	3
47	DV	0	3
49	BX	0	4
49	DX	0	4
All	All	38	55

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	669	G	C4'-C3'	-11.30	1.40	1.53
31	DA	669	G	C4'-C3'	-10.33	1.41	1.53
31	BA	1300	U	C4'-C3'	-9.89	1.42	1.53
31	BA	1332	G	N9-C4	-9.70	1.30	1.38
31	DA	783	A	N9-C4	-9.28	1.32	1.37

The worst 5 of 2162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BA	1332	G	N3-C4-C5	18.18	137.69	128.60
31	DA	1779	U	C5-C6-N1	-17.02	114.19	122.70
31	BA	1779	U	C5-C6-N1	-16.17	114.61	122.70
31	BA	1332	G	N3-C4-N9	-15.97	116.42	126.00
31	BA	1332	G	C2-N3-C4	-15.30	104.25	111.90

5 of 38 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	BA	100	G	C1'
31	BA	472	A	C3'
31	BA	669	G	C4',C3',C1'
31	BA	945	A	C1'
31	BA	1300	U	C4',C3',C1'

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B1	30	VAL	Peptide
24	B2	55	ARG	Peptide
27	B5	51	TYR	Peptide
28	B6	47	THR	Peptide
33	BD	47	GLY	Peptide

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	32329	0	16318	1597	0
1	CA	32329	0	16318	1553	0
2	AB	1901	0	1951	215	0
2	CB	1901	0	1951	207	0
3	AC	1613	0	1677	116	0
3	CC	1613	0	1677	116	0
4	AD	1703	0	1765	190	0
4	CD	1703	0	1764	192	0
5	AE	1147	0	1207	101	0
5	CE	1147	0	1207	100	0
6	AF	843	0	857	96	0
6	CF	843	0	857	98	0
7	AG	1257	0	1296	75	0
7	CG	1257	0	1296	75	0
8	AH	1116	0	1177	101	0
8	CH	1116	0	1177	99	0
9	AI	1011	0	1042	101	0
9	CI	1011	0	1042	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	105	0
10	CJ	795	0	840	102	0
11	AK	885	0	904	63	0
11	CK	885	0	904	68	0
12	AL	971	0	1057	100	0
12	CL	971	0	1057	103	0
13	AM	921	0	976	88	0
13	CM	921	0	976	91	0
14	AN	492	0	530	47	0
14	CN	492	0	529	46	0
15	AO	734	0	771	76	0
15	CO	734	0	771	78	0
16	AP	701	0	720	91	0
16	CP	701	0	720	97	0
17	AQ	824	0	891	66	0
17	CQ	824	0	891	55	0
18	AR	574	0	644	76	0
18	CR	574	0	644	78	0
19	AS	630	0	652	51	0
19	CS	630	0	652	52	0
20	AT	763	0	861	82	0
20	CT	763	0	861	73	0
21	AU	209	0	221	9	0
21	CU	209	0	221	9	0
22	B0	650	0	654	55	0
22	D0	650	0	654	57	0
23	B1	693	0	764	146	0
23	D1	693	0	764	143	0
24	B2	421	0	461	119	0
24	D2	421	0	461	123	0
25	B3	468	0	523	32	0
25	D3	468	0	523	41	0
26	B4	157	0	69	20	0
26	D4	157	0	69	21	0
27	B5	459	0	480	94	0
27	D5	459	0	480	86	0
28	B6	381	0	390	102	0
28	D6	381	0	390	97	0
29	B7	419	0	467	37	0
29	D7	419	0	467	39	0
30	B8	508	0	576	158	0
30	D8	508	0	576	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BA	58698	0	29590	2607	0
31	DA	58698	0	29591	2784	0
32	BB	2551	0	1295	145	0
32	DB	2551	0	1295	156	0
33	BD	2105	0	2182	325	0
33	DD	2105	0	2182	333	0
34	BE	1564	0	1629	240	0
34	DE	1564	0	1629	249	0
35	BF	1624	0	1677	182	0
35	DF	1624	0	1677	185	0
36	BG	1474	0	1534	190	0
36	DG	1474	0	1534	187	0
37	BH	1223	0	1282	162	0
37	DH	1223	0	1282	157	0
38	BI	1132	0	1218	120	0
38	DI	1132	0	1218	125	0
39	BN	1105	0	1180	218	0
39	DN	1105	0	1180	229	0
40	BO	933	0	996	77	0
40	DO	933	0	996	86	0
41	BP	1114	0	1187	302	0
41	DP	1114	0	1187	289	0
42	BQ	1080	0	1127	165	0
42	DQ	1080	0	1127	176	0
43	BR	960	0	1021	135	0
43	DR	960	0	1021	132	0
44	BS	771	0	832	149	0
44	DS	771	0	832	139	0
45	BT	1100	0	1164	210	0
45	DT	1100	0	1164	201	0
46	BU	958	0	1015	145	0
46	DU	958	0	1015	151	0
47	BV	779	0	851	224	0
47	DV	779	0	851	225	0
48	BW	896	0	953	76	0
48	DW	896	0	953	84	0
49	BX	726	0	778	168	0
49	DX	726	0	778	164	0
50	BY	776	0	870	177	0
50	DY	776	0	870	178	0
51	BZ	1404	0	1432	153	0
51	DZ	1404	0	1432	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AA	56	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	BA	368	0	0	0	0
52	BB	7	0	0	0	0
52	BD	1	0	0	0	0
52	BE	1	0	0	0	0
52	BF	1	0	0	0	0
52	BP	2	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	2	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	53	0	0	0	0
52	D1	1	0	0	0	0
52	D5	2	0	0	0	0
52	DA	332	0	0	0	0
52	DB	4	0	0	0	0
52	DD	1	0	0	0	0
52	DE	1	0	0	0	0
52	DF	1	0	0	0	0
52	DP	1	0	0	0	0
52	DQ	1	0	0	0	0
52	DR	1	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	2	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	20	0	10	0	0
55	DA	20	0	10	0	0
All	All	277987	0	189127	18994	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

The worst 5 of 18994 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)
27:B5:46:CYS:SG	27:B5:47:PRO:HD2	1.78	1.22
31:BA:1899:G:H22	31:BA:1902:C:N4	1.41	1.18
30:B8:32:LEU:CB	30:B8:35:GLN:H	1.57	1.17
32:DB:20:C:H2'	32:DB:21:G:H5''	1.25	1.17
1:CA:1442:G:O2'	1:CA:1442(A):G:H5''	1.43	1.16

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	155 (66%)	61 (26%)	17 (7%)	1	6
2	CB	233/256 (91%)	155 (66%)	60 (26%)	18 (8%)	1	6
3	AC	205/239 (86%)	148 (72%)	46 (22%)	11 (5%)	2	14
3	CC	205/239 (86%)	148 (72%)	45 (22%)	12 (6%)	2	11
4	AD	206/209 (99%)	129 (63%)	57 (28%)	20 (10%)	1	3
4	CD	206/209 (99%)	131 (64%)	55 (27%)	20 (10%)	1	3
5	AE	149/162 (92%)	103 (69%)	36 (24%)	10 (7%)	1	8
5	CE	149/162 (92%)	104 (70%)	36 (24%)	9 (6%)	2	11
6	AF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	2	15
6	CF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	2	15
7	AG	153/156 (98%)	123 (80%)	28 (18%)	2 (1%)	15	53
7	CG	153/156 (98%)	124 (81%)	27 (18%)	2 (1%)	15	53
8	AH	136/138 (99%)	98 (72%)	25 (18%)	13 (10%)	1	3
8	CH	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	1	4
9	AI	123/128 (96%)	89 (72%)	26 (21%)	8 (6%)	1	8
9	CI	123/128 (96%)	91 (74%)	24 (20%)	8 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/105 (92%)	78 (80%)	15 (16%)	4 (4%)	3	20
10	CJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	2	15
11	AK	117/129 (91%)	92 (79%)	23 (20%)	2 (2%)	11	46
11	CK	117/129 (91%)	90 (77%)	25 (21%)	2 (2%)	11	46
12	AL	123/135 (91%)	85 (69%)	25 (20%)	13 (11%)	0	3
12	CL	123/135 (91%)	82 (67%)	27 (22%)	14 (11%)	0	2
13	AM	107/126 (85%)	80 (75%)	21 (20%)	6 (6%)	2	13
13	CM	107/126 (85%)	81 (76%)	19 (18%)	7 (6%)	1	8
14	AN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	11	46
14	CN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	11	46
15	AO	86/89 (97%)	65 (76%)	14 (16%)	7 (8%)	1	5
15	CO	86/89 (97%)	64 (74%)	16 (19%)	6 (7%)	1	7
16	AP	82/88 (93%)	51 (62%)	18 (22%)	13 (16%)	0	1
16	CP	82/88 (93%)	52 (63%)	18 (22%)	12 (15%)	0	1
17	AQ	98/105 (93%)	79 (81%)	11 (11%)	8 (8%)	1	5
17	CQ	98/105 (93%)	78 (80%)	13 (13%)	7 (7%)	1	7
18	AR	68/88 (77%)	49 (72%)	14 (21%)	5 (7%)	1	6
18	CR	68/88 (77%)	46 (68%)	16 (24%)	6 (9%)	1	4
19	AS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	1	4
19	CS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	1	4
20	AT	97/106 (92%)	70 (72%)	18 (19%)	9 (9%)	1	4
20	CT	97/106 (92%)	68 (70%)	20 (21%)	9 (9%)	1	4
21	AU	23/27 (85%)	17 (74%)	5 (22%)	1 (4%)	3	19
21	CU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1	4
22	B0	83/85 (98%)	69 (83%)	10 (12%)	4 (5%)	3	17
22	D0	83/85 (98%)	68 (82%)	11 (13%)	4 (5%)	3	17
23	B1	87/98 (89%)	47 (54%)	24 (28%)	16 (18%)	0	0
23	D1	87/98 (89%)	46 (53%)	24 (28%)	17 (20%)	0	0
24	B2	49/72 (68%)	23 (47%)	14 (29%)	12 (24%)	0	0
24	D2	49/72 (68%)	22 (45%)	15 (31%)	12 (24%)	0	0
25	B3	58/60 (97%)	50 (86%)	8 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D3	58/60 (97%)	48 (83%)	10 (17%)	0	100	100
26	B4	30/71 (42%)	4 (13%)	14 (47%)	12 (40%)	0	0
26	D4	30/71 (42%)	3 (10%)	15 (50%)	12 (40%)	0	0
27	B5	57/60 (95%)	43 (75%)	4 (7%)	10 (18%)	0	1
27	D5	57/60 (95%)	42 (74%)	6 (10%)	9 (16%)	0	1
28	B6	41/54 (76%)	21 (51%)	6 (15%)	14 (34%)	0	0
28	D6	41/54 (76%)	21 (51%)	7 (17%)	13 (32%)	0	0
29	B7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
29	D7	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	B8	62/65 (95%)	41 (66%)	12 (19%)	9 (14%)	0	1
30	D8	62/65 (95%)	42 (68%)	12 (19%)	8 (13%)	0	1
33	BD	270/276 (98%)	211 (78%)	44 (16%)	15 (6%)	2	13
33	DD	270/276 (98%)	208 (77%)	46 (17%)	16 (6%)	2	11
34	BE	203/206 (98%)	147 (72%)	31 (15%)	25 (12%)	0	2
34	DE	203/206 (98%)	144 (71%)	37 (18%)	22 (11%)	0	2
35	BF	206/210 (98%)	158 (77%)	34 (16%)	14 (7%)	1	7
35	DF	206/210 (98%)	154 (75%)	36 (18%)	16 (8%)	1	6
36	BG	177/182 (97%)	125 (71%)	35 (20%)	17 (10%)	1	3
36	DG	177/182 (97%)	126 (71%)	34 (19%)	17 (10%)	1	3
37	BH	158/180 (88%)	102 (65%)	31 (20%)	25 (16%)	0	1
37	DH	158/180 (88%)	101 (64%)	31 (20%)	26 (16%)	0	1
38	BI	144/148 (97%)	98 (68%)	30 (21%)	16 (11%)	0	2
38	DI	144/148 (97%)	99 (69%)	33 (23%)	12 (8%)	1	5
39	BN	137/140 (98%)	89 (65%)	28 (20%)	20 (15%)	0	1
39	DN	137/140 (98%)	92 (67%)	25 (18%)	20 (15%)	0	1
40	BO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	11	46
40	DO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	7	34
41	BP	144/150 (96%)	71 (49%)	33 (23%)	40 (28%)	0	0
41	DP	144/150 (96%)	70 (49%)	33 (23%)	41 (28%)	0	0
42	BQ	134/141 (95%)	97 (72%)	21 (16%)	16 (12%)	0	2
42	DQ	134/141 (95%)	92 (69%)	25 (19%)	17 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BR	115/118 (98%)	86 (75%)	22 (19%)	7 (6%)	2	11
43	DR	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	2	11
44	BS	97/112 (87%)	45 (46%)	22 (23%)	30 (31%)	0	0
44	DS	97/112 (87%)	44 (45%)	22 (23%)	31 (32%)	0	0
45	BT	130/146 (89%)	91 (70%)	21 (16%)	18 (14%)	0	1
45	DT	130/146 (89%)	91 (70%)	21 (16%)	18 (14%)	0	1
46	BU	115/118 (98%)	89 (77%)	18 (16%)	8 (7%)	1	7
46	DU	115/118 (98%)	86 (75%)	21 (18%)	8 (7%)	1	7
47	BV	97/101 (96%)	54 (56%)	18 (19%)	25 (26%)	0	0
47	DV	97/101 (96%)	53 (55%)	19 (20%)	25 (26%)	0	0
48	BW	111/113 (98%)	85 (77%)	17 (15%)	9 (8%)	1	5
48	DW	111/113 (98%)	83 (75%)	19 (17%)	9 (8%)	1	5
49	BX	91/96 (95%)	47 (52%)	23 (25%)	21 (23%)	0	0
49	DX	91/96 (95%)	48 (53%)	23 (25%)	20 (22%)	0	0
50	BY	99/110 (90%)	47 (48%)	22 (22%)	30 (30%)	0	0
50	DY	99/110 (90%)	44 (44%)	25 (25%)	30 (30%)	0	0
51	BZ	175/206 (85%)	123 (70%)	32 (18%)	20 (11%)	0	2
51	DZ	175/206 (85%)	121 (69%)	36 (21%)	18 (10%)	1	3
All	All	11148/12060 (92%)	7786 (70%)	2170 (20%)	1192 (11%)	0	2

