wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:02 PM GMT

PDB ID	:	4V5A
Title	:	Structure of the Ribosome Recycling Factor bound to the Thermus thermophilus 70S ribosome with mRNA, ASL-Phe and tRNA-fMet
Authors	:	Weixlbaumer, A.; Petry, S.; Dunham, C.M.; Selmer, M.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2007-06-28
Resolution	:	3.50 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:

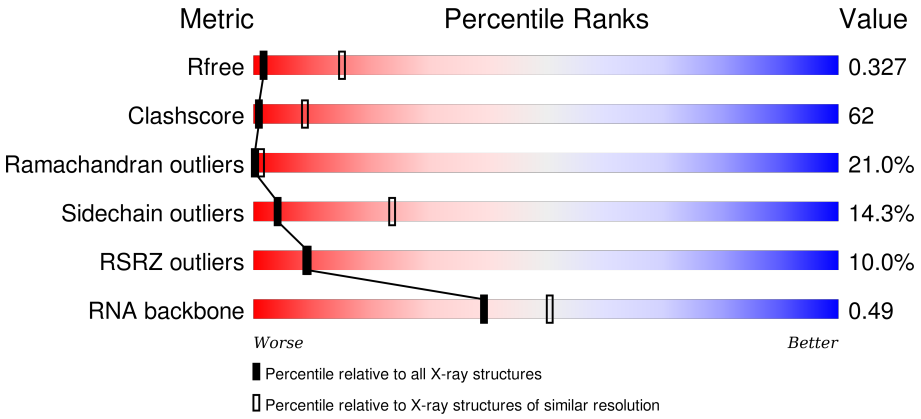
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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	11% 13% 73% 12% ••
1	CA	1522	13% 13% 73% 13% •
2	AB	256	9% 16% 50% 25% • 8%
2	CB	256	8% 16% 50% 25% • 8%

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Mol	Chain	Length	Quality of chain
3	AC	239	6% 17% 52% 15% 13%
3	CC	239	7% 18% 51% 15% 13%
4	AD	209	2% 12% 61% 24%
4	CD	209	% 12% 59% 25%
5	AE	162	2% 19% 56% 17% 7%
5	CE	162	4% 19% 56% 17% 7%
6	AF	101	2% 18% 65% 17%
6	CF	101	17% 65% 18%
7	AG	156	10% 17% 65% 16%
7	CG	156	12% 17% 65% 16%
8	AH	138	% 17% 64% 18%
8	CH	138	% 16% 64% 19%
9	AI	128	3% 13% 70% 15%
9	CI	128	22% 13% 70% 16%
10	AJ	105	4% 20% 60% 13% 6%
10	CJ	105	16% 19% 60% 14% 6%
11	AK	129	10% 16% 62% 12% 8%
11	CK	129	7% 19% 59% 12% 8%
12	AL	135	% 17% 57% 16% 7%
12	CL	135	% 19% 55% 17% 7%
13	AM	126	16% 19% 63% 17%
13	CM	126	10% 19% 64% 14%
14	AN	61	3% 18% 64% 15%
14	CN	61	2% 25% 57% 15%
15	AO	89	% 11% 73% 13%

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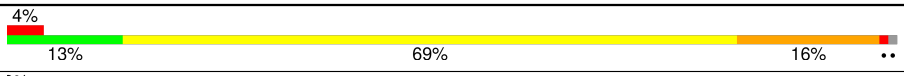
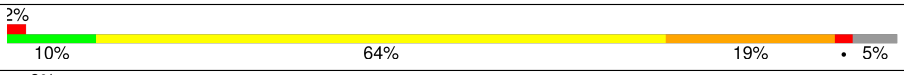
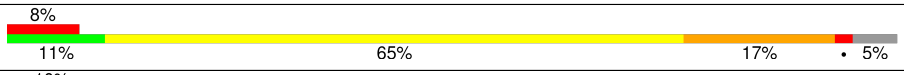
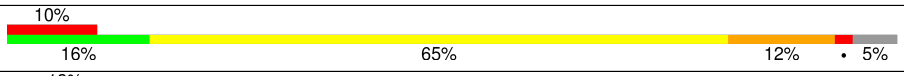
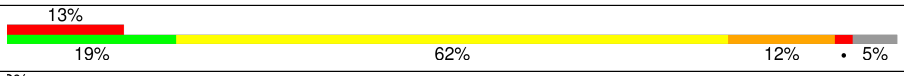
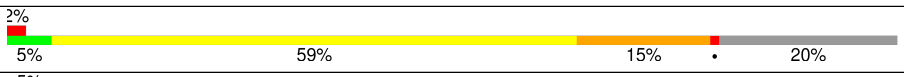
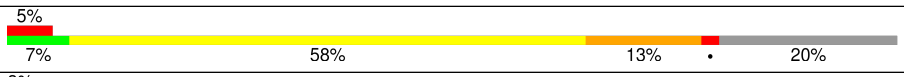
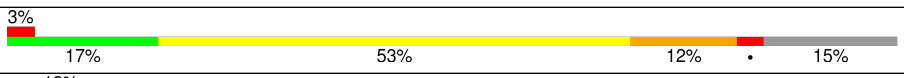
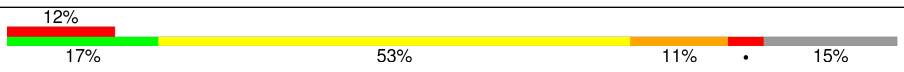
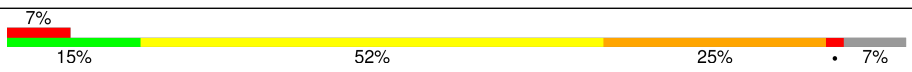
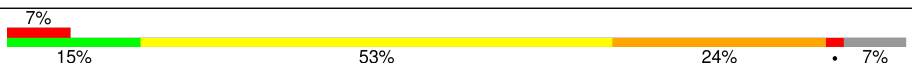
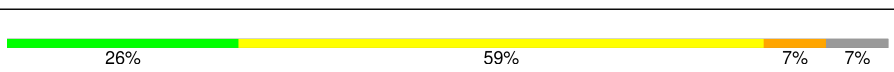
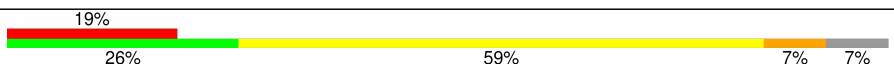
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
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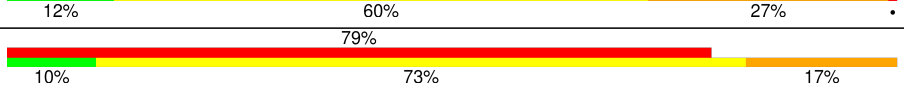
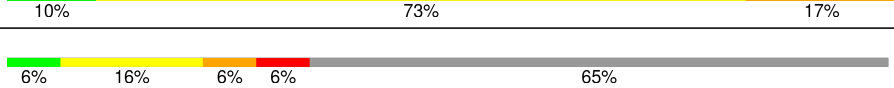
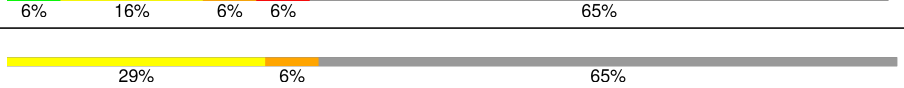
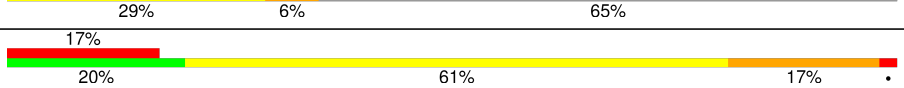
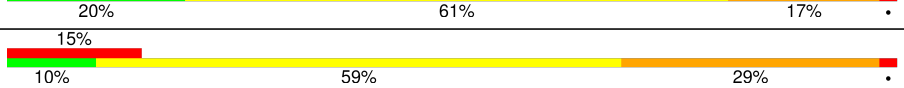
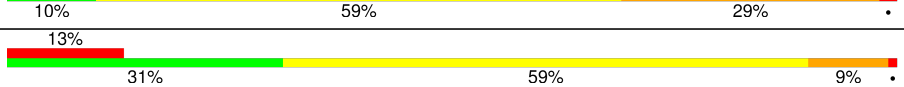
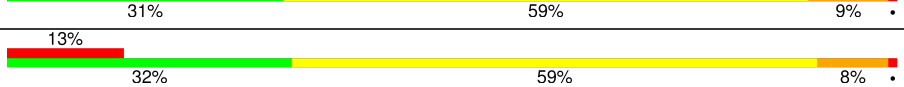
22	CV	76	
23	AW	77	
23	CW	77	
24	AX	31	
24	CX	31	
25	AY	185	
25	CY	185	
26	B0	85	
26	D0	85	
27	B1	98	
27	D1	98	

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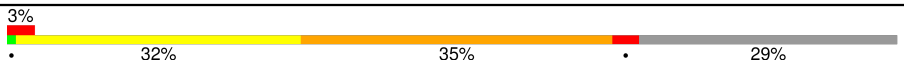
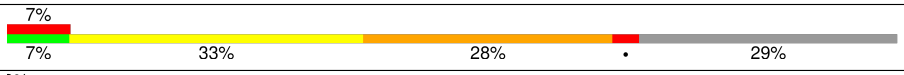
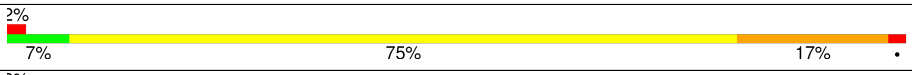
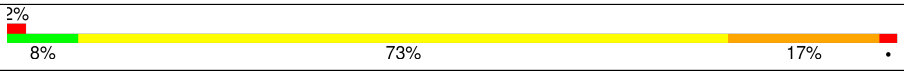
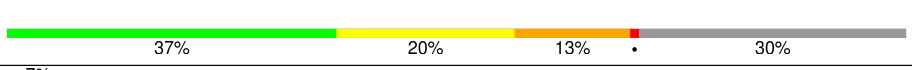
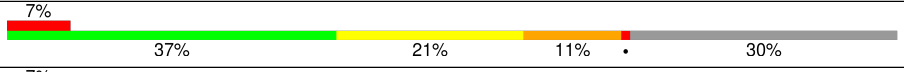
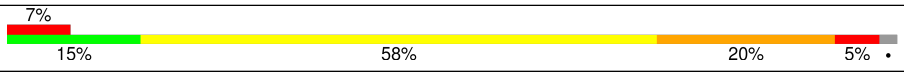
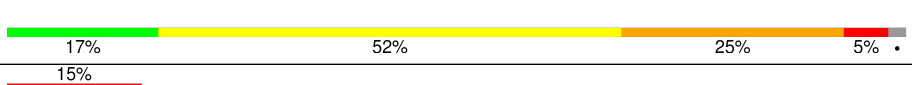
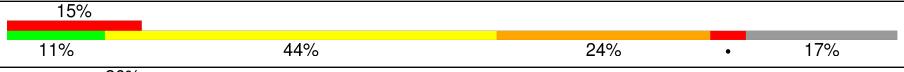
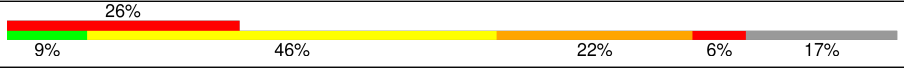
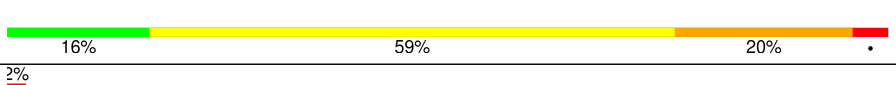
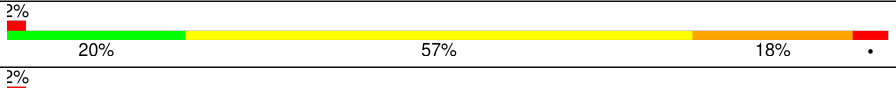
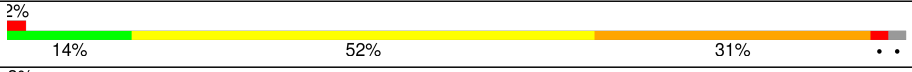
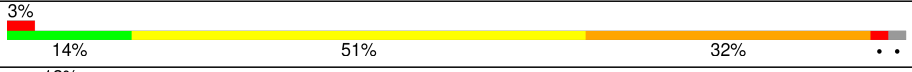
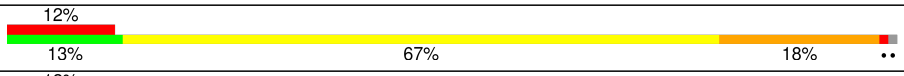
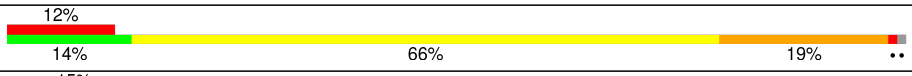
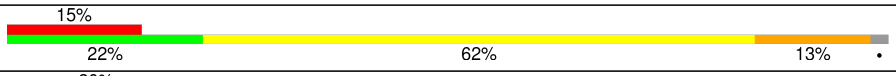
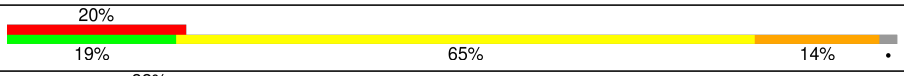
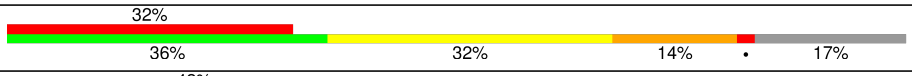
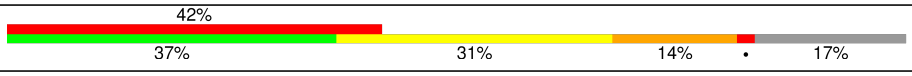
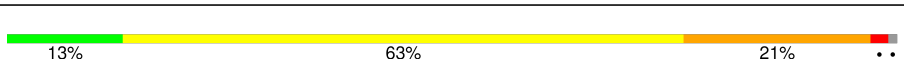
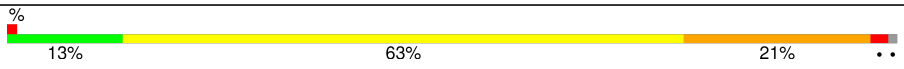
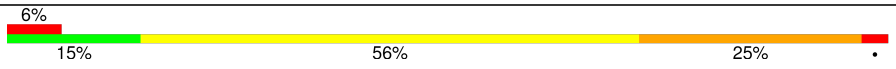
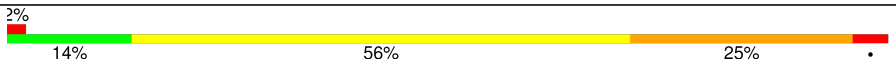
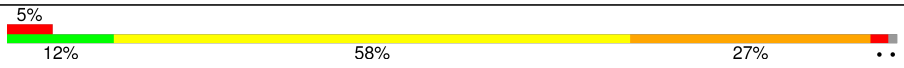
Mol	Chain	Length	Quality of chain
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	BA	2782	
35	DA	2782	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	
39	DE	206	
40	BF	210	

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Mol	Chain	Length	Quality of chain
40	DF	210	3% 11% 58% 28%
41	BG	182	12% 12% 61% 24%
41	DG	182	15% 7% 58% 31%
42	BH	180	13% 16% 47% 23% 11%
42	DH	180	4% 16% 49% 22% 11%
43	BI	148	10% 10% 59% 29%
43	DI	148	30% 11% 58% 29%
44	BN	140	5% 10% 58% 27%
44	DN	140	3% 9% 58% 28%
45	BO	122	2% 10% 61% 26%
45	DO	122	10% 62% 25%
46	BP	150	7% 11% 48% 31% 7%
46	DP	150	6% 11% 49% 31% 7%
47	BQ	141	5% 12% 52% 32%
47	DQ	141	2% 11% 55% 30%
48	BR	118	10% 48% 36% 5%
48	DR	118	8% 53% 33% 5%
49	BS	112	7% 9% 46% 29% 5% 12%
49	DS	112	19% 10% 43% 29% 6% 12%
50	BT	146	3% 13% 47% 30% 5% 5%
50	DT	146	5% 12% 48% 30% 5%
51	BU	118	3% 14% 59% 23%
51	DU	118	4% 9% 64% 23%
52	BV	101	16% 7% 53% 35% 5%
52	DV	101	9% 8% 50% 37% 5%

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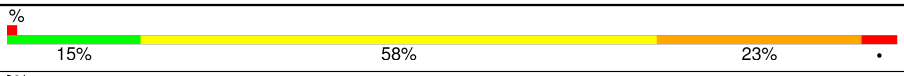
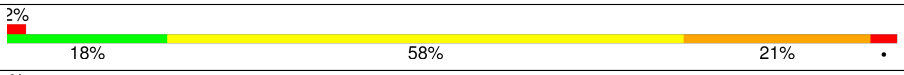
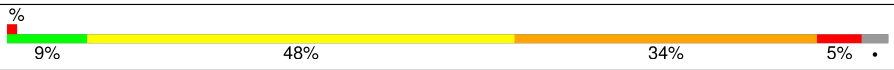
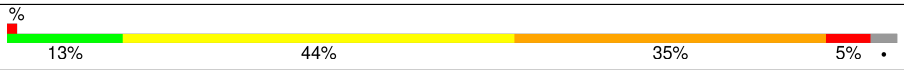
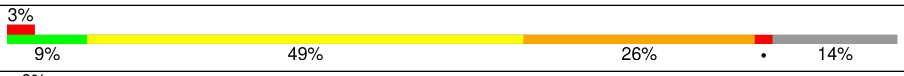
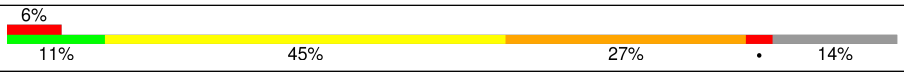
Mol	Chain	Length	Quality of chain
53	BW	113	
53	DW	113	
54	BX	96	
54	DX	96	
55	BY	110	
55	DY	110	
56	BZ	206	
56	DZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	1613	-	-	-	X
57	MG	AA	1695	-	-	-	X
57	MG	AA	1720	-	-	-	X
57	MG	AA	1734	-	-	-	X
57	MG	AA	1797	-	-	-	X
57	MG	AW	119	-	-	-	X
57	MG	BA	3025	-	-	-	X
57	MG	BA	3029	-	-	-	X
57	MG	BA	3048	-	-	-	X
57	MG	BA	3051	-	-	-	X
57	MG	BA	3101	-	-	-	X
57	MG	BA	3120	-	-	-	X
57	MG	BA	3125	-	-	-	X
57	MG	BA	3129	-	-	-	X
57	MG	BA	3143	-	-	-	X
57	MG	BA	3166	-	-	-	X
57	MG	BA	3167	-	-	-	X
57	MG	BA	3177	-	-	-	X
57	MG	BA	3189	-	-	-	X
57	MG	BA	3196	-	-	-	X
57	MG	BA	3210	-	-	-	X
57	MG	BA	3261	-	-	-	X
57	MG	BA	3268	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3274	-	-	-	X
57	MG	BA	3346	-	-	-	X
57	MG	BA	3352	-	-	-	X
57	MG	BA	3379	-	-	-	X
57	MG	BA	3389	-	-	-	X
57	MG	BA	3397	-	-	-	X
57	MG	BA	3409	-	-	-	X
57	MG	BA	3412	-	-	-	X
57	MG	BA	3432	-	-	-	X
57	MG	BD	301	-	-	-	X
57	MG	BO	201	-	-	-	X
57	MG	BP	202	-	-	-	X
57	MG	CA	1613	-	-	-	X
57	MG	CA	1624	-	-	-	X
57	MG	CA	1630	-	-	-	X
57	MG	CA	1634	-	-	-	X
57	MG	CA	1639	-	-	-	X
57	MG	CA	1686	-	-	-	X
57	MG	CA	1687	-	-	-	X
57	MG	CA	1690	-	-	-	X
57	MG	CA	1696	-	-	-	X
57	MG	CA	1699	-	-	-	X
57	MG	CA	1700	-	-	-	X
57	MG	CA	1707	-	-	-	X
57	MG	CA	1711	-	-	-	X
57	MG	CA	1712	-	-	-	X
57	MG	CA	1716	-	-	-	X
57	MG	CA	1736	-	-	-	X
57	MG	CA	1746	-	-	-	X
57	MG	CA	1763	-	-	-	X
57	MG	CA	1801	-	-	-	X
57	MG	CA	1805	-	-	-	X
57	MG	CN	101	-	-	-	X
57	MG	CW	119	-	-	-	X
57	MG	DA	3008	-	-	-	X
57	MG	DA	3012	-	-	-	X
57	MG	DA	3023	-	-	-	X
57	MG	DA	3027	-	-	-	X
57	MG	DA	3046	-	-	-	X
57	MG	DA	3048	-	-	-	X
57	MG	DA	3049	-	-	-	X
57	MG	DA	3063	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3066	-	-	-	X
57	MG	DA	3069	-	-	-	X
57	MG	DA	3071	-	-	-	X
57	MG	DA	3092	-	-	-	X
57	MG	DA	3094	-	-	-	X
57	MG	DA	3106	-	-	-	X
57	MG	DA	3118	-	-	-	X
57	MG	DA	3138	-	-	-	X
57	MG	DA	3141	-	-	-	X
57	MG	DA	3142	-	-	-	X
57	MG	DA	3149	-	-	-	X
57	MG	DA	3192	-	-	-	X
57	MG	DA	3232	-	-	-	X
57	MG	DA	3238	-	-	-	X
57	MG	DA	3256	-	-	-	X
57	MG	DA	3262	-	-	-	X
57	MG	DA	3282	-	-	-	X
57	MG	DA	3293	-	-	-	X
57	MG	DA	3308	-	-	-	X
57	MG	DA	3309	-	-	-	X
57	MG	DA	3313	-	-	-	X
57	MG	DA	3315	-	-	-	X
57	MG	DA	3318	-	-	-	X
57	MG	DA	3358	-	-	-	X
57	MG	DA	3375	-	-	-	X
57	MG	DA	3377	-	-	-	X
57	MG	DA	3387	-	-	-	X
57	MG	DA	3388	-	-	-	X
57	MG	DA	3396	-	-	-	X
57	MG	DA	3408	-	-	-	X
57	MG	DA	3419	-	-	-	X
57	MG	DA	3421	-	-	-	X
57	MG	DA	3429	-	-	-	X
57	MG	DB	214	-	-	-	X
57	MG	DP	201	-	-	-	X
57	MG	DU	202	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 290487 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

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

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

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

- Molecule 22 is a RNA chain called P-SITE RNA ASL-PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	17	Total	C	N	O	P	0	0	0
			362	163	68	115	16			
22	CV	17	Total	C	N	O	P	0	0	0
			362	163	68	115	16			

- Molecule 23 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			
23	CW	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0	0
			230	104	38	78	10			
24	CX	11	Total	C	N	O	P	0	0	0
			230	104	38	78	10			

- Molecule 25 is a protein called RIBOSOME RECYCLING FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
25	CY	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	85	Total	C	N	O	S	0	0	0
			652	403	137	111	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	D0	85	Total	C	N	O	S	0	0	0
			652	403	137	111	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	6	ALA	GLY	CONFLICT	UNP P60493
B0	8	ALA	GLY	CONFLICT	UNP P60493
D0	6	ALA	GLY	CONFLICT	UNP P60493
D0	8	ALA	GLY	CONFLICT	UNP P60493

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
30	B4	50	Total	C	N	O	0	0	1
			242	143	50	49			
30	D4	50	Total	C	N	O	0	0	1
			242	143	50	49			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2767	Total	C	N	O	P	0	0	0
			59601	26526	11153	19156	2766			
35	DA	2767	Total	C	N	O	P	0	0	0
			59601	26526	11153	19156	2766			

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

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
37	DC	191	Total	C	N	O	0	0	1
			1143	692	221	230			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	106	ALA	GLY	CONFLICT	UNP Q5SLP7
DC	132	ALA	GLY	CONFLICT	UNP Q5SLP7

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

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

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

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

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

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

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

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

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

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BA	445	Total Mg 445 445	0	0
57	AK	1	Total Mg 1 1	0	0
57	DF	5	Total Mg 5 5	0	0
57	CV	4	Total Mg 4 4	0	0
57	D2	2	Total Mg 2 2	0	0
57	BE	1	Total Mg 1 1	0	0
57	AW	23	Total Mg 23 23	0	0
57	DU	3	Total Mg 3 3	0	0
57	B1	4	Total Mg 4 4	0	0
57	BP	3	Total Mg 3 3	0	0
57	AX	5	Total Mg 5 5	0	0
57	CN	1	Total Mg 1 1	0	0
57	DN	2	Total Mg 2 2	0	0
57	CA	208	Total Mg 208 208	0	0
57	B5	2	Total Mg 2 2	0	0
57	BB	20	Total Mg 20 20	0	0
57	AE	2	Total Mg 2 2	0	0
57	DG	1	Total Mg 1 1	0	0
57	D3	1	Total Mg 1 1	0	0
57	BF	4	Total Mg 4 4	0	0
57	AV	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BX	2	Total Mg 2 2	0	0
57	B2	2	Total Mg 2 2	0	0
57	AA	204	Total Mg 204 204	0	0
57	D7	1	Total Mg 1 1	0	0
57	CX	4	Total Mg 4 4	0	0
57	DV	1	Total Mg 1 1	0	0
57	AM	1	Total Mg 1 1	0	0
57	BU	2	Total Mg 2 2	0	0
57	AD	2	Total Mg 2 2	0	0
57	BN	4	Total Mg 4 4	0	0
57	DH	1	Total Mg 1 1	0	0
57	BG	1	Total Mg 1 1	0	0
57	DS	1	Total Mg 1 1	0	0
57	DE	2	Total Mg 2 2	0	0
57	B3	1	Total Mg 1 1	0	0
57	DX	3	Total Mg 3 3	0	0
57	DA	441	Total Mg 441 441	0	0
57	B7	1	Total Mg 1 1	0	0
57	AL	2	Total Mg 2 2	0	0
57	AG	1	Total Mg 1 1	0	0
57	BO	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	D1	4	Total Mg 4 4	0	0
57	DP	4	Total Mg 4 4	0	0
57	CW	23	Total Mg 23 23	0	0
57	D5	1	Total Mg 1 1	0	0
57	BD	3	Total Mg 3 3	0	0
57	CE	3	Total Mg 3 3	0	0
57	CG	1	Total Mg 1 1	0	0
57	DD	3	Total Mg 3 3	0	0
57	CL	2	Total Mg 2 2	0	0
57	DB	19	Total Mg 19 19	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

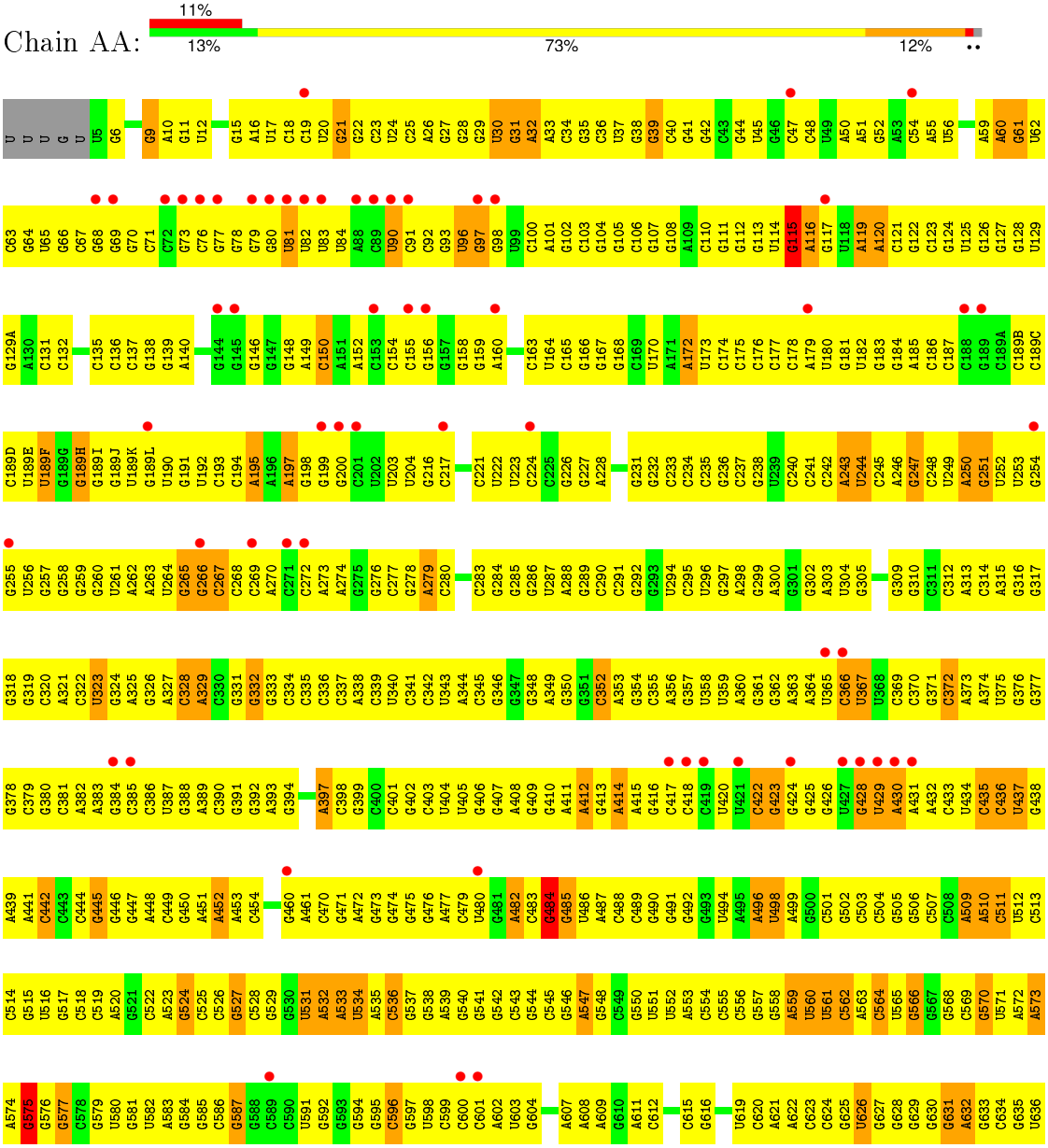
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	CN	1	Total Zn 1 1	0	0
58	AD	1	Total Zn 1 1	0	0
58	CD	1	Total Zn 1 1	0	0
58	AN	1	Total Zn 1 1	0	0

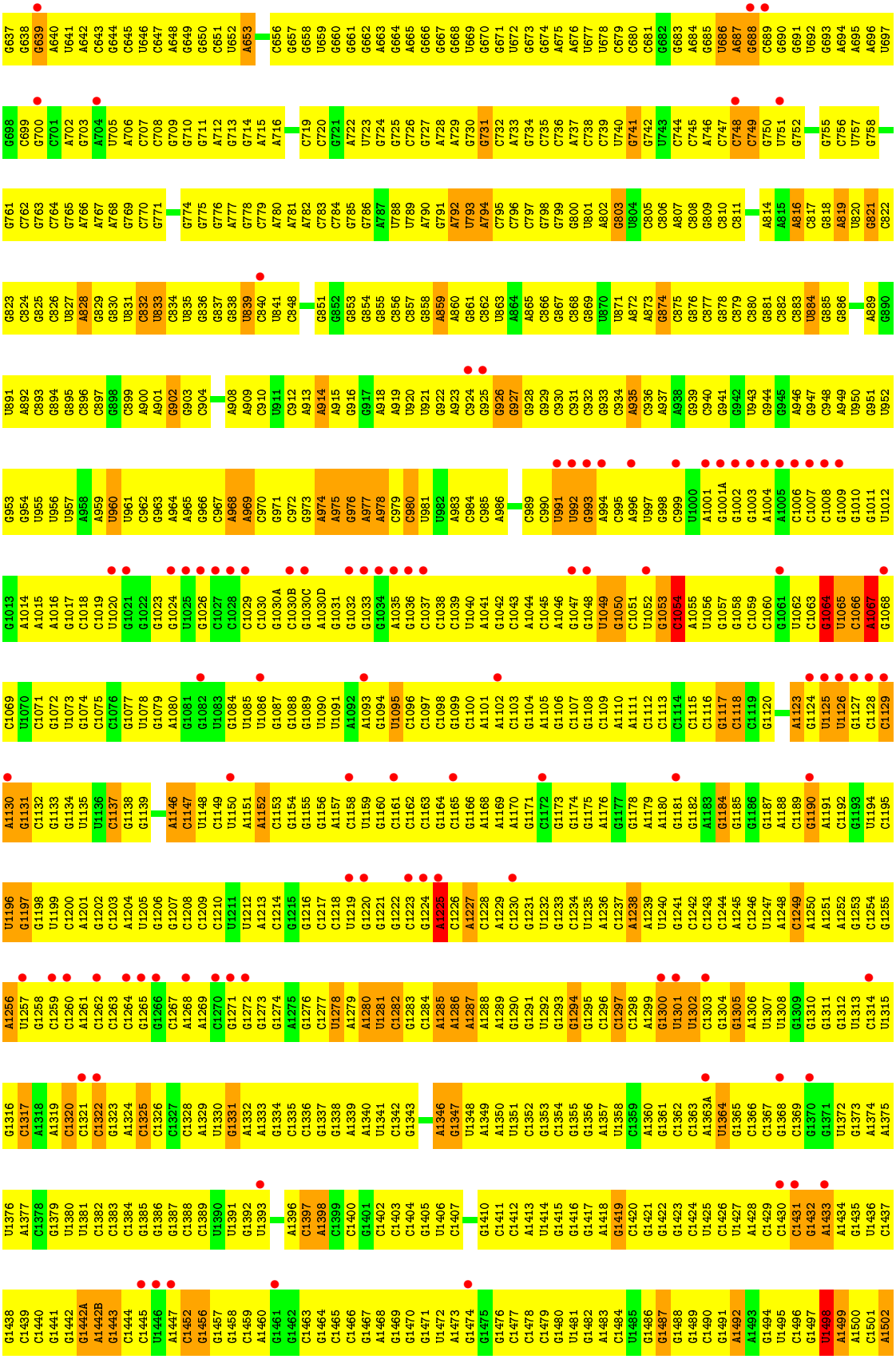
3 Residue-property plots (i)

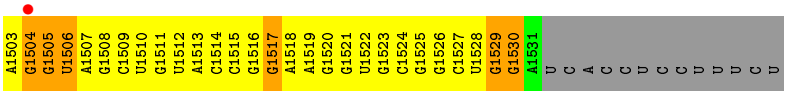
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 RRNA

Chain AA:

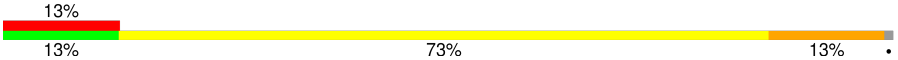


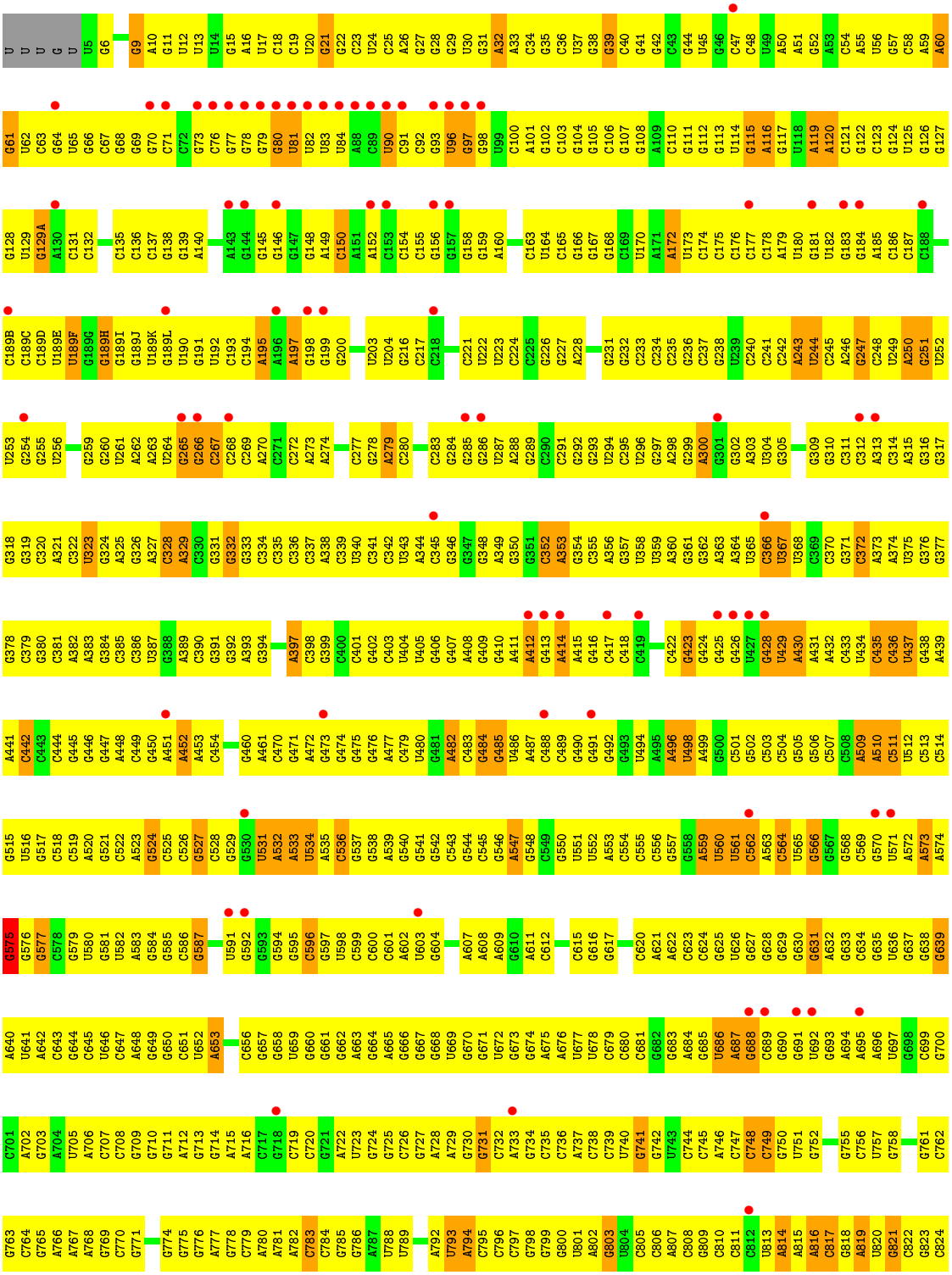

G637 G638 G639 A640 U641 A642 C643 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 C656 G657 G658 U659 G660 G661 G662 A663 G664 A665 G666 G667 G668 U669 G670 G671 U672 G673 G674 A675 A676 U677 U678 C679 C680 C681 G682 G683 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697
G698 C699 G700 C701 A702 G703 A704 U705 A706 C707 C708 G709 G710 G711 A712 G713 G714 A715 A716 C719 C720 G721 A722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 A733 G734 C735 C736 A737 C738 C739 U740 G741 U742 U743 C744 C745 A746 C747 C748 C749 G750 U751 G752 G755 C756 U757 G758
G761 C762 G763 C764 G765 A766 A767 A768 G769 C770 G771 G774 G775 G776 A777 G778 C779 A780 A781 A782 C783 C784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 C795 C796 C797 G798 G799 G800 U801 A802 G803 U804 C805 C806 A807 C808 G809 C810 C811 A814 A815 A816 C817 G818 A819 U820 G821 C822
G823 C824 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U839 C840 U841 C848 G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 G878 G879 C880 G881 G882 C883 U884 G885 G886 A889 G890
U891 A892 C893 G894 G895 C896 C897 G898 C899 A900 A901 G902 G903 C904 A908 A909 C910 U911 C912 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 G941 G942 U943 G944 G945 A946 G947 C948 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 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012
G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B C1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 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 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1115 C1116 G1117 C1118 C1119 G1120 A1123 G1124 U1125 U1126 G1127 C1128 C1129
A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 C1163 C1164 C1165 G1166 A1168 A1169 A1170 G1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1185 G1186 G1187 A1188 C1189 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 U1235 A1236 C1237 A1238 A1239 U1240 G1241 C1242 C1243 C1244 A1245 C1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 C1254 G1255
A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1263 C1264 G1265 G1266 C1267 A1268 A1269 C1270 G1271 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 C1290 G1291 U1292 G1293 G1294 G1295 C1296 C1297 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 G1311 G1312 U1313 C1314 U1315
G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327 C1328 A1329 U1330 G1331 A1332 A1333 G1334 C1335 C1336 G1337 G1338 A1339 A1340 U1341 C1342 G1343 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 C1354 G1355 G1356 A1357 U1358 C1359 A1360 G1361 C1362 C1363 A1363A U1364 G1365 C1366 C1367 G1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375
U1376 A1377 C1378 G1379 U1380 U1381 C1382 C1383 C1384 G1385 G1386 G1387 C1388 C1389 U1390 U1391 G1392 U1393 A1396 G1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1407 G1410 C1411 C1412 A1413 U1414 G1415 G1416 G1417 A1418 G1419 G1420 G1421 G1422 G1423 C1424 U1425 U1426 U1427 A1428 C1429 C1430 C1431 G1432 A1433 A1434 G1435 U1436 C1437
G1438 C1439 C1440 G1441 G1442 G1442A A1442B G1443 C1444 C1445 U1446 A1447 C1452 G1456 G1457 G1458 C1459 A1460 G1461 G1462 C1463 G1464 C1465 C1466 G1467 A1468 G1469 G1470 G1471 U1472 G1473 G1474 G1475 G1476 C1477 C1478 C1479 G1480 U1481 G1482 A1483 C1484 U1485 G1486 G1487 G1488 G1489 C1490 G1491 A1492 A1493 G1494 U1495 C1496 G1497 U1498 A1499 A1500 C1501 A1502

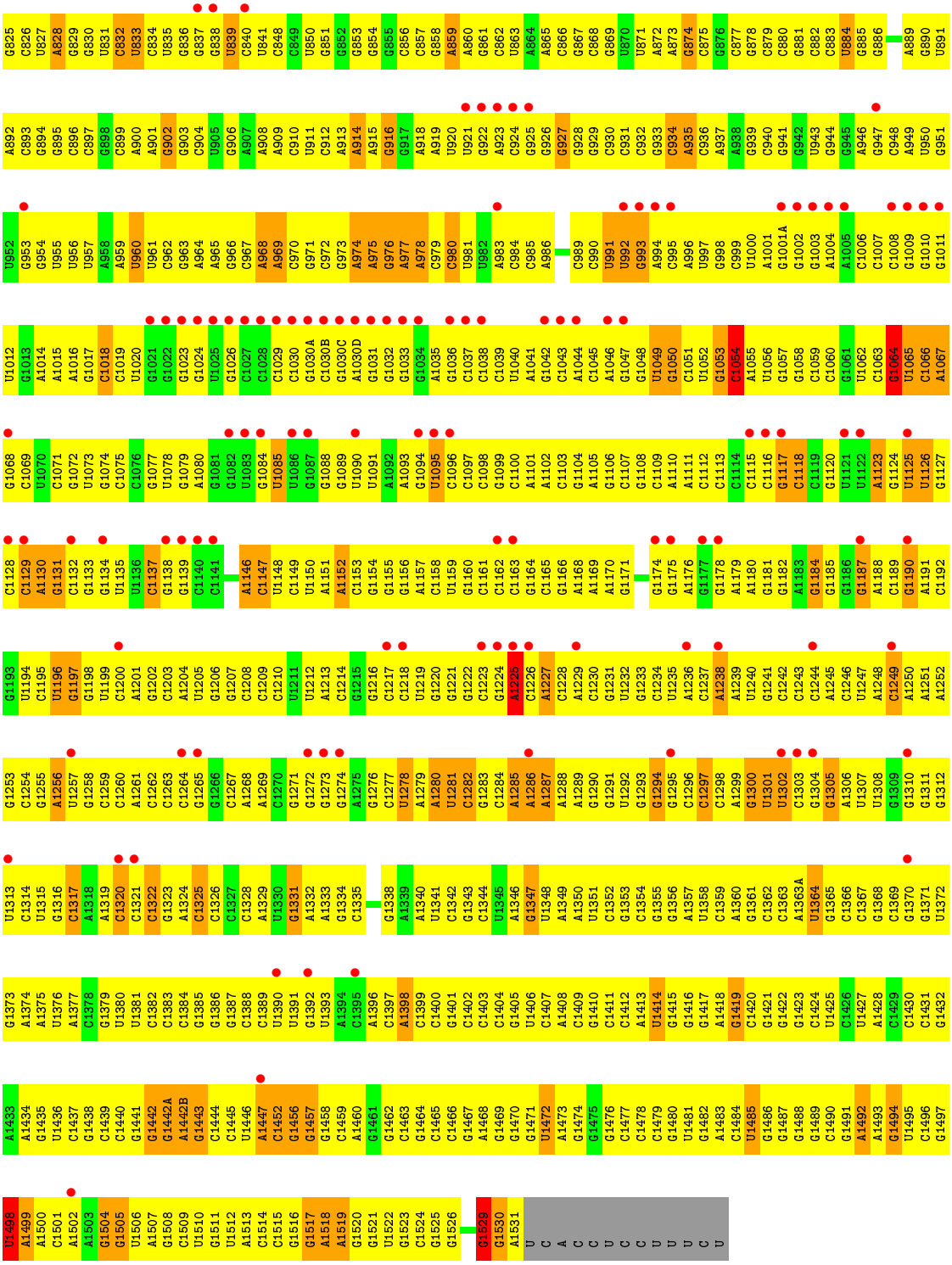


- Molecule 1: 16S RRNA

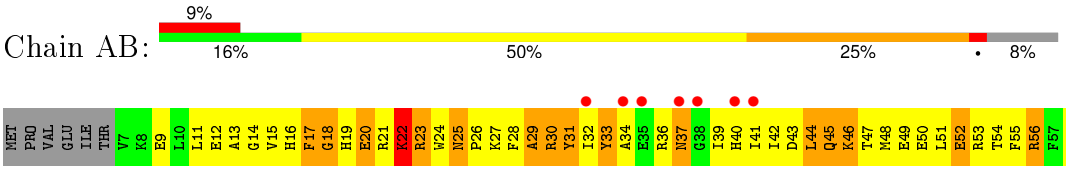
Chain CA:

