wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:09 PM GMT

PDB ID	:	4V67
Title	:	Crystal structure of a translation termination complex formed with release factor RF2.
Authors	:	Korostelev, A.; Asahara, H.; Lancaster, L.; Laurberg, M.; Hirschi, A.; Noller, H.F.
Deposited on	:	2008-10-27
Resolution	:	3.00 Å(reported)

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

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

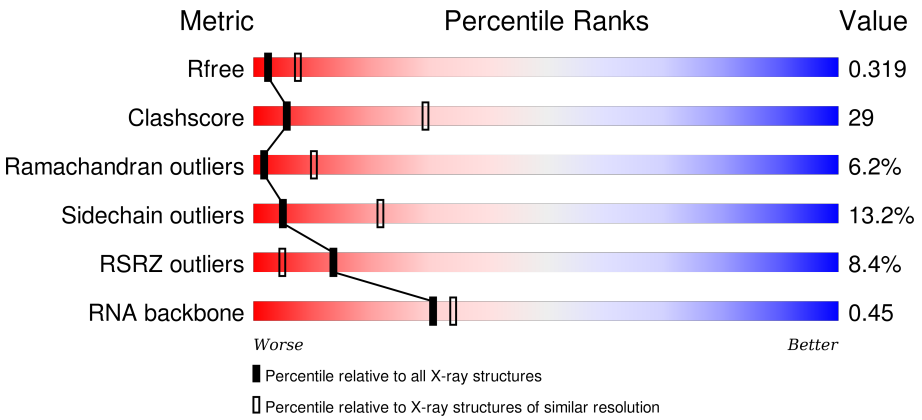
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	1525	% 33% 49% 14% • •
1	CA	1525	2% 31% 51% 13% • •
2	AY	77	38% 45% 17%
2	AZ	77	25% 36% 47% 16% •

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Mol	Chain	Length	Quality of chain
2	CY	77	43% 42% 16%
2	CZ	77	31% 35% 48% 16%
3	AV	27	4% 11% 15% 7% 63%
3	CV	27	7% 15% 7% 11% 63%
4	AB	256	10% 33% 52% 7% 9%
4	CB	256	12% 32% 51% 8% 9%
5	AC	239	5% 31% 47% 7% 14%
5	CC	239	6% 31% 48% 7% 14%
6	AD	209	8% 42% 49% 8%
6	CD	209	10% 45% 46% 8%
7	AE	162	6% 40% 42% 11% 7%
7	CE	162	2% 40% 43% 10% 7%
8	AF	101	2% 48% 48% 5%
8	CF	101	% 48% 49%
9	AG	156	6% 47% 49%
9	CG	156	6% 48% 48%
10	AH	138	3% 46% 46% 7%
10	CH	138	5% 46% 46% 6%
11	AI	128	13% 34% 53% 11%
11	CI	128	23% 34% 53% 10%
12	AJ	105	22% 31% 49% 11% 7%
12	CJ	105	24% 34% 46% 11% 7%
13	AK	129	5% 32% 49% 7% 12%
13	CK	129	12% 33% 49% 6% 12%
14	AL	134	3% 28% 51% 10% 9%

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Mol	Chain	Length	Quality of chain
14	CL	134	8% 31% 49% 10% • 9%
15	AM	126	11% 37% 47% 9% • 7%
15	CM	126	16% 35% 49% 8% • 7%
16	AN	61	13% 48% 44% 5% • •
16	CN	61	16% 43% 49% 5% • •
17	AO	89	% 42% 49% 8% •
17	CO	89	2% 43% 49% 7% •
18	AP	88	9% 33% 56% 6% 6%
18	CP	88	33% 33% 57% 5% 6%
19	AQ	105	% 35% 51% 8% 6%
19	CQ	105	8% 38% 48% 9% 6%
20	AR	88	5% 31% 42% 7% 20%
20	CR	88	14% 30% 40% 9% • 20%
21	AS	93	35% 26% 42% 14% • 16%
21	CS	93	29% 26% 42% 14% • 16%
22	AT	106	6% 28% 56% 9% 7%
22	CT	106	21% 28% 57% 8% 7%
23	AU	27	81% 33% 52% • 11%
23	CU	27	89% 33% 52% • 11%
24	AX	378	20% 34% 51% 10% • •
24	CX	378	24% 34% 52% 9% • •
25	BA	2894	3% 31% 48% 17% • •
25	DA	2894	3% 31% 48% 17% • •
26	BB	124	32% 50% 10% • •
26	DB	124	5% 33% 51% 10% • •