5 of 1192 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	18	GLY
2	AB	20	GLU
2	AB	106	LYS
2	AB	165	VAL
2	AB	195	ASP

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	170 (84%)	32 (16%)	3	15
2	CB	202/220 (92%)	168 (83%)	34 (17%)	2	13
3	AC	160/188 (85%)	153 (96%)	7 (4%)	35	74
3	CC	160/188 (85%)	153 (96%)	7 (4%)	35	74
4	AD	180/181 (99%)	156 (87%)	24 (13%)	5	21
4	CD	180/181 (99%)	156 (87%)	24 (13%)	5	21
5	AE	115/123 (94%)	95 (83%)	20 (17%)	2	12
5	CE	115/123 (94%)	95 (83%)	20 (17%)	2	12
6	AF	90/90 (100%)	79 (88%)	11 (12%)	6	25
6	CF	90/90 (100%)	78 (87%)	12 (13%)	5	21
7	AG	126/127 (99%)	122 (97%)	4 (3%)	46	82
7	CG	126/127 (99%)	122 (97%)	4 (3%)	46	82
8	AH	119/119 (100%)	106 (89%)	13 (11%)	8	30
8	CH	119/119 (100%)	106 (89%)	13 (11%)	8	30
9	AI	98/99 (99%)	90 (92%)	8 (8%)	14	46
9	CI	98/99 (99%)	90 (92%)	8 (8%)	14	46
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	7	28
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	7	28
11	AK	90/99 (91%)	82 (91%)	8 (9%)	12	42
11	CK	90/99 (91%)	83 (92%)	7 (8%)	16	49
12	AL	104/111 (94%)	92 (88%)	12 (12%)	7	28
12	CL	104/111 (94%)	91 (88%)	13 (12%)	6	24
13	AM	93/101 (92%)	87 (94%)	6 (6%)	21	58
13	CM	93/101 (92%)	87 (94%)	6 (6%)	21	58
14	AN	49/50 (98%)	45 (92%)	4 (8%)	14	46
14	CN	49/50 (98%)	45 (92%)	4 (8%)	14	46
15	AO	79/80 (99%)	68 (86%)	11 (14%)	4	19
15	CO	79/80 (99%)	68 (86%)	11 (14%)	4	19
16	AP	72/74 (97%)	58 (81%)	14 (19%)	2	9
16	CP	72/74 (97%)	59 (82%)	13 (18%)	2	11
17	AQ	94/97 (97%)	82 (87%)	12 (13%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	82 (87%)	12 (13%)	5	23
18	AR	61/77 (79%)	55 (90%)	6 (10%)	10	36
18	CR	61/77 (79%)	55 (90%)	6 (10%)	10	36
19	AS	69/80 (86%)	62 (90%)	7 (10%)	9	34
19	CS	69/80 (86%)	62 (90%)	7 (10%)	9	34
20	AT	76/82 (93%)	68 (90%)	8 (10%)	8	32
20	CT	76/82 (93%)	68 (90%)	8 (10%)	8	32
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
22	B0	61/67 (91%)	53 (87%)	8 (13%)	5	22
22	D0	61/67 (91%)	53 (87%)	8 (13%)	5	22
23	B1	73/83 (88%)	53 (73%)	20 (27%)	0	2
23	D1	73/83 (88%)	55 (75%)	18 (25%)	1	3
24	B2	46/67 (69%)	33 (72%)	13 (28%)	0	2
24	D2	46/67 (69%)	33 (72%)	13 (28%)	0	2
25	B3	51/52 (98%)	45 (88%)	6 (12%)	6	26
25	D3	51/52 (98%)	44 (86%)	7 (14%)	4	20
27	B5	51/52 (98%)	40 (78%)	11 (22%)	1	6
27	D5	51/52 (98%)	38 (74%)	13 (26%)	1	3
28	B6	43/52 (83%)	27 (63%)	16 (37%)	0	1
28	D6	43/52 (83%)	28 (65%)	15 (35%)	0	1
29	B7	41/42 (98%)	33 (80%)	8 (20%)	2	9
29	D7	41/42 (98%)	32 (78%)	9 (22%)	1	6
30	B8	53/55 (96%)	40 (76%)	13 (24%)	1	4
30	D8	53/55 (96%)	41 (77%)	12 (23%)	1	5
33	BD	213/218 (98%)	166 (78%)	47 (22%)	1	5
33	DD	213/218 (98%)	165 (78%)	48 (22%)	1	5
34	BE	165/166 (99%)	122 (74%)	43 (26%)	0	3
34	DE	165/166 (99%)	122 (74%)	43 (26%)	0	3
35	BF	165/166 (99%)	134 (81%)	31 (19%)	2	10
35	DF	165/166 (99%)	137 (83%)	28 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BG	155/156 (99%)	134 (86%)	21 (14%)	5	20
36	DG	155/156 (99%)	134 (86%)	21 (14%)	5	20
37	BH	132/148 (89%)	105 (80%)	27 (20%)	1	7
37	DH	132/148 (89%)	105 (80%)	27 (20%)	1	7
38	BI	122/124 (98%)	104 (85%)	18 (15%)	4	17
38	DI	122/124 (98%)	104 (85%)	18 (15%)	4	17
39	BN	117/119 (98%)	79 (68%)	38 (32%)	0	1
39	DN	117/119 (98%)	79 (68%)	38 (32%)	0	1
40	BO	100/100 (100%)	81 (81%)	19 (19%)	2	10
40	DO	100/100 (100%)	81 (81%)	19 (19%)	2	10
41	BP	112/116 (97%)	72 (64%)	40 (36%)	0	1
41	DP	112/116 (97%)	72 (64%)	40 (36%)	0	1
42	BQ	106/111 (96%)	86 (81%)	20 (19%)	2	10
42	DQ	106/111 (96%)	85 (80%)	21 (20%)	1	8
43	BR	100/101 (99%)	81 (81%)	19 (19%)	2	10
43	DR	100/101 (99%)	80 (80%)	20 (20%)	1	8
44	BS	77/88 (88%)	53 (69%)	24 (31%)	0	2
44	DS	77/88 (88%)	54 (70%)	23 (30%)	0	2
45	BT	116/127 (91%)	81 (70%)	35 (30%)	0	2
45	DT	116/127 (91%)	81 (70%)	35 (30%)	0	2
46	BU	92/94 (98%)	79 (86%)	13 (14%)	4	19
46	DU	92/94 (98%)	79 (86%)	13 (14%)	4	19
47	BV	82/82 (100%)	53 (65%)	29 (35%)	0	1
47	DV	82/82 (100%)	53 (65%)	29 (35%)	0	1
48	BW	91/92 (99%)	70 (77%)	21 (23%)	1	5
48	DW	91/92 (99%)	71 (78%)	20 (22%)	1	6
49	BX	74/78 (95%)	54 (73%)	20 (27%)	0	3
49	DX	74/78 (95%)	53 (72%)	21 (28%)	0	2
50	BY	84/91 (92%)	60 (71%)	24 (29%)	0	2
50	DY	84/91 (92%)	61 (73%)	23 (27%)	0	2
51	BZ	155/179 (87%)	130 (84%)	25 (16%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	DZ	155/179 (87%)	130 (84%)	25 (16%)	3 14
All	All	9322/9876 (94%)	7670 (82%)	1652 (18%)	2 11

5 of 1652 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BW	60	ASN
7	CG	36	LYS
46	DU	66	ASN
49	BX	49	VAL
2	CB	90	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 277 such sidechains are listed below:

Mol	Chain	Res	Type
48	BW	40	ASN
6	CF	18	GLN
45	DT	90	GLN
48	BW	62	HIS
2	CB	204	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	280 (18%)	31 (2%)
1	CA	1503/1522 (98%)	283 (18%)	31 (2%)
31	BA	2723/2787 (97%)	712 (26%)	70 (2%)
31	DA	2723/2787 (97%)	706 (25%)	69 (2%)
32	BB	118/122 (96%)	34 (28%)	1 (0%)
32	DB	118/122 (96%)	35 (29%)	1 (0%)
All	All	8688/8862 (98%)	2050 (23%)	203 (2%)

5 of 2050 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	41	G

5 of 203 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	2439	A
1	CA	429	U
31	DA	1934	C
31	BA	2689	U
1	CA	60	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 853 ligands modelled in this entry, 851 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	CLM	BA	3370	54	18,20,20	0.75	0	22,27,27	0.86	0
55	CLM	DA	3334	54	18,20,20	0.75	0	22,27,27	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	CLM	BA	3370	54	-	0/22/22/22	0/1/1/1
55	CLM	DA	3334	54	-	0/22/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	3
13	AM	3
47	DV	1
36	DG	1
36	BG	1
9	AI	1
9	CI	1
47	BV	1
28	D6	1
28	B6	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CM	69:GLU	C	70:LEU	N	5.35
1	AM	69:GLU	C	70:LEU	N	5.34
1	BG	112:PRO	C	113:ARG	N	4.53
1	DG	112:PRO	C	113:ARG	N	4.53
1	CM	112:GLY	C	113:PRO	N	4.49