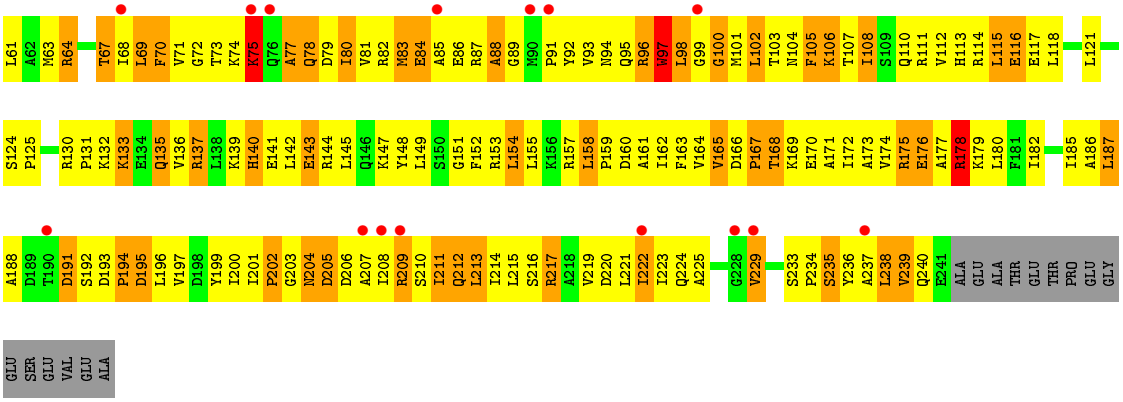






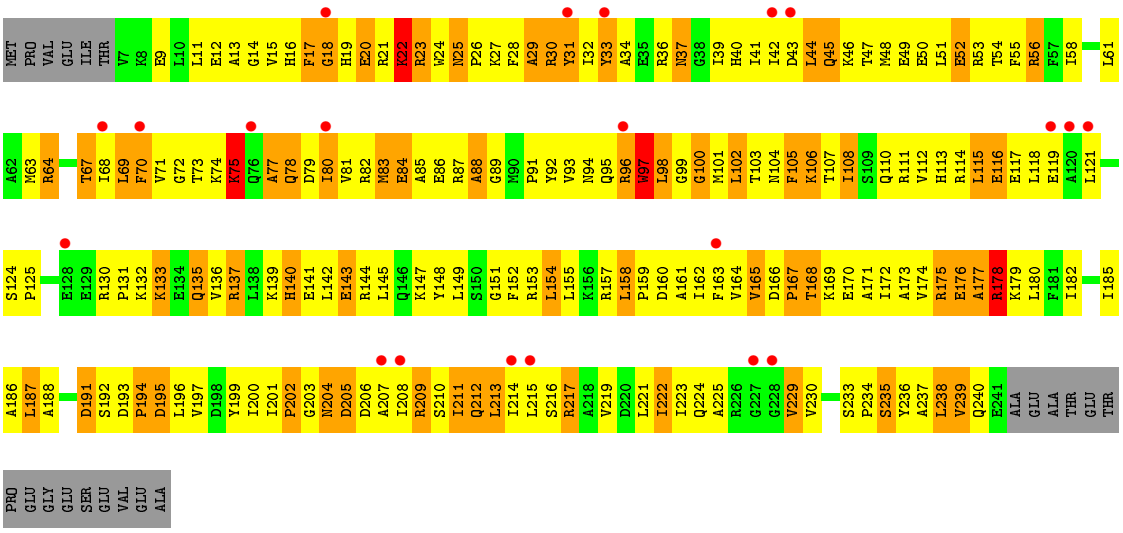
• Molecule 2: 30S RIBOSOMAL PROTEIN S2





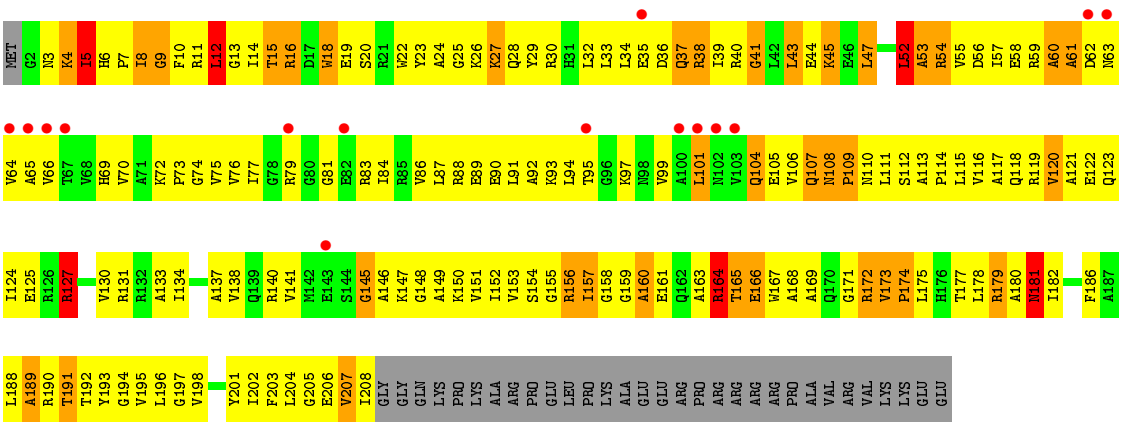
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CB:



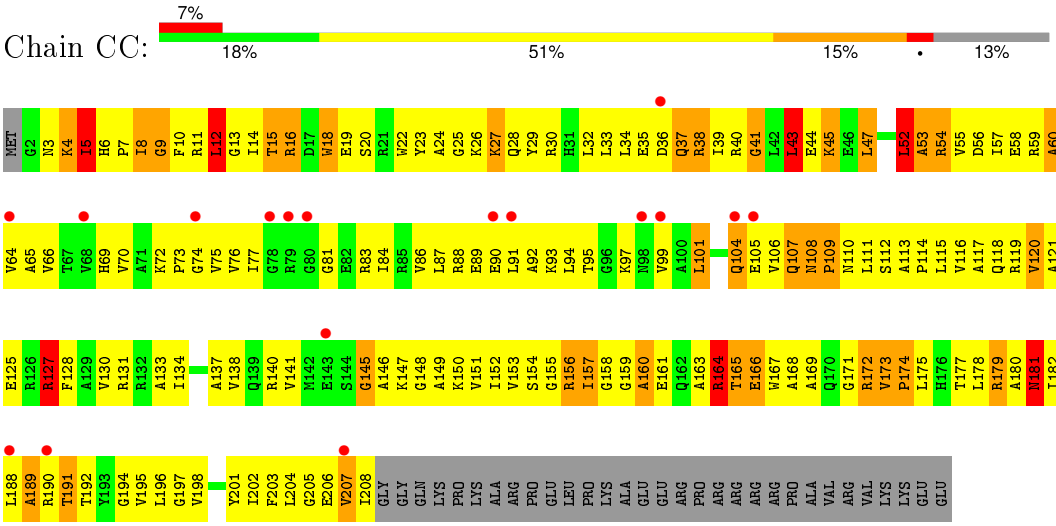
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



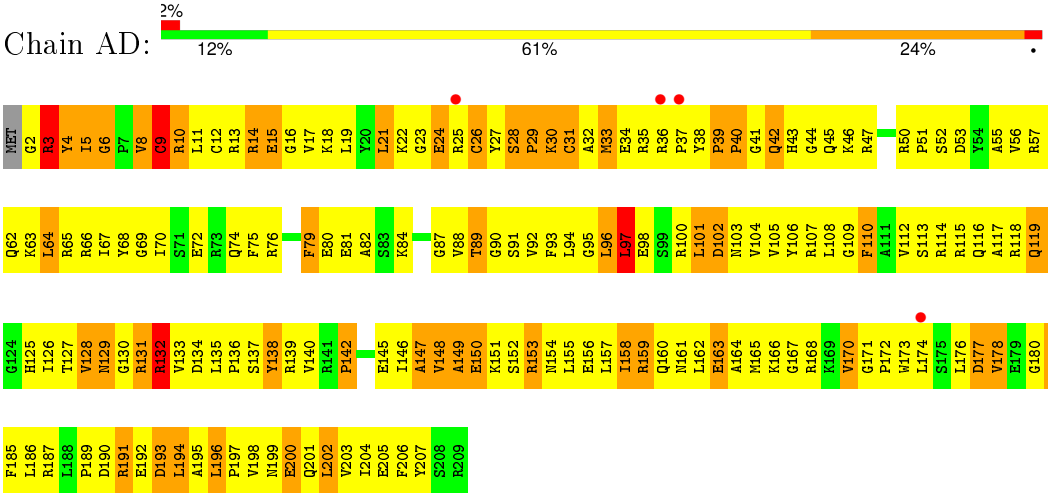
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:



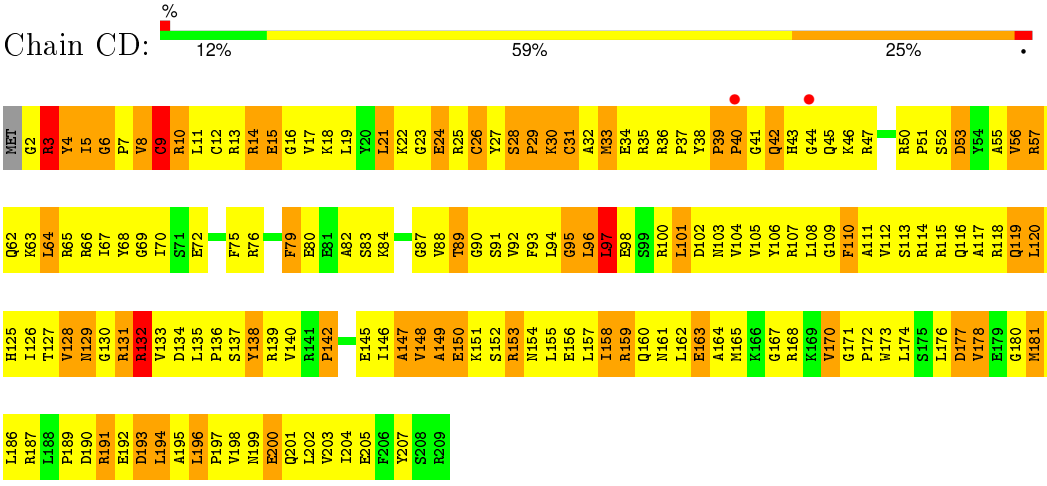
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



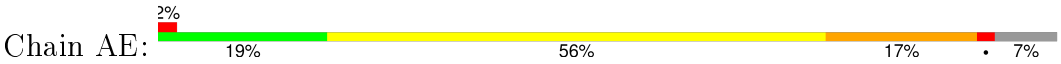
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

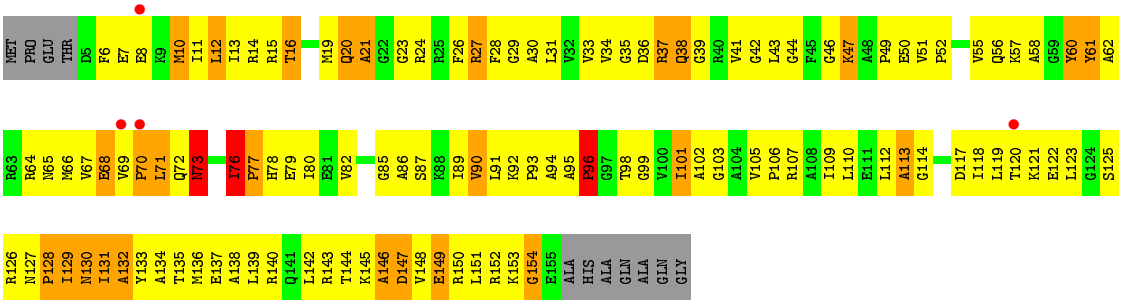
Chain CD:



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

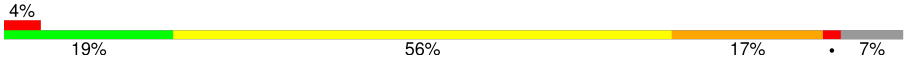
Chain AE:





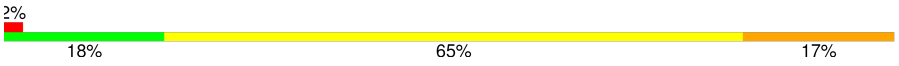
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



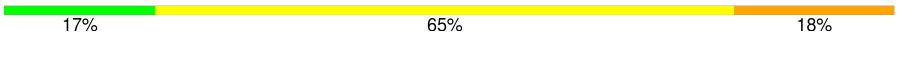
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



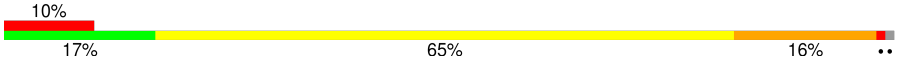
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

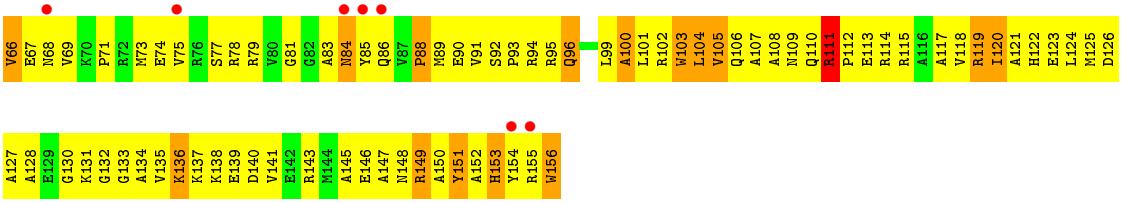
Chain CF:



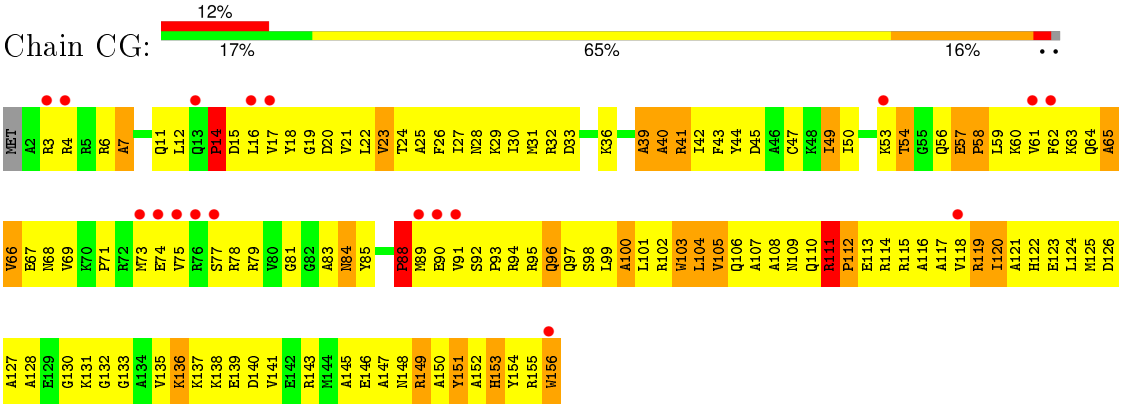
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:

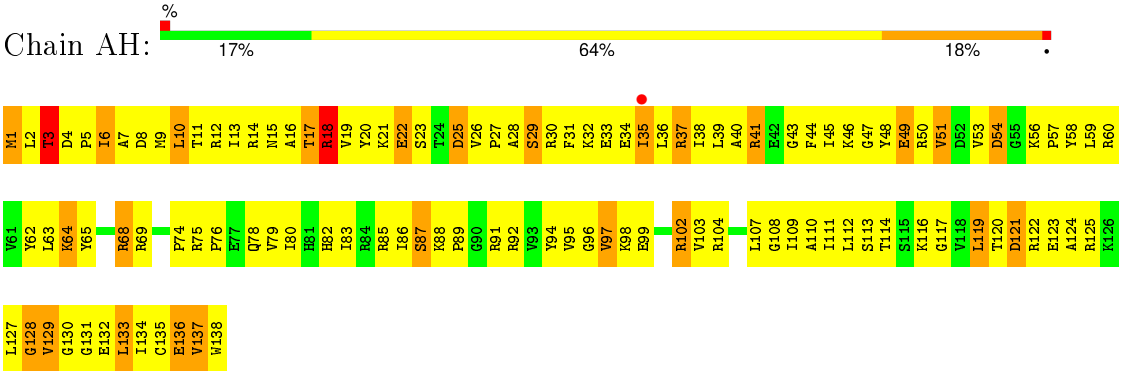




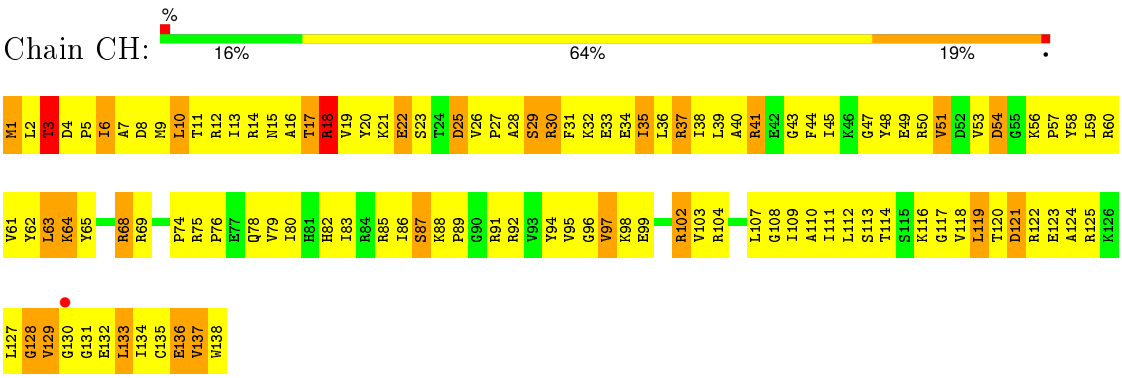
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



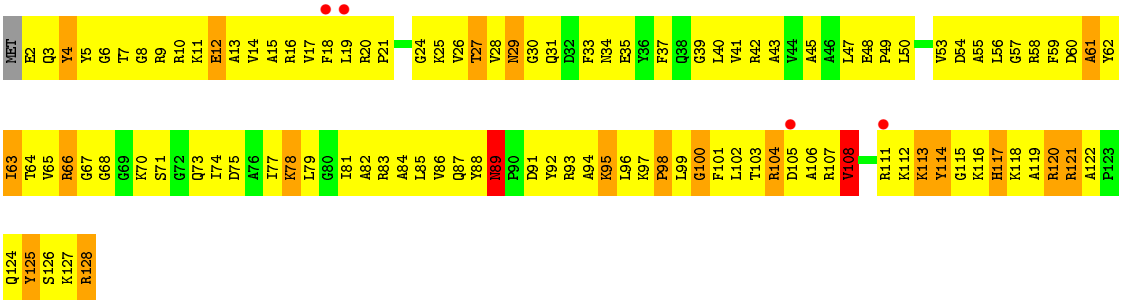
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

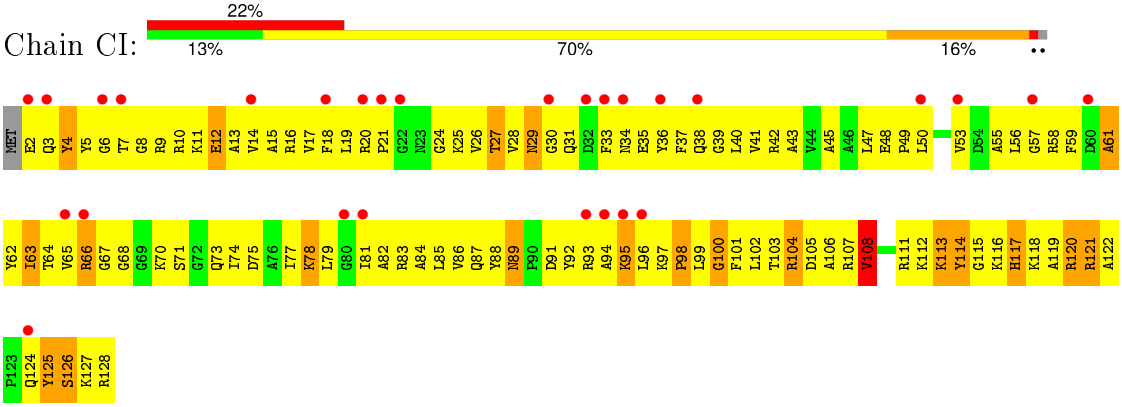


• Molecule 9: 30S RIBOSOMAL PROTEIN S9



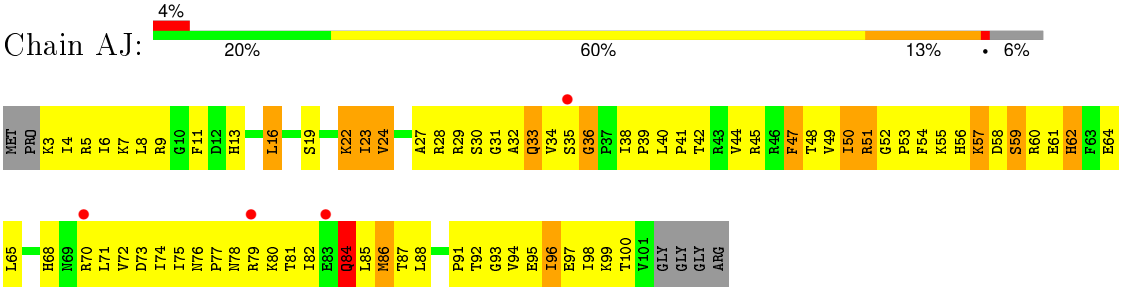
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



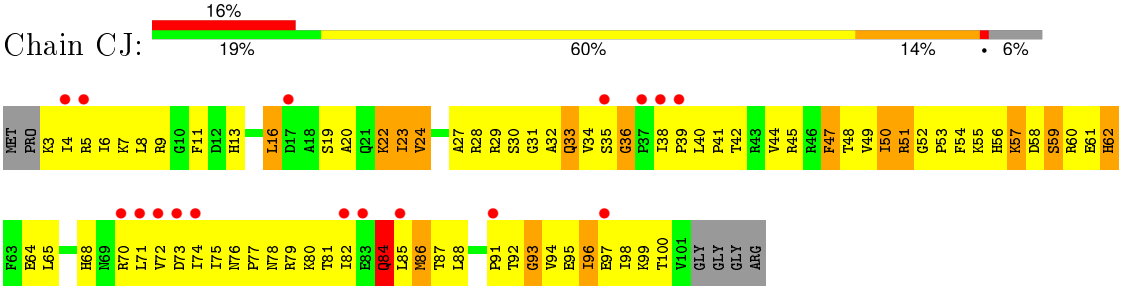
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



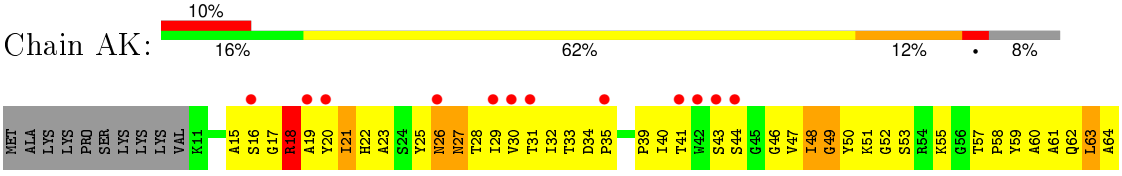
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

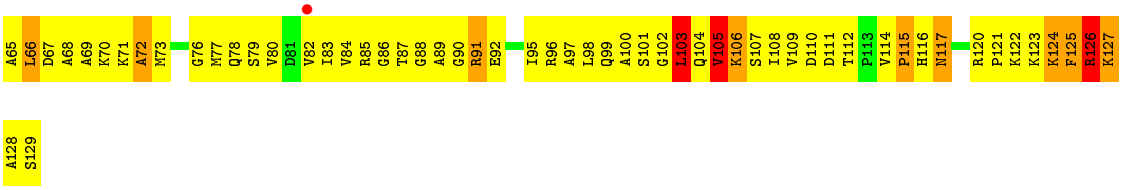
Chain CJ:



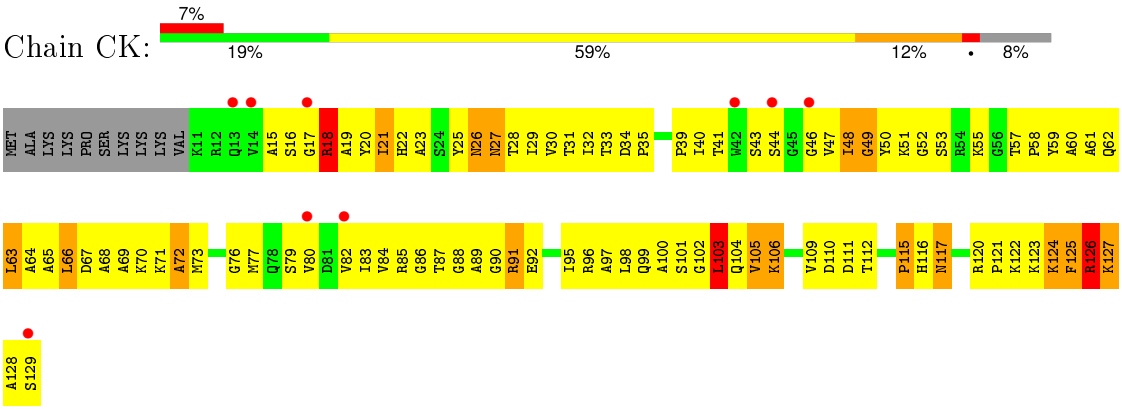
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:

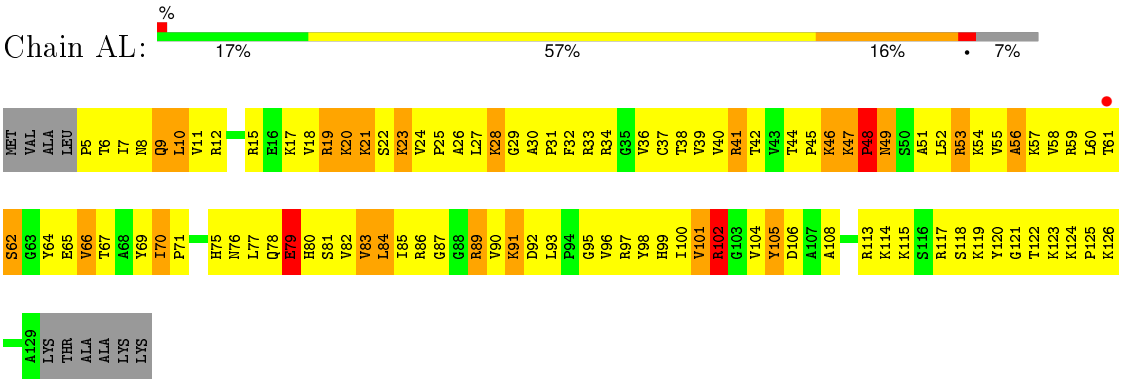




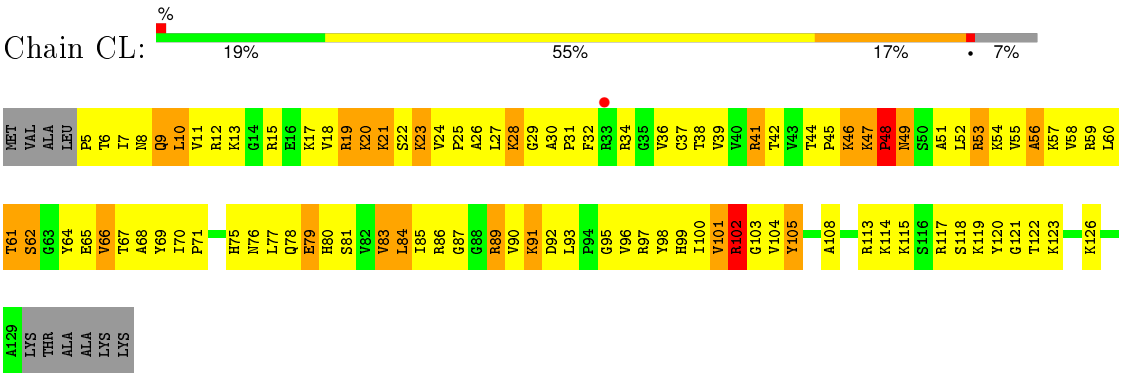
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



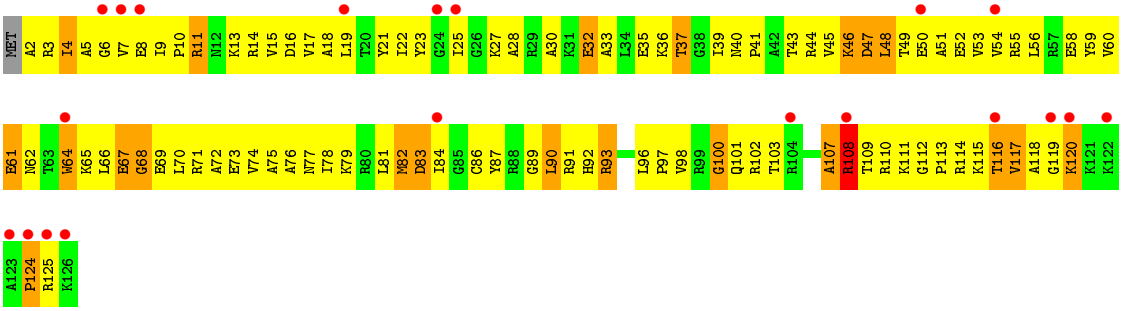
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

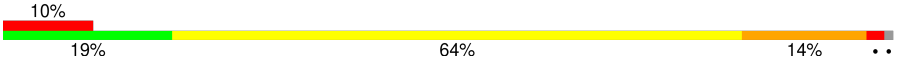


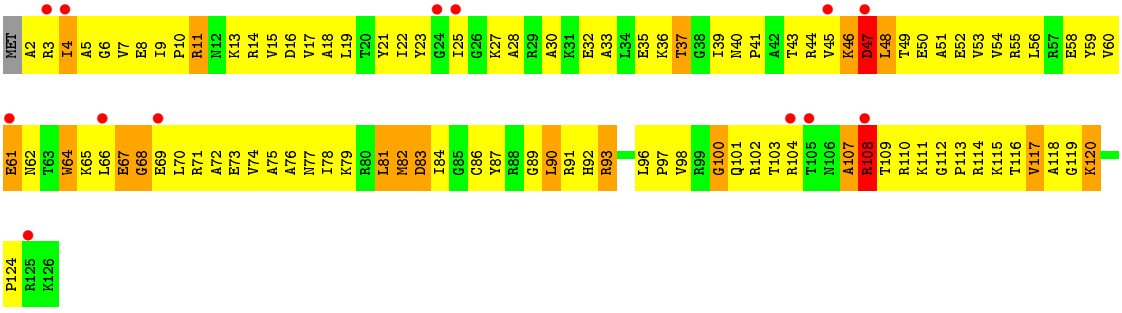
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

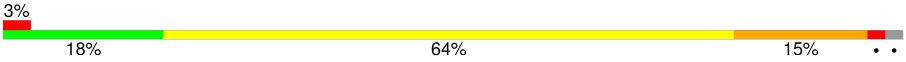
Chain CM:





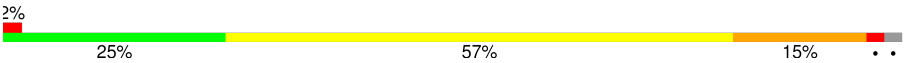
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

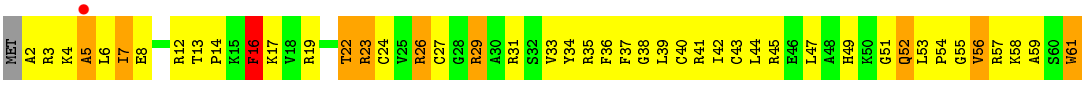
Chain AN:



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

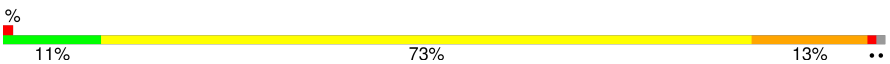
Chain CN:

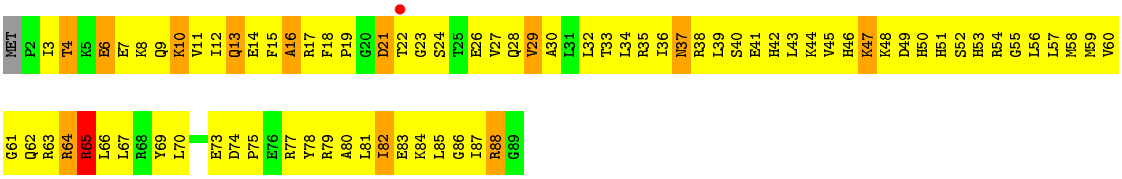




• Molecule 15: 30S RIBOSOMAL PROTEIN S15

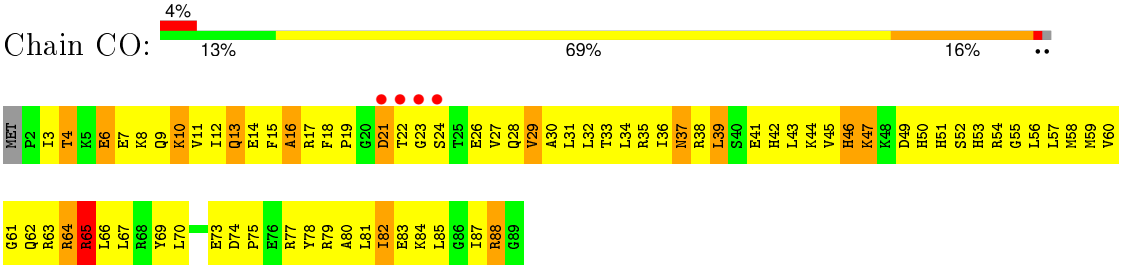
Chain AO:





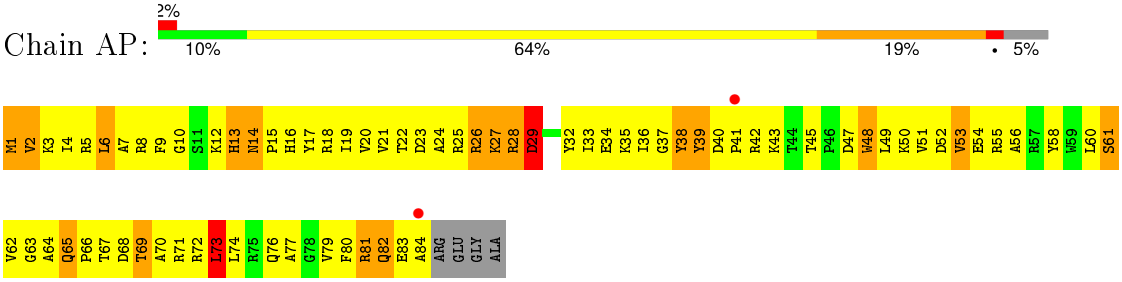
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



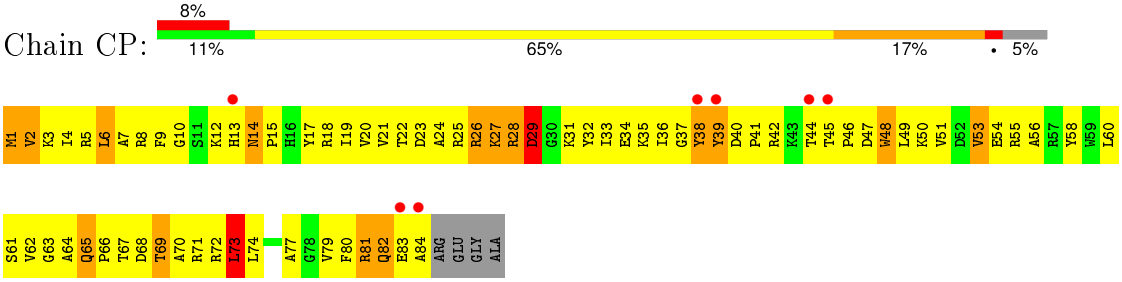
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



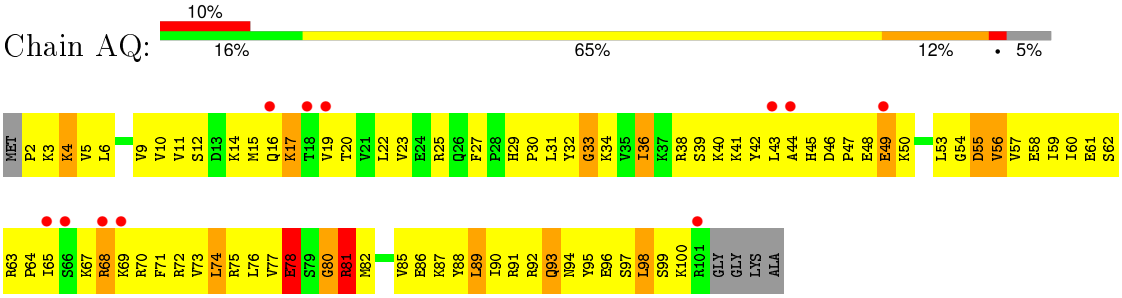
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



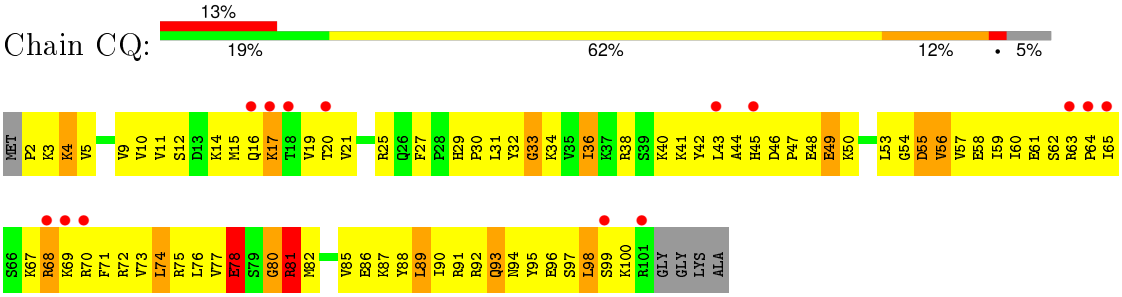
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



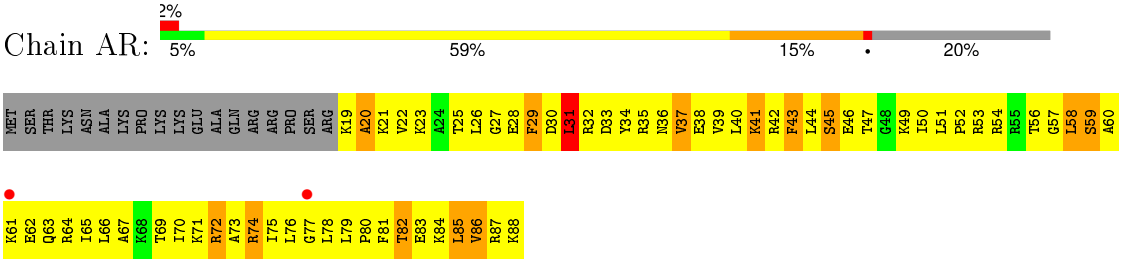
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



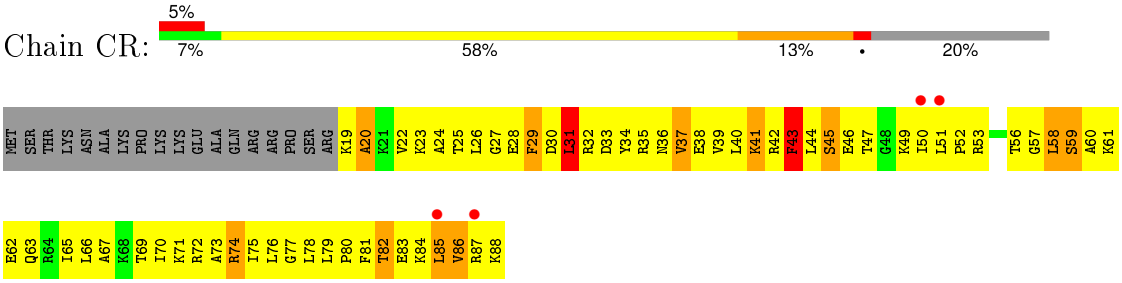
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



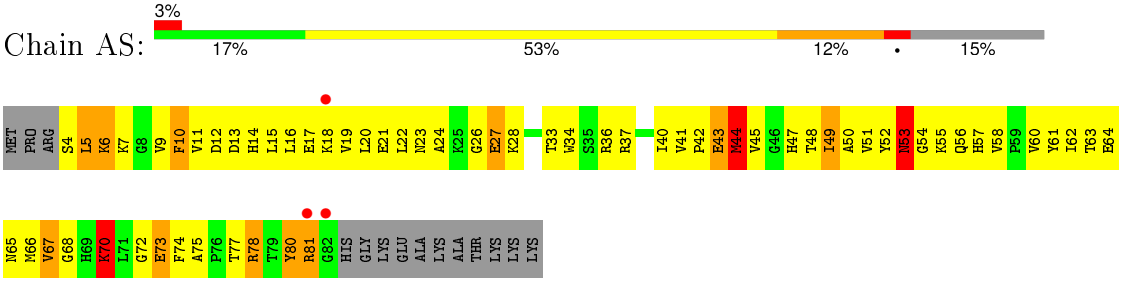
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



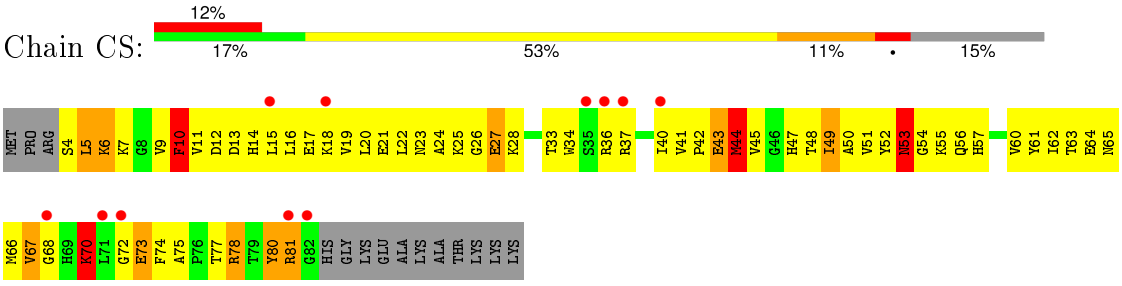
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



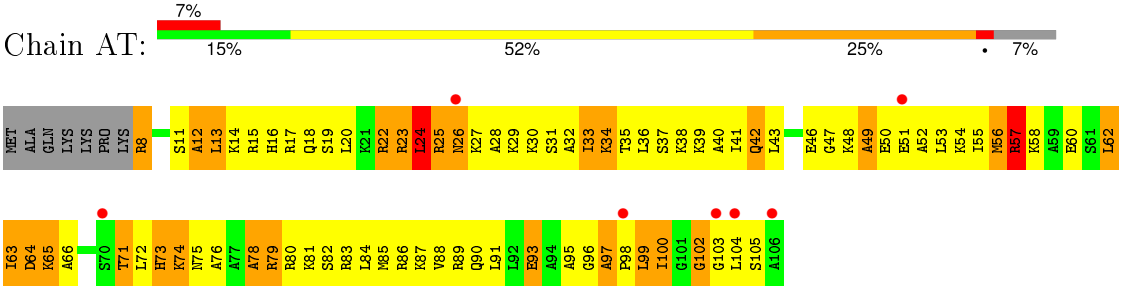
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



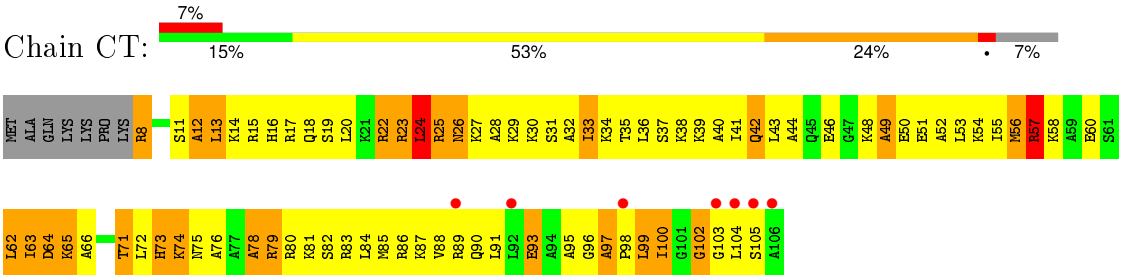
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



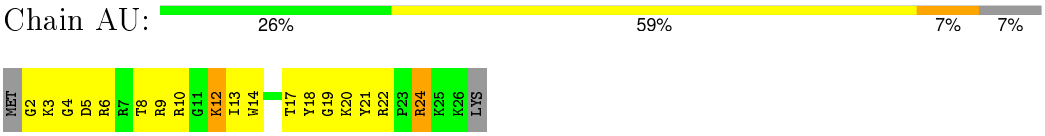
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:



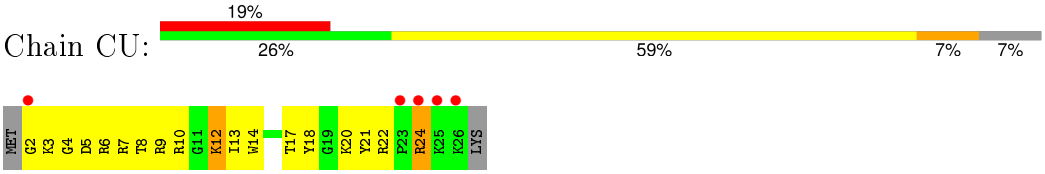
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



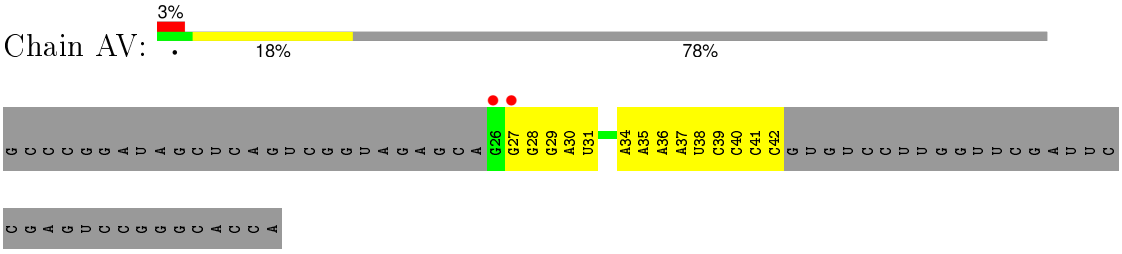
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



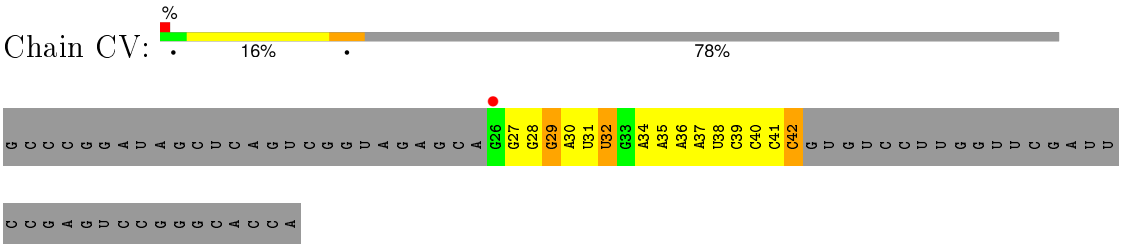
- Molecule 22: P-SITE RNA ASL-PHE

Chain AV:



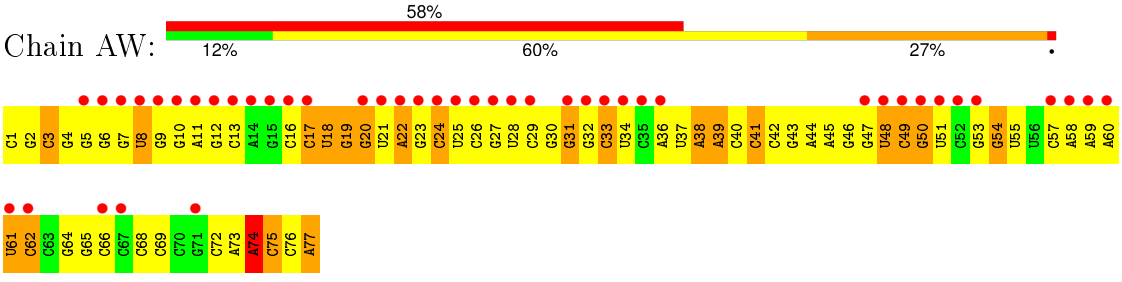
- Molecule 22: P-SITE RNA ASL-PHE

Chain CV:



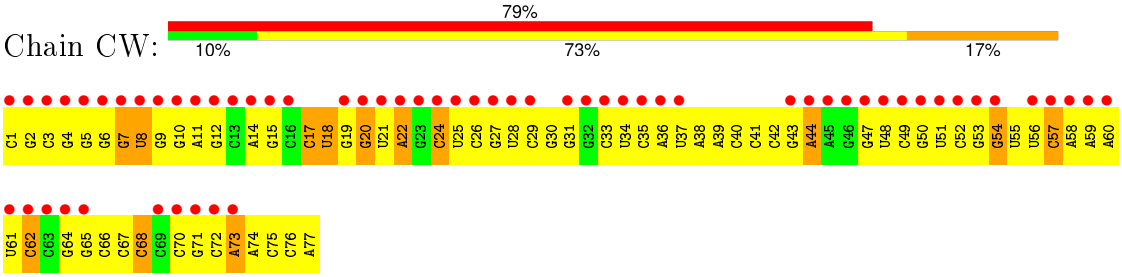
- Molecule 23: TRNA-FMET

Chain AW:



• Molecule 23: TRNA-FMET

Chain CW:



• Molecule 24: MRNA

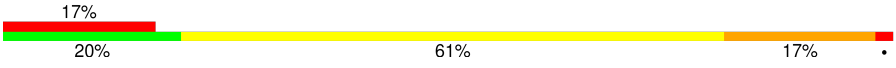
Chain AX:

• Molecule 24: MRNA

Chain CX:

• Molecule 25: RIBOSOME RECYCLING FACTOR

Chain AY:

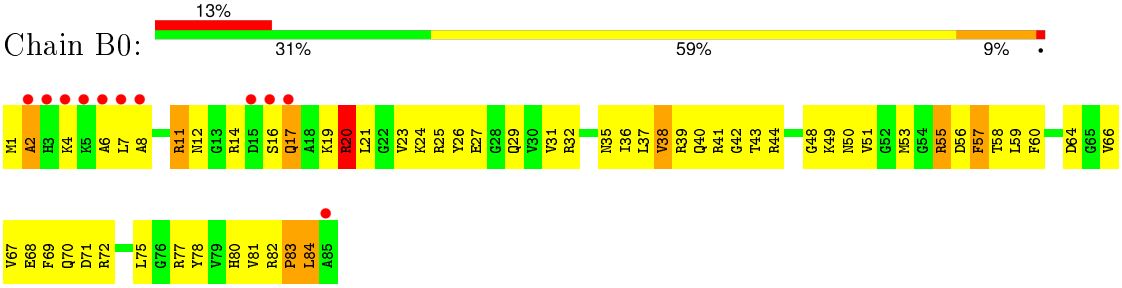


• Molecule 25: RIBOSOME RECYCLING FACTOR

Chain CY:

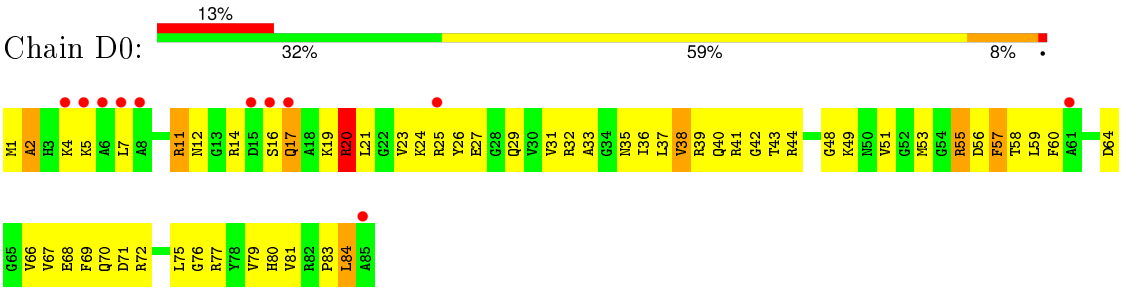
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



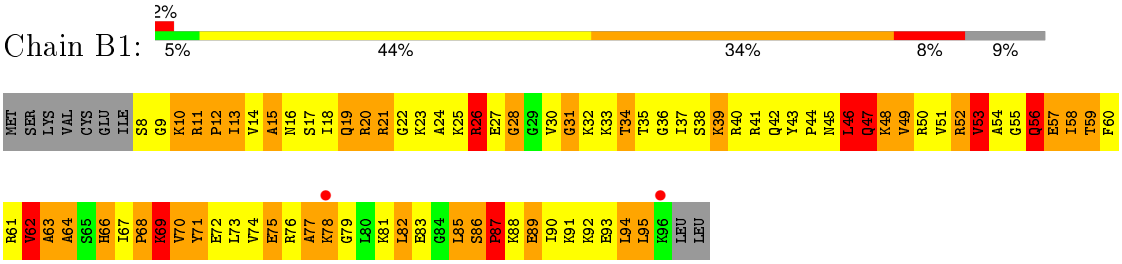
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0:



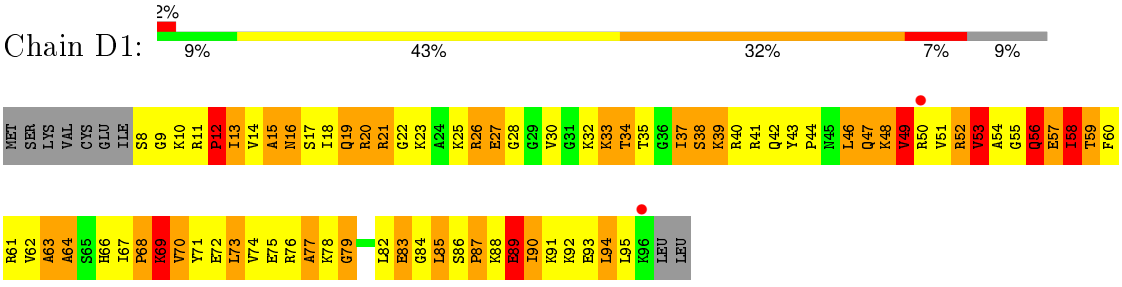
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1:



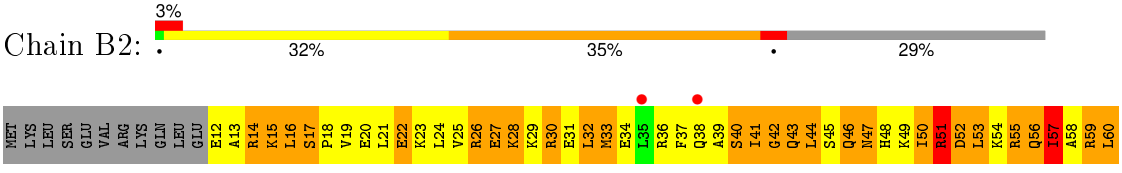
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain D1:



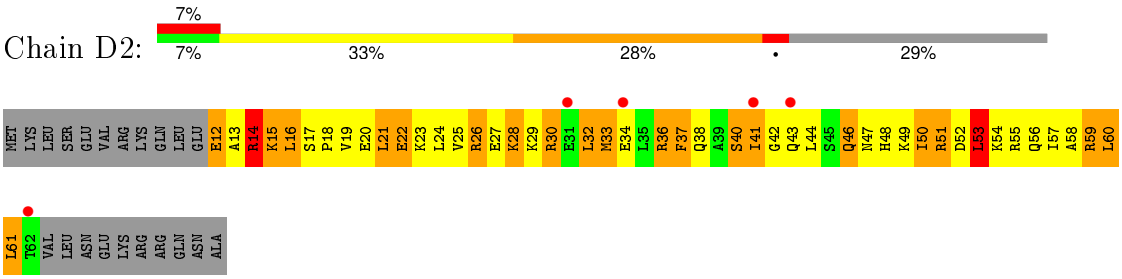
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain B2:



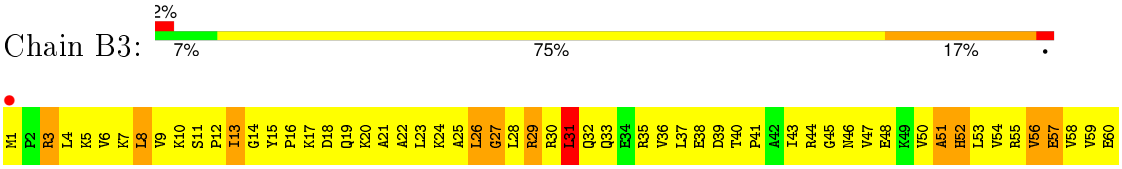
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain D2:



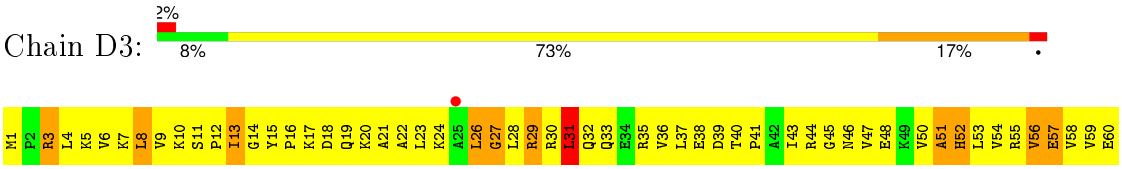
• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:



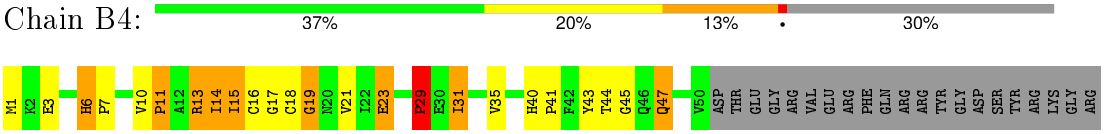
• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain D3:



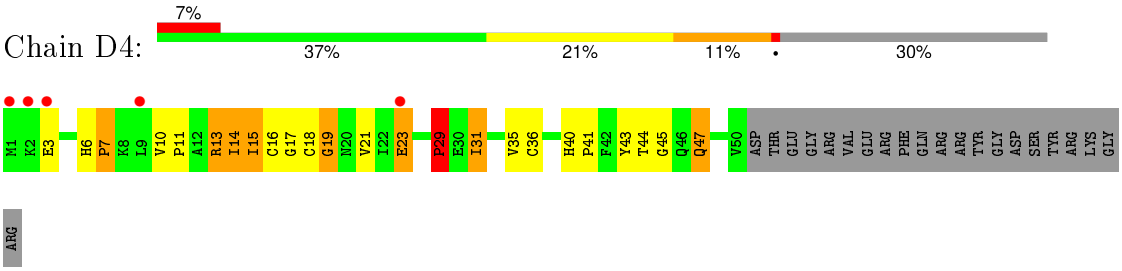
• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4:



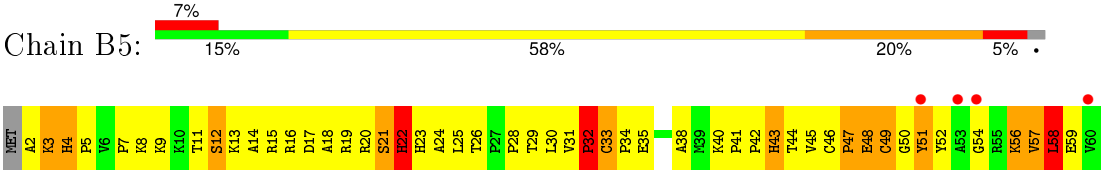
• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain D4:



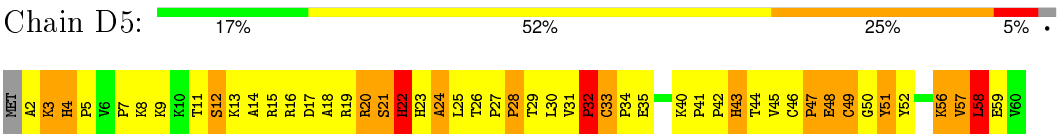
• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain B5:



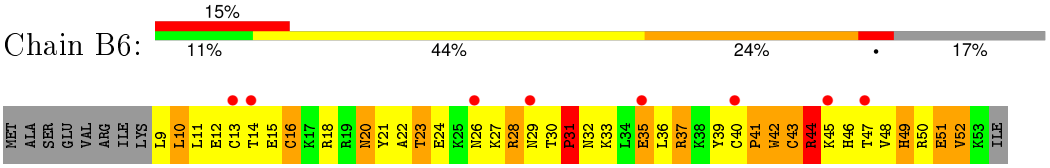
• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain D5:



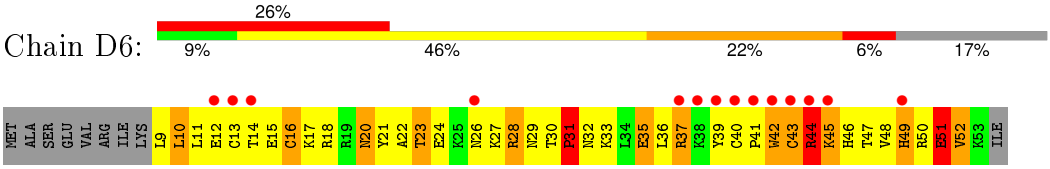
- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain B6:



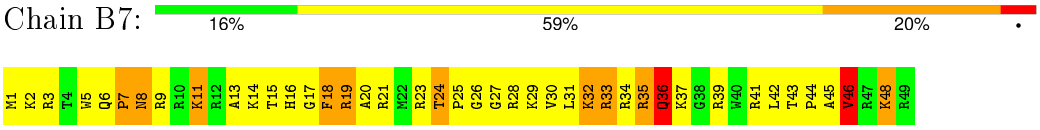
- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain D6:



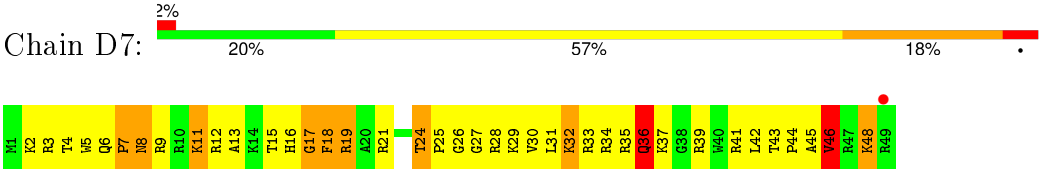
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7:



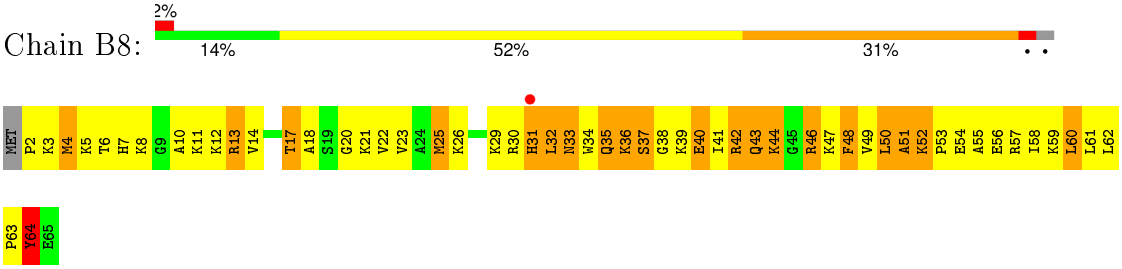
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7:



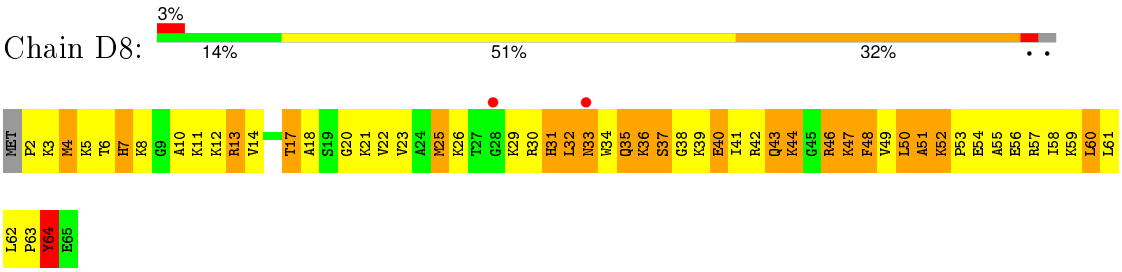
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain B8:



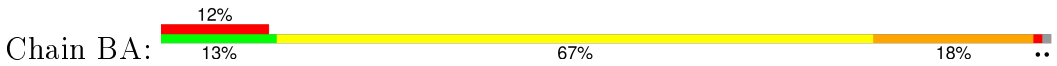
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

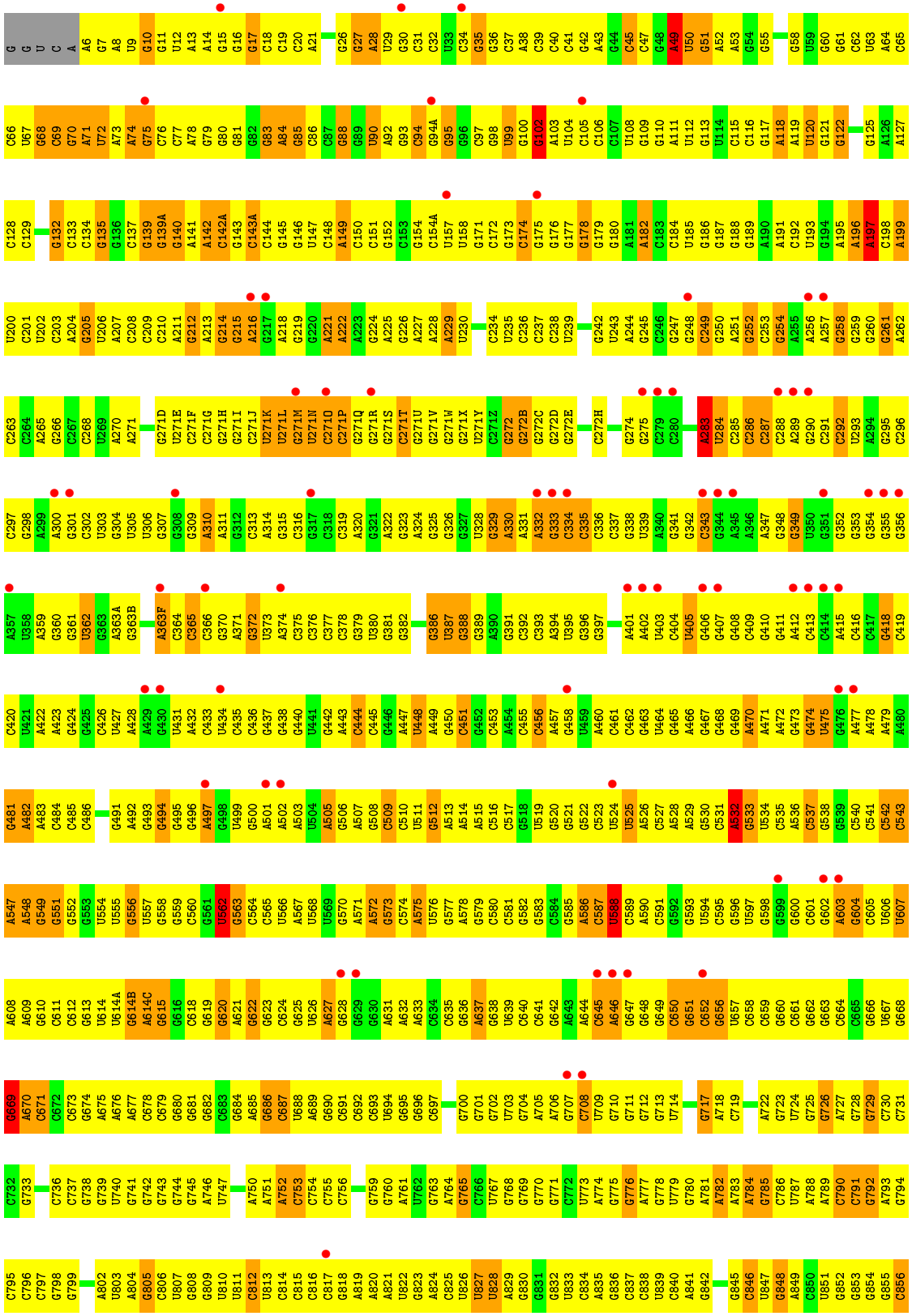
Chain D8:

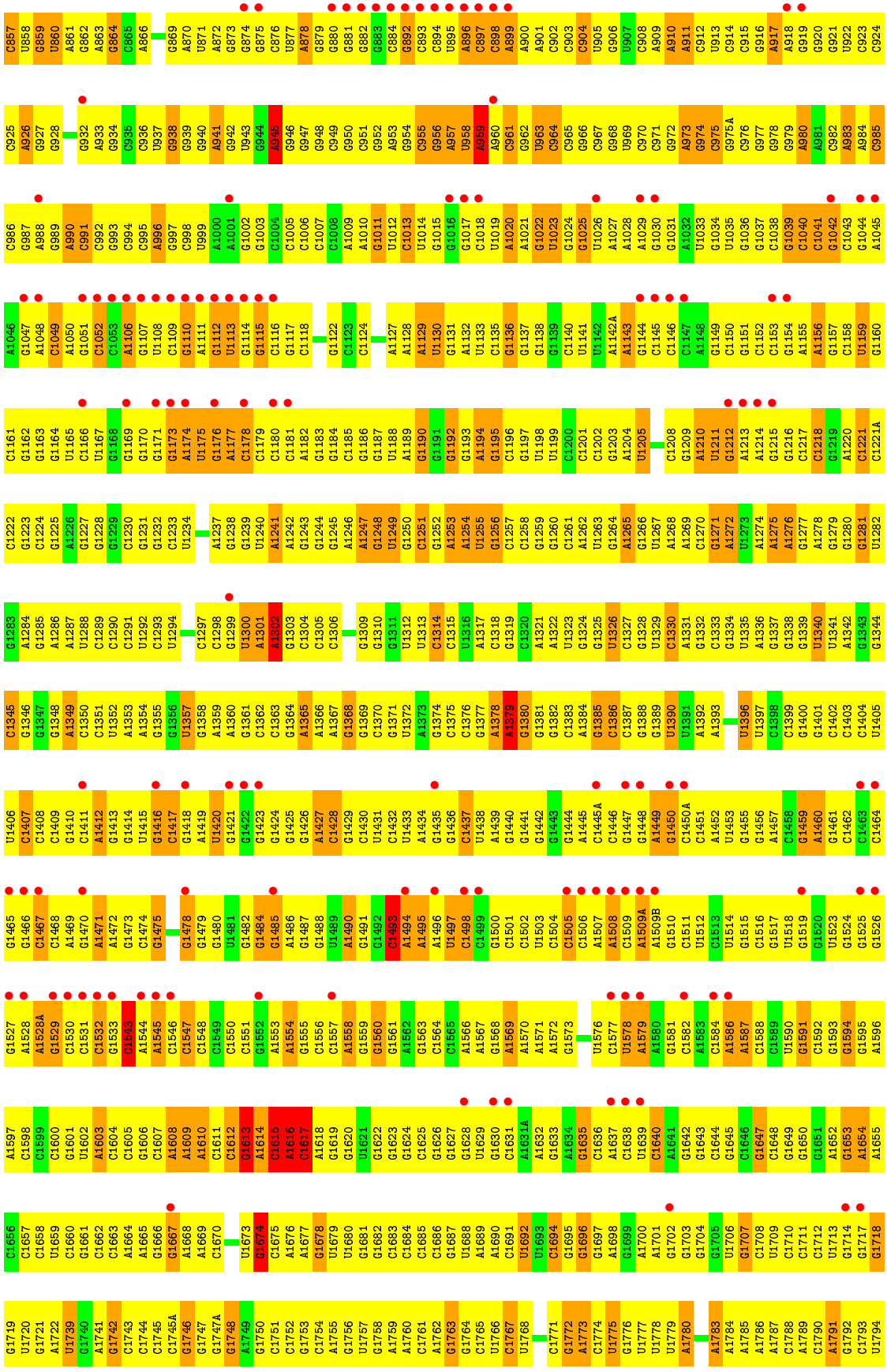


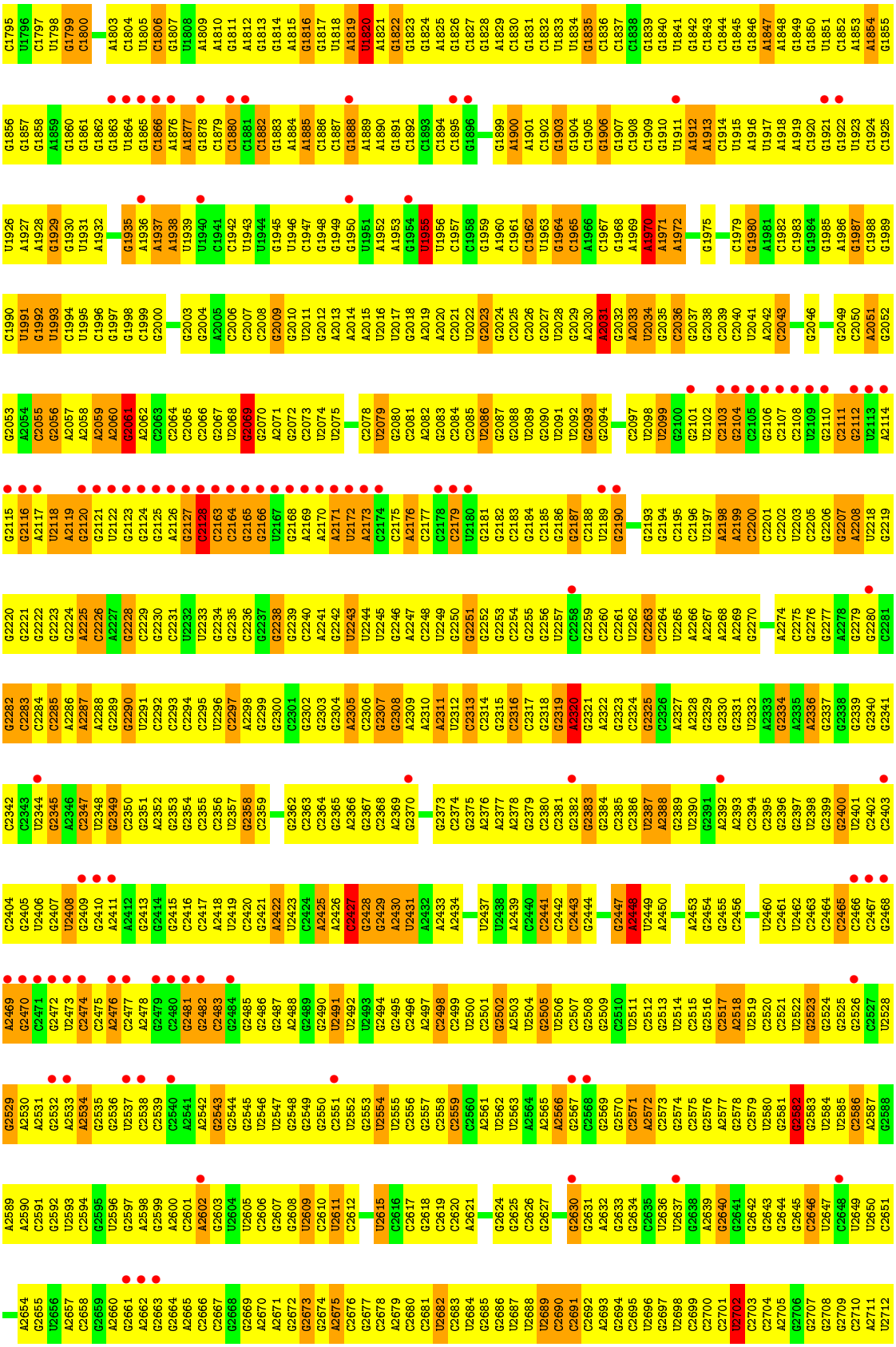
• Molecule 35: 23S RIBOSOMAL RNA

Chain BA:





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G1856 G1857 G1858 A1859 G1860 G1861 G1862 G1863 U1864 G1865 C1866 A1876 A1877 G1878 C1879 C1880 C1881 C1882 G1883 A1884 A1885 C1886 C1887 G1888 A1889 A1890 G1891 C1892 C1893 C1894 C1895 G1896 G1899 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907 C1908 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925
U1926 A1927 A1928 G1929 G1930 U1931 A1932 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1943 U1944 G1945 U1946 C1947 G1948 G1949 G1950 U1951 A1952 A1953 G1954 U1955 U1956 C1957 C1958 G1959 A1960 C1961 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1975 C1979 G1980 A1981 C1982 C1983 G1984 G1985 A1986 G1987 C1988 C1924 G1989
C1990 U1991 G1992 U1993 C1994 U1995 C1996 G1997 G1998 C1999 G2000 G2003 G2004 A2005 C2006 C2007 C2008 G2009 G2010 U2011 G2012 A2013 A2014 A2015 U2016 U2017 G2018 A2019 A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 G2046 G2049 C2050 A2051 G2052
G2053 A2054 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 G2070 A2071 G2072 C2073 U2074 U2075 C2078 U2079 G2080 C2081 A2082 G2083 C2084 C2085 U2086 G2087 G2088 U2089 G2090 U2091 U2092 G2093 G2094 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114
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G2220 G2221 G2222 G2223 G2224 A2225 C2226 A2227 G2228 C2229 G2230 C2231 U2232 U2233 G2234 G2235 C2236 G2237 G2238 G2239 C2240 A2241 C2242 U2243 U2244 U2245 G2246 A2247 C2248 U2249 G2250 G2251 G2252 G2253 C2254 G2255 G2256 U2257 C2258 G2259 C2260 C2261 U2262 C2263 C2264 U2265 A2266 A2267 A2268 A2269 G2270 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2281
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A2469 G2470 C2471 G2472 U2473 C2474 C2475 A2476 C2477 A2478 G2479 C2480 G2481 G2482 C2483 G2484 G2485 G2486 G2487 A2488 G2489 G2490 U2491 U2492 U2493 G2494 G2495 C2496 A2497 G2498 C2499 U2500 C2501 G2502 A2503 U2504 G2505 U2506 C2507 G2508 G2509 G2510 U2511 C2512 G2513 U2514 C2515 G2516 C2517 A2518 U2519 C2520 C2521 U2522 G2523 G2524 G2525 G2526 C2527 U2528
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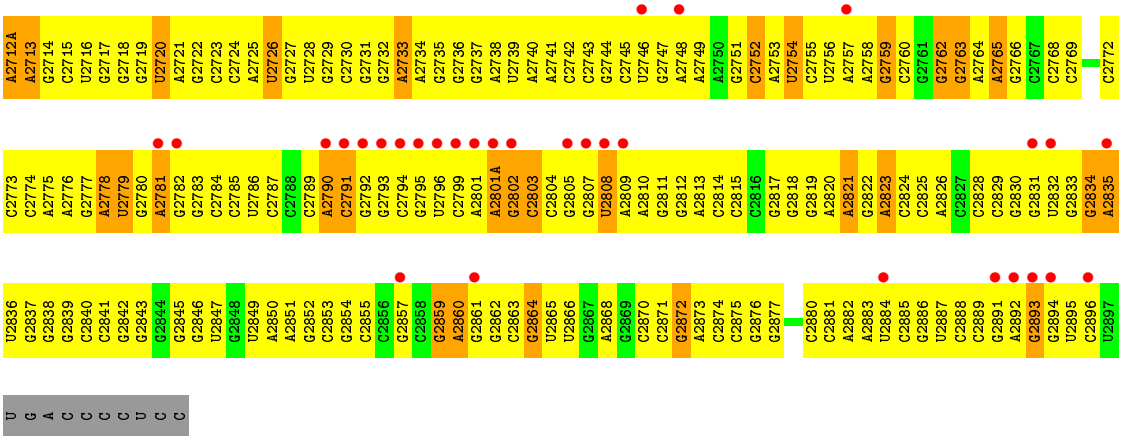
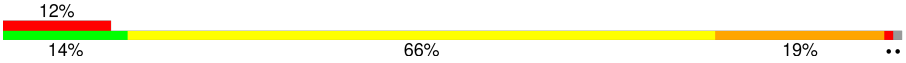
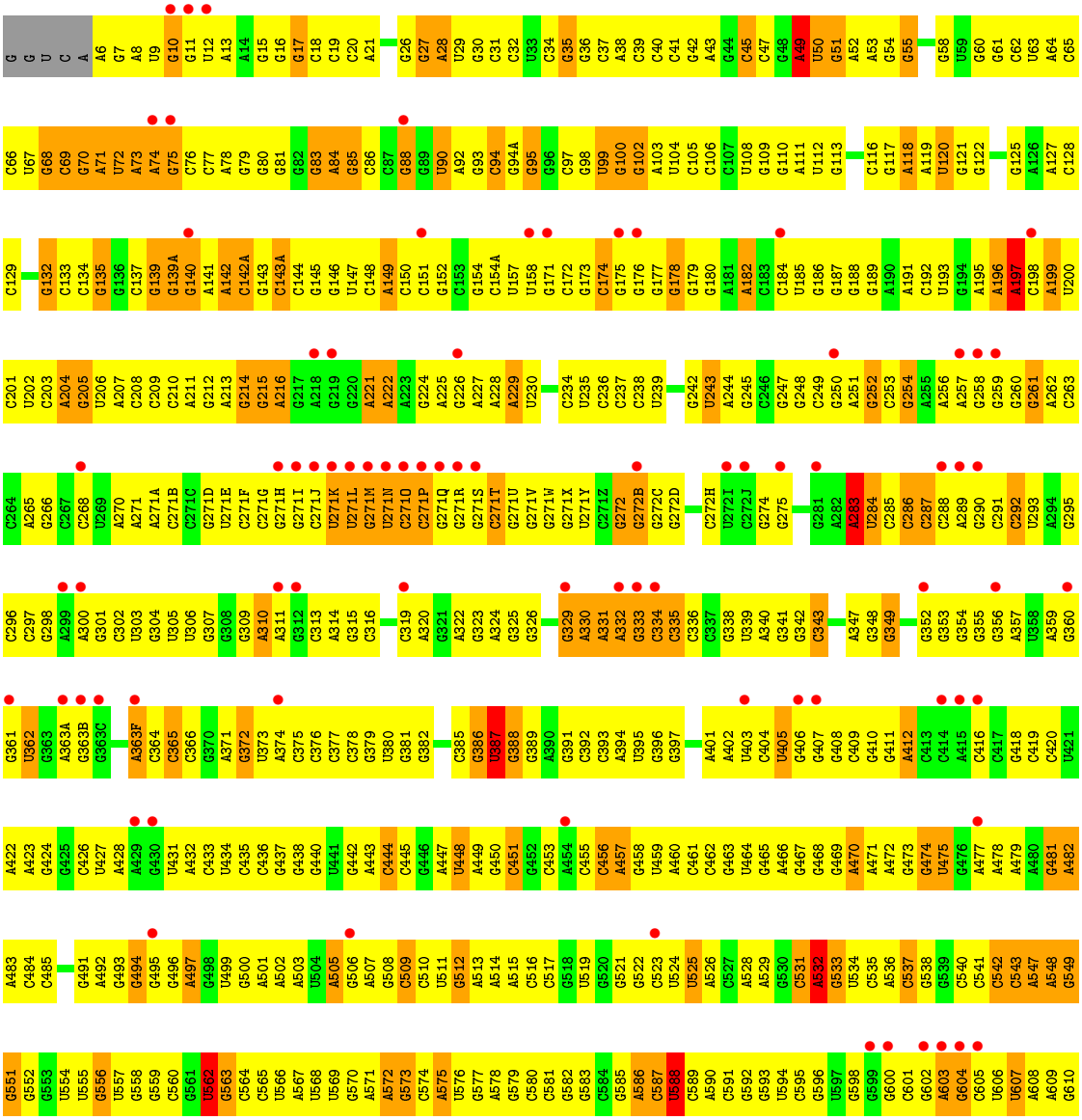
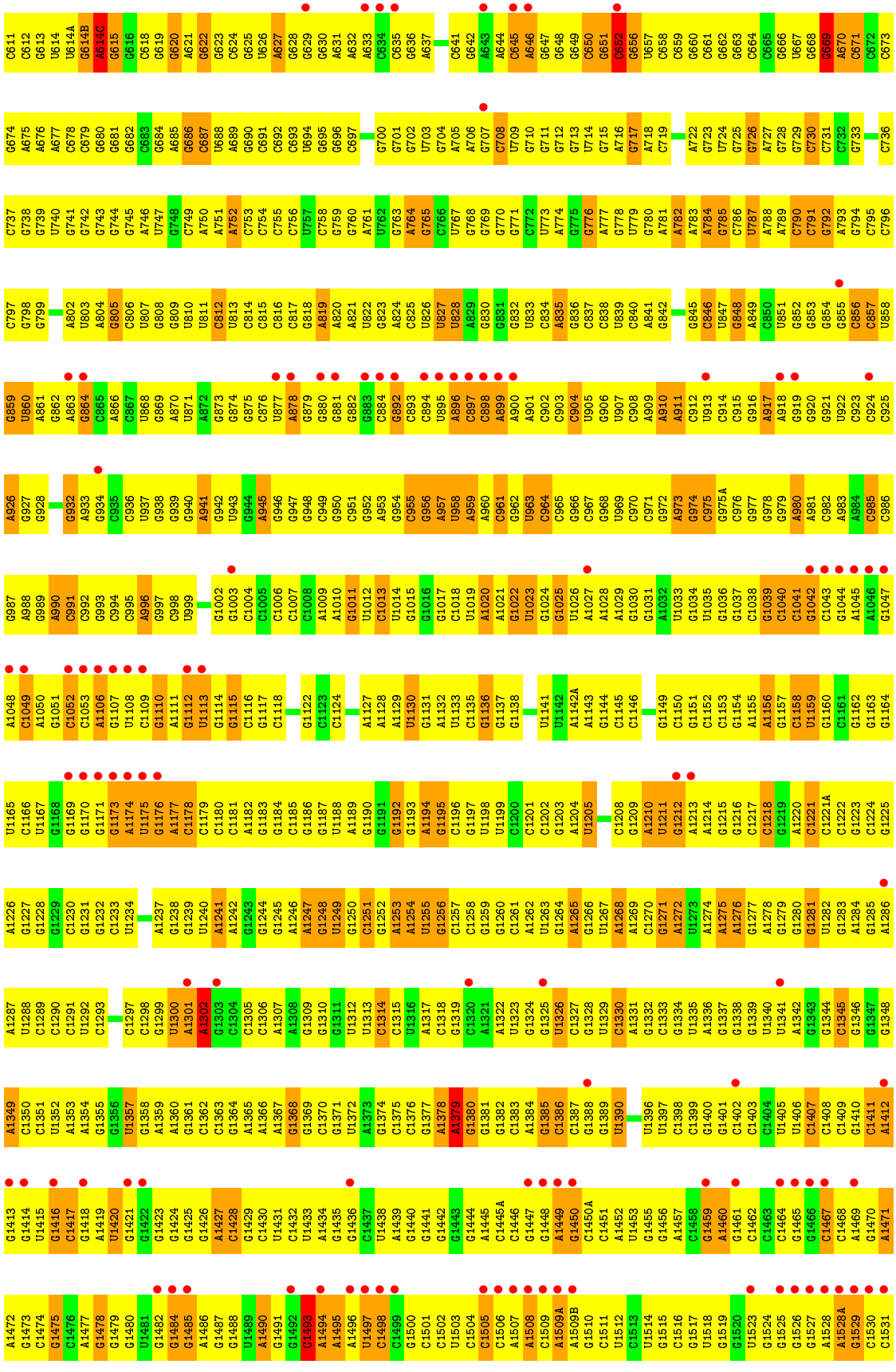


