wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:06 PM GMT

PDB ID	:	4V8G
Title	:	Crystal structure of RMF bound to the 70S ribosome.
Authors	:	Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on	:	2011-12-11
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 (i) symbol.

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

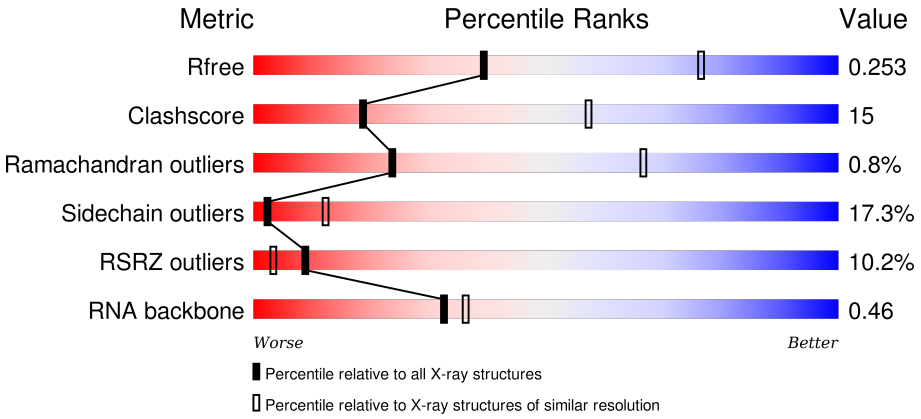
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 <=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	20% 28% 42% 22% 7%
1	CA	1522	15% 30% 44% 20%
2	AB	256	7% 39% 41% 9% 11%
2	CB	256	11% 39% 40% 11% 11%

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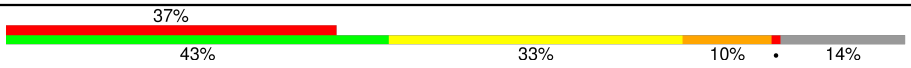
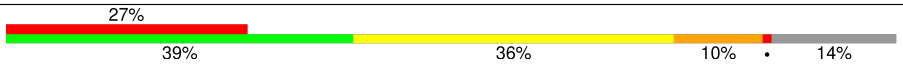
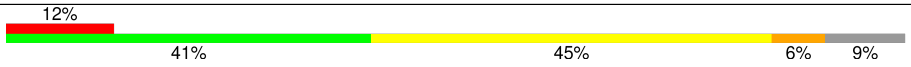
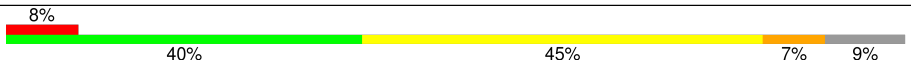
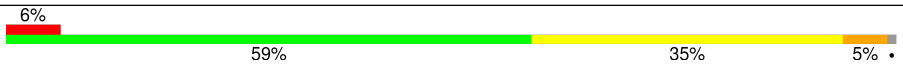
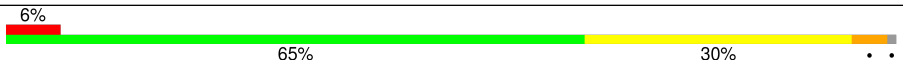
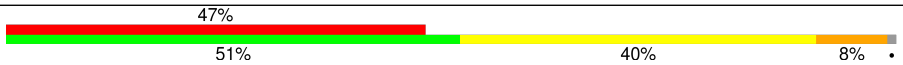
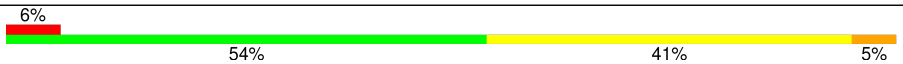
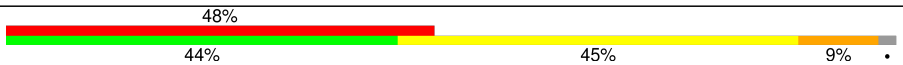
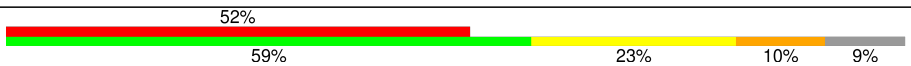
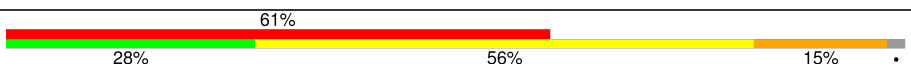
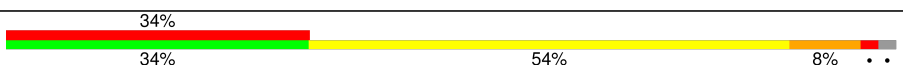
Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	7% 52% 43%
16	AP	88	30% 43% 40% 10% 7%
16	CP	88	7% 48% 32% 13% 7%
17	AQ	105	6% 61% 30% 6%
17	CQ	105	3% 56% 35% 6%
18	AR	88	13% 42% 32% 23%
18	CR	88	22% 44% 28% 5% 23%
19	AS	93	43% 41% 32% 13% 13%
19	CS	93	52% 51% 30% 5% 13%
20	AT	106	8% 42% 43% 5% 8%
20	CT	106	13% 50% 35% 6% 8%
21	AU	27	70% 26% 37% 22% 15%
21	CU	27	44% 48% 30% 7% 15%
22	AV	61	5% 57% 28% 13%
22	CV	61	3% 51% 23% 11% 13%
23	BA	2915	3% 33% 40% 18% 5%
23	DA	2915	4% 38% 39% 17%
24	BB	122	29% 49% 17%
24	DB	122	38% 45% 15%
25	BD	276	63% 31% 5%
25	DD	276	62% 30% 7%
26	BE	206	67% 25% 5%
26	DE	206	63% 27% 8%
27	BF	210	% 62% 28% 7%
27	DF	210	56% 34% 6%

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Mol	Chain	Length	Quality of chain
28	BG	182	11% 53% 40% 7%
28	DG	182	24% 53% 39% 8%
29	BH	180	% 66% 27%
29	DH	180	13% 66% 28%
30	BI	148	% 47% 41% 11%
30	DI	148	11% 57% 28% 13%
31	BN	140	58% 34% 8%
31	DN	140	% 56% 35% 8%
32	BO	122	69% 28%
32	DO	122	63% 34%
33	BP	150	64% 28% 7%
33	DP	150	2% 64% 30% 5%
34	BQ	141	% 69% 26% 5%
34	DQ	141	58% 35% 6%
35	BR	118	71% 22% 7%
35	DR	118	63% 33%
36	BS	112	54% 35% 10%
36	DS	112	4% 50% 41% 7%
37	BT	146	51% 31% 8% 10%
37	DT	146	% 51% 30% 8% 10%
38	BU	118	% 70% 25%
38	DU	118	2% 66% 29%
39	BV	101	61% 32% 6%
39	DV	101	57% 35% 8%
40	BW	113	73% 23%

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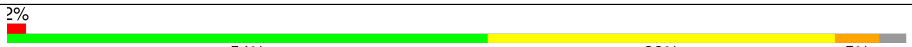
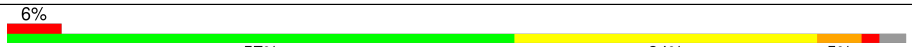
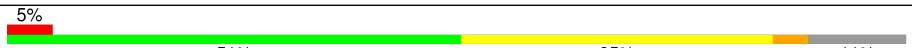
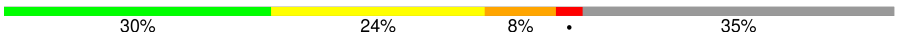
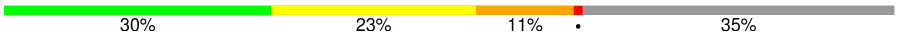
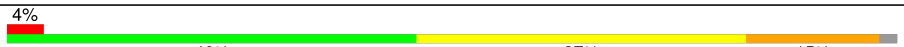
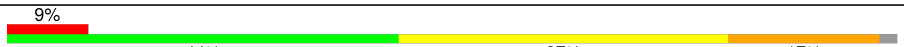
Mol	Chain	Length	Quality of chain
40	DW	113	
41	BX	96	
41	DX	96	
42	BY	110	
42	DY	110	
43	BZ	206	
43	DZ	206	
44	B0	85	
44	D0	85	
45	B1	98	
45	D1	98	
46	B2	72	
46	D2	72	
47	B3	60	
47	D3	60	
48	B4	71	
48	D4	71	
49	B5	60	
49	D5	60	
50	B6	54	
50	D6	54	
51	B7	49	
51	D7	49	
52	B8	65	
52	D8	65	

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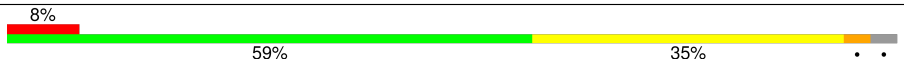
Mol	Chain	Length	Quality of chain
53	B9	37	
53	D9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	1604	-	-	-	X
54	MG	AA	1613	-	-	-	X
54	MG	AA	1615	-	-	-	X
54	MG	AA	1621	-	-	-	X
54	MG	AA	1627	-	-	-	X
54	MG	AA	1631	-	-	-	X
54	MG	AA	1640	-	-	-	X
54	MG	AA	1645	-	-	-	X
54	MG	AA	1657	-	-	-	X
54	MG	AA	1659	-	-	-	X
54	MG	AA	1660	-	-	-	X
54	MG	B3	101	-	-	-	X
54	MG	BA	3001	-	-	-	X
54	MG	BA	3003	-	-	-	X
54	MG	BA	3021	-	-	-	X
54	MG	BA	3031	-	-	-	X
54	MG	BA	3033	-	-	-	X
54	MG	BA	3034	-	-	-	X
54	MG	BA	3037	-	-	-	X
54	MG	BA	3039	-	-	-	X
54	MG	BA	3046	-	-	-	X
54	MG	BA	3047	-	-	-	X
54	MG	BA	3053	-	-	-	X
54	MG	BA	3071	-	-	-	X
54	MG	BA	3074	-	-	-	X
54	MG	BA	3078	-	-	-	X
54	MG	BA	3080	-	-	-	X
54	MG	BA	3108	-	-	-	X
54	MG	BA	3109	-	-	-	X
54	MG	BA	3113	-	-	-	X
54	MG	BA	3117	-	-	-	X
54	MG	BA	3119	-	-	-	X
54	MG	BA	3127	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3129	-	-	-	X
54	MG	BA	3133	-	-	-	X
54	MG	BA	3142	-	-	-	X
54	MG	BA	3160	-	-	-	X
54	MG	BA	3161	-	-	-	X
54	MG	BA	3187	-	-	-	X
54	MG	BA	3189	-	-	-	X
54	MG	BA	3197	-	-	-	X
54	MG	BA	3199	-	-	-	X
54	MG	BA	3219	-	-	-	X
54	MG	BA	3228	-	-	-	X
54	MG	BA	3230	-	-	-	X
54	MG	BA	3234	-	-	-	X
54	MG	BA	3236	-	-	-	X
54	MG	BA	3239	-	-	-	X
54	MG	BA	3244	-	-	-	X
54	MG	BA	3253	-	-	-	X
54	MG	BA	3254	-	-	-	X
54	MG	BA	3302	-	-	-	X
54	MG	BA	3307	-	-	-	X
54	MG	BA	3308	-	-	-	X
54	MG	BA	3311	-	-	-	X
54	MG	BA	3330	-	-	-	X
54	MG	BA	3333	-	-	-	X
54	MG	BA	3368	-	-	-	X
54	MG	BA	3387	-	-	-	X
54	MG	BA	3396	-	-	-	X
54	MG	BA	3408	-	-	-	X
54	MG	BA	3423	-	-	-	X
54	MG	BA	3424	-	-	-	X
54	MG	BA	3426	-	-	-	X
54	MG	BA	3427	-	-	-	X
54	MG	BA	3434	-	-	-	X
54	MG	BA	3435	-	-	-	X
54	MG	BA	3441	-	-	-	X
54	MG	BA	3448	-	-	-	X
54	MG	BA	3455	-	-	-	X
54	MG	BA	3461	-	-	-	X
54	MG	BA	3473	-	-	-	X
54	MG	BA	3475	-	-	-	X
54	MG	BA	3500	-	-	-	X
54	MG	BA	3504	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3512	-	-	-	X
54	MG	BA	3513	-	-	-	X
54	MG	BA	3517	-	-	-	X
54	MG	BA	3519	-	-	-	X
54	MG	BA	3526	-	-	-	X
54	MG	BA	3551	-	-	-	X
54	MG	BA	3557	-	-	-	X
54	MG	BA	3562	-	-	-	X
54	MG	BB	201	-	-	-	X
54	MG	BB	204	-	-	-	X
54	MG	BB	205	-	-	-	X
54	MG	BD	302	-	-	-	X
54	MG	BE	301	-	-	-	X
54	MG	BQ	202	-	-	-	X
54	MG	BR	201	-	-	-	X
54	MG	CA	1601	-	-	-	X
54	MG	CA	1602	-	-	-	X
54	MG	CA	1612	-	-	-	X
54	MG	CA	1613	-	-	-	X
54	MG	CA	1617	-	-	-	X
54	MG	CA	1618	-	-	-	X
54	MG	CA	1623	-	-	-	X
54	MG	CA	1626	-	-	-	X
54	MG	CA	1628	-	-	-	X
54	MG	CA	1631	-	-	-	X
54	MG	CA	1636	-	-	-	X
54	MG	CA	1638	-	-	-	X
54	MG	CA	1655	-	-	-	X
54	MG	DA	3003	-	-	-	X
54	MG	DA	3006	-	-	-	X
54	MG	DA	3011	-	-	-	X
54	MG	DA	3019	-	-	-	X
54	MG	DA	3020	-	-	-	X
54	MG	DA	3027	-	-	-	X
54	MG	DA	3032	-	-	-	X
54	MG	DA	3040	-	-	-	X
54	MG	DA	3044	-	-	-	X
54	MG	DA	3059	-	-	-	X
54	MG	DA	3062	-	-	-	X
54	MG	DA	3070	-	-	-	X
54	MG	DA	3072	-	-	-	X
54	MG	DA	3073	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3074	-	-	-	X
54	MG	DA	3079	-	-	-	X
54	MG	DA	3084	-	-	-	X
54	MG	DA	3085	-	-	-	X
54	MG	DA	3086	-	-	-	X
54	MG	DA	3092	-	-	-	X
54	MG	DA	3098	-	-	-	X
54	MG	DA	3099	-	-	-	X
54	MG	DA	3115	-	-	-	X
54	MG	DA	3116	-	-	-	X
54	MG	DA	3118	-	-	-	X
54	MG	DA	3120	-	-	-	X
54	MG	DA	3121	-	-	-	X
54	MG	DA	3124	-	-	-	X
54	MG	DA	3128	-	-	-	X
54	MG	DA	3130	-	-	-	X
54	MG	DA	3133	-	-	-	X
54	MG	DA	3138	-	-	-	X
54	MG	DA	3142	-	-	-	X
54	MG	DA	3144	-	-	-	X
54	MG	DA	3146	-	-	-	X
54	MG	DA	3149	-	-	-	X
54	MG	DA	3168	-	-	-	X
54	MG	DA	3169	-	-	-	X
54	MG	DA	3170	-	-	-	X
54	MG	DA	3177	-	-	-	X
54	MG	DA	3185	-	-	-	X
54	MG	DA	3188	-	-	-	X
54	MG	DA	3202	-	-	-	X
54	MG	DA	3204	-	-	-	X
54	MG	DA	3207	-	-	-	X
54	MG	DA	3208	-	-	-	X
54	MG	DA	3217	-	-	-	X
54	MG	DA	3219	-	-	-	X
54	MG	DA	3233	-	-	-	X
54	MG	DA	3236	-	-	-	X
54	MG	DA	3242	-	-	-	X
54	MG	DA	3247	-	-	-	X
54	MG	DA	3267	-	-	-	X
54	MG	DA	3279	-	-	-	X
54	MG	DA	3280	-	-	-	X
54	MG	DA	3290	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3291	-	-	-	X
54	MG	DA	3297	-	-	-	X
54	MG	DA	3303	-	-	-	X
54	MG	DA	3309	-	-	-	X
54	MG	DA	3324	-	-	-	X
54	MG	DA	3340	-	-	-	X
54	MG	DA	3341	-	-	-	X
54	MG	DA	3349	-	-	-	X
54	MG	DA	3354	-	-	-	X
54	MG	DA	3372	-	-	-	X
54	MG	DA	3374	-	-	-	X
54	MG	DA	3385	-	-	-	X
54	MG	DA	3390	-	-	-	X
54	MG	DA	3394	-	-	-	X
54	MG	DA	3395	-	-	-	X
54	MG	DA	3396	-	-	-	X
54	MG	DA	3410	-	-	-	X
54	MG	DB	201	-	-	-	X
54	MG	DF	301	-	-	-	X
54	MG	DP	201	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 283930 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1505	Total	C	N	O	P	0	0	0
			32353	14399	5995	10454	1505			
1	CA	1501	Total	C	N	O	P	0	0	0
			32270	14362	5983	10424	1501			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	5			
2	CB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	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
			1526	963	283	274	6			
4	CD	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	6			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	3			
6	CF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	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
			1164	726	224	208	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	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
			1045	665	188	190	2			
8	CH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	125	Total	C	N	O	0	0	0
			852	533	163	156			
9	CI	125	Total	C	N	O	0	0	0
			852	533	163	156			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	96	Total	C	N	O	0	0	0
			663	410	132	121			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O	0	0	0
			663	410	132	121			

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			
11	CK	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0	0
			905	567	178	159	1			
12	CL	122	Total	C	N	O	S	0	0	0
			905	567	178	159	1			

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			804	497	164	142	1			
13	CM	114	Total	C	N	O	S	0	0	0
			804	497	164	142	1			

- 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
			478	303	99	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			478	303	99	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
			724	453	143	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			
16	CP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			514	329	98	87			
18	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			
19	CS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	97	Total	C	N	O	S	0	0	0
			713	438	152	121	2			
20	CT	97	Total	C	N	O	S	0	0	0
			713	438	152	121	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a protein called Ribosome modulation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	53	Total	C	N	O	S	0	0	0
			333	204	66	61	2			
22	CV	53	Total	C	N	O	S	0	0	0
			353	218	67	66	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	56	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	57	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	58	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	59	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	60	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	61	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	56	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	57	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	58	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	59	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	60	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	61	HIS	-	EXPRESSION TAG	UNP P0AFW2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2809	Total	C	N	O	P	0	0	0
			60512	26930	11328	19446	2808			
23	DA	2814	Total	C	N	O	P	0	0	0
			60620	26978	11348	19481	2813			

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 25 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
25	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 26 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			
26	DE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 27 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			
27	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			

- Molecule 28 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			
28	DG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 29 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			
29	DH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 30 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	146	Total	C	N	O	S	0	0	0
			1040	669	180	190	1			
30	DI	146	Total	C	N	O	S	0	0	0
			1038	668	180	189	1			

- Molecule 31 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			
31	DN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 32 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			
32	DO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 33 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			
33	DP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 34 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
35	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 36 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BS	110	Total	C	N	O	0	0	0
			865	544	172	149			
36	DS	110	Total	C	N	O	0	0	0
			865	544	172	149			

- Molecule 37 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
37	DT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
38	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 39 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BV	100	Total	C	N	O	S	0	0	0
			760	490	136	133	1			
39	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

- Molecule 41 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
41	DX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
42	DY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 43 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			
43	DZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 44 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
44	D0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 45 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			
45	D1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 46 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
46	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 47 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	B3	59	Total	C	N	O	0	0	0
			458	293	87	78			
47	D3	59	Total	C	N	O	0	0	0
			458	293	87	78			

- Molecule 48 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
48	D4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 49 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
49	D5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 50 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
50	D6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 51 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
51	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 52 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
52	D8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 53 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			
53	D9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	618	Total	Mg	0	0
			618	618		
54	CA	69	Total	Mg	0	0
			69	69		
54	DF	2	Total	Mg	0	0
			2	2		
54	B8	3	Total	Mg	0	0
			3	3		
54	BE	6	Total	Mg	0	0
			6	6		
54	B1	1	Total	Mg	0	0
			1	1		
54	BP	1	Total	Mg	0	0
			1	1		
54	D6	1	Total	Mg	0	0
			1	1		
54	B5	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	BB	17	Total Mg 17 17	0	0
54	D8	1	Total Mg 1 1	0	0
54	B9	1	Total Mg 1 1	0	0
54	BF	2	Total Mg 2 2	0	0
54	B2	2	Total Mg 2 2	0	0
54	AA	106	Total Mg 106 106	0	0
54	BQ	3	Total Mg 3 3	0	0
54	D7	1	Total Mg 1 1	0	0
54	BU	2	Total Mg 2 2	0	0
54	AD	1	Total Mg 1 1	0	0
54	DD	1	Total Mg 1 1	0	0
54	B3	2	Total Mg 2 2	0	0
54	BR	2	Total Mg 2 2	0	0
54	DA	430	Total Mg 430 430	0	0
54	BV	1	Total Mg 1 1	0	0
54	DE	1	Total Mg 1 1	0	0
54	DP	1	Total Mg 1 1	0	0
54	BD	3	Total Mg 3 3	0	0
54	B0	2	Total Mg 2 2	0	0
54	BW	1	Total Mg 1 1	0	0
54	DB	5	Total Mg 5 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	B5	1	Total Zn 1 1	0	0
55	B4	1	Total Zn 1 1	0	0
55	AD	1	Total Zn 1 1	0	0
55	CD	1	Total Zn 1 1	0	0
55	B9	1	Total Zn 1 1	0	0
55	BY	1	Total Zn 1 1	0	0
55	DY	1	Total Zn 1 1	0	0
55	D5	1	Total Zn 1 1	0	0
55	D4	1	Total Zn 1 1	0	0
55	AN	1	Total Zn 1 1	0	0
55	CN	1	Total Zn 1 1	0	0
55	D6	1	Total Zn 1 1	0	0
55	D9	1	Total Zn 1 1	0	0
55	B6	1	Total Zn 1 1	0	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	145	Total O 145 145	0	0
56	AF	1	Total O 1 1	0	0
56	AK	1	Total O 1 1	0	0
56	AQ	1	Total O 1 1	0	0
56	BA	1422	Total O 1422 1422	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	BB	31	Total O 31 31	0	0
56	BD	10	Total O 10 10	0	0
56	BE	8	Total O 8 8	0	0
56	BF	11	Total O 11 11	0	0
56	BH	2	Total O 2 2	0	0
56	BN	2	Total O 2 2	0	0
56	BO	3	Total O 3 3	0	0
56	BP	6	Total O 6 6	0	0
56	BQ	2	Total O 2 2	0	0
56	BR	6	Total O 6 6	0	0
56	BT	1	Total O 1 1	0	0
56	BU	2	Total O 2 2	0	0
56	BV	2	Total O 2 2	0	0
56	BW	4	Total O 4 4	0	0
56	BX	2	Total O 2 2	0	0
56	BY	1	Total O 1 1	0	0
56	B0	4	Total O 4 4	0	0
56	B3	1	Total O 1 1	0	0
56	B4	1	Total O 1 1	0	0
56	B5	3	Total O 3 3	0	0
56	B7	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

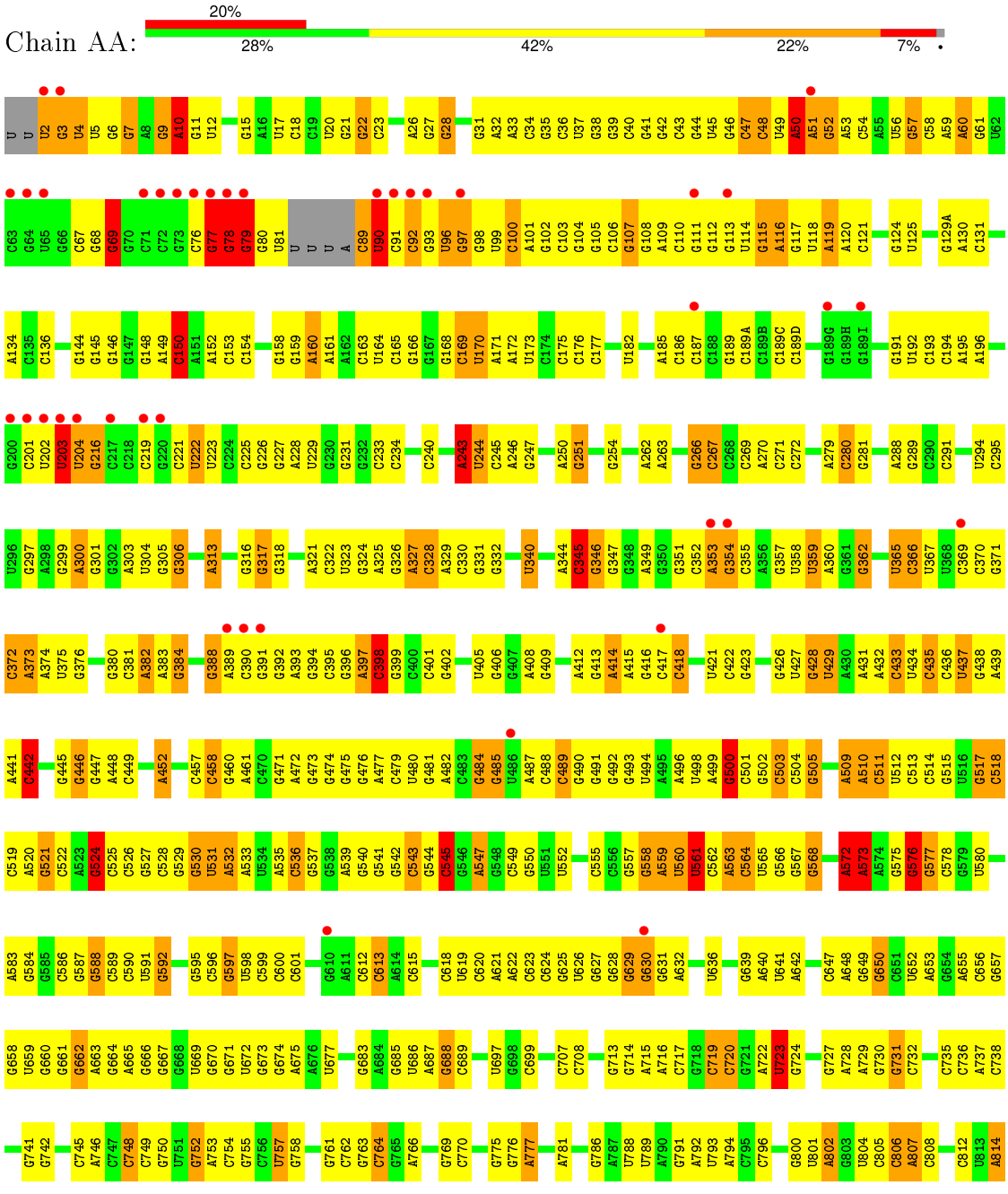
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	B8	7	Total O 7 7	0	0
56	B9	2	Total O 2 2	0	0
56	CA	119	Total O 119 119	0	0
56	CD	1	Total O 1 1	0	0
56	CK	2	Total O 2 2	0	0
56	CP	1	Total O 1 1	0	0
56	CT	2	Total O 2 2	0	0
56	DA	696	Total O 696 696	0	0
56	DB	9	Total O 9 9	0	0
56	DD	3	Total O 3 3	0	0
56	DE	2	Total O 2 2	0	0
56	DF	5	Total O 5 5	0	0
56	DP	5	Total O 5 5	0	0
56	DQ	2	Total O 2 2	0	0
56	DR	1	Total O 1 1	0	0
56	DV	1	Total O 1 1	0	0
56	DX	1	Total O 1 1	0	0
56	DY	1	Total O 1 1	0	0
56	D0	1	Total O 1 1	0	0
56	D1	2	Total O 2 2	0	0

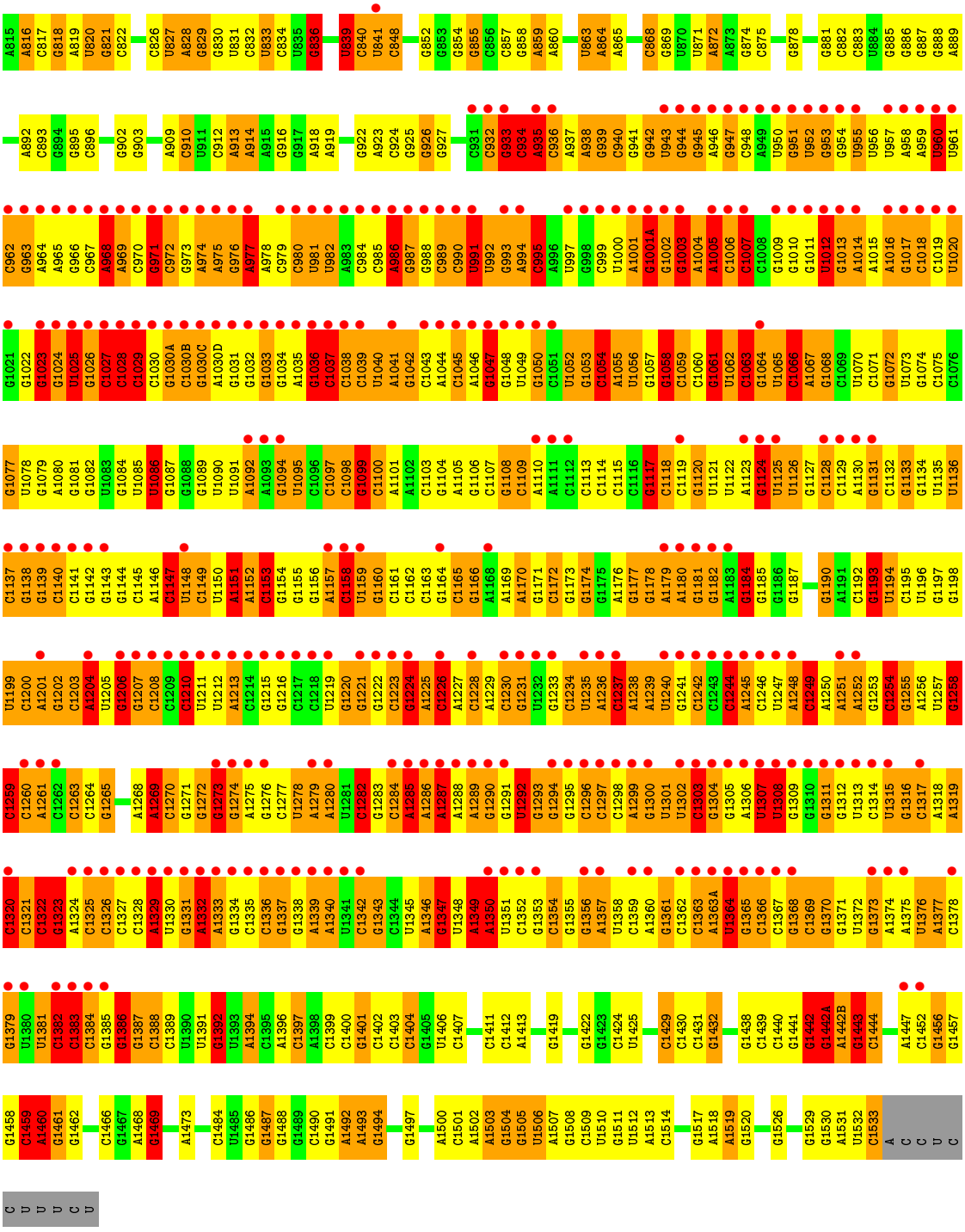
3 Residue-property plots (i)

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

- Molecule 1: 16S Ribosomal RNA

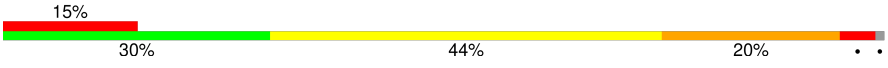
Chain AA:

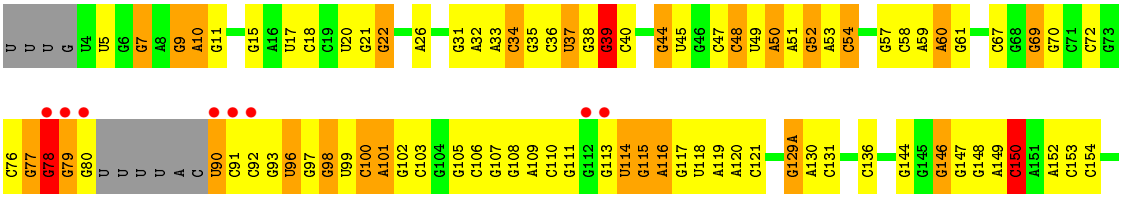


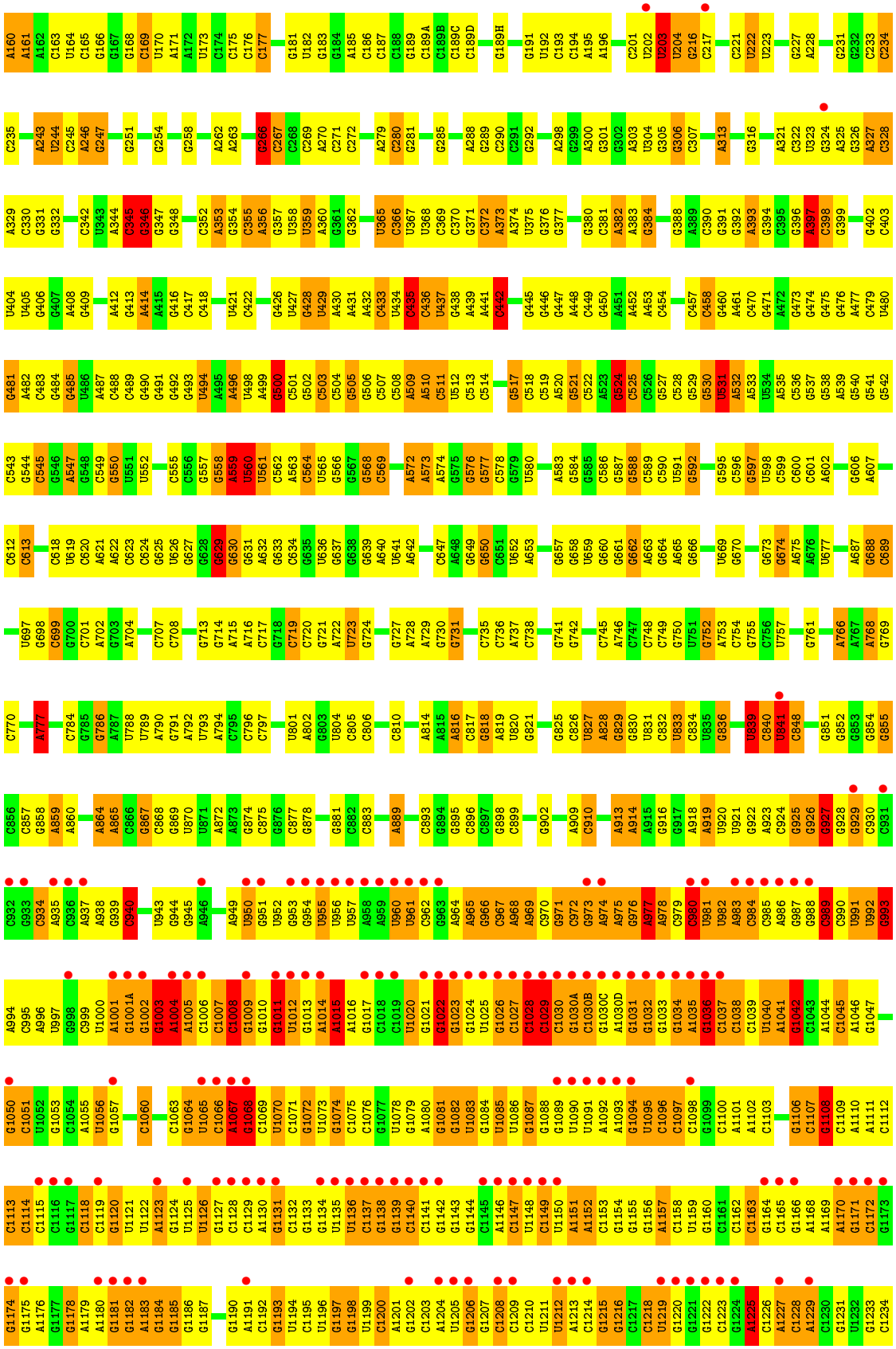


• Molecule 1: 16S Ribosomal RNA

Chain CA:



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C235 A243 U244 C245 A246 G247 G251 G254 G258 A262 A263 C266 C267 C268 C269 A270 C271 C272 A279 C280 G281 G285 A288 C289 C290 C291 C292 A298 C299 A300 G301 G302 A303 U304 G305 G306 C307 A313 G316 A321 C322 U323 G324 A325 G326 A327 C328
A329 C330 G331 G332 C342 U343 A344 C345 G346 G347 G348 C352 A353 G354 C355 A356 G357 U358 U359 A360 G361 G362 U365 C366 U367 U368 C369 C370 G371 C372 A373 A374 U375 G376 G377 G380 C381 A382 A383 G384 G388 A389 C390 G391 G392 A393 G394 C395 G396 A397 G398 G399 G402 C403
U404 U405 G406 G407 A408 G409 A412 G413 A414 A415 G416 C417 C418 U421 C422 G426 U427 G428 U429 A430 A431 A432 C433 U434 C435 C436 U437 G438 A439 A441 C442 G445 G446 G447 A448 G449 G450 A451 A452 A453 C454 C457 C458 G460 A461 C470 G471 A472 G473 G474 G475 G476 A477 C479 U480
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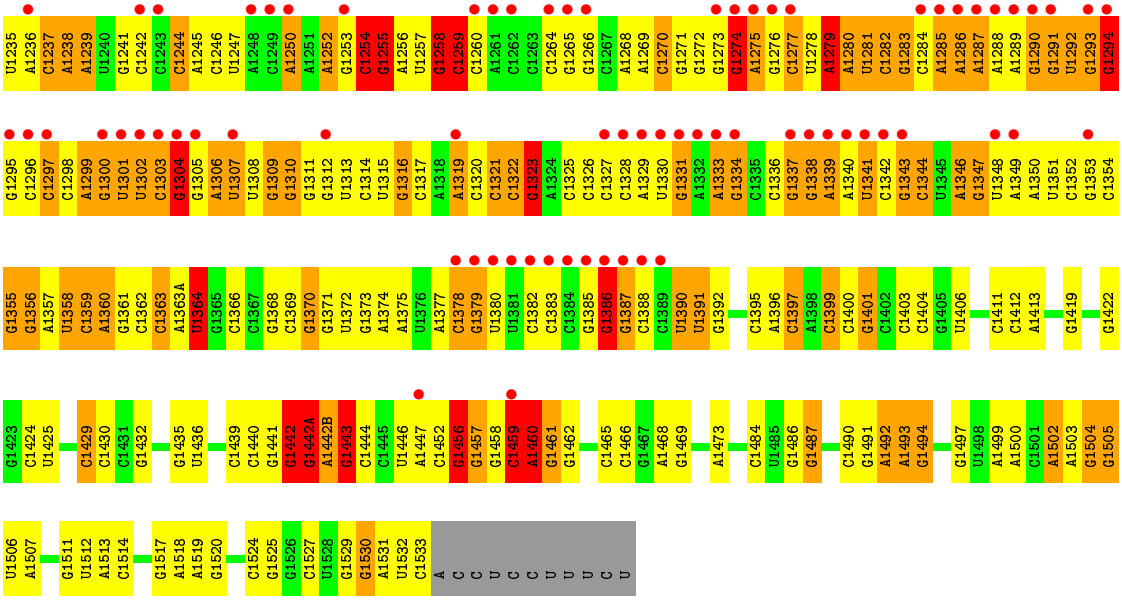
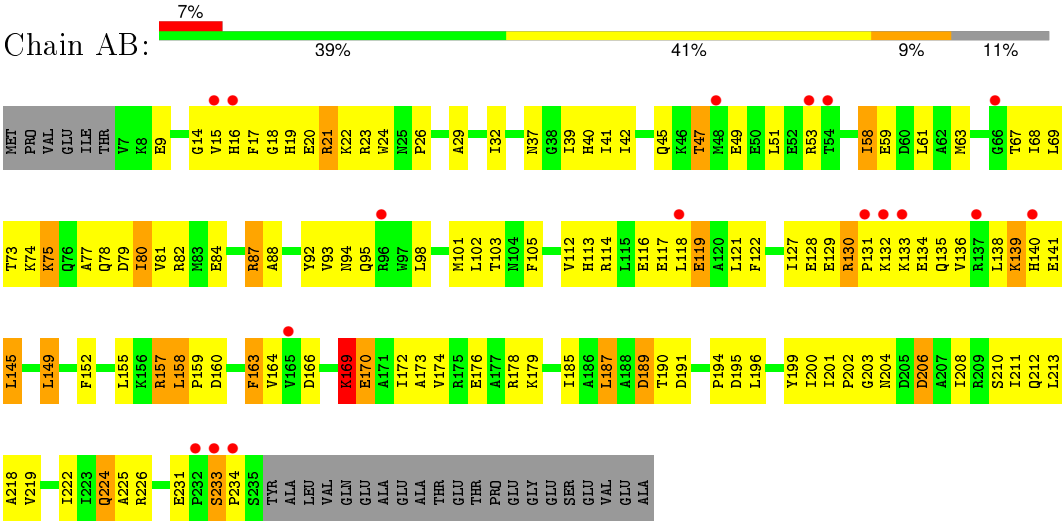
C543 G544 C545 G546 A547 G548 C549 G550 U551 U552 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 U565 G566 G567 G568 C569 A572 A573 A574 G575 G576 G577 C578 G579 U580 A583 G584 G585 C586 G587 G588 C589 C590 U591 G592 G595 C596 G597 U598 C599 C600 C601 A602 G606 A607
C612 G613 C618 U619 C620 A621 A622 C623 C624 G625 U626 G627 G628 G629 G630 G631 A632 G633 C634 G635 U636 G637 G638 G639 A640 U641 A642 C647 A648 G649 G650 C651 U652 A653 G657 G658 U659 G660 G661 G662 A663 G664 A665 G666 U669 G670 G673 G674 A675 A676 U677 A687 G688 C689
U697 G698 C699 G700 C701 A702 G703 A704 C707 C708 G713 G714 A715 A716 C717 G718 C719 C720 G721 A722 U723 G724 G727 A728 A729 G730 G731 C735 C736 A737 C738 G741 G742 C745 A746 C747 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G761 A766 A767 A768 G769
C770 A771 C784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 C795 C796 C797 U801 A802 G803 U804 C805 C806 C810 A814 A815 A816 C817 G818 A819 U820 G821 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 U839 C840 U841 G848 G851 G852 G853 G854 G855
C856 C857 G858 A859 A860 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 G878 G881 C882 C883 A889 C893 G894 G895 C896 C897 G898 G899 G902 A909 C910 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 A923 C924 G925 G926 G927 G928 G929 C930 C931
C932 G933 C934 A935 C936 A937 A938 G939 C940 U943 G944 G945 A946 A949 U950 G951 U952 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 G987 G988 C989 C990 U991 U992 G993
A994 C995 A996 U997 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 C1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 A1024 U1025 G1026 C1027 C1028 C1029 C1030 C1030A C1030B C1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047
G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 C1060 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 C1075 C1076 G1077 U1078 G1079 A1080 G1081 G1082 U1083 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1106 C1107 G1108 C1109 A1110 A1111 C1112
C1113 C1114 C1115 C1116 G1117 C1118 C1119 G1120 U1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 G1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1164 C1165 G1166 A1168 A1169 A1170 G1171 C1172 G1173
G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1185 G1186 G1187 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234



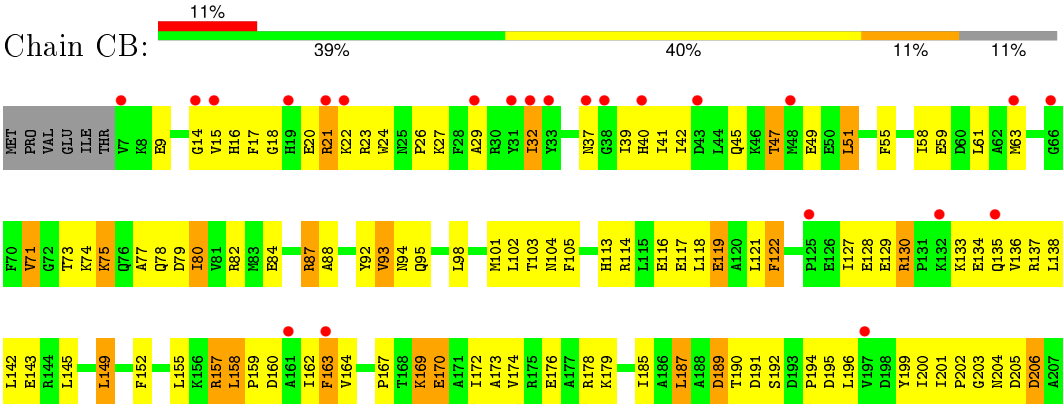
• Molecule 2: 30S Ribosomal Protein S2

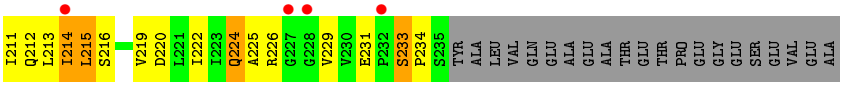
Chain AB:



• Molecule 2: 30S Ribosomal Protein S2

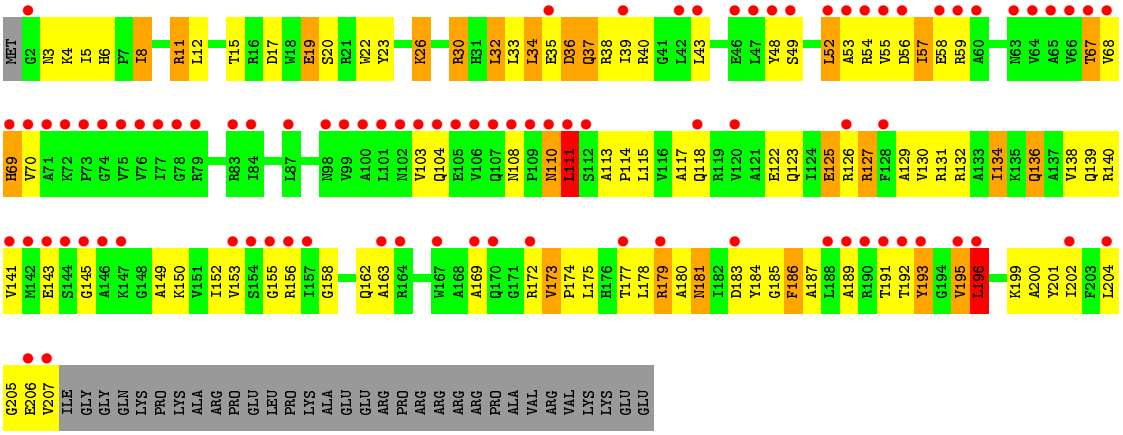
Chain CB:





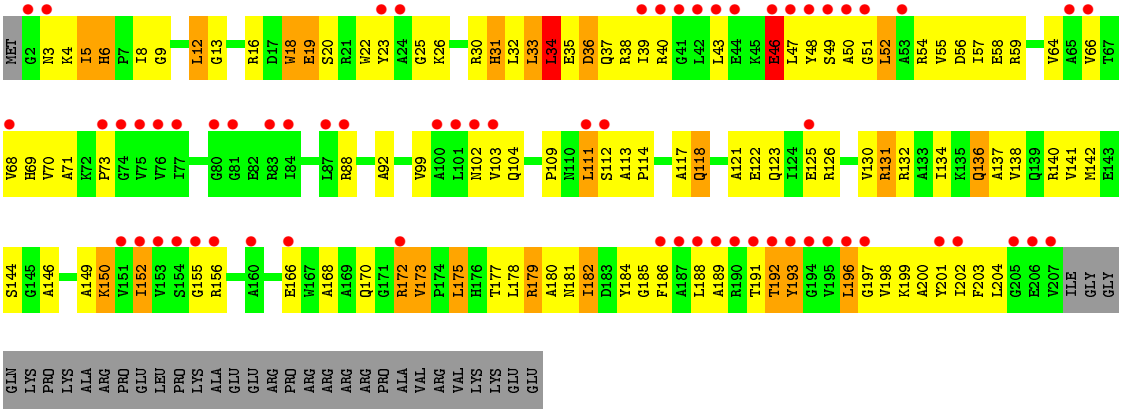
- Molecule 3: 30S Ribosomal Protein S3

Chain AC:



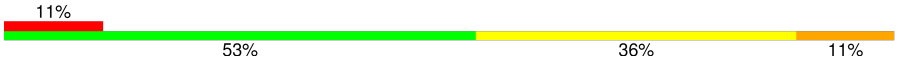
- Molecule 3: 30S Ribosomal Protein S3

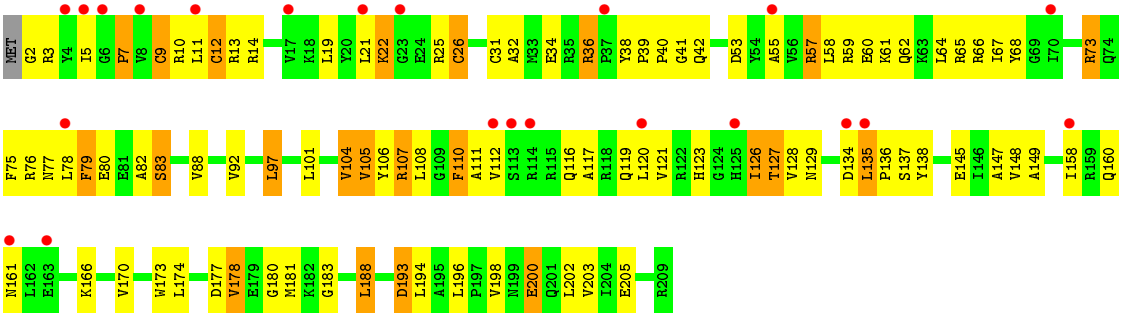
Chain CC:



- Molecule 4: 30S Ribosomal Protein S4

Chain AD:





- Molecule 4: 30S Ribosomal Protein S4

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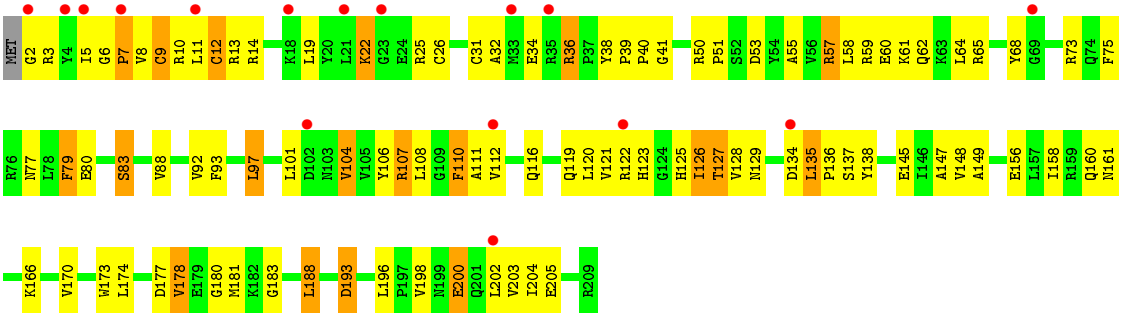
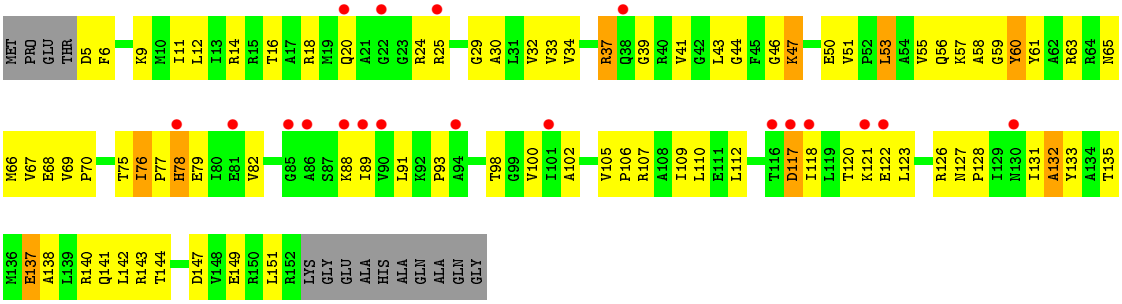


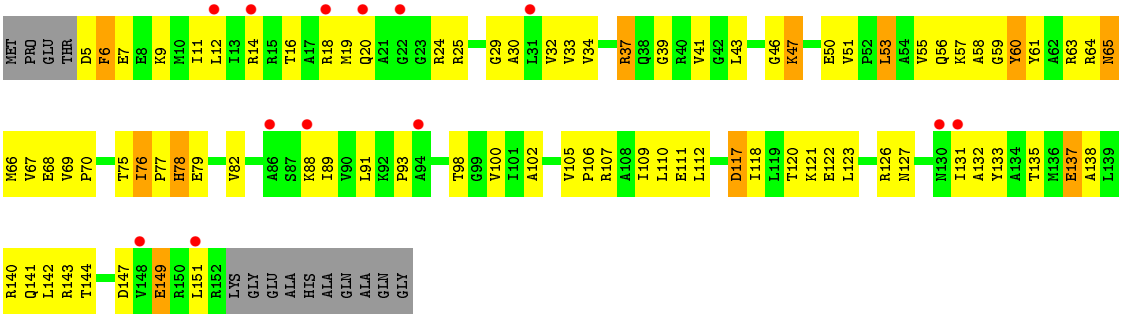
- Molecule 5: 30S Ribosomal Protein S5

Chain AE:



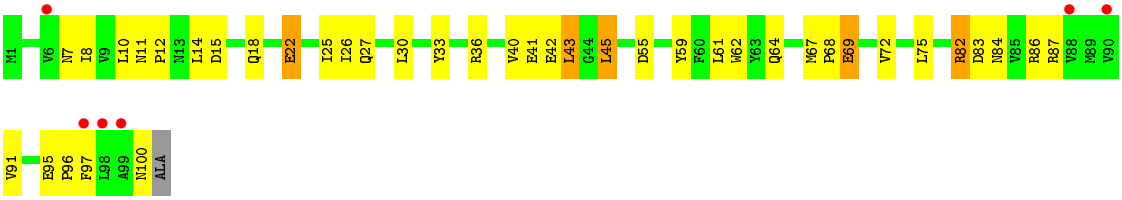
- Molecule 5: 30S Ribosomal Protein S5

Chain CE:



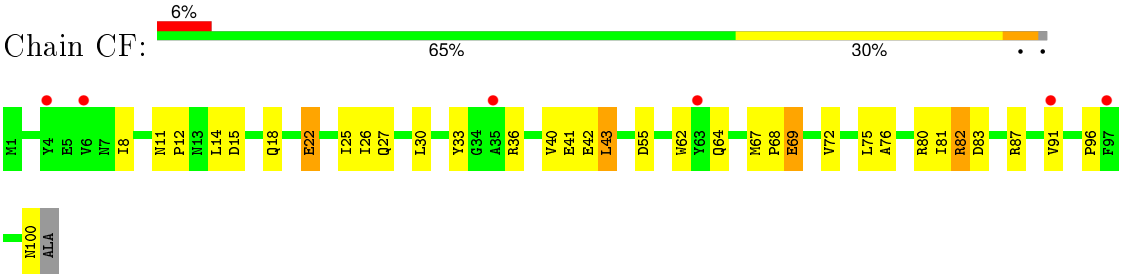
- Molecule 6: 30S Ribosomal Protein S6

Chain AF:



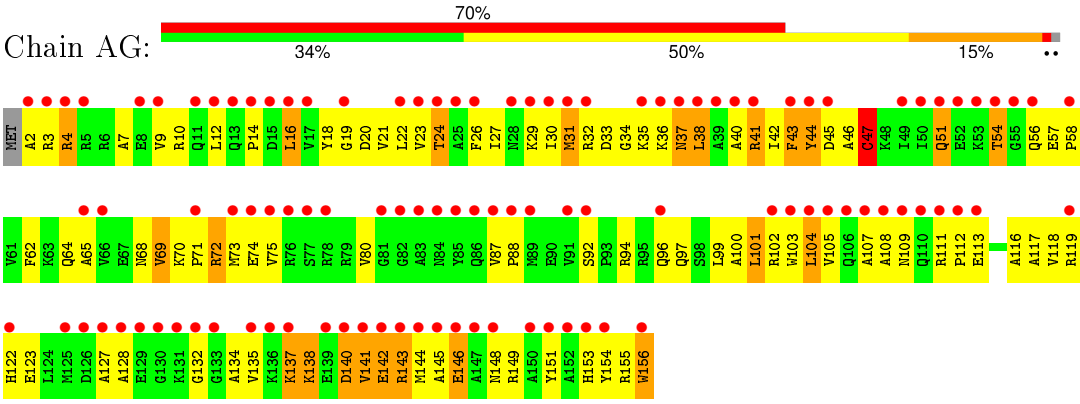
- Molecule 6: 30S Ribosomal Protein S6

Chain CF:



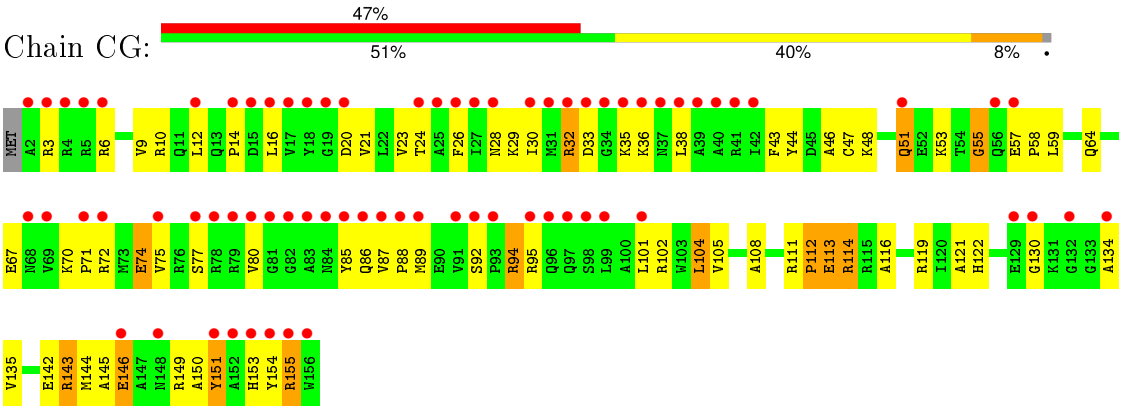
- Molecule 7: 30S Ribosomal Protein S7

Chain AG:



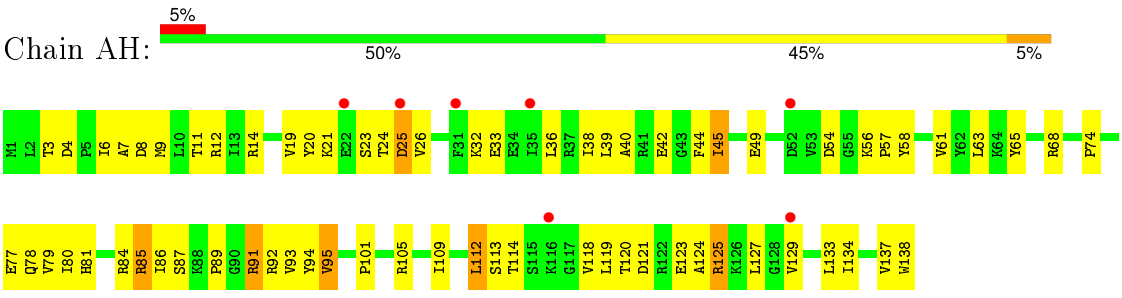
- Molecule 7: 30S Ribosomal Protein S7

Chain CG:



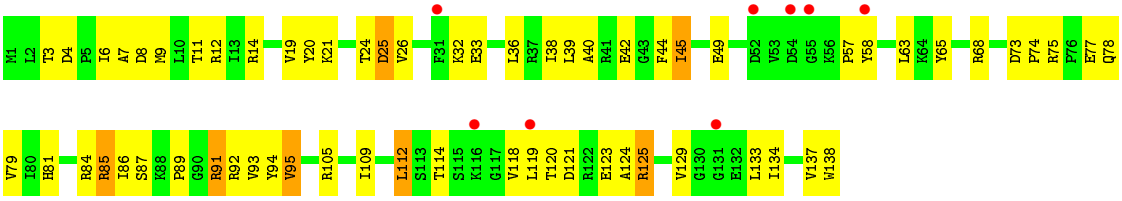
- Molecule 8: 30S Ribosomal Protein S8

Chain AH:



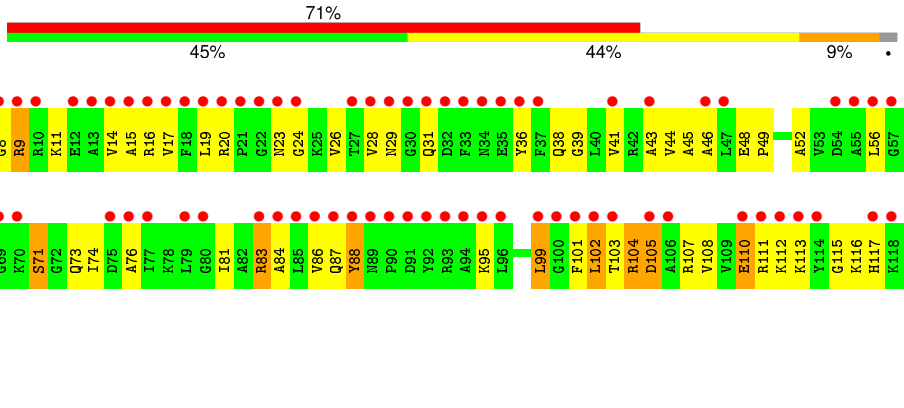
- Molecule 8: 30S Ribosomal Protein S8

Chain CH:



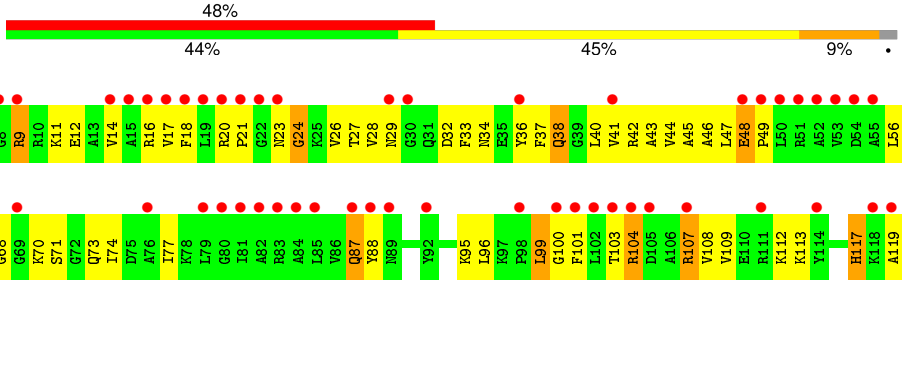
• Molecule 9: 30S Ribosomal Protein S9

Chain AI:



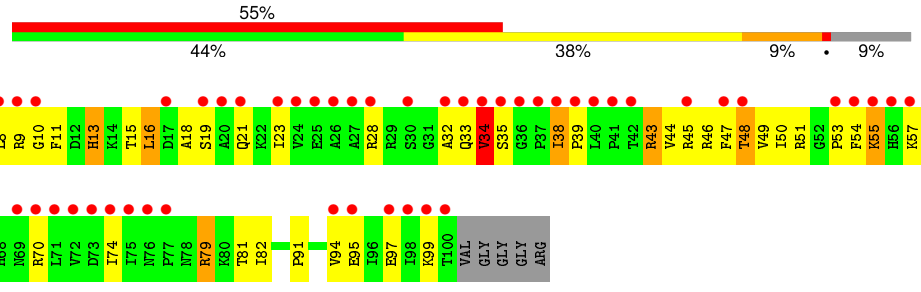
• Molecule 9: 30S Ribosomal Protein S9

Chain CI:



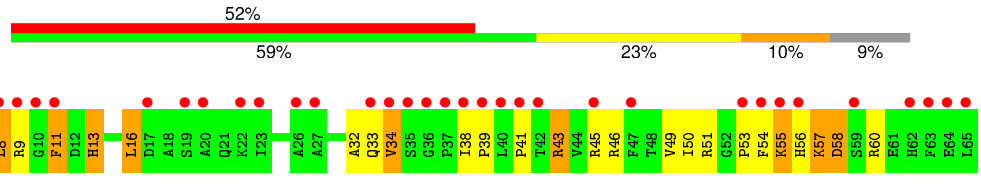
• Molecule 10: 30S Ribosomal Protein S10

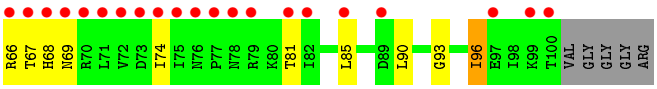
Chain AJ:



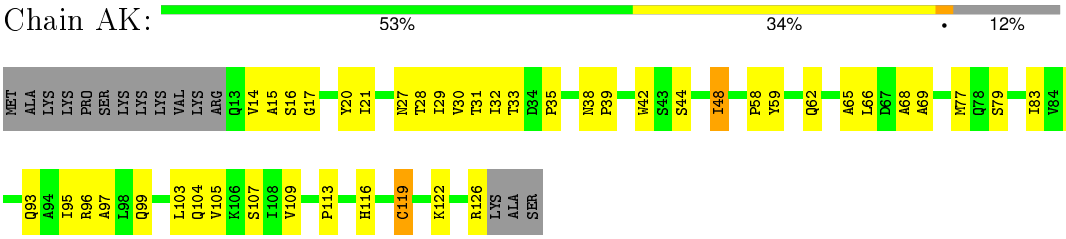
• Molecule 10: 30S Ribosomal Protein S10

Chain CJ:

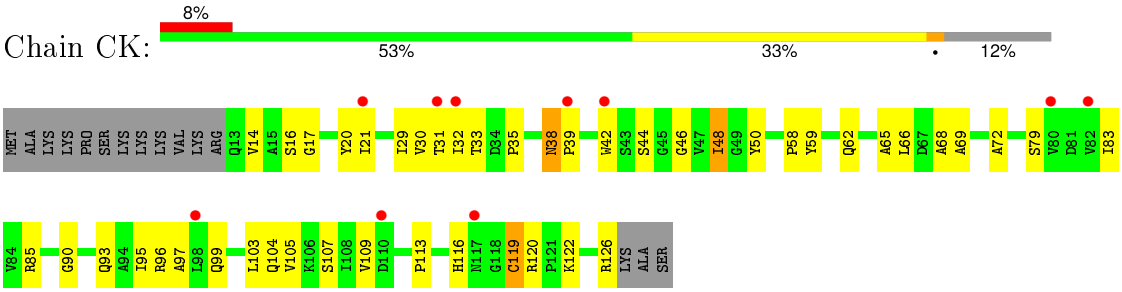




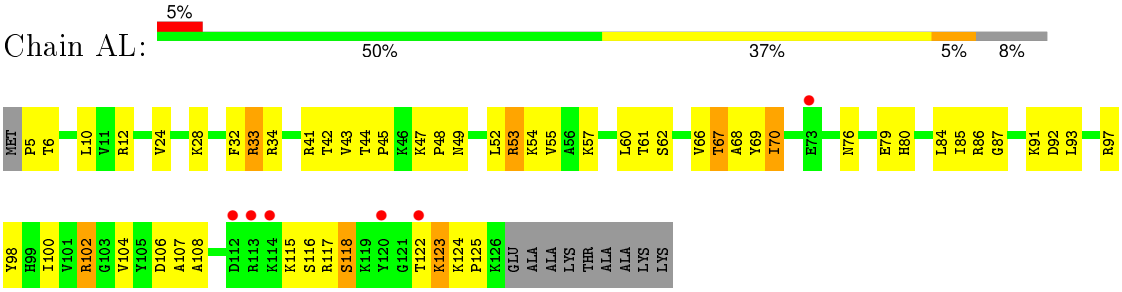
• Molecule 11: 30S Ribosomal Protein S11



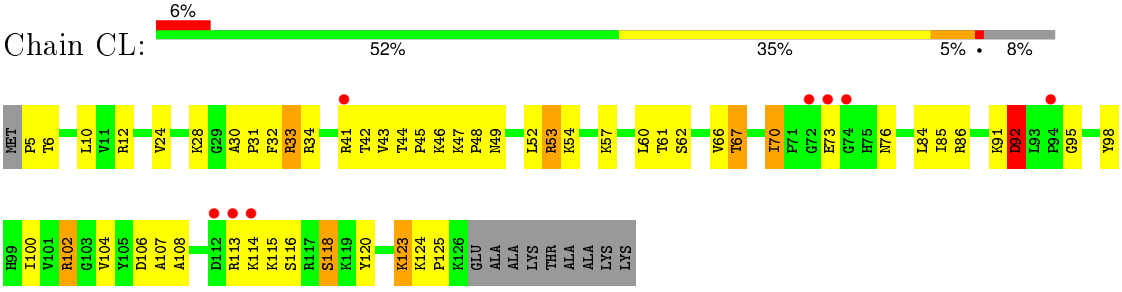
• Molecule 11: 30S Ribosomal Protein S11



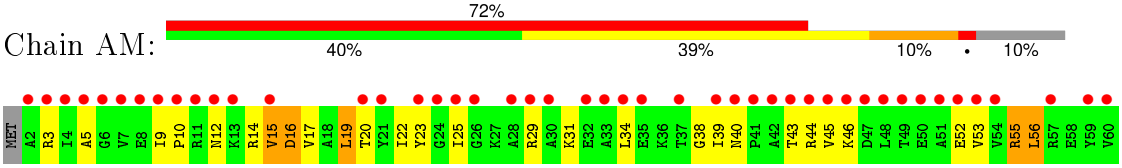
• Molecule 12: 30S Ribosomal Protein S12

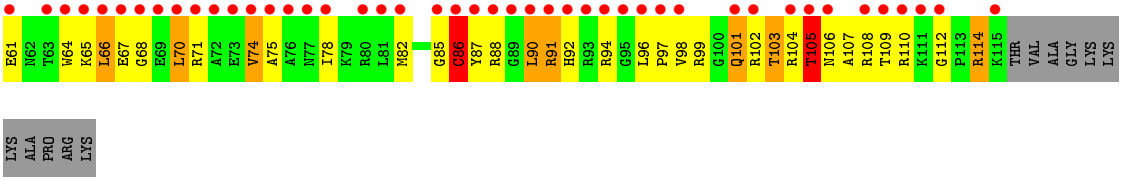


• Molecule 12: 30S Ribosomal Protein S12



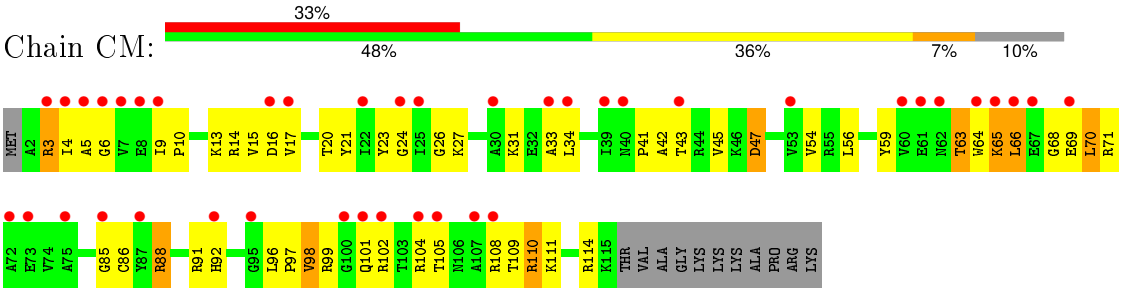
• Molecule 13: 30S Ribosomal Protein S13





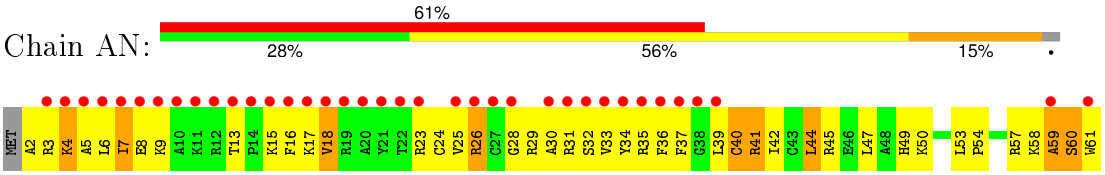
• Molecule 13: 30S Ribosomal Protein S13

Chain CM:



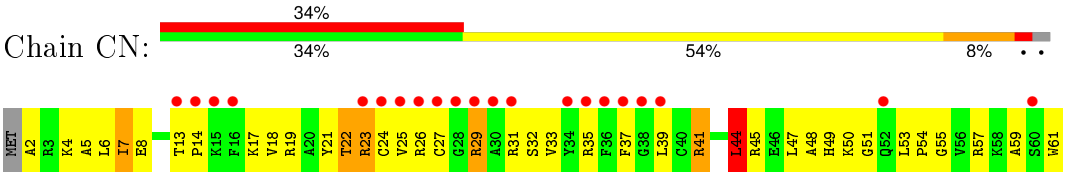
• Molecule 14: 30S Ribosomal Protein S14

Chain AN:



• Molecule 14: 30S Ribosomal Protein S14

Chain CN:



• Molecule 15: 30S Ribosomal Protein S15

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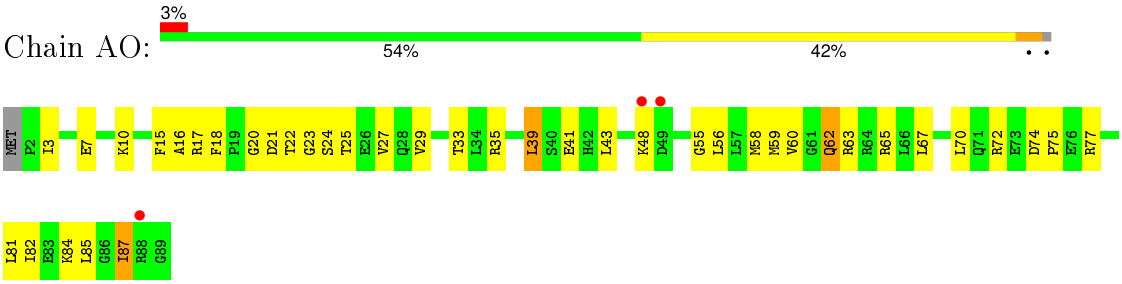

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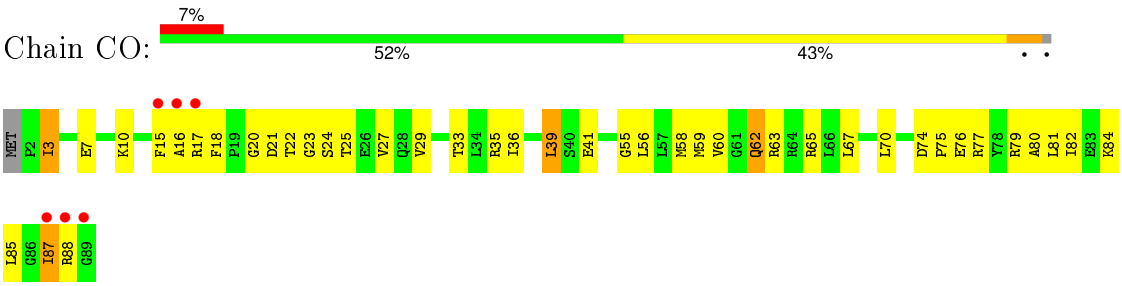

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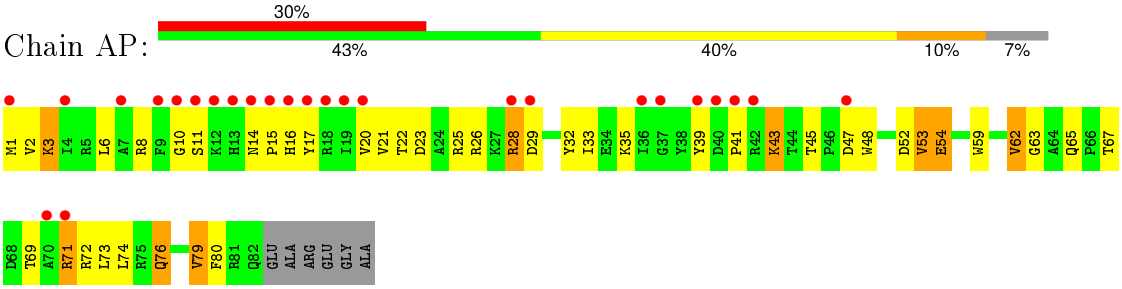