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	1.16	299 (19%) 1 1	42, 106, 199, 201	0
1	CA	1504/1522 (98%)	0.98	256 (17%) 2 1	46, 105, 198, 201	0
2	AB	235/256 (91%)	0.75	38 (16%) 3 1	83, 146, 188, 195	0
2	CB	235/256 (91%)	0.94	52 (22%) 1 1	84, 149, 187, 196	0
3	AC	207/239 (86%)	1.18	53 (25%) 1 1	97, 158, 187, 194	0
3	CC	207/239 (86%)	1.23	54 (26%) 1 1	98, 160, 187, 194	0
4	AD	208/209 (99%)	0.38	9 (4%) 39 16	72, 112, 165, 186	0
4	CD	208/209 (99%)	0.22	4 (1%) 70 41	70, 111, 164, 185	0
5	AE	151/162 (93%)	0.46	11 (7%) 18 6	59, 97, 151, 194	0
5	CE	151/162 (93%)	0.48	8 (5%) 30 12	64, 98, 153, 194	0
6	AF	101/101 (100%)	0.24	6 (5%) 26 10	66, 111, 160, 183	0
6	CF	101/101 (100%)	0.20	4 (3%) 42 17	67, 113, 160, 188	0
7	AG	155/156 (99%)	1.84	59 (38%) 0 0	124, 172, 192, 197	0
7	CG	155/156 (99%)	2.00	59 (38%) 0 0	125, 172, 192, 198	0
8	AH	138/138 (100%)	0.09	4 (2%) 55 26	67, 102, 147, 162	0
8	CH	138/138 (100%)	0.16	2 (1%) 78 51	66, 102, 147, 163	0
9	AI	127/128 (99%)	2.54	65 (51%) 0 0	125, 179, 196, 199	0
9	CI	127/128 (99%)	2.46	60 (47%) 0 0	126, 180, 197, 199	0
10	AJ	99/105 (94%)	3.12	57 (57%) 0 0	122, 175, 196, 198	0
10	CJ	99/105 (94%)	2.88	58 (58%) 0 0	121, 176, 197, 199	0
11	AK	119/129 (92%)	0.71	18 (15%) 3 1	63, 105, 164, 188	0
11	CK	119/129 (92%)	0.83	16 (13%) 4 1	65, 104, 168, 191	0
12	AL	125/135 (92%)	0.36	5 (4%) 42 17	57, 89, 154, 198	0
12	CL	125/135 (92%)	0.60	13 (10%) 8 3	55, 89, 158, 198	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	115/126 (91%)	2.76	66 (57%) 0 0	136, 190, 198, 200	0
13	CM	115/126 (91%)	2.65	63 (54%) 0 0	136, 188, 197, 199	0
14	AN	60/61 (98%)	1.74	22 (36%) 0 0	113, 167, 193, 196	0
14	CN	60/61 (98%)	1.36	15 (25%) 1 1	112, 168, 191, 196	0
15	AO	88/89 (98%)	0.14	4 (4%) 37 15	59, 91, 149, 155	0
15	CO	88/89 (98%)	0.15	2 (2%) 64 33	63, 92, 150, 157	0
16	AP	84/88 (95%)	0.99	16 (19%) 2 1	77, 101, 161, 188	0
16	CP	84/88 (95%)	0.53	5 (5%) 25 9	78, 100, 154, 186	0
17	AQ	100/105 (95%)	0.20	4 (4%) 42 17	62, 93, 138, 158	0
17	CQ	100/105 (95%)	0.17	3 (3%) 54 25	59, 92, 140, 157	0
18	AR	70/88 (79%)	0.39	3 (4%) 39 16	73, 98, 167, 197	0
18	CR	70/88 (79%)	0.98	7 (10%) 9 4	74, 100, 167, 196	0
19	AS	79/93 (84%)	4.31	64 (81%) 0 0	142, 191, 198, 199	0
19	CS	79/93 (84%)	3.65	60 (75%) 0 0	142, 190, 198, 199	0
20	AT	99/106 (93%)	0.21	4 (4%) 42 17	73, 110, 157, 186	0
20	CT	99/106 (93%)	0.42	10 (10%) 9 3	74, 108, 156, 189	0
21	AU	25/27 (92%)	4.56	19 (76%) 0 0	138, 175, 193, 196	0
21	CU	25/27 (92%)	3.50	18 (72%) 0 0	135, 172, 193, 195	0
22	B0	85/85 (100%)	0.73	8 (9%) 11 4	34, 59, 182, 197	0
22	D0	85/85 (100%)	0.66	13 (15%) 3 1	40, 64, 178, 197	0
23	B1	89/98 (90%)	0.39	3 (3%) 49 21	37, 64, 141, 187	0
23	D1	89/98 (90%)	0.20	5 (5%) 28 11	40, 66, 142, 191	0
24	B2	51/72 (70%)	0.92	8 (15%) 3 1	49, 87, 184, 193	0
24	D2	51/72 (70%)	0.55	8 (15%) 3 1	50, 91, 183, 195	0
25	B3	60/60 (100%)	0.08	1 (1%) 73 45	36, 56, 132, 180	0
25	D3	60/60 (100%)	0.43	5 (8%) 14 5	42, 61, 138, 178	0
26	B4	32/71 (45%)	0.02	1 (3%) 52 24	109, 156, 186, 191	0
26	D4	32/71 (45%)	0.24	1 (3%) 52 24	112, 161, 188, 195	0
27	B5	59/60 (98%)	0.71	6 (10%) 9 3	25, 47, 180, 195	0
27	D5	59/60 (98%)	0.38	6 (10%) 9 3	28, 50, 184, 195	0
28	B6	45/54 (83%)	0.82	5 (11%) 7 3	36, 70, 133, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	0.93	11 (24%) 1 1	42, 74, 138, 184	0
29	B7	49/49 (100%)	0.32	1 (2%) 68 39	26, 33, 117, 170	0
29	D7	49/49 (100%)	0.36	1 (2%) 68 39	27, 37, 118, 170	0
30	B8	64/65 (98%)	0.48	7 (10%) 7 3	34, 57, 138, 181	0
30	D8	64/65 (98%)	0.21	4 (6%) 23 9	38, 59, 139, 183	0
31	BA	2725/2787 (97%)	0.43	78 (2%) 55 26	26, 46, 145, 201	0
31	DA	2725/2787 (97%)	0.24	106 (3%) 43 18	27, 51, 149, 201	0
32	BB	119/122 (97%)	0.59	4 (3%) 49 21	39, 91, 140, 185	0
32	DB	119/122 (97%)	0.83	16 (13%) 4 1	48, 95, 154, 190	0
33	BD	272/276 (98%)	-0.08	3 (1%) 82 58	27, 47, 100, 177	0
33	DD	272/276 (98%)	-0.13	3 (1%) 82 58	29, 50, 104, 181	0
34	BE	205/206 (99%)	0.18	7 (3%) 49 21	25, 52, 145, 189	0
34	DE	205/206 (99%)	-0.01	5 (2%) 62 32	29, 56, 142, 189	0
35	BF	208/210 (99%)	0.48	15 (7%) 18 7	24, 58, 180, 197	0
35	DF	208/210 (99%)	0.41	16 (7%) 16 6	27, 63, 178, 197	0
36	BG	181/182 (99%)	1.22	41 (22%) 1 1	87, 145, 189, 199	0
36	DG	181/182 (99%)	2.00	77 (42%) 0 0	91, 153, 193, 199	0
37	BH	160/180 (88%)	0.41	8 (5%) 32 13	62, 102, 150, 193	0
37	DH	160/180 (88%)	1.13	40 (25%) 1 1	70, 110, 157, 195	0
38	BI	146/148 (98%)	0.54	14 (9%) 10 4	52, 143, 185, 195	0
38	DI	146/148 (98%)	3.36	68 (46%) 0 0	56, 156, 188, 198	0
39	BN	139/140 (99%)	0.22	5 (3%) 46 20	32, 60, 140, 187	0
39	DN	139/140 (99%)	-0.05	6 (4%) 39 16	38, 65, 142, 188	0
40	BO	122/122 (100%)	-0.18	0 100 100	32, 52, 105, 141	0
40	DO	122/122 (100%)	-0.43	0 100 100	35, 55, 111, 146	0
41	BP	146/150 (97%)	0.82	10 (6%) 20 7	22, 79, 148, 199	0
41	DP	146/150 (97%)	0.49	9 (6%) 24 9	27, 81, 150, 198	0
42	BQ	136/141 (96%)	0.55	9 (6%) 22 7	39, 64, 150, 189	0
42	DQ	136/141 (96%)	0.41	8 (5%) 26 10	43, 69, 149, 190	0
43	BR	117/118 (99%)	0.01	1 (0%) 85 64	28, 44, 113, 143	0
43	DR	117/118 (99%)	-0.15	2 (1%) 73 45	30, 49, 115, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	0.47	6 (6%) 25 9	53, 98, 141, 178	0
44	DS	99/112 (88%)	1.17	26 (26%) 1 1	63, 103, 146, 180	0
45	BT	132/146 (90%)	0.34	8 (6%) 25 9	42, 73, 157, 191	0
45	DT	132/146 (90%)	0.17	8 (6%) 25 9	46, 77, 159, 194	0
46	BU	117/118 (99%)	0.27	2 (1%) 73 45	23, 50, 114, 190	0
46	DU	117/118 (99%)	0.15	2 (1%) 73 45	32, 56, 119, 193	0
47	BV	101/101 (100%)	0.84	8 (7%) 15 5	32, 91, 171, 194	0
47	DV	101/101 (100%)	0.80	15 (14%) 3 1	35, 97, 169, 195	0
48	BW	113/113 (100%)	-0.18	1 (0%) 85 64	28, 40, 101, 168	0
48	DW	113/113 (100%)	-0.31	2 (1%) 71 43	31, 43, 106, 175	0
49	BX	93/96 (96%)	0.37	4 (4%) 39 16	36, 65, 142, 184	0
49	DX	93/96 (96%)	0.04	2 (2%) 65 35	42, 69, 147, 185	0
50	BY	101/110 (91%)	1.17	19 (18%) 2 1	39, 91, 191, 199	0
50	DY	101/110 (91%)	0.98	21 (20%) 1 1	40, 96, 191, 199	0
51	BZ	177/206 (85%)	0.24	4 (2%) 64 33	56, 100, 150, 175	0
51	DZ	177/206 (85%)	0.52	13 (7%) 18 6	63, 103, 153, 179	0
All	All	20064/20922 (95%)	0.68	2381 (11%) 6 2	22, 84, 190, 201	0