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Mol	Chain	Length	Quality of chain
27	BD	276	3% 36% 50% 11% • •
27	DD	276	% 36% 51% 10% • •
28	BE	206	6% 44% 45% 10% •
28	DE	206	14% 44% 45% 10% •
29	BF	210	3% 36% 50% 10% •
29	DF	210	3% 37% 48% 11% •
30	BG	182	18% 25% 61% 13% • •
30	DG	182	17% 25% 60% 13% • •
31	BH	180	20% 26% 52% 9% • 12%
31	DH	180	9% 24% 53% 10% • 12%
32	BI	148	11% 32% 52% 14% •
32	DI	148	5% 41% 45% 13% •
33	BK	147	52% 30% 59% 12%
33	DK	147	73% 31% 58% 12%
34	BN	163	7% 27% 43% 13% • 16%
34	DN	163	3% 26% 44% 13% • 16%
35	BO	122	43% 48% 10%
35	DO	122	46% 45% 9%
36	BP	150	9% 22% 45% 24% 6% •
36	DP	150	6% 21% 47% 24% 6% •
37	BQ	141	6% 24% 57% 12% • 5%
37	DQ	141	9% 28% 53% 12% • 5%
38	BR	118	31% 54% 14% •
38	DR	118	2% 31% 58% 10% •
39	BS	112	19% 25% 46% 14% • 13%

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Mol	Chain	Length	Quality of chain
39	DS	112	38% 24% 47% 14% • 13%
40	BT	146	10% 34% 45% 14% • 6%
40	DT	146	16% 36% 42% 14% • 6%
41	BU	118	4% 36% 53% 10% •
41	DU	118	18% 35% 53% 11% •
42	BV	101	7% 43% 40% 14% •
42	DV	101	8% 44% 41% 12% •
43	BW	113	% 40% 51% 8% •
43	DW	113	4% 38% 52% 9% •
44	BX	96	5% 33% 49% 14% •
44	DX	96	9% 36% 46% 14% •
45	BY	110	23% 31% 39% 19% • 9%
45	DY	110	15% 27% 41% 19% • 9%
46	BZ	206	8% 40% 44% 7% 9%
46	DZ	206	16% 40% 43% 8% 9%
47	B0	85	32% 48% 9% 11%
47	D0	85	2% 31% 49% 9% 11%
48	B1	98	4% 24% 43% 21% • 10%
48	D1	98	4% 21% 46% 21% • 10%
49	B2	72	3% 21% 42% 22% • 14%
49	D2	72	6% 17% 46% 22% • 14%
50	B3	60	12% 45% 52% • •
50	D3	60	3% 48% 47% • •
51	B4	97	2% 10% 14% 5% • 69%
51	D4	97	9% 16% • • 69%

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Mol	Chain	Length	Quality of chain
52	B5	60	3% 33% 43% 10% 13%
52	D5	60	3% 33% 47% 7% 13%
53	B6	54	59% 7% 52% 22% 19%
53	D6	54	67% 9% 50% 22% 19%
54	B7	49	22% 49% 41% 8%
54	D7	49	12% 47% 45% 6%
55	B8	65	12% 31% 51% 14%
55	D8	65	8% 29% 51% 15%