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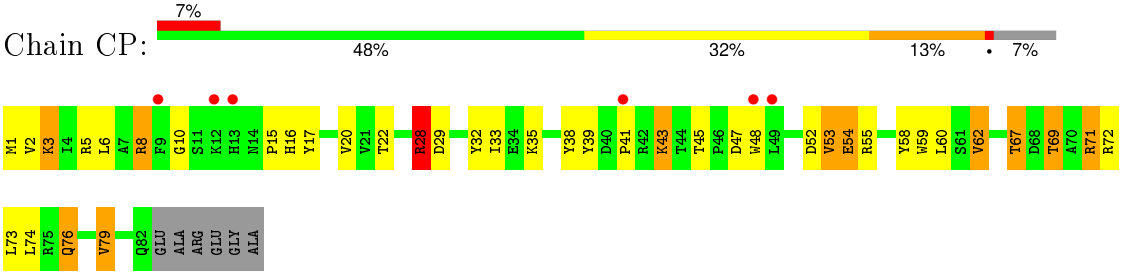

• Molecule 17: 30S Ribosomal Protein S17

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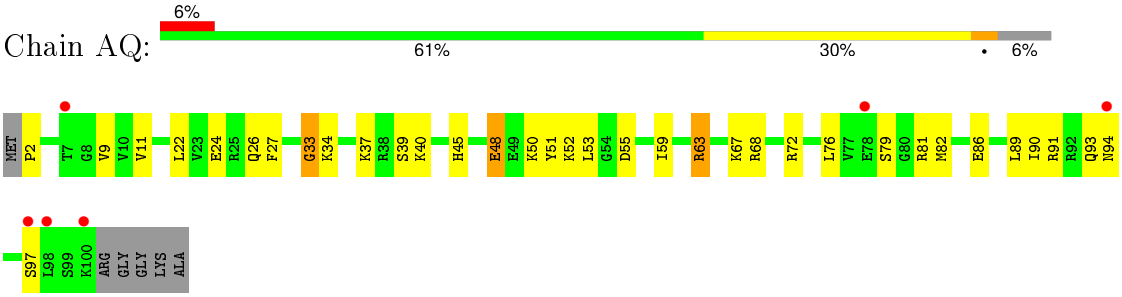

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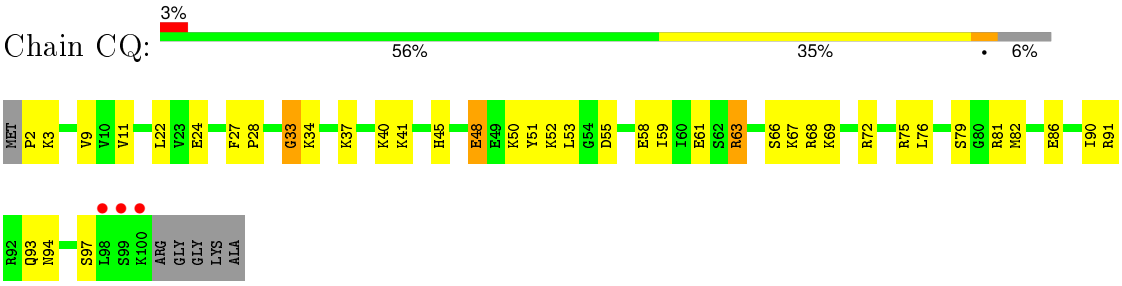

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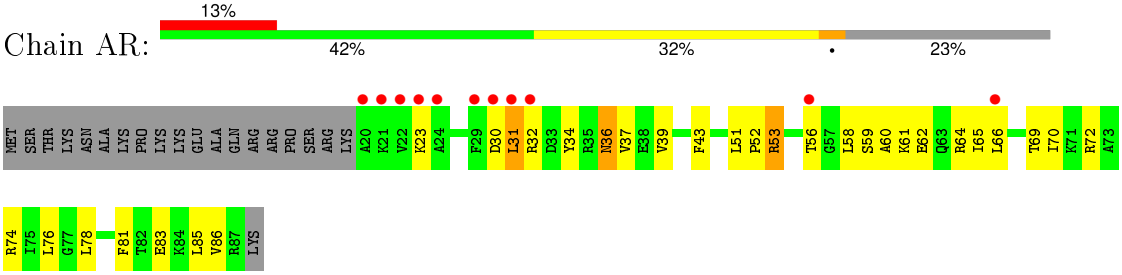

- Molecule 18: 30S Ribosomal Protein S18

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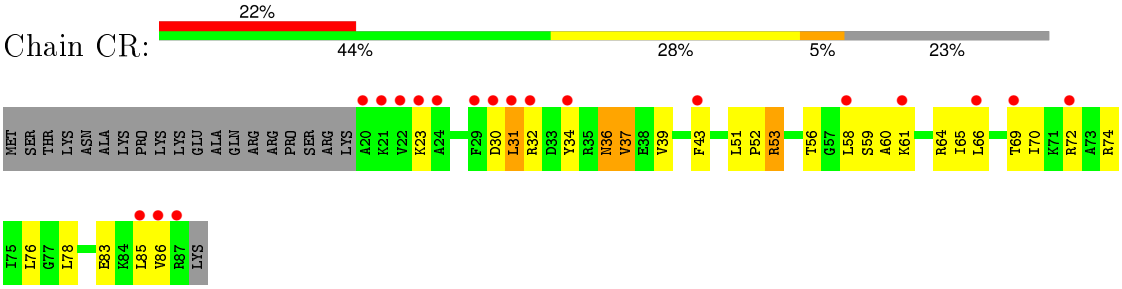

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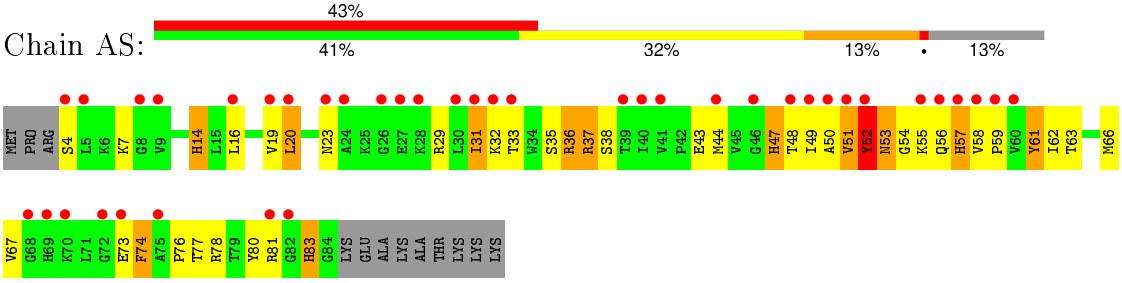

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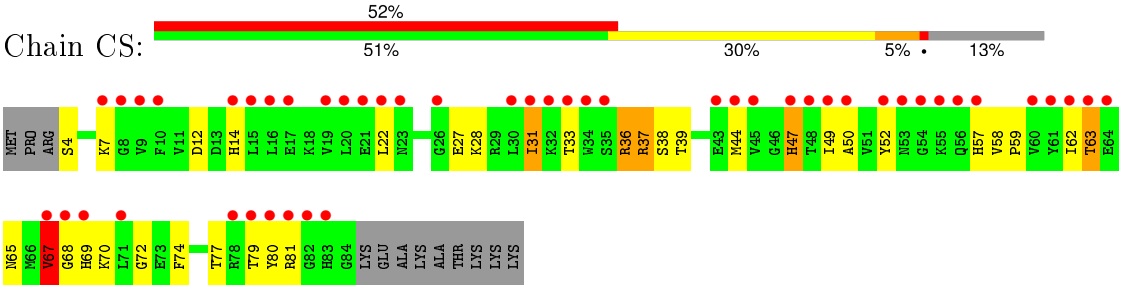

- Molecule 20: 30S Ribosomal Protein S20

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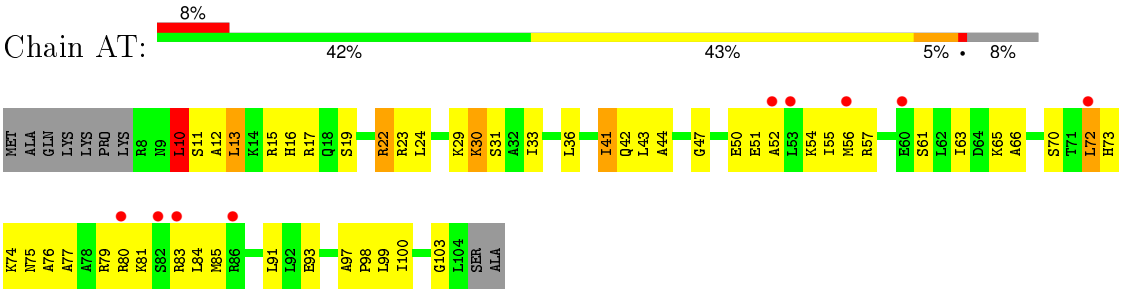

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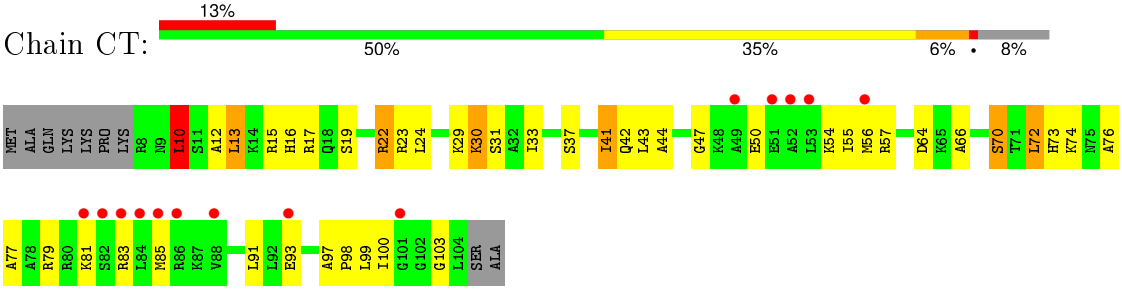

- Molecule 21: 30S Ribosomal Protein THX

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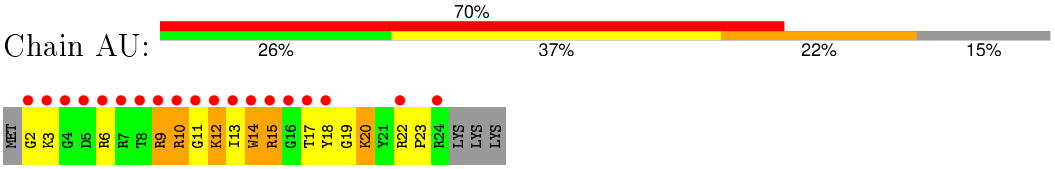

- Molecule 21: 30S Ribosomal Protein THX

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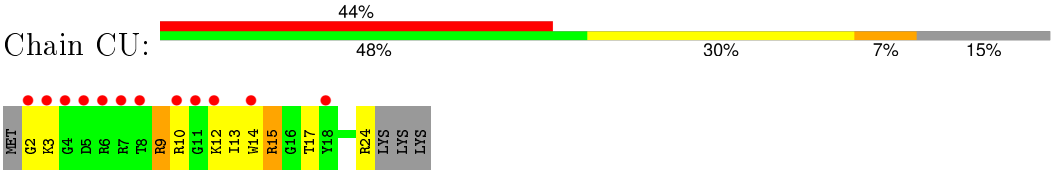

- Molecule 22: Ribosome modulation factor

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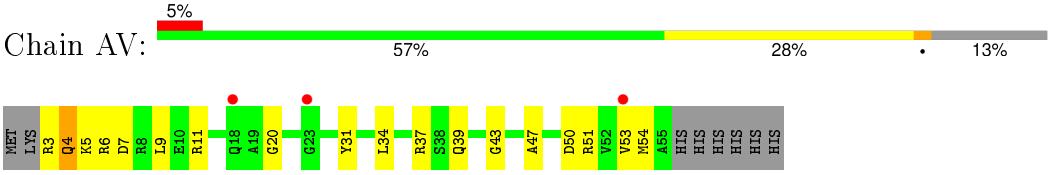

- Molecule 22: Ribosome modulation factor

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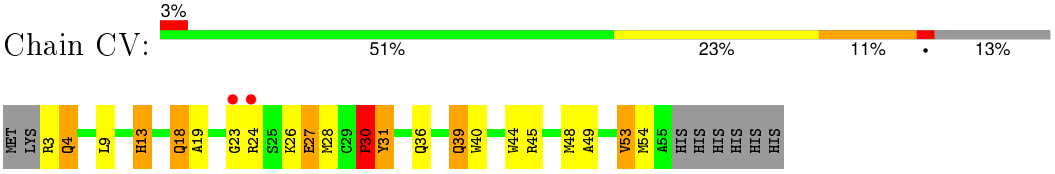

- Molecule 23: 23S Ribosomal RNA

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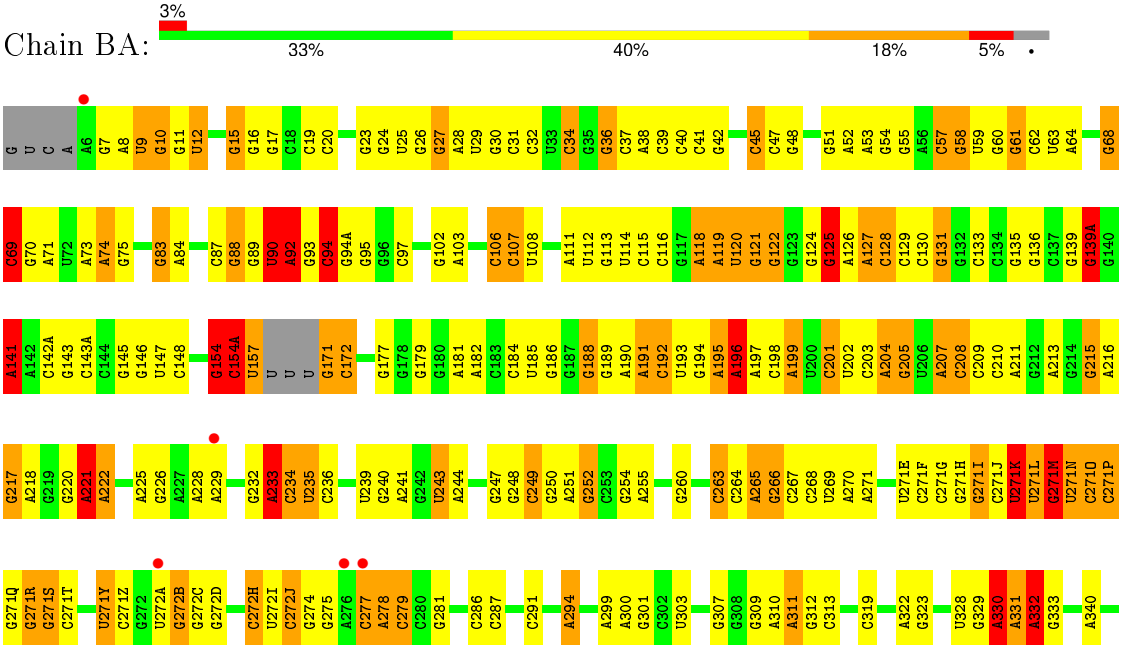

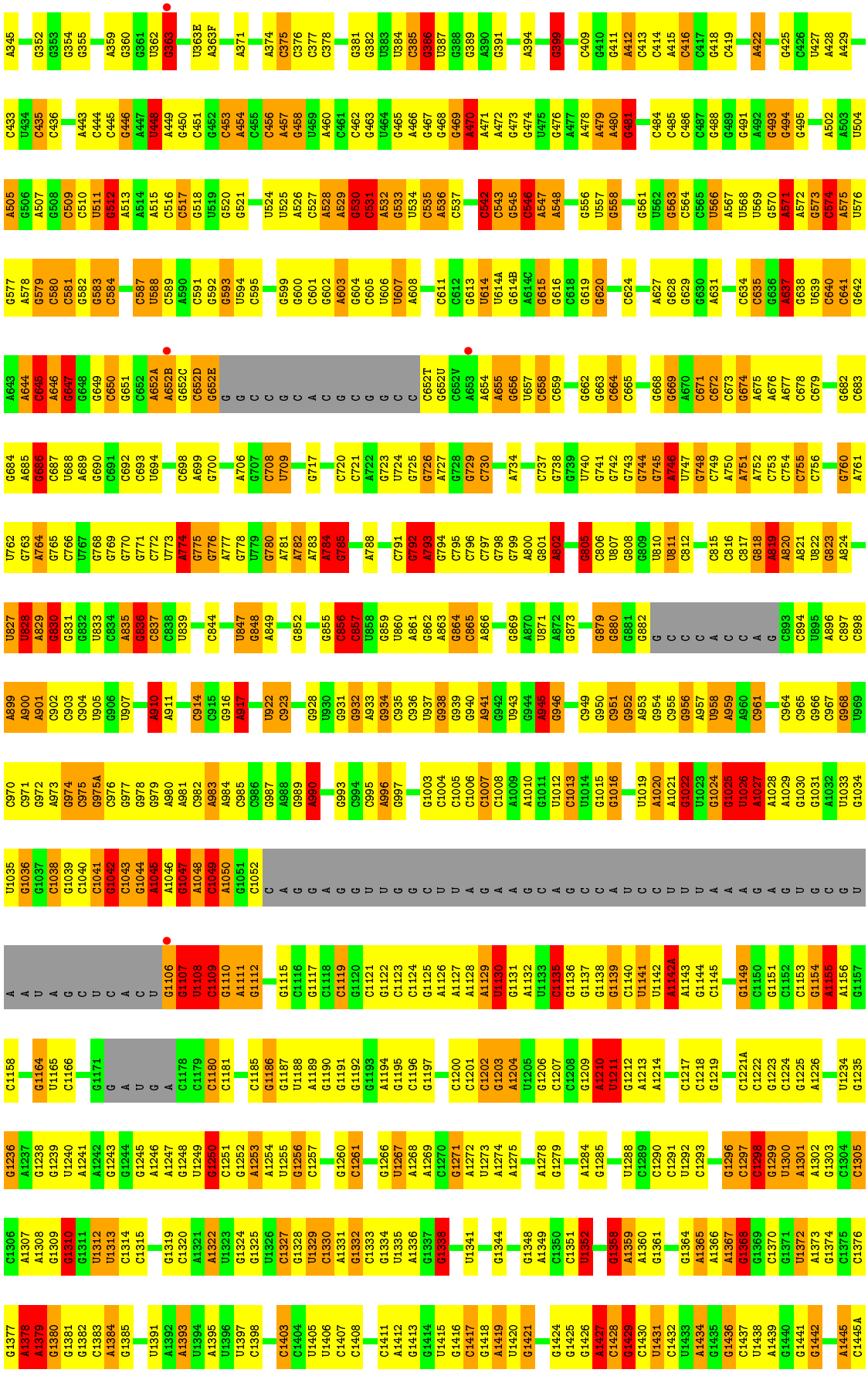
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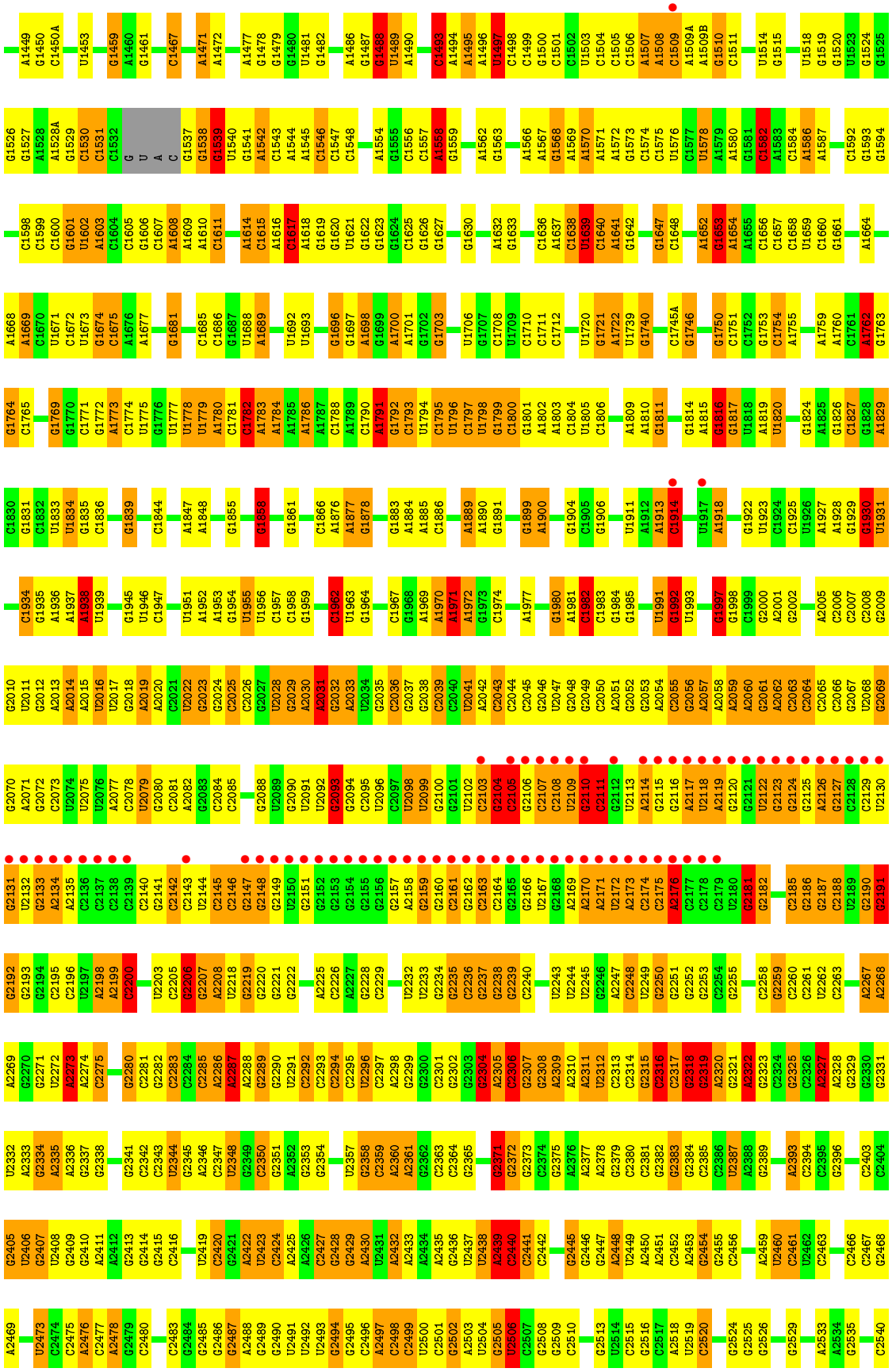

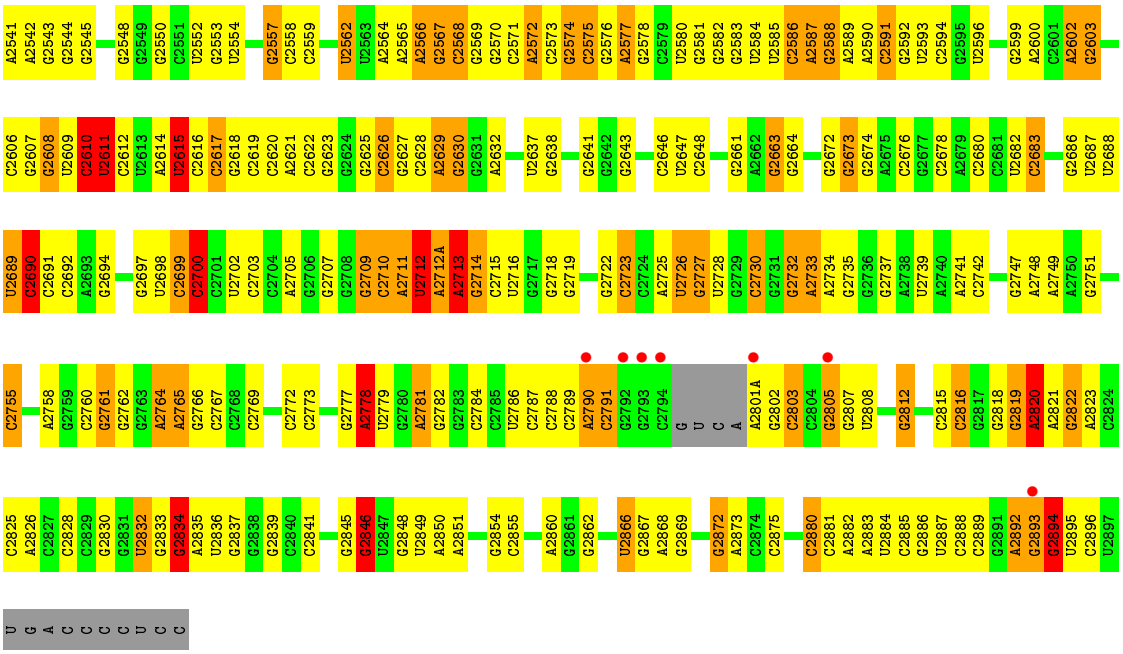

• Molecule 23: 23S Ribosomal RNA

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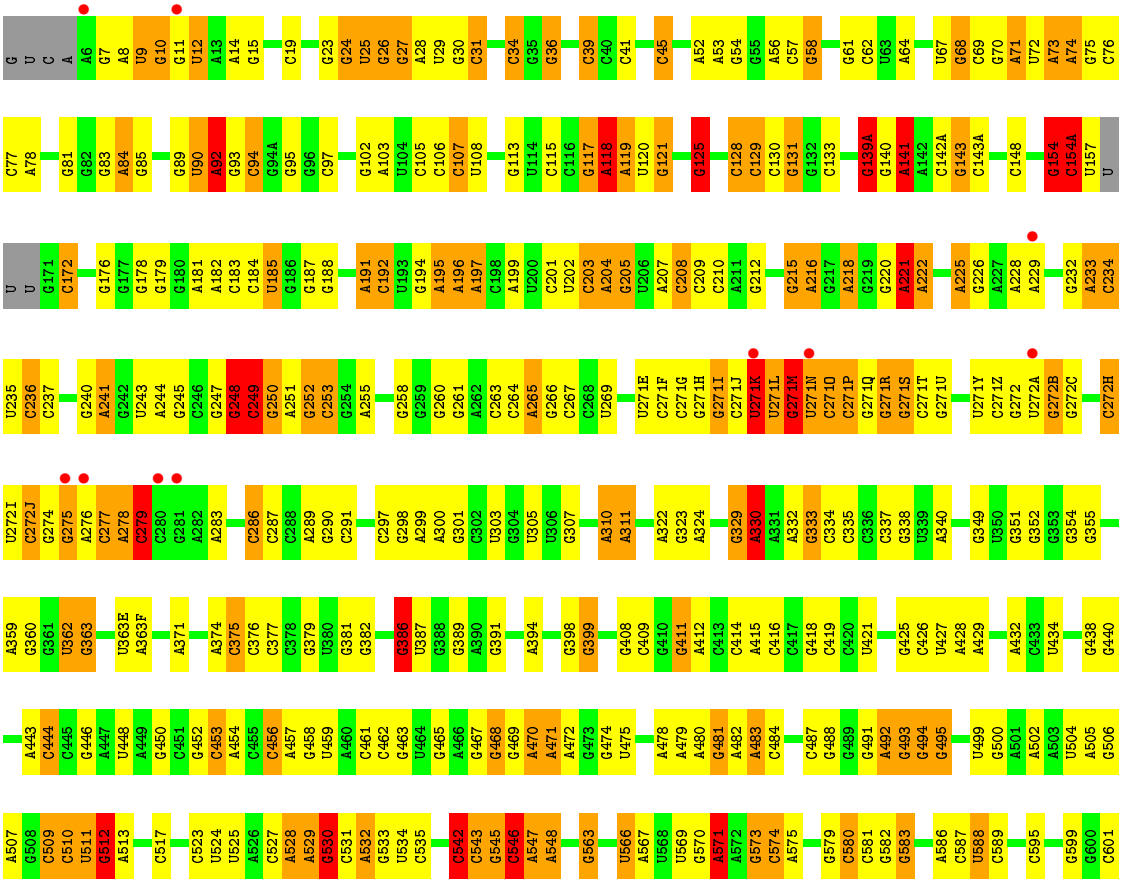

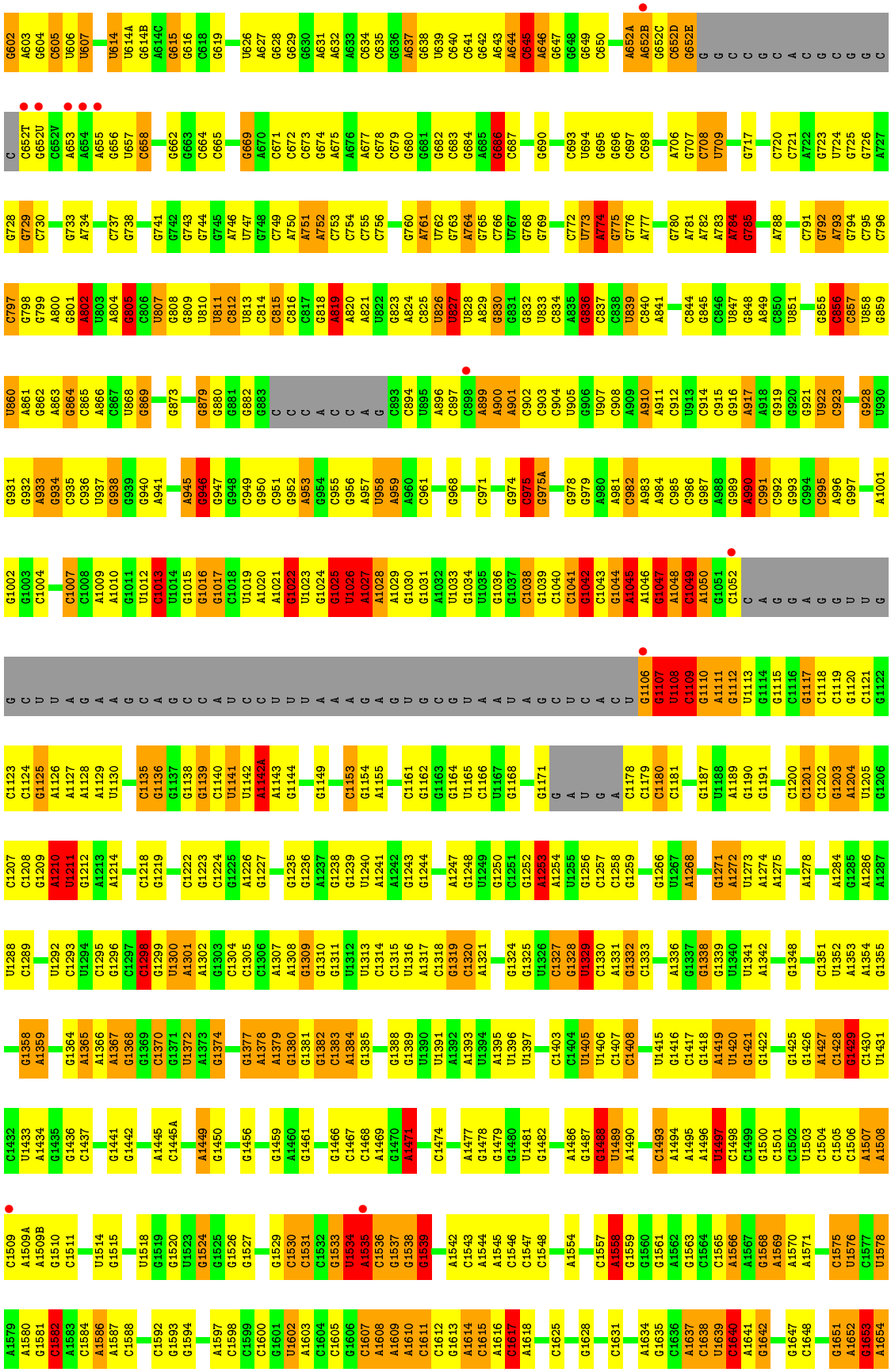

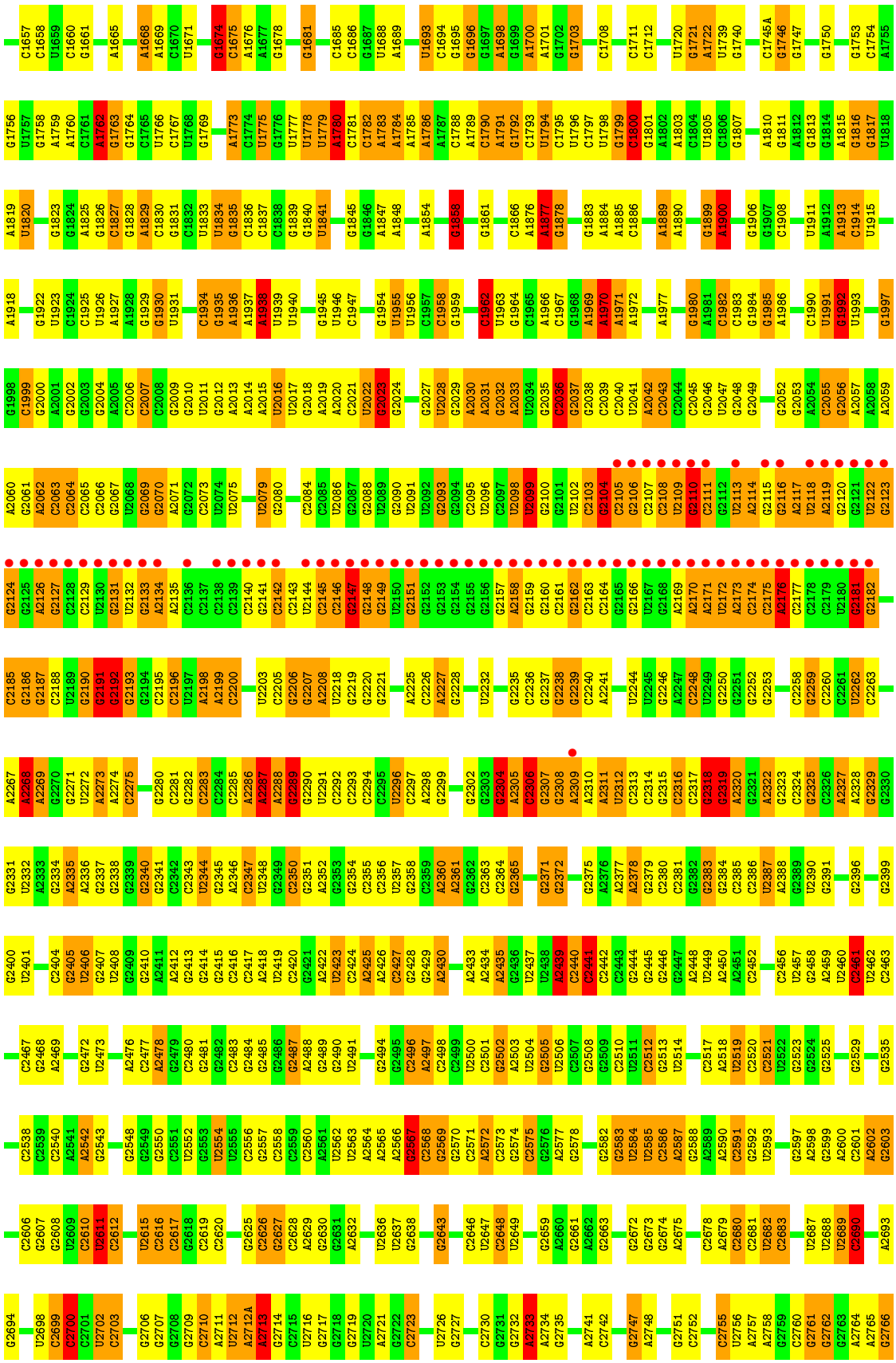
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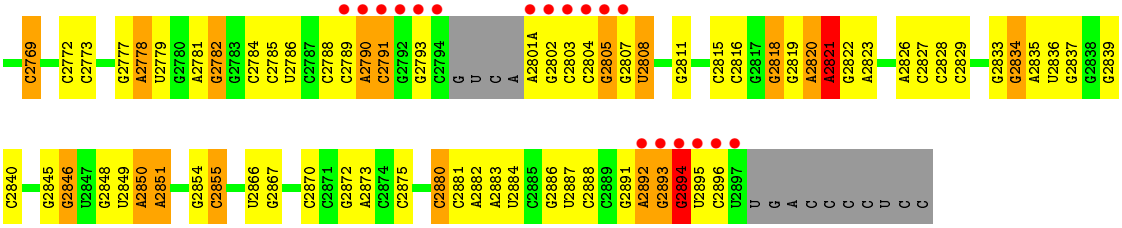
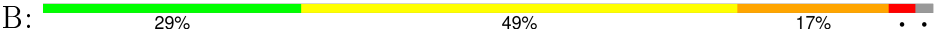
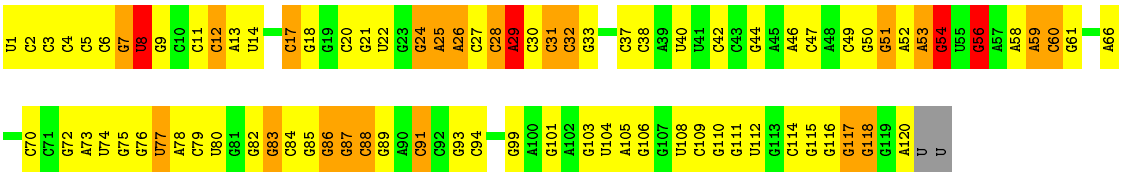


• Molecule 24: 5S Ribosomal RNA

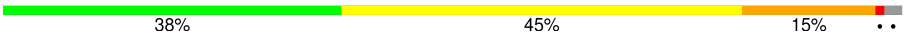
Chain BB:

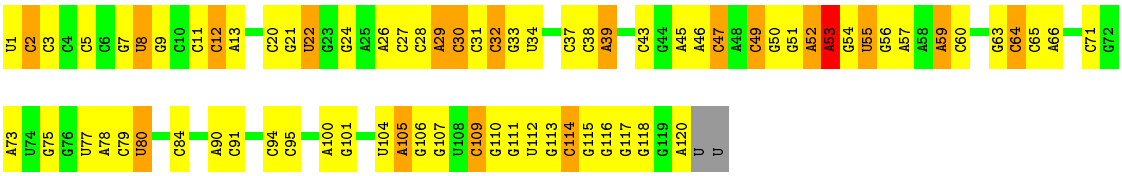




• Molecule 24: 5S Ribosomal RNA

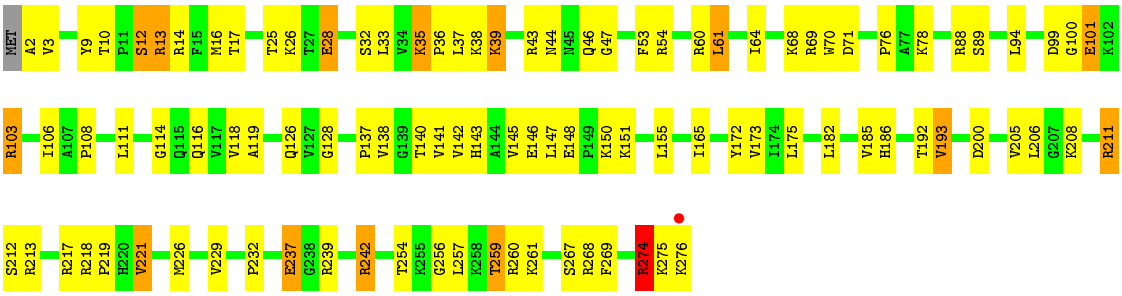
Chain DB:





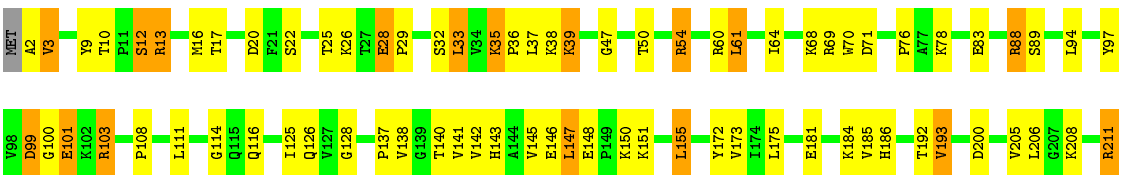
• Molecule 25: 50S Ribosomal Protein L2

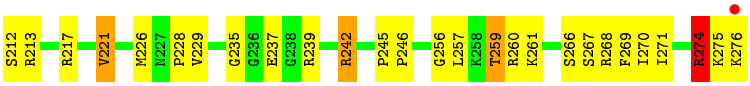
Chain BD:



• Molecule 25: 50S Ribosomal Protein L2

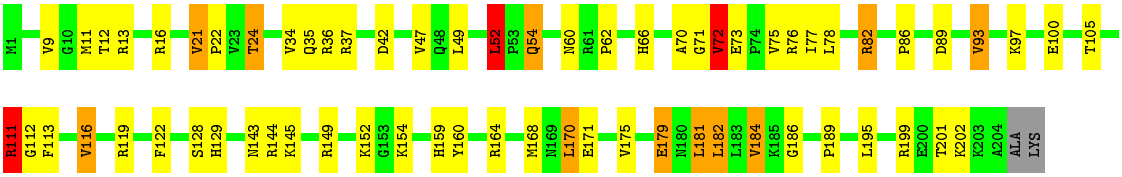
Chain DD:





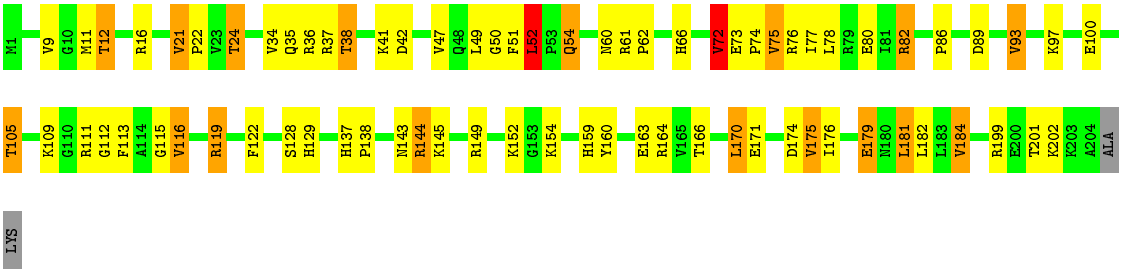
• Molecule 26: 50S Ribosomal Protein L3

Chain BE:



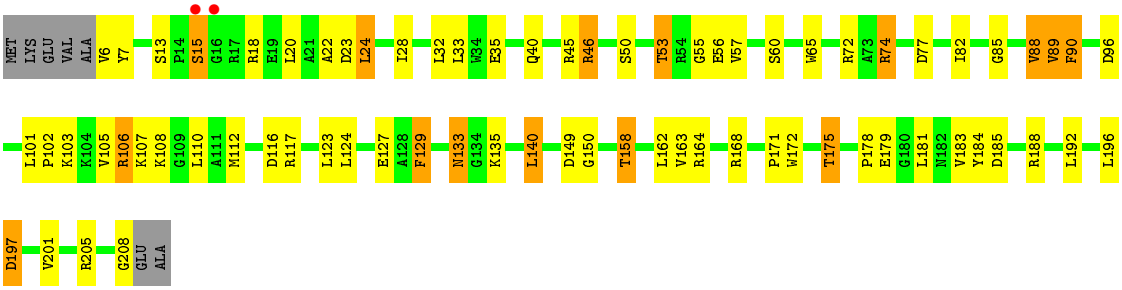
• Molecule 26: 50S Ribosomal Protein L3

Chain DE:



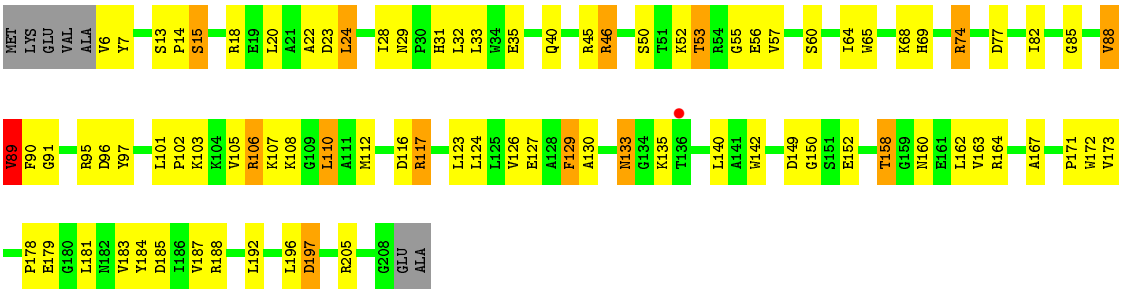
• Molecule 27: 50S Ribosomal Protein L4

Chain BF:



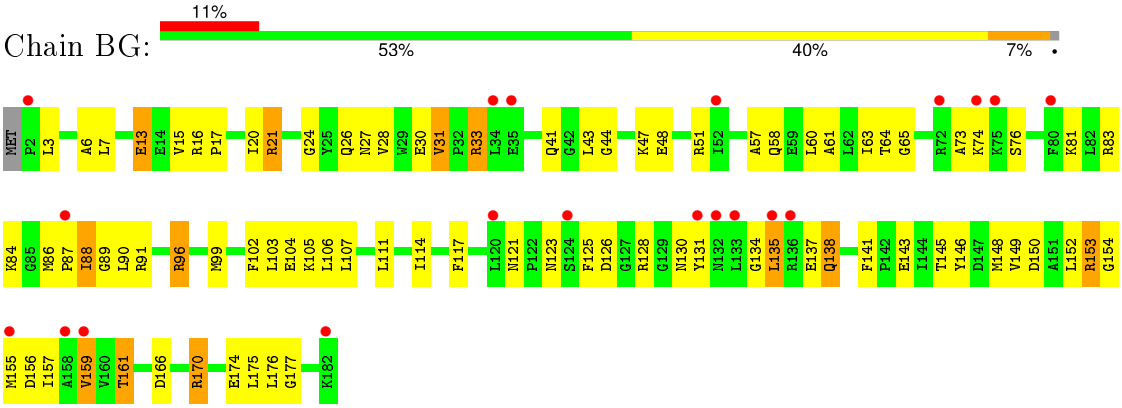
• Molecule 27: 50S Ribosomal Protein L4

Chain DF:



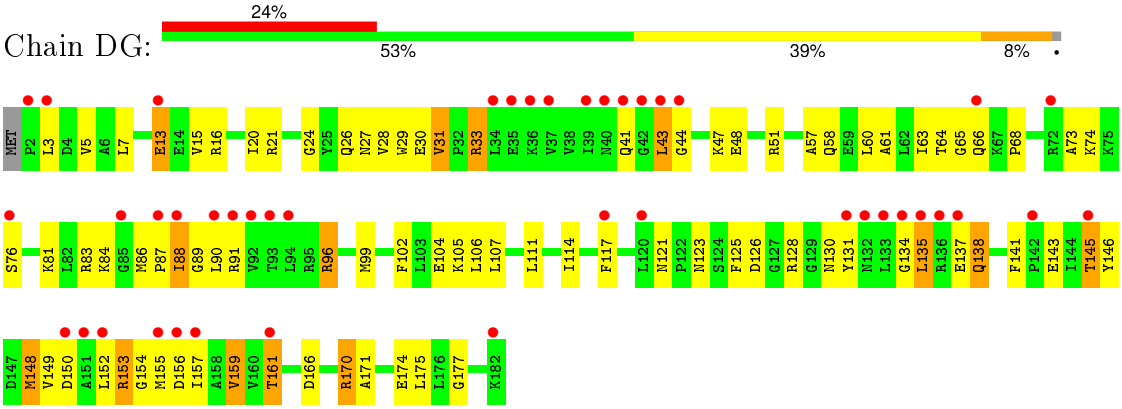
• Molecule 28: 50S Ribosomal Protein L5

Chain BG:



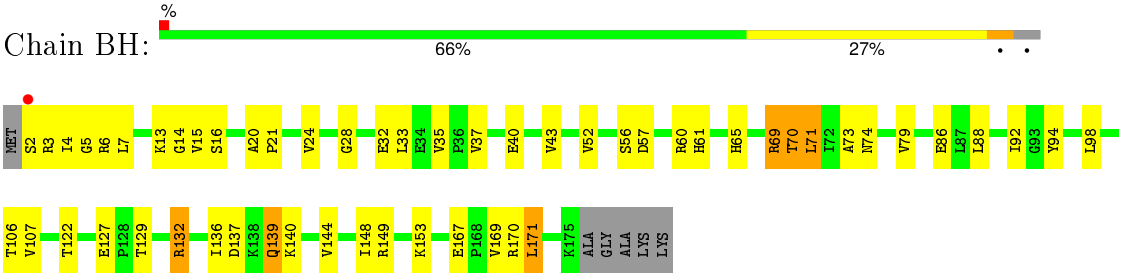
• Molecule 28: 50S Ribosomal Protein L5

Chain DG:



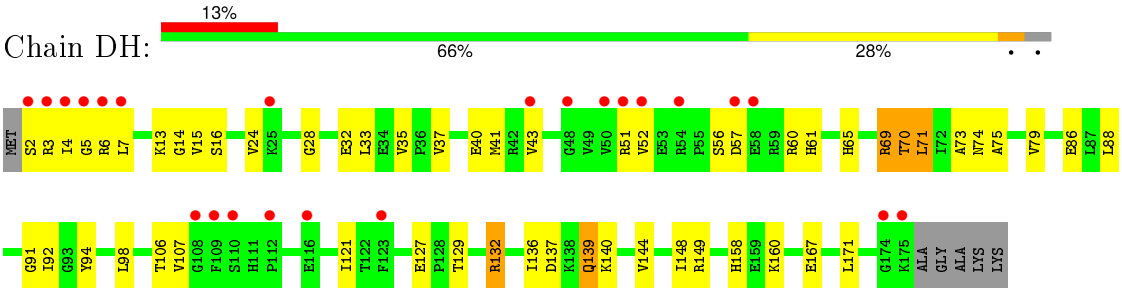
• Molecule 29: 50S Ribosomal Protein L6

Chain BH:



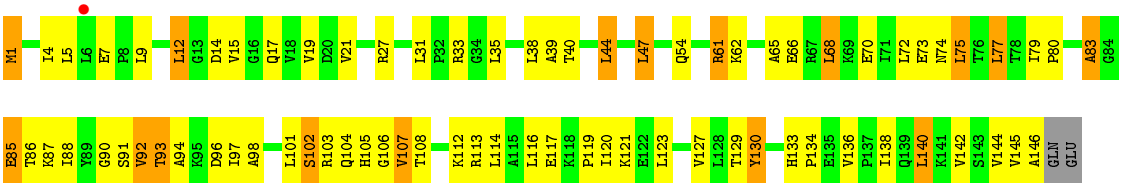
• Molecule 29: 50S Ribosomal Protein L6

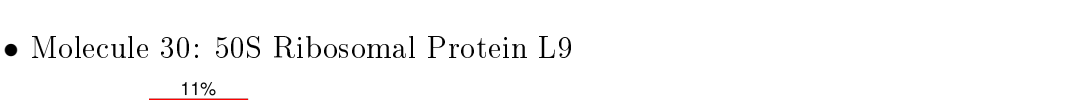
Chain DH:



• Molecule 30: 50S Ribosomal Protein L9

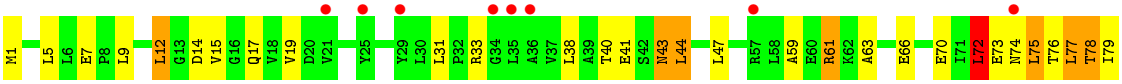
Chain BI:





• Molecule 30: 50S Ribosomal Protein L9

Chain DI:

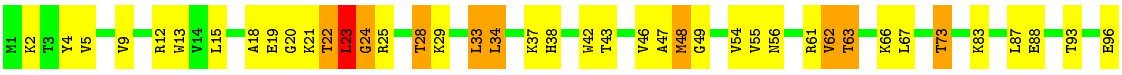


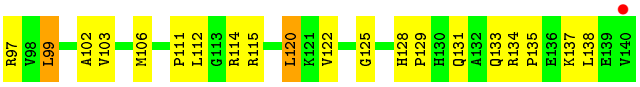
• Molecule 31: 50S Ribosomal Protein L13

Chain BN:

• Molecule 31: 50S Ribosomal Protein L13

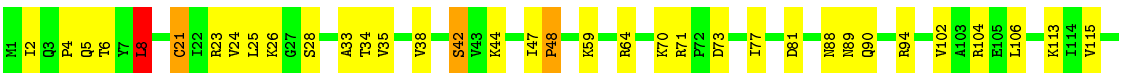
Chain DN:





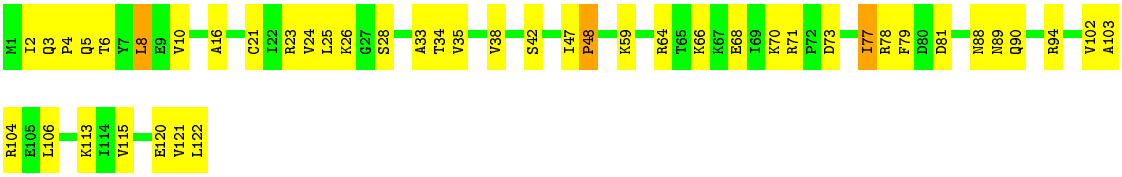
• Molecule 32: 50S Ribosomal Protein L14

Chain BO:



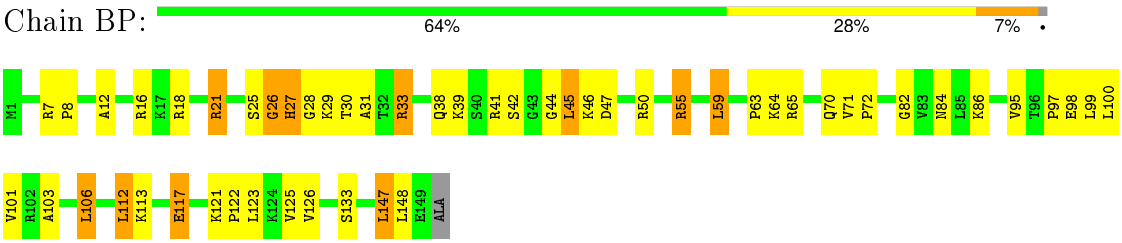
• Molecule 32: 50S Ribosomal Protein L14

Chain DO:



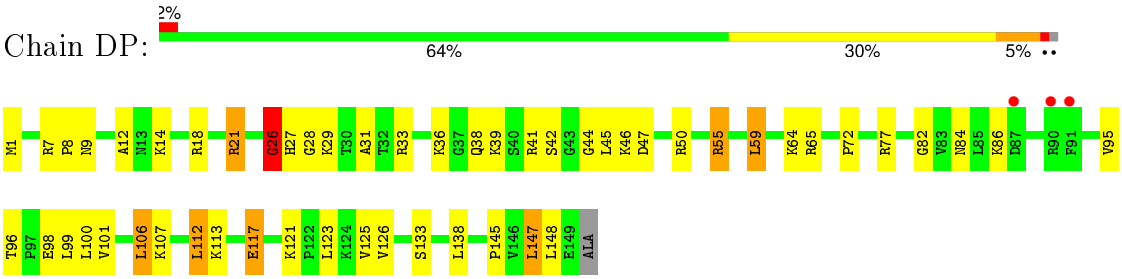
• Molecule 33: 50S Ribosomal Protein L15

Chain BP:



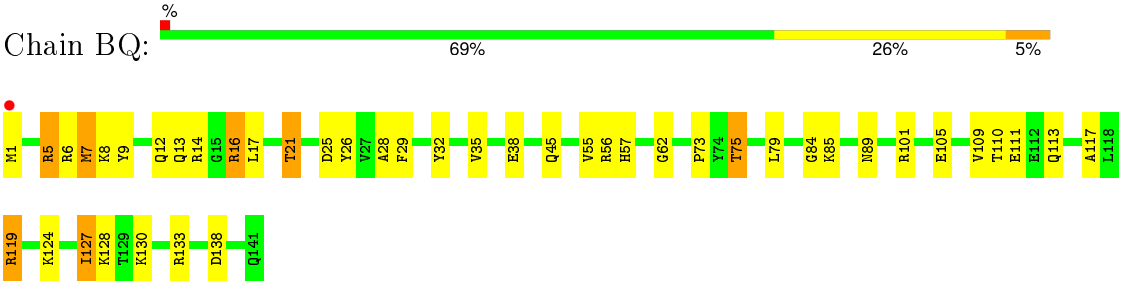
• Molecule 33: 50S Ribosomal Protein L15

Chain DP:



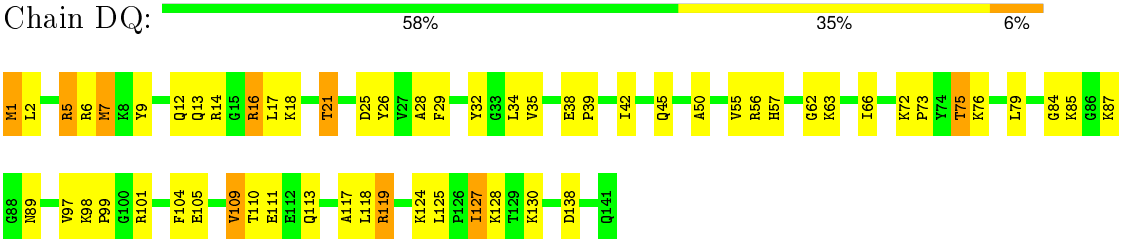
• Molecule 34: 50S Ribosomal Protein L16

Chain BQ:



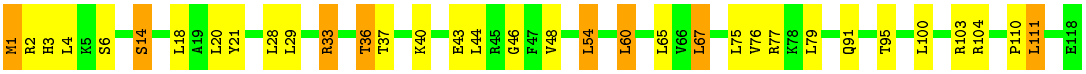
• Molecule 34: 50S Ribosomal Protein L16

Chain DQ:



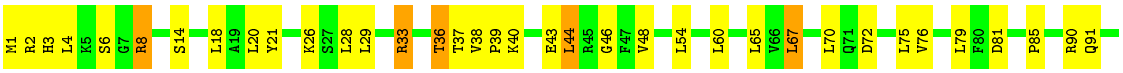
• Molecule 35: 50S Ribosomal Protein L17

Chain BR:



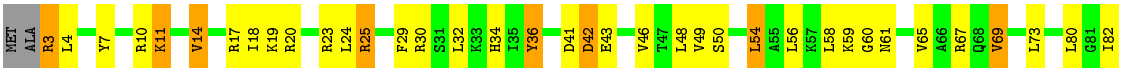
- Molecule 35: 50S Ribosomal Protein L17

Chain DR:



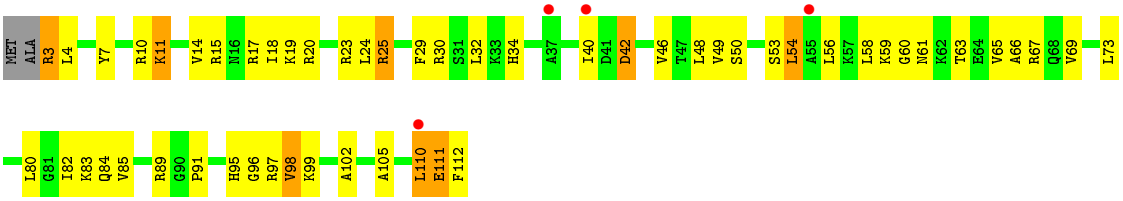
- Molecule 36: 50S Ribosomal Protein L18

Chain BS:



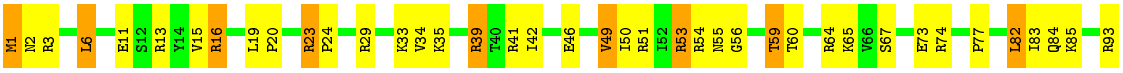
- Molecule 36: 50S Ribosomal Protein L18

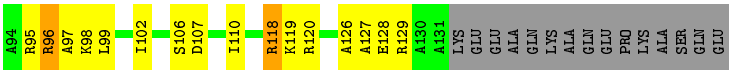
Chain DS:



- Molecule 37: 50S Ribosomal Protein L19

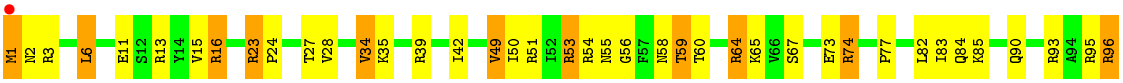
Chain BT:





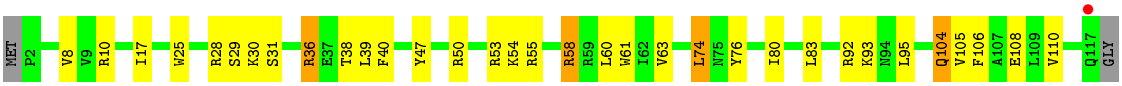
- Molecule 37: 50S Ribosomal Protein L19

Chain DT:



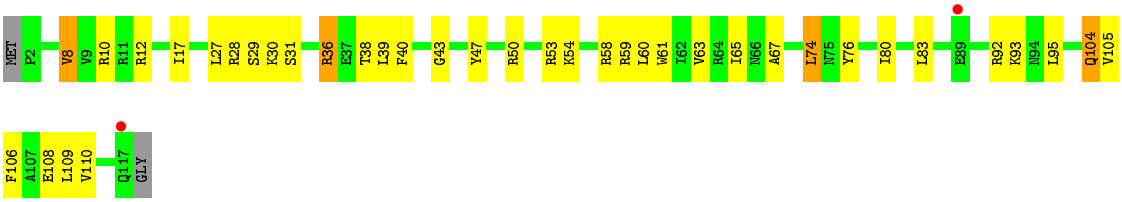
• Molecule 38: 50S Ribosomal Protein L20

Chain BU:



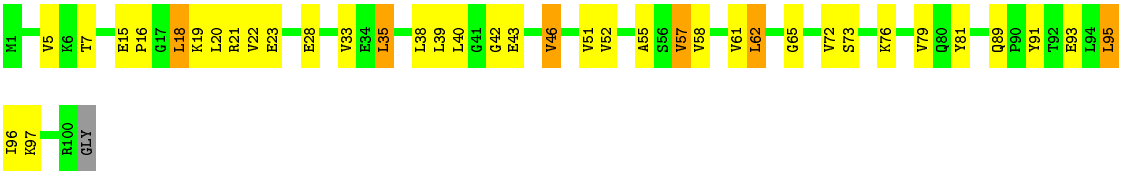
• Molecule 38: 50S Ribosomal Protein L20

Chain DU:



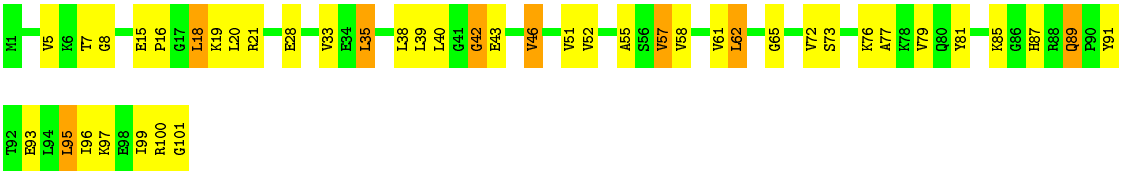
• Molecule 39: 50S Ribosomal Protein L21

Chain BV:



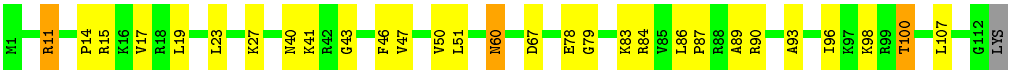
• Molecule 39: 50S Ribosomal Protein L21

Chain DV:



• Molecule 40: 50S Ribosomal Protein L22

Chain BW:

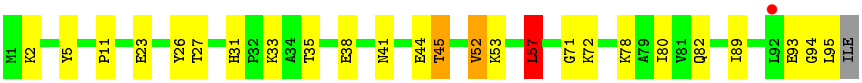


• Molecule 40: 50S Ribosomal Protein L22

Chain DW:

• Molecule 41: 50S Ribosomal Protein L23

Chain BX:

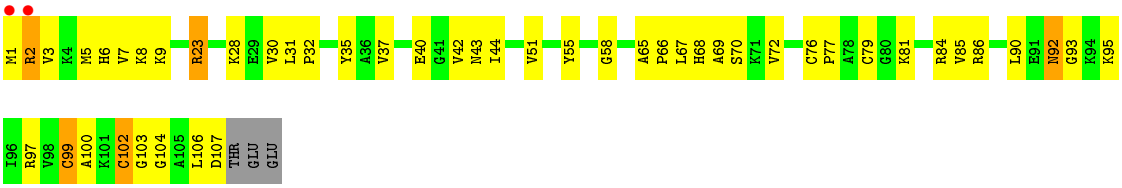


• Molecule 41: 50S Ribosomal Protein L23

Chain DX:

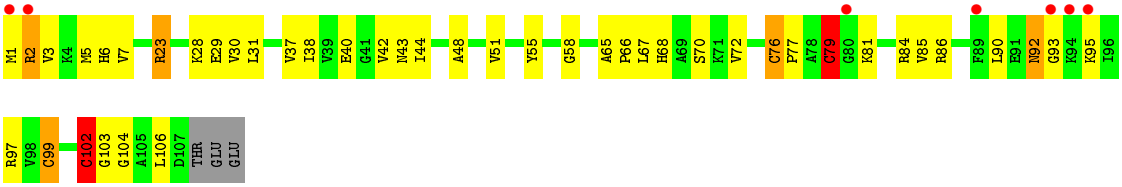
• Molecule 42: 50S Ribosomal Protein L24

Chain BY:



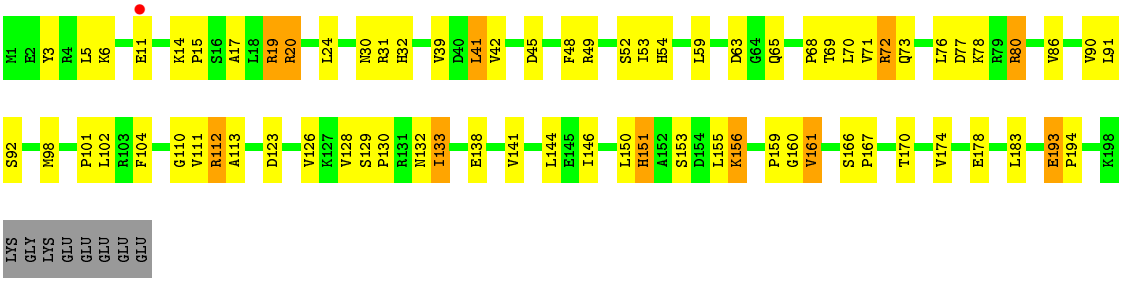
• Molecule 42: 50S Ribosomal Protein L24

Chain DY:



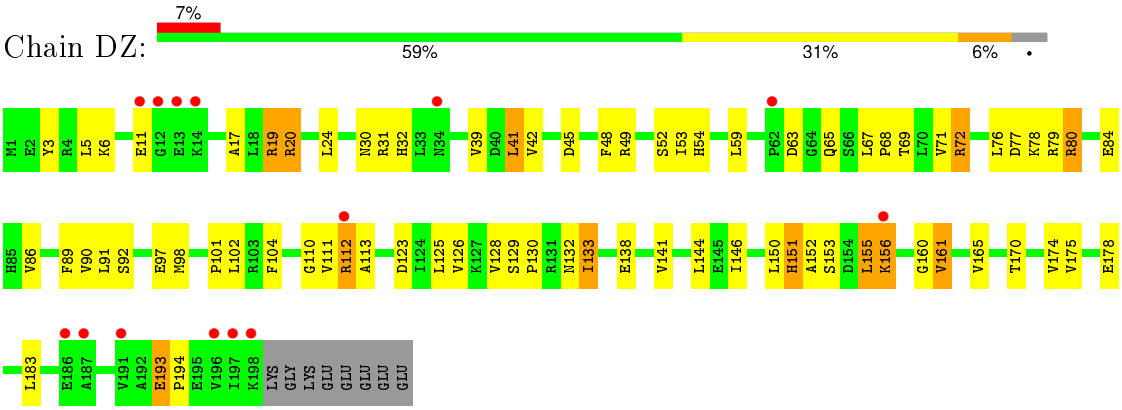
• Molecule 43: 50S Ribosomal Protein L25

Chain BZ:



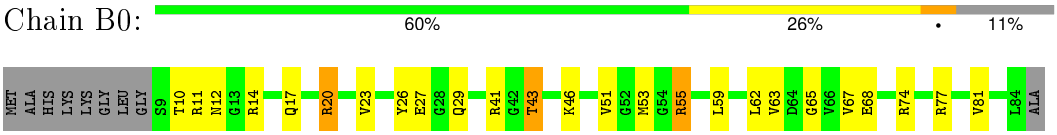
• Molecule 43: 50S Ribosomal Protein L25

Chain DZ:



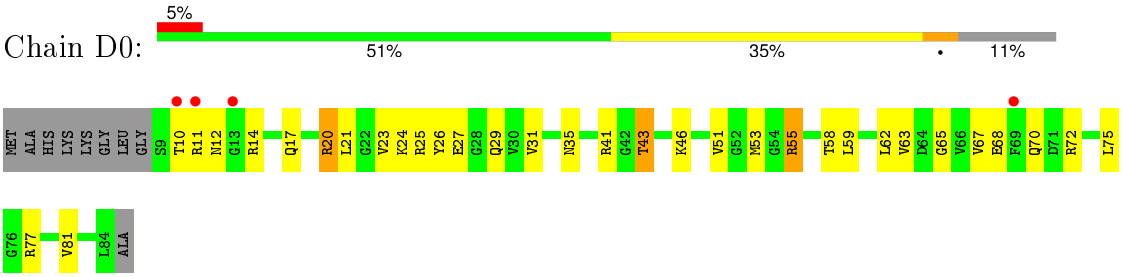
- Molecule 44: 50S Ribosomal Protein L27

Chain B0:



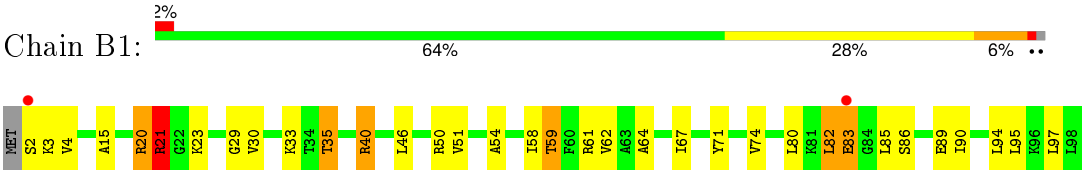
- Molecule 44: 50S Ribosomal Protein L27

Chain D0:



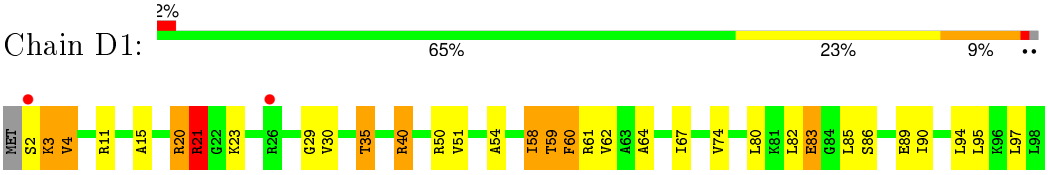
- Molecule 45: 50S Ribosomal Protein L28

Chain B1:



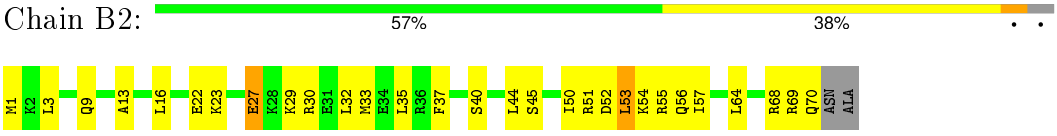
- Molecule 45: 50S Ribosomal Protein L28

Chain D1:



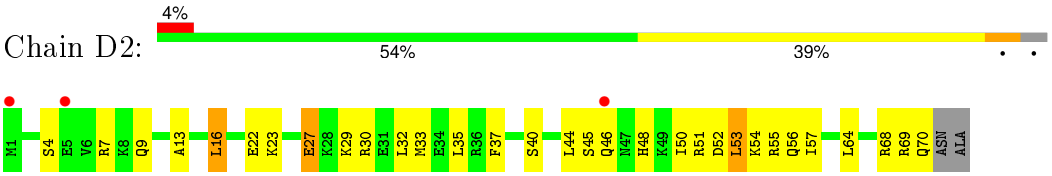
- Molecule 46: 50S Ribosomal Protein L29

Chain B2:



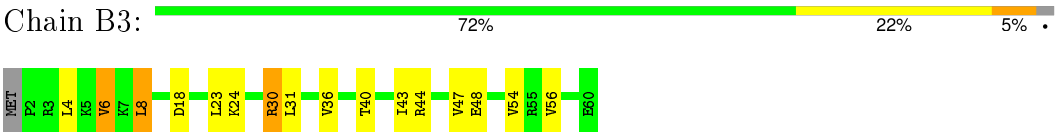
- Molecule 46: 50S Ribosomal Protein L29

Chain D2:



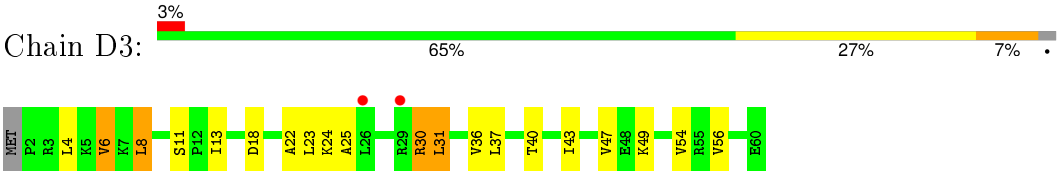
• Molecule 47: 50S Ribosomal Protein L30

Chain B3:



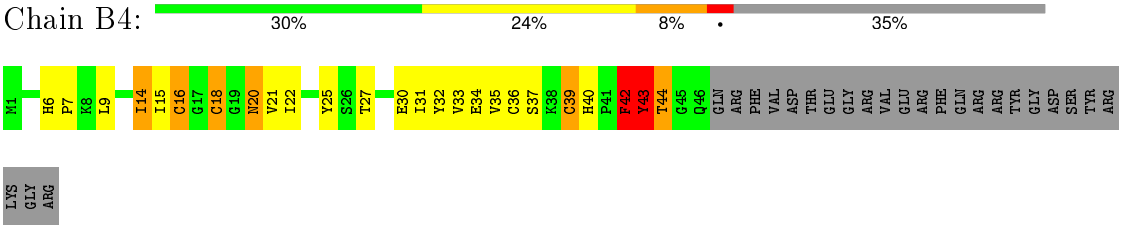
• Molecule 47: 50S Ribosomal Protein L30

Chain D3:



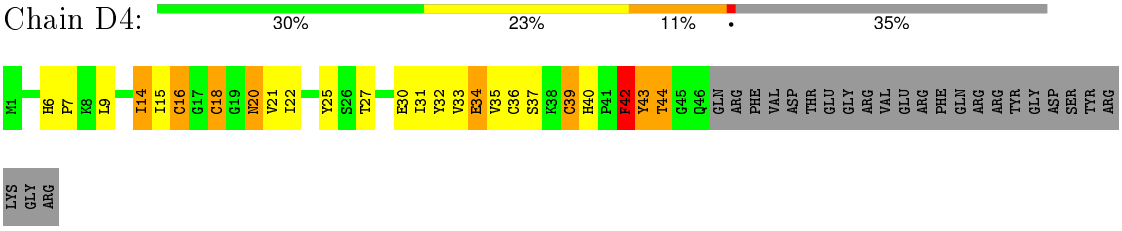
• Molecule 48: 50S Ribosomal Protein L31

Chain B4:



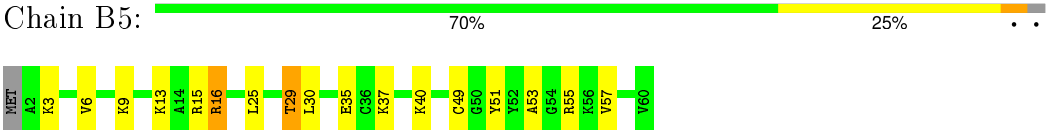
• Molecule 48: 50S Ribosomal Protein L31

Chain D4:



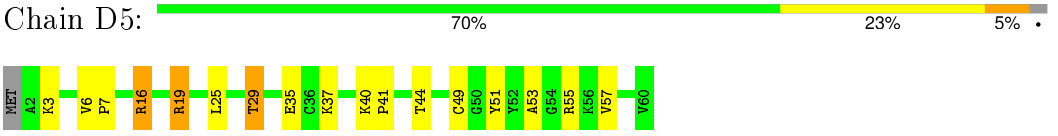
• Molecule 49: 50S Ribosomal Protein L32

Chain B5:



• Molecule 49: 50S Ribosomal Protein L32

Chain D5:

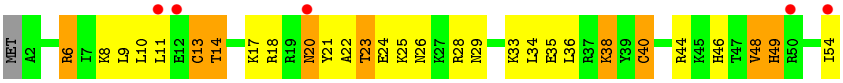


- Molecule 50: 50S Ribosomal Protein L33

Chain B6:

- Molecule 50: 50S Ribosomal Protein L33

Chain D6:

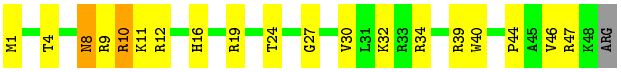


- Molecule 51: 50S Ribosomal Protein L34

Chain B7:

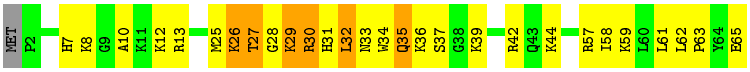
- Molecule 51: 50S Ribosomal Protein L34

Chain D7:



- Molecule 52: 50S Ribosomal Protein L35

Chain B8:

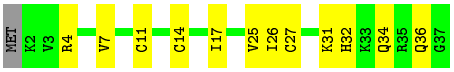


- Molecule 52: 50S Ribosomal Protein L35

Chain D8:

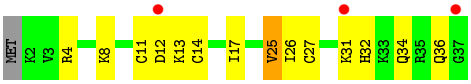
- Molecule 53: 50S Ribosomal Protein L36

Chain B9:



- Molecule 53: 50S Ribosomal Protein L36

Chain D9:


MET
K2
V3
R4
K8
C11
D12
K13
C14
I17
V25
I26
C27
K31
H32
K33
Q34
R36
Q36
G37

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.24Å 451.44Å 621.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.00 49.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.75-3.00) 98.0 (49.75-3.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.218 , 0.254 0.218 , 0.253	Depositor DCC
R_{free} test set	57194 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	68.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 1142037 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	283930	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AA	0.99	24/36215 (0.1%)	1.43	546/56522 (1.0%)
1	CA	0.91	21/36123 (0.1%)	1.38	452/56379 (0.8%)
2	AB	0.59	0/1809	0.73	1/2450 (0.0%)
2	CB	0.61	0/1809	0.73	1/2450 (0.0%)
3	AC	0.72	0/1474	0.82	2/2003 (0.1%)
3	CC	0.68	0/1474	0.79	2/2003 (0.1%)
4	AD	0.69	3/1556 (0.2%)	0.76	2/2113 (0.1%)
4	CD	0.64	2/1556 (0.1%)	0.74	2/2113 (0.1%)
5	AE	0.58	0/1121	0.79	0/1517
5	CE	0.58	0/1121	0.78	1/1517 (0.1%)
6	AF	0.55	0/790	0.71	0/1077
6	CF	0.54	0/790	0.70	0/1077
7	AG	0.83	0/1183	0.89	1/1599 (0.1%)
7	CG	0.72	0/1183	0.77	0/1599
8	AH	0.51	0/1065	0.67	0/1445
8	CH	0.50	0/1065	0.67	0/1445
9	AI	0.84	0/867	0.84	0/1180
9	CI	0.74	0/867	0.84	1/1180 (0.1%)
10	AJ	0.78	0/676	0.86	0/924
10	CJ	0.75	0/676	0.88	2/924 (0.2%)
11	AK	0.51	0/843	0.71	0/1144
11	CK	0.53	0/843	0.69	0/1144
12	AL	0.56	0/921	0.74	0/1247
12	CL	0.54	0/921	0.73	0/1247
13	AM	0.92	0/814	0.92	2/1107 (0.2%)
13	CM	0.72	0/814	0.83	0/1107
14	AN	0.79	0/487	0.93	0/649
14	CN	0.66	0/487	0.71	1/649 (0.2%)
15	AO	0.52	0/735	0.72	0/981
15	CO	0.52	0/735	0.72	0/981
16	AP	0.56	0/667	0.82	0/905
16	CP	0.54	0/667	0.84	1/905 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.56	0/836	0.72	0/1117
17	CQ	0.57	0/836	0.72	0/1117
18	AR	0.54	0/519	0.79	0/699
18	CR	0.56	0/519	0.79	0/699
19	AS	0.92	0/574	0.92	0/781
19	CS	0.69	0/574	0.81	0/781
20	AT	0.54	0/715	0.78	0/947
20	CT	0.52	0/715	0.77	0/947
21	AU	0.78	0/203	0.77	0/266
21	CU	0.73	0/203	0.68	0/266
22	AV	0.63	0/339	0.75	0/464
22	CV	0.65	0/360	0.85	1/492 (0.2%)
23	BA	1.60	727/67771 (1.1%)	1.72	2179/105789 (2.1%)
23	DA	1.16	149/67893 (0.2%)	1.60	1664/105982 (1.6%)
24	BB	1.11	3/2878 (0.1%)	1.57	62/4490 (1.4%)
24	DB	0.97	4/2878 (0.1%)	1.46	37/4490 (0.8%)
25	BD	0.88	3/2186 (0.1%)	0.96	0/2944
25	DD	0.80	2/2186 (0.1%)	0.91	1/2944 (0.0%)
26	BE	0.89	0/1588	0.96	3/2145 (0.1%)
26	DE	0.75	0/1588	0.92	0/2145
27	BF	0.88	1/1615 (0.1%)	0.86	0/2188
27	DF	0.70	0/1615	0.90	2/2188 (0.1%)
28	BG	0.53	0/1393	0.71	0/1892
28	DG	0.59	0/1393	0.71	0/1892
29	BH	0.68	0/1343	0.80	3/1820 (0.2%)
29	DH	0.60	0/1343	0.77	2/1820 (0.1%)
30	BI	0.64	0/1055	0.83	0/1445
30	DI	0.65	0/1053	0.84	1/1442 (0.1%)
31	BN	0.86	0/1139	0.87	2/1538 (0.1%)
31	DN	0.65	0/1139	0.87	1/1538 (0.1%)
32	BO	0.79	1/933 (0.1%)	0.86	1/1257 (0.1%)
32	DO	0.70	0/933	0.86	1/1257 (0.1%)
33	BP	0.80	0/1148	0.93	1/1529 (0.1%)
33	DP	0.67	0/1148	0.93	2/1529 (0.1%)
34	BQ	0.79	0/1143	0.89	0/1527
34	DQ	0.70	0/1143	0.86	0/1527
35	BR	0.82	0/982	0.94	2/1312 (0.2%)
35	DR	0.74	0/982	0.93	2/1312 (0.2%)
36	BS	0.65	0/875	0.88	0/1168
36	DS	0.66	0/875	0.84	0/1168
37	BT	0.74	0/1077	0.87	0/1444
37	DT	0.66	0/1077	0.85	0/1444
38	BU	1.02	0/977	0.89	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DU	0.79	0/977	0.88	0/1301
39	BV	0.89	0/771	0.84	0/1037
39	DV	0.70	0/782	0.84	1/1049 (0.1%)
40	BW	1.04	0/891	0.99	2/1197 (0.2%)
40	DW	0.87	0/891	0.91	0/1197
41	BX	0.87	0/756	0.88	1/1016 (0.1%)
41	DX	0.78	0/756	0.84	1/1016 (0.1%)
42	BY	0.81	0/798	0.88	0/1073
42	DY	0.72	1/798 (0.1%)	0.87	1/1073 (0.1%)
43	BZ	0.62	0/1555	0.82	1/2118 (0.0%)
43	DZ	0.63	0/1555	0.80	1/2118 (0.0%)
44	B0	0.83	0/602	0.86	0/804
44	D0	0.73	0/602	0.81	0/804
45	B1	0.80	0/752	1.00	3/1003 (0.3%)
45	D1	0.77	0/752	0.99	2/1003 (0.2%)
46	B2	0.81	0/590	0.82	0/781
46	D2	0.71	0/590	0.83	0/781
47	B3	0.79	0/463	0.86	1/623 (0.2%)
47	D3	0.64	0/463	0.82	0/623
48	B4	0.64	0/358	0.82	1/487 (0.2%)
48	D4	0.70	0/358	0.82	1/487 (0.2%)
49	B5	1.01	0/469	0.99	1/634 (0.2%)
49	D5	0.75	0/469	0.95	1/634 (0.2%)
50	B6	0.84	1/456 (0.2%)	0.86	0/609
50	D6	0.92	2/456 (0.4%)	0.89	2/609 (0.3%)
51	B7	1.07	0/426	1.16	2/561 (0.4%)
51	D7	0.92	0/426	1.00	0/561
52	B8	0.88	0/516	1.00	2/679 (0.3%)
52	D8	0.73	1/516 (0.2%)	0.92	1/679 (0.1%)
53	B9	0.85	0/300	0.91	0/395
53	D9	0.68	0/300	0.83	0/395
All	All	1.12	945/304490 (0.3%)	1.42	5009/455973 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	3
2	CB	0	3
3	AC	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	CC	0	2
5	CE	0	1
7	AG	0	4
7	CG	0	1
9	AI	0	2
9	CI	0	1
10	AJ	0	3
12	AL	0	1
12	CL	0	1
13	AM	0	3
13	CM	0	1
14	AN	0	3
17	AQ	0	1
17	CQ	0	1
19	AS	0	1
20	AT	0	2
20	CT	0	1
22	CV	0	3
25	BD	0	1
25	DD	0	1
26	BE	0	2
26	DE	0	1
27	BF	0	2
27	DF	0	3
28	BG	0	1
28	DG	0	1
30	BI	0	1
30	DI	0	1
31	BN	0	1
31	DN	0	2
32	BO	0	1
32	DO	0	1
33	BP	0	4
33	DP	0	2
36	BS	0	2
36	DS	0	1
37	BT	0	1
37	DT	0	1
41	BX	0	1
41	DX	0	1
42	BY	0	1
42	DY	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	BZ	0	1
45	B1	0	1
45	D1	0	1
48	B4	0	3
48	D4	0	2
52	D8	0	2
All	All	0	83

The worst 5 of 945 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1459	C	N1-C2	17.17	1.57	1.40
1	AA	1459	C	N1-C2	16.97	1.57	1.40
1	AA	1442(A)	G	N9-C4	16.14	1.50	1.38
1	CA	1442(A)	G	N9-C4	15.91	1.50	1.38
23	DA	528	A	N9-C4	-14.88	1.28	1.37

The worst 5 of 5009 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CA	1442(A)	G	N3-C4-C5	-27.29	114.95	128.60
1	CA	1459	C	N3-C2-O2	-27.00	103.00	121.90
1	AA	1442(A)	G	N3-C4-C5	-26.82	115.19	128.60
1	CA	1459	C	C6-N1-C2	-26.34	109.77	120.30
1	AA	1459	C	N3-C2-O2	-25.91	103.77	121.90

There are no chirality outliers.

5 of 83 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	128	GLU	Peptide
2	AB	14	GLY	Peptide
2	AB	71	VAL	Peptide
3	AC	186	PHE	Peptide
7	AG	19	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	32353	0	16329	1267	0
1	CA	32270	0	16287	987	1
2	AB	1775	0	1743	99	0
2	CB	1775	0	1743	93	0
3	AC	1450	0	1314	80	0
3	CC	1450	0	1314	99	0
4	AD	1526	0	1417	79	0
4	CD	1526	0	1415	91	0
5	AE	1105	0	1130	55	0
5	CE	1105	0	1130	60	0
6	AF	777	0	737	26	0
6	CF	777	0	737	24	0
7	AG	1164	0	1106	100	0
7	CG	1164	0	1106	54	0
8	AH	1045	0	1033	52	0
8	CH	1045	0	1033	52	0
9	AI	852	0	742	69	0
9	CI	852	0	742	62	0
10	AJ	663	0	558	56	0
10	CJ	663	0	558	30	0
11	AK	828	0	822	28	0
11	CK	828	0	822	31	0
12	AL	905	0	916	44	0
12	CL	905	0	916	44	0
13	AM	804	0	752	62	0
13	CM	804	0	752	48	0
14	AN	478	0	497	50	0
14	CN	478	0	497	35	0
15	AO	724	0	749	25	0
15	CO	724	0	749	29	0
16	AP	651	0	638	33	0
16	CP	651	0	638	35	0
17	AQ	823	0	891	16	0
17	CQ	823	0	891	18	0
18	AR	514	0	530	24	0
18	CR	514	0	530	24	0
19	AS	560	0	466	41	0
19	CS	560	0	466	23	0
20	AT	713	0	766	36	0
20	CT	713	0	766	30	0
21	AU	199	0	208	26	0
21	CU	199	0	208	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AV	333	0	235	14	0
22	CV	353	0	266	13	0
23	BA	60512	0	30492	877	0
23	DA	60620	0	30560	944	0
24	BB	2573	0	1304	45	0
24	DB	2573	0	1304	52	0
25	BD	2136	0	2218	67	0
25	DD	2136	0	2218	68	0
26	BE	1555	0	1607	39	0
26	DE	1555	0	1607	52	0
27	BF	1580	0	1621	51	0
27	DF	1580	0	1621	65	0
28	BG	1368	0	1324	51	0
28	DG	1368	0	1324	56	0
29	BH	1317	0	1376	30	0
29	DH	1317	0	1376	31	0
30	BI	1040	0	1045	55	1
30	DI	1038	0	1040	38	0
31	BN	1112	0	1180	37	0
31	DN	1112	0	1180	37	0
32	BO	923	0	981	24	0
32	DO	923	0	981	29	0
33	BP	1131	0	1201	38	0
33	DP	1131	0	1201	39	0
34	BQ	1122	0	1179	33	0
34	DQ	1122	0	1179	45	0
35	BR	968	0	1033	22	0
35	DR	968	0	1033	29	0
36	BS	865	0	905	46	0
36	DS	865	0	905	52	0
37	BT	1063	0	1103	41	0
37	DT	1063	0	1103	40	0
38	BU	959	0	1019	24	0
38	DU	959	0	1019	29	0
39	BV	760	0	816	20	0
39	DV	771	0	830	24	0
40	BW	881	0	935	17	0
40	DW	881	0	935	21	0
41	BX	742	0	799	17	0
41	DX	742	0	799	18	0
42	BY	785	0	828	31	0
42	DY	785	0	828	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BZ	1522	0	1511	49	0
43	DZ	1522	0	1511	52	0
44	B0	594	0	604	23	0
44	D0	594	0	604	31	0
45	B1	745	0	804	31	0
45	D1	745	0	804	31	0
46	B2	588	0	643	19	0
46	D2	588	0	643	24	0
47	B3	458	0	503	9	0
47	D3	458	0	503	13	0
48	B4	349	0	336	20	0
48	D4	349	0	336	20	0
49	B5	455	0	472	14	0
49	D5	455	0	472	17	0
50	B6	449	0	462	19	0
50	D6	449	0	462	18	0
51	B7	418	0	467	11	0
51	D7	418	0	467	15	0
52	B8	509	0	565	23	0
52	D8	509	0	565	28	0
53	B9	297	0	316	8	0
53	D9	297	0	316	10	0
54	AA	106	0	0	0	0
54	AD	1	0	0	0	0
54	B0	2	0	0	0	0
54	B1	1	0	0	0	0
54	B2	2	0	0	0	0
54	B3	2	0	0	0	0
54	B5	2	0	0	0	0
54	B8	3	0	0	0	0
54	B9	1	0	0	0	0
54	BA	618	0	0	0	0
54	BB	17	0	0	0	0
54	BD	3	0	0	0	0
54	BE	6	0	0	0	0
54	BF	2	0	0	0	0
54	BP	1	0	0	0	0
54	BQ	3	0	0	0	0
54	BR	2	0	0	0	0
54	BU	2	0	0	0	0
54	BV	1	0	0	0	0
54	BW	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	CA	69	0	0	0	0
54	D6	1	0	0	0	0
54	D7	1	0	0	0	0
54	D8	1	0	0	0	0
54	DA	430	0	0	0	0
54	DB	5	0	0	0	0
54	DD	1	0	0	0	0
54	DE	1	0	0	0	0
54	DF	2	0	0	0	0
54	DP	1	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	B4	1	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B9	1	0	0	0	0
55	BY	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
55	D4	1	0	0	0	0
55	D5	1	0	0	0	0
55	D6	1	0	0	0	0
55	D9	1	0	0	0	0
55	DY	1	0	0	0	0
56	AA	145	0	0	23	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AQ	1	0	0	0	0
56	B0	4	0	0	0	0
56	B3	1	0	0	0	0
56	B4	1	0	0	0	0
56	B5	3	0	0	1	0
56	B7	3	0	0	0	0
56	B8	7	0	0	0	0
56	B9	2	0	0	1	0
56	BA	1422	0	0	86	0
56	BB	31	0	0	1	0
56	BD	10	0	0	4	0
56	BE	8	0	0	0	0
56	BF	11	0	0	0	0
56	BH	2	0	0	0	0
56	BN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BO	3	0	0	0	0
56	BP	6	0	0	0	0
56	BQ	2	0	0	0	0
56	BR	6	0	0	0	0
56	BT	1	0	0	0	0
56	BU	2	0	0	0	0
56	BV	2	0	0	0	0
56	BW	4	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	CA	119	0	0	13	0
56	CD	1	0	0	0	0
56	CK	2	0	0	0	0
56	CP	1	0	0	0	0
56	CT	2	0	0	0	0
56	D0	1	0	0	0	0
56	D1	2	0	0	0	0
56	DA	696	0	0	56	0
56	DB	9	0	0	0	0
56	DD	3	0	0	0	0
56	DE	2	0	0	0	0
56	DF	5	0	0	0	0
56	DP	5	0	0	0	0
56	DQ	2	0	0	0	0
56	DR	1	0	0	0	0
56	DV	1	0	0	0	0
56	DX	1	0	0	0	0
56	DY	1	0	0	0	0
All	All	283930	0	186520	7011	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 7011 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)
1:AA:1303:C:N4	1:AA:1334:G:H1	1.41	1.17
23:BA:2296:U:O4	23:BA:2335:A:N6	1.76	1.15
23:DA:2296:U:O4	23:DA:2335:A:N6	1.79	1.15
1:AA:1003:G:H1	1:AA:1037:C:N4	1.46	1.14
1:AA:559:A:H4'	1:AA:560:U:H3'	1.35	1.07

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BI:91:SER:OG	1:CA:368:U:OP1[3_654]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	227/256 (89%)	188 (83%)	37 (16%)	2 (1%)	21	64
2	CB	227/256 (89%)	192 (85%)	33 (14%)	2 (1%)	21	64
3	AC	204/239 (85%)	179 (88%)	25 (12%)	0	100	100
3	CC	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	AD	206/209 (99%)	179 (87%)	25 (12%)	2 (1%)	19	61
4	CD	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	19	61
5	AE	146/162 (90%)	125 (86%)	20 (14%)	1 (1%)	26	70
5	CE	146/162 (90%)	126 (86%)	20 (14%)	0	100	100
6	AF	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
6	CF	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
7	AG	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	15	53
7	CG	153/156 (98%)	128 (84%)	23 (15%)	2 (1%)	15	53
8	AH	136/138 (99%)	122 (90%)	14 (10%)	0	100	100
8	CH	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	AI	123/128 (96%)	106 (86%)	15 (12%)	2 (2%)	12	48
9	CI	123/128 (96%)	109 (89%)	12 (10%)	2 (2%)	12	48
10	AJ	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	9	40
10	CJ	94/105 (90%)	74 (79%)	18 (19%)	2 (2%)	9	40
11	AK	112/129 (87%)	100 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CK	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
12	AL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	24	66
12	CL	120/132 (91%)	107 (89%)	11 (9%)	2 (2%)	11	46
13	AM	112/126 (89%)	82 (73%)	27 (24%)	3 (3%)	6	32
13	CM	112/126 (89%)	84 (75%)	27 (24%)	1 (1%)	21	64
14	AN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	15
14	CN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	11	46
15	AO	86/89 (97%)	71 (83%)	15 (17%)	0	100	100
15	CO	86/89 (97%)	72 (84%)	14 (16%)	0	100	100
16	AP	80/88 (91%)	69 (86%)	9 (11%)	2 (2%)	7	34
16	CP	80/88 (91%)	71 (89%)	7 (9%)	2 (2%)	7	34
17	AQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
17	CQ	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
18	CR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
19	AS	79/93 (85%)	62 (78%)	16 (20%)	1 (1%)	15	53
19	CS	79/93 (85%)	60 (76%)	16 (20%)	3 (4%)	4	22
20	AT	95/106 (90%)	82 (86%)	10 (10%)	3 (3%)	5	27
20	CT	95/106 (90%)	81 (85%)	11 (12%)	3 (3%)	5	27
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
22	AV	51/61 (84%)	42 (82%)	9 (18%)	0	100	100
22	CV	51/61 (84%)	34 (67%)	14 (28%)	3 (6%)	2	11
25	BD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	39	80
25	DD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	39	80
26	BE	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	19	61
26	DE	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	19	61
27	BF	201/210 (96%)	187 (93%)	13 (6%)	1 (0%)	34	76
27	DF	201/210 (96%)	188 (94%)	12 (6%)	1 (0%)	34	76
28	BG	179/182 (98%)	151 (84%)	28 (16%)	0	100	100
28	DG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	30	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	BH	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	16 56
29	DH	172/180 (96%)	158 (92%)	12 (7%)	2 (1%)	16 56
30	BI	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	9 40
30	DI	144/148 (97%)	113 (78%)	29 (20%)	2 (1%)	14 51
31	BN	138/140 (99%)	128 (93%)	6 (4%)	4 (3%)	6 29
31	DN	138/140 (99%)	126 (91%)	7 (5%)	5 (4%)	4 24
32	BO	120/122 (98%)	113 (94%)	7 (6%)	0	100 100
32	DO	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
33	BP	147/150 (98%)	134 (91%)	12 (8%)	1 (1%)	26 70
33	DP	147/150 (98%)	134 (91%)	13 (9%)	0	100 100
34	BQ	139/141 (99%)	127 (91%)	12 (9%)	0	100 100
34	DQ	139/141 (99%)	125 (90%)	14 (10%)	0	100 100
35	BR	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
35	DR	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
36	BS	108/112 (96%)	96 (89%)	11 (10%)	1 (1%)	21 64
36	DS	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	21 64
37	BT	129/146 (88%)	125 (97%)	4 (3%)	0	100 100
37	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100 100
38	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
38	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
39	BV	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
39	DV	99/101 (98%)	94 (95%)	5 (5%)	0	100 100
40	BW	110/113 (97%)	106 (96%)	4 (4%)	0	100 100
40	DW	110/113 (97%)	106 (96%)	4 (4%)	0	100 100
41	BX	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
41	DX	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
42	BY	105/110 (96%)	94 (90%)	9 (9%)	2 (2%)	10 43
42	DY	105/110 (96%)	95 (90%)	8 (8%)	2 (2%)	10 43
43	BZ	196/206 (95%)	178 (91%)	15 (8%)	3 (2%)	13 50
43	DZ	196/206 (95%)	177 (90%)	16 (8%)	3 (2%)	13 50
44	B0	74/85 (87%)	71 (96%)	3 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	D0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	B1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
45	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	58
46	B2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
46	D2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
47	B3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
47	D3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
48	B4	44/71 (62%)	37 (84%)	7 (16%)	0	100	100
48	D4	44/71 (62%)	38 (86%)	6 (14%)	0	100	100
49	B5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	D5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
50	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
50	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
51	B7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	8	38
51	D7	46/49 (94%)	45 (98%)	0	1 (2%)	8	38
52	B8	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	12	48
52	D8	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	5	27
53	B9	34/37 (92%)	34 (100%)	0	0	100	100
53	D9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	11473/12250 (94%)	10289 (90%)	1089 (10%)	95 (1%)	24	66

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	AM	91	ARG
33	BP	27	HIS
12	CL	92	ASP
31	DN	23	LEU
31	DN	24	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	177/220 (80%)	135 (76%)	42 (24%)	1 4
2	CB	177/220 (80%)	135 (76%)	42 (24%)	1 4
3	AC	114/188 (61%)	74 (65%)	40 (35%)	0 1
3	CC	114/188 (61%)	78 (68%)	36 (32%)	0 1
4	AD	141/181 (78%)	113 (80%)	28 (20%)	1 8
4	CD	141/181 (78%)	114 (81%)	27 (19%)	2 10
5	AE	108/123 (88%)	84 (78%)	24 (22%)	1 5
5	CE	108/123 (88%)	84 (78%)	24 (22%)	1 5
6	AF	76/90 (84%)	68 (90%)	8 (10%)	8 32
6	CF	76/90 (84%)	69 (91%)	7 (9%)	11 40
7	AG	103/127 (81%)	68 (66%)	35 (34%)	0 1
7	CG	103/127 (81%)	77 (75%)	26 (25%)	1 3
8	AH	103/119 (87%)	83 (81%)	20 (19%)	2 9
8	CH	103/119 (87%)	84 (82%)	19 (18%)	2 10
9	AI	62/99 (63%)	49 (79%)	13 (21%)	1 7
9	CI	62/99 (63%)	48 (77%)	14 (23%)	1 5
10	AJ	53/92 (58%)	41 (77%)	12 (23%)	1 5
10	CJ	53/92 (58%)	39 (74%)	14 (26%)	0 3
11	AK	81/99 (82%)	70 (86%)	11 (14%)	5 20
11	CK	81/99 (82%)	70 (86%)	11 (14%)	5 20
12	AL	91/109 (84%)	80 (88%)	11 (12%)	6 25
12	CL	91/109 (84%)	79 (87%)	12 (13%)	5 22
13	AM	64/101 (63%)	45 (70%)	19 (30%)	0 2
13	CM	64/101 (63%)	49 (77%)	15 (23%)	1 4
14	AN	46/50 (92%)	37 (80%)	9 (20%)	1 9
14	CN	46/50 (92%)	33 (72%)	13 (28%)	0 2
15	AO	77/80 (96%)	70 (91%)	7 (9%)	12 41
15	CO	77/80 (96%)	71 (92%)	6 (8%)	16 49
16	AP	63/74 (85%)	47 (75%)	16 (25%)	1 3
16	CP	63/74 (85%)	47 (75%)	16 (25%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	AQ	94/97 (97%)	80 (85%)	14 (15%)	4 17
17	CQ	94/97 (97%)	80 (85%)	14 (15%)	4 17
18	AR	49/77 (64%)	43 (88%)	6 (12%)	6 25
18	CR	49/77 (64%)	42 (86%)	7 (14%)	4 19
19	AS	43/80 (54%)	24 (56%)	19 (44%)	0 0
19	CS	43/80 (54%)	32 (74%)	11 (26%)	0 3
20	AT	65/82 (79%)	56 (86%)	9 (14%)	4 20
20	CT	65/82 (79%)	55 (85%)	10 (15%)	3 16
21	AU	18/22 (82%)	11 (61%)	7 (39%)	0 0
21	CU	18/22 (82%)	13 (72%)	5 (28%)	0 2
22	AV	16/50 (32%)	13 (81%)	3 (19%)	2 10
22	CV	21/50 (42%)	14 (67%)	7 (33%)	0 1
25	BD	215/218 (99%)	181 (84%)	34 (16%)	3 15
25	DD	215/218 (99%)	180 (84%)	35 (16%)	3 14
26	BE	163/166 (98%)	138 (85%)	25 (15%)	3 16
26	DE	163/166 (98%)	135 (83%)	28 (17%)	2 12
27	BF	159/166 (96%)	133 (84%)	26 (16%)	3 14
27	DF	159/166 (96%)	133 (84%)	26 (16%)	3 14
28	BG	128/156 (82%)	106 (83%)	22 (17%)	2 12
28	DG	128/156 (82%)	106 (83%)	22 (17%)	2 12
29	BH	141/148 (95%)	127 (90%)	14 (10%)	10 35
29	DH	141/148 (95%)	127 (90%)	14 (10%)	10 35
30	BI	99/124 (80%)	75 (76%)	24 (24%)	1 4
30	DI	98/124 (79%)	67 (68%)	31 (32%)	0 1
31	BN	117/119 (98%)	92 (79%)	25 (21%)	1 6
31	DN	117/119 (98%)	93 (80%)	24 (20%)	1 7
32	BO	98/100 (98%)	90 (92%)	8 (8%)	14 46
32	DO	98/100 (98%)	90 (92%)	8 (8%)	14 46
33	BP	114/116 (98%)	98 (86%)	16 (14%)	4 19
33	DP	114/116 (98%)	100 (88%)	14 (12%)	6 25
34	BQ	111/111 (100%)	95 (86%)	16 (14%)	4 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	DQ	111/111 (100%)	96 (86%)	15 (14%)	5 20
35	BR	101/101 (100%)	82 (81%)	19 (19%)	2 10
35	DR	101/101 (100%)	83 (82%)	18 (18%)	2 11
36	BS	84/88 (96%)	69 (82%)	15 (18%)	2 11
36	DS	84/88 (96%)	72 (86%)	12 (14%)	4 19
37	BT	110/127 (87%)	95 (86%)	15 (14%)	5 20
37	DT	110/127 (87%)	92 (84%)	18 (16%)	3 14
38	BU	93/94 (99%)	84 (90%)	9 (10%)	10 37
38	DU	93/94 (99%)	84 (90%)	9 (10%)	10 37
39	BV	79/82 (96%)	62 (78%)	17 (22%)	1 6
39	DV	80/82 (98%)	64 (80%)	16 (20%)	1 8
40	BW	89/92 (97%)	78 (88%)	11 (12%)	6 24
40	DW	89/92 (97%)	76 (85%)	13 (15%)	4 18
41	BX	75/78 (96%)	70 (93%)	5 (7%)	20 57
41	DX	75/78 (96%)	70 (93%)	5 (7%)	20 57
42	BY	80/91 (88%)	66 (82%)	14 (18%)	2 12
42	DY	80/91 (88%)	63 (79%)	17 (21%)	1 6
43	BZ	159/179 (89%)	141 (89%)	18 (11%)	7 28
43	DZ	159/179 (89%)	141 (89%)	18 (11%)	7 28
44	B0	59/67 (88%)	54 (92%)	5 (8%)	13 45
44	D0	59/67 (88%)	54 (92%)	5 (8%)	13 45
45	B1	78/83 (94%)	67 (86%)	11 (14%)	4 19
45	D1	78/83 (94%)	67 (86%)	11 (14%)	4 19
46	B2	65/67 (97%)	59 (91%)	6 (9%)	11 40
46	D2	65/67 (97%)	58 (89%)	7 (11%)	8 30
47	B3	49/52 (94%)	43 (88%)	6 (12%)	6 25
47	D3	49/52 (94%)	42 (86%)	7 (14%)	4 19
48	B4	39/63 (62%)	29 (74%)	10 (26%)	0 3
48	D4	39/63 (62%)	29 (74%)	10 (26%)	0 3
49	B5	50/52 (96%)	45 (90%)	5 (10%)	9 34
49	D5	50/52 (96%)	45 (90%)	5 (10%)	9 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	B6	50/52 (96%)	39 (78%)	11 (22%)	1 6
50	D6	50/52 (96%)	37 (74%)	13 (26%)	0 3
51	B7	41/42 (98%)	32 (78%)	9 (22%)	1 6
51	D7	41/42 (98%)	34 (83%)	7 (17%)	2 12
52	B8	52/55 (94%)	43 (83%)	9 (17%)	2 12
52	D8	52/55 (94%)	43 (83%)	9 (17%)	2 12
53	B9	32/34 (94%)	29 (91%)	3 (9%)	11 39
53	D9	32/34 (94%)	29 (91%)	3 (9%)	11 39
All	All	8753/10166 (86%)	7236 (83%)	1517 (17%)	2 12

5 of 1517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	B0	20	ARG
4	CD	97	LEU
41	DX	45	THR
46	B2	53	LEU
2	CB	58	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
9	CI	38	GLN
15	CO	37	ASN
42	DY	6	HIS
9	CI	73	GLN
10	CJ	33	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	425 (28%)	31 (2%)
1	CA	1499/1522 (98%)	383 (25%)	29 (1%)
23	BA	2802/2915 (96%)	556 (19%)	62 (2%)
23	DA	2808/2915 (96%)	552 (19%)	63 (2%)
24	BB	119/122 (97%)	21 (17%)	0
24	DB	119/122 (97%)	21 (17%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	8850/9118 (97%)	1958 (22%)	185 (2%)

5 of 1958 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	10	A
1	AA	22	G

5 of 185 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2308	G
1	CA	484	G
23	DA	2126	A
23	BA	2439	A
1	CA	7	G

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 1302 ligands modelled in this entry, 1302 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1505/1522 (98%)	1.14	310 (20%) 1 1	52, 116, 177, 188	0
1	CA	1501/1522 (98%)	0.67	221 (14%) 3 1	53, 112, 168, 181	0
2	AB	229/256 (89%)	0.35	18 (7%) 15 5	114, 135, 150, 160	0
2	CB	229/256 (89%)	0.65	27 (11%) 6 2	113, 135, 150, 160	0
3	AC	206/239 (86%)	1.90	89 (43%) 0 0	122, 148, 164, 172	0
3	CC	206/239 (86%)	1.54	64 (31%) 1 0	119, 140, 153, 162	0
4	AD	208/209 (99%)	0.44	22 (10%) 8 3	100, 116, 133, 143	0
4	CD	208/209 (99%)	0.22	16 (7%) 16 6	95, 111, 129, 142	0
5	AE	148/162 (91%)	0.46	19 (12%) 5 2	85, 109, 124, 129	0
5	CE	148/162 (91%)	0.46	13 (8%) 12 4	87, 108, 124, 132	0
6	AF	100/101 (99%)	-0.05	6 (6%) 25 9	88, 102, 122, 136	0
6	CF	100/101 (99%)	0.11	6 (6%) 25 9	93, 107, 123, 135	0
7	AG	155/156 (99%)	3.65	109 (70%) 0 0	134, 156, 166, 168	0
7	CG	155/156 (99%)	2.21	73 (47%) 0 0	118, 144, 151, 158	0
8	AH	138/138 (100%)	0.10	7 (5%) 32 12	93, 111, 121, 131	0
8	CH	138/138 (100%)	0.17	8 (5%) 26 10	89, 110, 120, 133	0
9	AI	125/128 (97%)	4.09	91 (72%) 0 0	131, 157, 170, 176	0
9	CI	125/128 (97%)	2.65	62 (49%) 0 0	129, 151, 161, 173	0
10	AJ	96/105 (91%)	3.70	58 (60%) 0 0	137, 155, 171, 176	0
10	CJ	96/105 (91%)	2.75	55 (57%) 0 0	130, 149, 161, 169	0
11	AK	114/129 (88%)	0.13	0 100 100	74, 109, 123, 127	0
11	CK	114/129 (88%)	0.39	10 (8%) 12 4	79, 109, 122, 124	0
12	AL	122/132 (92%)	0.19	6 (4%) 33 13	72, 95, 111, 120	0
12	CL	122/132 (92%)	0.31	8 (6%) 22 7	72, 92, 106, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	114/126 (90%)	4.62	91 (79%) 0 0	147, 160, 171, 177	0
13	CM	114/126 (90%)	2.04	41 (35%) 0 0	124, 145, 155, 158	0
14	AN	60/61 (98%)	3.98	37 (61%) 0 0	134, 160, 169, 174	0
14	CN	60/61 (98%)	1.93	21 (35%) 0 0	136, 146, 152, 155	0
15	AO	88/89 (98%)	0.03	3 (3%) 49 21	78, 103, 120, 131	0
15	CO	88/89 (98%)	0.09	6 (6%) 20 7	79, 102, 122, 129	0
16	AP	82/88 (93%)	1.32	26 (31%) 1 0	98, 112, 132, 138	0
16	CP	82/88 (93%)	0.56	6 (7%) 18 6	89, 105, 123, 132	0
17	AQ	99/105 (94%)	0.40	6 (6%) 25 9	86, 99, 113, 118	0
17	CQ	99/105 (94%)	0.04	3 (3%) 54 25	84, 98, 113, 117	0
18	AR	68/88 (77%)	0.71	11 (16%) 3 1	93, 104, 138, 141	0
18	CR	68/88 (77%)	1.17	19 (27%) 1 0	95, 107, 138, 143	0
19	AS	81/93 (87%)	3.02	40 (49%) 0 0	131, 164, 174, 179	0
19	CS	81/93 (87%)	2.70	48 (59%) 0 0	125, 146, 153, 155	0
20	AT	97/106 (91%)	0.55	9 (9%) 11 4	90, 106, 127, 131	0
20	CT	97/106 (91%)	0.70	14 (14%) 3 1	84, 103, 125, 132	0
21	AU	23/27 (85%)	6.87	19 (82%) 0 0	147, 161, 169, 174	0
21	CU	23/27 (85%)	2.53	12 (52%) 0 0	130, 145, 153, 154	0
22	AV	53/61 (86%)	0.17	3 (5%) 27 10	93, 105, 121, 143	0
22	CV	53/61 (86%)	-0.38	2 (3%) 44 18	90, 115, 141, 151	0
23	BA	2809/2915 (96%)	0.06	87 (3%) 52 24	31, 50, 134, 186	0
23	DA	2814/2915 (96%)	-0.11	112 (3%) 42 17	34, 56, 138, 189	0
24	BB	120/122 (98%)	-0.35	0 100 100	46, 72, 94, 119	0
24	DB	120/122 (98%)	-0.22	0 100 100	63, 90, 111, 129	0
25	BD	275/276 (99%)	-0.31	1 (0%) 93 80	34, 52, 69, 117	0
25	DD	275/276 (99%)	-0.40	1 (0%) 93 80	36, 55, 72, 119	0
26	BE	204/206 (99%)	-0.17	0 100 100	32, 55, 78, 95	0
26	DE	204/206 (99%)	-0.31	0 100 100	35, 61, 84, 101	0
27	BF	203/210 (96%)	-0.26	2 (0%) 84 60	30, 60, 92, 136	0
27	DF	203/210 (96%)	-0.24	1 (0%) 91 76	34, 67, 96, 136	0
28	BG	181/182 (99%)	0.46	20 (11%) 7 3	80, 120, 143, 152	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DG	181/182 (99%)	1.20	43 (23%) 1 1	92, 126, 146, 156	0
29	BH	174/180 (96%)	-0.17	1 (0%) 90 73	58, 79, 97, 110	0
29	DH	174/180 (96%)	0.46	23 (13%) 4 2	70, 92, 107, 122	0
30	BI	146/148 (98%)	-0.12	1 (0%) 89 70	57, 90, 108, 120	0
30	DI	146/148 (98%)	0.52	16 (10%) 7 3	60, 108, 127, 131	0
31	BN	140/140 (100%)	-0.32	0 100 100	39, 55, 83, 98	0
31	DN	140/140 (100%)	-0.55	1 (0%) 89 70	45, 63, 89, 101	0
32	BO	122/122 (100%)	-0.24	0 100 100	43, 58, 79, 85	0
32	DO	122/122 (100%)	-0.42	0 100 100	46, 62, 82, 86	0
33	BP	149/150 (99%)	0.04	0 100 100	34, 63, 98, 109	0
33	DP	149/150 (99%)	-0.20	3 (2%) 68 39	38, 70, 102, 111	0
34	BQ	141/141 (100%)	-0.15	1 (0%) 89 70	43, 61, 77, 91	0
34	DQ	141/141 (100%)	-0.19	0 100 100	47, 67, 85, 94	0
35	BR	118/118 (100%)	-0.25	0 100 100	38, 50, 70, 78	0
35	DR	118/118 (100%)	-0.33	0 100 100	42, 55, 73, 82	0
36	BS	110/112 (98%)	0.08	0 100 100	58, 75, 93, 101	0
36	DS	110/112 (98%)	0.13	4 (3%) 46 20	64, 82, 99, 110	0
37	BT	131/146 (89%)	-0.25	0 100 100	51, 63, 98, 117	0
37	DT	131/146 (89%)	-0.37	1 (0%) 87 67	55, 67, 101, 118	0
38	BU	116/118 (98%)	-0.16	1 (0%) 85 64	35, 48, 69, 81	0
38	DU	116/118 (98%)	-0.12	2 (1%) 73 45	40, 56, 76, 86	0
39	BV	100/101 (99%)	-0.26	0 100 100	34, 62, 81, 91	0
39	DV	101/101 (100%)	-0.05	0 100 100	40, 72, 90, 98	0
40	BW	112/113 (99%)	-0.40	0 100 100	36, 43, 64, 102	0
40	DW	112/113 (99%)	-0.59	0 100 100	40, 48, 69, 95	0
41	BX	95/96 (98%)	-0.16	1 (1%) 82 58	41, 51, 74, 98	0
41	DX	95/96 (98%)	-0.45	0 100 100	47, 56, 80, 102	0
42	BY	107/110 (97%)	-0.21	2 (1%) 70 41	52, 64, 89, 107	0
42	DY	107/110 (97%)	0.16	7 (6%) 22 8	59, 72, 96, 116	0
43	BZ	198/206 (96%)	-0.15	1 (0%) 91 76	65, 85, 111, 126	0
43	DZ	198/206 (96%)	0.23	14 (7%) 19 7	73, 92, 115, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	B0	76/85 (89%)	-0.30	0 100 100	48, 55, 71, 87	0
44	D0	76/85 (89%)	0.29	4 (5%) 30 12	53, 61, 76, 90	0
45	B1	97/98 (98%)	-0.15	2 (2%) 67 36	37, 57, 89, 103	0
45	D1	97/98 (98%)	-0.22	2 (2%) 67 36	41, 61, 91, 108	0
46	B2	70/72 (97%)	-0.13	0 100 100	50, 66, 84, 103	0
46	D2	70/72 (97%)	0.08	3 (4%) 39 16	55, 71, 88, 112	0
47	B3	59/60 (98%)	-0.30	0 100 100	43, 57, 85, 101	0
47	D3	59/60 (98%)	0.24	2 (3%) 49 21	49, 64, 92, 112	0
48	B4	46/71 (64%)	-0.56	0 100 100	106, 141, 151, 154	0
48	D4	46/71 (64%)	0.07	0 100 100	113, 141, 152, 163	0
49	B5	59/60 (98%)	-0.35	0 100 100	33, 51, 68, 89	0
49	D5	59/60 (98%)	-0.37	0 100 100	37, 55, 73, 95	0
50	B6	53/54 (98%)	0.29	2 (3%) 44 18	53, 61, 75, 78	0
50	D6	53/54 (98%)	0.57	5 (9%) 11 4	56, 65, 79, 82	0
51	B7	48/49 (97%)	0.08	3 (6%) 23 9	32, 37, 61, 78	0
51	D7	48/49 (97%)	-0.10	0 100 100	36, 40, 64, 83	0
52	B8	64/65 (98%)	-0.08	0 100 100	42, 49, 58, 70	0
52	D8	64/65 (98%)	-0.43	0 100 100	46, 53, 62, 72	0
53	B9	36/37 (97%)	0.12	0 100 100	49, 59, 72, 83	0
53	D9	36/37 (97%)	0.61	3 (8%) 14 5	58, 68, 81, 91	0
All	All	20542/21368 (96%)	0.38	2087 (10%) 9 3	30, 80, 160, 189	0