The worst 5 of 2381 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BF	208	GLY	24.4
42	BQ	140	ALA	19.2
38	DI	100	ALA	19.2
42	DQ	140	ALA	17.4
1	AA	88	A	17.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
52	MG	BA	3109	1/1	0.91	0.82	121.71	40,40,40,40	0
52	MG	DA	3106	1/1	0.79	0.90	86.86	53,53,53,53	0
52	MG	BA	3319	1/1	0.88	0.48	57.47	46,46,46,46	0
52	MG	DA	3312	1/1	0.83	0.59	52.48	45,45,45,45	0
52	MG	BA	3355	1/1	0.77	0.85	47.71	51,51,51,51	0
52	MG	BA	3230	1/1	0.92	0.76	47.57	37,37,37,37	0
52	MG	DA	3099	1/1	0.95	0.63	45.60	34,34,34,34	0
52	MG	DA	3094	1/1	0.92	0.69	45.25	38,38,38,38	0
52	MG	DA	3055	1/1	0.86	0.52	40.04	34,34,34,34	0
52	MG	CA	1625	1/1	0.81	0.56	37.14	59,59,59,59	0
52	MG	DA	3092	1/1	0.97	0.70	36.69	47,47,47,47	0
52	MG	BA	3047	1/1	0.97	0.56	35.83	22,22,22,22	0
52	MG	BA	3039	1/1	0.93	0.72	35.38	37,37,37,37	0
52	MG	DA	3040	1/1	0.93	0.95	33.80	58,58,58,58	0
52	MG	BA	3080	1/1	0.93	0.67	31.67	14,14,14,14	0
52	MG	BA	3072	1/1	0.66	0.56	31.44	41,41,41,41	0
52	MG	BA	3124	1/1	0.88	0.43	28.86	39,39,39,39	0
52	MG	BA	3171	1/1	0.73	0.77	28.33	35,35,35,35	0
52	MG	BA	3095	1/1	0.96	0.44	28.31	38,38,38,38	0
52	MG	DA	3089	1/1	0.92	0.61	28.14	31,31,31,31	0
52	MG	BA	3088	1/1	0.69	0.40	28.13	33,33,33,33	0
52	MG	BA	3285	1/1	0.95	0.41	26.56	35,35,35,35	0
52	MG	BA	3041	1/1	0.92	0.43	26.54	24,24,24,24	0
52	MG	BA	3202	1/1	0.91	0.61	26.36	35,35,35,35	0
52	MG	CA	1627	1/1	0.80	0.75	26.28	81,81,81,81	0
52	MG	BA	3127	1/1	0.81	0.50	25.87	44,44,44,44	0
52	MG	BA	3216	1/1	0.97	0.53	25.75	35,35,35,35	0
52	MG	BA	3156	1/1	0.97	0.49	25.37	12,12,12,12	0
52	MG	DA	3080	1/1	0.94	0.82	25.16	30,30,30,30	0
52	MG	BA	3038	1/1	0.94	0.48	23.76	17,17,17,17	0
52	MG	DA	3135	1/1	0.88	0.68	23.50	39,39,39,39	0
52	MG	BA	3012	1/1	0.97	0.47	23.41	38,38,38,38	0
52	MG	DA	3039	1/1	0.97	0.53	23.36	48,48,48,48	0
52	MG	DA	3090	1/1	0.82	0.34	23.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3006	1/1	0.88	0.57	21.56	38,38,38,38	0
52	MG	CA	1648	1/1	0.90	0.90	21.10	53,53,53,53	0
52	MG	DA	3001	1/1	0.89	0.43	21.05	45,45,45,45	0
52	MG	DA	3052	1/1	0.91	0.51	20.80	36,36,36,36	0
52	MG	DA	3216	1/1	0.86	0.56	20.73	45,45,45,45	0
52	MG	BA	3049	1/1	0.87	0.56	20.61	23,23,23,23	0
52	MG	BA	3343	1/1	0.96	0.55	20.49	40,40,40,40	0
52	MG	AA	1631	1/1	0.90	0.62	20.45	52,52,52,52	0
52	MG	BA	3006	1/1	0.96	0.62	20.40	33,33,33,33	0
52	MG	DA	3049	1/1	0.92	0.55	20.14	42,42,42,42	0
52	MG	DA	3093	1/1	0.98	0.48	20.10	44,44,44,44	0
52	MG	BA	3144	1/1	0.94	0.60	19.85	29,29,29,29	0
52	MG	DA	3122	1/1	0.95	0.67	19.69	40,40,40,40	0
52	MG	DA	3166	1/1	0.74	0.62	19.64	64,64,64,64	0
52	MG	BA	3037	1/1	0.98	0.50	19.57	1,1,1,1	0
52	MG	AA	1623	1/1	0.98	0.46	19.56	31,31,31,31	0
52	MG	BA	3052	1/1	0.95	0.53	19.16	23,23,23,23	0
52	MG	BA	3125	1/1	0.97	0.53	18.85	18,18,18,18	0
52	MG	DA	3074	1/1	0.69	0.59	18.83	54,54,54,54	0
52	MG	DA	3098	1/1	0.94	0.47	18.75	34,34,34,34	0
52	MG	BA	3092	1/1	0.98	0.50	18.75	19,19,19,19	0
52	MG	BA	3023	1/1	0.95	0.39	18.60	13,13,13,13	0
52	MG	BA	3182	1/1	0.95	0.49	18.48	37,37,37,37	0
52	MG	DA	3188	1/1	0.90	0.62	18.26	43,43,43,43	0
52	MG	AA	1617	1/1	0.95	0.52	18.22	57,57,57,57	0
52	MG	DA	3016	1/1	0.88	0.59	17.97	29,29,29,29	0
52	MG	BA	3117	1/1	0.91	0.31	17.92	50,50,50,50	0
52	MG	DA	3008	1/1	0.90	0.40	17.85	33,33,33,33	0
52	MG	BA	3325	1/1	0.86	0.63	17.85	53,53,53,53	0
52	MG	DA	3214	1/1	0.85	0.42	17.72	39,39,39,39	0
52	MG	BA	3051	1/1	0.98	0.50	17.67	19,19,19,19	0
52	MG	BA	3009	1/1	0.82	0.55	17.59	38,38,38,38	0
52	MG	DA	3047	1/1	0.85	0.55	17.58	33,33,33,33	0
52	MG	BA	3094	1/1	0.82	0.57	17.49	30,30,30,30	0
52	MG	DA	3141	1/1	0.96	0.54	17.32	35,35,35,35	0
52	MG	DA	3150	1/1	0.91	0.51	17.03	32,32,32,32	0
52	MG	BA	3175	1/1	0.65	0.64	16.97	43,43,43,43	0
52	MG	BA	3040	1/1	0.94	0.64	16.80	37,37,37,37	0
52	MG	BA	3074	1/1	0.79	0.50	16.69	48,48,48,48	0
52	MG	DA	3178	1/1	0.97	0.41	16.60	30,30,30,30	0
52	MG	BA	3360	1/1	0.82	0.51	16.29	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3174	1/1	0.97	0.48	15.88	29,29,29,29	0
52	MG	BA	3167	1/1	0.66	0.54	15.82	51,51,51,51	0
52	MG	BA	3213	1/1	0.98	0.47	15.81	17,17,17,17	0
52	MG	DA	3234	1/1	0.84	0.71	15.67	60,60,60,60	0
52	MG	BA	3032	1/1	0.98	0.34	15.54	15,15,15,15	0
52	MG	AA	1607	1/1	0.94	0.72	15.46	47,47,47,47	0
52	MG	BA	3061	1/1	0.92	0.38	15.23	35,35,35,35	0
52	MG	DA	3046	1/1	0.98	0.51	15.21	34,34,34,34	0
52	MG	AA	1629	1/1	0.83	0.35	15.04	49,49,49,49	0
52	MG	DA	3010	1/1	0.96	0.36	15.02	35,35,35,35	0
52	MG	BA	3008	1/1	0.95	0.45	14.71	27,27,27,27	0
52	MG	DA	3061	1/1	0.89	0.42	14.67	34,34,34,34	0
52	MG	BA	3001	1/1	0.93	0.37	14.63	36,36,36,36	0
52	MG	DA	3320	1/1	0.96	0.41	14.57	31,31,31,31	0
52	MG	BA	3150	1/1	0.69	0.43	14.56	40,40,40,40	0
52	MG	DA	3222	1/1	0.81	0.52	14.54	41,41,41,41	0
52	MG	BA	3323	1/1	0.82	0.63	14.41	42,42,42,42	0
52	MG	BA	3162	1/1	0.92	0.30	14.32	45,45,45,45	0
52	MG	DA	3171	1/1	0.99	0.35	14.15	26,26,26,26	0
52	MG	BA	3028	1/1	0.98	0.48	14.12	24,24,24,24	0
52	MG	DA	3260	1/1	0.89	0.48	14.04	34,34,34,34	0
52	MG	DA	3002	1/1	0.95	0.48	13.85	22,22,22,22	0
52	MG	BA	3090	1/1	0.92	0.42	13.76	14,14,14,14	0
52	MG	AA	1652	1/1	0.88	0.73	13.73	44,44,44,44	0
55	CLM	BA	3370	20/20	0.90	0.46	13.67	90,90,90,90	0
52	MG	BA	3096	1/1	0.97	0.43	13.58	16,16,16,16	0
52	MG	DA	3023	1/1	0.95	0.48	13.48	27,27,27,27	0
52	MG	BA	3066	1/1	0.96	0.44	13.36	34,34,34,34	0
52	MG	DA	3091	1/1	0.98	0.43	13.21	11,11,11,11	0
52	MG	BA	3298	1/1	0.92	0.36	12.96	41,41,41,41	0
52	MG	DA	3038	1/1	0.95	0.57	12.94	25,25,25,25	0
52	MG	DA	3289	1/1	0.78	0.45	12.80	53,53,53,53	0
52	MG	BA	3002	1/1	0.96	0.54	12.76	23,23,23,23	0
52	MG	BA	3313	1/1	0.72	0.66	12.60	56,56,56,56	0
52	MG	BA	3010	1/1	0.97	0.41	12.28	37,37,37,37	0
55	CLM	DA	3334	20/20	0.82	0.50	12.23	90,90,90,90	0
52	MG	DA	3017	1/1	0.96	0.45	12.04	37,37,37,37	0
52	MG	BA	3063	1/1	0.92	0.54	11.95	45,45,45,45	0
52	MG	DA	3168	1/1	0.94	0.55	11.90	32,32,32,32	0
52	MG	DA	3145	1/1	0.93	0.55	11.71	40,40,40,40	0
52	MG	DA	3283	1/1	0.78	0.65	11.65	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3071	1/1	0.96	0.54	11.63	31,31,31,31	0
52	MG	DA	3044	1/1	0.97	0.36	11.36	35,35,35,35	0
52	MG	BA	3142	1/1	0.97	0.41	10.79	26,26,26,26	0
52	MG	BA	3347	1/1	0.86	0.43	10.61	47,47,47,47	0
52	MG	BA	3326	1/1	0.82	0.43	10.60	40,40,40,40	0
52	MG	DA	3056	1/1	0.94	0.30	10.56	24,24,24,24	0
52	MG	BA	3294	1/1	0.97	0.56	10.32	40,40,40,40	0
52	MG	BA	3123	1/1	0.97	0.38	10.32	40,40,40,40	0
52	MG	DA	3109	1/1	0.91	0.34	10.16	48,48,48,48	0
52	MG	BA	3060	1/1	0.95	0.36	10.13	31,31,31,31	0
52	MG	DA	3041	1/1	0.96	0.33	9.94	29,29,29,29	0
52	MG	BA	3242	1/1	0.97	0.40	9.91	33,33,33,33	0
52	MG	AA	1625	1/1	0.95	0.58	9.86	40,40,40,40	0
52	MG	DA	3009	1/1	0.82	0.43	9.74	47,47,47,47	0
52	MG	DA	3020	1/1	0.98	0.60	9.59	33,33,33,33	0
52	MG	BA	3280	1/1	0.95	0.39	9.53	41,41,41,41	0
52	MG	BA	3100	1/1	0.98	0.39	9.45	23,23,23,23	0
52	MG	BA	3277	1/1	0.89	0.34	9.45	10,10,10,10	0
52	MG	BA	3016	1/1	0.94	0.34	9.36	11,11,11,11	0
52	MG	DA	3290	1/1	0.73	0.55	9.35	55,55,55,55	0
52	MG	CA	1637	1/1	0.86	0.35	9.34	65,65,65,65	0
52	MG	DA	3032	1/1	0.91	0.37	9.20	31,31,31,31	0
52	MG	BA	3075	1/1	0.84	0.47	9.07	38,38,38,38	0
52	MG	BA	3021	1/1	0.95	0.44	9.05	19,19,19,19	0
52	MG	DA	3075	1/1	0.80	0.45	8.96	38,38,38,38	0
52	MG	DA	3183	1/1	0.93	0.45	8.82	35,35,35,35	0
52	MG	BA	3191	1/1	0.97	0.42	8.73	19,19,19,19	0
52	MG	BA	3101	1/1	0.94	0.35	8.71	24,24,24,24	0
52	MG	CA	1610	1/1	0.83	0.27	8.63	66,66,66,66	0
52	MG	DA	3012	1/1	0.98	0.48	8.58	26,26,26,26	0
52	MG	DA	3146	1/1	0.95	0.34	8.55	37,37,37,37	0
52	MG	BA	3250	1/1	0.88	0.70	8.49	48,48,48,48	0
52	MG	BA	3111	1/1	0.87	0.55	8.37	41,41,41,41	0
52	MG	BA	3196	1/1	0.89	0.40	8.26	26,26,26,26	0
52	MG	DA	3034	1/1	0.98	0.37	8.23	38,38,38,38	0
52	MG	AA	1642	1/1	0.93	0.34	8.21	46,46,46,46	0
52	MG	BA	3148	1/1	0.88	0.48	8.10	23,23,23,23	0
52	MG	BA	3179	1/1	0.97	0.46	8.04	25,25,25,25	0
52	MG	CA	1613	1/1	0.89	0.35	8.02	58,58,58,58	0
54	K	DA	3333	1/1	0.84	0.30	8.00	62,62,62,62	0
52	MG	CA	1609	1/1	0.94	0.34	8.00	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3097	1/1	0.96	0.37	7.96	30,30,30,30	0