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
56	MG	AA	1613	-	-	-	X
56	MG	AA	1674	-	-	-	X
56	MG	AA	1686	-	-	-	X
56	MG	AA	1713	-	-	-	X
56	MG	AA	1725	-	-	-	X
56	MG	AA	1752	-	-	-	X
56	MG	AA	1768	-	-	-	X
56	MG	AA	1772	-	-	-	X
56	MG	AA	1782	-	-	-	X
56	MG	AA	1785	-	-	-	X
56	MG	AA	1793	-	-	-	X
56	MG	AA	1838	-	-	-	X
56	MG	AA	1874	-	-	-	X
56	MG	AA	1879	-	-	-	X
56	MG	AA	1893	-	-	-	X
56	MG	AA	1900	-	-	-	X
56	MG	AA	1903	-	-	-	X
56	MG	AA	1920	-	-	-	X
56	MG	AA	1975	-	-	-	X
56	MG	AA	1979	-	-	-	X
56	MG	AA	2009	-	-	-	X
56	MG	AA	2017	-	-	-	X
56	MG	AC	302	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AX	407	-	-	-	X
56	MG	AX	413	-	-	-	X
56	MG	AY	123	-	-	-	X
56	MG	BA	3007	-	-	-	X
56	MG	BA	3008	-	-	-	X
56	MG	BA	3009	-	-	-	X
56	MG	BA	3024	-	-	-	X
56	MG	BA	3042	-	-	-	X
56	MG	BA	3054	-	-	-	X
56	MG	BA	3073	-	-	-	X
56	MG	BA	3075	-	-	-	X
56	MG	BA	3077	-	-	-	X
56	MG	BA	3130	-	-	-	X
56	MG	BA	3131	-	-	-	X
56	MG	BA	3132	-	-	-	X
56	MG	BA	3143	-	-	-	X
56	MG	BA	3148	-	-	-	X
56	MG	BA	3150	-	-	-	X
56	MG	BA	3167	-	-	-	X
56	MG	BA	3168	-	-	-	X
56	MG	BA	3173	-	-	-	X
56	MG	BA	3197	-	-	-	X
56	MG	BA	3214	-	-	-	X
56	MG	BA	3218	-	-	-	X
56	MG	BA	3220	-	-	-	X
56	MG	BA	3234	-	-	-	X
56	MG	BA	3236	-	-	-	X
56	MG	BA	3266	-	-	-	X
56	MG	BA	3267	-	-	-	X
56	MG	BA	3270	-	-	-	X
56	MG	BA	3283	-	-	-	X
56	MG	BA	3294	-	-	-	X
56	MG	BA	3304	-	-	-	X
56	MG	BA	3311	-	-	-	X
56	MG	BA	3320	-	-	-	X
56	MG	BA	3330	-	-	-	X
56	MG	BA	3349	-	-	-	X
56	MG	BA	3350	-	-	-	X
56	MG	BA	3356	-	-	-	X
56	MG	BA	3361	-	-	-	X
56	MG	BA	3362	-	-	-	X
56	MG	BA	3368	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3376	-	-	-	X
56	MG	BA	3407	-	-	-	X
56	MG	BA	3416	-	-	-	X
56	MG	BA	3426	-	-	-	X
56	MG	BA	3428	-	-	-	X
56	MG	BA	3436	-	-	-	X
56	MG	BA	3460	-	-	-	X
56	MG	BA	3465	-	-	-	X
56	MG	BA	3467	-	-	-	X
56	MG	BA	3471	-	-	-	X
56	MG	BA	3521	-	-	-	X
56	MG	BA	3538	-	-	-	X
56	MG	BA	3549	-	-	-	X
56	MG	BA	3590	-	-	-	X
56	MG	BA	3594	-	-	-	X
56	MG	BA	3595	-	-	-	X
56	MG	BA	3597	-	-	-	X
56	MG	BA	3610	-	-	-	X
56	MG	BA	3611	-	-	-	X
56	MG	BA	3627	-	-	-	X
56	MG	BA	3633	-	-	-	X
56	MG	BA	3652	-	-	-	X
56	MG	BA	3662	-	-	-	X
56	MG	BA	3664	-	-	-	X
56	MG	BA	3667	-	-	-	X