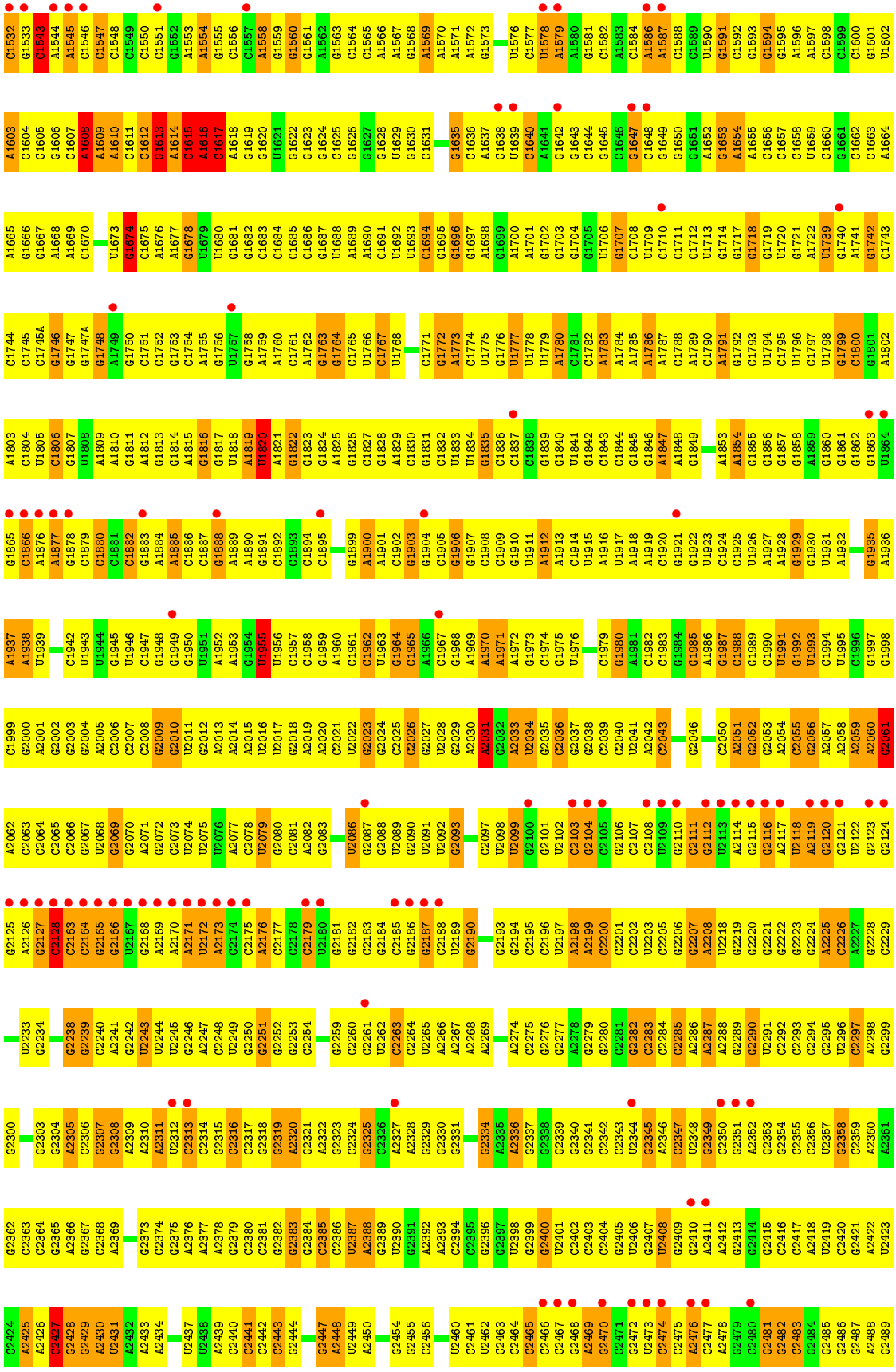
• Molecule 35: 23S RIBOSOMAL RNA

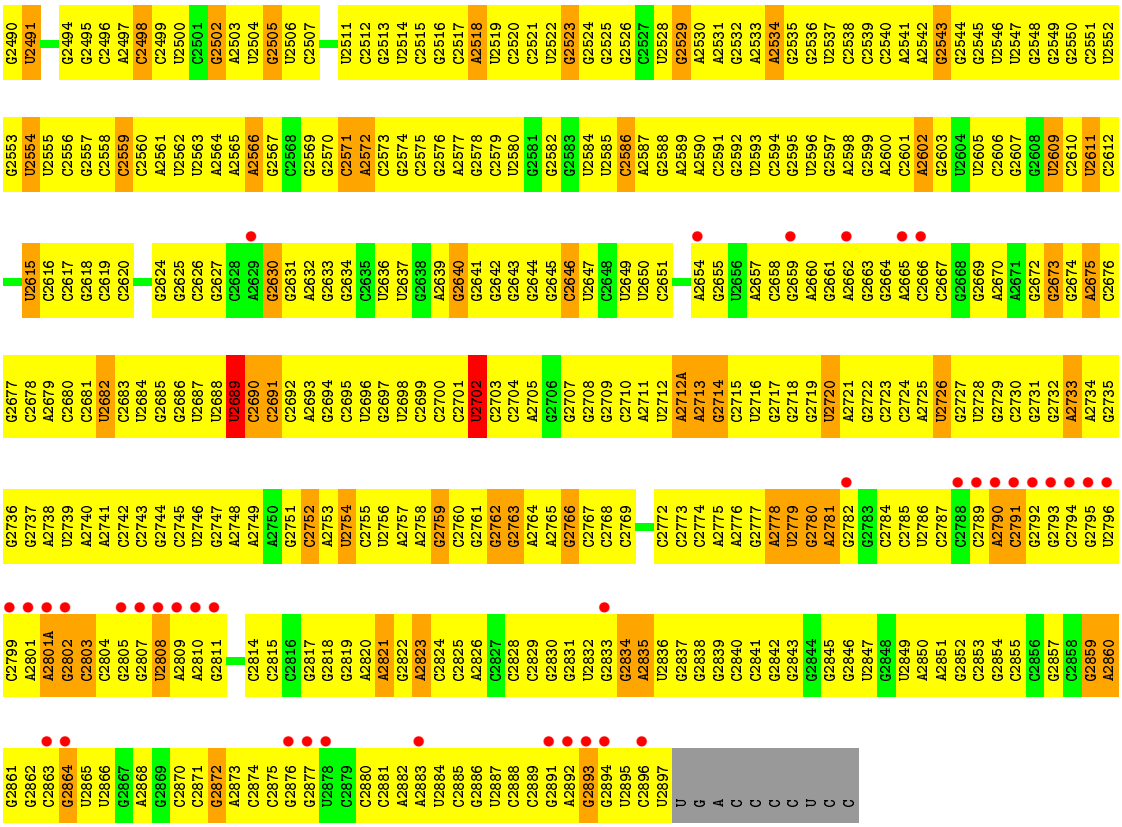
Chain DA:





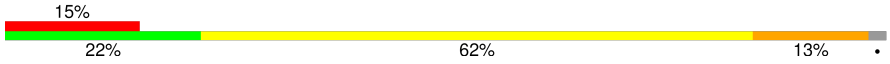


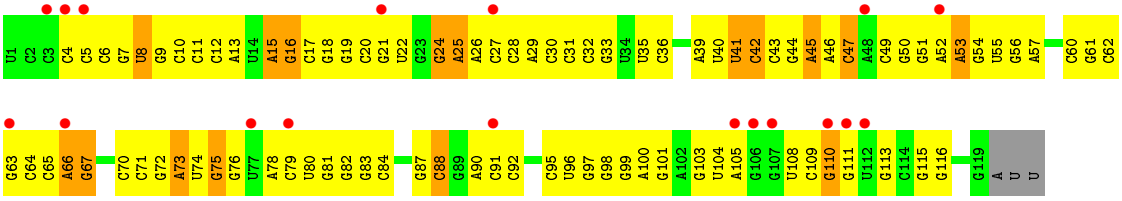




- Molecule 36: 5S RIBOSOMAL RNA

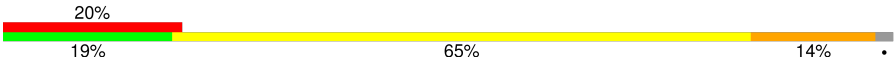
Chain BB:

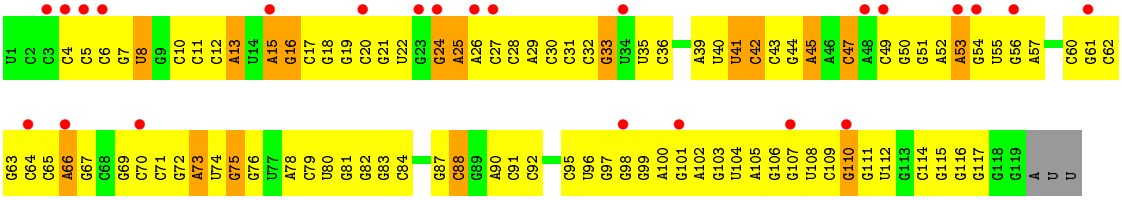




- Molecule 36: 5S RIBOSOMAL RNA

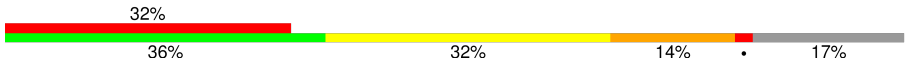
Chain DB:

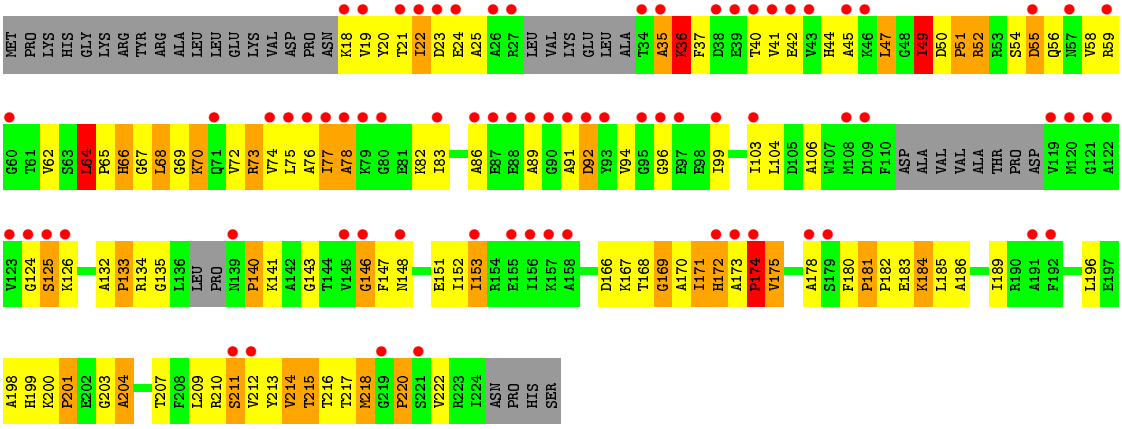




- Molecule 37: 50S RIBOSOMAL PROTEIN L1

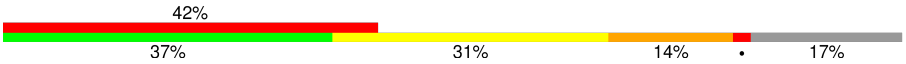
Chain BC:

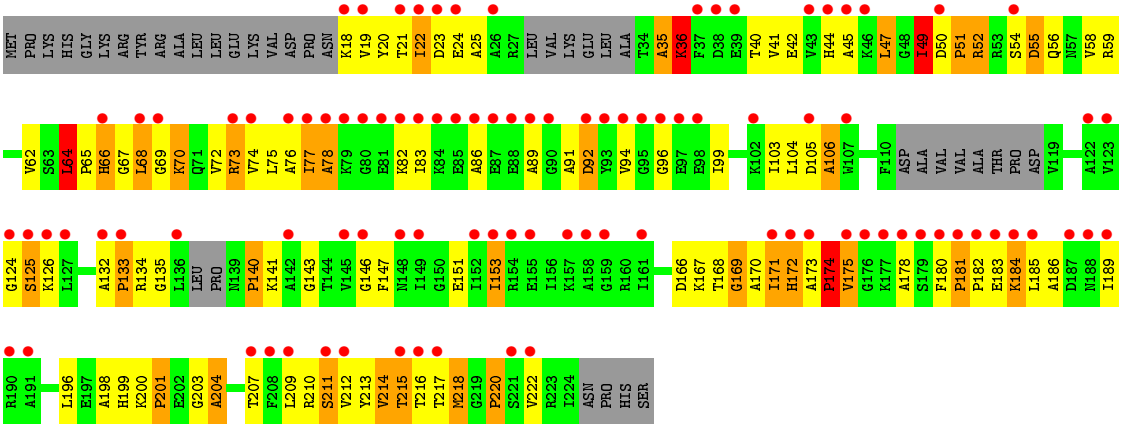




• Molecule 37: 50S RIBOSOMAL PROTEIN L1

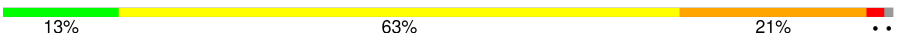
Chain DC:

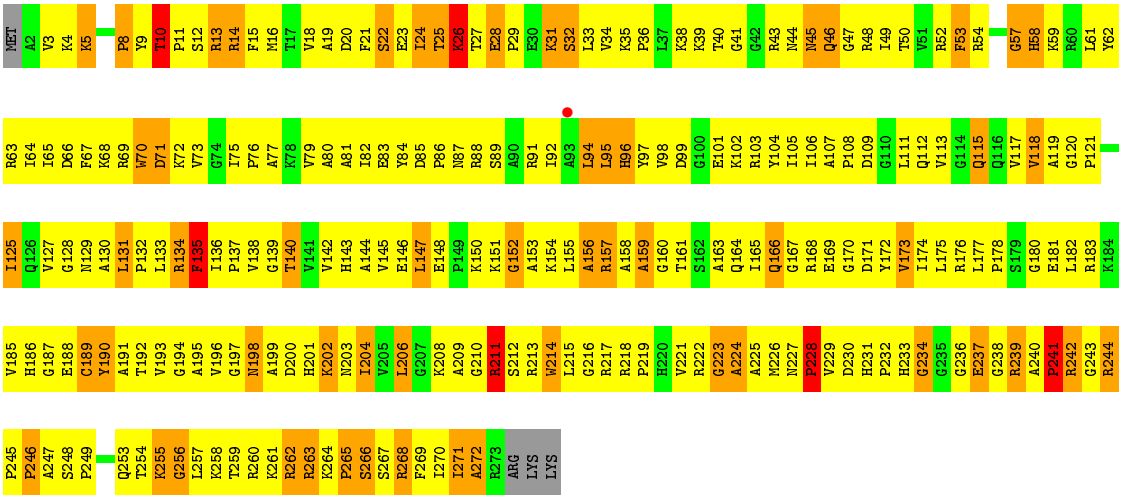




• Molecule 38: 50S RIBOSOMAL PROTEIN L2

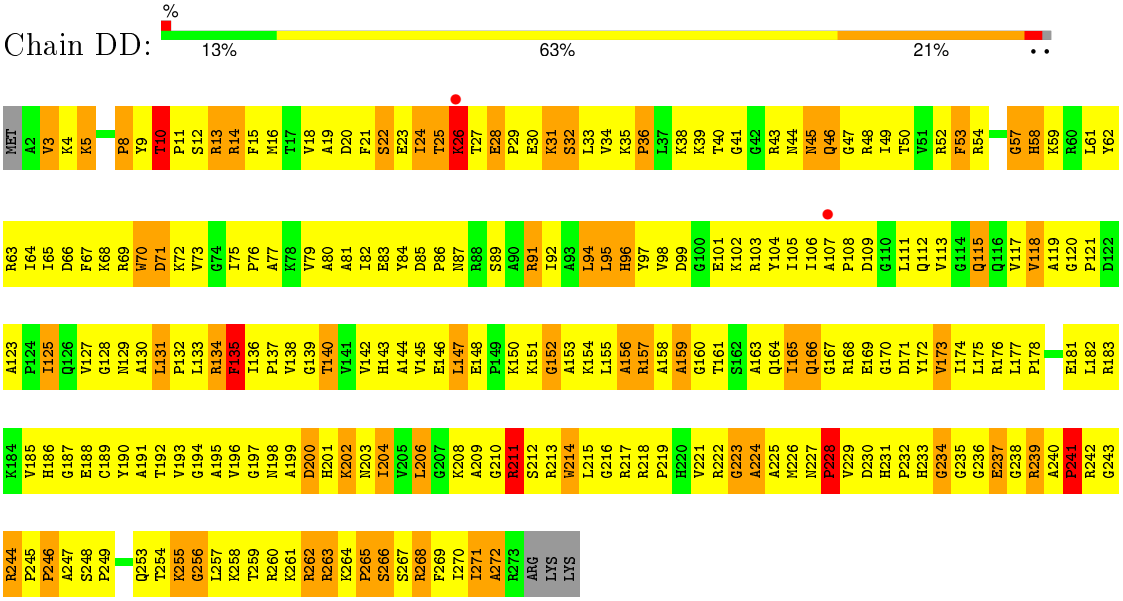
Chain BD:





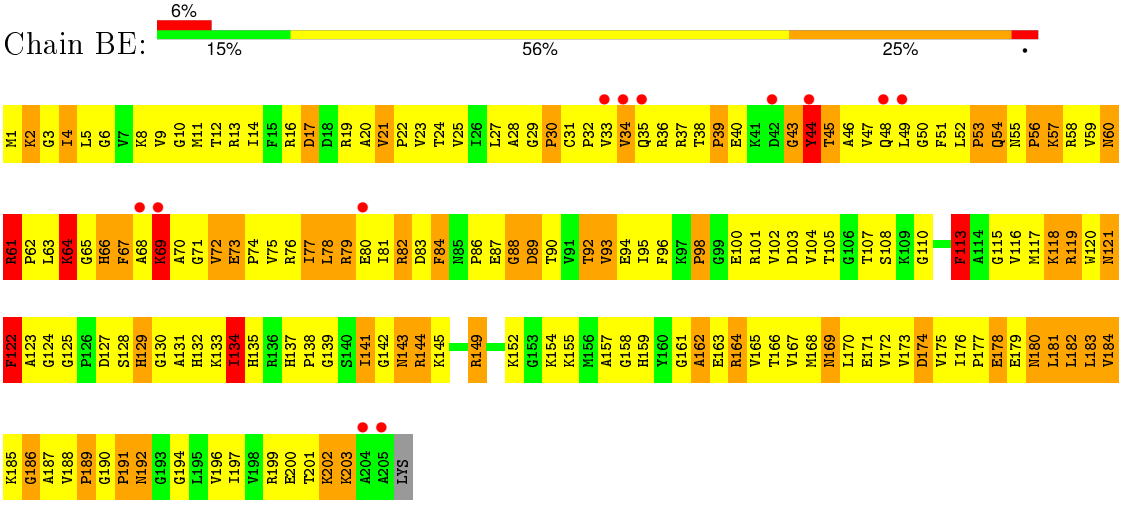
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD:



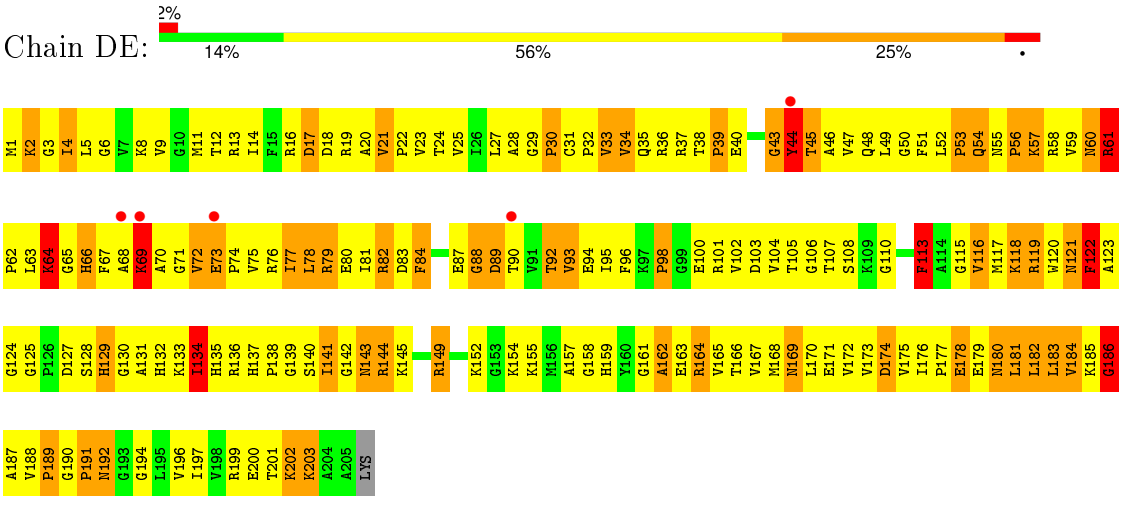
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:



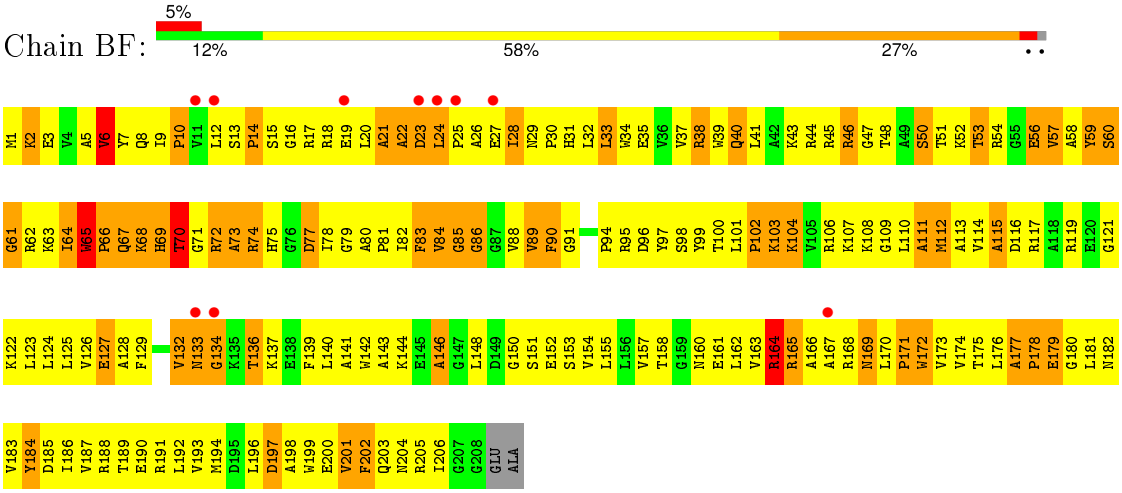
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain DE:



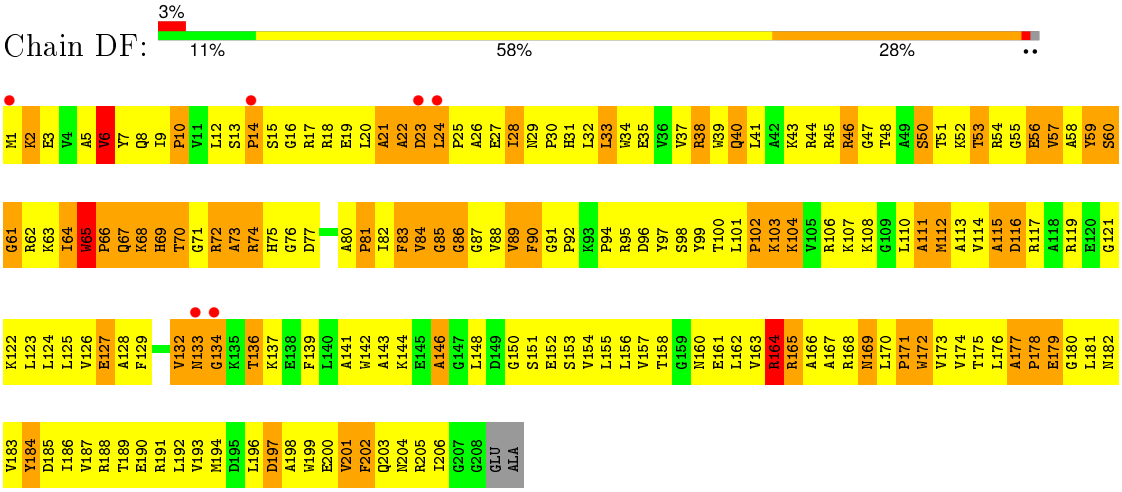
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF:



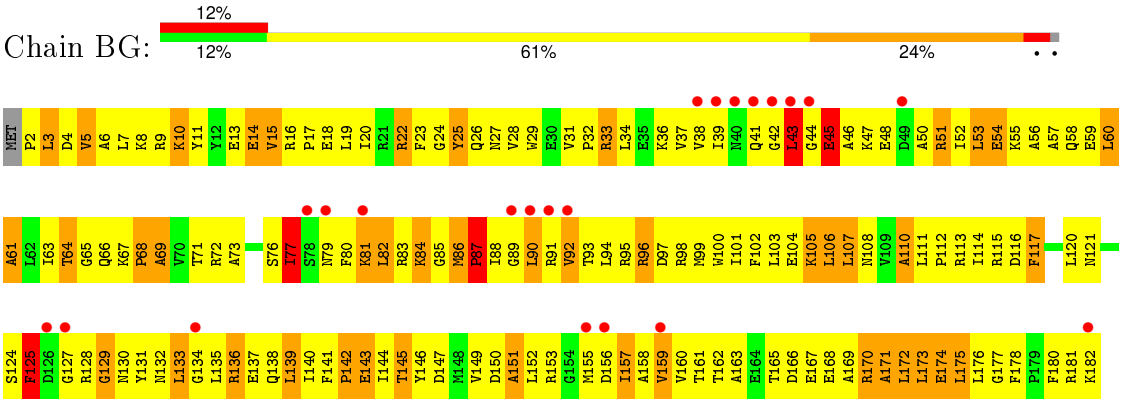
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain DF:



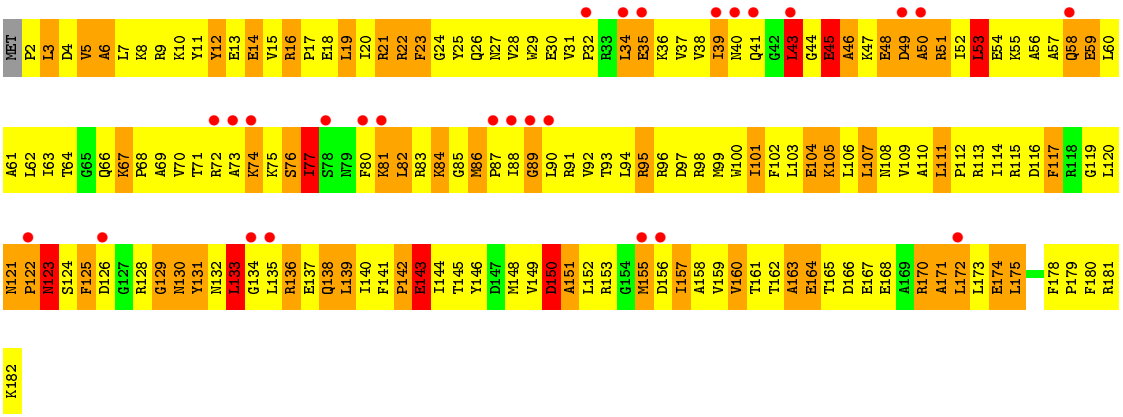
• Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain BG:



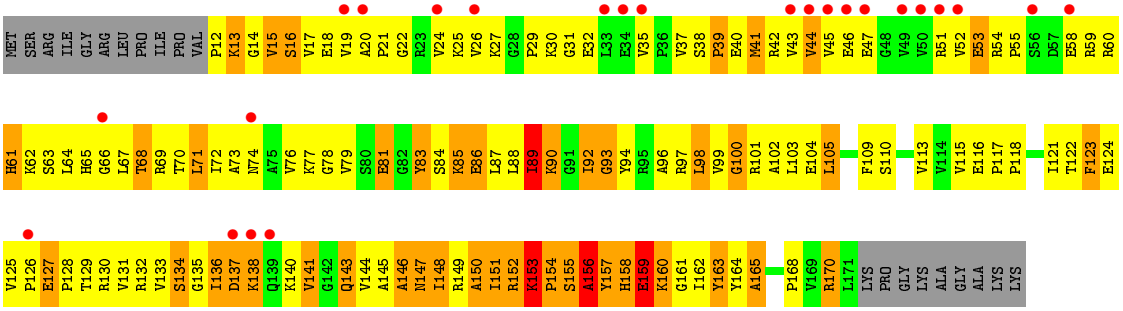
• Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain DG:



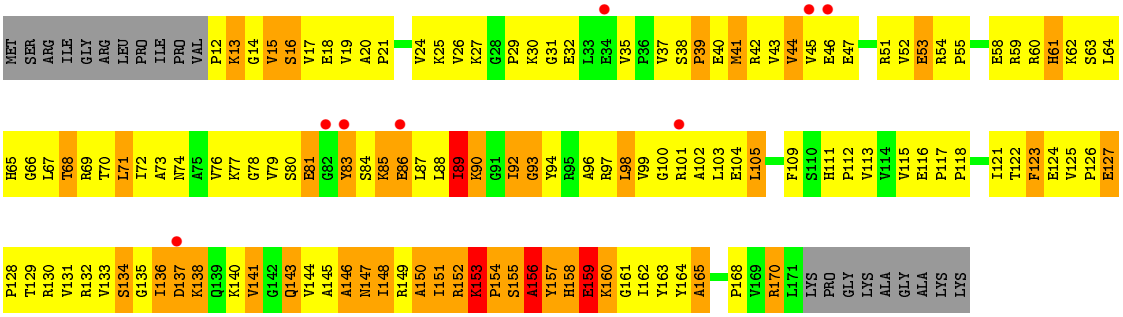
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:



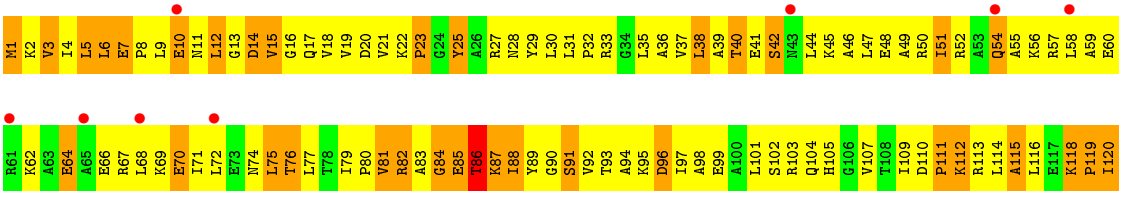
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

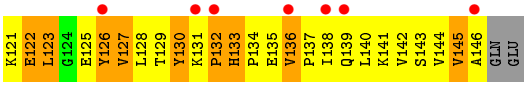
Chain DH:



• Molecule 43: 50S RIBOSOMAL PROTEIN L9

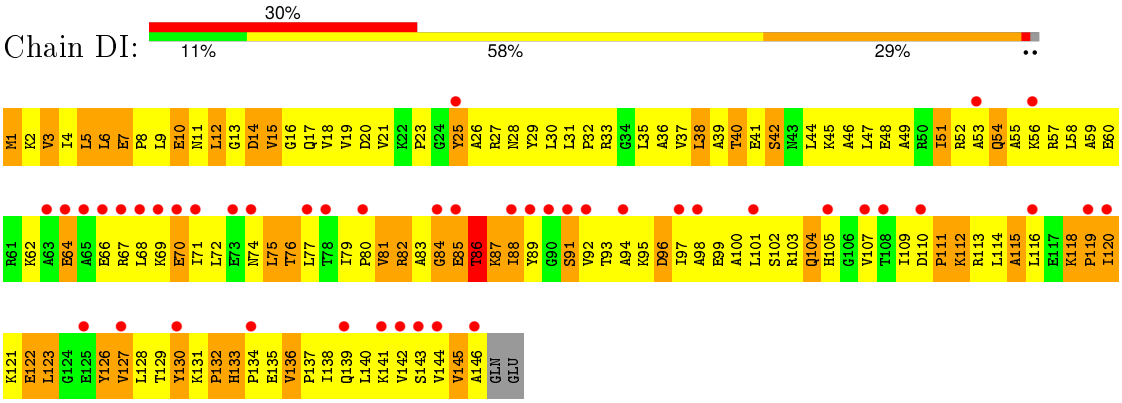
Chain BI:





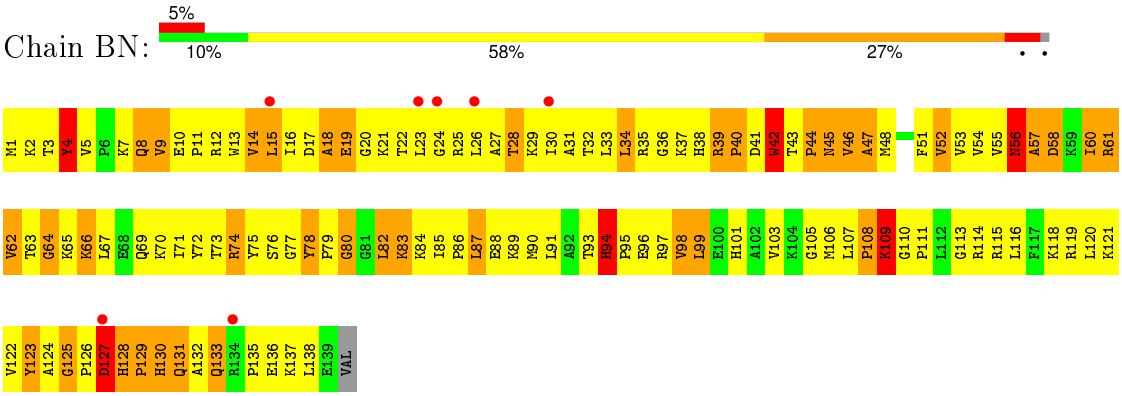
• Molecule 43: 50S RIBOSOMAL PROTEIN L9

Chain DI:



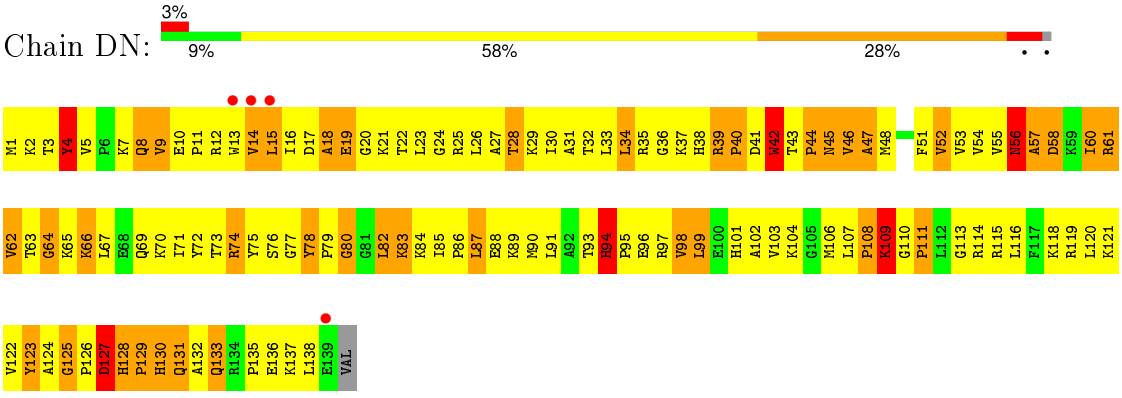
• Molecule 44: 50S RIBOSOMAL PROTEIN L13

Chain BN:



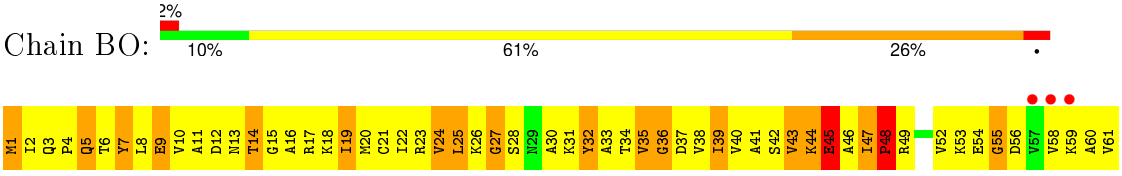
• Molecule 44: 50S RIBOSOMAL PROTEIN L13

Chain DN:



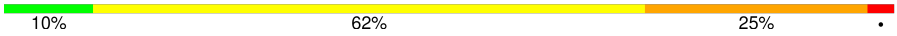
• Molecule 45: 50S RIBOSOMAL PROTEIN L14

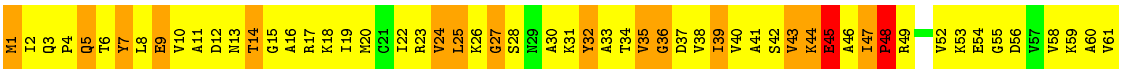
Chain BO:



• Molecule 45: 50S RIBOSOMAL PROTEIN L14

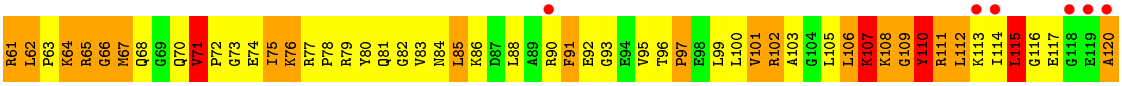
Chain DO:

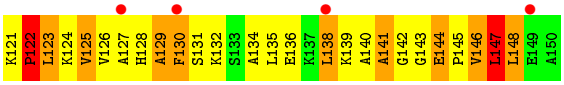




• Molecule 46: 50S RIBOSOMAL PROTEIN L15

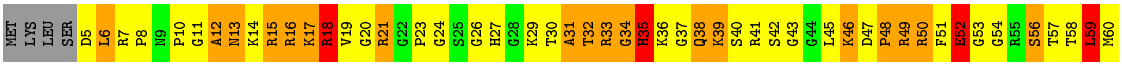
Chain BP:

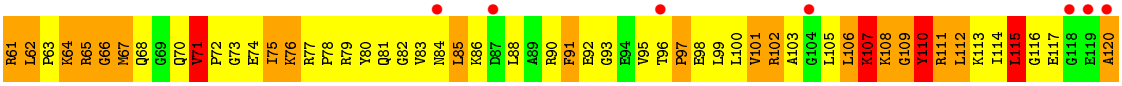


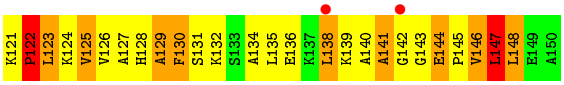


• Molecule 46: 50S RIBOSOMAL PROTEIN L15

Chain DP:

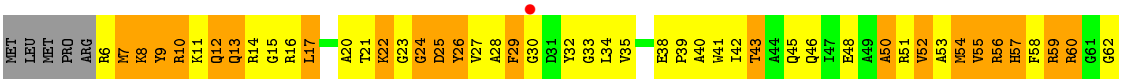


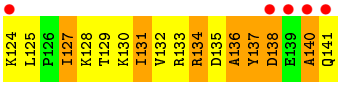




• Molecule 47: 50S RIBOSOMAL PROTEIN L16

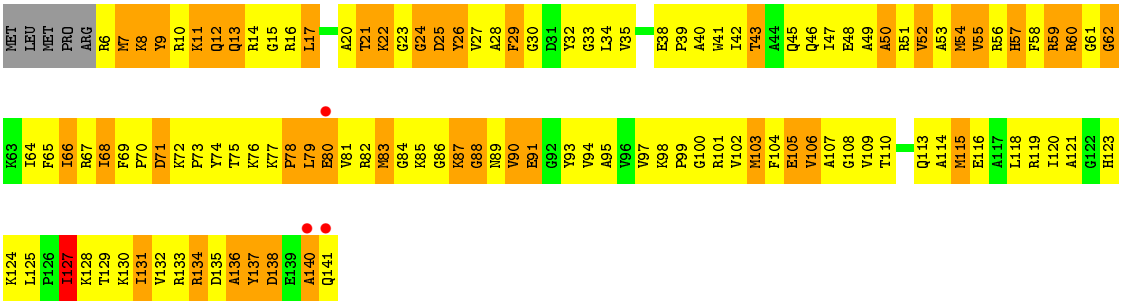
Chain BQ:





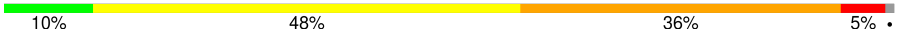
- Molecule 47: 50S RIBOSOMAL PROTEIN L16

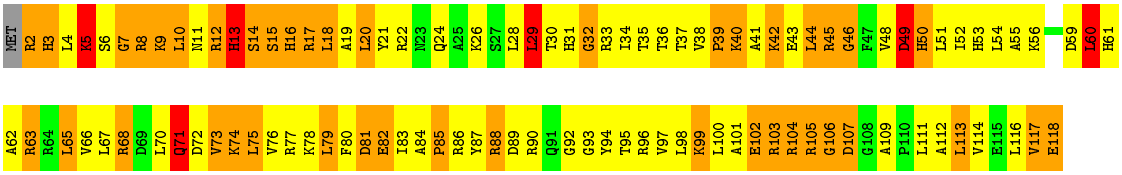
Chain DQ:



- Molecule 48: 50S RIBOSOMAL PROTEIN L17

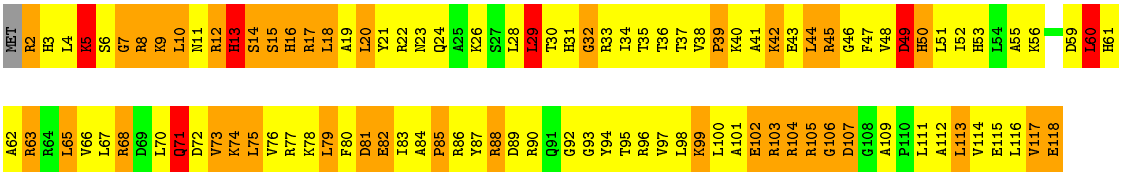
Chain BR:





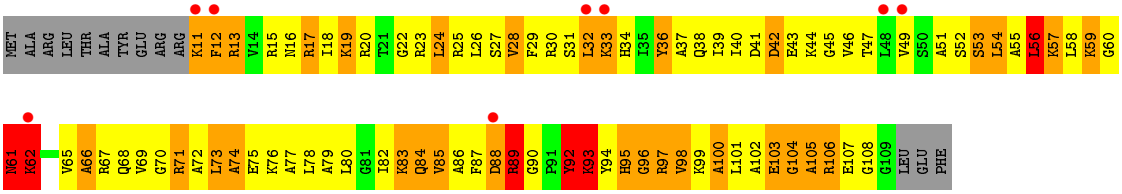
- Molecule 48: 50S RIBOSOMAL PROTEIN L17

Chain DR:



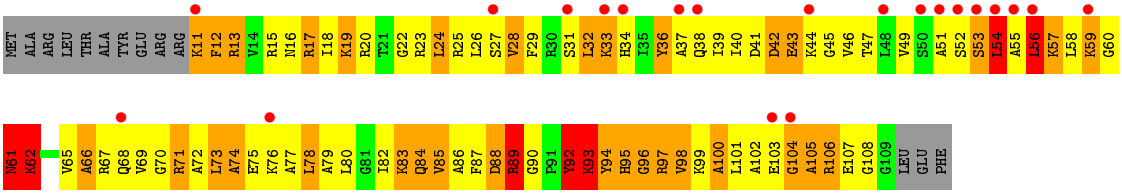
- Molecule 49: 50S RIBOSOMAL PROTEIN L18

Chain BS:



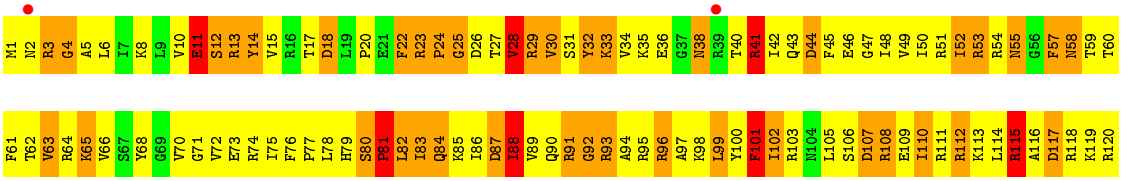
- Molecule 49: 50S RIBOSOMAL PROTEIN L18

Chain DS:



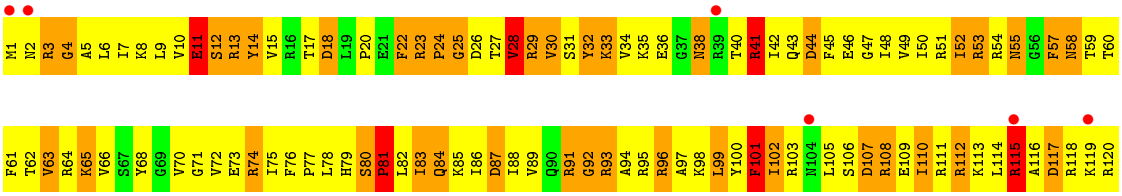
• Molecule 50: 50S RIBOSOMAL PROTEIN L19

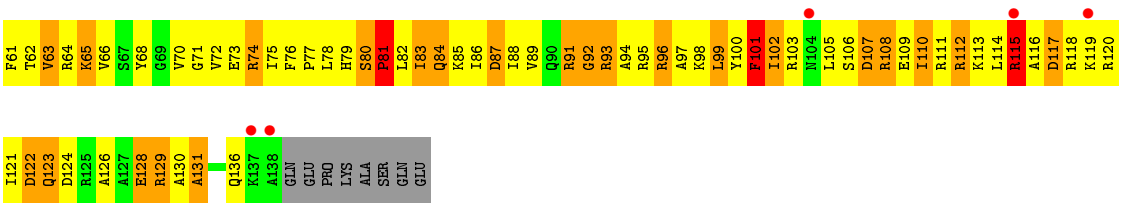
Chain BT:



• Molecule 50: 50S RIBOSOMAL PROTEIN L19

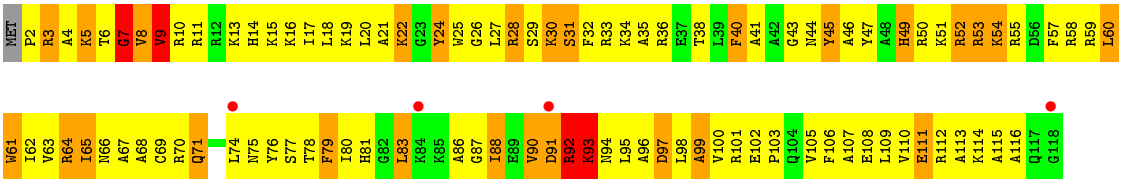
Chain DT:





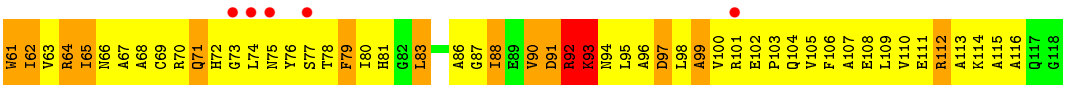
• Molecule 51: 50S RIBOSOMAL PROTEIN L20

Chain BU:



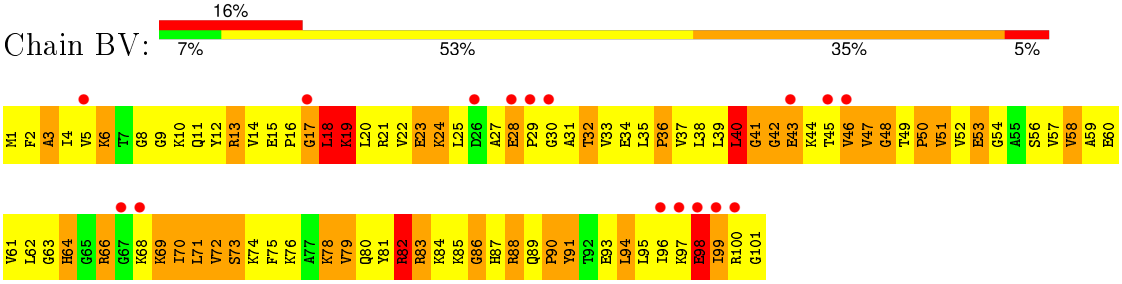
• Molecule 51: 50S RIBOSOMAL PROTEIN L20

Chain DU:



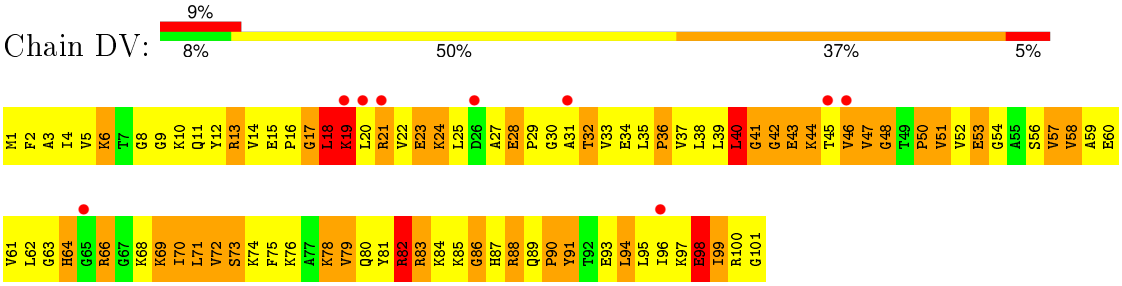
• Molecule 52: 50S RIBOSOMAL PROTEIN L21

Chain BV:



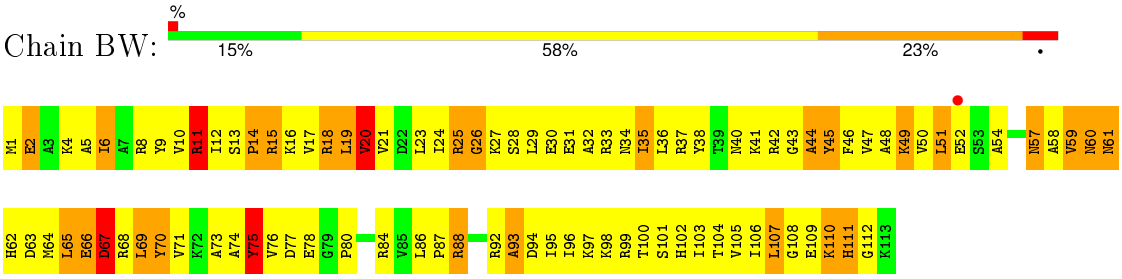
• Molecule 52: 50S RIBOSOMAL PROTEIN L21

Chain DV:



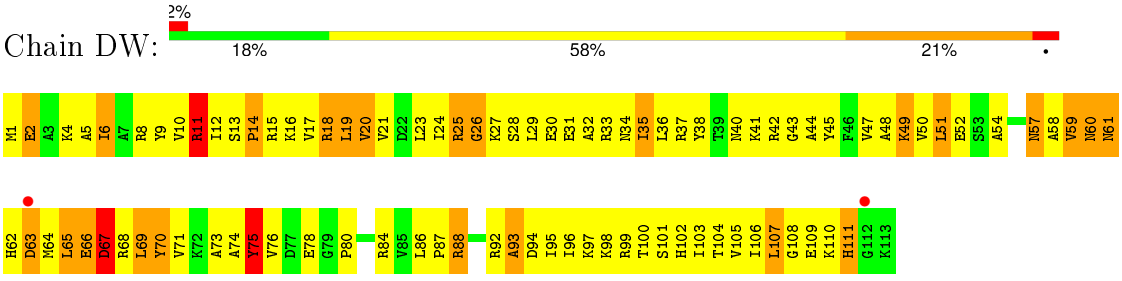
• Molecule 53: 50S RIBOSOMAL PROTEIN L22

Chain BW:



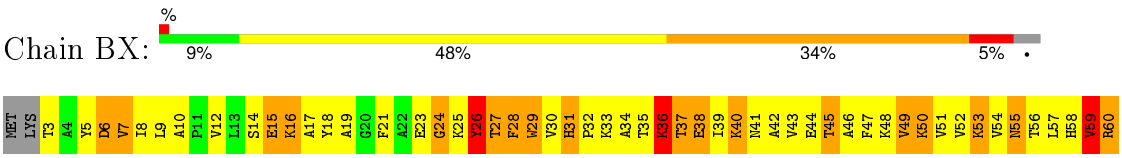
• Molecule 53: 50S RIBOSOMAL PROTEIN L22

Chain DW:



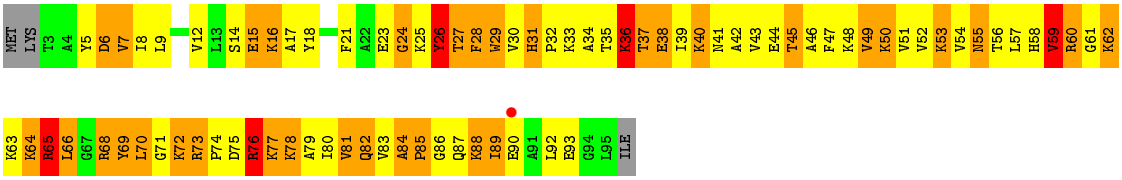
• Molecule 54: 50S RIBOSOMAL PROTEIN L23

Chain BX:



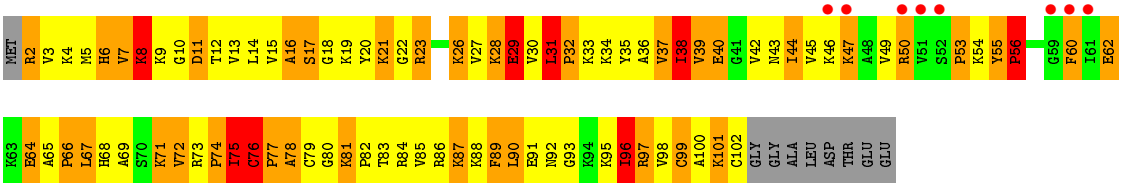
• Molecule 54: 50S RIBOSOMAL PROTEIN L23

Chain DX:



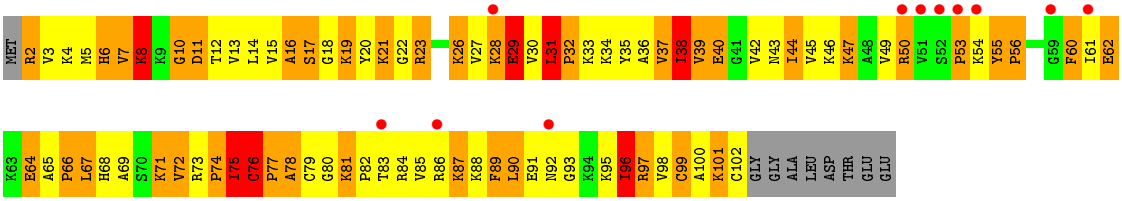
• Molecule 55: 50S RIBOSOMAL PROTEIN L24

Chain BY:



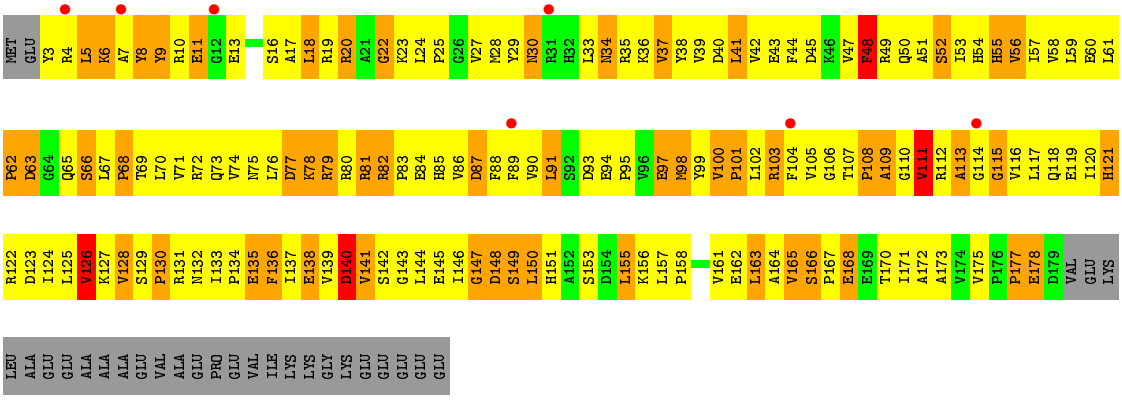
• Molecule 55: 50S RIBOSOMAL PROTEIN L24

Chain DY:



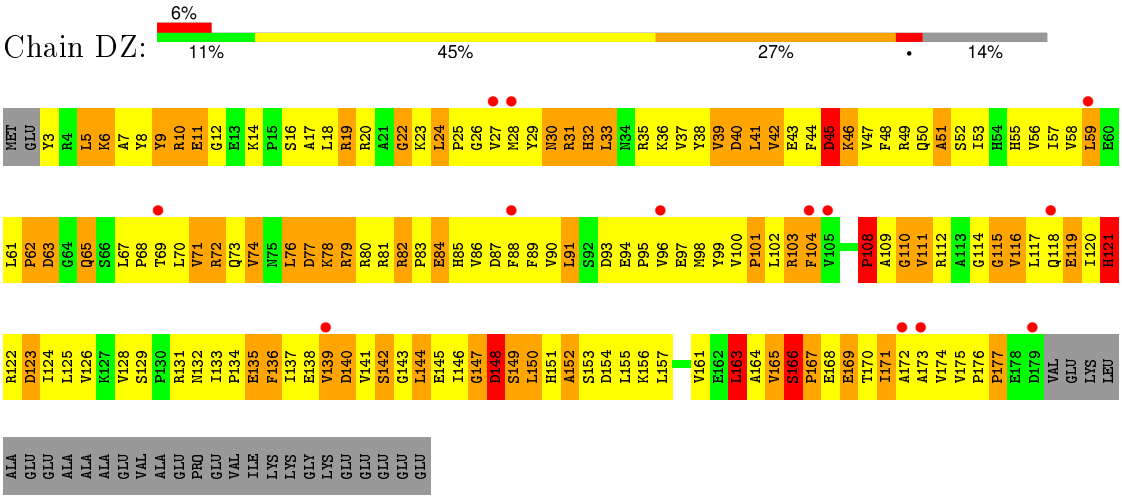
• Molecule 56: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



• Molecule 56: 50S RIBOSOMAL PROTEIN L25

Chain DZ:


6%
11%
45%
27%
14%
MET GLU Y3 R4 L5 K6 A7 Y8 Y9 R10 E11 G12 E13 K14 P15 S16 A17 L18 R19 R20 A21 G22 K23 L24 P25 G26 V27 M28 Y29 N30 R31 H32 L33 N34 R35 K36 V37 Y38 V39 D40 L41 V42 E43 F44 D45 K46 V47 F48 R49 Q50 A51 S52 I53 H54 H55 V56 I57 V58 L59 E60
L61 P62 D63 G64 Q65 S66 L67 P68 T69 L70 V71 R72 Q73 V74 N75 L76 D77 K78 R79 R80 R81 R82 P83 E84 H85 V86 D87 F88 F89 V90 L91 S92 D93 E94 P95 V96 E97 M98 Y99 V100 P101 L102 R103 F104 V105 P108 A109 G110 V111 R112 A113 G114 G115 V116 L117 Q118 E119 I120 H121
R122 D123 I124 L125 V126 K127 V128 S129 P130 R131 N132 I133 P134 E135 F136 I137 E138 V139 D140 V141 S142 G143 L144 E145 I146 G147 D148 S149 L150 H151 A152 S153 D154 L155 K156 L157 V161 E162 L163 A164 V165 S166 P167 E168 E169 T170 I171 A172 A173 V174 V175 P176 P177 E178 D179 VAL GLU LYS LEU
ALA GLU GLU GLU ALA ALA ALA GLU VAL VAL ALA GLU PRO GLU VAL ILE LYS LYS GLY LYS GLU GLU GLU GLU GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	212.41Å 450.11Å 630.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 49.89 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.50) 98.9 (49.89-3.50)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.265 , 0.326 0.266 , 0.327	Depositor DCC
R_{free} test set	33921 reflections (4.80%)	DCC
Wilson B-factor (Å^2)	81.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 93.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Outliers	0 of 744195 reflections	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	290487	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: 5MU, 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	0.49	0/36190	0.72	11/56486 (0.0%)
1	CA	0.49	0/36190	0.72	5/56486 (0.0%)
2	AB	0.37	0/1936	0.65	0/2611
2	CB	0.36	0/1936	0.64	0/2611
3	AC	0.37	0/1637	0.63	0/2207
3	CC	0.35	0/1637	0.63	0/2207
4	AD	0.43	0/1733	0.68	0/2318
4	CD	0.42	0/1733	0.68	0/2318
5	AE	0.41	0/1163	0.68	0/1566
5	CE	0.41	0/1163	0.68	0/1566
6	AF	0.36	0/856	0.67	0/1154
6	CF	0.39	0/856	0.68	0/1154
7	AG	0.35	0/1276	0.63	0/1709
7	CG	0.34	0/1276	0.62	0/1709
8	AH	0.36	0/1136	0.66	0/1527
8	CH	0.37	0/1136	0.67	0/1527
9	AI	0.35	0/1027	0.63	0/1372
9	CI	0.34	0/1027	0.62	0/1372
10	AJ	0.38	0/808	0.66	0/1087
10	CJ	0.37	0/808	0.65	0/1087
11	AK	0.37	0/900	0.66	0/1213
11	CK	0.37	0/900	0.67	0/1213
12	AL	0.44	0/987	0.72	0/1322
12	CL	0.42	0/987	0.72	0/1322
13	AM	0.33	0/994	0.59	0/1322
13	CM	0.32	0/994	0.60	0/1322
14	AN	0.39	0/501	0.68	0/664
14	CN	0.37	0/501	0.67	0/664
15	AO	0.36	0/745	0.64	0/992
15	CO	0.36	0/745	0.63	0/992
16	AP	0.47	0/717	0.74	0/965
16	CP	0.43	0/717	0.73	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.41	0/837	0.71	0/1119
17	CQ	0.40	0/837	0.71	0/1119
18	AR	0.39	0/579	0.72	0/768
18	CR	0.41	0/579	0.73	0/768
19	AS	0.36	0/643	0.61	0/867
19	CS	0.36	0/643	0.60	0/867
20	AT	0.34	0/765	0.69	0/1007
20	CT	0.33	0/765	0.69	0/1007
21	AU	0.44	0/213	0.64	0/279
21	CU	0.42	0/213	0.63	0/279
22	AV	0.66	0/405	0.77	0/630
22	CV	0.61	0/405	0.77	1/630 (0.2%)
23	AW	0.43	0/1810	0.73	0/2821
23	CW	0.46	0/1810	0.72	0/2821
24	AX	0.70	0/256	0.93	0/397
24	CX	0.68	0/256	0.91	0/397
25	AY	0.40	0/1497	0.71	0/2017
25	CY	0.44	0/1497	0.72	0/2017
26	B0	0.39	0/660	0.64	0/882
26	D0	0.40	0/660	0.64	0/882
27	B1	0.57	0/700	1.00	1/931 (0.1%)
27	D1	0.55	0/700	0.96	3/931 (0.3%)
28	B2	0.49	0/423	0.97	2/560 (0.4%)
28	D2	0.52	0/423	0.91	1/560 (0.2%)
29	B3	0.39	0/473	0.68	0/636
29	D3	0.40	0/473	0.68	0/636
30	B4	0.43	0/241	0.80	3/334 (0.9%)
30	D4	0.44	0/241	0.80	4/334 (1.2%)
31	B5	0.37	0/473	0.69	0/639
31	D5	0.38	0/473	0.71	0/639
32	B6	0.45	0/387	0.63	0/517
32	D6	0.42	0/387	0.63	0/517
33	B7	0.53	0/427	0.83	0/563
33	D7	0.53	0/427	0.84	1/563 (0.2%)
34	B8	0.51	0/516	0.89	1/681 (0.1%)
34	D8	0.49	0/516	0.88	1/681 (0.1%)
35	BA	0.57	2/66757 (0.0%)	0.76	19/104221 (0.0%)
35	DA	0.61	3/66757 (0.0%)	0.76	19/104221 (0.0%)
36	BB	0.40	0/2853	0.70	0/4451
36	DB	0.39	0/2853	0.70	0/4451
37	BC	0.36	0/1145	0.68	7/1556 (0.4%)
37	DC	0.36	0/1146	0.68	7/1558 (0.4%)
38	BD	0.47	0/2155	0.84	2/2907 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DD	0.49	0/2155	0.84	2/2907 (0.1%)
39	BE	0.44	0/1597	0.78	1/2155 (0.0%)
39	DE	0.47	0/1597	0.79	1/2155 (0.0%)
40	BF	0.46	1/1659 (0.1%)	0.72	0/2246
40	DF	0.46	1/1659 (0.1%)	0.72	0/2246
41	BG	0.39	0/1498	0.76	2/2013 (0.1%)
41	DG	0.38	0/1498	0.76	0/2013
42	BH	0.37	0/1246	0.72	1/1684 (0.1%)
42	DH	0.40	0/1246	0.73	1/1684 (0.1%)
43	BI	0.39	0/1147	0.72	0/1553
43	DI	0.40	0/1147	0.71	0/1553
44	BN	0.40	0/1132	0.74	0/1527
44	DN	0.45	0/1132	0.75	0/1527
45	BO	0.47	0/943	0.78	0/1269
45	DO	0.49	0/943	0.80	0/1269
46	BP	0.42	0/1131	0.94	5/1504 (0.3%)
46	DP	0.40	0/1131	0.94	5/1504 (0.3%)
47	BQ	0.41	0/1100	0.76	0/1470
47	DQ	0.42	0/1100	0.78	0/1470
48	BR	0.39	0/974	0.75	0/1302
48	DR	0.42	0/974	0.77	0/1302
49	BS	0.42	0/779	0.71	0/1038
49	DS	0.39	0/779	0.70	0/1038
50	BT	0.44	0/1156	0.77	1/1544 (0.1%)
50	DT	0.45	0/1156	0.77	1/1544 (0.1%)
51	BU	0.40	0/975	0.75	1/1297 (0.1%)
51	DU	0.46	0/975	0.77	1/1297 (0.1%)
52	BV	0.41	0/789	0.74	1/1054 (0.1%)
52	DV	0.42	0/789	0.75	1/1054 (0.1%)
53	BW	0.42	0/907	0.67	0/1216
53	DW	0.42	0/907	0.66	0/1216
54	BX	0.47	0/740	0.88	2/995 (0.2%)
54	DX	0.47	0/740	0.89	2/995 (0.2%)
55	BY	0.43	0/789	0.78	0/1053
55	DY	0.44	0/789	0.77	0/1053
56	BZ	0.40	0/1436	0.74	0/1951
56	DZ	0.40	0/1436	0.77	1/1951 (0.1%)
All	All	0.51	7/313639 (0.0%)	0.74	117/468340 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	17
1	CA	0	20
22	CV	0	2
23	AW	0	1
24	AX	0	3
35	BA	1	69
35	DA	1	63
All	All	2	175

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1543	C	N1-C2	5.59	1.45	1.40
40	DF	65	TRP	CB-CG	-5.48	1.40	1.50
35	DA	1543	C	N1-C2	5.43	1.45	1.40
35	DA	652	C	C3'-O3'	5.38	1.49	1.42
35	BA	652	C	C3'-O3'	5.30	1.49	1.42

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	DA	2128	C	C2'-C3'-O3'	10.31	132.19	109.50
35	BA	2128	C	C2'-C3'-O3'	10.29	132.14	109.50
46	BP	52	GLU	N-CA-C	8.91	135.05	111.00
46	DP	52	GLU	N-CA-C	8.80	134.76	111.00
38	BD	238	GLY	N-CA-C	-8.62	91.56	113.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	2128	C	C3'
35	DA	2128	C	C3'

5 of 175 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	21	G	Sidechain
1	AA	265	G	Sidechain
1	AA	323	U	Sidechain
1	AA	445	G	Sidechain
1	AA	96	U	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16313	2049	0
1	CA	32329	0	16314	2039	0
2	AB	1901	0	1951	382	0
2	CB	1901	0	1951	378	0
3	AC	1613	0	1677	256	0
3	CC	1613	0	1677	246	0
4	AD	1703	0	1763	346	0
4	CD	1703	0	1764	336	0
5	AE	1147	0	1207	211	0
5	CE	1147	0	1207	202	0
6	AF	843	0	857	151	0
6	CF	843	0	857	157	0
7	AG	1257	0	1296	235	0
7	CG	1257	0	1296	216	0
8	AH	1116	0	1177	231	0
8	CH	1116	0	1177	233	0
9	AI	1011	0	1041	208	0
9	CI	1011	0	1041	209	0
10	AJ	795	0	840	153	0
10	CJ	795	0	840	154	0
11	AK	885	0	904	179	0
11	CK	885	0	904	180	0
12	AL	971	0	1057	210	0
12	CL	971	0	1057	196	0
13	AM	988	0	1055	163	0
13	CM	988	0	1055	156	0
14	AN	492	0	529	95	0
14	CN	492	0	530	89	0
15	AO	734	0	771	111	0
15	CO	734	0	771	117	0
16	AP	701	0	720	157	0
16	CP	701	0	720	146	0
17	AQ	824	0	891	140	0
17	CQ	824	0	891	138	0
18	AR	574	0	644	138	0
18	CR	574	0	644	133	0
19	AS	630	0	652	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	630	0	652	138	0
20	AT	763	0	861	133	0
20	CT	763	0	861	125	0
21	AU	209	0	221	30	0
21	CU	209	0	221	28	0
22	AV	362	0	186	23	0
22	CV	362	0	186	20	0
23	AW	1641	0	836	105	0
23	CW	1641	0	839	72	0
24	AX	230	0	118	12	0
24	CX	230	0	117	16	0
25	AY	1478	0	1526	283	0
25	CY	1478	0	1526	303	0
26	B0	652	0	658	102	0
26	D0	652	0	658	87	0
27	B1	693	0	764	248	0
27	D1	693	0	763	241	0
28	B2	421	0	461	118	0
28	D2	421	0	461	146	0
29	B3	468	0	523	86	0
29	D3	468	0	523	82	0
30	B4	242	0	103	14	0
30	D4	242	0	103	10	0
31	B5	459	0	480	103	0
31	D5	459	0	480	107	0
32	B6	381	0	390	69	0
32	D6	381	0	390	72	0
33	B7	419	0	467	75	0
33	D7	419	0	467	72	0
34	B8	508	0	576	154	0
34	D8	508	0	576	143	0
35	BA	59601	0	30029	3753	1
35	DA	59601	0	30026	3760	0
36	BB	2551	0	1294	137	1
36	DB	2551	0	1294	155	0
37	BC	1142	0	861	85	0
37	DC	1143	0	865	78	0
38	BD	2105	0	2182	497	0
38	DD	2105	0	2182	503	0
39	BE	1564	0	1629	382	0
39	DE	1564	0	1629	393	0
40	BF	1624	0	1677	349	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DF	1624	0	1676	353	0
41	BG	1474	0	1534	336	0
41	DG	1474	0	1534	441	0
42	BH	1223	0	1282	242	0
42	DH	1223	0	1282	245	0
43	BI	1132	0	1218	227	0
43	DI	1132	0	1218	225	0
44	BN	1105	0	1180	277	0
44	DN	1105	0	1180	291	0
45	BO	933	0	996	234	0
45	DO	933	0	996	237	0
46	BP	1114	0	1187	382	0
46	DP	1114	0	1187	378	0
47	BQ	1080	0	1127	274	0
47	DQ	1080	0	1127	259	0
48	BR	960	0	1021	221	0
48	DR	960	0	1021	220	0
49	BS	771	0	832	201	0
49	DS	771	0	832	207	0
50	BT	1142	0	1202	320	0
50	DT	1142	0	1202	325	0
51	BU	958	0	1014	245	0
51	DU	958	0	1014	256	0
52	BV	779	0	851	231	0
52	DV	779	0	851	234	0
53	BW	896	0	953	174	0
53	DW	896	0	953	164	0
54	BX	726	0	778	251	0
54	DX	726	0	777	252	0
55	BY	776	0	870	205	0
55	DY	776	0	870	208	0
56	BZ	1404	0	1432	353	0
56	DZ	1404	0	1432	318	0
57	AA	204	0	0	0	0
57	AD	2	0	0	0	0
57	AE	2	0	0	0	0
57	AG	1	0	0	0	0
57	AK	1	0	0	0	0
57	AL	2	0	0	0	0
57	AM	1	0	0	0	0
57	AV	4	0	0	0	0
57	AW	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AX	5	0	0	0	0
57	B1	4	0	0	0	0
57	B2	2	0	0	0	0
57	B3	1	0	0	0	0
57	B5	2	0	0	0	0
57	B7	1	0	0	0	0
57	BA	445	0	0	1	0
57	BB	20	0	0	0	0
57	BD	3	0	0	0	0
57	BE	1	0	0	0	0
57	BF	4	0	0	0	0
57	BG	1	0	0	0	0
57	BN	4	0	0	0	0
57	BO	1	0	0	0	0
57	BP	3	0	0	0	0
57	BU	2	0	0	1	0
57	BX	2	0	0	0	0
57	CA	208	0	0	0	0
57	CE	3	0	0	0	0
57	CG	1	0	0	0	0
57	CL	2	0	0	0	0
57	CN	1	0	0	0	0
57	CV	4	0	0	0	0
57	CW	23	0	0	0	0
57	CX	4	0	0	0	0
57	D1	4	0	0	0	0
57	D2	2	0	0	0	0
57	D3	1	0	0	0	0
57	D5	1	0	0	0	0
57	D7	1	0	0	0	0
57	DA	441	0	0	0	0
57	DB	19	0	0	0	0
57	DD	3	0	0	0	0
57	DE	2	0	0	0	0
57	DF	5	0	0	0	0
57	DG	1	0	0	0	0
57	DH	1	0	0	0	0
57	DN	2	0	0	0	0
57	DP	4	0	0	0	0
57	DS	1	0	0	0	0
57	DU	3	0	0	0	0
57	DV	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DX	3	0	0	0	0
58	AD	1	0	0	0	0
58	AN	1	0	0	0	0
58	CD	1	0	0	0	0
58	CN	1	0	0	0	0
All	All	290487	0	197331	30328	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 62.

The worst 5 of 30328 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)
53:BW:29:LEU:HD21	53:BW:33:ARG:HE	1.07	1.20
55:DY:45:VAL:HA	55:DY:62:GLU:HG2	1.20	1.20
35:DA:2758:A:H2'	35:DA:2759:G:H5"	1.25	1.19
1:CA:1442(A):G:H3'	1:CA:1442(B):A:H5"	1.22	1.18
43:BI:91:SER:HB2	43:BI:119:PRO:HB2	1.21	1.18

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)
35:BA:1593:G:O2'	36:BB:54:G:OP1[1_655]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	233/256 (91%)	114 (49%)	69 (30%)	50 (22%)	0 1
2	CB	233/256 (91%)	114 (49%)	68 (29%)	51 (22%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	AC	205/239 (86%)	119 (58%)	50 (24%)	36 (18%)	0 2
3	CC	205/239 (86%)	121 (59%)	47 (23%)	37 (18%)	0 2
4	AD	206/209 (99%)	101 (49%)	62 (30%)	43 (21%)	0 1
4	CD	206/209 (99%)	101 (49%)	61 (30%)	44 (21%)	0 1
5	AE	149/162 (92%)	85 (57%)	44 (30%)	20 (13%)	0 5
5	CE	149/162 (92%)	84 (56%)	45 (30%)	20 (13%)	0 5
6	AF	99/101 (98%)	61 (62%)	23 (23%)	15 (15%)	0 3
6	CF	99/101 (98%)	60 (61%)	24 (24%)	15 (15%)	0 3
7	AG	153/156 (98%)	97 (63%)	31 (20%)	25 (16%)	0 3
7	CG	153/156 (98%)	97 (63%)	31 (20%)	25 (16%)	0 3
8	AH	136/138 (99%)	78 (57%)	39 (29%)	19 (14%)	0 4
8	CH	136/138 (99%)	79 (58%)	37 (27%)	20 (15%)	0 4
9	AI	121/128 (94%)	80 (66%)	27 (22%)	14 (12%)	0 7
9	CI	121/128 (94%)	79 (65%)	27 (22%)	15 (12%)	0 6
10	AJ	97/105 (92%)	64 (66%)	23 (24%)	10 (10%)	1 9
10	CJ	97/105 (92%)	64 (66%)	22 (23%)	11 (11%)	0 7
11	AK	117/129 (91%)	69 (59%)	31 (26%)	17 (14%)	0 4
11	CK	117/129 (91%)	68 (58%)	32 (27%)	17 (14%)	0 4
12	AL	123/135 (91%)	78 (63%)	28 (23%)	17 (14%)	0 4
12	CL	123/135 (91%)	77 (63%)	27 (22%)	19 (15%)	0 3
13	AM	113/126 (90%)	59 (52%)	35 (31%)	19 (17%)	0 3
13	CM	113/126 (90%)	60 (53%)	34 (30%)	19 (17%)	0 3
14	AN	58/61 (95%)	38 (66%)	12 (21%)	8 (14%)	0 4
14	CN	58/61 (95%)	38 (66%)	12 (21%)	8 (14%)	0 4
15	AO	86/89 (97%)	48 (56%)	26 (30%)	12 (14%)	0 4
15	CO	86/89 (97%)	49 (57%)	26 (30%)	11 (13%)	0 5
16	AP	82/88 (93%)	45 (55%)	24 (29%)	13 (16%)	0 3
16	CP	82/88 (93%)	45 (55%)	24 (29%)	13 (16%)	0 3
17	AQ	98/105 (93%)	66 (67%)	19 (19%)	13 (13%)	0 5
17	CQ	98/105 (93%)	65 (66%)	20 (20%)	13 (13%)	0 5
18	AR	68/88 (77%)	38 (56%)	18 (26%)	12 (18%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	CR	68/88 (77%)	37 (54%)	20 (29%)	11 (16%)	0 3
19	AS	77/93 (83%)	49 (64%)	19 (25%)	9 (12%)	0 7
19	CS	77/93 (83%)	49 (64%)	19 (25%)	9 (12%)	0 7
20	AT	97/106 (92%)	46 (47%)	29 (30%)	22 (23%)	0 1
20	CT	97/106 (92%)	46 (47%)	30 (31%)	21 (22%)	0 1
21	AU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1 12
21	CU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1 12
25	AY	183/185 (99%)	115 (63%)	44 (24%)	24 (13%)	0 5
25	CY	183/185 (99%)	81 (44%)	54 (30%)	48 (26%)	0 1
26	B0	83/85 (98%)	61 (74%)	13 (16%)	9 (11%)	0 8
26	D0	83/85 (98%)	59 (71%)	15 (18%)	9 (11%)	0 8
27	B1	87/98 (89%)	34 (39%)	22 (25%)	31 (36%)	0 0
27	D1	87/98 (89%)	41 (47%)	22 (25%)	24 (28%)	0 0
28	B2	49/72 (68%)	14 (29%)	21 (43%)	14 (29%)	0 0
28	D2	49/72 (68%)	16 (33%)	20 (41%)	13 (26%)	0 0
29	B3	58/60 (97%)	34 (59%)	15 (26%)	9 (16%)	0 3
29	D3	58/60 (97%)	34 (59%)	15 (26%)	9 (16%)	0 3
30	B4	48/71 (68%)	8 (17%)	23 (48%)	17 (35%)	0 0
30	D4	48/71 (68%)	8 (17%)	22 (46%)	18 (38%)	0 0
31	B5	57/60 (95%)	28 (49%)	14 (25%)	15 (26%)	0 1
31	D5	57/60 (95%)	28 (49%)	12 (21%)	17 (30%)	0 0
32	B6	41/54 (76%)	21 (51%)	11 (27%)	9 (22%)	0 1
32	D6	41/54 (76%)	21 (51%)	11 (27%)	9 (22%)	0 1
33	B7	47/49 (96%)	29 (62%)	9 (19%)	9 (19%)	0 2
33	D7	47/49 (96%)	29 (62%)	10 (21%)	8 (17%)	0 3
34	B8	62/65 (95%)	25 (40%)	22 (36%)	15 (24%)	0 1
34	D8	62/65 (95%)	26 (42%)	21 (34%)	15 (24%)	0 1
37	BC	183/229 (80%)	79 (43%)	49 (27%)	55 (30%)	0 0
37	DC	183/229 (80%)	79 (43%)	49 (27%)	55 (30%)	0 0
38	BD	270/276 (98%)	158 (58%)	62 (23%)	50 (18%)	0 2
38	DD	270/276 (98%)	159 (59%)	62 (23%)	49 (18%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
39	BE	203/206 (98%)	110 (54%)	46 (23%)	47 (23%)	0 1
39	DE	203/206 (98%)	111 (55%)	44 (22%)	48 (24%)	0 1
40	BF	206/210 (98%)	109 (53%)	53 (26%)	44 (21%)	0 1
40	DF	206/210 (98%)	108 (52%)	53 (26%)	45 (22%)	0 1
41	BG	177/182 (97%)	89 (50%)	48 (27%)	40 (23%)	0 1
41	DG	177/182 (97%)	89 (50%)	41 (23%)	47 (27%)	0 0
42	BH	158/180 (88%)	78 (49%)	44 (28%)	36 (23%)	0 1
42	DH	158/180 (88%)	80 (51%)	44 (28%)	34 (22%)	0 1
43	BI	144/148 (97%)	80 (56%)	36 (25%)	28 (19%)	0 2
43	DI	144/148 (97%)	80 (56%)	37 (26%)	27 (19%)	0 2
44	BN	137/140 (98%)	64 (47%)	40 (29%)	33 (24%)	0 1
44	DN	137/140 (98%)	65 (47%)	39 (28%)	33 (24%)	0 1
45	BO	120/122 (98%)	73 (61%)	24 (20%)	23 (19%)	0 2
45	DO	120/122 (98%)	74 (62%)	24 (20%)	22 (18%)	0 2
46	BP	144/150 (96%)	77 (54%)	27 (19%)	40 (28%)	0 0
46	DP	144/150 (96%)	75 (52%)	29 (20%)	40 (28%)	0 0
47	BQ	134/141 (95%)	70 (52%)	37 (28%)	27 (20%)	0 1
47	DQ	134/141 (95%)	72 (54%)	35 (26%)	27 (20%)	0 1
48	BR	115/118 (98%)	54 (47%)	26 (23%)	35 (30%)	0 0
48	DR	115/118 (98%)	53 (46%)	29 (25%)	33 (29%)	0 0
49	BS	97/112 (87%)	34 (35%)	27 (28%)	36 (37%)	0 0
49	DS	97/112 (87%)	34 (35%)	28 (29%)	35 (36%)	0 0
50	BT	136/146 (93%)	79 (58%)	26 (19%)	31 (23%)	0 1
50	DT	136/146 (93%)	78 (57%)	29 (21%)	29 (21%)	0 1
51	BU	115/118 (98%)	50 (44%)	39 (34%)	26 (23%)	0 1
51	DU	115/118 (98%)	51 (44%)	38 (33%)	26 (23%)	0 1
52	BV	97/101 (96%)	39 (40%)	21 (22%)	37 (38%)	0 0
52	DV	97/101 (96%)	39 (40%)	22 (23%)	36 (37%)	0 0
53	BW	111/113 (98%)	62 (56%)	27 (24%)	22 (20%)	0 2
53	DW	111/113 (98%)	60 (54%)	34 (31%)	17 (15%)	0 3
54	BX	91/96 (95%)	39 (43%)	24 (26%)	28 (31%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
54	DX	91/96 (95%)	38 (42%)	25 (28%)	28 (31%)	0 0
55	BY	99/110 (90%)	36 (36%)	29 (29%)	34 (34%)	0 0
55	DY	99/110 (90%)	38 (38%)	25 (25%)	36 (36%)	0 0
56	BZ	175/206 (85%)	87 (50%)	41 (23%)	47 (27%)	0 0
56	DZ	175/206 (85%)	92 (53%)	46 (26%)	37 (21%)	0 1
All	All	11936/12888 (93%)	6356 (53%)	3078 (26%)	2502 (21%)	0 1

5 of 2502 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	20	GLU
2	AB	22	LYS
2	AB	29	ALA
2	AB	30	ARG
2	AB	37	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	202/220 (92%)	177 (88%)	25 (12%)	6 29
2	CB	202/220 (92%)	177 (88%)	25 (12%)	6 29
3	AC	160/188 (85%)	142 (89%)	18 (11%)	7 34
3	CC	160/188 (85%)	142 (89%)	18 (11%)	7 34
4	AD	180/181 (99%)	155 (86%)	25 (14%)	4 25
4	CD	180/181 (99%)	156 (87%)	24 (13%)	5 26
5	AE	115/123 (94%)	99 (86%)	16 (14%)	4 25
5	CE	115/123 (94%)	99 (86%)	16 (14%)	4 25
6	AF	90/90 (100%)	86 (96%)	4 (4%)	35 73
6	CF	90/90 (100%)	86 (96%)	4 (4%)	35 73
7	AG	126/127 (99%)	118 (94%)	8 (6%)	22 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	CG	126/127 (99%)	116 (92%)	10 (8%)	15 53
8	AH	119/119 (100%)	108 (91%)	11 (9%)	11 45
8	CH	119/119 (100%)	108 (91%)	11 (9%)	11 45
9	AI	98/99 (99%)	83 (85%)	15 (15%)	3 21
9	CI	98/99 (99%)	85 (87%)	13 (13%)	5 26
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	15 52
10	CJ	88/92 (96%)	81 (92%)	7 (8%)	15 52
11	AK	90/99 (91%)	80 (89%)	10 (11%)	8 35
11	CK	90/99 (91%)	81 (90%)	9 (10%)	9 41
12	AL	104/111 (94%)	91 (88%)	13 (12%)	6 29
12	CL	104/111 (94%)	93 (89%)	11 (11%)	8 38
13	AM	99/101 (98%)	92 (93%)	7 (7%)	18 58
13	CM	99/101 (98%)	92 (93%)	7 (7%)	18 58
14	AN	49/50 (98%)	45 (92%)	4 (8%)	14 51
14	CN	49/50 (98%)	45 (92%)	4 (8%)	14 51
15	AO	79/80 (99%)	71 (90%)	8 (10%)	9 40
15	CO	79/80 (99%)	70 (89%)	9 (11%)	7 33
16	AP	72/74 (97%)	61 (85%)	11 (15%)	3 21
16	CP	72/74 (97%)	61 (85%)	11 (15%)	3 21
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	22 62
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	22 62
18	AR	61/77 (79%)	56 (92%)	5 (8%)	14 51
18	CR	61/77 (79%)	55 (90%)	6 (10%)	10 42
19	AS	69/80 (86%)	57 (83%)	12 (17%)	2 14
19	CS	69/80 (86%)	56 (81%)	13 (19%)	2 11
20	AT	76/82 (93%)	65 (86%)	11 (14%)	4 23
20	CT	76/82 (93%)	65 (86%)	11 (14%)	4 23
21	AU	19/22 (86%)	18 (95%)	1 (5%)	28 67
21	CU	19/22 (86%)	18 (95%)	1 (5%)	28 67
25	AY	157/157 (100%)	135 (86%)	22 (14%)	4 24
25	CY	157/157 (100%)	142 (90%)	15 (10%)	10 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	B0	61/67 (91%)	57 (93%)	4 (7%)	21 61
26	D0	61/67 (91%)	57 (93%)	4 (7%)	21 61
27	B1	73/83 (88%)	54 (74%)	19 (26%)	0 4
27	D1	73/83 (88%)	50 (68%)	23 (32%)	0 3
28	B2	46/67 (69%)	31 (67%)	15 (33%)	0 2
28	D2	46/67 (69%)	34 (74%)	12 (26%)	0 4
29	B3	51/52 (98%)	48 (94%)	3 (6%)	24 65
29	D3	51/52 (98%)	48 (94%)	3 (6%)	24 65
31	B5	51/52 (98%)	42 (82%)	9 (18%)	2 13
31	D5	51/52 (98%)	43 (84%)	8 (16%)	3 19
32	B6	43/52 (83%)	34 (79%)	9 (21%)	1 8
32	D6	43/52 (83%)	34 (79%)	9 (21%)	1 8
33	B7	41/42 (98%)	34 (83%)	7 (17%)	2 15
33	D7	41/42 (98%)	34 (83%)	7 (17%)	2 15
34	B8	53/55 (96%)	45 (85%)	8 (15%)	3 21
34	D8	53/55 (96%)	45 (85%)	8 (15%)	3 21
37	BC	61/181 (34%)	56 (92%)	5 (8%)	14 51
37	DC	61/181 (34%)	57 (93%)	4 (7%)	21 61
38	BD	213/218 (98%)	186 (87%)	27 (13%)	5 28
38	DD	213/218 (98%)	186 (87%)	27 (13%)	5 28
39	BE	165/166 (99%)	142 (86%)	23 (14%)	4 25
39	DE	165/166 (99%)	141 (86%)	24 (14%)	4 23
40	BF	165/166 (99%)	142 (86%)	23 (14%)	4 25
40	DF	165/166 (99%)	142 (86%)	23 (14%)	4 25
41	BG	155/156 (99%)	137 (88%)	18 (12%)	7 33
41	DG	155/156 (99%)	127 (82%)	28 (18%)	2 12
42	BH	132/148 (89%)	115 (87%)	17 (13%)	5 27
42	DH	132/148 (89%)	116 (88%)	16 (12%)	6 30
43	BI	122/124 (98%)	103 (84%)	19 (16%)	3 20
43	DI	122/124 (98%)	103 (84%)	19 (16%)	3 20
44	BN	117/119 (98%)	100 (86%)	17 (14%)	4 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	DN	117/119 (98%)	99 (85%)	18 (15%)	3 20
45	BO	100/100 (100%)	80 (80%)	20 (20%)	1 9
45	DO	100/100 (100%)	79 (79%)	21 (21%)	1 8
46	BP	112/116 (97%)	84 (75%)	28 (25%)	1 4
46	DP	112/116 (97%)	84 (75%)	28 (25%)	1 4
47	BQ	106/111 (96%)	86 (81%)	20 (19%)	2 10
47	DQ	106/111 (96%)	88 (83%)	18 (17%)	2 15
48	BR	100/101 (99%)	80 (80%)	20 (20%)	1 9
48	DR	100/101 (99%)	80 (80%)	20 (20%)	1 9
49	BS	77/88 (88%)	63 (82%)	14 (18%)	2 12
49	DS	77/88 (88%)	62 (80%)	15 (20%)	2 10
50	BT	120/127 (94%)	89 (74%)	31 (26%)	0 4
50	DT	120/127 (94%)	89 (74%)	31 (26%)	0 4
51	BU	92/94 (98%)	80 (87%)	12 (13%)	5 27
51	DU	92/94 (98%)	81 (88%)	11 (12%)	6 30
52	BV	82/82 (100%)	68 (83%)	14 (17%)	2 15
52	DV	82/82 (100%)	68 (83%)	14 (17%)	2 15
53	BW	91/92 (99%)	78 (86%)	13 (14%)	4 24
53	DW	91/92 (99%)	78 (86%)	13 (14%)	4 24
54	BX	74/78 (95%)	59 (80%)	15 (20%)	1 9
54	DX	74/78 (95%)	58 (78%)	16 (22%)	1 7
55	BY	84/91 (92%)	63 (75%)	21 (25%)	1 4
55	DY	84/91 (92%)	63 (75%)	21 (25%)	1 4
56	BZ	155/179 (87%)	134 (86%)	21 (14%)	5 26
56	DZ	155/179 (87%)	124 (80%)	31 (20%)	1 9
All	All	9778/10552 (93%)	8384 (86%)	1394 (14%)	4 24

5 of 1394 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	BW	70	TYR
7	CG	54	THR
51	DU	3	ARG

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Mol	Chain	Res	Type
55	BY	2	ARG
2	CB	115	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 303 such sidechains are listed below:

Mol	Chain	Res	Type
50	BT	123	GLN
4	CD	201	GLN
49	DS	16	ASN
51	BU	94	ASN
2	CB	37	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	210 (13%)	31 (2%)
1	CA	1503/1522 (98%)	214 (14%)	29 (1%)
22	AV	16/76 (21%)	0	0
22	CV	16/76 (21%)	0	0
23	AW	76/77 (98%)	26 (34%)	0
23	CW	76/77 (98%)	20 (26%)	0
24	AX	10/31 (32%)	3 (30%)	0
24	CX	10/31 (32%)	2 (20%)	0
35	BA	2766/2782 (99%)	577 (20%)	57 (2%)
35	DA	2766/2782 (99%)	580 (20%)	57 (2%)
36	BB	118/122 (96%)	19 (16%)	1 (0%)
36	DB	118/122 (96%)	19 (16%)	1 (0%)
All	All	8978/9220 (97%)	1670 (18%)	176 (1%)

5 of 1670 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 176 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2225	A
1	CA	366	C
35	DA	1992	G
35	BA	2290	G
1	CA	30	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	5MU	AW	55	23	12,22,23	1.36	3 (25%)	14,32,35	4.56	3 (21%)
23	5MU	CW	55	23	12,22,23	1.39	3 (25%)	14,32,35	4.50	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	AW	55	23	-	0/3/25/26	0/2/2/2
23	5MU	CW	55	23	-	0/3/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CW	55	5MU	C6-C5	-2.18	1.34	1.40
23	AW	55	5MU	C6-C5	-2.05	1.34	1.40
23	CW	55	5MU	C6-N1	2.42	1.38	1.35
23	AW	55	5MU	C6-N1	2.46	1.38	1.35
23	AW	55	5MU	C4-N3	3.16	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	55	5MU	C5-C4-N3	-9.04	115.07	125.14
23	CW	55	5MU	C5-C4-N3	-8.87	115.26	125.14
23	AW	55	5MU	C5M-C5-C6	2.06	122.77	118.62
23	CW	55	5MU	C5M-C5-C6	2.08	122.80	118.62
23	CW	55	5MU	C4-N3-C2	14.02	127.36	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	55	5MU	1	0
23	CW	55	5MU	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1486 ligands modelled in this entry, 1486 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	AI	2
9	CI	2
52	DV	1
41	DG	1
41	BG	1
52	BV	1
32	D6	1
32	B6	1

The worst 5 of 20 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	46:HIS	C	47:THR	N	6.15
1	D6	46:HIS	C	47:THR	N	6.12
1	CI	53:VAL	C	54:ASP	N	5.30
1	AI	53:VAL	C	54:ASP	N	5.29
1	DG	112:PRO	C	113:ARG	N	4.36