52	MG	BA	3165	1/1	0.95	0.30	7.88	26,26,26,26	0
52	MG	BA	3119	1/1	0.94	0.40	7.45	34,34,34,34	0
52	MG	CA	1621	1/1	0.90	0.43	7.43	50,50,50,50	0
52	MG	BA	3055	1/1	0.98	0.41	7.38	19,19,19,19	0
52	MG	DA	3156	1/1	0.86	0.35	7.31	51,51,51,51	0
52	MG	DA	3229	1/1	0.96	0.55	7.18	36,36,36,36	0
52	MG	BA	3350	1/1	0.83	0.38	7.13	54,54,54,54	0
52	MG	DA	3267	1/1	0.80	0.45	7.12	46,46,46,46	0
52	MG	DA	3108	1/1	0.96	0.47	6.81	39,39,39,39	0
52	MG	AA	1624	1/1	0.83	0.49	6.74	59,59,59,59	0
52	MG	DA	3058	1/1	0.91	0.34	6.56	42,42,42,42	0
52	MG	BA	3046	1/1	0.91	0.37	6.55	24,24,24,24	0
52	MG	CA	1647	1/1	0.97	0.28	6.53	49,49,49,49	0
52	MG	BA	3058	1/1	0.96	0.29	6.30	30,30,30,30	0
52	MG	BA	3224	1/1	0.94	0.31	6.24	27,27,27,27	0
52	MG	CA	1620	1/1	0.93	0.34	6.13	45,45,45,45	0
52	MG	DA	3053	1/1	0.98	0.46	6.11	21,21,21,21	0
52	MG	DA	3165	1/1	0.84	0.28	6.07	38,38,38,38	0
52	MG	DA	3028	1/1	0.96	0.33	6.05	34,34,34,34	0
52	MG	BA	3070	1/1	0.95	0.35	5.90	24,24,24,24	0
52	MG	DA	3124	1/1	0.56	0.29	5.88	49,49,49,49	0
52	MG	BA	3112	1/1	0.88	0.25	5.79	14,14,14,14	0
52	MG	DA	3223	1/1	0.89	0.62	5.76	37,37,37,37	0
52	MG	DA	3138	1/1	0.96	0.37	5.54	31,31,31,31	0
52	MG	DA	3303	1/1	0.72	0.28	5.53	43,43,43,43	0
52	MG	DU	201	1/1	0.79	0.47	5.47	60,60,60,60	0
52	MG	DA	3030	1/1	0.92	0.26	5.46	37,37,37,37	0
52	MG	DA	3057	1/1	0.95	0.32	5.33	32,32,32,32	0
52	MG	BF	301	1/1	0.66	0.40	5.33	43,43,43,43	0
52	MG	DA	3115	1/1	0.87	0.27	5.30	47,47,47,47	0
52	MG	AA	1608	1/1	0.93	0.45	5.28	70,70,70,70	0
52	MG	BA	3308	1/1	0.93	0.37	5.18	45,45,45,45	0
52	MG	BA	3261	1/1	0.97	0.26	5.11	27,27,27,27	0
52	MG	BQ	202	1/1	0.87	0.35	5.08	37,37,37,37	0
52	MG	BA	3316	1/1	0.95	0.35	5.07	41,41,41,41	0
52	MG	DA	3070	1/1	0.92	0.32	4.95	35,35,35,35	0
52	MG	DA	3060	1/1	0.95	0.31	4.94	46,46,46,46	0
52	MG	CA	1612	1/1	0.92	0.34	4.94	48,48,48,48	0
52	MG	BA	3071	1/1	0.94	0.44	4.87	22,22,22,22	0
52	MG	DA	3120	1/1	0.93	0.29	4.84	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3237	1/1	0.80	0.50	4.84	42,42,42,42	0
52	MG	AA	1651	1/1	0.85	0.32	4.72	45,45,45,45	0
52	MG	BA	3283	1/1	0.91	0.36	4.66	50,50,50,50	0
52	MG	DA	3245	1/1	0.81	0.19	4.62	65,65,65,65	0
52	MG	BA	3284	1/1	0.94	0.28	4.60	39,39,39,39	0
52	MG	DF	301	1/1	0.85	0.41	4.53	53,53,53,53	0
52	MG	AA	1614	1/1	0.96	0.33	4.39	47,47,47,47	0
52	MG	BA	3044	1/1	0.95	0.28	4.25	9,9,9,9	0
52	MG	BA	3020	1/1	0.96	0.35	4.16	8,8,8,8	0
52	MG	BA	3053	1/1	0.97	0.43	4.10	6,6,6,6	0
52	MG	DA	3285	1/1	0.87	0.20	3.84	33,33,33,33	0
52	MG	DA	3121	1/1	0.92	0.28	3.80	49,49,49,49	0
52	MG	DA	3018	1/1	0.95	0.33	3.80	29,29,29,29	0
52	MG	DA	3063	1/1	0.92	0.39	3.56	38,38,38,38	0
52	MG	CA	1607	1/1	0.92	0.46	3.50	46,46,46,46	0
52	MG	DA	3159	1/1	0.79	0.24	3.48	40,40,40,40	0
52	MG	BA	3361	1/1	0.77	0.32	3.42	52,52,52,52	0
52	MG	DA	3123	1/1	0.81	0.22	3.35	38,38,38,38	0
52	MG	DA	3148	1/1	0.93	0.29	3.32	51,51,51,51	0
52	MG	BA	3200	1/1	0.88	0.33	3.30	12,12,12,12	0
52	MG	DA	3116	1/1	0.88	0.28	3.18	45,45,45,45	0
52	MG	BA	3351	1/1	0.79	0.30	3.16	48,48,48,48	0
52	MG	DA	3118	1/1	0.88	0.33	2.99	43,43,43,43	0
52	MG	BA	3236	1/1	0.92	0.25	2.92	31,31,31,31	0
52	MG	BA	3327	1/1	0.92	0.29	2.74	48,48,48,48	0
52	MG	D1	101	1/1	0.93	0.34	2.63	47,47,47,47	0
52	MG	DA	3184	1/1	0.77	0.29	2.58	32,32,32,32	0
52	MG	BA	3287	1/1	0.92	0.34	2.56	27,27,27,27	0
52	MG	BA	3057	1/1	0.94	0.29	2.55	37,37,37,37	0
52	MG	BA	3034	1/1	0.96	0.23	2.45	45,45,45,45	0
52	MG	DA	3248	1/1	0.92	0.32	2.41	33,33,33,33	0
52	MG	DX	101	1/1	0.84	0.25	2.27	45,45,45,45	0
52	MG	BA	3321	1/1	0.90	0.31	2.26	33,33,33,33	0
52	MG	DA	3210	1/1	0.85	0.23	2.09	46,46,46,46	0
52	MG	DA	3186	1/1	0.97	0.25	2.08	42,42,42,42	0
52	MG	DA	3140	1/1	0.94	0.47	1.95	42,42,42,42	0
52	MG	BD	301	1/1	0.96	0.43	1.93	25,25,25,25	0
52	MG	BU	201	1/1	0.97	0.36	1.89	25,25,25,25	0
52	MG	AA	1641	1/1	0.90	0.22	1.84	64,64,64,64	0
52	MG	BA	3252	1/1	0.94	0.22	1.79	50,50,50,50	0
52	MG	DA	3043	1/1	0.97	0.25	1.56	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DD	301	1/1	0.85	0.44	1.55	32,32,32,32	0
52	MG	B1	101	1/1	0.92	0.32	1.41	25,25,25,25	0
52	MG	BR	201	1/1	0.98	0.39	1.38	7,7,7,7	0
52	MG	BA	3135	1/1	0.97	0.23	1.27	30,30,30,30	0
52	MG	DA	3201	1/1	0.78	0.23	1.25	43,43,43,43	0
52	MG	BA	3091	1/1	0.94	0.25	1.25	14,14,14,14	0
52	MG	BA	3126	1/1	0.97	0.21	1.08	29,29,29,29	0
52	MG	AA	1615	1/1	0.91	0.21	1.04	35,35,35,35	0
52	MG	BX	101	1/1	0.92	0.26	1.01	21,21,21,21	0
52	MG	BA	3113	1/1	0.78	0.21	0.89	26,26,26,26	0
52	MG	BA	3121	1/1	0.98	0.27	0.80	34,34,34,34	0
52	MG	DA	3110	1/1	0.87	0.22	0.80	50,50,50,50	0
52	MG	DA	3237	1/1	0.95	0.26	0.69	57,57,57,57	0
52	MG	AA	1611	1/1	0.77	0.18	0.63	72,72,72,72	0
52	MG	DA	3200	1/1	0.92	0.19	0.62	37,37,37,37	0
52	MG	DA	3301	1/1	0.89	0.20	0.57	15,15,15,15	0
52	MG	DA	3326	1/1	0.89	0.21	0.56	49,49,49,49	0
52	MG	BA	3352	1/1	0.87	0.27	0.56	51,51,51,51	0
52	MG	DA	3126	1/1	0.86	0.16	0.54	36,36,36,36	0
52	MG	DA	3288	1/1	0.90	0.22	0.42	42,42,42,42	0
52	MG	BA	3281	1/1	0.94	0.21	0.40	41,41,41,41	0
52	MG	DA	3220	1/1	0.89	0.20	0.39	40,40,40,40	0
52	MG	DA	3179	1/1	0.93	0.33	0.38	29,29,29,29	0
52	MG	DA	3225	1/1	0.80	0.20	0.36	37,37,37,37	0
52	MG	BA	3264	1/1	0.95	0.24	-0.00	11,11,11,11	0
52	MG	BA	3214	1/1	0.97	0.20	-0.11	23,23,23,23	0
52	MG	DA	3240	1/1	0.96	0.18	-0.20	40,40,40,40	0
52	MG	CA	1653	1/1	0.90	0.19	-0.31	47,47,47,47	0
53	ZN	AD	301	1/1	0.99	0.28	-0.33	109,109,109,109	0
53	ZN	CD	301	1/1	0.96	0.28	-0.43	107,107,107,107	0
52	MG	AA	1627	1/1	0.95	0.20	-0.44	60,60,60,60	0
52	MG	BA	3215	1/1	0.81	0.20	-0.49	10,10,10,10	0
52	MG	BA	3303	1/1	0.95	0.23	-0.55	37,37,37,37	0
52	MG	DA	3315	1/1	0.91	0.17	-0.80	43,43,43,43	0
52	MG	AA	1610	1/1	0.95	0.21	-0.83	33,33,33,33	0
52	MG	DA	3247	1/1	0.99	0.15	-0.84	37,37,37,37	0
52	MG	DA	3277	1/1	0.89	0.17	-0.96	38,38,38,38	0
53	ZN	AN	101	1/1	0.92	0.15	-1.00	144,144,144,144	0
52	MG	BA	3149	1/1	0.98	0.19	-1.14	8,8,8,8	0
52	MG	BA	3243	1/1	0.86	0.20	-1.16	30,30,30,30	0
52	MG	DA	3062	1/1	0.97	0.16	-1.19	24,24,24,24	0
52	MG	DA	3125	1/1	0.91	0.16	-1.22	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	ZN	CN	101	1/1	0.98	0.16	-1.30	136,136,136,136	0
52	MG	BA	3312	1/1	0.92	0.20	-1.33	41,41,41,41	0
52	MG	DA	3230	1/1	0.94	0.15	-1.39	25,25,25,25	0
52	MG	BA	3197	1/1	0.94	0.18	-1.44	27,27,27,27	0
52	MG	BA	3087	1/1	0.97	0.20	-1.55	10,10,10,10	0
52	MG	BA	3043	1/1	0.99	0.18	-1.56	32,32,32,32	0
52	MG	BA	3262	1/1	0.97	0.15	-1.59	30,30,30,30	0
52	MG	BA	3129	1/1	0.96	0.19	-1.59	33,33,33,33	0
52	MG	BA	3152	1/1	0.94	0.12	-1.66	49,49,49,49	0
52	MG	BB	207	1/1	0.95	0.20	-1.71	58,58,58,58	0
52	MG	BA	3062	1/1	0.82	0.17	-1.72	30,30,30,30	0
52	MG	BA	3130	1/1	0.95	0.13	-1.74	36,36,36,36	0
52	MG	BA	3239	1/1	0.92	0.17	-1.76	32,32,32,32	0
52	MG	BA	3181	1/1	0.78	0.15	-1.90	32,32,32,32	0
52	MG	CA	1652	1/1	0.87	0.15	-1.91	61,61,61,61	0
52	MG	DA	3170	1/1	0.83	0.15	-1.97	42,42,42,42	0
52	MG	AA	1656	1/1	0.80	0.17	-2.03	62,62,62,62	0
52	MG	AA	1635	1/1	0.66	0.14	-2.12	53,53,53,53	0
52	MG	DA	3327	1/1	0.83	0.14	-2.22	41,41,41,41	0
52	MG	BA	3292	1/1	0.73	0.14	-2.30	41,41,41,41	0
52	MG	AA	1616	1/1	0.94	0.08	-2.36	57,57,57,57	0
52	MG	BA	3263	1/1	0.93	0.17	-2.58	29,29,29,29	0
52	MG	DA	3087	1/1	0.97	0.12	-2.61	24,24,24,24	0
52	MG	DA	3113	1/1	0.93	0.09	-2.70	59,59,59,59	0
52	MG	BA	3234	1/1	0.81	0.19	-2.93	16,16,16,16	0
52	MG	BA	3256	1/1	0.93	0.12	-3.03	24,24,24,24	0
52	MG	BA	3116	1/1	0.81	0.11	-3.38	41,41,41,41	0
52	MG	BB	203	1/1	0.83	0.11	-3.85	55,55,55,55	0
52	MG	CA	1623	1/1	0.96	0.12	-3.86	50,50,50,50	0
52	MG	BA	3251	1/1	0.97	0.17	-3.87	40,40,40,40	0
52	MG	DB	203	1/1	0.90	0.14	-4.03	73,73,73,73	0
52	MG	DA	3246	1/1	0.90	0.10	-4.20	43,43,43,43	0
52	MG	AA	1646	1/1	0.86	0.12	-4.45	48,48,48,48	0
52	MG	BA	3296	1/1	0.88	0.07	-4.56	36,36,36,36	0
52	MG	CA	1640	1/1	0.96	0.12	-4.61	53,53,53,53	0
52	MG	CA	1631	1/1	0.86	0.08	-4.98	71,71,71,71	0
54	K	BA	3369	1/1	0.91	0.16	-5.83	41,41,41,41	0
52	MG	BA	3056	1/1	0.83	0.16	-6.13	20,20,20,20	0
52	MG	BA	3248	1/1	0.85	0.35	-	33,33,33,33	0
52	MG	DA	3325	1/1	0.79	0.56	-	46,46,46,46	0
52	MG	CA	1608	1/1	0.74	0.33	-	68,68,68,68	0