56	MG	BA	3673	-	-	-	X
56	MG	BA	3709	-	-	-	X
56	MG	BA	3722	-	-	-	X
56	MG	BA	3724	-	-	-	X
56	MG	BA	3736	-	-	-	X
56	MG	BA	3739	-	-	-	X
56	MG	BA	3746	-	-	-	X
56	MG	BA	3751	-	-	-	X
56	MG	BA	3753	-	-	-	X
56	MG	BA	3808	-	-	-	X
56	MG	BA	3832	-	-	-	X
56	MG	BA	3840	-	-	-	X
56	MG	BA	3863	-	-	-	X
56	MG	BA	3865	-	-	-	X
56	MG	BA	3867	-	-	-	X
56	MG	BA	3872	-	-	-	X
56	MG	BA	3879	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3898	-	-	-	X
56	MG	BA	3900	-	-	-	X
56	MG	BA	3904	-	-	-	X
56	MG	BD	5001	-	-	-	X
56	MG	BD	5002	-	-	-	X
56	MG	BF	302	-	-	-	X
56	MG	BF	303	-	-	-	X
56	MG	BO	205	-	-	-	X
56	MG	CA	1623	-	-	-	X
56	MG	CA	1639	-	-	-	X
56	MG	CA	1653	-	-	-	X
56	MG	CA	1655	-	-	-	X
56	MG	CA	1663	-	-	-	X
56	MG	CA	1689	-	-	-	X
56	MG	CA	1697	-	-	-	X
56	MG	CA	1710	-	-	-	X
56	MG	CA	1712	-	-	-	X
56	MG	CA	1736	-	-	-	X
56	MG	CA	1749	-	-	-	X
56	MG	CA	1757	-	-	-	X
56	MG	CA	1769	-	-	-	X
56	MG	CA	1785	-	-	-	X
56	MG	CA	1788	-	-	-	X
56	MG	CA	1793	-	-	-	X
56	MG	DA	3004	-	-	-	X
56	MG	DA	3013	-	-	-	X
56	MG	DA	3028	-	-	-	X
56	MG	DA	3047	-	-	-	X
56	MG	DA	3051	-	-	-	X
56	MG	DA	3053	-	-	-	X
56	MG	DA	3062	-	-	-	X
56	MG	DA	3069	-	-	-	X
56	MG	DA	3074	-	-	-	X
56	MG	DA	3085	-	-	-	X
56	MG	DA	3092	-	-	-	X
56	MG	DA	3101	-	-	-	X
56	MG	DA	3120	-	-	-	X
56	MG	DA	3129	-	-	-	X
56	MG	DA	3131	-	-	-	X
56	MG	DA	3132	-	-	-	X
56	MG	DA	3134	-	-	-	X
56	MG	DA	3148	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3149	-	-	-	X
56	MG	DA	3159	-	-	-	X
56	MG	DA	3180	-	-	-	X
56	MG	DA	3190	-	-	-	X
56	MG	DA	3204	-	-	-	X
56	MG	DA	3207	-	-	-	X
56	MG	DA	3216	-	-	-	X
56	MG	DA	3257	-	-	-	X
56	MG	DA	3264	-	-	-	X
56	MG	DA	3269	-	-	-	X
56	MG	DA	3286	-	-	-	X
56	MG	DA	3287	-	-	-	X
56	MG	DA	3297	-	-	-	X
56	MG	DA	3315	-	-	-	X
56	MG	DA	3330	-	-	-	X
56	MG	DA	3332	-	-	-	X
56	MG	DA	3335	-	-	-	X
56	MG	DA	3339	-	-	-	X
56	MG	DA	3344	-	-	-	X
56	MG	DA	3409	-	-	-	X
56	MG	DA	3417	-	-	-	X
56	MG	DA	3418	-	-	-	X
56	MG	DA	3422	-	-	-	X
56	MG	DA	3423	-	-	-	X
56	MG	DA	3424	-	-	-	X
56	MG	DA	3442	-	-	-	X
56	MG	DA	3444	-	-	-	X
56	MG	DA	3445	-	-	-	X
56	MG	DA	3447	-	-	-	X
56	MG	DA	3451	-	-	-	X
56	MG	DA	3468	-	-	-	X
56	MG	DA	3470	-	-	-	X
56	MG	DA	3488	-	-	-	X
56	MG	DD	5005	-	-	-	X