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	1504/1522 (98%)	0.68	162 (10%) 8 7	15, 82, 177, 200	0
1	CA	1504/1522 (98%)	0.84	195 (12%) 5 5	20, 90, 190, 200	0
2	AB	235/256 (91%)	0.24	22 (9%) 11 10	19, 113, 188, 200	0
2	CB	235/256 (91%)	0.25	21 (8%) 12 10	26, 127, 188, 200	0
3	AC	207/239 (86%)	0.14	15 (7%) 18 15	11, 98, 175, 200	0
3	CC	207/239 (86%)	0.30	17 (8%) 14 12	38, 121, 183, 200	0
4	AD	208/209 (99%)	-0.20	4 (1%) 70 60	13, 75, 145, 200	0
4	CD	208/209 (99%)	-0.20	2 (0%) 84 76	25, 89, 155, 200	0
5	AE	151/162 (93%)	-0.20	4 (2%) 59 49	21, 73, 158, 190	0
5	CE	151/162 (93%)	0.14	6 (3%) 42 33	26, 89, 157, 200	0
6	AF	101/101 (100%)	-0.11	2 (1%) 68 59	19, 100, 151, 189	0
6	CF	101/101 (100%)	-0.21	0 100 100	16, 83, 141, 170	0
7	AG	155/156 (99%)	0.18	15 (9%) 10 9	34, 104, 175, 194	0
7	CG	155/156 (99%)	0.33	18 (11%) 6 6	53, 123, 185, 200	0
8	AH	138/138 (100%)	-0.28	1 (0%) 89 82	33, 81, 145, 190	0
8	CH	138/138 (100%)	-0.34	1 (0%) 89 82	30, 91, 147, 165	0
9	AI	127/128 (99%)	0.03	4 (3%) 52 43	27, 123, 180, 200	0
9	CI	127/128 (99%)	0.84	28 (22%) 1 1	43, 140, 195, 200	0
10	AJ	99/105 (94%)	0.25	4 (4%) 42 33	47, 120, 180, 200	0
10	CJ	99/105 (94%)	1.03	17 (17%) 2 2	65, 140, 189, 200	0
11	AK	119/129 (92%)	0.30	13 (10%) 7 7	13, 78, 163, 187	0
11	CK	119/129 (92%)	0.33	9 (7%) 17 14	30, 86, 164, 200	0
12	AL	125/135 (92%)	-0.33	1 (0%) 87 80	19, 71, 146, 200	0
12	CL	125/135 (92%)	-0.24	1 (0%) 87 80	12, 75, 143, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	125/126 (99%)	0.56	20 (16%) 3 3	56, 124, 183, 200	0
13	CM	125/126 (99%)	0.34	13 (10%) 8 8	41, 140, 199, 200	0
14	AN	60/61 (98%)	-0.09	2 (3%) 50 41	38, 94, 181, 200	0
14	CN	60/61 (98%)	0.09	1 (1%) 73 64	57, 117, 171, 189	0
15	AO	88/89 (98%)	-0.33	1 (1%) 82 73	11, 84, 147, 172	0
15	CO	88/89 (98%)	-0.14	4 (4%) 37 29	18, 88, 146, 167	0
16	AP	84/88 (95%)	-0.19	2 (2%) 62 52	17, 64, 135, 200	0
16	CP	84/88 (95%)	0.24	7 (8%) 14 12	32, 90, 139, 199	0
17	AQ	100/105 (95%)	0.13	11 (11%) 7 7	15, 81, 143, 200	0
17	CQ	100/105 (95%)	0.25	14 (14%) 4 4	20, 84, 134, 200	0
18	AR	70/88 (79%)	0.12	2 (2%) 55 45	33, 87, 156, 200	0
18	CR	70/88 (79%)	0.03	4 (5%) 27 21	17, 79, 137, 170	0
19	AS	79/93 (84%)	0.17	3 (3%) 44 36	60, 134, 200, 200	0
19	CS	79/93 (84%)	0.49	11 (13%) 4 4	76, 140, 200, 200	0
20	AT	99/106 (93%)	0.14	7 (7%) 19 15	21, 91, 178, 200	0
20	CT	99/106 (93%)	0.01	7 (7%) 19 15	45, 102, 167, 197	0
21	AU	25/27 (92%)	0.08	0 100 100	59, 114, 161, 200	0
21	CU	25/27 (92%)	0.98	5 (20%) 1 2	58, 131, 182, 200	0
22	AV	17/76 (22%)	0.70	2 (11%) 6 6	55, 68, 122, 125	0
22	CV	17/76 (22%)	0.36	1 (5%) 26 20	56, 73, 128, 131	0
23	AW	76/77 (98%)	3.51	45 (59%) 0 0	63, 179, 200, 200	0
23	CW	76/77 (98%)	4.90	61 (80%) 0 0	62, 191, 200, 200	0
24	AX	11/31 (35%)	-0.00	0 100 100	23, 72, 120, 172	0
24	CX	11/31 (35%)	-0.01	0 100 100	41, 63, 93, 196	0
25	AY	185/185 (100%)	0.63	31 (16%) 2 2	27, 99, 167, 200	0
25	CY	185/185 (100%)	0.42	28 (15%) 3 3	9, 93, 166, 198	0
26	B0	85/85 (100%)	0.61	11 (12%) 5 5	21, 80, 184, 199	0
26	D0	85/85 (100%)	0.66	11 (12%) 5 5	39, 95, 174, 200	0
27	B1	89/98 (90%)	-0.27	2 (2%) 65 55	5, 64, 138, 193	0
27	D1	89/98 (90%)	-0.46	2 (2%) 65 55	5, 62, 133, 200	0
28	B2	51/72 (70%)	-0.27	2 (3%) 43 35	44, 103, 157, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	D2	51/72 (70%)	0.16	5 (9%) 10 9	24, 93, 168, 200	0
29	B3	60/60 (100%)	-0.10	1 (1%) 73 64	15, 81, 158, 200	0
29	D3	60/60 (100%)	-0.12	1 (1%) 73 64	21, 85, 167, 200	0
30	B4	50/71 (70%)	-0.15	0 100 100	71, 144, 192, 200	0
30	D4	50/71 (70%)	0.21	5 (10%) 9 9	86, 167, 192, 200	0
31	B5	59/60 (98%)	0.11	4 (6%) 20 16	22, 84, 184, 200	0
31	D5	59/60 (98%)	-0.32	0 100 100	6, 74, 191, 200	0
32	B6	45/54 (83%)	0.85	8 (17%) 2 2	53, 122, 184, 200	0
32	D6	45/54 (83%)	1.49	14 (31%) 1 1	54, 147, 188, 200	0
33	B7	49/49 (100%)	-0.21	0 100 100	5, 47, 114, 200	0
33	D7	49/49 (100%)	-0.35	1 (2%) 68 59	3, 44, 105, 176	0
34	B8	64/65 (98%)	-0.15	1 (1%) 74 65	7, 53, 145, 200	0
34	D8	64/65 (98%)	-0.10	2 (3%) 52 43	27, 73, 140, 185	0
35	BA	2767/2782 (99%)	0.73	331 (11%) 6 6	9, 65, 172, 200	0
35	DA	2767/2782 (99%)	0.73	324 (11%) 6 6	6, 62, 169, 200	0
36	BB	119/122 (97%)	1.08	18 (15%) 3 3	60, 102, 160, 189	0
36	DB	119/122 (97%)	1.15	24 (20%) 1 2	69, 140, 188, 200	0
37	BC	191/229 (83%)	2.12	74 (38%) 0 0	76, 175, 200, 200	0
37	DC	191/229 (83%)	2.60	97 (50%) 0 0	120, 180, 200, 200	0
38	BD	272/276 (98%)	-0.36	1 (0%) 93 90	8, 56, 122, 200	0
38	DD	272/276 (98%)	-0.43	2 (0%) 89 82	1, 47, 114, 200	0
39	BE	205/206 (99%)	0.15	12 (5%) 26 20	10, 75, 160, 200	0
39	DE	205/206 (99%)	-0.11	5 (2%) 62 52	7, 64, 153, 199	0
40	BF	208/210 (99%)	-0.05	10 (4%) 34 27	1, 69, 164, 200	0
40	DF	208/210 (99%)	-0.12	6 (2%) 55 45	6, 75, 170, 200	0
41	BG	181/182 (99%)	0.31	22 (12%) 5 6	36, 107, 171, 200	0
41	DG	181/182 (99%)	0.80	27 (14%) 3 3	45, 135, 191, 200	0
42	BH	160/180 (88%)	0.64	24 (15%) 3 3	47, 145, 200, 200	0
42	DH	160/180 (88%)	0.12	8 (5%) 32 25	36, 110, 180, 200	0
43	BI	146/148 (98%)	0.32	15 (10%) 9 8	25, 112, 184, 200	0
43	DI	146/148 (98%)	1.76	45 (30%) 1 1	17, 134, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BN	139/140 (99%)	-0.08	7 (5%) 32 25	37, 98, 160, 200	0
44	DN	139/140 (99%)	-0.28	4 (2%) 55 45	19, 76, 152, 195	0
45	BO	122/122 (100%)	-0.22	3 (2%) 61 50	15, 63, 116, 133	0
45	DO	122/122 (100%)	-0.38	0 100 100	10, 49, 100, 128	0
46	BP	146/150 (97%)	0.09	10 (6%) 20 16	6, 84, 167, 200	0
46	DP	146/150 (97%)	0.15	9 (6%) 24 19	18, 93, 168, 199	0
47	BQ	136/141 (96%)	0.02	7 (5%) 32 24	26, 90, 187, 200	0
47	DQ	136/141 (96%)	-0.21	3 (2%) 65 55	16, 73, 158, 200	0
48	BR	117/118 (99%)	-0.44	0 100 100	8, 66, 138, 198	0
48	DR	117/118 (99%)	-0.40	0 100 100	8, 64, 136, 180	0
49	BS	99/112 (88%)	0.25	8 (8%) 15 12	32, 105, 186, 200	0
49	DS	99/112 (88%)	1.03	21 (21%) 1 1	62, 133, 182, 200	0
50	BT	138/146 (94%)	-0.09	4 (2%) 55 45	21, 96, 190, 200	0
50	DT	138/146 (94%)	-0.04	8 (5%) 26 21	17, 84, 173, 200	0
51	BU	117/118 (99%)	-0.22	4 (3%) 49 40	15, 79, 161, 182	0
51	DU	117/118 (99%)	-0.17	5 (4%) 39 30	12, 65, 141, 194	0
52	BV	101/101 (100%)	0.58	16 (15%) 3 3	26, 106, 188, 200	0
52	DV	101/101 (100%)	0.12	9 (8%) 12 10	29, 100, 178, 200	0
53	BW	113/113 (100%)	-0.41	1 (0%) 85 78	8, 55, 134, 200	0
53	DW	113/113 (100%)	-0.31	2 (1%) 71 62	16, 66, 148, 200	0
54	BX	93/96 (96%)	-0.32	1 (1%) 82 73	12, 83, 163, 200	0
54	DX	93/96 (96%)	-0.32	1 (1%) 82 73	18, 79, 147, 185	0
55	BY	101/110 (91%)	0.05	8 (7%) 15 13	16, 94, 187, 200	0
55	DY	101/110 (91%)	0.38	11 (10%) 7 7	21, 108, 187, 200	0
56	BZ	177/206 (85%)	-0.09	7 (3%) 42 33	46, 113, 178, 200	0
56	DZ	177/206 (85%)	0.25	13 (7%) 18 14	11, 114, 180, 200	0
All	All	21176/22108 (95%)	0.43	2121 (10%) 9 9	1, 84, 184, 200	0

The worst 5 of 2121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BA	897	C	18.3
35	DA	2109	U	18.2

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Mol	Chain	Res	Type	RSRZ
35	DA	897	C	17.9
43	DI	143	SER	17.6
23	CW	7	G	14.5

6.2 Non-standard residues in protein, DNA, RNA chains (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
23	5MU	CW	55	21/22	0.20	0.72	-	177,200,200,200	0
23	5MU	AW	55	21/22	0.84	0.25	-	130,173,200,200	0