52	MG	BB	202	1/1	0.96	0.34	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3213	1/1	0.95	0.42	-	26,26,26,26	0
52	MG	DA	3035	1/1	0.92	0.45	-	31,31,31,31	0
52	MG	DA	3257	1/1	0.84	0.36	-	46,46,46,46	0
52	MG	BA	3362	1/1	0.48	0.38	-	50,50,50,50	0
52	MG	BA	3254	1/1	0.94	0.70	-	34,34,34,34	0
52	MG	BA	3247	1/1	0.75	0.56	-	35,35,35,35	0
52	MG	DA	3174	1/1	0.94	0.34	-	54,54,54,54	0
52	MG	BA	3133	1/1	0.99	0.31	-	25,25,25,25	0
52	MG	DA	3167	1/1	0.70	0.26	-	63,63,63,63	0
52	MG	AA	1649	1/1	0.74	0.26	-	76,76,76,76	0
52	MG	BA	3089	1/1	0.88	0.39	-	15,15,15,15	0
52	MG	DA	3117	1/1	0.94	0.12	-	54,54,54,54	0
52	MG	DA	3095	1/1	0.92	0.41	-	47,47,47,47	0
52	MG	CA	1630	1/1	0.78	0.61	-	66,66,66,66	0
52	MG	BA	3136	1/1	0.96	0.50	-	22,22,22,22	0
52	MG	DA	3294	1/1	0.94	0.18	-	46,46,46,46	0
52	MG	BA	3106	1/1	0.94	0.57	-	37,37,37,37	0
52	MG	BA	3205	1/1	0.88	0.50	-	34,34,34,34	0
52	MG	DA	3241	1/1	0.91	0.12	-	54,54,54,54	0
52	MG	DA	3029	1/1	0.84	0.23	-	43,43,43,43	0
52	MG	BA	3143	1/1	0.94	0.63	-	29,29,29,29	0
52	MG	BA	3166	1/1	0.91	0.19	-	27,27,27,27	0
52	MG	BA	3245	1/1	0.92	0.52	-	52,52,52,52	0
52	MG	AA	1606	1/1	0.97	0.60	-	86,86,86,86	0
52	MG	DA	3051	1/1	0.92	0.51	-	29,29,29,29	0
52	MG	BQ	201	1/1	0.98	0.22	-	18,18,18,18	0
52	MG	BA	3338	1/1	0.83	0.38	-	50,50,50,50	0
52	MG	BA	3170	1/1	0.92	0.65	-	36,36,36,36	0
52	MG	DA	3105	1/1	0.86	0.20	-	39,39,39,39	0
52	MG	CA	1638	1/1	0.80	1.28	-	64,64,64,64	0
52	MG	CA	1604	1/1	0.87	0.32	-	67,67,67,67	0
52	MG	DA	3078	1/1	0.99	0.50	-	31,31,31,31	0
52	MG	DA	3316	1/1	0.90	0.21	-	62,62,62,62	0
52	MG	AA	1620	1/1	0.83	0.61	-	52,52,52,52	0
52	MG	DA	3164	1/1	0.86	0.56	-	41,41,41,41	0
52	MG	BA	3083	1/1	0.92	0.55	-	34,34,34,34	0
52	MG	BA	3093	1/1	0.82	0.99	-	50,50,50,50	0
52	MG	DA	3013	1/1	0.95	0.46	-	10,10,10,10	0
52	MG	BA	3206	1/1	0.92	0.56	-	29,29,29,29	0
52	MG	BA	3099	1/1	0.95	0.30	-	34,34,34,34	0
52	MG	CA	1645	1/1	0.88	0.35	-	45,45,45,45	0
52	MG	DA	3197	1/1	0.95	0.47	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3155	1/1	0.88	0.32	-	39,39,39,39	0
52	MG	BA	3187	1/1	0.97	0.61	-	33,33,33,33	0
52	MG	BA	3232	1/1	0.88	0.31	-	27,27,27,27	0
52	MG	DA	3329	1/1	0.80	0.34	-	51,51,51,51	0
52	MG	BA	3183	1/1	0.98	0.38	-	43,43,43,43	0
52	MG	BA	3114	1/1	0.96	0.49	-	21,21,21,21	0
52	MG	DA	3232	1/1	0.48	0.87	-	63,63,63,63	0
52	MG	BA	3235	1/1	0.91	0.56	-	38,38,38,38	0
52	MG	BA	3270	1/1	0.94	0.54	-	26,26,26,26	0
52	MG	DA	3273	1/1	0.95	0.28	-	39,39,39,39	0
52	MG	DA	3180	1/1	0.78	0.50	-	38,38,38,38	0
52	MG	BA	3227	1/1	0.92	0.61	-	22,22,22,22	0
52	MG	DA	3151	1/1	0.97	0.44	-	40,40,40,40	0
52	MG	DA	3153	1/1	0.78	0.77	-	73,73,73,73	0
52	MG	BA	3188	1/1	0.90	0.51	-	36,36,36,36	0
52	MG	BA	3120	1/1	0.95	0.42	-	25,25,25,25	0
52	MG	AA	1630	1/1	0.84	0.53	-	49,49,49,49	0
52	MG	BA	3131	1/1	0.75	0.52	-	45,45,45,45	0
52	MG	DR	201	1/1	0.93	0.45	-	34,34,34,34	0
52	MG	AA	1613	1/1	0.83	0.29	-	62,62,62,62	0
52	MG	DA	3259	1/1	0.84	0.51	-	79,79,79,79	0
52	MG	DA	3067	1/1	0.91	0.29	-	35,35,35,35	0
52	MG	DA	3004	1/1	0.96	0.25	-	19,19,19,19	0
52	MG	DA	3129	1/1	0.95	0.32	-	36,36,36,36	0
52	MG	DA	3309	1/1	0.36	0.17	-	66,66,66,66	0
52	MG	AA	1634	1/1	0.91	0.64	-	51,51,51,51	0
52	MG	DA	3310	1/1	0.59	0.45	-	56,56,56,56	0
52	MG	BA	3357	1/1	0.92	0.40	-	44,44,44,44	0
52	MG	BA	3354	1/1	0.89	0.38	-	40,40,40,40	0
52	MG	DA	3322	1/1	0.78	0.39	-	45,45,45,45	0
52	MG	BA	3031	1/1	0.96	0.22	-	39,39,39,39	0
52	MG	DA	3208	1/1	0.79	0.57	-	34,34,34,34	0
52	MG	DA	3317	1/1	0.98	0.06	-	48,48,48,48	0
52	MG	BA	3198	1/1	0.81	0.89	-	62,62,62,62	0
52	MG	DA	3096	1/1	0.91	0.47	-	61,61,61,61	0
52	MG	BA	3158	1/1	0.95	0.35	-	9,9,9,9	0
52	MG	BA	3221	1/1	0.84	0.25	-	31,31,31,31	0
52	MG	BA	3104	1/1	0.93	0.18	-	22,22,22,22	0
52	MG	BA	3138	1/1	0.97	0.38	-	4,4,4,4	0
52	MG	DA	3275	1/1	0.93	0.60	-	51,51,51,51	0
52	MG	CA	1626	1/1	0.72	0.48	-	68,68,68,68	0
52	MG	BA	3033	1/1	0.92	0.30	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3252	1/1	0.73	0.47	-	57,57,57,57	0
52	MG	DA	3176	1/1	0.87	0.20	-	66,66,66,66	0
52	MG	BA	3315	1/1	0.88	0.23	-	43,43,43,43	0
52	MG	BA	3067	1/1	0.97	0.56	-	28,28,28,28	0
52	MG	DA	3005	1/1	0.94	0.19	-	49,49,49,49	0
52	MG	BA	3128	1/1	0.62	0.91	-	45,45,45,45	0
52	MG	BA	3293	1/1	0.95	0.36	-	47,47,47,47	0
52	MG	BA	3336	1/1	0.76	0.34	-	49,49,49,49	0
52	MG	DA	3212	1/1	0.93	0.21	-	33,33,33,33	0
52	MG	BP	202	1/1	0.94	0.28	-	0,0,0,0	0
52	MG	AA	1650	1/1	0.89	0.56	-	49,49,49,49	0
52	MG	DA	3205	1/1	0.98	0.70	-	39,39,39,39	0
52	MG	DA	3266	1/1	0.90	0.61	-	45,45,45,45	0
52	MG	BA	3328	1/1	0.94	0.29	-	27,27,27,27	0
52	MG	CA	1605	1/1	0.92	0.29	-	68,68,68,68	0
52	MG	BA	3222	1/1	0.96	0.58	-	20,20,20,20	0
52	MG	DA	3224	1/1	0.95	0.61	-	41,41,41,41	0
52	MG	DA	3076	1/1	0.97	0.23	-	23,23,23,23	0
52	MG	BA	3048	1/1	0.94	0.55	-	22,22,22,22	0
52	MG	DA	3258	1/1	0.94	0.24	-	38,38,38,38	0
52	MG	BA	3022	1/1	0.95	0.36	-	37,37,37,37	0
52	MG	DA	3236	1/1	0.67	0.56	-	71,71,71,71	0
52	MG	AA	1601	1/1	0.96	0.22	-	50,50,50,50	0
52	MG	BA	3139	1/1	0.84	0.67	-	30,30,30,30	0
52	MG	BA	3013	1/1	0.91	0.41	-	7,7,7,7	0
52	MG	BA	3098	1/1	0.66	0.34	-	59,59,59,59	0
52	MG	DA	3235	1/1	0.89	0.28	-	48,48,48,48	0
52	MG	BA	3103	1/1	0.91	0.36	-	27,27,27,27	0
52	MG	DA	3279	1/1	0.94	0.59	-	44,44,44,44	0
52	MG	B5	102	1/1	0.94	0.59	-	44,44,44,44	0
52	MG	AA	1643	1/1	0.49	1.02	-	66,66,66,66	0
52	MG	DA	3068	1/1	0.96	0.44	-	57,57,57,57	0
52	MG	DA	3173	1/1	0.80	0.77	-	57,57,57,57	0
52	MG	DA	3293	1/1	0.81	0.74	-	54,54,54,54	0
52	MG	BA	3211	1/1	0.96	0.29	-	30,30,30,30	0
52	MG	DA	3324	1/1	0.95	0.17	-	38,38,38,38	0
52	MG	DA	3254	1/1	0.93	0.19	-	46,46,46,46	0
52	MG	BA	3334	1/1	0.95	0.40	-	39,39,39,39	0
52	MG	DA	3131	1/1	0.92	0.28	-	55,55,55,55	0
52	MG	DA	3286	1/1	0.93	0.43	-	43,43,43,43	0
52	MG	BA	3137	1/1	0.94	0.32	-	34,34,34,34	0
52	MG	BA	3209	1/1	0.85	0.39	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3318	1/1	0.92	0.36	-	43,43,43,43	0
52	MG	DA	3270	1/1	0.84	0.43	-	55,55,55,55	0
52	MG	BA	3054	1/1	0.95	0.29	-	48,48,48,48	0
52	MG	CA	1622	1/1	0.88	0.45	-	46,46,46,46	0
52	MG	BA	3274	1/1	0.82	0.46	-	33,33,33,33	0
52	MG	BA	3017	1/1	0.99	0.46	-	27,27,27,27	0
52	MG	CA	1629	1/1	0.95	0.16	-	57,57,57,57	0
52	MG	BA	3201	1/1	0.91	0.63	-	31,31,31,31	0
52	MG	DA	3026	1/1	0.92	0.42	-	55,55,55,55	0
52	MG	DA	3244	1/1	0.93	0.62	-	36,36,36,36	0
52	MG	BA	3172	1/1	0.96	0.53	-	18,18,18,18	0
52	MG	BA	3030	1/1	0.96	0.26	-	17,17,17,17	0
52	MG	DA	3253	1/1	0.98	0.59	-	32,32,32,32	0
52	MG	DA	3307	1/1	0.97	0.32	-	42,42,42,42	0
52	MG	BA	3275	1/1	0.98	0.46	-	29,29,29,29	0
52	MG	BA	3210	1/1	0.97	0.51	-	29,29,29,29	0
52	MG	DA	3085	1/1	0.83	0.17	-	19,19,19,19	0
52	MG	BA	3015	1/1	0.98	0.36	-	29,29,29,29	0
52	MG	DA	3025	1/1	0.79	0.44	-	46,46,46,46	0
52	MG	CA	1628	1/1	0.85	0.63	-	50,50,50,50	0
52	MG	BA	3255	1/1	0.85	0.44	-	54,54,54,54	0
52	MG	BA	3115	1/1	0.86	0.44	-	34,34,34,34	0
52	MG	DA	3022	1/1	0.95	0.29	-	38,38,38,38	0
52	MG	DA	3084	1/1	0.98	0.45	-	31,31,31,31	0
52	MG	BA	3324	1/1	0.91	0.44	-	53,53,53,53	0
52	MG	DA	3181	1/1	0.97	0.67	-	29,29,29,29	0
52	MG	DA	3154	1/1	0.90	0.52	-	51,51,51,51	0
52	MG	BA	3286	1/1	0.87	0.51	-	44,44,44,44	0
52	MG	AA	1622	1/1	0.89	0.46	-	40,40,40,40	0
52	MG	CA	1617	1/1	0.94	0.53	-	48,48,48,48	0
52	MG	DA	3111	1/1	0.98	0.63	-	39,39,39,39	0
52	MG	BA	3079	1/1	0.98	0.24	-	36,36,36,36	0
52	MG	BA	3344	1/1	0.92	0.09	-	56,56,56,56	0
52	MG	AA	1647	1/1	0.94	0.47	-	46,46,46,46	0
52	MG	BA	3358	1/1	0.79	0.50	-	59,59,59,59	0
52	MG	CA	1601	1/1	0.91	0.20	-	61,61,61,61	0
52	MG	DA	3162	1/1	0.97	0.52	-	50,50,50,50	0
52	MG	DA	3263	1/1	0.82	0.29	-	65,65,65,65	0
52	MG	AA	1612	1/1	0.82	0.59	-	56,56,56,56	0
52	MG	DA	3300	1/1	0.94	0.47	-	54,54,54,54	0
52	MG	CA	1624	1/1	0.93	0.40	-	50,50,50,50	0
52	MG	DA	3175	1/1	0.82	0.48	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3300	1/1	0.84	0.41	-	45,45,45,45	0
52	MG	BA	3346	1/1	0.71	0.12	-	63,63,63,63	0
52	MG	BA	3147	1/1	0.95	0.57	-	28,28,28,28	0
52	MG	DA	3302	1/1	0.86	0.24	-	39,39,39,39	0
52	MG	DA	3137	1/1	0.83	0.17	-	69,69,69,69	0
52	MG	BA	3335	1/1	0.88	0.42	-	57,57,57,57	0
52	MG	DA	3073	1/1	0.98	0.30	-	27,27,27,27	0
52	MG	DA	3185	1/1	0.92	0.47	-	49,49,49,49	0
52	MG	DA	3136	1/1	0.87	0.36	-	48,48,48,48	0