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 301148 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
			Total	C	N	O	P			
1	AA	1504	32332	14391	5994	10444	1503	0	0	0
1	CA	1504	32332	14391	5994	10444	1503	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	466	G	C	CONFLICT	GB 155076
CA	466	G	C	CONFLICT	GB 155076

- Molecule 2 is a RNA chain called P AND E-SITE TRNA(FMET).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AZ	77	1640	732	297	535	76	0	0	0
2	AY	77	1640	732	297	535	76	0	0	0
2	CZ	77	1640	732	297	535	76	0	0	0
2	CY	77	1640	732	297	535	76	0	0	0

- Molecule 3 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	AV	10	214	98	44	63	9	0	0	0
3	CV	10	214	98	44	63	9	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AB	234	1900	1213	341	341	5	0	0	0
4	CB	234	1900	1213	341	341	5	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AC	206	1612	1016	314	281	1	0	0	0
5	CC	206	1612	1016	314	281	1	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	AE	151	1155	729	218	204	4	0	0	0
7	CE	151	1155	729	218	204	4	0	0	0

- Molecule 8 is a protein called 30S ribosomal protein S6.

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

- Molecule 9 is a protein called 30S ribosomal protein S7.

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

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

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AJ	98	794	499	156	138	1	0	0	0
			Total	C	N	O	S			
12	CJ	98	794	499	156	138	1	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AK	114	842	522	159	158	3	0	0	0
			Total	C	N	O	S			
13	CK	114	842	522	159	158	3	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AL	122	956	603	193	159	1	0	0	0
			Total	C	N	O	S			
14	CL	122	956	603	193	159	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	ALA	-	INSERTION	UNP P61941
AL	3	LEU	-	INSERTION	UNP P61941
CL	2	ALA	-	INSERTION	UNP P61941
CL	3	LEU	-	INSERTION	UNP P61941

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AM	117	933	577	192	162	2	0	0	0
			Total	C	N	O	S			
15	CM	117	933	577	192	162	2	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S14.

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

- Molecule 17 is a protein called 30S ribosomal protein S15.

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

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	AP	83	700	443	139	117	1	0	0	0
			Total	C	N	O	S			
18	CP	83	700	443	139	117	1	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AQ	99	823	528	152	141	2	0	0	0
19	CQ	99	823	528	152	141	2	0	0	0

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	AS	78	629	403	114	110	2	0	0	0
21	CS	78	629	403	114	110	2	0	0	0

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	AT	99	762	469	162	129	2	0	0	0
22	CT	99	762	469	162	129	2	0	0	0

- Molecule 23 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
23	AU	24	208	128	50	30	0	0	0
23	CU	24	208	128	50	30	0	0	0

- Molecule 24 is a protein called Bacterial peptide chain release factor 2 (RF-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	AX	362	2876	1794	518	556	8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	CX	362	2876	1794	518	556	8	0	0	0

- Molecule 25 is a RNA chain called 23S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	BA	2879	61997	27594	11582	19943	2878	0	0	0
			Total	C	N	O	P			
25	DA	2879	61997	27594	11582	19943	2878	0	0	0

- Molecule 26 is a RNA chain called 5S RRNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	BD	271	2104	1329	416	356	3	0	0	0
			Total	C	N	O	S			
27	DD	271	2104	1329	416	356	3	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	BE	204	1563	988	299	270	6	0	0	0
			Total	C	N	O	S			
28	DE	204	1563	988	299	270	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	BF	202	1586	1011	297	275	3	0	0	0
			Total	C	N	O	S			
29	DF	202	1586	1011	297	275	3	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	1	MET	-	INSERTION	UNP Q72I05
BF	2	LYS	-	INSERTION	UNP Q72I05
BF	3	GLU	-	INSERTION	UNP Q72I05
BF	4	VAL	-	INSERTION	UNP Q72I05
BF	5	ALA	-	INSERTION	UNP Q72I05
DF	1	MET	-	INSERTION	UNP Q72I05
DF	2	LYS	-	INSERTION	UNP Q72I05
DF	3	GLU	-	INSERTION	UNP Q72I05
DF	4	VAL	-	INSERTION	UNP Q72I05
DF	5	ALA	-	INSERTION	UNP Q72I05