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
57	MG	DA	3049	1/1	0.76	0.99	51.73	43,43,43,43	0
57	MG	CA	1696	1/1	0.99	0.65	25.39	52,52,52,52	0
57	MG	DA	3388	1/1	0.93	0.75	24.70	39,39,39,39	0
57	MG	CA	1690	1/1	0.87	0.59	23.16	20,20,20,20	1
57	MG	DA	3141	1/1	0.84	0.67	20.40	1,1,1,1	1
57	MG	BA	3051	1/1	0.97	0.56	17.43	1,1,1,1	0
57	MG	BA	3125	1/1	0.92	0.45	17.02	1,1,1,1	0
57	MG	AA	1695	1/1	0.93	0.45	16.17	42,42,42,42	0
57	MG	AA	1734	1/1	0.78	0.79	15.77	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	DA	3262	1/1	0.72	1.47	14.36	79,79,79,79	1
57	MG	DA	3048	1/1	0.88	0.83	13.25	56,56,56,56	1
57	MG	BA	3129	1/1	0.87	0.31	12.65	8,8,8,8	1
57	MG	BA	3389	1/1	0.91	0.65	12.29	31,31,31,31	0
57	MG	DA	3429	1/1	0.97	0.74	12.24	36,36,36,36	1
57	MG	CA	1801	1/1	0.82	1.28	12.20	2,2,2,2	1
57	MG	DA	3012	1/1	0.92	0.41	11.78	1,1,1,1	0
57	MG	CA	1711	1/1	0.89	0.43	11.56	37,37,37,37	1
57	MG	DA	3092	1/1	0.97	0.41	11.47	1,1,1,1	0
57	MG	DA	3358	1/1	0.76	0.71	11.40	11,11,11,11	1
57	MG	BA	3210	1/1	0.95	1.18	10.11	10,10,10,10	1
57	MG	DA	3419	1/1	0.93	0.60	10.06	58,58,58,58	0
57	MG	BA	3352	1/1	0.98	0.94	10.01	44,44,44,44	1
57	MG	DA	3046	1/1	0.93	0.41	9.62	1,1,1,1	0
57	MG	DA	3377	1/1	0.93	0.84	9.56	62,62,62,62	1
57	MG	DP	201	1/1	0.90	0.67	9.23	1,1,1,1	1
57	MG	DB	214	1/1	0.96	0.95	9.23	25,25,25,25	1
57	MG	BA	3379	1/1	0.51	1.27	9.10	50,50,50,50	1
57	MG	AA	1797	1/1	0.82	0.71	9.10	9,9,9,9	1
57	MG	DA	3282	1/1	0.80	0.41	9.00	1,1,1,1	1
57	MG	CA	1686	1/1	0.65	0.46	8.69	49,49,49,49	0
57	MG	DA	3396	1/1	0.86	0.60	8.41	14,14,14,14	0
57	MG	BA	3346	1/1	0.90	0.38	8.13	43,43,43,43	0
57	MG	DA	3308	1/1	0.97	0.58	8.07	3,3,3,3	0
57	MG	DA	3023	1/1	0.97	0.40	7.98	1,1,1,1	0
57	MG	DA	3008	1/1	0.93	0.41	7.71	1,1,1,1	0
57	MG	BA	3409	1/1	0.89	0.40	7.65	5,5,5,5	0
57	MG	BA	3143	1/1	0.92	0.45	7.26	1,1,1,1	1
57	MG	DA	3309	1/1	0.92	0.35	7.06	44,44,44,44	0
57	MG	DA	3094	1/1	0.96	0.60	6.95	1,1,1,1	1
57	MG	DA	3192	1/1	0.87	0.60	6.93	27,27,27,27	0
57	MG	CA	1639	1/1	0.94	0.44	6.55	34,34,34,34	0
57	MG	DA	3238	1/1	0.94	0.39	6.50	1,1,1,1	0
57	MG	DA	3138	1/1	0.86	0.26	6.28	17,17,17,17	0
57	MG	BA	3196	1/1	0.96	0.43	6.19	19,19,19,19	0
57	MG	CA	1736	1/1	0.77	0.46	6.15	71,71,71,71	0
57	MG	DA	3106	1/1	0.98	0.37	6.05	1,1,1,1	0
57	MG	DA	3066	1/1	0.98	0.32	6.02	1,1,1,1	0
57	MG	CA	1624	1/1	0.95	0.69	6.00	40,40,40,40	0
57	MG	DA	3063	1/1	0.97	0.44	6.00	1,1,1,1	0
57	MG	DA	3149	1/1	0.91	0.70	5.90	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	DA	3069	1/1	0.88	0.35	5.88	21,21,21,21	0
57	MG	DA	3293	1/1	0.96	0.32	5.77	1,1,1,1	1
57	MG	CN	101	1/1	0.73	0.51	5.69	65,65,65,65	0
57	MG	DA	3027	1/1	0.97	0.48	5.67	55,55,55,55	1
57	MG	DA	3315	1/1	0.98	0.32	5.46	6,6,6,6	0
57	MG	CA	1634	1/1	0.95	0.42	5.40	25,25,25,25	0
57	MG	DA	3375	1/1	0.98	0.51	5.36	74,74,74,74	1
57	MG	CA	1712	1/1	0.91	0.49	5.15	19,19,19,19	0
57	MG	CA	1746	1/1	0.14	0.92	5.01	74,74,74,74	0
57	MG	AA	1720	1/1	0.79	0.50	4.82	91,91,91,91	0
57	MG	DU	202	1/1	0.96	0.69	4.52	1,1,1,1	1
57	MG	CA	1700	1/1	0.92	0.25	4.42	10,10,10,10	0
57	MG	CA	1805	1/1	0.94	0.38	4.41	1,1,1,1	0
57	MG	BA	3048	1/1	0.98	0.47	4.12	1,1,1,1	0
57	MG	DA	3256	1/1	0.98	0.38	4.12	1,1,1,1	0
57	MG	BA	3120	1/1	0.88	0.42	4.10	38,38,38,38	0
57	MG	CA	1613	1/1	0.92	0.69	3.83	10,10,10,10	1
57	MG	BA	3397	1/1	0.72	0.41	3.69	44,44,44,44	0
57	MG	BA	3167	1/1	0.80	0.29	3.64	50,50,50,50	0
57	MG	DA	3387	1/1	0.89	0.25	3.51	33,33,33,33	1
57	MG	BA	3029	1/1	0.87	0.63	3.50	1,1,1,1	1
57	MG	CA	1716	1/1	0.89	0.79	3.47	75,75,75,75	0
57	MG	BA	3025	1/1	0.96	0.30	3.41	3,3,3,3	0
57	MG	BA	3432	1/1	0.96	0.33	3.29	47,47,47,47	0
57	MG	DA	3232	1/1	0.96	0.42	3.22	1,1,1,1	0
57	MG	BD	301	1/1	0.97	0.27	3.20	1,1,1,1	0
57	MG	BP	202	1/1	0.96	0.54	3.15	9,9,9,9	1
57	MG	BA	3166	1/1	0.83	0.28	3.10	66,66,66,66	0
57	MG	DA	3313	1/1	0.96	0.28	3.10	5,5,5,5	0
57	MG	BA	3177	1/1	0.96	0.26	3.03	36,36,36,36	1
57	MG	BA	3101	1/1	0.67	0.45	2.87	1,1,1,1	1
57	MG	DA	3421	1/1	0.99	0.43	2.85	40,40,40,40	0
57	MG	BA	3261	1/1	0.98	0.43	2.80	1,1,1,1	0
57	MG	CA	1687	1/1	0.88	0.43	2.77	42,42,42,42	0
57	MG	CA	1707	1/1	0.74	0.34	2.76	32,32,32,32	0
57	MG	DA	3408	1/1	0.95	0.27	2.63	1,1,1,1	0
57	MG	DA	3142	1/1	0.98	0.28	2.60	21,21,21,21	0
57	MG	AA	1613	1/1	0.89	0.48	2.55	11,11,11,11	1
57	MG	DA	3071	1/1	0.93	0.38	2.32	1,1,1,1	0
57	MG	DA	3118	1/1	0.96	0.20	2.26	9,9,9,9	0
57	MG	CA	1630	1/1	0.96	0.33	2.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3274	1/1	0.87	0.26	2.13	55,55,55,55	0
57	MG	BO	201	1/1	0.94	0.41	1.98	1,1,1,1	1
57	MG	DN	202	1/1	0.75	0.29	1.95	31,31,31,31	1
57	MG	CA	1699	1/1	0.97	0.50	1.88	6,6,6,6	1
57	MG	BA	3412	1/1	0.54	0.49	1.86	34,34,34,34	1
57	MG	DA	3229	1/1	0.98	0.24	1.72	1,1,1,1	0
57	MG	BA	3069	1/1	0.99	0.28	1.69	1,1,1,1	0
57	MG	AA	1732	1/1	0.94	0.28	1.67	31,31,31,31	0
57	MG	AW	119	1/1	0.88	1.01	1.66	71,71,71,71	1
57	MG	BA	3009	1/1	0.92	0.35	1.65	1,1,1,1	0
57	MG	DU	201	1/1	0.97	0.29	1.59	77,77,77,77	1
57	MG	BA	3361	1/1	0.96	0.30	1.58	1,1,1,1	1
57	MG	DA	3014	1/1	0.93	0.24	1.56	14,14,14,14	0
57	MG	BA	3013	1/1	0.99	0.28	1.49	1,1,1,1	0
57	MG	DA	3389	1/1	0.93	0.26	1.41	33,33,33,33	1
57	MG	CA	1671	1/1	0.95	0.32	1.33	21,21,21,21	0
57	MG	BA	3198	1/1	0.94	0.26	1.32	4,4,4,4	0
57	MG	BA	3318	1/1	0.94	0.32	1.27	1,1,1,1	0
57	MG	CA	1763	1/1	0.88	0.48	1.24	15,15,15,15	0
57	MG	BA	3047	1/1	0.97	0.25	1.24	1,1,1,1	0
57	MG	DA	3288	1/1	0.96	0.25	1.23	7,7,7,7	1
57	MG	DA	3120	1/1	0.99	0.20	1.22	1,1,1,1	1
57	MG	AA	1705	1/1	0.80	0.30	1.19	38,38,38,38	0
57	MG	BA	3027	1/1	0.98	0.25	1.14	1,1,1,1	1
57	MG	DA	3180	1/1	0.93	0.38	1.14	47,47,47,47	0
57	MG	CG	201	1/1	0.81	0.34	1.11	10,10,10,10	1
57	MG	DA	3412	1/1	0.98	0.29	1.10	12,12,12,12	0
57	MG	BA	3268	1/1	0.96	0.44	1.05	30,30,30,30	0
57	MG	DA	3123	1/1	0.99	0.22	0.97	1,1,1,1	0
57	MG	BA	3182	1/1	0.92	0.30	0.94	13,13,13,13	0
57	MG	BA	3189	1/1	0.80	0.93	0.89	87,87,87,87	0
57	MG	BA	3243	1/1	0.99	0.25	0.87	1,1,1,1	0
57	MG	AA	1735	1/1	0.90	0.25	0.85	15,15,15,15	0
57	MG	B1	101	1/1	0.95	0.30	0.84	27,27,27,27	0
57	MG	CA	1636	1/1	0.96	0.23	0.82	1,1,1,1	0
57	MG	BA	3263	1/1	0.90	0.29	0.75	29,29,29,29	0
57	MG	BA	3173	1/1	0.97	0.29	0.74	24,24,24,24	0
57	MG	BA	3400	1/1	0.96	0.22	0.73	1,1,1,1	0
57	MG	AA	1635	1/1	0.96	0.24	0.70	2,2,2,2	0
57	MG	DA	3385	1/1	0.80	0.39	0.69	44,44,44,44	0
57	MG	BF	301	1/1	0.96	0.38	0.68	14,14,14,14	0
57	MG	AA	1796	1/1	0.95	0.19	0.68	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	AA	1712	1/1	0.87	0.31	0.64	50,50,50,50	0
57	MG	DA	3022	1/1	0.89	0.26	0.55	28,28,28,28	1
57	MG	BA	3118	1/1	0.94	0.24	0.54	33,33,33,33	1
57	MG	DA	3199	1/1	0.95	0.23	0.50	5,5,5,5	0
57	MG	DA	3305	1/1	0.98	0.21	0.48	1,1,1,1	0
57	MG	BA	3068	1/1	0.99	0.20	0.41	1,1,1,1	0
57	MG	BA	3130	1/1	0.88	0.28	0.38	1,1,1,1	1
57	MG	DA	3213	1/1	0.95	0.24	0.33	24,24,24,24	0
57	MG	DA	3089	1/1	0.98	0.21	0.33	3,3,3,3	0
57	MG	DA	3268	1/1	0.89	0.22	0.32	24,24,24,24	0
57	MG	DE	301	1/1	0.99	0.20	0.28	1,1,1,1	1
57	MG	DA	3175	1/1	0.99	0.27	0.26	43,43,43,43	1
57	MG	BA	3140	1/1	0.93	0.24	0.22	24,24,24,24	1
57	MG	BA	3079	1/1	0.95	0.20	0.13	1,1,1,1	0
57	MG	BA	3151	1/1	0.98	0.26	0.12	1,1,1,1	0
57	MG	BA	3408	1/1	0.87	0.25	0.08	21,21,21,21	0
57	MG	DA	3030	1/1	0.99	0.20	0.03	2,2,2,2	0
57	MG	AA	1658	1/1	0.97	0.24	0.02	1,1,1,1	0
57	MG	BA	3161	1/1	0.99	0.19	-0.03	7,7,7,7	1
57	MG	DA	3083	1/1	0.99	0.24	-0.07	22,22,22,22	0
57	MG	DA	3052	1/1	0.97	0.16	-0.13	1,1,1,1	0
57	MG	AA	1691	1/1	0.93	0.28	-0.13	69,69,69,69	0
57	MG	AA	1708	1/1	0.96	0.19	-0.16	37,37,37,37	0
57	MG	AA	1794	1/1	0.92	0.28	-0.19	40,40,40,40	0
57	MG	CA	1739	1/1	0.90	0.27	-0.20	32,32,32,32	0
57	MG	BA	3271	1/1	0.94	0.21	-0.21	9,9,9,9	0
57	MG	BA	3004	1/1	0.95	0.19	-0.23	31,31,31,31	1
57	MG	DA	3085	1/1	0.98	0.17	-0.24	1,1,1,1	0
57	MG	BA	3065	1/1	0.97	0.18	-0.24	7,7,7,7	0
58	ZN	AN	101	1/1	0.99	0.23	-0.24	143,143,143,143	0
57	MG	AA	1623	1/1	0.92	0.23	-0.29	16,16,16,16	0
57	MG	DA	3318	1/1	0.89	0.62	-0.29	7,7,7,7	1
57	MG	AA	1758	1/1	0.87	0.20	-0.29	11,11,11,11	0
57	MG	BA	3085	1/1	0.94	0.20	-0.32	1,1,1,1	0
57	MG	BA	3144	1/1	0.94	0.18	-0.36	40,40,40,40	0
57	MG	BA	3277	1/1	0.93	0.21	-0.37	28,28,28,28	1
57	MG	DA	3197	1/1	0.98	0.24	-0.38	3,3,3,3	0
57	MG	BE	301	1/1	0.97	0.23	-0.39	1,1,1,1	1
57	MG	BA	3122	1/1	0.97	0.20	-0.39	1,1,1,1	1
57	MG	AA	1709	1/1	0.95	0.18	-0.40	3,3,3,3	0
57	MG	BU	201	1/1	0.93	0.25	-0.41	12,12,12,12	1
57	MG	BA	3204	1/1	0.87	0.26	-0.42	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3061	1/1	0.97	0.22	-0.45	3,3,3,3	0
57	MG	BA	3057	1/1	0.99	0.16	-0.46	7,7,7,7	0
57	MG	BX	102	1/1	0.93	0.18	-0.50	1,1,1,1	1
57	MG	BA	3239	1/1	0.92	0.20	-0.50	14,14,14,14	1
57	MG	BA	3250	1/1	0.87	0.16	-0.51	24,24,24,24	0
57	MG	CA	1715	1/1	0.59	0.20	-0.57	55,55,55,55	0
57	MG	AA	1610	1/1	0.94	0.19	-0.58	29,29,29,29	0
57	MG	BA	3422	1/1	0.87	0.20	-0.58	30,30,30,30	0
57	MG	DA	3045	1/1	0.94	0.21	-0.60	10,10,10,10	0
57	MG	AA	1624	1/1	0.96	0.24	-0.64	9,9,9,9	0
57	MG	CW	119	1/1	0.82	0.69	-0.66	57,57,57,57	1
57	MG	DA	3010	1/1	0.94	0.17	-0.72	1,1,1,1	0
57	MG	BA	3094	1/1	0.94	0.15	-0.74	25,25,25,25	1
57	MG	BP	203	1/1	0.98	0.32	-0.77	1,1,1,1	1
57	MG	BA	3387	1/1	0.92	0.16	-0.77	42,42,42,42	0
57	MG	AA	1692	1/1	0.98	0.19	-0.77	3,3,3,3	1
57	MG	DA	3059	1/1	0.95	0.18	-0.77	1,1,1,1	0
57	MG	DA	3057	1/1	0.92	0.18	-0.77	3,3,3,3	0
57	MG	CA	1631	1/1	0.90	0.23	-0.84	57,57,57,57	0
57	MG	AA	1607	1/1	0.96	0.16	-0.85	1,1,1,1	0
57	MG	DA	3384	1/1	0.96	0.16	-0.86	1,1,1,1	1
57	MG	BA	3411	1/1	0.84	0.22	-0.87	99,99,99,99	1
57	MG	DA	3306	1/1	0.96	0.14	-0.89	1,1,1,1	0
57	MG	AA	1690	1/1	0.96	0.16	-0.90	40,40,40,40	0
57	MG	CA	1761	1/1	0.87	0.22	-0.94	1,1,1,1	1
57	MG	BN	201	1/1	0.98	0.18	-0.96	47,47,47,47	1
57	MG	AA	1670	1/1	0.98	0.20	-0.97	22,22,22,22	0
57	MG	DF	302	1/1	0.95	0.21	-0.98	15,15,15,15	0
57	MG	AA	1698	1/1	0.90	0.15	-0.98	1,1,1,1	0
57	MG	BA	3076	1/1	0.97	0.20	-0.99	1,1,1,1	0
57	MG	DA	3348	1/1	0.98	0.12	-1.01	9,9,9,9	1
57	MG	BA	3201	1/1	0.94	0.20	-1.03	31,31,31,31	0
57	MG	DA	3186	1/1	0.98	0.18	-1.03	24,24,24,24	0
57	MG	BA	3015	1/1	0.95	0.15	-1.04	6,6,6,6	0
57	MG	DA	3171	1/1	0.96	0.18	-1.05	33,33,33,33	0
57	MG	DA	3386	1/1	0.97	0.14	-1.07	19,19,19,19	0
57	MG	BA	3191	1/1	0.90	0.19	-1.08	23,23,23,23	0
57	MG	DD	301	1/1	0.99	0.19	-1.11	1,1,1,1	0
57	MG	BA	3188	1/1	0.83	0.16	-1.16	12,12,12,12	0
57	MG	BA	3236	1/1	0.99	0.15	-1.17	1,1,1,1	0
57	MG	BA	3016	1/1	0.99	0.14	-1.20	31,31,31,31	1
57	MG	AA	1685	1/1	0.96	0.13	-1.21	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3135	1/1	0.94	0.17	-1.23	38,38,38,38	0
57	MG	DA	3398	1/1	0.95	0.18	-1.23	13,13,13,13	1
57	MG	DA	3399	1/1	0.96	0.15	-1.24	19,19,19,19	0
57	MG	BA	3414	1/1	0.98	0.17	-1.28	20,20,20,20	0
57	MG	DA	3410	1/1	0.95	0.16	-1.28	31,31,31,31	1
57	MG	BX	101	1/1	0.95	0.21	-1.29	26,26,26,26	1
57	MG	BA	3193	1/1	0.97	0.14	-1.30	1,1,1,1	0
57	MG	BA	3017	1/1	0.99	0.12	-1.32	3,3,3,3	1
57	MG	B1	103	1/1	0.95	0.15	-1.34	1,1,1,1	0
57	MG	AA	1689	1/1	0.98	0.14	-1.34	6,6,6,6	0
57	MG	D7	101	1/1	0.97	0.12	-1.34	93,93,93,93	1
57	MG	CA	1629	1/1	0.93	0.11	-1.36	2,2,2,2	1
57	MG	DA	3189	1/1	0.94	0.17	-1.40	59,59,59,59	0
57	MG	BA	3336	1/1	0.93	0.19	-1.42	8,8,8,8	1
57	MG	BA	3424	1/1	0.98	0.15	-1.43	37,37,37,37	0
57	MG	AA	1662	1/1	0.98	0.09	-1.47	41,41,41,41	1
58	ZN	CN	102	1/1	0.98	0.14	-1.48	114,114,114,114	0
57	MG	BA	3087	1/1	0.98	0.09	-1.48	18,18,18,18	0
57	MG	BA	3433	1/1	0.97	0.14	-1.53	33,33,33,33	0
57	MG	CA	1621	1/1	0.97	0.16	-1.57	31,31,31,31	0
57	MG	DA	3047	1/1	0.98	0.15	-1.58	1,1,1,1	0
57	MG	DX	101	1/1	0.98	0.11	-1.59	52,52,52,52	1
57	MG	BA	3212	1/1	0.99	0.06	-1.61	2,2,2,2	0
57	MG	BA	3077	1/1	0.98	0.14	-1.62	1,1,1,1	0
57	MG	CA	1664	1/1	0.91	0.10	-1.63	54,54,54,54	1
57	MG	CX	104	1/1	0.98	0.14	-1.64	39,39,39,39	0
57	MG	BA	3021	1/1	0.98	0.16	-1.64	2,2,2,2	0
57	MG	CA	1792	1/1	0.71	0.15	-1.66	16,16,16,16	1
57	MG	DA	3133	1/1	0.96	0.16	-1.66	9,9,9,9	0
57	MG	DA	3109	1/1	0.98	0.08	-1.74	17,17,17,17	0
57	MG	CA	1625	1/1	0.96	0.17	-1.74	23,23,23,23	0
57	MG	DA	3272	1/1	0.98	0.16	-1.75	5,5,5,5	0
57	MG	AA	1697	1/1	0.97	0.21	-1.76	17,17,17,17	1
57	MG	CL	201	1/1	0.96	0.09	-1.77	1,1,1,1	0
57	MG	DP	203	1/1	0.95	0.17	-1.78	1,1,1,1	1
57	MG	DA	3393	1/1	0.97	0.14	-1.80	1,1,1,1	1
57	MG	DA	3007	1/1	0.95	0.17	-1.80	14,14,14,14	0
57	MG	BA	3187	1/1	0.98	0.09	-1.83	1,1,1,1	0
57	MG	DA	3113	1/1	0.96	0.14	-1.87	1,1,1,1	0
57	MG	DA	3195	1/1	0.91	0.16	-1.88	15,15,15,15	0
57	MG	AA	1713	1/1	0.94	0.13	-1.90	25,25,25,25	0
57	MG	B7	101	1/1	0.97	0.08	-1.90	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	DA	3239	1/1	0.99	0.14	-1.95	4,4,4,4	0
57	MG	BA	3032	1/1	0.98	0.15	-1.97	1,1,1,1	0
57	MG	DA	3078	1/1	0.99	0.16	-1.99	58,58,58,58	1
57	MG	DA	3075	1/1	0.98	0.15	-1.99	1,1,1,1	0
57	MG	BA	3116	1/1	0.98	0.13	-2.00	13,13,13,13	0
57	MG	BA	3311	1/1	0.98	0.12	-2.01	1,1,1,1	0
57	MG	CA	1782	1/1	0.85	0.13	-2.12	28,28,28,28	0
58	ZN	AD	303	1/1	1.00	0.20	-2.13	26,26,26,26	0
57	MG	DA	3200	1/1	0.97	0.17	-2.13	2,2,2,2	0
57	MG	AA	1693	1/1	0.82	0.10	-2.13	80,80,80,80	0
57	MG	AM	201	1/1	0.96	0.12	-2.14	28,28,28,28	0
57	MG	CA	1608	1/1	0.98	0.11	-2.17	17,17,17,17	0
57	MG	CA	1638	1/1	0.96	0.11	-2.19	6,6,6,6	0
57	MG	CA	1694	1/1	0.90	0.13	-2.20	59,59,59,59	0
57	MG	BA	3111	1/1	0.95	0.06	-2.21	1,1,1,1	0
58	ZN	CD	301	1/1	1.00	0.22	-2.23	35,35,35,35	0
57	MG	AA	1684	1/1	0.93	0.11	-2.27	25,25,25,25	0
57	MG	BA	3091	1/1	0.93	0.17	-2.28	1,1,1,1	0
57	MG	AA	1759	1/1	0.94	0.14	-2.29	20,20,20,20	0
57	MG	DA	3077	1/1	0.98	0.11	-2.33	1,1,1,1	0
57	MG	DA	3183	1/1	0.99	0.10	-2.34	11,11,11,11	0
57	MG	CA	1800	1/1	0.99	0.09	-2.38	9,9,9,9	0
57	MG	CA	1708	1/1	0.97	0.15	-2.39	99,99,99,99	0
57	MG	CA	1609	1/1	0.99	0.21	-2.39	62,62,62,62	0
57	MG	BA	3302	1/1	0.96	0.05	-2.41	19,19,19,19	1
57	MG	AA	1628	1/1	0.97	0.14	-2.42	1,1,1,1	1
57	MG	DA	3093	1/1	0.97	0.10	-2.43	9,9,9,9	0
57	MG	CA	1637	1/1	0.96	0.15	-2.45	47,47,47,47	0
57	MG	BA	3095	1/1	0.99	0.12	-2.48	1,1,1,1	0
57	MG	DA	3255	1/1	0.98	0.08	-2.51	1,1,1,1	0
57	MG	DA	3129	1/1	0.97	0.18	-2.53	1,1,1,1	0
57	MG	CA	1693	1/1	0.93	0.08	-2.58	14,14,14,14	1
57	MG	BA	3115	1/1	0.97	0.11	-2.59	3,3,3,3	0
57	MG	DA	3433	1/1	0.96	0.18	-2.60	28,28,28,28	1
57	MG	CA	1660	1/1	0.93	0.16	-2.63	8,8,8,8	0
57	MG	CA	1723	1/1	0.98	0.18	-2.70	10,10,10,10	1
57	MG	DD	302	1/1	0.99	0.13	-2.71	2,2,2,2	0
57	MG	DA	3040	1/1	0.95	0.13	-2.75	1,1,1,1	0
57	MG	CA	1627	1/1	0.98	0.09	-2.81	5,5,5,5	0
57	MG	BA	3063	1/1	0.96	0.13	-2.82	6,6,6,6	0
57	MG	BA	3185	1/1	0.97	0.09	-2.84	1,1,1,1	0
57	MG	BA	3054	1/1	0.97	0.14	-2.85	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	D1	103	1/1	0.99	0.08	-2.86	33,33,33,33	0
57	MG	AA	1629	1/1	0.93	0.11	-2.87	22,22,22,22	0
57	MG	BA	3295	1/1	0.93	0.12	-2.90	1,1,1,1	0
57	MG	BA	3319	1/1	0.99	0.11	-3.08	1,1,1,1	0
57	MG	BA	3245	1/1	0.91	0.10	-3.15	52,52,52,52	1
57	MG	DA	3208	1/1	1.00	0.11	-3.17	14,14,14,14	0
57	MG	DA	3035	1/1	0.95	0.10	-3.19	48,48,48,48	0
57	MG	BA	3108	1/1	0.97	0.09	-3.28	25,25,25,25	0
57	MG	DA	3019	1/1	0.99	0.10	-3.29	23,23,23,23	0
57	MG	DP	204	1/1	0.95	0.13	-3.31	15,15,15,15	1
57	MG	AA	1777	1/1	0.91	0.13	-3.32	6,6,6,6	0
57	MG	DA	3167	1/1	0.97	0.11	-3.40	12,12,12,12	0
57	MG	AA	1626	1/1	0.96	0.09	-3.42	1,1,1,1	0
57	MG	AA	1703	1/1	0.90	0.13	-3.50	22,22,22,22	0
57	MG	AA	1678	1/1	0.98	0.07	-3.75	13,13,13,13	0
57	MG	CA	1691	1/1	0.97	0.09	-3.81	1,1,1,1	0
57	MG	DA	3074	1/1	0.98	0.07	-3.93	2,2,2,2	0
57	MG	DA	3003	1/1	0.96	0.09	-3.96	1,1,1,1	1
57	MG	DA	3201	1/1	0.93	0.14	-4.12	15,15,15,15	0
57	MG	BA	3244	1/1	0.99	0.14	-4.13	1,1,1,1	0
57	MG	CA	1705	1/1	0.94	0.11	-4.21	5,5,5,5	0
57	MG	DA	3061	1/1	0.99	0.09	-4.48	31,31,31,31	0
57	MG	BB	207	1/1	0.96	0.04	-4.92	11,11,11,11	0
57	MG	CA	1714	1/1	0.97	0.10	-5.35	53,53,53,53	0
57	MG	BA	3278	1/1	0.98	0.07	-5.46	8,8,8,8	0
57	MG	AA	1636	1/1	0.97	0.07	-6.08	16,16,16,16	0
57	MG	DA	3015	1/1	0.99	0.05	-7.31	1,1,1,1	1
57	MG	BA	3242	1/1	0.97	0.11	-9.09	1,1,1,1	0
57	MG	BA	3089	1/1	0.93	0.57	-	6,6,6,6	1
57	MG	B1	104	1/1	0.97	0.18	-	62,62,62,62	0
57	MG	BA	3338	1/1	0.92	0.17	-	46,46,46,46	0
57	MG	BA	3350	1/1	0.93	0.34	-	70,70,70,70	0
57	MG	BA	3158	1/1	0.83	0.35	-	32,32,32,32	0
57	MG	AA	1784	1/1	0.97	0.42	-	43,43,43,43	1
57	MG	CA	1781	1/1	0.95	0.20	-	1,1,1,1	1
57	MG	BA	3066	1/1	0.96	0.15	-	20,20,20,20	0
57	MG	BA	3042	1/1	0.98	0.18	-	1,1,1,1	0
57	MG	AA	1733	1/1	0.79	0.43	-	5,5,5,5	1
57	MG	CA	1669	1/1	0.95	0.41	-	32,32,32,32	0
57	MG	DA	3265	1/1	0.93	0.52	-	70,70,70,70	0
57	MG	BA	3176	1/1	0.89	0.57	-	21,21,21,21	1
57	MG	DA	3101	1/1	0.70	0.44	-	17,17,17,17	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	AA	1615	1/1	0.67	1.36	-	47,47,47,47	0
57	MG	AA	1714	1/1	0.98	0.18	-	23,23,23,23	0
57	MG	AA	1762	1/1	0.66	0.44	-	58,58,58,58	0
57	MG	AW	113	1/1	0.77	0.27	-	60,60,60,60	0
57	MG	CW	115	1/1	0.46	0.85	-	93,93,93,93	1
57	MG	AW	115	1/1	0.87	0.40	-	19,19,19,19	1
57	MG	BA	3390	1/1	0.81	0.57	-	24,24,24,24	0
57	MG	CW	103	1/1	0.89	0.75	-	61,61,61,61	1
57	MG	CA	1651	1/1	0.85	0.36	-	50,50,50,50	1
57	MG	DA	3317	1/1	0.87	0.40	-	78,78,78,78	1
57	MG	DA	3042	1/1	0.88	0.22	-	17,17,17,17	1
57	MG	BA	3052	1/1	0.99	0.10	-	51,51,51,51	0
57	MG	BA	3106	1/1	0.97	0.17	-	19,19,19,19	1
57	MG	DF	305	1/1	0.85	0.30	-	1,1,1,1	1
57	MG	CA	1799	1/1	0.98	0.28	-	39,39,39,39	1
57	MG	DA	3079	1/1	0.99	0.09	-	5,5,5,5	0
57	MG	DA	3349	1/1	0.94	0.22	-	10,10,10,10	1
57	MG	BA	3190	1/1	0.96	0.14	-	17,17,17,17	0
57	MG	BA	3155	1/1	0.96	0.16	-	37,37,37,37	0
57	MG	DA	3437	1/1	0.95	0.27	-	59,59,59,59	1
57	MG	BA	3307	1/1	0.94	0.36	-	35,35,35,35	0
57	MG	BA	3073	1/1	0.94	0.47	-	1,1,1,1	0
57	MG	AA	1740	1/1	0.94	0.13	-	35,35,35,35	0
57	MG	DA	3369	1/1	0.90	0.45	-	142,142,142,142	1
57	MG	BA	3232	1/1	0.86	0.34	-	30,30,30,30	0
57	MG	BA	3266	1/1	0.88	0.83	-	65,65,65,65	0
57	MG	DA	3158	1/1	0.97	0.13	-	23,23,23,23	0
57	MG	AA	1804	1/1	0.96	0.26	-	20,20,20,20	0
57	MG	AW	102	1/1	0.76	0.39	-	82,82,82,82	1
57	MG	BB	201	1/1	0.99	0.06	-	32,32,32,32	1
57	MG	AA	1768	1/1	0.97	0.23	-	7,7,7,7	0
57	MG	AW	122	1/1	0.90	0.33	-	47,47,47,47	0
57	MG	CE	202	1/1	0.70	0.49	-	85,85,85,85	1
57	MG	DA	3104	1/1	0.98	0.14	-	9,9,9,9	1
57	MG	DA	3212	1/1	0.12	0.72	-	86,86,86,86	1
57	MG	BA	3314	1/1	0.97	0.47	-	23,23,23,23	0
57	MG	DA	3271	1/1	0.79	0.49	-	113,113,113,113	1
57	MG	DA	3245	1/1	0.86	0.57	-	67,67,67,67	0
57	MG	DA	3205	1/1	0.94	0.08	-	13,13,13,13	0
57	MG	CA	1605	1/1	0.99	0.08	-	18,18,18,18	0
57	MG	BA	3124	1/1	0.99	0.09	-	7,7,7,7	0
57	MG	CA	1661	1/1	0.98	0.43	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3378	1/1	0.96	0.15	-	31,31,31,31	0
57	MG	AA	1656	1/1	0.93	0.26	-	31,31,31,31	0
57	MG	DA	3039	1/1	0.97	0.14	-	2,2,2,2	0
57	MG	CA	1789	1/1	0.98	0.25	-	73,73,73,73	0
57	MG	DA	3154	1/1	0.81	0.42	-	83,83,83,83	1
57	MG	CA	1806	1/1	0.90	0.29	-	35,35,35,35	0
57	MG	AA	1639	1/1	0.94	0.29	-	8,8,8,8	1
57	MG	DA	3269	1/1	0.91	0.53	-	57,57,57,57	1
57	MG	BN	202	1/1	0.92	0.62	-	3,3,3,3	1
57	MG	AA	1787	1/1	0.92	0.19	-	53,53,53,53	1
57	MG	AA	1786	1/1	0.97	0.11	-	1,1,1,1	1
57	MG	AA	1782	1/1	0.90	0.30	-	47,47,47,47	0
57	MG	CA	1654	1/1	0.93	0.24	-	1,1,1,1	0
57	MG	DB	206	1/1	0.91	0.22	-	72,72,72,72	0
57	MG	BA	3428	1/1	0.97	0.11	-	1,1,1,1	0
57	MG	DA	3363	1/1	0.71	0.44	-	13,13,13,13	1
57	MG	CA	1783	1/1	0.73	0.10	-	33,33,33,33	1
57	MG	BA	3436	1/1	1.00	0.18	-	6,6,6,6	1
57	MG	AA	1779	1/1	0.94	0.25	-	1,1,1,1	1
57	MG	BA	3102	1/1	0.78	0.38	-	21,21,21,21	1
57	MG	AA	1765	1/1	0.90	0.13	-	41,41,41,41	0
57	MG	AV	103	1/1	0.77	0.14	-	70,70,70,70	0
57	MG	BB	212	1/1	0.96	0.14	-	1,1,1,1	1
57	MG	DA	3009	1/1	0.95	0.27	-	1,1,1,1	1
57	MG	BA	3211	1/1	0.98	0.17	-	50,50,50,50	1
57	MG	BA	3186	1/1	0.97	0.17	-	5,5,5,5	1
57	MG	DA	3196	1/1	0.96	0.34	-	7,7,7,7	1
57	MG	CA	1767	1/1	0.77	1.31	-	94,94,94,94	0
57	MG	CA	1676	1/1	0.97	0.20	-	43,43,43,43	1
57	MG	BB	202	1/1	0.94	0.18	-	9,9,9,9	1
57	MG	DA	3084	1/1	0.93	0.22	-	13,13,13,13	0
57	MG	AA	1775	1/1	0.95	0.18	-	14,14,14,14	1
57	MG	CA	1649	1/1	0.78	0.23	-	14,14,14,14	1
57	MG	AW	120	1/1	0.93	0.31	-	58,58,58,58	1
57	MG	DA	3289	1/1	0.87	0.53	-	36,36,36,36	0
57	MG	BA	3200	1/1	0.98	0.14	-	5,5,5,5	1
57	MG	BA	3330	1/1	0.85	0.14	-	35,35,35,35	0
57	MG	BA	3178	1/1	0.86	0.37	-	38,38,38,38	0
57	MG	CA	1730	1/1	0.92	0.24	-	1,1,1,1	0
57	MG	DF	301	1/1	0.96	0.19	-	38,38,38,38	1
57	MG	BA	3258	1/1	0.86	0.17	-	32,32,32,32	0
57	MG	AW	116	1/1	0.85	0.30	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	DA	3221	1/1	0.62	0.79	-	79,79,79,79	1
57	MG	DA	3244	1/1	0.98	0.13	-	57,57,57,57	0
57	MG	DA	3392	1/1	0.82	0.50	-	46,46,46,46	0
57	MG	BA	3308	1/1	0.93	0.96	-	30,30,30,30	1
57	MG	AA	1801	1/1	0.97	0.35	-	1,1,1,1	0
57	MG	DB	201	1/1	0.87	0.23	-	22,22,22,22	1
57	MG	BA	3299	1/1	0.79	1.04	-	26,26,26,26	1
57	MG	CA	1698	1/1	0.94	0.11	-	22,22,22,22	0
57	MG	BA	3282	1/1	0.87	0.32	-	72,72,72,72	0
57	MG	DA	3121	1/1	0.99	0.38	-	20,20,20,20	0
57	MG	BB	210	1/1	0.66	0.88	-	68,68,68,68	1
57	MG	DA	3425	1/1	0.95	0.26	-	19,19,19,19	0
57	MG	DA	3251	1/1	0.99	0.22	-	10,10,10,10	1
57	MG	BA	3150	1/1	0.89	0.25	-	22,22,22,22	0
57	MG	BA	3435	1/1	0.90	0.38	-	85,85,85,85	0
57	MG	BA	3026	1/1	0.94	0.17	-	8,8,8,8	0
57	MG	DA	3406	1/1	0.88	0.82	-	57,57,57,57	0
57	MG	DA	3211	1/1	0.95	0.17	-	39,39,39,39	1
57	MG	CW	113	1/1	0.55	0.68	-	68,68,68,68	1
57	MG	DA	3184	1/1	0.98	0.19	-	1,1,1,1	0
57	MG	DA	3299	1/1	0.71	0.51	-	13,13,13,13	1
57	MG	CA	1770	1/1	0.67	1.18	-	78,78,78,78	1
57	MG	D1	101	1/1	0.97	0.46	-	55,55,55,55	0
57	MG	AA	1704	1/1	0.92	0.21	-	11,11,11,11	0
57	MG	CA	1795	1/1	0.99	0.14	-	34,34,34,34	0
57	MG	AA	1649	1/1	0.99	0.09	-	56,56,56,56	0
57	MG	BA	3296	1/1	0.97	0.26	-	11,11,11,11	0
57	MG	BA	3213	1/1	0.90	0.41	-	49,49,49,49	1
57	MG	DA	3252	1/1	0.83	0.34	-	89,89,89,89	0
57	MG	BA	3137	1/1	0.88	0.72	-	7,7,7,7	0
57	MG	DA	3156	1/1	0.93	0.21	-	21,21,21,21	0
57	MG	CA	1675	1/1	0.92	0.84	-	47,47,47,47	1
57	MG	BA	3355	1/1	0.98	0.10	-	37,37,37,37	0
57	MG	DA	3418	1/1	0.95	0.62	-	24,24,24,24	1
57	MG	BA	3018	1/1	0.52	0.26	-	35,35,35,35	0
57	MG	CA	1642	1/1	0.96	0.13	-	2,2,2,2	0
57	MG	CA	1657	1/1	0.85	0.44	-	67,67,67,67	0
57	MG	DA	3225	1/1	0.85	0.16	-	35,35,35,35	0
57	MG	AA	1707	1/1	0.90	0.52	-	53,53,53,53	0
57	MG	CA	1744	1/1	0.83	0.18	-	33,33,33,33	0
57	MG	BA	3439	1/1	0.88	0.38	-	25,25,25,25	0
57	MG	DA	3227	1/1	0.91	0.43	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3053	1/1	0.84	0.14	-	1,1,1,1	0
57	MG	DA	3260	1/1	0.96	0.31	-	8,8,8,8	1
57	MG	AA	1729	1/1	0.95	0.10	-	19,19,19,19	0
57	MG	DA	3096	1/1	0.98	0.30	-	1,1,1,1	0
57	MG	CA	1769	1/1	0.93	0.23	-	28,28,28,28	0
57	MG	DA	3428	1/1	0.93	0.55	-	17,17,17,17	0
57	MG	BA	3413	1/1	0.94	0.36	-	21,21,21,21	1
57	MG	DA	3361	1/1	0.49	0.50	-	88,88,88,88	0
57	MG	DA	3146	1/1	0.95	0.17	-	3,3,3,3	0
57	MG	DA	3297	1/1	0.97	0.35	-	11,11,11,11	1
57	MG	CA	1667	1/1	0.98	0.27	-	8,8,8,8	0
57	MG	BA	3364	1/1	0.93	0.19	-	12,12,12,12	0
57	MG	AA	1633	1/1	0.94	0.30	-	26,26,26,26	0
57	MG	BA	3257	1/1	0.91	0.24	-	42,42,42,42	0
57	MG	BA	3070	1/1	0.96	0.28	-	24,24,24,24	0
57	MG	CX	101	1/1	0.99	0.07	-	56,56,56,56	1
57	MG	BA	3337	1/1	0.81	0.68	-	1,1,1,1	1
57	MG	AA	1725	1/1	0.87	0.50	-	48,48,48,48	0
57	MG	DA	3416	1/1	0.98	0.15	-	1,1,1,1	1
57	MG	DA	3321	1/1	0.79	0.36	-	85,85,85,85	0
57	MG	DA	3243	1/1	0.99	0.10	-	18,18,18,18	0
57	MG	DA	3219	1/1	0.93	0.70	-	21,21,21,21	1
57	MG	BA	3404	1/1	0.93	0.19	-	108,108,108,108	0
57	MG	BA	3276	1/1	0.88	0.82	-	34,34,34,34	1
57	MG	BA	3287	1/1	0.67	0.43	-	45,45,45,45	1
57	MG	AW	104	1/1	0.97	0.09	-	14,14,14,14	1
57	MG	BA	3043	1/1	0.94	0.19	-	26,26,26,26	0
57	MG	BB	215	1/1	0.90	0.25	-	49,49,49,49	1
57	MG	AA	1750	1/1	0.97	0.11	-	42,42,42,42	0
57	MG	DA	3168	1/1	0.96	0.86	-	36,36,36,36	1
57	MG	CA	1748	1/1	0.82	0.62	-	97,97,97,97	1
57	MG	BA	3199	1/1	0.95	0.47	-	5,5,5,5	1
57	MG	BA	3351	1/1	0.88	0.36	-	68,68,68,68	1
57	MG	BA	3289	1/1	0.79	0.37	-	60,60,60,60	1
57	MG	DA	3370	1/1	0.71	0.47	-	100,100,100,100	1
57	MG	CA	1611	1/1	0.96	0.10	-	22,22,22,22	0
57	MG	DA	3237	1/1	0.96	0.33	-	22,22,22,22	0
57	MG	DA	3037	1/1	0.92	0.17	-	1,1,1,1	0
57	MG	BB	204	1/1	0.75	0.74	-	76,76,76,76	1
57	MG	CA	1681	1/1	0.50	0.48	-	96,96,96,96	1
57	MG	DA	3128	1/1	0.97	0.12	-	1,1,1,1	1
57	MG	AA	1710	1/1	0.92	0.40	-	113,113,113,113	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3349	1/1	0.93	0.34	-	86,86,86,86	0
57	MG	AE	201	1/1	0.93	0.19	-	28,28,28,28	0
57	MG	AA	1645	1/1	0.90	0.21	-	14,14,14,14	1
57	MG	BA	3380	1/1	0.92	0.16	-	63,63,63,63	0
57	MG	BA	3001	1/1	0.91	0.38	-	8,8,8,8	0
57	MG	BA	3371	1/1	0.98	0.28	-	53,53,53,53	1
57	MG	BA	3402	1/1	0.81	0.22	-	13,13,13,13	1
57	MG	BA	3440	1/1	0.88	0.13	-	33,33,33,33	0
57	MG	DA	3099	1/1	0.98	0.29	-	1,1,1,1	1
57	MG	DA	3179	1/1	0.93	0.40	-	52,52,52,52	1
57	MG	DA	3051	1/1	0.96	0.18	-	1,1,1,1	0
57	MG	BA	3030	1/1	0.84	0.34	-	56,56,56,56	1
57	MG	CA	1650	1/1	0.88	0.26	-	98,98,98,98	1
57	MG	DA	3345	1/1	0.92	0.15	-	2,2,2,2	1
57	MG	AW	105	1/1	0.96	0.52	-	82,82,82,82	0
57	MG	AX	102	1/1	0.97	0.19	-	4,4,4,4	0
57	MG	AA	1751	1/1	0.98	0.24	-	14,14,14,14	0
57	MG	BA	3119	1/1	0.97	0.19	-	4,4,4,4	0
57	MG	AA	1781	1/1	0.84	0.33	-	7,7,7,7	1
57	MG	DA	3286	1/1	0.94	0.40	-	12,12,12,12	0
57	MG	AA	1738	1/1	0.90	0.42	-	18,18,18,18	1
57	MG	DA	3292	1/1	0.85	0.38	-	45,45,45,45	0
57	MG	DB	210	1/1	0.94	0.21	-	49,49,49,49	1
57	MG	CA	1740	1/1	0.96	0.36	-	44,44,44,44	0
57	MG	BA	3267	1/1	0.91	0.24	-	34,34,34,34	0
57	MG	BA	3099	1/1	0.94	0.28	-	45,45,45,45	1
57	MG	DA	3436	1/1	0.79	0.71	-	41,41,41,41	0
57	MG	BA	3230	1/1	0.88	0.22	-	22,22,22,22	0
57	MG	BA	3445	1/1	0.83	0.51	-	25,25,25,25	1
57	MG	BA	3110	1/1	0.96	0.19	-	32,32,32,32	1
57	MG	DA	3371	1/1	0.62	0.19	-	35,35,35,35	1
57	MG	DA	3224	1/1	0.90	0.25	-	65,65,65,65	1
57	MG	BA	3418	1/1	0.84	0.39	-	41,41,41,41	1
57	MG	DA	3274	1/1	0.94	0.05	-	65,65,65,65	0
57	MG	BA	3343	1/1	0.81	0.28	-	33,33,33,33	0
57	MG	DA	3324	1/1	0.91	0.15	-	40,40,40,40	0
57	MG	CW	110	1/1	0.06	2.12	-	66,66,66,66	1
57	MG	DA	3228	1/1	0.94	0.56	-	41,41,41,41	0
57	MG	CA	1697	1/1	0.76	0.36	-	59,59,59,59	1
57	MG	CA	1737	1/1	0.55	0.66	-	1,1,1,1	1
57	MG	AX	101	1/1	0.89	0.28	-	15,15,15,15	1
57	MG	AA	1752	1/1	0.90	0.29	-	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	DA	3119	1/1	0.98	0.31	-	1,1,1,1	0
57	MG	BA	3134	1/1	0.99	0.07	-	1,1,1,1	0
57	MG	CA	1689	1/1	0.98	0.09	-	87,87,87,87	0
57	MG	BA	3430	1/1	0.96	0.29	-	1,1,1,1	1
57	MG	DA	3164	1/1	0.93	0.09	-	72,72,72,72	0
57	MG	AW	118	1/1	0.12	0.30	-	69,69,69,69	1
57	MG	DA	3137	1/1	0.98	0.15	-	5,5,5,5	1
57	MG	BA	3256	1/1	0.97	0.18	-	1,1,1,1	1
57	MG	BA	3291	1/1	0.94	0.15	-	7,7,7,7	0
57	MG	BA	3335	1/1	0.91	0.37	-	1,1,1,1	1
57	MG	DA	3097	1/1	0.97	0.12	-	55,55,55,55	1
57	MG	DA	3435	1/1	0.89	0.24	-	48,48,48,48	0
57	MG	DA	3351	1/1	0.98	0.28	-	11,11,11,11	1
57	MG	DA	3423	1/1	0.90	0.23	-	49,49,49,49	0
57	MG	DA	3266	1/1	0.96	0.20	-	17,17,17,17	1
57	MG	DA	3374	1/1	0.96	0.15	-	28,28,28,28	0
57	MG	BA	3002	1/1	0.75	0.40	-	16,16,16,16	1
57	MG	CA	1644	1/1	0.93	0.24	-	31,31,31,31	0
57	MG	BA	3395	1/1	0.89	0.28	-	1,1,1,1	1
57	MG	BA	3062	1/1	0.99	0.24	-	1,1,1,1	0
57	MG	DA	3082	1/1	0.97	0.14	-	20,20,20,20	0
57	MG	DA	3242	1/1	0.78	0.19	-	100,100,100,100	1
57	MG	CA	1612	1/1	0.92	0.27	-	75,75,75,75	0
57	MG	BA	3056	1/1	0.99	0.09	-	1,1,1,1	0
57	MG	DV	201	1/1	0.96	0.15	-	1,1,1,1	0
57	MG	AW	108	1/1	0.69	1.08	-	24,24,24,24	1
57	MG	AA	1643	1/1	0.94	0.24	-	43,43,43,43	0
57	MG	DA	3401	1/1	0.97	0.30	-	49,49,49,49	1
57	MG	BA	3373	1/1	0.83	0.29	-	1,1,1,1	1
57	MG	AA	1723	1/1	0.86	0.22	-	55,55,55,55	0
57	MG	BA	3138	1/1	0.98	0.21	-	12,12,12,12	0
57	MG	BA	3290	1/1	0.93	1.13	-	33,33,33,33	1
57	MG	BB	217	1/1	0.70	0.24	-	49,49,49,49	0
57	MG	AA	1683	1/1	0.84	0.42	-	1,1,1,1	1
57	MG	BA	3072	1/1	0.97	0.34	-	100,100,100,100	0
57	MG	CA	1656	1/1	0.94	0.16	-	19,19,19,19	1
57	MG	DA	3379	1/1	0.96	0.16	-	47,47,47,47	0
57	MG	AA	1686	1/1	0.88	0.24	-	61,61,61,61	0
57	MG	CA	1765	1/1	0.73	0.68	-	85,85,85,85	0
57	MG	BA	3022	1/1	0.98	0.48	-	1,1,1,1	0
57	MG	AA	1647	1/1	0.98	0.10	-	17,17,17,17	1
57	MG	AA	1650	1/1	0.50	1.83	-	20,20,20,20	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3092	1/1	0.98	0.17	-	5,5,5,5	0
57	MG	BA	3038	1/1	0.92	0.34	-	22,22,22,22	1
57	MG	DA	3354	1/1	0.92	0.25	-	6,6,6,6	1
57	MG	DA	3362	1/1	0.91	0.27	-	15,15,15,15	0
57	MG	BA	3084	1/1	0.98	0.17	-	1,1,1,1	1
57	MG	DA	3281	1/1	0.67	0.49	-	64,64,64,64	0
57	MG	CA	1726	1/1	0.70	0.33	-	36,36,36,36	0
57	MG	AA	1803	1/1	0.92	0.24	-	9,9,9,9	0
57	MG	BA	3050	1/1	0.99	0.15	-	1,1,1,1	1
57	MG	DA	3323	1/1	0.86	0.14	-	63,63,63,63	1
57	MG	BA	3194	1/1	0.97	0.43	-	19,19,19,19	0
57	MG	CA	1745	1/1	0.88	0.21	-	112,112,112,112	1
57	MG	DA	3105	1/1	0.98	0.10	-	26,26,26,26	0
57	MG	CA	1640	1/1	0.84	0.27	-	65,65,65,65	1
57	MG	AA	1761	1/1	0.92	0.18	-	13,13,13,13	0
57	MG	BA	3224	1/1	0.91	1.25	-	80,80,80,80	0
57	MG	AA	1773	1/1	0.90	0.81	-	16,16,16,16	1
57	MG	CA	1688	1/1	0.97	0.37	-	21,21,21,21	0
57	MG	DF	304	1/1	0.98	0.23	-	66,66,66,66	0
57	MG	DA	3058	1/1	0.95	0.22	-	42,42,42,42	0
57	MG	BA	3327	1/1	0.74	0.13	-	46,46,46,46	1
57	MG	AA	1741	1/1	0.87	0.29	-	48,48,48,48	0
57	MG	AA	1724	1/1	0.91	0.22	-	34,34,34,34	1
57	MG	BA	3241	1/1	0.88	0.50	-	27,27,27,27	0
57	MG	DA	3029	1/1	0.97	0.14	-	1,1,1,1	0
57	MG	DA	3253	1/1	0.94	0.52	-	25,25,25,25	0
57	MG	BB	213	1/1	0.64	0.78	-	33,33,33,33	1
57	MG	AA	1666	1/1	0.85	0.41	-	47,47,47,47	0
57	MG	B5	101	1/1	0.97	0.23	-	1,1,1,1	0
57	MG	DA	3130	1/1	0.97	0.09	-	33,33,33,33	0
57	MG	CW	111	1/1	-0.29	0.57	-	136,136,136,136	1
57	MG	CA	1713	1/1	0.92	0.26	-	40,40,40,40	1
57	MG	BA	3123	1/1	0.92	0.58	-	35,35,35,35	0
57	MG	AW	121	1/1	0.80	0.49	-	63,63,63,63	0
57	MG	BA	3376	1/1	0.99	0.05	-	15,15,15,15	0
57	MG	BA	3396	1/1	0.94	0.57	-	15,15,15,15	0
57	MG	BA	3096	1/1	0.99	0.32	-	1,1,1,1	1
57	MG	BA	3270	1/1	0.77	0.22	-	6,6,6,6	0
57	MG	AA	1731	1/1	0.96	0.12	-	79,79,79,79	1
57	MG	DA	3422	1/1	0.61	0.23	-	62,62,62,62	0
57	MG	AA	1747	1/1	0.94	0.27	-	5,5,5,5	0
57	MG	CA	1653	1/1	0.91	0.11	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BB	203	1/1	0.85	0.25	-	60,60,60,60	0
57	MG	DA	3294	1/1	0.96	0.18	-	73,73,73,73	1
57	MG	AA	1668	1/1	0.84	0.31	-	18,18,18,18	0
57	MG	DA	3103	1/1	0.94	0.30	-	1,1,1,1	0
57	MG	BA	3362	1/1	0.85	0.28	-	38,38,38,38	0
57	MG	AA	1778	1/1	0.97	0.09	-	16,16,16,16	1
57	MG	DB	211	1/1	0.95	0.15	-	1,1,1,1	1
57	MG	DA	3216	1/1	0.95	0.10	-	28,28,28,28	1
57	MG	BA	3279	1/1	0.87	0.25	-	35,35,35,35	1
57	MG	BA	3019	1/1	0.95	0.48	-	1,1,1,1	0
57	MG	AA	1609	1/1	0.90	0.34	-	7,7,7,7	1
57	MG	BA	3234	1/1	0.98	0.18	-	12,12,12,12	0
57	MG	BA	3401	1/1	0.93	0.68	-	42,42,42,42	0
57	MG	DA	3438	1/1	0.83	1.20	-	48,48,48,48	1
57	MG	AA	1651	1/1	0.92	0.16	-	32,32,32,32	0
57	MG	BA	3246	1/1	0.93	0.32	-	23,23,23,23	1
57	MG	DA	3135	1/1	0.79	0.87	-	12,12,12,12	0
57	MG	BA	3286	1/1	0.73	0.43	-	32,32,32,32	1
57	MG	CA	1659	1/1	0.90	0.15	-	34,34,34,34	1
57	MG	AA	1760	1/1	0.87	0.23	-	37,37,37,37	0
57	MG	DA	3147	1/1	0.93	0.21	-	22,22,22,22	0
57	MG	DA	3270	1/1	0.63	1.08	-	47,47,47,47	1
57	MG	AW	109	1/1	0.83	0.29	-	37,37,37,37	1
57	MG	CV	103	1/1	0.96	0.05	-	44,44,44,44	0
57	MG	BA	3075	1/1	0.97	0.35	-	6,6,6,6	1
57	MG	BA	3434	1/1	0.86	0.20	-	60,60,60,60	0
57	MG	BA	3358	1/1	0.95	0.30	-	22,22,22,22	0
57	MG	DA	3076	1/1	0.98	0.33	-	1,1,1,1	0
57	MG	DA	3241	1/1	0.68	0.86	-	50,50,50,50	0
57	MG	DA	3178	1/1	0.98	0.15	-	1,1,1,1	1
57	MG	AA	1742	1/1	0.86	0.14	-	36,36,36,36	0
57	MG	DA	3072	1/1	0.99	0.09	-	1,1,1,1	1
57	MG	DA	3080	1/1	0.99	0.09	-	1,1,1,1	1
57	MG	DA	3073	1/1	0.99	0.21	-	1,1,1,1	1
57	MG	DA	3222	1/1	0.99	0.23	-	3,3,3,3	1
57	MG	BA	3425	1/1	0.93	0.12	-	23,23,23,23	0
57	MG	DA	3329	1/1	0.45	1.32	-	62,62,62,62	1
57	MG	DA	3153	1/1	0.98	0.15	-	1,1,1,1	0
57	MG	DA	3001	1/1	0.95	0.23	-	49,49,49,49	0
57	MG	BN	204	1/1	0.78	0.36	-	20,20,20,20	1
57	MG	BA	3206	1/1	0.78	0.36	-	1,1,1,1	1
57	MG	CA	1677	1/1	0.94	0.20	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	DA	3328	1/1	0.88	0.62	-	63,63,63,63	0
57	MG	AA	1763	1/1	0.94	0.64	-	40,40,40,40	1
57	MG	DA	3343	1/1	0.82	0.40	-	1,1,1,1	1
57	MG	CW	102	1/1	0.78	0.27	-	38,38,38,38	1
57	MG	BA	3149	1/1	0.96	0.18	-	36,36,36,36	0
57	MG	AA	1618	1/1	0.97	0.17	-	1,1,1,1	0
57	MG	DA	3110	1/1	0.97	0.15	-	1,1,1,1	1
57	MG	CA	1776	1/1	0.94	0.21	-	32,32,32,32	0
57	MG	BA	3008	1/1	0.95	0.35	-	19,19,19,19	0
57	MG	BA	3367	1/1	0.90	0.45	-	37,37,37,37	0
57	MG	DA	3108	1/1	0.98	0.19	-	13,13,13,13	0
57	MG	BA	3197	1/1	0.92	0.20	-	25,25,25,25	1
57	MG	AA	1653	1/1	0.76	0.77	-	93,93,93,93	1
57	MG	DA	3273	1/1	0.60	0.43	-	97,97,97,97	1
57	MG	DA	3431	1/1	0.85	0.12	-	16,16,16,16	0
57	MG	BA	3383	1/1	0.93	0.96	-	39,39,39,39	1
57	MG	BA	3443	1/1	0.83	0.14	-	49,49,49,49	0
57	MG	DA	3356	1/1	0.95	0.17	-	57,57,57,57	0
57	MG	BA	3247	1/1	0.99	0.27	-	26,26,26,26	1
57	MG	DA	3064	1/1	0.99	0.09	-	18,18,18,18	0
57	MG	CA	1741	1/1	0.91	0.21	-	1,1,1,1	1
57	MG	CA	1793	1/1	0.83	0.64	-	74,74,74,74	0
57	MG	AA	1789	1/1	0.28	0.45	-	111,111,111,111	0
57	MG	DA	3223	1/1	0.93	0.61	-	12,12,12,12	1
57	MG	BA	3260	1/1	0.95	0.44	-	1,1,1,1	0
57	MG	DA	3336	1/1	0.83	0.31	-	60,60,60,60	0
57	MG	DA	3018	1/1	0.89	0.39	-	12,12,12,12	0
57	MG	DB	205	1/1	0.93	0.40	-	5,5,5,5	1
57	MG	B3	101	1/1	0.98	0.20	-	14,14,14,14	0
57	MG	BA	3333	1/1	0.91	0.10	-	41,41,41,41	0
57	MG	AA	1757	1/1	0.94	0.33	-	51,51,51,51	1
57	MG	AA	1769	1/1	0.74	1.21	-	48,48,48,48	0
57	MG	CW	109	1/1	0.51	0.37	-	30,30,30,30	1
57	MG	DA	3430	1/1	0.94	0.21	-	13,13,13,13	0
57	MG	D2	2601	1/1	0.76	0.47	-	73,73,73,73	1
57	MG	BA	3128	1/1	0.88	0.27	-	1,1,1,1	0
57	MG	CA	1641	1/1	0.85	0.14	-	17,17,17,17	0
57	MG	DA	3127	1/1	0.60	0.54	-	57,57,57,57	0
57	MG	DA	3087	1/1	0.81	0.47	-	17,17,17,17	1
57	MG	DA	3335	1/1	0.97	0.12	-	7,7,7,7	1
57	MG	DA	3114	1/1	0.97	0.13	-	1,1,1,1	0
57	MG	CW	117	1/1	0.54	0.26	-	57,57,57,57	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	AA	1627	1/1	0.96	0.48	-	9,9,9,9	0
57	MG	BF	302	1/1	0.91	0.78	-	15,15,15,15	1
57	MG	BA	3431	1/1	0.91	0.58	-	12,12,12,12	0
57	MG	DA	3407	1/1	0.87	0.28	-	9,9,9,9	0
57	MG	DA	3088	1/1	0.97	0.51	-	1,1,1,1	1
57	MG	CA	1808	1/1	0.88	0.41	-	43,43,43,43	1
57	MG	DA	3174	1/1	0.76	0.55	-	50,50,50,50	1
57	MG	BA	3427	1/1	0.96	0.29	-	99,99,99,99	1
57	MG	DA	3344	1/1	0.91	0.15	-	20,20,20,20	0
57	MG	BA	3321	1/1	0.86	0.12	-	51,51,51,51	0
57	MG	DA	3296	1/1	0.75	0.67	-	33,33,33,33	1