The worst 5 of 2087 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AM	43	THR	24.2
14	AN	13	THR	23.5
9	CI	7	THR	17.9
10	AJ	72	VAL	17.3
21	AU	11	GLY	15.8

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3118	1/1	0.98	0.44	68.52	44,44,44,44	0
54	MG	DA	3177	1/1	0.85	0.84	65.87	59,59,59,59	0
54	MG	DA	3086	1/1	0.94	0.63	65.25	54,54,54,54	0
54	MG	DA	3121	1/1	0.84	0.65	63.87	53,53,53,53	0
54	MG	AA	1645	1/1	0.95	0.86	37.87	77,77,77,77	0
54	MG	AA	1657	1/1	0.92	0.53	37.73	81,81,81,81	0
54	MG	DA	3138	1/1	0.91	0.74	34.50	60,60,60,60	0
54	MG	AA	1660	1/1	0.92	0.96	33.56	91,91,91,91	0
54	MG	DA	3120	1/1	0.88	0.71	33.13	52,52,52,52	0
54	MG	AA	1621	1/1	0.93	0.98	31.45	80,80,80,80	0
54	MG	CA	1631	1/1	0.71	1.00	27.74	88,88,88,88	0
54	MG	DA	3207	1/1	0.93	0.42	26.99	53,53,53,53	0
54	MG	CA	1601	1/1	0.95	0.37	26.79	50,50,50,50	0
54	MG	BA	3078	1/1	0.90	0.35	25.99	38,38,38,38	0
54	MG	BA	3080	1/1	0.98	0.52	24.42	42,42,42,42	0
54	MG	DA	3074	1/1	0.96	0.50	23.40	38,38,38,38	0
54	MG	BA	3308	1/1	0.86	0.54	22.91	51,51,51,51	0
54	MG	CA	1613	1/1	0.87	1.05	22.74	71,71,71,71	0
54	MG	DA	3185	1/1	0.95	0.46	22.73	47,47,47,47	0
54	MG	CA	1617	1/1	0.93	0.90	21.27	70,70,70,70	0
54	MG	DA	3242	1/1	0.90	0.55	20.44	38,38,38,38	0
54	MG	BA	3001	1/1	0.89	0.43	20.32	56,56,56,56	0
54	MG	BA	3160	1/1	0.89	0.38	19.52	46,46,46,46	0
54	MG	BA	3455	1/1	0.97	0.34	18.50	42,42,42,42	0
54	MG	DA	3144	1/1	0.95	0.30	18.04	42,42,42,42	0
54	MG	BE	301	1/1	0.88	0.53	16.84	43,43,43,43	0
54	MG	BA	3396	1/1	0.81	0.43	16.76	23,23,23,23	0
54	MG	DA	3208	1/1	0.90	0.43	16.00	52,52,52,52	0
54	MG	AA	1615	1/1	0.90	0.37	14.76	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DP	201	1/1	0.79	0.78	14.68	58,58,58,58	0
54	MG	BA	3033	1/1	0.96	0.36	14.59	40,40,40,40	0
54	MG	DA	3279	1/1	0.98	0.33	14.39	40,40,40,40	0
54	MG	BR	201	1/1	0.83	0.60	14.29	58,58,58,58	0
54	MG	BA	3244	1/1	0.88	0.46	14.22	45,45,45,45	0
54	MG	DA	3099	1/1	0.93	0.26	14.15	40,40,40,40	0
54	MG	DA	3385	1/1	0.97	0.36	14.13	49,49,49,49	0
54	MG	BA	3113	1/1	0.94	0.40	14.07	35,35,35,35	0
54	MG	DA	3003	1/1	0.92	0.35	13.81	35,35,35,35	0
54	MG	BA	3557	1/1	0.98	0.49	13.78	42,42,42,42	0
54	MG	DA	3027	1/1	0.93	0.42	13.70	51,51,51,51	0
54	MG	DA	3236	1/1	0.98	0.54	13.25	44,44,44,44	0
54	MG	DA	3372	1/1	0.94	0.33	13.18	40,40,40,40	0
54	MG	BA	3473	1/1	0.95	0.44	13.17	59,59,59,59	0
54	MG	BA	3129	1/1	0.95	0.40	12.86	49,49,49,49	0
54	MG	BA	3234	1/1	0.98	0.33	12.31	34,34,34,34	0
54	MG	BA	3333	1/1	0.94	0.30	12.28	36,36,36,36	0
54	MG	DA	3116	1/1	0.96	0.40	12.03	46,46,46,46	0
54	MG	DA	3204	1/1	0.97	0.30	11.97	37,37,37,37	0
54	MG	CA	1618	1/1	0.93	0.37	11.70	75,75,75,75	0
54	MG	DA	3070	1/1	0.92	0.33	11.65	53,53,53,53	0
54	MG	DA	3146	1/1	0.92	0.44	11.41	35,35,35,35	0
54	MG	BA	3034	1/1	0.77	0.29	11.39	46,46,46,46	0
54	MG	DA	3309	1/1	0.97	0.47	11.22	48,48,48,48	0
54	MG	BQ	202	1/1	0.92	0.36	11.07	53,53,53,53	0
54	MG	BA	3031	1/1	0.85	0.39	10.76	41,41,41,41	0
54	MG	AA	1627	1/1	0.76	0.50	10.61	70,70,70,70	0
54	MG	DA	3133	1/1	0.85	0.39	10.54	78,78,78,78	0
54	MG	BA	3003	1/1	0.90	0.34	10.43	29,29,29,29	0
54	MG	DA	3124	1/1	0.96	0.47	10.41	35,35,35,35	0
54	MG	BA	3161	1/1	0.89	0.34	10.34	54,54,54,54	0
54	MG	AA	1659	1/1	0.84	0.45	10.15	62,62,62,62	0
54	MG	DA	3142	1/1	0.91	0.25	9.80	46,46,46,46	0
54	MG	BA	3046	1/1	0.90	0.28	9.79	49,49,49,49	0
54	MG	BA	3228	1/1	0.97	0.38	9.36	26,26,26,26	0
54	MG	BA	3368	1/1	0.99	0.30	9.24	34,34,34,34	0
54	MG	DA	3394	1/1	0.94	0.33	9.02	56,56,56,56	0
54	MG	DA	3085	1/1	0.93	0.45	9.00	51,51,51,51	0
54	MG	BA	3197	1/1	0.90	0.31	8.99	62,62,62,62	0
54	MG	DA	3247	1/1	0.95	0.37	8.88	52,52,52,52	0
54	MG	CA	1636	1/1	0.69	0.42	8.87	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3475	1/1	0.89	0.22	8.78	53,53,53,53	0
54	MG	BA	3074	1/1	0.90	0.38	8.47	55,55,55,55	0
54	MG	BA	3519	1/1	0.82	0.33	8.33	90,90,90,90	0
54	MG	CA	1612	1/1	0.59	0.42	8.26	84,84,84,84	0
54	MG	BA	3562	1/1	0.82	0.33	8.16	43,43,43,43	0
54	MG	BA	3408	1/1	0.97	0.32	8.12	34,34,34,34	0
54	MG	BA	3142	1/1	0.83	0.53	8.05	53,53,53,53	0
54	MG	BA	3109	1/1	0.94	0.25	7.93	57,57,57,57	0
54	MG	DA	3149	1/1	0.98	0.38	7.88	36,36,36,36	0
54	MG	DA	3006	1/1	0.86	0.28	7.85	44,44,44,44	0
54	MG	DA	3098	1/1	0.66	0.29	7.82	62,62,62,62	0
54	MG	DA	3032	1/1	0.96	0.30	7.22	43,43,43,43	0
54	MG	DA	3168	1/1	0.94	0.29	7.04	42,42,42,42	0
54	MG	CA	1602	1/1	0.94	0.58	6.98	82,82,82,82	0
54	MG	DA	3115	1/1	0.95	0.41	6.94	39,39,39,39	0
54	MG	CA	1638	1/1	0.61	0.37	6.89	71,71,71,71	0
54	MG	BA	3330	1/1	0.88	0.28	6.64	36,36,36,36	0
54	MG	BA	3053	1/1	0.89	0.34	6.52	53,53,53,53	0
54	MG	CA	1628	1/1	0.94	0.27	6.48	55,55,55,55	0
54	MG	DA	3340	1/1	0.95	0.38	6.28	44,44,44,44	0
54	MG	DA	3280	1/1	0.98	0.26	6.24	40,40,40,40	0
54	MG	DA	3062	1/1	0.81	0.22	6.10	65,65,65,65	0
54	MG	BA	3117	1/1	0.93	0.26	6.08	31,31,31,31	0
54	MG	BA	3187	1/1	0.91	0.27	6.05	30,30,30,30	0
54	MG	BA	3526	1/1	0.93	0.29	6.04	28,28,28,28	0
54	MG	B3	101	1/1	0.89	0.43	6.01	60,60,60,60	0
54	MG	DB	201	1/1	0.85	0.28	5.94	75,75,75,75	0
54	MG	BA	3219	1/1	0.91	0.33	5.87	62,62,62,62	0
54	MG	DA	3374	1/1	0.90	0.26	5.83	44,44,44,44	0
54	MG	AA	1640	1/1	0.94	0.50	5.76	80,80,80,80	0
54	MG	BA	3512	1/1	0.96	0.33	5.62	45,45,45,45	0
54	MG	DA	3291	1/1	0.82	0.33	5.62	43,43,43,43	0
54	MG	DA	3073	1/1	0.88	0.21	5.53	54,54,54,54	0
54	MG	DA	3349	1/1	0.89	0.30	5.52	54,54,54,54	0
54	MG	BA	3021	1/1	0.96	0.27	5.52	33,33,33,33	0
54	MG	DA	3219	1/1	0.90	0.30	5.48	38,38,38,38	0
54	MG	BA	3435	1/1	0.92	0.28	5.42	36,36,36,36	0
54	MG	DA	3233	1/1	0.95	0.32	5.36	43,43,43,43	0
54	MG	BA	3189	1/1	0.94	0.28	5.17	46,46,46,46	0
54	MG	BA	3047	1/1	0.97	0.28	4.94	50,50,50,50	0
54	MG	BA	3504	1/1	0.99	0.39	4.80	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3448	1/1	0.90	0.26	4.78	33,33,33,33	0
54	MG	DA	3059	1/1	0.93	0.27	4.73	55,55,55,55	0
54	MG	DA	3170	1/1	0.95	0.25	4.70	52,52,52,52	0
54	MG	DA	3040	1/1	0.84	0.31	4.68	50,50,50,50	0
54	MG	BA	3199	1/1	0.95	0.23	4.68	31,31,31,31	0
54	MG	DA	3092	1/1	0.95	0.23	4.58	63,63,63,63	0
54	MG	BA	3239	1/1	0.91	0.27	4.53	38,38,38,38	0
54	MG	BA	3434	1/1	0.95	0.38	4.51	36,36,36,36	0
54	MG	BA	3517	1/1	0.84	0.26	4.32	51,51,51,51	0
54	MG	BA	3230	1/1	0.95	0.38	4.31	50,50,50,50	0
54	MG	DA	3396	1/1	0.88	0.24	4.29	37,37,37,37	0
54	MG	BA	3551	1/1	0.95	0.26	4.28	40,40,40,40	0
54	MG	BA	3108	1/1	0.94	0.26	4.24	56,56,56,56	0
54	MG	DA	3341	1/1	0.89	0.24	4.18	39,39,39,39	0
54	MG	DA	3395	1/1	0.95	0.26	4.13	37,37,37,37	0
54	MG	BA	3441	1/1	0.97	0.25	4.06	35,35,35,35	0
54	MG	DA	3084	1/1	0.82	0.30	4.02	62,62,62,62	0
54	MG	BA	3427	1/1	0.96	0.22	4.01	32,32,32,32	0
54	MG	BA	3039	1/1	0.83	0.31	3.93	44,44,44,44	0
54	MG	CA	1623	1/1	0.81	0.89	3.84	73,73,73,73	0
54	MG	DA	3130	1/1	0.81	0.24	3.84	59,59,59,59	0
54	MG	BA	3311	1/1	0.95	0.27	3.83	60,60,60,60	0
54	MG	DA	3020	1/1	0.97	0.20	3.74	39,39,39,39	0
54	MG	BA	3133	1/1	0.95	0.30	3.70	31,31,31,31	0
54	MG	BA	3302	1/1	0.94	0.28	3.64	45,45,45,45	0
54	MG	BA	3253	1/1	0.96	0.23	3.57	38,38,38,38	0
54	MG	BA	3254	1/1	0.90	0.21	3.54	67,67,67,67	0
54	MG	AA	1613	1/1	0.91	0.25	3.52	74,74,74,74	0
54	MG	BA	3071	1/1	0.92	0.20	3.51	49,49,49,49	0
54	MG	DA	3354	1/1	0.93	0.27	3.49	41,41,41,41	0
54	MG	BB	205	1/1	0.98	0.29	3.48	57,57,57,57	0
54	MG	BB	201	1/1	0.95	0.22	3.45	61,61,61,61	0
54	MG	DA	3044	1/1	0.89	0.22	3.42	51,51,51,51	0
54	MG	DA	3072	1/1	0.92	0.36	3.39	50,50,50,50	0
54	MG	DA	3188	1/1	0.95	0.23	3.26	54,54,54,54	0
54	MG	DA	3019	1/1	0.92	0.20	3.24	41,41,41,41	0
54	MG	DA	3267	1/1	0.97	0.19	3.19	59,59,59,59	0
54	MG	BA	3500	1/1	0.86	0.21	3.15	33,33,33,33	0
54	MG	CA	1626	1/1	0.92	0.26	3.13	86,86,86,86	0
54	MG	DA	3169	1/1	0.97	0.25	3.10	39,39,39,39	0
54	MG	CA	1655	1/1	0.89	0.28	3.05	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3387	1/1	0.95	0.25	3.04	33,33,33,33	0
54	MG	AA	1604	1/1	0.55	0.32	3.03	81,81,81,81	0
54	MG	DA	3217	1/1	0.78	0.26	2.98	69,69,69,69	0
54	MG	DA	3324	1/1	0.92	0.20	2.88	64,64,64,64	0
54	MG	BA	3037	1/1	0.89	0.22	2.83	52,52,52,52	0
54	MG	DA	3290	1/1	0.95	0.24	2.82	42,42,42,42	0
54	MG	DA	3297	1/1	0.82	0.22	2.81	66,66,66,66	0
54	MG	BA	3424	1/1	0.99	0.23	2.75	32,32,32,32	0
54	MG	DA	3128	1/1	0.80	0.29	2.68	72,72,72,72	0
54	MG	BA	3127	1/1	0.92	0.23	2.59	51,51,51,51	0
54	MG	BA	3513	1/1	0.80	0.21	2.56	66,66,66,66	0
54	MG	DA	3011	1/1	0.85	0.22	2.55	46,46,46,46	0
54	MG	BA	3119	1/1	0.94	0.22	2.55	39,39,39,39	0
54	MG	DF	301	1/1	0.97	0.37	2.55	58,58,58,58	0
54	MG	DA	3410	1/1	0.82	0.18	2.47	72,72,72,72	0
54	MG	BA	3426	1/1	0.96	0.22	2.46	28,28,28,28	0
54	MG	BA	3461	1/1	0.98	0.23	2.40	38,38,38,38	0
54	MG	BA	3236	1/1	0.95	0.21	2.32	50,50,50,50	0
54	MG	DA	3303	1/1	0.94	0.19	2.29	37,37,37,37	0
54	MG	BA	3423	1/1	0.97	0.22	2.27	30,30,30,30	0
54	MG	DA	3390	1/1	0.83	0.17	2.27	69,69,69,69	0
54	MG	DA	3202	1/1	0.98	0.23	2.25	37,37,37,37	0
54	MG	DA	3079	1/1	0.91	0.20	2.22	60,60,60,60	0
54	MG	BA	3307	1/1	0.98	0.20	2.04	29,29,29,29	0
54	MG	BB	204	1/1	0.82	0.20	2.03	67,67,67,67	0
54	MG	BD	302	1/1	0.98	0.28	2.02	38,38,38,38	0
54	MG	BA	3180	1/1	0.89	0.25	2.00	51,51,51,51	0
54	MG	DA	3325	1/1	0.97	0.26	1.97	36,36,36,36	0
54	MG	DA	3302	1/1	0.94	0.26	1.96	36,36,36,36	0
54	MG	BA	3489	1/1	0.89	0.20	1.93	38,38,38,38	0
54	MG	CA	1632	1/1	0.95	0.29	1.91	65,65,65,65	0
54	MG	BA	3178	1/1	0.81	0.18	1.81	58,58,58,58	0
54	MG	BB	213	1/1	0.84	0.21	1.77	69,69,69,69	0
54	MG	DA	3402	1/1	0.95	0.22	1.75	59,59,59,59	0
54	MG	DA	3028	1/1	0.92	0.20	1.75	53,53,53,53	0
54	MG	DA	3304	1/1	0.96	0.18	1.75	38,38,38,38	0
54	MG	DA	3342	1/1	0.80	0.24	1.74	41,41,41,41	0
54	MG	DA	3406	1/1	0.85	0.25	1.72	35,35,35,35	0
54	MG	BA	3407	1/1	0.92	0.22	1.72	35,35,35,35	0
54	MG	DA	3135	1/1	0.92	0.26	1.68	44,44,44,44	0
54	MG	BA	3390	1/1	0.98	0.22	1.61	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3428	1/1	0.93	0.24	1.58	35,35,35,35	0
54	MG	DA	3066	1/1	0.88	0.18	1.57	56,56,56,56	0
54	MG	BA	3417	1/1	0.95	0.21	1.42	37,37,37,37	0
54	MG	DA	3353	1/1	0.94	0.20	1.37	40,40,40,40	0
54	MG	BA	3422	1/1	0.87	0.23	1.35	27,27,27,27	0
54	MG	BA	3222	1/1	0.95	0.19	1.35	51,51,51,51	0
54	MG	AA	1605	1/1	0.78	0.29	1.35	74,74,74,74	0
54	MG	CA	1653	1/1	0.68	0.24	1.28	83,83,83,83	0
54	MG	BA	3351	1/1	0.54	0.24	1.28	57,57,57,57	0
54	MG	CA	1607	1/1	0.92	0.25	1.26	72,72,72,72	0
54	MG	BA	3367	1/1	0.97	0.21	1.26	33,33,33,33	0
54	MG	BA	3107	1/1	0.87	0.13	1.15	49,49,49,49	0
54	MG	BA	3451	1/1	0.98	0.23	1.15	34,34,34,34	0
54	MG	BA	3030	1/1	0.88	0.25	1.13	37,37,37,37	0
54	MG	DA	3095	1/1	0.82	0.21	1.08	71,71,71,71	0
54	MG	BA	3007	1/1	0.94	0.22	1.07	36,36,36,36	0
54	MG	B9	102	1/1	0.96	0.31	0.98	45,45,45,45	0
54	MG	B8	102	1/1	0.85	0.33	0.94	61,61,61,61	0
54	MG	BA	3057	1/1	0.95	0.20	0.93	46,46,46,46	0
54	MG	BA	3131	1/1	0.96	0.19	0.93	44,44,44,44	0
54	MG	DA	3226	1/1	0.93	0.22	0.76	53,53,53,53	0
54	MG	DA	3064	1/1	0.90	0.18	0.71	53,53,53,53	0
54	MG	BA	3193	1/1	0.93	0.19	0.71	50,50,50,50	0
54	MG	DA	3012	1/1	0.76	0.21	0.70	60,60,60,60	0
54	MG	BA	3465	1/1	0.89	0.20	0.68	38,38,38,38	0
54	MG	DA	3222	1/1	0.94	0.26	0.60	47,47,47,47	0
54	MG	BA	3048	1/1	0.96	0.20	0.53	42,42,42,42	0
54	MG	DA	3004	1/1	0.99	0.14	0.48	59,59,59,59	0
54	MG	DA	3370	1/1	0.94	0.19	0.45	51,51,51,51	0
54	MG	BA	3412	1/1	0.89	0.21	0.43	41,41,41,41	0
54	MG	AA	1674	1/1	0.93	0.20	0.41	73,73,73,73	0
54	MG	DA	3408	1/1	0.86	0.15	0.36	65,65,65,65	0
54	MG	DA	3356	1/1	0.97	0.20	0.26	42,42,42,42	0
54	MG	AA	1631	1/1	0.91	0.41	0.26	64,64,64,64	0
54	MG	DA	3405	1/1	0.94	0.17	0.25	70,70,70,70	0
54	MG	BB	215	1/1	0.73	0.18	0.25	77,77,77,77	0
54	MG	BA	3345	1/1	0.95	0.16	0.24	45,45,45,45	0
54	MG	DA	3240	1/1	0.92	0.21	0.22	67,67,67,67	0
54	MG	AA	1703	1/1	0.91	0.20	0.20	89,89,89,89	0
54	MG	BA	3164	1/1	0.96	0.17	0.20	39,39,39,39	0
54	MG	DA	3041	1/1	0.87	0.19	0.20	49,49,49,49	0
54	MG	BA	3410	1/1	0.94	0.20	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3292	1/1	0.93	0.18	0.10	39,39,39,39	0
55	ZN	CD	301	1/1	0.90	0.32	0.07	96,96,96,96	0
54	MG	BA	3432	1/1	0.96	0.18	0.02	31,31,31,31	0
54	MG	BA	3221	1/1	0.97	0.17	-0.02	51,51,51,51	0
54	MG	BA	3456	1/1	0.79	0.13	-0.08	89,89,89,89	0
54	MG	AD	302	1/1	0.92	0.17	-0.09	120,120,120,120	0
54	MG	DA	3018	1/1	0.92	0.16	-0.10	42,42,42,42	0
54	MG	BA	3094	1/1	0.94	0.17	-0.11	41,41,41,41	0
54	MG	DA	3427	1/1	0.96	0.16	-0.15	40,40,40,40	0
54	MG	DA	3013	1/1	0.94	0.16	-0.25	41,41,41,41	0
54	MG	BA	3157	1/1	0.88	0.15	-0.30	46,46,46,46	0
54	MG	BA	3553	1/1	0.73	0.18	-0.36	70,70,70,70	0
54	MG	BB	202	1/1	0.83	0.14	-0.36	46,46,46,46	0
55	ZN	BY	201	1/1	0.95	0.13	-0.39	74,74,74,74	0
54	MG	BA	3232	1/1	0.91	0.14	-0.43	54,54,54,54	0
54	MG	BE	304	1/1	0.91	0.17	-0.47	32,32,32,32	0
54	MG	AA	1694	1/1	0.85	0.19	-0.50	110,110,110,110	0
55	ZN	AD	301	1/1	0.93	0.24	-0.53	107,107,107,107	0
54	MG	DA	3412	1/1	0.93	0.16	-0.55	45,45,45,45	0
54	MG	BA	3429	1/1	0.95	0.17	-0.65	29,29,29,29	0
54	MG	DD	301	1/1	0.97	0.15	-0.67	40,40,40,40	0
54	MG	AA	1636	1/1	0.94	0.18	-0.70	86,86,86,86	0
54	MG	DA	3269	1/1	0.91	0.15	-0.73	54,54,54,54	0
54	MG	BA	3149	1/1	0.95	0.14	-0.74	49,49,49,49	0
54	MG	BA	3438	1/1	0.96	0.17	-0.76	38,38,38,38	0
54	MG	DA	3278	1/1	0.62	0.16	-0.76	46,46,46,46	0
54	MG	CA	1644	1/1	0.98	0.15	-0.80	74,74,74,74	0
55	ZN	B5	103	1/1	0.99	0.14	-0.83	58,58,58,58	0
54	MG	BA	3552	1/1	0.97	0.18	-0.87	38,38,38,38	0
54	MG	BA	3416	1/1	0.95	0.17	-0.89	46,46,46,46	0
54	MG	DA	3014	1/1	0.88	0.10	-0.95	52,52,52,52	0
55	ZN	DY	201	1/1	0.84	0.09	-0.99	128,128,128,128	0
54	MG	DA	3322	1/1	0.96	0.15	-1.02	35,35,35,35	0
54	MG	DA	3285	1/1	0.98	0.13	-1.05	52,52,52,52	0
54	MG	BA	3406	1/1	0.97	0.18	-1.07	40,40,40,40	0
54	MG	DA	3094	1/1	0.97	0.12	-1.12	39,39,39,39	0
55	ZN	B6	101	1/1	0.98	0.12	-1.14	54,54,54,54	0
55	ZN	D5	101	1/1	0.98	0.07	-1.19	65,65,65,65	0
54	MG	BA	3603	1/1	0.98	0.19	-1.21	30,30,30,30	0
54	MG	BA	3029	1/1	0.87	0.15	-1.24	83,83,83,83	0
54	MG	CA	1641	1/1	0.90	0.19	-1.25	74,74,74,74	0
54	MG	BA	3238	1/1	0.97	0.16	-1.28	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3389	1/1	0.95	0.14	-1.28	58,58,58,58	0
54	MG	AA	1697	1/1	0.69	0.16	-1.31	75,75,75,75	0
55	ZN	AN	101	1/1	0.37	0.14	-1.34	213,213,213,213	0
54	MG	BA	3304	1/1	0.95	0.17	-1.36	27,27,27,27	0
54	MG	BA	3320	1/1	0.76	0.15	-1.38	57,57,57,57	0
54	MG	DA	3360	1/1	0.49	0.13	-1.40	63,63,63,63	0
54	MG	BA	3314	1/1	0.58	0.16	-1.40	71,71,71,71	0
54	MG	DA	3376	1/1	0.87	0.13	-1.40	43,43,43,43	0
54	MG	BA	3515	1/1	0.94	0.12	-1.47	46,46,46,46	0
55	ZN	CN	101	1/1	0.65	0.17	-1.49	188,188,188,188	0
54	MG	BA	3511	1/1	0.90	0.16	-1.54	33,33,33,33	0
54	MG	CA	1666	1/1	0.89	0.09	-1.56	131,131,131,131	0
54	MG	BA	3386	1/1	0.78	0.12	-1.59	77,77,77,77	0
54	MG	BA	3570	1/1	0.98	0.17	-1.62	36,36,36,36	0
55	ZN	D6	101	1/1	0.96	0.10	-1.67	86,86,86,86	0
54	MG	BA	3006	1/1	0.88	0.17	-1.69	44,44,44,44	0
54	MG	BA	3397	1/1	0.93	0.18	-1.72	31,31,31,31	0
55	ZN	D4	101	1/1	0.83	0.05	-1.72	176,176,176,176	0
54	MG	BA	3023	1/1	0.84	0.12	-1.75	52,52,52,52	0
54	MG	DA	3355	1/1	0.83	0.11	-1.81	37,37,37,37	0
54	MG	BA	3309	1/1	0.97	0.16	-1.81	38,38,38,38	0
54	MG	DA	3296	1/1	0.91	0.12	-1.82	50,50,50,50	0
54	MG	DA	3306	1/1	0.85	0.11	-1.84	88,88,88,88	0
54	MG	BA	3156	1/1	0.94	0.15	-1.89	57,57,57,57	0
54	MG	BA	3357	1/1	0.90	0.15	-1.91	47,47,47,47	0
55	ZN	D9	101	1/1	0.97	0.05	-1.95	87,87,87,87	0
54	MG	BA	3355	1/1	0.94	0.16	-1.99	54,54,54,54	0
54	MG	DA	3329	1/1	0.86	0.12	-1.99	47,47,47,47	0
54	MG	DA	3058	1/1	0.81	0.11	-2.00	51,51,51,51	0
54	MG	BA	3485	1/1	0.95	0.15	-2.04	60,60,60,60	0
54	MG	BA	3105	1/1	0.87	0.12	-2.04	40,40,40,40	0
55	ZN	B9	101	1/1	0.98	0.13	-2.04	69,69,69,69	0
54	MG	DA	3375	1/1	0.92	0.14	-2.09	50,50,50,50	0
54	MG	DA	3276	1/1	0.97	0.12	-2.10	51,51,51,51	0
55	ZN	B4	101	1/1	0.65	0.06	-2.10	200,200,200,200	0
54	MG	DA	3183	1/1	0.94	0.13	-2.13	50,50,50,50	0
54	MG	AA	1664	1/1	0.93	0.15	-2.18	85,85,85,85	0
54	MG	BA	3378	1/1	0.98	0.12	-2.20	38,38,38,38	0
54	MG	DA	3274	1/1	0.96	0.10	-2.21	35,35,35,35	0
54	MG	DA	3299	1/1	0.80	0.14	-2.22	54,54,54,54	0
54	MG	DA	3333	1/1	0.96	0.06	-2.27	53,53,53,53	0
54	MG	DA	3377	1/1	0.96	0.10	-2.39	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3312	1/1	0.92	0.09	-2.45	67,67,67,67	0
54	MG	DA	3315	1/1	0.88	0.13	-2.47	59,59,59,59	0
54	MG	BA	3402	1/1	0.92	0.08	-2.52	47,47,47,47	0
54	MG	BA	3528	1/1	0.96	0.12	-2.54	43,43,43,43	0
54	MG	BA	3479	1/1	0.93	0.17	-2.55	35,35,35,35	0
54	MG	DA	3288	1/1	0.97	0.12	-2.56	37,37,37,37	0
54	MG	CA	1643	1/1	0.74	0.06	-2.60	109,109,109,109	0
54	MG	BA	3331	1/1	0.98	0.16	-2.64	51,51,51,51	0
54	MG	DA	3363	1/1	0.73	0.10	-2.65	72,72,72,72	0
54	MG	BA	3038	1/1	0.96	0.10	-2.70	36,36,36,36	0
54	MG	DA	3352	1/1	0.99	0.10	-2.74	61,61,61,61	0
54	MG	BA	3576	1/1	0.97	0.12	-2.81	41,41,41,41	0
54	MG	AA	1693	1/1	0.92	0.10	-2.82	78,78,78,78	0
54	MG	AA	1691	1/1	0.79	0.10	-2.88	58,58,58,58	0
54	MG	BA	3022	1/1	0.89	0.09	-2.88	57,57,57,57	0
54	MG	BE	306	1/1	0.93	0.09	-2.89	56,56,56,56	0
54	MG	BA	3491	1/1	0.94	0.14	-2.90	65,65,65,65	0
54	MG	CA	1654	1/1	0.98	0.11	-2.93	95,95,95,95	0
54	MG	DA	3104	1/1	0.88	0.11	-2.94	57,57,57,57	0
54	MG	BA	3025	1/1	0.96	0.11	-3.02	52,52,52,52	0
54	MG	AA	1704	1/1	0.93	0.11	-3.03	90,90,90,90	0
54	MG	CA	1627	1/1	0.88	0.13	-3.14	79,79,79,79	0
54	MG	DA	3418	1/1	0.99	0.07	-3.28	39,39,39,39	0
54	MG	BA	3421	1/1	0.97	0.14	-3.34	36,36,36,36	0
54	MG	DA	3281	1/1	0.99	0.09	-3.49	36,36,36,36	0
54	MG	DA	3270	1/1	0.98	0.11	-3.51	34,34,34,34	0
54	MG	AA	1617	1/1	0.93	0.11	-3.52	82,82,82,82	0
54	MG	BA	3484	1/1	0.98	0.12	-3.52	40,40,40,40	0
54	MG	BA	3505	1/1	0.92	0.07	-3.55	76,76,76,76	0
54	MG	BA	3596	1/1	0.98	0.13	-3.58	46,46,46,46	0
54	MG	BA	3404	1/1	0.94	0.11	-3.59	46,46,46,46	0
54	MG	BA	3398	1/1	0.97	0.17	-3.62	36,36,36,36	0
54	MG	DA	3010	1/1	0.96	0.15	-3.82	43,43,43,43	0
54	MG	BA	3403	1/1	0.98	0.13	-3.87	44,44,44,44	0
54	MG	BA	3605	1/1	0.98	0.12	-3.94	30,30,30,30	0
54	MG	BA	3560	1/1	0.99	0.12	-4.06	29,29,29,29	0
54	MG	DA	3382	1/1	0.92	0.10	-4.07	53,53,53,53	0
54	MG	BA	3295	1/1	0.91	0.11	-4.15	44,44,44,44	0
54	MG	BA	3327	1/1	0.86	0.17	-4.16	34,34,34,34	0
54	MG	BA	3321	1/1	0.96	0.11	-4.39	65,65,65,65	0
54	MG	BA	3602	1/1	0.99	0.09	-4.58	24,24,24,24	0
54	MG	BA	3385	1/1	0.97	0.10	-4.70	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1689	1/1	0.98	0.09	-4.75	55,55,55,55	0
54	MG	BA	3409	1/1	0.97	0.18	-5.40	26,26,26,26	0
54	MG	CA	1652	1/1	0.98	0.10	-5.43	65,65,65,65	0
54	MG	BA	3019	1/1	0.94	0.11	-5.67	39,39,39,39	0
54	MG	BA	3177	1/1	0.98	0.10	-6.08	45,45,45,45	0
54	MG	BA	3532	1/1	0.89	0.09	-6.20	35,35,35,35	0
54	MG	BA	3376	1/1	0.95	0.11	-6.34	55,55,55,55	0
54	MG	BA	3597	1/1	0.99	0.09	-6.45	26,26,26,26	0
54	MG	BA	3379	1/1	0.96	0.06	-7.10	56,56,56,56	0
54	MG	BA	3516	1/1	0.97	0.14	-7.21	39,39,39,39	0
54	MG	BA	3020	1/1	0.97	0.10	-7.55	34,34,34,34	0
54	MG	BA	3601	1/1	0.98	0.06	-7.68	33,33,33,33	0
54	MG	BA	3540	1/1	0.98	0.06	-9.15	61,61,61,61	0
54	MG	BA	3312	1/1	0.96	0.09	-10.41	50,50,50,50	0
54	MG	BA	3354	1/1	0.96	0.06	-11.89	49,49,49,49	0
54	MG	BA	3494	1/1	0.94	0.47	-	44,44,44,44	0
54	MG	BA	3174	1/1	0.76	0.39	-	71,71,71,71	0
54	MG	BA	3618	1/1	0.77	0.18	-	85,85,85,85	0
54	MG	AA	1649	1/1	0.93	0.20	-	66,66,66,66	0
54	MG	AA	1658	1/1	0.94	0.16	-	60,60,60,60	0
54	MG	BA	3118	1/1	0.79	0.88	-	57,57,57,57	0
54	MG	BA	3181	1/1	0.91	0.21	-	48,48,48,48	0
54	MG	BA	3425	1/1	0.88	0.14	-	37,37,37,37	0
54	MG	DA	3286	1/1	0.92	0.16	-	50,50,50,50	0
54	MG	DA	3150	1/1	0.96	0.38	-	41,41,41,41	0
54	MG	BA	3229	1/1	0.96	0.36	-	51,51,51,51	0
54	MG	DA	3225	1/1	0.94	0.26	-	64,64,64,64	0
54	MG	AA	1648	1/1	0.94	0.20	-	62,62,62,62	0
54	MG	DA	3249	1/1	0.95	0.37	-	67,67,67,67	0
54	MG	DA	3415	1/1	0.89	0.10	-	89,89,89,89	0
54	MG	DA	3126	1/1	0.81	0.12	-	80,80,80,80	0
54	MG	BA	3581	1/1	0.83	0.14	-	47,47,47,47	0
54	MG	CA	1630	1/1	0.92	0.47	-	72,72,72,72	0
54	MG	DA	3065	1/1	0.92	0.19	-	58,58,58,58	0
54	MG	BA	3049	1/1	0.94	0.19	-	54,54,54,54	0
54	MG	BA	3530	1/1	0.89	0.11	-	84,84,84,84	0
54	MG	BA	3436	1/1	0.89	0.33	-	38,38,38,38	0
54	MG	DA	3428	1/1	0.94	0.12	-	81,81,81,81	0
54	MG	BA	3617	1/1	0.76	0.15	-	93,93,93,93	0
54	MG	DA	3198	1/1	0.91	0.17	-	55,55,55,55	0
54	MG	BA	3477	1/1	0.98	0.08	-	45,45,45,45	0
54	MG	BA	3604	1/1	0.97	0.07	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3187	1/1	0.91	0.66	-	47,47,47,47	0
54	MG	AA	1675	1/1	0.67	0.40	-	73,73,73,73	0
54	MG	BA	3082	1/1	0.84	0.28	-	71,71,71,71	0
54	MG	BA	3430	1/1	0.98	0.22	-	30,30,30,30	0
54	MG	AA	1638	1/1	0.79	0.24	-	78,78,78,78	0
54	MG	BE	302	1/1	0.89	0.21	-	52,52,52,52	0
54	MG	BA	3076	1/1	0.77	0.13	-	70,70,70,70	0
54	MG	BA	3115	1/1	0.96	0.36	-	43,43,43,43	0
54	MG	DA	3419	1/1	0.98	0.08	-	50,50,50,50	0