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	BG	181	1475	943	268	260	4	0	0	0
30	DG	181	1475	943	268	260	4	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	BH	159	1222	773	228	220	1	0	0	0
31	DH	159	1222	773	228	220	1	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	BI	145	1132	724	200	207	1	0	0	0
32	DI	145	1132	724	200	207	1	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	BK	147	1088	692	191	199	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	DK	147	1088	692	191	199	6	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	BN	137	1096	707	205	181	3	0	0	0
			Total	C	N	O	S			
34	DN	137	1096	707	205	181	3	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	1	MET	-	INSERTION	UNP Q72IN1
BN	2	VAL	-	INSERTION	UNP Q72IN1
BN	3	LYS	-	INSERTION	UNP Q72IN1
BN	4	SER	-	INSERTION	UNP Q72IN1
BN	5	SER	-	INSERTION	UNP Q72IN1
BN	6	LEU	-	INSERTION	UNP Q72IN1
BN	7	ALA	-	INSERTION	UNP Q72IN1
BN	8	PHE	-	INSERTION	UNP Q72IN1
BN	9	LEU	-	INSERTION	UNP Q72IN1
BN	10	ARG	-	INSERTION	UNP Q72IN1
BN	11	GLY	-	INSERTION	UNP Q72IN1
BN	12	PRO	-	INSERTION	UNP Q72IN1
BN	13	PRO	-	INSERTION	UNP Q72IN1
BN	14	ILE	-	INSERTION	UNP Q72IN1
BN	15	PRO	-	INSERTION	UNP Q72IN1
BN	16	ARG	-	INSERTION	UNP Q72IN1
BN	17	GLN	-	INSERTION	UNP Q72IN1
BN	18	GLU	-	INSERTION	UNP Q72IN1
BN	19	GLN	-	INSERTION	UNP Q72IN1
BN	20	ARG	-	INSERTION	UNP Q72IN1
BN	21	ARG	-	INSERTION	UNP Q72IN1
BN	22	ALA	-	INSERTION	UNP Q72IN1
BN	23	LEU	-	INSERTION	UNP Q72IN1
BN	24	VAL	-	INSERTION	UNP Q72IN1
DN	1	MET	-	INSERTION	UNP Q72IN1
DN	2	VAL	-	INSERTION	UNP Q72IN1
DN	3	LYS	-	INSERTION	UNP Q72IN1
DN	4	SER	-	INSERTION	UNP Q72IN1

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Chain	Residue	Modelled	Actual	Comment	Reference
DN	5	SER	-	INSERTION	UNP Q72IN1
DN	6	LEU	-	INSERTION	UNP Q72IN1
DN	7	ALA	-	INSERTION	UNP Q72IN1
DN	8	PHE	-	INSERTION	UNP Q72IN1
DN	9	LEU	-	INSERTION	UNP Q72IN1
DN	10	ARG	-	INSERTION	UNP Q72IN1
DN	11	GLY	-	INSERTION	UNP Q72IN1
DN	12	PRO	-	INSERTION	UNP Q72IN1
DN	13	PRO	-	INSERTION	UNP Q72IN1
DN	14	ILE	-	INSERTION	UNP Q72IN1
DN	15	PRO	-	INSERTION	UNP Q72IN1
DN	16	ARG	-	INSERTION	UNP Q72IN1
DN	17	GLN	-	INSERTION	UNP Q72IN1
DN	18	GLU	-	INSERTION	UNP Q72IN1
DN	19	GLN	-	INSERTION	UNP Q72IN1
DN	20	ARG	-	INSERTION	UNP Q72IN1
DN	21	ARG	-	INSERTION	UNP Q72IN1
DN	22	ALA	-	INSERTION	UNP Q72IN1
DN	23	LEU	-	INSERTION	UNP Q72IN1
DN	24	VAL	-	INSERTION	UNP Q72IN1