57	MG	AA	1630	1/1	0.99	0.16	-	19,19,19,19	0
57	MG	BA	3306	1/1	0.87	0.87	-	50,50,50,50	0
57	MG	BA	3195	1/1	0.99	0.13	-	39,39,39,39	1
57	MG	BA	3407	1/1	0.90	0.41	-	10,10,10,10	0
57	MG	BA	3058	1/1	0.88	0.44	-	3,3,3,3	1
57	MG	BA	3329	1/1	0.95	0.56	-	61,61,61,61	0
57	MG	AA	1660	1/1	0.98	0.33	-	17,17,17,17	0
57	MG	BA	3208	1/1	0.97	0.22	-	23,23,23,23	1
57	MG	DA	3155	1/1	0.96	0.37	-	21,21,21,21	0
57	MG	BA	3322	1/1	0.74	0.78	-	21,21,21,21	1
57	MG	CA	1652	1/1	0.93	0.49	-	1,1,1,1	1
57	MG	BA	3005	1/1	0.79	0.36	-	25,25,25,25	0
57	MG	AW	114	1/1	0.80	0.16	-	78,78,78,78	0
57	MG	AA	1603	1/1	0.85	0.23	-	20,20,20,20	0
57	MG	CE	201	1/1	0.94	0.67	-	78,78,78,78	0
57	MG	BA	3180	1/1	0.94	0.45	-	1,1,1,1	1
57	MG	CA	1601	1/1	0.99	0.11	-	21,21,21,21	1
57	MG	CA	1754	1/1	0.77	0.32	-	42,42,42,42	0
57	MG	DA	3062	1/1	0.98	0.54	-	21,21,21,21	0
57	MG	DA	3198	1/1	0.98	0.15	-	11,11,11,11	0
57	MG	CW	105	1/1	0.90	1.01	-	79,79,79,79	1
57	MG	AA	1785	1/1	0.80	0.15	-	19,19,19,19	0
57	MG	AA	1625	1/1	0.89	0.43	-	31,31,31,31	0
57	MG	DA	3182	1/1	0.98	0.19	-	1,1,1,1	1
57	MG	BA	3035	1/1	0.59	0.39	-	67,67,67,67	1
57	MG	BA	3353	1/1	0.92	0.54	-	41,41,41,41	1
57	MG	DA	3131	1/1	0.95	0.13	-	22,22,22,22	0
57	MG	CA	1803	1/1	0.81	0.30	-	83,83,83,83	0
57	MG	CA	1790	1/1	0.96	0.18	-	19,19,19,19	0
57	MG	BA	3384	1/1	0.98	0.15	-	1,1,1,1	1
57	MG	CA	1665	1/1	0.98	0.48	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	AD	301	1/1	0.93	0.21	-	15,15,15,15	1
57	MG	DE	302	1/1	0.91	0.37	-	50,50,50,50	0
57	MG	DA	3194	1/1	0.89	0.39	-	57,57,57,57	0
57	MG	DA	3424	1/1	0.81	0.21	-	31,31,31,31	1
57	MG	CA	1646	1/1	0.77	0.44	-	56,56,56,56	0
57	MG	BA	3003	1/1	0.96	0.34	-	68,68,68,68	1
57	MG	DA	3415	1/1	0.85	0.38	-	3,3,3,3	1
57	MG	DX	103	1/1	0.79	0.35	-	48,48,48,48	1
57	MG	DA	3017	1/1	0.95	0.07	-	11,11,11,11	0
57	MG	BA	3145	1/1	0.91	0.30	-	4,4,4,4	0
57	MG	BA	3359	1/1	0.93	0.39	-	21,21,21,21	1
57	MG	DA	3112	1/1	0.97	0.41	-	1,1,1,1	0
57	MG	CA	1798	1/1	0.92	0.39	-	43,43,43,43	1
57	MG	BA	3071	1/1	0.98	0.14	-	20,20,20,20	0
57	MG	AA	1642	1/1	0.95	0.14	-	26,26,26,26	0
57	MG	AA	1634	1/1	0.92	0.10	-	28,28,28,28	0
57	MG	BA	3153	1/1	0.71	0.35	-	35,35,35,35	1
57	MG	DA	3140	1/1	0.63	0.44	-	25,25,25,25	0
57	MG	BA	3323	1/1	0.88	0.35	-	74,74,74,74	0
57	MG	DA	3322	1/1	0.87	0.19	-	34,34,34,34	1
57	MG	BA	3255	1/1	0.96	0.17	-	25,25,25,25	0
57	MG	CW	120	1/1	0.93	0.27	-	20,20,20,20	1
57	MG	BA	3339	1/1	0.93	0.39	-	3,3,3,3	0
57	MG	AA	1716	1/1	0.68	0.26	-	60,60,60,60	0
57	MG	BA	3218	1/1	0.99	0.08	-	50,50,50,50	0
57	MG	CA	1607	1/1	0.93	0.25	-	54,54,54,54	0
57	MG	CA	1757	1/1	0.93	0.65	-	35,35,35,35	0
57	MG	BA	3399	1/1	0.94	0.23	-	56,56,56,56	1
57	MG	BA	3083	1/1	0.98	0.15	-	18,18,18,18	0
57	MG	BA	3320	1/1	0.89	0.23	-	37,37,37,37	1
57	MG	DA	3032	1/1	0.95	0.20	-	23,23,23,23	0
57	MG	BA	3081	1/1	0.99	0.14	-	1,1,1,1	0
57	MG	BA	3345	1/1	0.93	0.84	-	1,1,1,1	1
57	MG	DA	3405	1/1	0.93	0.35	-	30,30,30,30	1
57	MG	CA	1632	1/1	0.91	0.23	-	36,36,36,36	0
57	MG	CA	1727	1/1	0.91	1.17	-	92,92,92,92	0
57	MG	DA	3148	1/1	0.96	0.21	-	26,26,26,26	0
57	MG	BA	3207	1/1	0.68	0.74	-	1,1,1,1	1
57	MG	BA	3301	1/1	0.95	0.12	-	24,24,24,24	0
57	MG	DA	3218	1/1	0.91	0.42	-	12,12,12,12	0
57	MG	AG	201	1/1	0.96	0.21	-	5,5,5,5	1
57	MG	AW	123	1/1	0.68	0.48	-	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3340	1/1	0.85	0.64	-	22,22,22,22	1
57	MG	DA	3125	1/1	0.99	0.39	-	4,4,4,4	1
57	MG	BA	3060	1/1	0.89	0.23	-	42,42,42,42	0
57	MG	DA	3160	1/1	0.98	0.18	-	1,1,1,1	1
57	MG	BA	3348	1/1	0.86	1.28	-	84,84,84,84	0
57	MG	AA	1687	1/1	0.89	0.14	-	61,61,61,61	0
57	MG	AA	1637	1/1	0.97	0.22	-	11,11,11,11	0
57	MG	AA	1802	1/1	0.93	0.22	-	18,18,18,18	0
57	MG	CA	1617	1/1	0.86	0.72	-	29,29,29,29	0
57	MG	DA	3161	1/1	0.76	0.31	-	112,112,112,112	0
57	MG	DA	3312	1/1	0.88	0.30	-	1,1,1,1	0
57	MG	AA	1772	1/1	0.94	0.57	-	52,52,52,52	0
57	MG	DA	3173	1/1	0.98	0.35	-	52,52,52,52	1
57	MG	AA	1798	1/1	0.60	0.69	-	52,52,52,52	1
57	MG	AX	105	1/1	0.95	0.14	-	35,35,35,35	0
57	MG	BA	3326	1/1	0.95	0.20	-	23,23,23,23	1
57	MG	BA	3317	1/1	0.98	0.12	-	60,60,60,60	0
57	MG	AV	101	1/1	0.87	0.37	-	46,46,46,46	0
57	MG	DA	3426	1/1	0.86	0.24	-	44,44,44,44	0
57	MG	DA	3098	1/1	0.98	0.14	-	5,5,5,5	0
57	MG	BA	3216	1/1	0.89	0.09	-	49,49,49,49	0
57	MG	DA	3026	1/1	0.91	0.67	-	1,1,1,1	0
57	MG	DA	3020	1/1	0.99	0.48	-	1,1,1,1	0
57	MG	BA	3044	1/1	0.95	0.38	-	36,36,36,36	0
57	MG	DA	3267	1/1	0.99	0.24	-	28,28,28,28	1
57	MG	DA	3086	1/1	0.91	0.46	-	1,1,1,1	1
57	MG	BA	3292	1/1	0.79	0.82	-	27,27,27,27	1
57	MG	BA	3126	1/1	0.95	0.33	-	1,1,1,1	0
57	MG	CA	1760	1/1	0.78	0.45	-	40,40,40,40	0
57	MG	BA	3012	1/1	0.97	0.12	-	38,38,38,38	0
57	MG	DA	3404	1/1	0.96	0.26	-	43,43,43,43	0
57	MG	CA	1720	1/1	0.94	0.14	-	4,4,4,4	1
57	MG	DA	3053	1/1	0.97	0.28	-	3,3,3,3	0
57	MG	DA	3172	1/1	0.99	0.14	-	17,17,17,17	1
57	MG	AA	1619	1/1	0.96	0.16	-	25,25,25,25	0
57	MG	AA	1764	1/1	0.83	0.26	-	35,35,35,35	0
57	MG	BA	3109	1/1	0.94	0.45	-	3,3,3,3	0
57	MG	BA	3214	1/1	0.94	0.16	-	106,106,106,106	1
57	MG	CW	116	1/1	0.24	0.73	-	107,107,107,107	0
57	MG	BA	3304	1/1	0.97	0.14	-	24,24,24,24	0
57	MG	AA	1756	1/1	0.96	0.15	-	58,58,58,58	0
57	MG	CA	1771	1/1	0.86	0.08	-	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	AA	1654	1/1	0.98	0.37	-	65,65,65,65	0
57	MG	DA	3376	1/1	0.93	0.22	-	1,1,1,1	0
57	MG	AA	1620	1/1	0.99	0.17	-	3,3,3,3	0
57	MG	BD	303	1/1	0.97	0.40	-	13,13,13,13	1
57	MG	DA	3337	1/1	0.93	0.31	-	92,92,92,92	0
57	MG	CW	121	1/1	0.88	0.36	-	28,28,28,28	1
57	MG	CV	104	1/1	0.85	0.35	-	45,45,45,45	1
57	MG	BA	3377	1/1	0.96	0.26	-	95,95,95,95	0
57	MG	CA	1779	1/1	0.95	0.43	-	34,34,34,34	0
57	MG	BA	3067	1/1	0.99	0.13	-	1,1,1,1	1
57	MG	CE	203	1/1	0.94	0.44	-	38,38,38,38	1
57	MG	AA	1721	1/1	0.92	0.43	-	44,44,44,44	0
57	MG	BA	3112	1/1	0.91	0.23	-	34,34,34,34	1
57	MG	DA	3261	1/1	0.97	0.37	-	30,30,30,30	0
57	MG	DA	3298	1/1	0.96	0.08	-	22,22,22,22	0
57	MG	CA	1717	1/1	0.93	0.15	-	1,1,1,1	0
57	MG	BA	3310	1/1	0.93	0.26	-	5,5,5,5	1
57	MG	BA	3393	1/1	0.93	0.22	-	14,14,14,14	0
57	MG	BA	3049	1/1	0.97	0.20	-	17,17,17,17	0
57	MG	CA	1738	1/1	0.74	0.94	-	67,67,67,67	0
57	MG	BA	3226	1/1	0.95	0.33	-	1,1,1,1	1
57	MG	DA	3441	1/1	0.80	1.08	-	44,44,44,44	1
57	MG	AA	1622	1/1	0.99	0.08	-	1,1,1,1	1
57	MG	DB	202	1/1	0.42	0.69	-	33,33,33,33	1
57	MG	DA	3068	1/1	0.95	0.26	-	24,24,24,24	0
57	MG	AA	1601	1/1	0.95	0.15	-	21,21,21,21	0
57	MG	AA	1672	1/1	0.97	0.17	-	24,24,24,24	0
57	MG	D2	2602	1/1	0.98	0.35	-	6,6,6,6	1
57	MG	AA	1792	1/1	0.83	0.52	-	56,56,56,56	0
57	MG	CA	1616	1/1	0.86	0.79	-	64,64,64,64	0
57	MG	BA	3202	1/1	0.96	0.21	-	14,14,14,14	0
57	MG	AA	1612	1/1	0.96	0.26	-	36,36,36,36	0
57	MG	DA	3028	1/1	0.93	0.12	-	59,59,59,59	1
57	MG	DA	3157	1/1	0.97	0.25	-	37,37,37,37	0
57	MG	BA	3148	1/1	0.97	0.28	-	8,8,8,8	0
57	MG	BA	3007	1/1	0.99	0.08	-	37,37,37,37	0
57	MG	DA	3314	1/1	0.97	0.37	-	1,1,1,1	1
57	MG	CA	1645	1/1	0.84	0.30	-	46,46,46,46	0
57	MG	BA	3183	1/1	0.96	0.76	-	52,52,52,52	0
57	MG	AA	1793	1/1	0.94	0.18	-	6,6,6,6	1
57	MG	DA	3143	1/1	0.98	0.39	-	24,24,24,24	0
57	MG	AA	1788	1/1	0.78	0.30	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	CA	1604	1/1	0.96	0.10	-	41,41,41,41	0
57	MG	CA	1768	1/1	0.91	0.58	-	5,5,5,5	1
57	MG	CA	1756	1/1	0.83	0.55	-	56,56,56,56	0
57	MG	BA	3392	1/1	0.58	0.19	-	70,70,70,70	0
57	MG	CA	1628	1/1	0.96	0.68	-	35,35,35,35	0
57	MG	BN	203	1/1	0.92	0.18	-	56,56,56,56	1
57	MG	CA	1791	1/1	0.97	0.13	-	1,1,1,1	1
57	MG	DA	3136	1/1	0.85	0.27	-	9,9,9,9	1
57	MG	DA	3132	1/1	0.98	0.08	-	34,34,34,34	0
57	MG	BA	3259	1/1	0.98	0.08	-	1,1,1,1	1
57	MG	CA	1786	1/1	0.60	0.49	-	39,39,39,39	1
57	MG	DA	3342	1/1	0.99	0.21	-	1,1,1,1	1
57	MG	BA	3203	1/1	0.88	0.27	-	10,10,10,10	0
57	MG	DA	3372	1/1	0.83	0.72	-	35,35,35,35	1
57	MG	DB	209	1/1	0.80	0.40	-	96,96,96,96	1
57	MG	CA	1623	1/1	0.69	0.34	-	84,84,84,84	1
57	MG	DA	3070	1/1	0.97	0.35	-	40,40,40,40	1
57	MG	DA	3214	1/1	0.71	0.35	-	64,64,64,64	1
57	MG	DA	3202	1/1	0.86	0.89	-	7,7,7,7	1
57	MG	AW	106	1/1	0.81	0.54	-	26,26,26,26	1
57	MG	CA	1774	1/1	0.86	0.32	-	74,74,74,74	0
57	MG	BA	3363	1/1	0.96	0.12	-	90,90,90,90	0
57	MG	BA	3391	1/1	0.91	0.33	-	30,30,30,30	0
57	MG	AA	1726	1/1	0.84	0.32	-	10,10,10,10	0
57	MG	BA	3248	1/1	0.94	0.17	-	10,10,10,10	0
57	MG	BA	3006	1/1	0.77	0.46	-	77,77,77,77	0
57	MG	BA	3354	1/1	0.96	0.15	-	58,58,58,58	0
57	MG	DB	215	1/1	0.90	0.32	-	63,63,63,63	1
57	MG	BA	3175	1/1	0.94	0.11	-	21,21,21,21	0
57	MG	AA	1754	1/1	0.89	0.29	-	49,49,49,49	1
57	MG	DA	3150	1/1	0.84	0.47	-	39,39,39,39	1
57	MG	CV	102	1/1	0.73	0.45	-	57,57,57,57	0
57	MG	BA	3136	1/1	0.97	0.29	-	1,1,1,1	0
57	MG	AA	1718	1/1	0.79	0.41	-	1,1,1,1	1
57	MG	BA	3225	1/1	0.83	0.91	-	67,67,67,67	0
57	MG	DB	212	1/1	0.66	0.28	-	55,55,55,55	0
57	MG	CA	1718	1/1	0.73	0.94	-	59,59,59,59	0
57	MG	CA	1807	1/1	0.99	0.20	-	1,1,1,1	0
57	MG	DH	201	1/1	0.67	0.53	-	12,12,12,12	1
57	MG	DA	3381	1/1	0.99	0.17	-	65,65,65,65	0
57	MG	CA	1620	1/1	0.94	0.13	-	34,34,34,34	0
57	MG	B1	102	1/1	0.87	0.22	-	7,7,7,7	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	CA	1683	1/1	0.92	0.45	-	19,19,19,19	0
57	MG	BA	3205	1/1	0.93	0.15	-	23,23,23,23	0
57	MG	AK	201	1/1	0.78	0.43	-	33,33,33,33	1
57	MG	BA	3020	1/1	0.91	0.24	-	21,21,21,21	0
57	MG	BU	202	1/1	0.97	0.26	-	18,18,18,18	1
57	MG	DA	3025	1/1	0.97	0.19	-	5,5,5,5	0
57	MG	BF	303	1/1	0.89	0.18	-	36,36,36,36	0
57	MG	BA	3405	1/1	0.86	0.36	-	22,22,22,22	0
57	MG	DA	3300	1/1	0.96	0.19	-	38,38,38,38	0
57	MG	BA	3344	1/1	0.98	0.17	-	1,1,1,1	1
57	MG	DA	3203	1/1	0.95	0.40	-	1,1,1,1	1
57	MG	BA	3275	1/1	0.92	0.14	-	37,37,37,37	0
57	MG	CA	1658	1/1	0.68	0.97	-	24,24,24,24	1
57	MG	BA	3300	1/1	0.96	0.28	-	1,1,1,1	1
57	MG	AA	1681	1/1	0.95	0.30	-	14,14,14,14	0
57	MG	BA	3107	1/1	0.91	0.18	-	23,23,23,23	0
57	MG	AA	1715	1/1	0.83	0.98	-	29,29,29,29	1
57	MG	DA	3226	1/1	0.94	0.33	-	48,48,48,48	0
57	MG	AA	1694	1/1	0.89	0.25	-	13,13,13,13	1
57	MG	BA	3313	1/1	0.97	0.40	-	18,18,18,18	0
57	MG	AA	1767	1/1	0.90	0.27	-	21,21,21,21	0
57	MG	CL	202	1/1	0.91	0.33	-	5,5,5,5	1
57	MG	BA	3316	1/1	0.74	0.60	-	1,1,1,1	1
57	MG	BF	304	1/1	0.82	0.35	-	9,9,9,9	1
57	MG	CA	1732	1/1	0.98	0.27	-	10,10,10,10	0
57	MG	BA	3406	1/1	0.91	0.45	-	19,19,19,19	0
57	MG	CA	1655	1/1	0.82	0.55	-	69,69,69,69	1
57	MG	AA	1667	1/1	0.94	0.38	-	17,17,17,17	0
57	MG	BA	3223	1/1	0.98	0.21	-	9,9,9,9	1
57	MG	DB	207	1/1	0.94	0.25	-	16,16,16,16	1
57	MG	CA	1804	1/1	0.76	0.32	-	45,45,45,45	0
57	MG	DA	3122	1/1	0.99	0.19	-	8,8,8,8	0
57	MG	DA	3169	1/1	0.98	0.33	-	1,1,1,1	1
57	MG	DA	3107	1/1	0.92	0.37	-	34,34,34,34	0
57	MG	AD	302	1/1	0.91	0.44	-	28,28,28,28	0
57	MG	DA	3394	1/1	0.95	0.17	-	30,30,30,30	1
57	MG	DA	3249	1/1	0.96	0.11	-	1,1,1,1	0
57	MG	BB	211	1/1	0.97	0.30	-	44,44,44,44	1
57	MG	BB	216	1/1	0.99	0.36	-	1,1,1,1	1
57	MG	CA	1643	1/1	0.77	0.99	-	73,73,73,73	1
57	MG	DA	3276	1/1	0.93	0.22	-	47,47,47,47	0
57	MG	BA	3156	1/1	0.89	0.64	-	12,12,12,12	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	DA	3352	1/1	0.95	0.27	-	123,123,123,123	1
57	MG	BA	3033	1/1	0.96	0.30	-	20,20,20,20	0
57	MG	BA	3113	1/1	0.95	0.29	-	1,1,1,1	0
57	MG	BA	3231	1/1	0.01	0.84	-	102,102,102,102	0
57	MG	DA	3159	1/1	0.70	0.30	-	21,21,21,21	0
57	MG	DA	3340	1/1	0.92	0.15	-	59,59,59,59	0
57	MG	CA	1692	1/1	0.82	0.32	-	74,74,74,74	1
57	MG	CA	1703	1/1	0.94	0.28	-	12,12,12,12	0
57	MG	CA	1701	1/1	0.96	0.24	-	3,3,3,3	0
57	MG	BA	3235	1/1	0.95	0.44	-	22,22,22,22	0
57	MG	CA	1797	1/1	0.79	1.54	-	82,82,82,82	1
57	MG	BA	3437	1/1	0.86	0.32	-	64,64,64,64	0
57	MG	CV	101	1/1	0.73	0.15	-	41,41,41,41	0
57	MG	AA	1671	1/1	0.85	0.33	-	47,47,47,47	0
57	MG	AA	1679	1/1	0.83	0.47	-	12,12,12,12	1
57	MG	BA	3147	1/1	0.98	0.73	-	1,1,1,1	1
57	MG	CA	1614	1/1	0.97	0.34	-	6,6,6,6	0
57	MG	DA	3188	1/1	0.98	0.19	-	26,26,26,26	0
57	MG	DA	3038	1/1	0.99	0.20	-	3,3,3,3	1
57	MG	CA	1663	1/1	0.98	0.57	-	15,15,15,15	1
57	MG	BA	3347	1/1	0.94	0.50	-	1,1,1,1	0
57	MG	DA	3005	1/1	0.92	0.11	-	22,22,22,22	0
57	MG	BB	205	1/1	0.99	0.11	-	6,6,6,6	1
57	MG	CA	1719	1/1	0.93	0.20	-	56,56,56,56	1
57	MG	BA	3034	1/1	0.98	0.13	-	15,15,15,15	0
57	MG	DA	3091	1/1	0.98	0.14	-	1,1,1,1	0
57	MG	DA	3285	1/1	0.85	0.53	-	13,13,13,13	1
57	MG	AA	1700	1/1	0.95	0.42	-	34,34,34,34	0
57	MG	BA	3272	1/1	0.93	0.15	-	1,1,1,1	1
57	MG	D3	101	1/1	0.88	0.27	-	42,42,42,42	0
57	MG	CA	1750	1/1	0.96	0.36	-	14,14,14,14	0
57	MG	CA	1678	1/1	0.95	0.10	-	4,4,4,4	0
57	MG	DX	102	1/1	0.96	0.26	-	23,23,23,23	1
57	MG	BA	3221	1/1	0.97	0.16	-	49,49,49,49	0
57	MG	DA	3411	1/1	0.95	0.17	-	19,19,19,19	0
57	MG	DB	204	1/1	0.87	0.43	-	89,89,89,89	1
57	MG	DA	3378	1/1	0.99	0.21	-	18,18,18,18	1
57	MG	AX	103	1/1	0.98	0.09	-	1,1,1,1	1
57	MG	BA	3332	1/1	0.91	0.37	-	64,64,64,64	0
57	MG	BA	3046	1/1	0.97	0.12	-	15,15,15,15	0
57	MG	CA	1794	1/1	0.82	0.68	-	68,68,68,68	0
57	MG	CW	106	1/1	0.47	1.15	-	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3086	1/1	0.93	0.52	-	1,1,1,1	0
57	MG	DA	3304	1/1	0.97	0.46	-	1,1,1,1	1
57	MG	DA	3002	1/1	0.99	0.12	-	6,6,6,6	1
57	MG	CA	1743	1/1	0.83	0.33	-	64,64,64,64	0
57	MG	BA	3420	1/1	0.99	0.12	-	10,10,10,10	0
57	MG	DA	3163	1/1	0.82	0.46	-	17,17,17,17	1
57	MG	DA	3117	1/1	0.94	0.34	-	5,5,5,5	0
57	MG	AW	111	1/1	0.42	0.32	-	76,76,76,76	1
57	MG	CA	1684	1/1	0.83	0.36	-	59,59,59,59	0
57	MG	AW	101	1/1	0.96	1.05	-	51,51,51,51	1
57	MG	DA	3207	1/1	0.86	0.54	-	36,36,36,36	1
57	MG	DA	3124	1/1	0.96	0.22	-	24,24,24,24	0
57	MG	DA	3284	1/1	0.94	0.38	-	18,18,18,18	0
57	MG	BA	3423	1/1	-0.04	0.63	-	54,54,54,54	1
57	MG	BD	302	1/1	0.98	0.26	-	1,1,1,1	0
57	MG	BA	3237	1/1	0.98	0.13	-	8,8,8,8	1
57	MG	CW	118	1/1	0.70	0.43	-	1,1,1,1	1
57	MG	DA	3181	1/1	0.83	0.36	-	47,47,47,47	1
57	MG	BA	3381	1/1	0.99	0.11	-	23,23,23,23	0
57	MG	CX	102	1/1	0.97	0.17	-	1,1,1,1	1
57	MG	BA	3172	1/1	0.97	0.30	-	100,100,100,100	1
57	MG	DA	3126	1/1	0.92	0.20	-	1,1,1,1	0
57	MG	CA	1731	1/1	0.54	0.49	-	54,54,54,54	0
57	MG	BA	3041	1/1	0.98	0.19	-	46,46,46,46	1
57	MG	DA	3320	1/1	0.82	0.55	-	75,75,75,75	0
57	MG	DA	3034	1/1	0.96	0.29	-	33,33,33,33	0
57	MG	BA	3341	1/1	0.93	0.16	-	4,4,4,4	1
57	MG	BA	3309	1/1	0.76	0.65	-	47,47,47,47	0
57	MG	BA	3114	1/1	0.96	0.28	-	1,1,1,1	0
57	MG	DA	3021	1/1	0.98	0.19	-	2,2,2,2	1
57	MG	DA	3325	1/1	0.85	0.26	-	72,72,72,72	0
57	MG	DA	3230	1/1	0.98	0.13	-	35,35,35,35	0
57	MG	CW	107	1/1	0.81	1.01	-	84,84,84,84	0
57	MG	BB	208	1/1	0.85	0.16	-	38,38,38,38	1
57	MG	DA	3338	1/1	0.92	0.30	-	16,16,16,16	1
57	MG	BA	3078	1/1	0.99	0.17	-	1,1,1,1	0
57	MG	BA	3369	1/1	0.83	0.15	-	50,50,50,50	0
57	MG	CA	1728	1/1	0.85	0.38	-	41,41,41,41	1
57	MG	DA	3391	1/1	0.95	0.12	-	19,19,19,19	0
57	MG	B2	602	1/1	0.95	0.25	-	1,1,1,1	1
57	MG	BA	3415	1/1	0.91	0.17	-	18,18,18,18	1
57	MG	DA	3417	1/1	1.00	0.10	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	AA	1799	1/1	0.52	0.36	-	58,58,58,58	1
57	MG	CA	1775	1/1	0.92	0.22	-	1,1,1,1	1
57	MG	AA	1674	1/1	0.91	0.21	-	30,30,30,30	1
57	MG	CA	1685	1/1	0.96	0.21	-	25,25,25,25	1
57	MG	CA	1752	1/1	0.96	0.23	-	85,85,85,85	0
57	MG	BA	3090	1/1	0.97	0.25	-	24,24,24,24	1
57	MG	AA	1783	1/1	0.99	0.09	-	39,39,39,39	1
57	MG	CA	1734	1/1	0.96	0.22	-	46,46,46,46	1
57	MG	DB	219	1/1	0.67	0.75	-	56,56,56,56	1
57	MG	DA	3185	1/1	0.99	0.16	-	19,19,19,19	0
57	MG	DA	3414	1/1	0.92	0.18	-	16,16,16,16	0
57	MG	BA	3444	1/1	0.94	0.65	-	15,15,15,15	1
57	MG	AA	1736	1/1	0.88	0.45	-	20,20,20,20	0
57	MG	BA	3251	1/1	0.57	0.52	-	64,64,64,64	0
57	MG	CA	1619	1/1	0.98	0.07	-	3,3,3,3	0
57	MG	BA	3372	1/1	0.89	0.34	-	20,20,20,20	1
57	MG	DA	3067	1/1	0.95	0.32	-	1,1,1,1	0
57	MG	DA	3275	1/1	0.85	0.89	-	2,2,2,2	1
57	MG	AA	1604	1/1	0.99	0.08	-	3,3,3,3	0
57	MG	BA	3374	1/1	0.85	0.94	-	28,28,28,28	1
57	MG	DA	3409	1/1	0.77	1.58	-	83,83,83,83	1
57	MG	BA	3368	1/1	0.90	0.20	-	1,1,1,1	1
57	MG	DA	3360	1/1	0.82	0.09	-	5,5,5,5	0
57	MG	CA	1796	1/1	-0.37	0.28	-	95,95,95,95	1
57	MG	BA	3394	1/1	0.94	0.36	-	7,7,7,7	1
57	MG	BA	3388	1/1	0.89	0.57	-	4,4,4,4	1
57	MG	DA	3170	1/1	0.93	0.31	-	26,26,26,26	1
57	MG	DA	3402	1/1	0.90	0.23	-	45,45,45,45	1
57	MG	AA	1669	1/1	0.89	0.42	-	5,5,5,5	0
57	MG	DB	217	1/1	0.96	0.05	-	53,53,53,53	1
57	MG	BA	3303	1/1	0.93	0.39	-	8,8,8,8	1
57	MG	CA	1622	1/1	0.90	0.23	-	39,39,39,39	0
57	MG	CA	1674	1/1	0.80	0.24	-	44,44,44,44	1
57	MG	BB	218	1/1	0.90	0.11	-	18,18,18,18	0
57	MG	DA	3332	1/1	0.81	0.34	-	41,41,41,41	1
57	MG	AA	1675	1/1	0.99	0.28	-	41,41,41,41	1
57	MG	BA	3417	1/1	0.84	0.54	-	17,17,17,17	1
57	MG	DA	3116	1/1	0.99	0.40	-	1,1,1,1	1
57	MG	AA	1701	1/1	0.87	0.59	-	8,8,8,8	1
57	MG	BA	3438	1/1	0.97	0.08	-	44,44,44,44	0
57	MG	BA	3356	1/1	0.88	0.30	-	3,3,3,3	1
57	MG	AA	1696	1/1	0.85	0.42	-	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	DB	218	1/1	0.82	0.25	-	30,30,30,30	1
57	MG	BA	3273	1/1	0.99	0.14	-	57,57,57,57	1
57	MG	DA	3220	1/1	0.79	0.79	-	86,86,86,86	0
57	MG	BA	3165	1/1	0.98	0.09	-	4,4,4,4	1
57	MG	BA	3082	1/1	0.97	0.17	-	1,1,1,1	1
57	MG	BA	3342	1/1	0.97	0.16	-	26,26,26,26	1
57	MG	BA	3366	1/1	0.93	0.54	-	38,38,38,38	1
57	MG	BA	3219	1/1	0.90	0.63	-	1,1,1,1	1
57	MG	BA	3285	1/1	0.83	0.54	-	40,40,40,40	0
57	MG	BA	3097	1/1	0.98	0.10	-	1,1,1,1	0
57	MG	DF	303	1/1	0.95	0.61	-	4,4,4,4	1
57	MG	DA	3397	1/1	0.98	0.31	-	1,1,1,1	0
57	MG	AA	1730	1/1	0.99	0.13	-	1,1,1,1	1
57	MG	DA	3193	1/1	0.97	0.12	-	1,1,1,1	1
57	MG	BA	3416	1/1	0.89	0.35	-	13,13,13,13	0
57	MG	CA	1618	1/1	0.99	0.07	-	22,22,22,22	1
57	MG	BA	3365	1/1	0.83	0.36	-	36,36,36,36	0
57	MG	DA	3333	1/1	0.95	0.10	-	15,15,15,15	0
57	MG	AA	1673	1/1	0.96	0.13	-	12,12,12,12	1
57	MG	BA	3305	1/1	0.96	0.09	-	37,37,37,37	0
57	MG	DA	3033	1/1	0.94	0.20	-	13,13,13,13	0
57	MG	BG	201	1/1	0.92	0.09	-	17,17,17,17	0
57	MG	BB	220	1/1	-0.38	1.19	-	71,71,71,71	1
57	MG	AA	1774	1/1	0.96	0.30	-	23,23,23,23	0
57	MG	AA	1614	1/1	0.95	0.59	-	11,11,11,11	0
57	MG	DA	3191	1/1	0.96	0.18	-	5,5,5,5	1
57	MG	DA	3139	1/1	0.79	0.60	-	53,53,53,53	0
57	MG	AA	1661	1/1	0.98	0.09	-	10,10,10,10	1
57	MG	DA	3287	1/1	0.96	0.14	-	28,28,28,28	0
57	MG	BA	3249	1/1	0.98	0.41	-	58,58,58,58	0
57	MG	BA	3174	1/1	0.95	0.19	-	1,1,1,1	1
57	MG	BA	3131	1/1	0.97	0.12	-	1,1,1,1	0
57	MG	DA	3055	1/1	0.96	0.08	-	1,1,1,1	0
57	MG	DA	3439	1/1	0.28	1.57	-	85,85,85,85	1
57	MG	CA	1668	1/1	0.79	0.27	-	43,43,43,43	0
57	MG	DA	3177	1/1	0.90	0.50	-	22,22,22,22	0
57	MG	BA	3088	1/1	0.86	0.31	-	1,1,1,1	1
57	MG	AA	1659	1/1	0.90	0.53	-	27,27,27,27	0
57	MG	BA	3283	1/1	0.99	0.16	-	2,2,2,2	0
57	MG	AA	1605	1/1	0.98	0.43	-	3,3,3,3	0
57	MG	DA	3250	1/1	0.96	0.18	-	1,1,1,1	0
57	MG	CA	1709	1/1	0.77	0.19	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	DA	3044	1/1	0.99	0.27	-	60,60,60,60	0
57	MG	DA	3166	1/1	0.88	0.35	-	43,43,43,43	0
57	MG	BA	3312	1/1	0.95	0.22	-	1,1,1,1	0
57	MG	BA	3403	1/1	0.97	0.21	-	55,55,55,55	1
57	MG	CA	1725	1/1	0.62	0.63	-	43,43,43,43	1
57	MG	CA	1722	1/1	0.98	0.09	-	1,1,1,1	1
57	MG	CA	1742	1/1	0.87	0.71	-	1,1,1,1	1
57	MG	DA	3432	1/1	0.93	0.41	-	50,50,50,50	0
57	MG	CA	1788	1/1	0.73	0.34	-	1,1,1,1	1
57	MG	BA	3264	1/1	0.83	1.21	-	66,66,66,66	0
57	MG	DA	3236	1/1	0.88	0.39	-	14,14,14,14	0
57	MG	CA	1704	1/1	0.82	0.81	-	62,62,62,62	0
57	MG	AA	1743	1/1	0.62	0.64	-	74,74,74,74	1
57	MG	DA	3347	1/1	0.99	0.31	-	35,35,35,35	1
57	MG	CA	1702	1/1	0.86	0.65	-	47,47,47,47	0
57	MG	AA	1744	1/1	0.93	0.43	-	22,22,22,22	0
57	MG	DA	3056	1/1	0.97	0.24	-	11,11,11,11	0
57	MG	BA	3297	1/1	0.90	0.26	-	12,12,12,12	0
57	MG	DA	3257	1/1	0.99	0.15	-	54,54,54,54	0
57	MG	DA	3050	1/1	0.98	0.45	-	136,136,136,136	1
57	MG	BA	3014	1/1	0.68	0.77	-	51,51,51,51	0
57	MG	AA	1664	1/1	0.97	0.21	-	4,4,4,4	0
57	MG	DA	3307	1/1	0.77	0.49	-	43,43,43,43	0
57	MG	BA	3023	1/1	0.97	0.10	-	1,1,1,1	1
57	MG	BA	3281	1/1	0.44	1.97	-	43,43,43,43	1
57	MG	AA	1755	1/1	0.91	0.25	-	47,47,47,47	0
57	MG	CA	1751	1/1	0.96	0.31	-	10,10,10,10	0
57	MG	DA	3434	1/1	0.70	0.38	-	98,98,98,98	0
57	MG	CA	1753	1/1	0.97	0.20	-	7,7,7,7	1
57	MG	AA	1749	1/1	0.72	0.45	-	1,1,1,1	1
57	MG	AA	1717	1/1	0.93	0.19	-	12,12,12,12	1
57	MG	BA	3294	1/1	0.85	0.54	-	55,55,55,55	0
57	MG	AA	1719	1/1	0.93	0.26	-	1,1,1,1	1
57	MG	AA	1617	1/1	0.95	0.11	-	6,6,6,6	1
57	MG	DA	3301	1/1	0.17	1.62	-	55,55,55,55	1
57	MG	BA	3024	1/1	0.98	0.45	-	44,44,44,44	1
57	MG	CA	1647	1/1	0.94	0.43	-	82,82,82,82	0
57	MG	DA	3102	1/1	0.89	0.17	-	3,3,3,3	0
57	MG	B2	601	1/1	0.97	0.53	-	22,22,22,22	0
57	MG	CA	1606	1/1	0.96	0.43	-	29,29,29,29	0
57	MG	DA	3190	1/1	0.97	0.41	-	32,32,32,32	0
57	MG	BA	3227	1/1	0.60	1.37	-	71,71,71,71	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3142	1/1	0.98	0.15	-	67,67,67,67	0
57	MG	BA	3105	1/1	0.98	0.17	-	1,1,1,1	0
57	MG	AA	1606	1/1	0.97	0.15	-	1,1,1,1	0
57	MG	CA	1772	1/1	0.91	0.18	-	60,60,60,60	0
57	MG	AA	1722	1/1	0.97	0.12	-	37,37,37,37	0
57	MG	AX	104	1/1	0.99	0.11	-	55,55,55,55	1
57	MG	BA	3064	1/1	0.98	0.30	-	1,1,1,1	0
57	MG	BA	3419	1/1	0.98	0.07	-	57,57,57,57	1
57	MG	BA	3181	1/1	0.95	0.09	-	17,17,17,17	0
57	MG	BA	3217	1/1	0.95	0.33	-	35,35,35,35	0
57	MG	AA	1677	1/1	0.96	0.12	-	42,42,42,42	0
57	MG	BA	3157	1/1	0.86	0.20	-	28,28,28,28	0
57	MG	DA	3403	1/1	0.91	0.49	-	47,47,47,47	1
57	MG	AA	1795	1/1	0.97	0.16	-	1,1,1,1	0
57	MG	BA	3398	1/1	0.96	0.10	-	11,11,11,11	0
57	MG	CA	1729	1/1	0.89	0.56	-	63,63,63,63	0
57	MG	BA	3133	1/1	0.96	0.22	-	1,1,1,1	0
57	MG	DB	216	1/1	0.82	0.28	-	54,54,54,54	0
57	MG	CA	1735	1/1	0.80	0.31	-	1,1,1,1	1
57	MG	BA	3121	1/1	0.95	0.35	-	30,30,30,30	0
57	MG	BA	3442	1/1	0.94	0.16	-	33,33,33,33	0
57	MG	B5	102	1/1	0.94	0.36	-	48,48,48,48	0
57	MG	DA	3295	1/1	0.57	0.23	-	79,79,79,79	0
57	MG	AA	1791	1/1	0.70	1.26	-	35,35,35,35	1
57	MG	BA	3098	1/1	0.97	0.15	-	1,1,1,1	0
57	MG	BA	3385	1/1	0.93	0.16	-	7,7,7,7	0
57	MG	DA	3373	1/1	0.93	0.26	-	74,74,74,74	0
57	MG	CA	1682	1/1	0.96	0.24	-	9,9,9,9	0
57	MG	CA	1673	1/1	0.69	0.11	-	57,57,57,57	0
57	MG	AA	1608	1/1	0.92	0.06	-	3,3,3,3	0
57	MG	AA	1706	1/1	0.45	0.57	-	58,58,58,58	1
57	MG	BA	3031	1/1	0.99	0.30	-	1,1,1,1	0
57	MG	DD	303	1/1	0.94	0.20	-	1,1,1,1	0
57	MG	BA	3170	1/1	0.99	0.09	-	1,1,1,1	1
57	MG	BA	3184	1/1	0.93	0.11	-	44,44,44,44	0
57	MG	BA	3037	1/1	0.95	0.25	-	27,27,27,27	0
57	MG	AA	1727	1/1	0.98	0.14	-	63,63,63,63	0
57	MG	BA	3284	1/1	0.89	0.30	-	12,12,12,12	1
57	MG	BA	3410	1/1	0.97	0.20	-	6,6,6,6	1
57	MG	BA	3179	1/1	0.92	0.18	-	30,30,30,30	0
57	MG	DA	3254	1/1	0.98	0.24	-	109,109,109,109	1
57	MG	DA	3151	1/1	0.97	0.20	-	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3228	1/1	0.93	0.24	-	50,50,50,50	0
57	MG	BA	3164	1/1	0.94	0.46	-	56,56,56,56	0
57	MG	BA	3159	1/1	0.93	0.40	-	1,1,1,1	0
57	MG	AA	1711	1/1	0.99	0.13	-	21,21,21,21	1
57	MG	AA	1663	1/1	0.90	0.59	-	36,36,36,36	0
57	MG	DA	3364	1/1	0.96	0.26	-	42,42,42,42	0
57	MG	DA	3036	1/1	0.96	0.46	-	13,13,13,13	1
57	MG	AA	1665	1/1	0.89	0.44	-	21,21,21,21	0
57	MG	DA	3413	1/1	0.97	0.10	-	10,10,10,10	1
57	MG	D1	102	1/1	0.88	0.33	-	51,51,51,51	0
57	MG	DA	3327	1/1	0.97	0.07	-	2,2,2,2	1
57	MG	D5	101	1/1	0.97	0.10	-	20,20,20,20	0
57	MG	BA	3331	1/1	0.91	0.14	-	11,11,11,11	1
57	MG	DA	3280	1/1	0.95	0.16	-	24,24,24,24	1
57	MG	AA	1699	1/1	0.97	0.07	-	1,1,1,1	1
57	MG	AA	1746	1/1	0.91	0.39	-	29,29,29,29	0
57	MG	CA	1670	1/1	0.95	0.13	-	23,23,23,23	0
57	MG	AA	1688	1/1	0.91	0.45	-	12,12,12,12	1
57	MG	AA	1657	1/1	0.98	0.17	-	8,8,8,8	1
57	MG	DA	3209	1/1	0.97	0.25	-	1,1,1,1	1
57	MG	AE	202	1/1	0.90	0.20	-	37,37,37,37	0
57	MG	BA	3252	1/1	0.91	0.31	-	23,23,23,23	0
57	MG	CW	123	1/1	0.42	0.33	-	1,1,1,1	1
57	MG	AL	202	1/1	0.96	0.20	-	1,1,1,1	0
57	MG	BA	3093	1/1	0.93	0.14	-	1,1,1,1	0
57	MG	BA	3104	1/1	0.97	0.10	-	1,1,1,1	0
57	MG	AA	1771	1/1	0.96	0.17	-	9,9,9,9	0
57	MG	DB	203	1/1	0.97	0.30	-	60,60,60,60	0
57	MG	DG	201	1/1	0.88	0.22	-	38,38,38,38	0
57	MG	BA	3229	1/1	0.78	0.20	-	39,39,39,39	0
57	MG	BA	3141	1/1	0.83	0.26	-	6,6,6,6	1
57	MG	DA	3145	1/1	0.93	0.47	-	56,56,56,56	1
57	MG	CA	1615	1/1	0.90	0.24	-	42,42,42,42	0
57	MG	DA	3346	1/1	0.75	0.44	-	115,115,115,115	0
57	MG	BA	3269	1/1	0.87	0.21	-	22,22,22,22	0
57	MG	AW	110	1/1	0.80	0.31	-	30,30,30,30	1
57	MG	AA	1748	1/1	0.80	0.18	-	73,73,73,73	0
57	MG	CA	1662	1/1	0.97	0.45	-	1,1,1,1	0
57	MG	CW	104	1/1	0.74	0.21	-	35,35,35,35	1
57	MG	BB	209	1/1	0.68	0.50	-	108,108,108,108	0
57	MG	DA	3233	1/1	0.93	0.29	-	1,1,1,1	1
57	MG	CA	1747	1/1	0.76	0.68	-	19,19,19,19	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	DA	3065	1/1	0.96	0.26	-	1,1,1,1	1
57	MG	DA	3395	1/1	0.91	0.65	-	1,1,1,1	0
57	MG	BA	3100	1/1	0.91	0.33	-	1,1,1,1	1
57	MG	DA	3111	1/1	0.98	0.14	-	4,4,4,4	0
57	MG	BA	3152	1/1	0.90	0.23	-	62,62,62,62	0
57	MG	AA	1621	1/1	0.92	0.12	-	3,3,3,3	0
57	MG	AA	1776	1/1	0.96	0.21	-	33,33,33,33	1
57	MG	BA	3254	1/1	0.98	0.05	-	5,5,5,5	0
57	MG	BA	3238	1/1	0.85	0.69	-	38,38,38,38	1
57	MG	DA	3357	1/1	0.94	0.07	-	52,52,52,52	0
57	MG	AA	1631	1/1	0.90	0.23	-	1,1,1,1	1
57	MG	AW	103	1/1	0.76	0.28	-	1,1,1,1	1
57	MG	BA	3370	1/1	0.91	0.31	-	37,37,37,37	0
57	MG	DA	3115	1/1	0.94	0.41	-	6,6,6,6	0
57	MG	DA	3279	1/1	0.82	0.46	-	75,75,75,75	0
57	MG	CA	1780	1/1	0.93	0.72	-	31,31,31,31	1
57	MG	DA	3400	1/1	0.79	0.80	-	61,61,61,61	1
57	MG	DA	3016	1/1	0.81	0.18	-	57,57,57,57	0
57	MG	BA	3421	1/1	0.92	0.67	-	39,39,39,39	1
57	MG	DA	3204	1/1	0.98	0.22	-	51,51,51,51	1
57	MG	DA	3355	1/1	0.79	0.19	-	42,42,42,42	1
57	MG	DA	3006	1/1	0.73	0.48	-	93,93,93,93	0
57	MG	BA	3429	1/1	0.92	0.16	-	32,32,32,32	0
57	MG	CA	1733	1/1	0.86	0.40	-	59,59,59,59	0
57	MG	CW	122	1/1	0.93	0.21	-	70,70,70,70	0
57	MG	DA	3326	1/1	0.75	0.82	-	96,96,96,96	1
57	MG	DA	3081	1/1	0.96	0.14	-	11,11,11,11	0
57	MG	CA	1759	1/1	0.31	2.40	-	108,108,108,108	1
57	MG	CA	1762	1/1	0.94	0.30	-	7,7,7,7	1
57	MG	CA	1602	1/1	0.70	0.62	-	72,72,72,72	0
57	MG	DA	3100	1/1	0.82	0.37	-	63,63,63,63	1
57	MG	DA	3152	1/1	0.78	0.66	-	62,62,62,62	1
57	MG	CA	1778	1/1	0.85	0.46	-	1,1,1,1	1
57	MG	BA	3280	1/1	0.90	0.23	-	72,72,72,72	0
57	MG	AA	1641	1/1	0.98	0.13	-	26,26,26,26	0
57	MG	BA	3045	1/1	0.98	0.23	-	1,1,1,1	1
57	MG	BA	3169	1/1	0.92	0.33	-	33,33,33,33	0
57	MG	BA	3324	1/1	0.67	0.34	-	56,56,56,56	0
57	MG	DA	3054	1/1	0.98	0.10	-	1,1,1,1	0
57	MG	AA	1728	1/1	0.93	0.16	-	34,34,34,34	0
57	MG	DA	3331	1/1	0.89	0.22	-	79,79,79,79	1
57	MG	DA	3316	1/1	0.83	0.40	-	14,14,14,14	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	AW	112	1/1	0.35	0.23	-	64,64,64,64	1
57	MG	DA	3060	1/1	0.98	0.23	-	1,1,1,1	0
57	MG	DA	3031	1/1	0.97	0.28	-	2,2,2,2	0
57	MG	AA	1648	1/1	0.93	0.17	-	3,3,3,3	1
57	MG	CA	1755	1/1	0.94	0.30	-	1,1,1,1	0
57	MG	DA	3162	1/1	0.95	0.14	-	2,2,2,2	1
57	MG	AL	201	1/1	0.95	0.15	-	1,1,1,1	1
57	MG	CW	108	1/1	0.86	0.43	-	28,28,28,28	1
57	MG	CA	1610	1/1	0.88	0.23	-	15,15,15,15	1
57	MG	BA	3315	1/1	0.83	0.55	-	87,87,87,87	0
57	MG	CA	1603	1/1	0.98	0.22	-	77,77,77,77	0
57	MG	DA	3283	1/1	0.96	0.21	-	7,7,7,7	1
57	MG	BA	3325	1/1	0.80	0.26	-	30,30,30,30	0
57	MG	BA	3028	1/1	0.97	0.41	-	1,1,1,1	0
57	MG	D1	104	1/1	0.59	0.56	-	74,74,74,74	1
57	MG	AA	1780	1/1	0.46	0.68	-	95,95,95,95	1
57	MG	DB	213	1/1	0.90	0.15	-	28,28,28,28	1
57	MG	DA	3367	1/1	0.72	0.56	-	95,95,95,95	1
57	MG	DA	3165	1/1	0.79	0.18	-	47,47,47,47	0
57	MG	AA	1640	1/1	0.83	0.33	-	18,18,18,18	0
57	MG	BA	3386	1/1	0.93	0.14	-	13,13,13,13	0
57	MG	DA	3013	1/1	0.95	0.51	-	7,7,7,7	1
57	MG	CA	1635	1/1	0.95	0.06	-	6,6,6,6	0
57	MG	DA	3427	1/1	0.97	0.22	-	1,1,1,1	0
57	MG	CA	1773	1/1	0.98	0.30	-	9,9,9,9	0
57	MG	DA	3258	1/1	0.80	0.67	-	23,23,23,23	1
57	MG	DA	3368	1/1	0.92	0.37	-	78,78,78,78	0
57	MG	DA	3248	1/1	0.94	0.33	-	5,5,5,5	1
57	MG	DA	3365	1/1	0.95	0.21	-	24,24,24,24	1
57	MG	DA	3215	1/1	0.71	0.58	-	17,17,17,17	1
57	MG	BA	3154	1/1	0.89	0.19	-	56,56,56,56	0
57	MG	BA	3293	1/1	0.96	0.10	-	19,19,19,19	0
57	MG	DA	3043	1/1	0.97	0.16	-	6,6,6,6	0
57	MG	AA	1611	1/1	0.92	0.13	-	24,24,24,24	0
57	MG	BA	3127	1/1	0.97	0.45	-	3,3,3,3	1
57	MG	BA	3059	1/1	0.97	0.12	-	9,9,9,9	0
57	MG	AA	1676	1/1	0.86	0.24	-	32,32,32,32	0
57	MG	BA	3328	1/1	0.90	0.13	-	33,33,33,33	0
57	MG	AA	1766	1/1	0.94	0.20	-	1,1,1,1	1
57	MG	DA	3353	1/1	0.98	0.25	-	107,107,107,107	1
57	MG	AA	1616	1/1	0.92	0.12	-	24,24,24,24	1
57	MG	DA	3247	1/1	0.94	0.30	-	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3209	1/1	0.92	0.08	-	18,18,18,18	0
57	MG	AA	1632	1/1	0.98	0.19	-	4,4,4,4	0
57	MG	DA	3380	1/1	0.98	0.10	-	16,16,16,16	1
57	MG	BA	3334	1/1	0.70	0.45	-	51,51,51,51	1
57	MG	CA	1724	1/1	0.87	0.36	-	51,51,51,51	0
57	MG	CA	1626	1/1	0.98	0.09	-	23,23,23,23	0
57	MG	CA	1758	1/1	0.78	0.39	-	21,21,21,21	1
57	MG	BA	3074	1/1	0.99	0.08	-	1,1,1,1	1
57	MG	AW	117	1/1	0.89	0.18	-	19,19,19,19	1
57	MG	DA	3440	1/1	0.88	0.40	-	80,80,80,80	0
57	MG	CA	1666	1/1	0.92	0.28	-	1,1,1,1	0
57	MG	AA	1680	1/1	0.79	0.33	-	53,53,53,53	0
57	MG	DA	3330	1/1	0.91	0.30	-	73,73,73,73	0
57	MG	DA	3011	1/1	0.99	0.11	-	42,42,42,42	0
57	MG	DU	203	1/1	0.90	0.25	-	49,49,49,49	1
57	MG	DA	3134	1/1	0.96	0.31	-	8,8,8,8	0
57	MG	AA	1638	1/1	0.95	0.41	-	39,39,39,39	0
57	MG	BP	201	1/1	0.96	0.28	-	11,11,11,11	1
57	MG	CX	103	1/1	0.88	0.28	-	45,45,45,45	1
57	MG	AA	1655	1/1	0.92	0.33	-	31,31,31,31	0
57	MG	CW	114	1/1	0.93	0.17	-	4,4,4,4	1
57	MG	DA	3259	1/1	0.99	0.19	-	22,22,22,22	0
57	MG	DA	3024	1/1	0.96	0.32	-	32,32,32,32	0
57	MG	CA	1679	1/1	0.93	0.21	-	22,22,22,22	0
57	MG	AA	1602	1/1	0.92	0.15	-	64,64,64,64	0
57	MG	BA	3382	1/1	0.97	0.06	-	38,38,38,38	0
57	MG	AA	1800	1/1	0.86	0.29	-	38,38,38,38	0
57	MG	DA	3264	1/1	0.92	0.24	-	25,25,25,25	0
57	MG	DA	3187	1/1	0.94	0.74	-	83,83,83,83	1
57	MG	CA	1802	1/1	0.82	1.37	-	39,39,39,39	0
57	MG	BA	3265	1/1	0.98	0.10	-	37,37,37,37	0
57	MG	DA	3235	1/1	0.99	0.12	-	7,7,7,7	1
57	MG	DA	3302	1/1	0.86	0.27	-	80,80,80,80	1
57	MG	CA	1710	1/1	0.98	0.18	-	16,16,16,16	0
57	MG	BA	3160	1/1	0.95	0.38	-	6,6,6,6	0
57	MG	CA	1764	1/1	0.85	0.08	-	49,49,49,49	0
57	MG	BA	3253	1/1	0.93	0.37	-	56,56,56,56	1
57	MG	DB	208	1/1	0.82	0.17	-	53,53,53,53	1
57	MG	BB	214	1/1	0.93	0.15	-	34,34,34,34	0
57	MG	DA	3311	1/1	0.97	0.22	-	11,11,11,11	1
57	MG	DA	3290	1/1	0.88	0.49	-	21,21,21,21	0
57	MG	DA	3144	1/1	0.91	0.21	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3240	1/1	0.98	0.20	-	8,8,8,8	0
57	MG	AA	1770	1/1	0.99	0.11	-	16,16,16,16	1
57	MG	CA	1777	1/1	0.97	0.13	-	47,47,47,47	0
57	MG	AA	1737	1/1	0.79	0.36	-	30,30,30,30	1
57	MG	CW	112	1/1	0.79	0.47	-	24,24,24,24	1
57	MG	AA	1745	1/1	0.97	0.35	-	79,79,79,79	0
57	MG	DA	3278	1/1	0.65	0.33	-	36,36,36,36	1
57	MG	CA	1706	1/1	0.90	0.42	-	47,47,47,47	1
57	MG	DA	3263	1/1	0.99	0.14	-	16,16,16,16	0
57	MG	AA	1652	1/1	0.94	0.45	-	11,11,11,11	0
57	MG	BA	3215	1/1	0.94	0.72	-	38,38,38,38	1
57	MG	BA	3117	1/1	0.92	0.19	-	8,8,8,8	0
57	MG	CA	1633	1/1	0.97	0.08	-	2,2,2,2	0
57	MG	DA	3095	1/1	0.99	0.10	-	1,1,1,1	0
57	MG	AW	107	1/1	0.97	0.76	-	57,57,57,57	0
57	MG	BA	3426	1/1	0.95	0.20	-	27,27,27,27	0
57	MG	DA	3004	1/1	0.78	0.84	-	64,64,64,64	0
57	MG	AA	1790	1/1	0.92	0.28	-	35,35,35,35	0
57	MG	AV	102	1/1	0.71	0.41	-	73,73,73,73	0
57	MG	CA	1721	1/1	0.92	0.19	-	17,17,17,17	1
57	MG	DA	3206	1/1	0.84	0.69	-	32,32,32,32	1
57	MG	CA	1784	1/1	0.93	0.23	-	1,1,1,1	1
57	MG	DA	3341	1/1	0.94	0.56	-	20,20,20,20	0
57	MG	DA	3420	1/1	0.92	0.26	-	14,14,14,14	1
57	MG	DA	3041	1/1	0.95	0.12	-	24,24,24,24	0
57	MG	DA	3366	1/1	0.69	0.40	-	46,46,46,46	1
57	MG	BA	3132	1/1	0.92	0.12	-	24,24,24,24	1
57	MG	DA	3350	1/1	0.98	0.55	-	73,73,73,73	1
57	MG	DS	201	1/1	0.88	0.21	-	1,1,1,1	1
57	MG	DA	3231	1/1	0.93	0.45	-	14,14,14,14	0
57	MG	DA	3310	1/1	0.91	0.86	-	7,7,7,7	1
57	MG	DA	3217	1/1	0.94	0.25	-	31,31,31,31	0
57	MG	AA	1702	1/1	0.84	0.49	-	57,57,57,57	0
57	MG	BA	3168	1/1	0.76	0.37	-	29,29,29,29	0
57	MG	BA	3360	1/1	0.94	0.27	-	10,10,10,10	0
57	MG	BA	3163	1/1	0.88	0.21	-	33,33,33,33	0
57	MG	DA	3334	1/1	0.98	0.22	-	30,30,30,30	0
57	MG	DA	3240	1/1	0.97	0.13	-	72,72,72,72	0
57	MG	DA	3383	1/1	0.97	0.15	-	42,42,42,42	1
57	MG	DA	3319	1/1	0.76	0.25	-	116,116,116,116	1
57	MG	BA	3162	1/1	0.99	0.23	-	54,54,54,54	1
57	MG	CW	101	1/1	0.83	1.80	-	83,83,83,83	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	AA	1646	1/1	0.88	0.43	-	29,29,29,29	0
57	MG	BA	3298	1/1	0.99	0.17	-	1,1,1,1	1
57	MG	BA	3036	1/1	0.97	0.40	-	18,18,18,18	0
57	MG	BA	3146	1/1	0.96	0.13	-	1,1,1,1	0
57	MG	AA	1753	1/1	0.92	0.41	-	48,48,48,48	0
57	MG	BA	3103	1/1	0.83	0.95	-	33,33,33,33	1
57	MG	DA	3303	1/1	0.79	0.54	-	4,4,4,4	0
57	MG	BB	206	1/1	0.88	0.70	-	13,13,13,13	1
57	MG	CA	1749	1/1	0.97	0.10	-	49,49,49,49	1
57	MG	DA	3277	1/1	0.94	0.17	-	22,22,22,22	0
57	MG	DA	3339	1/1	0.90	0.50	-	1,1,1,1	1
57	MG	DA	3234	1/1	0.99	0.11	-	88,88,88,88	1
57	MG	AA	1682	1/1	0.87	0.22	-	46,46,46,46	0
57	MG	DN	201	1/1	0.95	0.18	-	21,21,21,21	1
57	MG	BA	3222	1/1	0.91	0.14	-	1,1,1,1	0
57	MG	BA	3010	1/1	0.81	0.91	-	17,17,17,17	1
57	MG	BA	3171	1/1	0.96	0.17	-	1,1,1,1	1
57	MG	CA	1680	1/1	0.89	0.23	-	75,75,75,75	1
57	MG	BB	219	1/1	0.94	0.46	-	73,73,73,73	1
57	MG	CA	1672	1/1	0.91	0.27	-	44,44,44,44	0
57	MG	BA	3011	1/1	0.94	0.42	-	15,15,15,15	0
57	MG	BA	3080	1/1	0.98	0.23	-	26,26,26,26	0
57	MG	BA	3357	1/1	0.98	0.17	-	105,105,105,105	1
57	MG	DA	3291	1/1	0.97	0.16	-	1,1,1,1	1
57	MG	BA	3055	1/1	0.98	0.16	-	1,1,1,1	0
57	MG	AA	1739	1/1	0.92	0.44	-	44,44,44,44	0
57	MG	CA	1785	1/1	0.44	0.42	-	112,112,112,112	0
57	MG	BA	3039	1/1	0.97	0.09	-	1,1,1,1	0
57	MG	BA	3040	1/1	0.94	0.09	-	16,16,16,16	0
57	MG	DA	3390	1/1	0.85	0.19	-	34,34,34,34	0
57	MG	BA	3233	1/1	0.96	0.30	-	1,1,1,1	0
57	MG	DA	3090	1/1	0.13	0.55	-	97,97,97,97	0
57	MG	AV	104	1/1	0.99	0.09	-	58,58,58,58	1
57	MG	DA	3210	1/1	0.94	0.11	-	93,93,93,93	1
57	MG	BA	3262	1/1	0.99	0.18	-	32,32,32,32	1
57	MG	CA	1766	1/1	0.98	0.16	-	1,1,1,1	0
57	MG	CA	1787	1/1	0.97	0.48	-	11,11,11,11	0
57	MG	BA	3192	1/1	0.95	0.46	-	15,15,15,15	0
57	MG	AA	1644	1/1	0.87	0.29	-	1,1,1,1	0
57	MG	BA	3375	1/1	0.89	0.14	-	62,62,62,62	0
57	MG	DA	3382	1/1	0.82	0.37	-	71,71,71,71	0
57	MG	BA	3220	1/1	0.99	0.16	-	16,16,16,16	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	BA	3441	1/1	0.84	0.19	-	6,6,6,6	1
57	MG	DA	3246	1/1	0.97	0.23	-	57,57,57,57	0
57	MG	DP	202	1/1	0.89	0.32	-	1,1,1,1	1
57	MG	DA	3359	1/1	0.94	0.17	-	40,40,40,40	0
57	MG	CA	1648	1/1	0.94	0.50	-	14,14,14,14	1
57	MG	BA	3139	1/1	0.93	0.39	-	8,8,8,8	1
57	MG	BA	3288	1/1	0.95	0.23	-	44,44,44,44	1
57	MG	DA	3176	1/1	0.62	0.62	-	77,77,77,77	0
57	MG	CA	1695	1/1	0.93	0.25	-	1,1,1,1	1

6.5 Other polymers (i)

There are no such residues in this entry.