54	MG	BA	3286	1/1	0.92	0.24	-	52,52,52,52	0
54	MG	BA	3482	1/1	0.98	0.18	-	58,58,58,58	0
54	MG	DA	3337	1/1	0.94	0.10	-	42,42,42,42	0
54	MG	BA	3442	1/1	0.97	0.15	-	31,31,31,31	0
54	MG	AA	1671	1/1	0.86	0.25	-	89,89,89,89	0
54	MG	DA	3265	1/1	0.95	0.21	-	39,39,39,39	0
54	MG	BA	3527	1/1	0.90	0.15	-	51,51,51,51	0
54	MG	BA	3050	1/1	0.89	0.23	-	46,46,46,46	0
54	MG	BA	3507	1/1	0.97	0.15	-	53,53,53,53	0
54	MG	DA	3068	1/1	0.95	0.23	-	48,48,48,48	0
54	MG	DA	3210	1/1	0.71	0.28	-	60,60,60,60	0
54	MG	AA	1678	1/1	0.74	0.45	-	75,75,75,75	0
54	MG	BA	3549	1/1	0.89	0.12	-	68,68,68,68	0
54	MG	BA	3279	1/1	0.92	0.17	-	54,54,54,54	0
54	MG	DA	3250	1/1	0.93	0.43	-	41,41,41,41	0
54	MG	DA	3266	1/1	0.95	0.09	-	58,58,58,58	0
54	MG	DA	3230	1/1	0.95	0.17	-	67,67,67,67	0
54	MG	BA	3388	1/1	0.88	0.17	-	54,54,54,54	0
54	MG	DA	3232	1/1	0.87	0.36	-	46,46,46,46	0
54	MG	BA	3064	1/1	0.88	0.27	-	45,45,45,45	0
54	MG	BA	3319	1/1	0.96	0.06	-	68,68,68,68	0
54	MG	AA	1667	1/1	0.80	0.28	-	63,63,63,63	0
54	MG	BA	3443	1/1	0.99	0.26	-	41,41,41,41	0
54	MG	DA	3272	1/1	0.96	0.18	-	47,47,47,47	0
54	MG	BA	3089	1/1	0.92	0.40	-	46,46,46,46	0
54	MG	CA	1667	1/1	0.87	0.14	-	64,64,64,64	0
54	MG	BA	3216	1/1	0.79	0.23	-	52,52,52,52	0
54	MG	BA	3125	1/1	0.94	0.23	-	50,50,50,50	0
54	MG	DA	3195	1/1	0.87	0.85	-	75,75,75,75	0
54	MG	CA	1605	1/1	0.83	0.32	-	74,74,74,74	0
54	MG	BE	303	1/1	0.96	0.14	-	54,54,54,54	0
54	MG	BA	3251	1/1	0.78	0.34	-	63,63,63,63	0
54	MG	DA	3026	1/1	0.85	0.16	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3109	1/1	0.78	0.26	-	70,70,70,70	0
54	MG	BA	3263	1/1	0.96	0.63	-	41,41,41,41	0
54	MG	BA	3220	1/1	0.76	0.24	-	79,79,79,79	0
54	MG	BA	3194	1/1	0.73	0.22	-	79,79,79,79	0
54	MG	CA	1621	1/1	0.83	0.27	-	64,64,64,64	0
54	MG	AA	1626	1/1	0.96	0.52	-	67,67,67,67	0
54	MG	DA	3031	1/1	0.95	0.45	-	43,43,43,43	0
54	MG	BA	3171	1/1	0.84	0.24	-	67,67,67,67	0
54	MG	BA	3574	1/1	0.98	0.06	-	41,41,41,41	0
54	MG	DA	3254	1/1	0.80	0.39	-	43,43,43,43	0
54	MG	BA	3287	1/1	0.95	0.45	-	65,65,65,65	0
54	MG	BA	3591	1/1	0.97	0.13	-	56,56,56,56	0
54	MG	DA	3139	1/1	0.88	0.49	-	65,65,65,65	0
54	MG	BA	3248	1/1	0.98	0.19	-	50,50,50,50	0
54	MG	BA	3168	1/1	0.95	0.39	-	52,52,52,52	0
54	MG	AA	1628	1/1	0.68	0.28	-	84,84,84,84	0
54	MG	DA	3075	1/1	0.68	0.45	-	71,71,71,71	0
54	MG	BA	3296	1/1	0.98	0.08	-	48,48,48,48	0
54	MG	DA	3244	1/1	0.89	0.46	-	35,35,35,35	0
54	MG	BA	3214	1/1	0.94	0.57	-	34,34,34,34	0
54	MG	DA	3206	1/1	0.65	0.18	-	75,75,75,75	0
54	MG	DA	3330	1/1	0.92	0.25	-	44,44,44,44	0
54	MG	BA	3203	1/1	0.94	0.31	-	69,69,69,69	0
54	MG	DA	3211	1/1	0.82	0.26	-	53,53,53,53	0
54	MG	DA	3411	1/1	0.90	0.15	-	90,90,90,90	0
54	MG	BA	3073	1/1	0.90	0.11	-	67,67,67,67	0
54	MG	DA	3100	1/1	0.95	0.32	-	61,61,61,61	0
54	MG	BA	3488	1/1	0.97	0.15	-	34,34,34,34	0
54	MG	AA	1629	1/1	0.93	0.15	-	63,63,63,63	0
54	MG	BA	3462	1/1	0.97	0.12	-	25,25,25,25	0
54	MG	DA	3143	1/1	0.67	0.55	-	62,62,62,62	0
54	MG	DA	3156	1/1	0.96	0.26	-	52,52,52,52	0
54	MG	BA	3061	1/1	0.90	0.51	-	64,64,64,64	0
54	MG	AA	1688	1/1	0.83	0.21	-	111,111,111,111	0
54	MG	DA	3253	1/1	0.96	0.30	-	42,42,42,42	0
54	MG	DA	3386	1/1	0.90	0.11	-	63,63,63,63	0
54	MG	BA	3610	1/1	0.95	0.06	-	56,56,56,56	0
54	MG	BA	3042	1/1	0.95	0.51	-	47,47,47,47	0
54	MG	DA	3316	1/1	0.88	0.12	-	75,75,75,75	0
54	MG	BA	3072	1/1	0.89	0.28	-	59,59,59,59	0
54	MG	BA	3508	1/1	0.95	0.12	-	40,40,40,40	0
54	MG	DA	3228	1/1	0.95	0.54	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3176	1/1	0.94	0.33	-	61,61,61,61	0
54	MG	BA	3347	1/1	0.91	0.22	-	55,55,55,55	0
54	MG	DA	3193	1/1	0.93	0.33	-	63,63,63,63	0
54	MG	BA	3155	1/1	0.90	0.36	-	64,64,64,64	0
54	MG	BA	3233	1/1	0.95	0.13	-	59,59,59,59	0
54	MG	DA	3379	1/1	0.65	0.09	-	94,94,94,94	0
54	MG	BA	3375	1/1	0.81	0.33	-	46,46,46,46	0
54	MG	AA	1652	1/1	0.72	0.67	-	82,82,82,82	0
54	MG	BA	3558	1/1	0.76	0.17	-	61,61,61,61	0
54	MG	DA	3141	1/1	0.81	0.53	-	74,74,74,74	0
54	MG	DA	3351	1/1	0.97	0.15	-	78,78,78,78	0
54	MG	DA	3399	1/1	0.94	0.41	-	60,60,60,60	0
54	MG	BA	3015	1/1	0.92	0.37	-	42,42,42,42	0
54	MG	BA	3176	1/1	0.87	0.50	-	69,69,69,69	0
54	MG	BF	301	1/1	0.91	0.40	-	56,56,56,56	0
54	MG	BA	3260	1/1	0.94	0.61	-	50,50,50,50	0
54	MG	BB	212	1/1	0.93	0.06	-	68,68,68,68	0
54	MG	BA	3054	1/1	0.94	0.15	-	52,52,52,52	0
54	MG	DA	3103	1/1	0.74	0.30	-	71,71,71,71	0
54	MG	DA	3346	1/1	0.66	0.10	-	89,89,89,89	0
54	MG	BB	214	1/1	0.83	0.17	-	67,67,67,67	0
54	MG	DA	3339	1/1	0.91	0.11	-	48,48,48,48	0
54	MG	DA	3275	1/1	0.96	0.12	-	48,48,48,48	0
54	MG	DA	3361	1/1	0.96	0.05	-	67,67,67,67	0
54	MG	BA	3358	1/1	0.90	0.07	-	64,64,64,64	0
54	MG	AA	1663	1/1	0.77	0.43	-	70,70,70,70	0
54	MG	DA	3049	1/1	0.89	0.30	-	58,58,58,58	0
54	MG	AA	1607	1/1	0.93	0.40	-	69,69,69,69	0
54	MG	BA	3135	1/1	0.80	0.45	-	54,54,54,54	0
54	MG	DA	3338	1/1	0.95	0.19	-	50,50,50,50	0
54	MG	BA	3469	1/1	0.77	0.25	-	77,77,77,77	0
54	MG	DA	3320	1/1	0.97	0.13	-	57,57,57,57	0
54	MG	BA	3269	1/1	0.88	0.27	-	54,54,54,54	0
54	MG	BA	3027	1/1	0.92	0.15	-	56,56,56,56	0
54	MG	DA	3310	1/1	0.76	0.29	-	56,56,56,56	0
54	MG	BA	3564	1/1	0.96	0.28	-	36,36,36,36	0
54	MG	BA	3011	1/1	0.81	0.58	-	50,50,50,50	0
54	MG	BA	3146	1/1	0.93	0.51	-	52,52,52,52	0
54	MG	BA	3166	1/1	0.81	0.48	-	58,58,58,58	0
54	MG	DA	3091	1/1	0.68	0.16	-	70,70,70,70	0
54	MG	BA	3144	1/1	0.89	0.36	-	54,54,54,54	0
54	MG	DA	3093	1/1	0.88	0.73	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3171	1/1	0.97	0.31	-	53,53,53,53	0
54	MG	BA	3440	1/1	0.97	0.09	-	63,63,63,63	0
54	MG	DA	3251	1/1	0.95	0.48	-	39,39,39,39	0
54	MG	AA	1683	1/1	0.82	0.30	-	139,139,139,139	0
54	MG	BA	3506	1/1	0.97	0.16	-	61,61,61,61	0
54	MG	DA	3234	1/1	0.95	0.48	-	56,56,56,56	0
54	MG	DA	3220	1/1	0.98	0.25	-	48,48,48,48	0
54	MG	DA	3023	1/1	0.82	0.49	-	61,61,61,61	0
54	MG	BA	3184	1/1	0.76	0.20	-	66,66,66,66	0
54	MG	AA	1687	1/1	0.73	0.14	-	70,70,70,70	0
54	MG	BA	3018	1/1	0.92	0.11	-	72,72,72,72	0
54	MG	DA	3148	1/1	0.92	0.42	-	70,70,70,70	0
54	MG	DA	3414	1/1	0.97	0.12	-	68,68,68,68	0
54	MG	DA	3307	1/1	0.98	0.22	-	39,39,39,39	0
54	MG	BA	3359	1/1	0.94	0.13	-	49,49,49,49	0
54	MG	BA	3352	1/1	0.97	0.09	-	53,53,53,53	0
54	MG	BA	3547	1/1	0.94	0.25	-	31,31,31,31	0
54	MG	BP	201	1/1	0.91	0.28	-	43,43,43,43	0
54	MG	BA	3062	1/1	0.84	0.08	-	69,69,69,69	0
54	MG	DA	3298	1/1	0.87	0.14	-	71,71,71,71	0
54	MG	BA	3413	1/1	0.95	0.28	-	31,31,31,31	0
54	MG	BA	3593	1/1	0.69	0.10	-	70,70,70,70	0
54	MG	DA	3182	1/1	0.88	0.28	-	59,59,59,59	0
54	MG	BA	3463	1/1	0.88	0.20	-	36,36,36,36	0
54	MG	BA	3316	1/1	0.90	0.32	-	34,34,34,34	0
54	MG	BA	3150	1/1	0.90	0.22	-	61,61,61,61	0
54	MG	DA	3218	1/1	0.96	0.71	-	53,53,53,53	0
54	MG	BA	3147	1/1	0.82	0.30	-	57,57,57,57	0
54	MG	CA	1657	1/1	0.91	0.23	-	86,86,86,86	0
54	MG	BA	3567	1/1	0.82	0.09	-	62,62,62,62	0
54	MG	CA	1619	1/1	0.61	0.46	-	69,69,69,69	0
54	MG	AA	1706	1/1	0.89	0.08	-	100,100,100,100	0
54	MG	DA	3293	1/1	0.91	0.29	-	50,50,50,50	0
54	MG	BA	3224	1/1	0.79	0.31	-	61,61,61,61	0
54	MG	DA	3404	1/1	0.99	0.07	-	53,53,53,53	0
54	MG	BA	3495	1/1	0.85	0.19	-	70,70,70,70	0
54	MG	CA	1651	1/1	0.95	0.17	-	61,61,61,61	0
54	MG	DA	3321	1/1	0.95	0.21	-	53,53,53,53	0
54	MG	BA	3101	1/1	0.91	0.28	-	51,51,51,51	0
54	MG	AA	1620	1/1	0.77	0.92	-	77,77,77,77	0
54	MG	DA	3332	1/1	0.98	0.05	-	62,62,62,62	0
54	MG	DA	3359	1/1	0.93	0.37	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3041	1/1	0.91	0.12	-	56,56,56,56	0
54	MG	BA	3539	1/1	0.97	0.06	-	61,61,61,61	0
54	MG	BA	3335	1/1	0.89	0.15	-	55,55,55,55	0
54	MG	BA	3453	1/1	0.94	0.17	-	74,74,74,74	0
54	MG	BA	3188	1/1	0.93	0.28	-	43,43,43,43	0
54	MG	DA	3255	1/1	0.97	0.37	-	63,63,63,63	0
54	MG	BA	3502	1/1	0.97	0.17	-	41,41,41,41	0
54	MG	DA	3161	1/1	0.87	0.47	-	55,55,55,55	0
54	MG	BA	3608	1/1	0.60	0.12	-	87,87,87,87	0
54	MG	BA	3490	1/1	0.96	0.27	-	53,53,53,53	0
54	MG	CA	1610	1/1	0.84	0.43	-	80,80,80,80	0
54	MG	DA	3362	1/1	0.85	0.11	-	63,63,63,63	0
54	MG	DA	3166	1/1	0.96	0.22	-	55,55,55,55	0
54	MG	BA	3079	1/1	0.81	0.27	-	68,68,68,68	0
54	MG	DA	3239	1/1	0.89	0.28	-	39,39,39,39	0
54	MG	BA	3349	1/1	0.96	0.13	-	39,39,39,39	0
54	MG	BA	3616	1/1	0.90	0.08	-	82,82,82,82	0
54	MG	BA	3400	1/1	0.94	0.19	-	34,34,34,34	0
54	MG	DA	3201	1/1	0.93	0.36	-	69,69,69,69	0
54	MG	BA	3235	1/1	0.94	0.12	-	45,45,45,45	0
54	MG	AA	1637	1/1	0.75	0.33	-	82,82,82,82	0
54	MG	BA	3058	1/1	0.96	0.10	-	56,56,56,56	0
54	MG	DA	3042	1/1	0.92	0.58	-	46,46,46,46	0
54	MG	DA	3191	1/1	0.95	0.26	-	50,50,50,50	0
54	MG	BA	3008	1/1	0.96	0.28	-	32,32,32,32	0
54	MG	DA	3106	1/1	0.81	0.33	-	56,56,56,56	0
54	MG	DA	3063	1/1	0.85	0.19	-	54,54,54,54	0
54	MG	BA	3369	1/1	0.91	0.31	-	74,74,74,74	0
54	MG	BA	3459	1/1	0.40	0.14	-	130,130,130,130	0
54	MG	DA	3089	1/1	0.75	0.38	-	82,82,82,82	0
54	MG	DA	3153	1/1	0.95	0.47	-	38,38,38,38	0
54	MG	BA	3538	1/1	0.84	0.13	-	70,70,70,70	0
54	MG	BA	3128	1/1	0.94	0.21	-	53,53,53,53	0
54	MG	D7	101	1/1	0.91	0.30	-	52,52,52,52	0
54	MG	BA	3250	1/1	0.90	0.23	-	47,47,47,47	0
54	MG	BA	3541	1/1	0.96	0.30	-	54,54,54,54	0
54	MG	BA	3542	1/1	0.92	0.23	-	60,60,60,60	0
54	MG	DA	3308	1/1	0.97	0.42	-	49,49,49,49	0
54	MG	AA	1665	1/1	0.54	0.53	-	86,86,86,86	0
54	MG	BE	305	1/1	0.97	0.22	-	32,32,32,32	0
54	MG	DA	3102	1/1	0.71	0.47	-	79,79,79,79	0
54	MG	BA	3365	1/1	0.84	0.10	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1646	1/1	0.86	0.38	-	73,73,73,73	0
54	MG	AA	1611	1/1	0.84	0.30	-	69,69,69,69	0
54	MG	BA	3582	1/1	0.96	0.12	-	54,54,54,54	0
54	MG	CA	1606	1/1	0.80	0.62	-	81,81,81,81	0
54	MG	DA	3105	1/1	0.92	0.55	-	33,33,33,33	0
54	MG	BA	3545	1/1	0.80	0.18	-	79,79,79,79	0
54	MG	DA	3212	1/1	0.94	0.26	-	38,38,38,38	0
54	MG	BA	3381	1/1	0.98	0.08	-	49,49,49,49	0
54	MG	DA	3077	1/1	0.78	0.21	-	66,66,66,66	0
54	MG	DA	3241	1/1	0.96	0.25	-	63,63,63,63	0
54	MG	DA	3384	1/1	0.93	0.21	-	57,57,57,57	0
54	MG	BA	3481	1/1	0.93	0.10	-	76,76,76,76	0
54	MG	DA	3287	1/1	0.97	0.07	-	46,46,46,46	0
54	MG	CA	1629	1/1	0.87	0.23	-	72,72,72,72	0
54	MG	DA	3257	1/1	0.92	0.62	-	59,59,59,59	0
54	MG	BA	3586	1/1	0.94	0.09	-	58,58,58,58	0
54	MG	AA	1601	1/1	0.91	0.29	-	68,68,68,68	0
54	MG	BA	3100	1/1	0.84	0.34	-	72,72,72,72	0
54	MG	CA	1603	1/1	0.94	0.28	-	73,73,73,73	0
54	MG	BA	3518	1/1	0.97	0.36	-	59,59,59,59	0
54	MG	BA	3566	1/1	0.95	0.21	-	40,40,40,40	0
54	MG	DA	3034	1/1	0.90	0.27	-	74,74,74,74	0
54	MG	BA	3318	1/1	0.92	0.24	-	73,73,73,73	0
54	MG	BA	3373	1/1	0.95	0.09	-	55,55,55,55	0
54	MG	DA	3345	1/1	0.86	0.27	-	100,100,100,100	0
54	MG	DA	3175	1/1	0.81	0.27	-	69,69,69,69	0
54	MG	BA	3140	1/1	0.89	0.46	-	59,59,59,59	0
54	MG	BA	3114	1/1	0.89	0.25	-	43,43,43,43	0
54	MG	BA	3124	1/1	0.90	0.23	-	68,68,68,68	0
54	MG	DA	3248	1/1	0.94	0.55	-	44,44,44,44	0
54	MG	DA	3200	1/1	0.81	0.19	-	67,67,67,67	0
54	MG	BA	3225	1/1	0.81	0.34	-	61,61,61,61	0
54	MG	DA	3331	1/1	0.95	0.17	-	69,69,69,69	0
54	MG	BA	3380	1/1	0.97	0.07	-	50,50,50,50	0
54	MG	AA	1680	1/1	0.92	0.17	-	83,83,83,83	0
54	MG	AA	1692	1/1	0.83	0.53	-	113,113,113,113	0
54	MG	BA	3299	1/1	0.98	0.22	-	38,38,38,38	0
54	MG	DA	3367	1/1	0.91	0.14	-	68,68,68,68	0
54	MG	BA	3278	1/1	0.96	0.25	-	43,43,43,43	0
54	MG	BB	203	1/1	0.94	0.19	-	80,80,80,80	0
54	MG	BA	3584	1/1	0.86	0.14	-	68,68,68,68	0
54	MG	DA	3318	1/1	0.93	0.07	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1606	1/1	0.84	0.90	-	74,74,74,74	0
54	MG	BA	3294	1/1	0.93	0.20	-	37,37,37,37	0
54	MG	DA	3422	1/1	0.95	0.10	-	75,75,75,75	0
54	MG	DA	3192	1/1	0.77	0.19	-	66,66,66,66	0
54	MG	DA	3009	1/1	0.94	0.26	-	54,54,54,54	0
54	MG	DA	3347	1/1	0.92	0.07	-	76,76,76,76	0
54	MG	BA	3353	1/1	0.95	0.13	-	28,28,28,28	0
54	MG	DA	3025	1/1	0.97	0.18	-	57,57,57,57	0
54	MG	DA	3157	1/1	0.92	0.33	-	69,69,69,69	0
54	MG	AA	1641	1/1	0.81	0.65	-	93,93,93,93	0
54	MG	BD	301	1/1	0.90	0.20	-	41,41,41,41	0
54	MG	DA	3184	1/1	0.94	0.44	-	39,39,39,39	0
54	MG	DA	3216	1/1	0.91	0.19	-	53,53,53,53	0
54	MG	AA	1612	1/1	0.86	0.36	-	76,76,76,76	0
54	MG	BA	3247	1/1	0.89	0.25	-	53,53,53,53	0
54	MG	BA	3313	1/1	0.98	0.12	-	42,42,42,42	0
54	MG	DA	3173	1/1	0.92	0.40	-	49,49,49,49	0
54	MG	BA	3391	1/1	0.96	0.28	-	38,38,38,38	0
54	MG	BA	3218	1/1	0.93	0.37	-	54,54,54,54	0
54	MG	BA	3589	1/1	0.92	0.06	-	70,70,70,70	0
54	MG	DA	3016	1/1	0.95	0.11	-	41,41,41,41	0
54	MG	D6	102	1/1	0.92	0.50	-	64,64,64,64	0
54	MG	BA	3266	1/1	0.93	0.77	-	48,48,48,48	0
54	MG	BA	3401	1/1	0.96	0.17	-	45,45,45,45	0
54	MG	BA	3341	1/1	0.88	0.08	-	69,69,69,69	0
54	MG	BA	3521	1/1	0.92	0.19	-	41,41,41,41	0
54	MG	BA	3383	1/1	0.95	0.17	-	71,71,71,71	0
54	MG	DA	3229	1/1	0.92	0.37	-	55,55,55,55	0
54	MG	BA	3024	1/1	0.87	0.29	-	48,48,48,48	0
54	MG	DA	3005	1/1	0.94	0.20	-	64,64,64,64	0
54	MG	AA	1685	1/1	0.95	0.11	-	77,77,77,77	0
54	MG	BA	3561	1/1	0.94	0.27	-	49,49,49,49	0
54	MG	BA	3342	1/1	0.94	0.08	-	57,57,57,57	0
54	MG	DA	3057	1/1	0.90	0.14	-	67,67,67,67	0
54	MG	CA	1661	1/1	0.78	0.27	-	100,100,100,100	0
54	MG	DA	3069	1/1	0.82	0.48	-	61,61,61,61	0
54	MG	BA	3476	1/1	0.98	0.23	-	44,44,44,44	0
54	MG	BA	3026	1/1	0.90	0.18	-	68,68,68,68	0
54	MG	DA	3295	1/1	0.92	0.17	-	42,42,42,42	0
54	MG	BA	3524	1/1	0.87	0.17	-	77,77,77,77	0
54	MG	DA	3235	1/1	0.96	0.33	-	36,36,36,36	0
54	MG	BA	3270	1/1	0.77	0.32	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3206	1/1	0.84	0.13	-	68,68,68,68	0
54	MG	CA	1669	1/1	0.83	0.10	-	117,117,117,117	0
54	MG	DA	3189	1/1	0.81	0.80	-	66,66,66,66	0
54	MG	DA	3051	1/1	0.94	0.15	-	43,43,43,43	0
54	MG	DA	3227	1/1	0.90	0.39	-	65,65,65,65	0
54	MG	BA	3487	1/1	0.67	0.22	-	94,94,94,94	0
54	MG	AA	1634	1/1	0.91	0.77	-	95,95,95,95	0
54	MG	BA	3578	1/1	0.98	0.21	-	60,60,60,60	0
54	MG	DA	3311	1/1	0.85	0.07	-	65,65,65,65	0
54	MG	DA	3403	1/1	0.88	0.18	-	49,49,49,49	0
54	MG	BA	3464	1/1	0.82	0.32	-	41,41,41,41	0
54	MG	AA	1677	1/1	0.90	0.89	-	81,81,81,81	0
54	MG	DA	3158	1/1	0.91	0.43	-	72,72,72,72	0
54	MG	DA	3081	1/1	0.86	0.23	-	52,52,52,52	0
54	MG	BA	3165	1/1	0.93	0.13	-	56,56,56,56	0
54	MG	B5	102	1/1	0.99	0.08	-	42,42,42,42	0
54	MG	DA	3147	1/1	0.95	0.68	-	78,78,78,78	0
54	MG	BA	3085	1/1	0.92	0.30	-	63,63,63,63	0
54	MG	BA	3356	1/1	0.90	0.28	-	59,59,59,59	0
54	MG	BV	201	1/1	0.80	0.36	-	74,74,74,74	0
54	MG	AA	1603	1/1	0.91	0.11	-	68,68,68,68	0
54	MG	DA	3401	1/1	0.91	0.07	-	85,85,85,85	0
54	MG	BA	3179	1/1	0.95	0.45	-	48,48,48,48	0
54	MG	BA	3446	1/1	0.94	0.10	-	40,40,40,40	0
54	MG	BA	3102	1/1	0.90	0.25	-	59,59,59,59	0
54	MG	BA	3568	1/1	0.96	0.14	-	60,60,60,60	0
54	MG	BA	3298	1/1	0.92	0.11	-	53,53,53,53	0
54	MG	BA	3533	1/1	0.90	0.19	-	48,48,48,48	0
54	MG	AA	1633	1/1	0.89	0.52	-	72,72,72,72	0
54	MG	BA	3445	1/1	0.93	0.09	-	56,56,56,56	0
54	MG	AA	1672	1/1	0.95	0.66	-	82,82,82,82	0
54	MG	DA	3024	1/1	0.88	0.41	-	49,49,49,49	0
54	MG	DA	3335	1/1	0.94	0.25	-	72,72,72,72	0
54	MG	BA	3273	1/1	0.89	0.22	-	66,66,66,66	0
54	MG	AA	1643	1/1	0.77	0.86	-	96,96,96,96	0
54	MG	BA	3418	1/1	0.93	0.09	-	54,54,54,54	0
54	MG	BA	3035	1/1	0.96	0.24	-	45,45,45,45	0
54	MG	DA	3039	1/1	0.97	0.28	-	41,41,41,41	0
54	MG	BA	3343	1/1	0.87	0.06	-	91,91,91,91	0
54	MG	DA	3423	1/1	0.83	0.14	-	79,79,79,79	0
54	MG	BA	3306	1/1	0.94	0.16	-	51,51,51,51	0
54	MG	DA	3271	1/1	0.94	0.10	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3119	1/1	0.92	0.61	-	57,57,57,57	0
54	MG	BB	210	1/1	0.86	0.14	-	67,67,67,67	0
54	MG	BA	3537	1/1	0.93	0.17	-	38,38,38,38	0
54	MG	DA	3131	1/1	0.95	0.28	-	39,39,39,39	0
54	MG	BA	3563	1/1	0.94	0.11	-	67,67,67,67	0
54	MG	DA	3256	1/1	0.82	0.58	-	59,59,59,59	0
54	MG	DA	3426	1/1	0.98	0.10	-	94,94,94,94	0
54	MG	DA	3137	1/1	0.96	0.57	-	64,64,64,64	0
54	MG	BA	3291	1/1	0.95	0.13	-	59,59,59,59	0
54	MG	BA	3588	1/1	0.93	0.25	-	86,86,86,86	0
54	MG	BA	3523	1/1	0.95	0.06	-	79,79,79,79	0
54	MG	BW	201	1/1	0.93	0.17	-	51,51,51,51	0
54	MG	BA	3120	1/1	0.88	0.31	-	42,42,42,42	0
54	MG	BA	3339	1/1	0.83	0.08	-	91,91,91,91	0
54	MG	DA	3164	1/1	0.96	0.23	-	46,46,46,46	0
54	MG	DA	3368	1/1	0.94	0.17	-	78,78,78,78	0
54	MG	BF	302	1/1	0.93	0.21	-	62,62,62,62	0
54	MG	BA	3284	1/1	0.95	0.13	-	40,40,40,40	0
54	MG	AA	1681	1/1	0.92	0.12	-	65,65,65,65	0
54	MG	DA	3348	1/1	0.93	0.12	-	85,85,85,85	0
54	MG	CA	1634	1/1	0.86	0.35	-	101,101,101,101	0
54	MG	BA	3529	1/1	0.78	0.28	-	86,86,86,86	0
54	MG	AA	1644	1/1	0.94	0.34	-	74,74,74,74	0
54	MG	BA	3077	1/1	0.88	0.59	-	43,43,43,43	0
54	MG	DA	3140	1/1	0.93	0.54	-	70,70,70,70	0
54	MG	DA	3260	1/1	0.91	0.50	-	44,44,44,44	0
54	MG	BA	3261	1/1	0.96	0.29	-	59,59,59,59	0
54	MG	CA	1620	1/1	0.96	0.32	-	57,57,57,57	0
54	MG	AA	1610	1/1	0.96	0.29	-	75,75,75,75	0
54	MG	BA	3450	1/1	0.87	0.13	-	71,71,71,71	0
54	MG	BA	3364	1/1	0.96	0.12	-	46,46,46,46	0
54	MG	AA	1661	1/1	0.73	0.80	-	77,77,77,77	0
54	MG	DA	3223	1/1	0.80	0.09	-	104,104,104,104	0
54	MG	BA	3103	1/1	0.91	0.47	-	67,67,67,67	0
54	MG	BA	3075	1/1	0.96	0.30	-	53,53,53,53	0
54	MG	DA	3172	1/1	0.82	0.27	-	50,50,50,50	0
54	MG	BA	3172	1/1	0.93	0.22	-	71,71,71,71	0
54	MG	DA	3179	1/1	0.94	0.27	-	62,62,62,62	0
54	MG	BA	3614	1/1	0.74	0.31	-	94,94,94,94	0
54	MG	BA	3569	1/1	0.81	0.27	-	68,68,68,68	0
54	MG	BA	3496	1/1	0.81	0.10	-	79,79,79,79	0
54	MG	AA	1656	1/1	0.59	0.83	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3315	1/1	0.72	0.17	-	84,84,84,84	0
54	MG	BA	3577	1/1	0.94	0.23	-	58,58,58,58	0
54	MG	DA	3424	1/1	0.86	0.14	-	130,130,130,130	0
54	MG	CA	1656	1/1	0.70	0.12	-	97,97,97,97	0
54	MG	BA	3536	1/1	0.85	0.09	-	82,82,82,82	0
54	MG	BA	3310	1/1	0.99	0.21	-	44,44,44,44	0
54	MG	BA	3257	1/1	0.69	0.40	-	64,64,64,64	0
54	MG	BA	3612	1/1	0.78	0.12	-	100,100,100,100	0
54	MG	DA	3357	1/1	0.82	0.14	-	53,53,53,53	0
54	MG	BA	3186	1/1	0.91	0.40	-	64,64,64,64	0
54	MG	BA	3478	1/1	0.90	0.16	-	92,92,92,92	0
54	MG	DA	3381	1/1	0.89	0.09	-	79,79,79,79	0
54	MG	DA	3336	1/1	0.79	0.16	-	87,87,87,87	0
54	MG	BA	3088	1/1	0.93	0.35	-	46,46,46,46	0
54	MG	BA	3452	1/1	0.95	0.11	-	62,62,62,62	0
54	MG	BA	3466	1/1	0.98	0.07	-	67,67,67,67	0
54	MG	DA	3082	1/1	0.76	0.41	-	51,51,51,51	0
54	MG	BA	3449	1/1	0.89	0.18	-	49,49,49,49	0
54	MG	AA	1632	1/1	0.85	0.52	-	93,93,93,93	0
54	MG	DA	3076	1/1	0.96	0.17	-	70,70,70,70	0
54	MG	DA	3180	1/1	0.93	0.24	-	78,78,78,78	0
54	MG	BB	217	1/1	0.99	0.25	-	42,42,42,42	0
54	MG	BA	3531	1/1	0.93	0.15	-	49,49,49,49	0
54	MG	BA	3503	1/1	0.72	0.22	-	68,68,68,68	0
54	MG	BA	3362	1/1	0.89	0.11	-	73,73,73,73	0
54	MG	DA	3197	1/1	0.88	0.65	-	66,66,66,66	0
54	MG	BA	3272	1/1	0.90	0.07	-	65,65,65,65	0
54	MG	BA	3599	1/1	0.97	0.09	-	50,50,50,50	0
54	MG	BA	3324	1/1	0.96	0.10	-	82,82,82,82	0
54	MG	BA	3012	1/1	0.94	0.20	-	34,34,34,34	0
54	MG	AA	1698	1/1	0.91	0.44	-	68,68,68,68	0
54	MG	DA	3021	1/1	0.93	0.24	-	53,53,53,53	0
54	MG	BA	3213	1/1	0.89	0.37	-	64,64,64,64	0
54	MG	AA	1650	1/1	0.88	0.27	-	70,70,70,70	0
54	MG	BA	3325	1/1	0.89	0.11	-	47,47,47,47	0
54	MG	DA	3022	1/1	0.97	0.36	-	52,52,52,52	0
54	MG	BA	3116	1/1	0.88	0.37	-	56,56,56,56	0
54	MG	DA	3300	1/1	0.98	0.20	-	62,62,62,62	0
54	MG	BA	3600	1/1	0.99	0.20	-	31,31,31,31	0
54	MG	DA	3107	1/1	0.77	0.20	-	47,47,47,47	0
54	MG	BA	3439	1/1	0.87	0.18	-	53,53,53,53	0
54	MG	BA	3190	1/1	0.96	0.31	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3585	1/1	0.94	0.24	-	54,54,54,54	0
54	MG	BA	3092	1/1	0.92	0.41	-	55,55,55,55	0
54	MG	AA	1690	1/1	0.93	0.12	-	59,59,59,59	0
54	MG	BA	3096	1/1	0.93	0.54	-	63,63,63,63	0
54	MG	BA	3415	1/1	0.88	0.12	-	49,49,49,49	0
54	MG	DA	3289	1/1	0.95	0.20	-	52,52,52,52	0
54	MG	AA	1679	1/1	0.84	0.35	-	64,64,64,64	0
54	MG	DA	3008	1/1	0.85	0.22	-	48,48,48,48	0
54	MG	BA	3550	1/1	0.98	0.28	-	37,37,37,37	0
54	MG	BA	3099	1/1	0.94	0.28	-	52,52,52,52	0
54	MG	DA	3258	1/1	0.92	0.10	-	56,56,56,56	0
54	MG	BA	3419	1/1	0.97	0.25	-	35,35,35,35	0
54	MG	DA	3430	1/1	0.97	0.05	-	72,72,72,72	0
54	MG	BA	3162	1/1	0.96	0.48	-	62,62,62,62	0
54	MG	BA	3182	1/1	0.95	0.09	-	69,69,69,69	0
54	MG	BA	3534	1/1	0.67	0.27	-	76,76,76,76	0
54	MG	AA	1701	1/1	0.93	0.12	-	96,96,96,96	0
54	MG	BA	3154	1/1	0.90	0.15	-	49,49,49,49	0
54	MG	BA	3609	1/1	0.98	0.18	-	51,51,51,51	0
54	MG	DA	3037	1/1	0.77	0.46	-	49,49,49,49	0
54	MG	BA	3433	1/1	0.94	0.14	-	35,35,35,35	0
54	MG	BA	3068	1/1	0.86	0.18	-	70,70,70,70	0
54	MG	BA	3374	1/1	0.57	0.14	-	75,75,75,75	0
54	MG	AA	1639	1/1	0.87	0.20	-	74,74,74,74	0
54	MG	B5	101	1/1	0.91	0.29	-	51,51,51,51	0
54	MG	BA	3384	1/1	0.80	0.11	-	62,62,62,62	0
54	MG	DB	203	1/1	0.93	0.48	-	61,61,61,61	0
54	MG	DA	3045	1/1	0.94	0.36	-	72,72,72,72	0
54	MG	DA	3391	1/1	0.83	0.14	-	67,67,67,67	0
54	MG	BA	3264	1/1	0.87	0.62	-	38,38,38,38	0
54	MG	BA	3158	1/1	0.89	0.35	-	51,51,51,51	0
54	MG	BA	3444	1/1	0.90	0.06	-	61,61,61,61	0
54	MG	BA	3431	1/1	0.98	0.25	-	34,34,34,34	0
54	MG	DA	3050	1/1	0.69	0.16	-	90,90,90,90	0
54	MG	DA	3096	1/1	0.93	0.42	-	46,46,46,46	0