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	BO	122	932	587	171	170	4	0	0	0
35	DO	122	932	587	171	170	4	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	BQ	134	1064	680	201	178	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	DQ	134	1064	680	201	178	5	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
39	BS	98	770	486	154	130	0	0	0
39	DS	98	770	486	154	130	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	BT	137	1143	713	234	195	1	0	0	0
40	DT	137	1143	713	234	195	1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	BU	117	964	610	202	151	1	0	0	0
41	DU	117	964	610	202	151	1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	BW	112	890	560	175	153	2	0	0	0
43	DW	112	890	560	175	153	2	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
44	BX	92	725	471	131	123	0	0	0
44	DX	92	725	471	131	123	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BY	100	775	500	148	123	4	0	0	0
45	DY	100	775	500	148	123	4	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	BZ	187	1482	945	264	271	2	0	0	0
46	DZ	187	1482	945	264	271	2	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	B0	76	605	376	126	102	1	0	0	0
47	D0	76	605	376	126	102	1	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
48	B1	88	694	435	141	118	0	0	0
48	D1	88	694	435	141	118	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	B2	62	520	325	102	91	2	0	0	0
49	D2	62	520	325	102	91	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	B3	59	467	298	90	78	1	0	0	0
50	D3	59	467	298	90	78	1	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	B4	30	225	142	36	43	4	0	0	0
51	D4	30	225	142	36	43	4	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B4	1	MET	-	INSERTION	UNP Q72JR0
B4	2	PRO	-	INSERTION	UNP Q72JR0
B4	3	LEU	-	INSERTION	UNP Q72JR0
B4	4	GLY	-	INSERTION	UNP Q72JR0
B4	5	VAL	-	INSERTION	UNP Q72JR0
B4	6	HIS	-	INSERTION	UNP Q72JR0
B4	7	PRO	-	INSERTION	UNP Q72JR0
B4	8	LEU	-	INSERTION	UNP Q72JR0
B4	9	TYR	-	INSERTION	UNP Q72JR0
B4	10	THR	-	INSERTION	UNP Q72JR0
B4	11	LYS	-	INSERTION	UNP Q72JR0

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Chain	Residue	Modelled	Actual	Comment	Reference
B4	12	ARG	-	INSERTION	UNP Q72JR0
B4	13	TRP	-	INSERTION	UNP Q72JR0
B4	14	LEU	-	INSERTION	UNP Q72JR0
B4	15	ALA	-	INSERTION	UNP Q72JR0
B4	16	HIS	-	INSERTION	UNP Q72JR0
B4	17	GLY	-	INSERTION	UNP Q72JR0
B4	18	GLN	-	INSERTION	UNP Q72JR0
B4	19	ASP	-	INSERTION	UNP Q72JR0
B4	20	ARG	-	INSERTION	UNP Q72JR0
B4	21	ALA	-	INSERTION	UNP Q72JR0
B4	22	LYS	-	INSERTION	UNP Q72JR0
B4	23	LYS	-	INSERTION	UNP Q72JR0
B4	24	GLU	-	INSERTION	UNP Q72JR0
B4	25	ALA	-	INSERTION	UNP Q72JR0
B4	26	ASN	-	INSERTION	UNP Q72JR0
B4	27	VAL	-	INSERTION	UNP Q72JR0
D4	1	MET	-	INSERTION	UNP Q72JR0
D4	2	PRO	-	INSERTION	UNP Q72JR0
D4	3	LEU	-	INSERTION	UNP Q72JR0
D4	4	GLY	-	INSERTION	UNP Q72JR0
D4	5	VAL	-	INSERTION	UNP Q72JR0
D4	6	HIS	-	INSERTION	UNP Q72JR0
D4	7	PRO	-	INSERTION	UNP Q72JR0
D4	8	LEU	-	INSERTION	UNP Q72JR0
D4	9	TYR	-	INSERTION	UNP Q72JR0
D4	10	THR	-	INSERTION	UNP Q72JR0
D4	11	LYS	-	INSERTION	UNP Q72JR0
D4	12	ARG	-	INSERTION	UNP Q72JR0
D4	13	TRP	-	INSERTION	UNP Q72JR0
D4	14	LEU	-	INSERTION	UNP Q72JR0
D4	15	ALA	-	INSERTION	UNP Q72JR0
D4	16	HIS	-	INSERTION	UNP Q72JR0
D4	17	GLY	-	INSERTION	UNP Q72JR0
D4	18	GLN	-	INSERTION	UNP Q72JR0
D4	19	ASP	-	INSERTION	UNP Q72JR0
D4	20	ARG	-	INSERTION	UNP Q72JR0
D4	21	ALA	-	INSERTION	UNP Q72JR0
D4	22	LYS	-	INSERTION	UNP Q72JR0
D4	23	LYS	-	INSERTION	UNP Q72JR0
D4	24	GLU	-	INSERTION	UNP Q72JR0
D4	25	ALA	-	INSERTION	UNP Q72JR0
D4	26	ASN	-	INSERTION	UNP Q72JR0