52	MG	BA	3186	1/1	0.94	0.50	-	38,38,38,38	0
52	MG	BA	3363	1/1	0.74	0.20	-	54,54,54,54	0
52	MG	DA	3328	1/1	0.74	0.52	-	61,61,61,61	0
52	MG	DA	3182	1/1	0.93	0.55	-	41,41,41,41	0
52	MG	DA	3042	1/1	0.94	0.24	-	29,29,29,29	0
52	MG	BA	3306	1/1	0.93	0.56	-	35,35,35,35	0
52	MG	CA	1606	1/1	0.85	0.86	-	52,52,52,52	0
52	MG	BA	3302	1/1	0.98	0.72	-	31,31,31,31	0
52	MG	BA	3271	1/1	0.72	0.16	-	53,53,53,53	0
52	MG	BA	3310	1/1	0.98	0.52	-	31,31,31,31	0
52	MG	DA	3144	1/1	0.94	0.60	-	43,43,43,43	0
52	MG	DA	3331	1/1	0.76	0.15	-	67,67,67,67	0
52	MG	DA	3128	1/1	0.93	0.23	-	29,29,29,29	0
52	MG	BA	3356	1/1	0.85	0.08	-	60,60,60,60	0
52	MG	DA	3321	1/1	0.99	0.06	-	41,41,41,41	0
52	MG	BA	3151	1/1	0.72	0.39	-	47,47,47,47	0
52	MG	DA	3299	1/1	0.88	0.18	-	41,41,41,41	0
52	MG	BA	3184	1/1	0.90	0.52	-	40,40,40,40	0
52	MG	AA	1637	1/1	0.77	0.69	-	51,51,51,51	0
52	MG	DA	3007	1/1	0.88	0.48	-	48,48,48,48	0
52	MG	BA	3320	1/1	0.83	1.16	-	52,52,52,52	0
52	MG	DA	3027	1/1	0.93	0.60	-	36,36,36,36	0
52	MG	DA	3227	1/1	0.90	0.23	-	47,47,47,47	0
52	MG	DA	3196	1/1	0.97	0.48	-	33,33,33,33	0
52	MG	DA	3276	1/1	0.89	0.85	-	44,44,44,44	0
52	MG	DA	3271	1/1	0.80	0.56	-	56,56,56,56	0
52	MG	BA	3208	1/1	0.97	0.32	-	17,17,17,17	0
52	MG	DA	3268	1/1	0.91	0.94	-	63,63,63,63	0
52	MG	DA	3284	1/1	0.92	0.72	-	49,49,49,49	0
52	MG	BA	3036	1/1	0.95	0.45	-	8,8,8,8	0
52	MG	DA	3161	1/1	0.95	0.16	-	44,44,44,44	0
52	MG	AA	1609	1/1	0.91	0.45	-	52,52,52,52	0
52	MG	DA	3187	1/1	0.77	0.57	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3035	1/1	0.96	0.33	-	18,18,18,18	0
52	MG	DA	3169	1/1	0.91	0.54	-	45,45,45,45	0
52	MG	BA	3065	1/1	0.96	0.29	-	28,28,28,28	0
52	MG	BA	3014	1/1	0.96	0.54	-	30,30,30,30	0
52	MG	DA	3079	1/1	0.98	0.22	-	36,36,36,36	0
52	MG	DA	3272	1/1	0.89	0.47	-	47,47,47,47	0
52	MG	DA	3133	1/1	0.62	0.12	-	55,55,55,55	0
52	MG	BA	3004	1/1	0.91	0.35	-	14,14,14,14	0
52	MG	CA	1643	1/1	0.91	0.29	-	42,42,42,42	0
52	MG	DA	3119	1/1	0.95	0.40	-	36,36,36,36	0
52	MG	BB	204	1/1	0.92	0.43	-	41,41,41,41	0
52	MG	BB	201	1/1	0.90	0.54	-	35,35,35,35	0
52	MG	DA	3107	1/1	0.90	0.44	-	15,15,15,15	0
52	MG	BA	3160	1/1	0.87	0.58	-	41,41,41,41	0
52	MG	BA	3266	1/1	0.94	0.44	-	37,37,37,37	0
52	MG	DA	3011	1/1	0.96	0.51	-	27,27,27,27	0
52	MG	CA	1614	1/1	0.86	0.63	-	57,57,57,57	0
52	MG	AA	1654	1/1	0.62	0.83	-	64,64,64,64	0
52	MG	AA	1640	1/1	0.95	0.47	-	60,60,60,60	0
52	MG	DA	3064	1/1	0.99	0.50	-	44,44,44,44	0
52	MG	DA	3036	1/1	0.97	0.46	-	12,12,12,12	0
52	MG	DA	3152	1/1	0.95	0.40	-	36,36,36,36	0
52	MG	DA	3215	1/1	0.89	0.28	-	27,27,27,27	0
52	MG	BA	3045	1/1	0.99	0.41	-	14,14,14,14	0
52	MG	BA	3340	1/1	0.88	0.22	-	39,39,39,39	0
52	MG	BA	3207	1/1	0.84	0.72	-	32,32,32,32	0
52	MG	DA	3255	1/1	0.97	0.45	-	49,49,49,49	0
52	MG	DA	3296	1/1	0.90	0.31	-	45,45,45,45	0
52	MG	DA	3195	1/1	0.77	0.48	-	36,36,36,36	0
52	MG	AA	1645	1/1	0.92	0.59	-	61,61,61,61	0
52	MG	BA	3260	1/1	0.91	0.29	-	13,13,13,13	0
52	MG	BA	3085	1/1	0.91	0.16	-	9,9,9,9	0
52	MG	BA	3146	1/1	0.92	0.40	-	33,33,33,33	0
52	MG	DB	202	1/1	0.88	0.41	-	60,60,60,60	0
52	MG	AA	1632	1/1	0.84	0.65	-	51,51,51,51	0
52	MG	BA	3228	1/1	0.90	0.42	-	27,27,27,27	0
52	MG	BA	3178	1/1	0.97	0.27	-	32,32,32,32	0
52	MG	CA	1644	1/1	0.97	0.25	-	43,43,43,43	0
52	MG	DA	3157	1/1	0.92	0.25	-	48,48,48,48	0
52	MG	BA	3220	1/1	0.95	0.69	-	22,22,22,22	0
52	MG	CA	1642	1/1	0.81	1.23	-	71,71,71,71	0
52	MG	BA	3339	1/1	0.94	0.34	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3076	1/1	0.95	0.23	-	21,21,21,21	0
52	MG	DA	3100	1/1	0.98	0.48	-	35,35,35,35	0
52	MG	BA	3364	1/1	0.88	0.35	-	64,64,64,64	0
52	MG	DA	3190	1/1	0.96	0.40	-	43,43,43,43	0
52	MG	DA	3323	1/1	0.91	0.67	-	62,62,62,62	0
52	MG	BA	3110	1/1	0.91	0.52	-	27,27,27,27	0
52	MG	DA	3238	1/1	0.98	0.30	-	36,36,36,36	0
52	MG	BA	3097	1/1	0.89	0.41	-	32,32,32,32	0
52	MG	BA	3268	1/1	0.96	0.52	-	38,38,38,38	0
52	MG	AA	1618	1/1	0.91	0.19	-	53,53,53,53	0
52	MG	BA	3007	1/1	0.72	0.70	-	40,40,40,40	0
52	MG	DA	3101	1/1	0.84	0.33	-	34,34,34,34	0
52	MG	BA	3240	1/1	0.86	0.38	-	50,50,50,50	0
52	MG	BA	3332	1/1	0.88	0.41	-	35,35,35,35	0
52	MG	DA	3054	1/1	0.83	0.28	-	55,55,55,55	0
52	MG	BA	3301	1/1	0.95	0.66	-	36,36,36,36	0
52	MG	CA	1646	1/1	0.94	0.79	-	58,58,58,58	0
52	MG	CA	1641	1/1	0.93	0.40	-	45,45,45,45	0
52	MG	BA	3190	1/1	0.96	0.55	-	36,36,36,36	0
52	MG	BA	3161	1/1	0.89	0.27	-	32,32,32,32	0
52	MG	BP	201	1/1	0.84	0.56	-	35,35,35,35	0
52	MG	DA	3081	1/1	0.97	0.56	-	24,24,24,24	0
52	MG	DA	3211	1/1	0.89	0.90	-	50,50,50,50	0
52	MG	DA	3226	1/1	0.92	0.65	-	55,55,55,55	0
52	MG	DA	3155	1/1	0.96	0.13	-	41,41,41,41	0
52	MG	CA	1618	1/1	0.91	0.46	-	58,58,58,58	0
52	MG	DA	3319	1/1	0.92	0.63	-	55,55,55,55	0
52	MG	DA	3050	1/1	0.95	0.34	-	33,33,33,33	0
52	MG	BA	3019	1/1	0.97	0.58	-	13,13,13,13	0
52	MG	DA	3217	1/1	0.97	0.13	-	36,36,36,36	0
52	MG	DA	3243	1/1	0.73	0.52	-	56,56,56,56	0
52	MG	CA	1619	1/1	0.95	0.53	-	40,40,40,40	0
52	MG	BA	3153	1/1	0.94	0.41	-	34,34,34,34	0
52	MG	BA	3305	1/1	0.83	0.27	-	54,54,54,54	0
52	MG	DA	3189	1/1	0.98	0.14	-	42,42,42,42	0
52	MG	BA	3073	1/1	0.97	0.28	-	7,7,7,7	0
52	MG	DA	3015	1/1	0.97	0.39	-	52,52,52,52	0
52	MG	DA	3193	1/1	0.89	0.74	-	40,40,40,40	0
52	MG	DA	3297	1/1	0.56	0.51	-	55,55,55,55	0
52	MG	DA	3112	1/1	0.95	0.44	-	28,28,28,28	0
52	MG	CA	1611	1/1	0.82	0.84	-	76,76,76,76	0
52	MG	DA	3251	1/1	0.90	0.18	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	AA	1653	1/1	0.91	0.33	-	46,46,46,46	0
52	MG	BE	301	1/1	0.92	0.49	-	16,16,16,16	0
52	MG	DA	3203	1/1	0.98	0.32	-	38,38,38,38	0
52	MG	BA	3290	1/1	0.96	0.28	-	40,40,40,40	0
52	MG	BA	3025	1/1	0.89	0.27	-	29,29,29,29	0
52	MG	DA	3031	1/1	0.98	0.17	-	51,51,51,51	0
52	MG	DA	3256	1/1	0.93	0.30	-	46,46,46,46	0
52	MG	DA	3024	1/1	0.96	0.40	-	47,47,47,47	0
52	MG	BA	3359	1/1	0.84	0.58	-	39,39,39,39	0
52	MG	BA	3367	1/1	0.86	0.10	-	47,47,47,47	0
52	MG	BA	3265	1/1	0.93	0.31	-	43,43,43,43	0
52	MG	BA	3217	1/1	0.95	0.35	-	34,34,34,34	0
52	MG	BA	3176	1/1	0.79	0.42	-	58,58,58,58	0
52	MG	DA	3104	1/1	0.98	0.43	-	41,41,41,41	0
52	MG	CA	1603	1/1	0.98	0.42	-	32,32,32,32	0
52	MG	BA	3317	1/1	0.87	0.36	-	53,53,53,53	0
52	MG	BA	3107	1/1	0.97	0.25	-	7,7,7,7	0
52	MG	DA	3239	1/1	0.85	0.77	-	41,41,41,41	0
52	MG	BA	3154	1/1	0.74	0.37	-	77,77,77,77	0
52	MG	BA	3329	1/1	0.93	0.33	-	49,49,49,49	0
52	MG	BA	3059	1/1	0.94	0.34	-	25,25,25,25	0
52	MG	BA	3331	1/1	0.87	0.53	-	37,37,37,37	0
52	MG	BA	3304	1/1	0.90	0.52	-	49,49,49,49	0
52	MG	DA	3127	1/1	0.84	0.20	-	33,33,33,33	0
52	MG	BA	3212	1/1	0.96	0.33	-	30,30,30,30	0
52	MG	DA	3313	1/1	0.90	0.67	-	48,48,48,48	0
52	MG	DA	3265	1/1	0.82	0.14	-	38,38,38,38	0
52	MG	DA	3088	1/1	0.93	0.48	-	40,40,40,40	0
52	MG	AA	1626	1/1	0.93	0.44	-	46,46,46,46	0
52	MG	BA	3289	1/1	0.79	0.27	-	44,44,44,44	0
52	MG	DA	3021	1/1	0.88	0.35	-	38,38,38,38	0
52	MG	DA	3209	1/1	0.98	0.40	-	51,51,51,51	0
52	MG	BA	3078	1/1	0.98	0.45	-	22,22,22,22	0
52	MG	CA	1635	1/1	0.87	0.79	-	73,73,73,73	0
52	MG	AA	1621	1/1	0.91	0.49	-	37,37,37,37	0
52	MG	BA	3258	1/1	0.86	0.24	-	21,21,21,21	0
52	MG	BA	3341	1/1	0.87	0.66	-	66,66,66,66	0
52	MG	BA	3204	1/1	0.90	0.26	-	36,36,36,36	0
52	MG	BA	3134	1/1	0.92	0.27	-	36,36,36,36	0
52	MG	DA	3231	1/1	0.91	0.55	-	54,54,54,54	0
52	MG	DA	3142	1/1	0.98	0.57	-	32,32,32,32	0
52	MG	BA	3082	1/1	0.96	0.33	-	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3218	1/1	0.93	0.33	-	30,30,30,30	0
52	MG	DA	3114	1/1	0.94	0.22	-	46,46,46,46	0
52	MG	BA	3225	1/1	0.87	0.60	-	32,32,32,32	0
52	MG	DA	3177	1/1	0.85	0.41	-	37,37,37,37	0
52	MG	BA	3333	1/1	0.91	0.48	-	50,50,50,50	0
52	MG	DA	3262	1/1	0.90	0.71	-	60,60,60,60	0
52	MG	BA	3345	1/1	0.84	0.25	-	43,43,43,43	0
52	MG	BA	3177	1/1	0.90	0.87	-	67,67,67,67	0
52	MG	BA	3288	1/1	0.88	0.52	-	46,46,46,46	0
52	MG	BA	3185	1/1	0.96	0.27	-	45,45,45,45	0
52	MG	BA	3122	1/1	0.93	0.51	-	37,37,37,37	0
52	MG	BA	3314	1/1	0.86	0.50	-	41,41,41,41	0
52	MG	BA	3157	1/1	0.95	0.44	-	13,13,13,13	0
52	MG	BA	3026	1/1	0.89	0.39	-	45,45,45,45	0
52	MG	BA	3249	1/1	0.86	0.32	-	54,54,54,54	0
52	MG	DA	3045	1/1	0.97	0.40	-	30,30,30,30	0
52	MG	D5	101	1/1	0.93	0.47	-	30,30,30,30	0
52	MG	DA	3083	1/1	0.95	0.45	-	37,37,37,37	0