54	MG	BA	3571	1/1	0.92	0.14	-	76,76,76,76	0
54	MG	BA	3056	1/1	0.95	0.40	-	48,48,48,48	0
54	MG	BA	3065	1/1	0.94	0.13	-	47,47,47,47	0
54	MG	BA	3252	1/1	0.95	0.24	-	44,44,44,44	0
54	MG	DA	3152	1/1	0.93	0.47	-	58,58,58,58	0
54	MG	DA	3048	1/1	0.75	0.47	-	53,53,53,53	0
54	MG	DA	3111	1/1	0.87	0.46	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3097	1/1	0.87	0.72	-	64,64,64,64	0
54	MG	DA	3056	1/1	0.87	0.44	-	61,61,61,61	0
54	MG	BA	3138	1/1	0.90	0.19	-	54,54,54,54	0
54	MG	BA	3322	1/1	0.95	0.13	-	45,45,45,45	0
54	MG	BA	3467	1/1	0.92	0.13	-	73,73,73,73	0
54	MG	DA	3035	1/1	0.82	0.64	-	68,68,68,68	0
54	MG	BA	3126	1/1	0.95	0.41	-	57,57,57,57	0
54	MG	DA	3387	1/1	0.81	0.09	-	71,71,71,71	0
54	MG	AA	1642	1/1	0.94	0.16	-	64,64,64,64	0
54	MG	BA	3215	1/1	0.96	0.14	-	61,61,61,61	0
54	MG	BA	3377	1/1	0.93	0.12	-	69,69,69,69	0
54	MG	DA	3194	1/1	0.93	0.55	-	77,77,77,77	0
54	MG	CA	1665	1/1	0.85	0.14	-	76,76,76,76	0
54	MG	DA	3167	1/1	0.94	0.10	-	59,59,59,59	0
54	MG	BA	3196	1/1	0.80	0.79	-	80,80,80,80	0
54	MG	DA	3407	1/1	0.94	0.25	-	59,59,59,59	0
54	MG	AA	1668	1/1	0.98	0.12	-	83,83,83,83	0
54	MG	BA	3005	1/1	0.95	0.14	-	42,42,42,42	0
54	MG	DA	3136	1/1	0.96	0.52	-	42,42,42,42	0
54	MG	BA	3573	1/1	0.96	0.09	-	55,55,55,55	0
54	MG	DA	3108	1/1	0.83	0.18	-	80,80,80,80	0
54	MG	BA	3044	1/1	0.92	0.16	-	49,49,49,49	0
54	MG	BA	3098	1/1	0.91	0.39	-	54,54,54,54	0
54	MG	B2	102	1/1	0.92	0.26	-	60,60,60,60	0
54	MG	BA	3212	1/1	0.95	0.16	-	47,47,47,47	0
54	MG	BA	3093	1/1	0.81	0.18	-	81,81,81,81	0
54	MG	BA	3492	1/1	0.88	0.15	-	78,78,78,78	0
54	MG	AA	1676	1/1	0.81	0.62	-	84,84,84,84	0
54	MG	BA	3595	1/1	0.89	0.09	-	82,82,82,82	0
54	MG	BA	3066	1/1	0.87	0.11	-	43,43,43,43	0
54	MG	CA	1642	1/1	0.96	0.08	-	87,87,87,87	0
54	MG	DA	3165	1/1	0.94	0.17	-	58,58,58,58	0
54	MG	DA	3047	1/1	0.60	0.44	-	65,65,65,65	0
54	MG	DA	3323	1/1	0.96	0.20	-	36,36,36,36	0
54	MG	BA	3414	1/1	0.89	0.28	-	26,26,26,26	0
54	MG	BA	3361	1/1	0.91	0.20	-	53,53,53,53	0
54	MG	BA	3470	1/1	0.97	0.23	-	35,35,35,35	0
54	MG	BA	3145	1/1	0.26	0.48	-	78,78,78,78	0
54	MG	DA	3429	1/1	0.95	0.16	-	44,44,44,44	0
54	MG	DA	3417	1/1	0.86	0.26	-	81,81,81,81	0
54	MG	BA	3167	1/1	0.82	0.35	-	68,68,68,68	0
54	MG	BU	201	1/1	0.81	0.41	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3364	1/1	0.93	0.12	-	67,67,67,67	0
54	MG	BA	3231	1/1	0.92	0.41	-	45,45,45,45	0
54	MG	BA	3134	1/1	0.95	0.45	-	44,44,44,44	0
54	MG	BB	206	1/1	0.93	0.15	-	62,62,62,62	0
54	MG	DA	3088	1/1	0.96	0.26	-	65,65,65,65	0
54	MG	CA	1604	1/1	0.95	0.19	-	110,110,110,110	0
54	MG	CA	1668	1/1	0.65	0.22	-	105,105,105,105	0
54	MG	DA	3215	1/1	0.92	0.24	-	58,58,58,58	0
54	MG	DA	3294	1/1	0.93	0.16	-	52,52,52,52	0
54	MG	BA	3382	1/1	0.94	0.08	-	58,58,58,58	0
54	MG	BA	3055	1/1	0.84	0.32	-	58,58,58,58	0
54	MG	CA	1660	1/1	0.81	0.15	-	106,106,106,106	0
54	MG	BA	3275	1/1	0.94	0.19	-	41,41,41,41	0
54	MG	DA	3159	1/1	0.92	0.62	-	59,59,59,59	0
54	MG	BA	3143	1/1	0.94	0.40	-	45,45,45,45	0
54	MG	BA	3211	1/1	0.95	0.19	-	53,53,53,53	0
54	MG	BA	3163	1/1	0.97	0.43	-	42,42,42,42	0
54	MG	BA	3245	1/1	0.99	0.12	-	36,36,36,36	0
54	MG	BA	3265	1/1	0.94	0.39	-	30,30,30,30	0
54	MG	DA	3145	1/1	0.97	0.44	-	47,47,47,47	0
54	MG	BA	3613	1/1	0.80	0.12	-	109,109,109,109	0
54	MG	AA	1608	1/1	0.80	0.15	-	90,90,90,90	0
54	MG	BA	3185	1/1	0.91	0.23	-	44,44,44,44	0
54	MG	BA	3002	1/1	0.86	0.19	-	98,98,98,98	0
54	MG	BA	3087	1/1	0.89	0.26	-	56,56,56,56	0
54	MG	BA	3063	1/1	0.83	0.21	-	84,84,84,84	0
54	MG	B2	101	1/1	0.83	0.26	-	75,75,75,75	0
54	MG	BA	3338	1/1	0.91	0.15	-	30,30,30,30	0
54	MG	BA	3317	1/1	0.97	0.09	-	51,51,51,51	0
54	MG	CA	1659	1/1	0.90	0.21	-	60,60,60,60	0
54	MG	CA	1662	1/1	0.88	0.18	-	95,95,95,95	0
54	MG	BA	3293	1/1	0.97	0.21	-	29,29,29,29	0
54	MG	BB	207	1/1	0.67	0.60	-	69,69,69,69	0
54	MG	BA	3280	1/1	0.39	0.44	-	89,89,89,89	0
54	MG	BA	3032	1/1	0.86	0.21	-	67,67,67,67	0
54	MG	DA	3129	1/1	0.84	0.35	-	78,78,78,78	0
54	MG	BA	3242	1/1	0.80	0.40	-	66,66,66,66	0
54	MG	BA	3598	1/1	0.95	0.13	-	39,39,39,39	0
54	MG	DA	3273	1/1	0.98	0.11	-	37,37,37,37	0
54	MG	BA	3285	1/1	0.89	0.55	-	59,59,59,59	0
54	MG	BA	3514	1/1	0.71	0.19	-	97,97,97,97	0
54	MG	DA	3190	1/1	0.74	0.34	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3213	1/1	0.90	0.13	-	64,64,64,64	0
54	MG	DA	3263	1/1	0.97	0.08	-	70,70,70,70	0
54	MG	BA	3204	1/1	0.90	0.18	-	47,47,47,47	0
54	MG	BA	3004	1/1	0.90	0.21	-	41,41,41,41	0
54	MG	BA	3346	1/1	0.96	0.07	-	45,45,45,45	0
54	MG	DA	3080	1/1	0.83	1.04	-	73,73,73,73	0
54	MG	DA	3110	1/1	0.98	0.08	-	46,46,46,46	0
54	MG	BA	3393	1/1	0.99	0.19	-	38,38,38,38	0
54	MG	BA	3255	1/1	0.94	0.58	-	65,65,65,65	0
54	MG	CA	1645	1/1	0.92	0.30	-	63,63,63,63	0
54	MG	BA	3336	1/1	0.95	0.12	-	46,46,46,46	0
54	MG	BA	3136	1/1	0.80	0.24	-	73,73,73,73	0
54	MG	BD	303	1/1	0.95	0.35	-	58,58,58,58	0
54	MG	CA	1608	1/1	0.70	0.45	-	67,67,67,67	0
54	MG	DA	3392	1/1	0.98	0.09	-	56,56,56,56	0
54	MG	DA	3261	1/1	0.91	0.42	-	56,56,56,56	0
54	MG	BA	3399	1/1	0.92	0.23	-	41,41,41,41	0
54	MG	BA	3084	1/1	0.95	0.17	-	56,56,56,56	0
54	MG	BA	3535	1/1	0.84	0.24	-	70,70,70,70	0
54	MG	DA	3378	1/1	0.90	0.14	-	98,98,98,98	0
54	MG	CA	1649	1/1	0.89	0.16	-	92,92,92,92	0
54	MG	BA	3198	1/1	0.94	0.25	-	29,29,29,29	0
54	MG	DE	301	1/1	0.94	0.51	-	37,37,37,37	0
54	MG	DA	3155	1/1	0.79	0.28	-	57,57,57,57	0
54	MG	AA	1635	1/1	0.95	0.21	-	71,71,71,71	0
54	MG	AA	1662	1/1	0.94	0.22	-	83,83,83,83	0
54	MG	BA	3297	1/1	0.83	0.17	-	35,35,35,35	0
54	MG	BA	3013	1/1	0.87	0.60	-	103,103,103,103	0
54	MG	DA	3343	1/1	0.94	0.17	-	35,35,35,35	0
54	MG	BU	202	1/1	0.92	0.53	-	62,62,62,62	0
54	MG	CA	1611	1/1	0.91	0.18	-	64,64,64,64	0
54	MG	DA	3224	1/1	0.89	0.35	-	80,80,80,80	0
54	MG	CA	1622	1/1	0.90	0.32	-	74,74,74,74	0
54	MG	BA	3340	1/1	0.78	0.21	-	65,65,65,65	0
54	MG	BA	3036	1/1	0.89	0.41	-	49,49,49,49	0
54	MG	BA	3615	1/1	0.93	0.06	-	91,91,91,91	0
54	MG	DA	3358	1/1	0.92	0.15	-	68,68,68,68	0
54	MG	DA	3400	1/1	0.69	0.33	-	95,95,95,95	0
54	MG	BA	3110	1/1	0.97	0.37	-	23,23,23,23	0
54	MG	DA	3371	1/1	0.93	0.19	-	50,50,50,50	0
54	MG	BA	3217	1/1	0.71	0.39	-	51,51,51,51	0
54	MG	CA	1625	1/1	0.86	0.37	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3389	1/1	0.92	0.20	-	33,33,33,33	0
54	MG	BA	3192	1/1	0.96	0.33	-	43,43,43,43	0
54	MG	BA	3363	1/1	0.73	0.26	-	74,74,74,74	0
54	MG	DA	3060	1/1	0.91	0.21	-	60,60,60,60	0
54	MG	BA	3195	1/1	0.68	0.31	-	84,84,84,84	0
54	MG	DA	3151	1/1	0.94	0.37	-	58,58,58,58	0
54	MG	BR	202	1/1	0.94	0.39	-	49,49,49,49	0
54	MG	BA	3282	1/1	0.94	0.28	-	43,43,43,43	0
54	MG	DA	3221	1/1	0.85	0.48	-	69,69,69,69	0
54	MG	BA	3592	1/1	0.91	0.08	-	51,51,51,51	0
54	MG	BA	3290	1/1	0.95	0.38	-	47,47,47,47	0
54	MG	AA	1614	1/1	0.98	0.23	-	62,62,62,62	0
54	MG	DA	3380	1/1	0.78	0.10	-	91,91,91,91	0
54	MG	BB	216	1/1	0.98	0.33	-	46,46,46,46	0
54	MG	BA	3223	1/1	0.95	0.18	-	57,57,57,57	0
54	MG	DA	3231	1/1	0.91	0.48	-	54,54,54,54	0
54	MG	BA	3337	1/1	0.89	0.24	-	33,33,33,33	0
54	MG	DA	3413	1/1	0.95	0.17	-	37,37,37,37	0
54	MG	DA	3090	1/1	0.94	0.25	-	53,53,53,53	0
54	MG	DA	3326	1/1	0.83	0.10	-	95,95,95,95	0
54	MG	DA	3314	1/1	0.91	0.23	-	54,54,54,54	0
54	MG	AA	1616	1/1	0.72	0.45	-	79,79,79,79	0
54	MG	D8	101	1/1	0.89	0.61	-	49,49,49,49	0
54	MG	BA	3141	1/1	0.90	0.27	-	65,65,65,65	0
54	MG	CA	1650	1/1	0.92	0.20	-	100,100,100,100	0
54	MG	BA	3510	1/1	0.94	0.17	-	33,33,33,33	0
54	MG	BA	3246	1/1	0.98	0.21	-	49,49,49,49	0
54	MG	AA	1651	1/1	0.89	0.86	-	69,69,69,69	0
54	MG	BA	3606	1/1	0.95	0.11	-	29,29,29,29	0
54	MG	BA	3183	1/1	0.46	0.28	-	76,76,76,76	0
54	MG	BA	3458	1/1	0.72	0.19	-	45,45,45,45	0
54	MG	BA	3328	1/1	0.95	0.20	-	27,27,27,27	0
54	MG	BQ	203	1/1	0.96	0.23	-	44,44,44,44	0
54	MG	DA	3038	1/1	0.95	0.33	-	39,39,39,39	0
54	MG	BA	3572	1/1	0.70	0.13	-	49,49,49,49	0
54	MG	DB	202	1/1	0.74	1.21	-	86,86,86,86	0
54	MG	AA	1630	1/1	0.64	0.51	-	76,76,76,76	0
54	MG	BB	209	1/1	0.84	0.17	-	79,79,79,79	0
54	MG	BA	3277	1/1	0.87	0.21	-	66,66,66,66	0
54	MG	BA	3360	1/1	0.86	0.17	-	53,53,53,53	0
54	MG	BA	3543	1/1	0.94	0.19	-	59,59,59,59	0
54	MG	BA	3069	1/1	0.92	0.52	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3015	1/1	0.82	0.39	-	71,71,71,71	0
54	MG	DA	3083	1/1	0.89	0.34	-	55,55,55,55	0
54	MG	DA	3262	1/1	0.91	0.16	-	46,46,46,46	0
54	MG	BA	3051	1/1	0.91	0.15	-	52,52,52,52	0
54	MG	DA	3117	1/1	0.96	0.35	-	34,34,34,34	0
54	MG	AA	1696	1/1	0.81	0.18	-	74,74,74,74	0
54	MG	DA	3071	1/1	0.84	0.34	-	60,60,60,60	0
54	MG	DA	3101	1/1	0.93	0.20	-	62,62,62,62	0
54	MG	BA	3009	1/1	0.83	0.23	-	59,59,59,59	0
54	MG	DA	3317	1/1	0.78	0.18	-	94,94,94,94	0
54	MG	BA	3202	1/1	0.98	0.53	-	65,65,65,65	0
54	MG	DA	3369	1/1	0.92	0.18	-	57,57,57,57	0
54	MG	BA	3344	1/1	0.82	0.10	-	52,52,52,52	0
54	MG	BA	3590	1/1	0.86	0.16	-	82,82,82,82	0
54	MG	BA	3205	1/1	0.65	0.41	-	61,61,61,61	0
54	MG	DA	3252	1/1	0.81	0.36	-	41,41,41,41	0
54	MG	BA	3191	1/1	0.88	0.14	-	45,45,45,45	0
54	MG	B8	103	1/1	0.98	0.14	-	51,51,51,51	0
54	MG	DA	3214	1/1	0.86	0.76	-	74,74,74,74	0
54	MG	DA	3238	1/1	0.95	0.61	-	52,52,52,52	0
54	MG	DA	3313	1/1	0.60	0.19	-	64,64,64,64	0
54	MG	BA	3305	1/1	0.97	0.10	-	37,37,37,37	0
54	MG	DA	3388	1/1	0.71	0.12	-	72,72,72,72	0
54	MG	BA	3611	1/1	0.93	0.07	-	70,70,70,70	0
54	MG	DA	3160	1/1	0.96	0.50	-	48,48,48,48	0
54	MG	BA	3334	1/1	0.86	0.16	-	43,43,43,43	0
54	MG	BA	3289	1/1	0.91	0.67	-	50,50,50,50	0
54	MG	BA	3259	1/1	0.89	0.31	-	51,51,51,51	0
54	MG	BA	3499	1/1	0.65	0.23	-	107,107,107,107	0
54	MG	BA	3227	1/1	0.93	0.20	-	42,42,42,42	0
54	MG	DA	3046	1/1	0.92	0.71	-	43,43,43,43	0
54	MG	B8	101	1/1	0.92	0.40	-	64,64,64,64	0
54	MG	BA	3040	1/1	0.90	0.23	-	33,33,33,33	0
54	MG	BA	3370	1/1	0.98	0.10	-	66,66,66,66	0
54	MG	BA	3208	1/1	0.93	0.29	-	54,54,54,54	0
54	MG	CA	1614	1/1	0.96	0.26	-	69,69,69,69	0
54	MG	DA	3061	1/1	0.93	0.38	-	52,52,52,52	0
54	MG	BA	3420	1/1	0.88	0.28	-	41,41,41,41	0
54	MG	DA	3283	1/1	0.97	0.14	-	48,48,48,48	0
54	MG	DA	3393	1/1	0.73	0.11	-	81,81,81,81	0
54	MG	BA	3067	1/1	0.89	0.36	-	35,35,35,35	0
54	MG	B3	102	1/1	0.94	0.28	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3087	1/1	0.94	0.31	-	58,58,58,58	0
54	MG	DA	3350	1/1	0.95	0.14	-	50,50,50,50	0
54	MG	DA	3186	1/1	0.90	0.24	-	42,42,42,42	0
54	MG	BA	3480	1/1	0.91	0.13	-	70,70,70,70	0
54	MG	AA	1647	1/1	0.96	0.34	-	61,61,61,61	0
54	MG	DA	3122	1/1	0.95	0.52	-	47,47,47,47	0
54	MG	DA	3154	1/1	0.97	0.83	-	62,62,62,62	0
54	MG	BA	3060	1/1	0.98	0.30	-	45,45,45,45	0
54	MG	DA	3373	1/1	0.99	0.27	-	38,38,38,38	0
54	MG	DA	3055	1/1	0.95	0.45	-	43,43,43,43	0
54	MG	CA	1615	1/1	0.83	0.62	-	76,76,76,76	0
54	MG	BA	3579	1/1	0.98	0.12	-	53,53,53,53	0
54	MG	DA	3174	1/1	0.91	0.46	-	60,60,60,60	0
54	MG	BA	3121	1/1	0.89	0.15	-	38,38,38,38	0
54	MG	BA	3371	1/1	0.88	0.10	-	67,67,67,67	0
54	MG	AA	1654	1/1	0.91	0.06	-	87,87,87,87	0
54	MG	BA	3472	1/1	0.95	0.21	-	29,29,29,29	0
54	MG	AA	1623	1/1	0.87	0.47	-	74,74,74,74	0
54	MG	DA	3383	1/1	0.87	0.25	-	63,63,63,63	0
54	MG	DA	3114	1/1	0.84	0.15	-	51,51,51,51	0
54	MG	CA	1664	1/1	0.91	0.16	-	94,94,94,94	0
54	MG	BA	3594	1/1	0.78	0.15	-	70,70,70,70	0
54	MG	CA	1609	1/1	0.71	0.88	-	70,70,70,70	0
54	MG	BA	3123	1/1	0.95	0.20	-	43,43,43,43	0
54	MG	DA	3237	1/1	0.94	0.51	-	39,39,39,39	0
54	MG	BA	3151	1/1	0.92	0.21	-	62,62,62,62	0
54	MG	BA	3112	1/1	0.95	0.40	-	47,47,47,47	0
54	MG	B0	102	1/1	0.89	0.17	-	56,56,56,56	0
54	MG	AA	1625	1/1	0.82	0.25	-	102,102,102,102	0
54	MG	BA	3326	1/1	0.96	0.14	-	30,30,30,30	0
54	MG	DA	3246	1/1	0.87	0.46	-	41,41,41,41	0
54	MG	CA	1658	1/1	0.89	0.17	-	83,83,83,83	0
54	MG	DA	3196	1/1	0.96	0.48	-	63,63,63,63	0
54	MG	AA	1669	1/1	0.90	0.37	-	96,96,96,96	0
54	MG	AA	1695	1/1	0.91	0.12	-	93,93,93,93	0
54	MG	BA	3268	1/1	0.97	0.29	-	44,44,44,44	0
54	MG	DA	3245	1/1	0.83	0.34	-	47,47,47,47	0
54	MG	DA	3409	1/1	0.91	0.06	-	79,79,79,79	0
54	MG	BA	3300	1/1	0.93	0.15	-	37,37,37,37	0
54	MG	BA	3501	1/1	0.91	0.11	-	61,61,61,61	0
54	MG	BA	3200	1/1	0.83	0.23	-	51,51,51,51	0
54	MG	AA	1624	1/1	0.91	0.88	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3033	1/1	0.78	0.30	-	68,68,68,68	0
54	MG	DA	3203	1/1	0.91	0.75	-	48,48,48,48	0
54	MG	AA	1653	1/1	0.82	0.61	-	80,80,80,80	0
54	MG	CA	1635	1/1	0.81	0.18	-	68,68,68,68	0
54	MG	BA	3483	1/1	0.97	0.16	-	57,57,57,57	0
54	MG	DA	3327	1/1	0.77	0.45	-	94,94,94,94	0
54	MG	BA	3525	1/1	0.92	0.07	-	112,112,112,112	0
54	MG	BA	3028	1/1	0.93	0.23	-	46,46,46,46	0
54	MG	AA	1670	1/1	0.89	0.16	-	115,115,115,115	0
54	MG	BA	3139	1/1	0.79	0.28	-	53,53,53,53	0
54	MG	BA	3394	1/1	0.94	0.10	-	29,29,29,29	0
54	MG	CA	1637	1/1	0.90	0.65	-	67,67,67,67	0
54	MG	BA	3548	1/1	0.96	0.20	-	41,41,41,41	0
54	MG	DA	3001	1/1	0.69	0.21	-	62,62,62,62	0
54	MG	DA	3264	1/1	0.98	0.21	-	46,46,46,46	0
54	MG	BB	208	1/1	0.86	0.32	-	70,70,70,70	0
54	MG	BA	3081	1/1	0.90	0.19	-	66,66,66,66	0
54	MG	DF	302	1/1	0.87	0.24	-	64,64,64,64	0
54	MG	BA	3587	1/1	0.78	0.08	-	66,66,66,66	0
54	MG	CA	1639	1/1	0.94	0.65	-	61,61,61,61	0
54	MG	CA	1647	1/1	0.98	0.14	-	78,78,78,78	0
54	MG	DA	3134	1/1	0.90	0.22	-	64,64,64,64	0
54	MG	BA	3274	1/1	0.79	0.14	-	81,81,81,81	0
54	MG	BA	3095	1/1	0.92	0.38	-	45,45,45,45	0
54	MG	AA	1705	1/1	0.96	0.14	-	68,68,68,68	0
54	MG	DA	3334	1/1	0.93	0.16	-	56,56,56,56	0
54	MG	BA	3267	1/1	0.79	0.55	-	53,53,53,53	0
54	MG	DA	3067	1/1	0.95	0.33	-	32,32,32,32	0
54	MG	BA	3447	1/1	0.94	0.28	-	37,37,37,37	0
54	MG	BA	3241	1/1	0.81	0.74	-	62,62,62,62	0
54	MG	DA	3277	1/1	0.96	0.12	-	42,42,42,42	0
54	MG	CA	1640	1/1	0.89	0.28	-	62,62,62,62	0
54	MG	DA	3420	1/1	0.87	0.09	-	97,97,97,97	0
54	MG	DA	3344	1/1	0.98	0.09	-	51,51,51,51	0
54	MG	BA	3468	1/1	0.94	0.15	-	38,38,38,38	0
54	MG	AA	1655	1/1	0.79	0.19	-	90,90,90,90	0
54	MG	BA	3303	1/1	0.98	0.20	-	36,36,36,36	0
54	MG	BA	3554	1/1	0.86	0.21	-	58,58,58,58	0
54	MG	BA	3152	1/1	0.69	0.24	-	73,73,73,73	0
54	MG	AA	1619	1/1	0.92	0.34	-	68,68,68,68	0
54	MG	BA	3097	1/1	0.86	0.38	-	58,58,58,58	0
54	MG	BA	3544	1/1	0.96	0.19	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3301	1/1	0.92	0.17	-	55,55,55,55	0
54	MG	DA	3078	1/1	0.93	0.44	-	53,53,53,53	0
54	MG	BA	3210	1/1	0.93	0.24	-	57,57,57,57	0
54	MG	AA	1702	1/1	0.66	0.21	-	97,97,97,97	0
54	MG	BA	3090	1/1	0.93	0.15	-	45,45,45,45	0
54	MG	DA	3132	1/1	0.97	0.41	-	49,49,49,49	0
54	MG	BA	3170	1/1	0.82	0.57	-	52,52,52,52	0
54	MG	DA	3284	1/1	0.95	0.16	-	61,61,61,61	0
54	MG	BA	3045	1/1	0.93	0.21	-	62,62,62,62	0
54	MG	DA	3416	1/1	0.95	0.13	-	32,32,32,32	0
54	MG	BA	3237	1/1	0.82	0.40	-	56,56,56,56	0
54	MG	AA	1682	1/1	0.73	0.18	-	111,111,111,111	0
54	MG	BA	3014	1/1	0.89	0.19	-	57,57,57,57	0
54	MG	BA	3486	1/1	0.88	0.10	-	48,48,48,48	0
54	MG	CA	1648	1/1	0.79	0.13	-	100,100,100,100	0
54	MG	BA	3575	1/1	0.98	0.07	-	54,54,54,54	0
54	MG	DA	3053	1/1	0.89	0.36	-	54,54,54,54	0
54	MG	BQ	201	1/1	0.93	0.20	-	49,49,49,49	0
54	MG	AA	1699	1/1	0.76	0.16	-	69,69,69,69	0
54	MG	AA	1609	1/1	0.59	0.32	-	91,91,91,91	0
54	MG	BA	3509	1/1	0.78	0.23	-	85,85,85,85	0
54	MG	B1	101	1/1	0.84	0.28	-	50,50,50,50	0
54	MG	BA	3137	1/1	0.91	0.17	-	38,38,38,38	0
54	MG	BA	3372	1/1	0.98	0.13	-	50,50,50,50	0
54	MG	DA	3123	1/1	0.83	0.20	-	56,56,56,56	0
54	MG	DA	3052	1/1	0.94	0.30	-	71,71,71,71	0
54	MG	DA	3112	1/1	0.78	0.34	-	60,60,60,60	0
54	MG	BA	3148	1/1	0.91	0.28	-	54,54,54,54	0
54	MG	DA	3125	1/1	0.89	0.43	-	66,66,66,66	0
54	MG	BA	3159	1/1	0.57	0.22	-	66,66,66,66	0
54	MG	DA	3425	1/1	0.94	0.07	-	60,60,60,60	0
54	MG	BA	3437	1/1	0.95	0.20	-	28,28,28,28	0
54	MG	BA	3522	1/1	0.89	0.56	-	68,68,68,68	0
54	MG	BA	3471	1/1	0.99	0.21	-	38,38,38,38	0
54	MG	BA	3520	1/1	0.93	0.23	-	67,67,67,67	0
54	MG	BA	3460	1/1	0.94	0.09	-	58,58,58,58	0
54	MG	DA	3259	1/1	0.91	0.59	-	64,64,64,64	0
54	MG	BA	3070	1/1	0.91	0.18	-	61,61,61,61	0
54	MG	BA	3474	1/1	0.87	0.20	-	66,66,66,66	0
54	MG	BA	3556	1/1	0.86	0.20	-	58,58,58,58	0
54	MG	CA	1616	1/1	0.92	0.42	-	72,72,72,72	0
54	MG	BA	3395	1/1	0.98	0.14	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3007	1/1	0.93	0.18	-	36,36,36,36	0
54	MG	BA	3301	1/1	0.94	0.05	-	62,62,62,62	0
54	MG	DA	3205	1/1	0.89	0.07	-	82,82,82,82	0
54	MG	BA	3262	1/1	0.97	0.38	-	32,32,32,32	0
54	MG	DA	3305	1/1	0.96	0.09	-	55,55,55,55	0
54	MG	BA	3052	1/1	0.92	0.26	-	61,61,61,61	0
54	MG	BA	3271	1/1	0.92	0.15	-	60,60,60,60	0
54	MG	BA	3493	1/1	0.95	0.19	-	52,52,52,52	0
54	MG	BA	3240	1/1	0.79	0.38	-	64,64,64,64	0
54	MG	BA	3323	1/1	0.99	0.09	-	40,40,40,40	0
54	MG	DA	3268	1/1	0.98	0.16	-	43,43,43,43	0
54	MG	BA	3249	1/1	0.89	0.30	-	70,70,70,70	0
54	MG	BA	3243	1/1	0.57	0.11	-	117,117,117,117	0
54	MG	DA	3113	1/1	0.93	0.37	-	42,42,42,42	0
54	MG	BA	3454	1/1	0.97	0.17	-	34,34,34,34	0
54	MG	DA	3163	1/1	0.95	0.38	-	56,56,56,56	0
54	MG	DA	3054	1/1	0.95	0.72	-	75,75,75,75	0
54	MG	BA	3292	1/1	0.97	0.20	-	44,44,44,44	0
54	MG	BA	3607	1/1	0.95	0.13	-	38,38,38,38	0
54	MG	AA	1622	1/1	0.77	0.72	-	67,67,67,67	0
54	MG	BA	3059	1/1	0.94	0.31	-	49,49,49,49	0
54	MG	DA	3002	1/1	0.92	0.70	-	67,67,67,67	0
54	MG	BA	3111	1/1	0.90	0.30	-	57,57,57,57	0
54	MG	DA	3397	1/1	0.92	0.05	-	65,65,65,65	0
54	MG	DA	3127	1/1	0.84	0.29	-	63,63,63,63	0
54	MG	BA	3010	1/1	0.95	0.20	-	48,48,48,48	0
54	MG	BA	3405	1/1	0.94	0.19	-	38,38,38,38	0
54	MG	DA	3366	1/1	0.97	0.14	-	35,35,35,35	0
54	MG	BA	3329	1/1	0.86	0.17	-	45,45,45,45	0
54	MG	BA	3392	1/1	0.84	0.11	-	55,55,55,55	0
54	MG	BA	3348	1/1	0.98	0.22	-	37,37,37,37	0
54	MG	AA	1673	1/1	0.80	0.30	-	67,67,67,67	0
54	MG	AA	1700	1/1	0.82	0.34	-	114,114,114,114	0
54	MG	BA	3104	1/1	0.98	0.21	-	48,48,48,48	0
54	MG	BA	3201	1/1	0.80	0.59	-	79,79,79,79	0
54	MG	BA	3332	1/1	0.88	0.28	-	60,60,60,60	0
54	MG	BA	3016	1/1	0.89	0.42	-	57,57,57,57	0
54	MG	BA	3173	1/1	0.89	0.29	-	65,65,65,65	0
54	MG	BA	3207	1/1	0.80	0.16	-	59,59,59,59	0
54	MG	DA	3181	1/1	0.86	0.67	-	51,51,51,51	0
54	MG	DA	3328	1/1	0.91	0.09	-	34,34,34,34	0
54	MG	BA	3283	1/1	0.86	0.55	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3030	1/1	0.85	0.17	-	52,52,52,52	0
54	MG	BA	3281	1/1	0.95	0.28	-	56,56,56,56	0
54	MG	BA	3132	1/1	0.93	0.31	-	31,31,31,31	0
54	MG	BA	3457	1/1	0.86	0.15	-	91,91,91,91	0
54	MG	CA	1624	1/1	0.75	0.42	-	82,82,82,82	0
54	MG	DA	3162	1/1	0.78	0.38	-	55,55,55,55	0
54	MG	DA	3319	1/1	0.97	0.10	-	59,59,59,59	0
54	MG	BA	3288	1/1	0.96	0.51	-	33,33,33,33	0
54	MG	BA	3555	1/1	0.91	0.31	-	49,49,49,49	0
54	MG	CA	1663	1/1	0.89	0.18	-	91,91,91,91	0
54	MG	BA	3122	1/1	0.83	0.33	-	56,56,56,56	0
54	MG	DA	3199	1/1	0.90	0.06	-	74,74,74,74	0
54	MG	BA	3350	1/1	0.93	0.18	-	60,60,60,60	0
54	MG	BA	3498	1/1	0.91	0.14	-	69,69,69,69	0
54	MG	BA	3580	1/1	0.94	0.08	-	61,61,61,61	0
54	MG	DA	3282	1/1	0.95	0.08	-	42,42,42,42	0
54	MG	BA	3130	1/1	0.89	0.38	-	32,32,32,32	0
54	MG	DA	3043	1/1	0.86	0.18	-	63,63,63,63	0
54	MG	AA	1618	1/1	0.91	0.13	-	69,69,69,69	0
54	MG	DB	204	1/1	0.98	0.14	-	74,74,74,74	0
54	MG	AA	1666	1/1	0.91	0.54	-	62,62,62,62	0
54	MG	B0	101	1/1	0.77	0.16	-	75,75,75,75	0
54	MG	BA	3017	1/1	0.93	0.14	-	47,47,47,47	0
54	MG	BA	3091	1/1	0.91	0.35	-	47,47,47,47	0
54	MG	DA	3398	1/1	0.98	0.12	-	52,52,52,52	0
54	MG	BA	3559	1/1	0.85	0.27	-	39,39,39,39	0
54	MG	BA	3106	1/1	0.87	0.41	-	48,48,48,48	0
54	MG	BB	211	1/1	0.96	0.09	-	51,51,51,51	0
54	MG	DA	3036	1/1	0.86	0.18	-	65,65,65,65	0
54	MG	BA	3169	1/1	0.73	0.48	-	60,60,60,60	0
54	MG	CA	1646	1/1	0.89	0.49	-	92,92,92,92	0
54	MG	DA	3365	1/1	0.95	0.08	-	50,50,50,50	0
54	MG	DA	3209	1/1	0.92	0.24	-	79,79,79,79	0
54	MG	BA	3153	1/1	0.89	0.32	-	53,53,53,53	0
54	MG	AA	1684	1/1	0.96	0.05	-	76,76,76,76	0
54	MG	AA	1602	1/1	0.86	0.28	-	111,111,111,111	0
54	MG	DA	3029	1/1	0.94	0.15	-	72,72,72,72	0
54	MG	BA	3565	1/1	0.75	0.28	-	90,90,90,90	0
54	MG	BA	3043	1/1	0.94	0.34	-	54,54,54,54	0
54	MG	BA	3258	1/1	0.95	0.44	-	56,56,56,56	0
54	MG	BA	3086	1/1	0.92	0.26	-	57,57,57,57	0
54	MG	BA	3083	1/1	0.95	0.47	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3497	1/1	0.94	0.17	-	55,55,55,55	0
54	MG	DA	3017	1/1	0.92	0.29	-	61,61,61,61	0
54	MG	DA	3243	1/1	0.96	0.36	-	53,53,53,53	0
54	MG	BA	3366	1/1	0.99	0.08	-	50,50,50,50	0
54	MG	DA	3178	1/1	0.96	0.47	-	58,58,58,58	0
54	MG	DA	3421	1/1	0.86	0.09	-	69,69,69,69	0
54	MG	BA	3175	1/1	0.90	0.35	-	70,70,70,70	0
54	MG	BA	3411	1/1	0.98	0.28	-	43,43,43,43	0
54	MG	AA	1686	1/1	0.91	0.19	-	115,115,115,115	0
54	MG	BA	3276	1/1	0.89	0.63	-	56,56,56,56	0
54	MG	BA	3226	1/1	0.88	0.31	-	62,62,62,62	0
54	MG	BA	3256	1/1	0.96	0.68	-	69,69,69,69	0
54	MG	CA	1633	1/1	0.96	0.25	-	71,71,71,71	0
54	MG	BA	3583	1/1	0.95	0.05	-	50,50,50,50	0
54	MG	BA	3546	1/1	0.90	0.09	-	57,57,57,57	0
54	MG	BA	3209	1/1	0.93	0.37	-	67,67,67,67	0
54	MG	DB	205	1/1	0.96	0.15	-	70,70,70,70	0

6.5 Other polymers

There are no such residues in this entry.