52	MG	BA	3368	1/1	0.86	0.07	-	60,60,60,60	0
52	MG	AA	1655	1/1	0.95	0.21	-	45,45,45,45	0
52	MG	DA	3308	1/1	0.93	0.15	-	43,43,43,43	0
52	MG	AA	1619	1/1	0.94	0.37	-	44,44,44,44	0
52	MG	DA	3274	1/1	0.78	0.42	-	71,71,71,71	0
52	MG	DA	3218	1/1	0.94	0.31	-	24,24,24,24	0
52	MG	BA	3349	1/1	0.62	0.78	-	65,65,65,65	0
52	MG	DA	3281	1/1	0.78	0.81	-	63,63,63,63	0
52	MG	DA	3019	1/1	0.95	0.63	-	25,25,25,25	0
52	MG	DA	3130	1/1	0.97	0.20	-	53,53,53,53	0
52	MG	BA	3084	1/1	0.99	0.37	-	5,5,5,5	0
52	MG	BA	3077	1/1	0.97	0.28	-	20,20,20,20	0
52	MG	DA	3311	1/1	0.95	0.28	-	29,29,29,29	0
52	MG	DE	301	1/1	0.95	0.43	-	31,31,31,31	0
52	MG	DA	3172	1/1	0.97	0.32	-	48,48,48,48	0
52	MG	BA	3192	1/1	0.96	0.34	-	17,17,17,17	0
52	MG	CA	1650	1/1	0.90	0.31	-	45,45,45,45	0
52	MG	CA	1632	1/1	0.95	0.35	-	56,56,56,56	0
52	MG	BA	3241	1/1	0.92	0.18	-	44,44,44,44	0
52	MG	BA	3233	1/1	0.96	0.29	-	20,20,20,20	0
52	MG	BA	3159	1/1	0.76	0.70	-	52,52,52,52	0
52	MG	AA	1603	1/1	0.93	0.38	-	43,43,43,43	0
52	MG	CA	1616	1/1	0.95	0.50	-	45,45,45,45	0
52	MG	AA	1639	1/1	0.93	0.35	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3273	1/1	0.99	0.20	-	3,3,3,3	0
52	MG	BA	3102	1/1	0.94	0.44	-	38,38,38,38	0
52	MG	BA	3011	1/1	0.98	0.47	-	17,17,17,17	0
52	MG	BA	3141	1/1	0.76	0.18	-	47,47,47,47	0
52	MG	CA	1602	1/1	0.91	0.57	-	40,40,40,40	0
52	MG	BA	3269	1/1	0.89	0.43	-	34,34,34,34	0
52	MG	DA	3086	1/1	0.88	0.20	-	34,34,34,34	0
52	MG	BA	3219	1/1	0.94	0.59	-	24,24,24,24	0
52	MG	BA	3337	1/1	0.79	0.47	-	32,32,32,32	0
52	MG	BA	3140	1/1	0.95	0.53	-	44,44,44,44	0
52	MG	DA	3103	1/1	0.88	0.56	-	33,33,33,33	0
52	MG	BA	3278	1/1	0.83	0.16	-	31,31,31,31	0
52	MG	BA	3272	1/1	0.91	0.44	-	36,36,36,36	0
52	MG	DA	3314	1/1	0.93	0.23	-	40,40,40,40	0
52	MG	DA	3077	1/1	0.96	0.27	-	38,38,38,38	0
52	MG	DA	3149	1/1	0.79	0.58	-	54,54,54,54	0
52	MG	BA	3309	1/1	0.90	0.58	-	49,49,49,49	0
52	MG	BA	3291	1/1	0.79	0.21	-	54,54,54,54	0
52	MG	DA	3072	1/1	0.84	0.89	-	71,71,71,71	0
52	MG	BA	3257	1/1	0.96	0.22	-	35,35,35,35	0
52	MG	DB	201	1/1	0.84	0.46	-	57,57,57,57	0
52	MG	BA	3342	1/1	0.94	1.38	-	69,69,69,69	0
52	MG	BA	3145	1/1	0.94	0.52	-	33,33,33,33	0
52	MG	BA	3365	1/1	0.84	0.36	-	43,43,43,43	0
52	MG	DA	3192	1/1	0.95	0.65	-	36,36,36,36	0
52	MG	DA	3048	1/1	0.93	0.48	-	30,30,30,30	0
52	MG	BA	3164	1/1	0.96	0.33	-	33,33,33,33	0
52	MG	BA	3297	1/1	0.96	0.34	-	31,31,31,31	0
52	MG	DA	3207	1/1	0.90	0.46	-	54,54,54,54	0
52	MG	BA	3307	1/1	0.74	0.35	-	38,38,38,38	0
52	MG	DA	3202	1/1	0.92	0.54	-	46,46,46,46	0
52	MG	DB	204	1/1	0.84	0.47	-	37,37,37,37	0
52	MG	CA	1633	1/1	0.90	0.87	-	50,50,50,50	0
52	MG	BA	3253	1/1	0.96	0.30	-	17,17,17,17	0
52	MG	BA	3081	1/1	0.99	0.43	-	7,7,7,7	0
52	MG	BA	3318	1/1	0.83	0.38	-	34,34,34,34	0
52	MG	BA	3003	1/1	0.86	0.80	-	44,44,44,44	0
52	MG	AA	1628	1/1	0.91	0.69	-	70,70,70,70	0
52	MG	BA	3193	1/1	0.93	0.55	-	46,46,46,46	0
52	MG	DA	3204	1/1	0.95	0.30	-	42,42,42,42	0
52	MG	DA	3278	1/1	0.83	0.52	-	54,54,54,54	0
52	MG	DA	3066	1/1	0.98	0.42	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3050	1/1	0.97	0.31	-	21,21,21,21	0
52	MG	BA	3276	1/1	0.84	0.36	-	35,35,35,35	0
52	MG	CA	1639	1/1	0.91	0.56	-	50,50,50,50	0
52	MG	BA	3027	1/1	0.95	0.49	-	25,25,25,25	0
52	MG	BA	3282	1/1	0.80	0.59	-	46,46,46,46	0
52	MG	BA	3068	1/1	0.97	0.60	-	35,35,35,35	0
52	MG	BA	3108	1/1	0.91	0.18	-	31,31,31,31	0
52	MG	DA	3134	1/1	0.97	0.54	-	28,28,28,28	0
52	MG	DA	3269	1/1	0.91	0.20	-	61,61,61,61	0
52	MG	AA	1604	1/1	0.70	0.32	-	62,62,62,62	0
52	MG	DA	3037	1/1	0.98	0.76	-	33,33,33,33	0
52	MG	DA	3191	1/1	0.91	0.44	-	38,38,38,38	0
52	MG	DA	3219	1/1	0.94	0.36	-	25,25,25,25	0
52	MG	BA	3311	1/1	0.94	0.20	-	38,38,38,38	0
52	MG	DA	3242	1/1	0.89	0.33	-	35,35,35,35	0
52	MG	BA	3199	1/1	0.86	0.40	-	42,42,42,42	0
52	MG	DA	3332	1/1	0.88	0.15	-	69,69,69,69	0
52	MG	AA	1644	1/1	0.77	0.41	-	68,68,68,68	0
52	MG	BA	3173	1/1	0.96	0.29	-	50,50,50,50	0
52	MG	DA	3282	1/1	0.90	0.23	-	61,61,61,61	0
52	MG	DA	3249	1/1	0.78	0.23	-	48,48,48,48	0
52	MG	DA	3059	1/1	0.97	0.41	-	24,24,24,24	0
52	MG	DA	3295	1/1	0.73	0.65	-	73,73,73,73	0
52	MG	DA	3194	1/1	0.97	0.35	-	22,22,22,22	0
52	MG	DQ	201	1/1	0.84	0.36	-	42,42,42,42	0
52	MG	BA	3163	1/1	0.95	0.51	-	53,53,53,53	0
52	MG	BA	3203	1/1	0.75	0.13	-	47,47,47,47	0
52	MG	DA	3306	1/1	0.88	0.43	-	54,54,54,54	0
52	MG	DP	201	1/1	0.95	0.18	-	19,19,19,19	0
52	MG	BA	3330	1/1	0.79	0.55	-	48,48,48,48	0
52	MG	DA	3082	1/1	0.97	0.48	-	44,44,44,44	0
52	MG	BA	3259	1/1	0.80	0.40	-	40,40,40,40	0
52	MG	BA	3005	1/1	0.98	0.36	-	26,26,26,26	0
52	MG	BA	3042	1/1	0.94	0.31	-	7,7,7,7	0
52	MG	BA	3169	1/1	0.91	0.34	-	33,33,33,33	0
52	MG	AA	1633	1/1	0.98	0.10	-	42,42,42,42	0
52	MG	CA	1615	1/1	0.95	0.39	-	64,64,64,64	0
52	MG	BA	3229	1/1	0.85	0.36	-	26,26,26,26	0
52	MG	DA	3305	1/1	0.67	0.99	-	46,46,46,46	0
52	MG	BA	3238	1/1	0.83	0.77	-	43,43,43,43	0
52	MG	DA	3292	1/1	0.91	0.32	-	52,52,52,52	0
52	MG	DA	3199	1/1	0.95	0.57	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3105	1/1	0.94	0.54	-	19,19,19,19	0
52	MG	BA	3366	1/1	0.86	0.14	-	52,52,52,52	0
52	MG	BA	3069	1/1	0.92	0.31	-	26,26,26,26	0
52	MG	AA	1602	1/1	0.98	0.56	-	32,32,32,32	0
52	MG	DA	3102	1/1	0.98	0.55	-	24,24,24,24	0
52	MG	BA	3295	1/1	0.96	0.23	-	35,35,35,35	0
52	MG	BA	3018	1/1	0.93	0.29	-	27,27,27,27	0
52	MG	DA	3228	1/1	0.95	0.23	-	38,38,38,38	0
52	MG	DA	3304	1/1	0.81	0.79	-	63,63,63,63	0
52	MG	BA	3024	1/1	0.99	0.33	-	20,20,20,20	0
52	MG	DA	3065	1/1	0.89	0.19	-	30,30,30,30	0
52	MG	BA	3353	1/1	0.98	0.12	-	31,31,31,31	0
52	MG	DA	3163	1/1	0.95	0.66	-	30,30,30,30	0
52	MG	DA	3160	1/1	0.91	0.59	-	51,51,51,51	0
52	MG	BA	3231	1/1	0.95	0.11	-	26,26,26,26	0
52	MG	AA	1605	1/1	0.91	0.38	-	71,71,71,71	0
52	MG	BA	3132	1/1	0.94	0.27	-	15,15,15,15	0
52	MG	BA	3322	1/1	0.89	0.50	-	41,41,41,41	0
52	MG	CA	1649	1/1	0.82	0.35	-	55,55,55,55	0
52	MG	DA	3287	1/1	0.82	1.19	-	61,61,61,61	0
52	MG	DA	3206	1/1	0.83	0.64	-	45,45,45,45	0
52	MG	DA	3291	1/1	0.95	0.20	-	36,36,36,36	0
52	MG	BA	3029	1/1	0.94	0.32	-	25,25,25,25	0
52	MG	DA	3139	1/1	0.95	0.82	-	43,43,43,43	0
52	MG	BA	3348	1/1	0.95	0.26	-	34,34,34,34	0
52	MG	BA	3279	1/1	0.86	0.36	-	39,39,39,39	0
52	MG	BA	3189	1/1	0.93	0.19	-	46,46,46,46	0
52	MG	CA	1651	1/1	0.91	0.69	-	51,51,51,51	0
52	MG	BA	3194	1/1	0.99	0.50	-	30,30,30,30	0
52	MG	DA	3132	1/1	0.86	0.77	-	53,53,53,53	0
52	MG	BA	3267	1/1	0.95	0.19	-	41,41,41,41	0
52	MG	DA	3014	1/1	0.88	0.40	-	71,71,71,71	0
52	MG	B5	101	1/1	0.95	0.39	-	28,28,28,28	0
52	MG	BA	3226	1/1	0.92	0.20	-	14,14,14,14	0
52	MG	DA	3147	1/1	0.95	0.26	-	43,43,43,43	0
52	MG	BA	3180	1/1	0.76	0.64	-	46,46,46,46	0
52	MG	DA	3198	1/1	0.90	0.31	-	37,37,37,37	0
52	MG	DA	3298	1/1	0.80	0.64	-	59,59,59,59	0
52	MG	BA	3064	1/1	0.95	0.48	-	41,41,41,41	0
52	MG	DA	3330	1/1	0.92	0.28	-	53,53,53,53	0
52	MG	BA	3223	1/1	0.95	0.43	-	25,25,25,25	0
52	MG	DA	3233	1/1	0.87	0.56	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3299	1/1	0.87	0.37	-	37,37,37,37	0
52	MG	DA	3003	1/1	0.91	0.71	-	39,39,39,39	0
52	MG	DA	3158	1/1	0.98	0.31	-	33,33,33,33	0
52	MG	DA	3250	1/1	0.87	0.35	-	56,56,56,56	0
52	MG	BB	205	1/1	0.88	0.16	-	59,59,59,59	0
52	MG	DA	3069	1/1	0.91	0.30	-	63,63,63,63	0
52	MG	BA	3086	1/1	0.97	0.35	-	27,27,27,27	0
52	MG	BA	3168	1/1	0.97	0.45	-	21,21,21,21	0
52	MG	DA	3261	1/1	0.96	0.06	-	51,51,51,51	0
52	MG	BA	3118	1/1	0.85	0.20	-	38,38,38,38	0
52	MG	BA	3246	1/1	0.79	0.37	-	40,40,40,40	0
52	MG	DA	3264	1/1	0.78	0.26	-	58,58,58,58	0
52	MG	AA	1638	1/1	0.82	0.52	-	69,69,69,69	0
52	MG	CA	1636	1/1	0.91	0.26	-	77,77,77,77	0
52	MG	DA	3033	1/1	0.97	0.29	-	31,31,31,31	0
52	MG	BR	202	1/1	0.86	0.68	-	31,31,31,31	0
52	MG	DA	3221	1/1	0.80	0.68	-	43,43,43,43	0
52	MG	DA	3143	1/1	0.92	0.42	-	40,40,40,40	0
52	MG	BA	3195	1/1	0.94	0.42	-	49,49,49,49	0
52	MG	BA	3244	1/1	0.87	0.36	-	50,50,50,50	0
52	MG	AA	1648	1/1	0.86	1.31	-	80,80,80,80	0
52	MG	DA	3280	1/1	0.71	0.42	-	70,70,70,70	0
52	MG	AA	1636	1/1	0.93	0.52	-	47,47,47,47	0
52	MG	BB	206	1/1	0.97	0.74	-	48,48,48,48	0
52	MG	CA	1634	1/1	0.93	0.16	-	47,47,47,47	0
52	MG	D5	102	1/1	0.86	0.51	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.