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Chain	Residue	Modelled	Actual	Comment	Reference
D4	27	VAL	-	INSERTION	UNP Q72JR0

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	B5	52	404	255	79	65	5	0	0	0
52	D5	52	404	255	79	65	5	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	B6	44	380	235	77	64	4	0	0	0
53	D6	44	380	235	77	64	4	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L34.

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

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	B8	63	507	326	101	78	2	0	0	0
55	D8	63	507	326	101	78	2	0	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	CZ	14	14	14	0	0
56	B4	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	BA	923	923	923	0	0
56	AK	7	7	7	0	0
56	DQ	2	2	2	0	0
56	AB	7	7	7	0	0
56	DF	1	1	1	0	0
56	B8	4	4	4	0	0
56	BE	6	6	6	0	0
56	DU	1	1	1	0	0
56	D8	1	1	1	0	0
56	B1	7	7	7	0	0
56	DY	1	1	1	0	0
56	AN	1	1	1	0	0
56	BP	2	2	2	0	0
56	AX	14	14	14	0	0
56	DN	1	1	1	0	0
56	BI	6	6	6	0	0
56	CY	14	14	14	0	0
56	CH	2	2	2	0	0
56	CA	222	222	222	0	0
56	B5	2	2	2	0	0
56	BB	35	35	35	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	AJ	1	1	1	0	0
56	BT	1	1	1	0	0
56	DO	2	2	2	0	0
56	AE	8	8	8	0	0
56	DG	2	2	2	0	0
56	CF	5	5	5	0	0
56	DT	1	1	1	0	0
56	BF	6	6	6	0	0
56	AV	3	3	3	0	0
56	BX	2	2	2	0	0
56	DA	491	491	491	0	0
56	B2	3	3	3	0	0
56	AA	428	428	428	0	0
56	BQ	6	6	6	0	0
56	CQ	1	1	1	0	0
56	D6	1	1	1	0	0
56	AR	1	1	1	0	0
56	B6	2	2	2	0	0
56	DI	1	1	1	0	0
56	AM	3	3	3	0	0
56	BU	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	DR	1	1	1	0	0
56	CC	1	1	1	0	0
56	AD	3	3	3	0	0
56	BN	4	4	4	0	0
56	CT	1	1	1	0	0
56	CG	2	2	2	0	0
56	BG	2	2	2	0	0
56	AI	1	1	1	0	0
56	BY	3	3	3	0	0
56	DE	1	1	1	0	0
56	BR	2	2	2	0	0
56	AZ	15	15	15	0	0
56	BK	3	3	3	0	0
56	DP	1	1	1	0	0
56	DD	9	9	9	0	0
56	AL	4	4	4	0	0
56	BV	3	3	3	0	0
56	AG	2	2	2	0	0
56	BO	5	5	5	0	0
56	AQ	1	1	1	0	0
56	D1	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	AH	2	2	2	0	0
56	BZ	1	1	1	0	0
56	CO	1	1	1	0	0
56	AC	4	4	4	0	0
56	BS	3	3	3	0	0
56	DB	12	12	12	0	0
56	CS	1	1	1	0	0
56	CB	2	2	2	0	0
56	BD	7	7	7	0	0
56	AT	2	2	2	0	0
56	CL	1	1	1	0	0
56	B0	3	3	3	0	0
56	AO	2	2	2	0	0
56	BW	2	2	2	0	0
56	AY	26	26	26	0	0
56	CK	3	3	3	0	0
56	AF	2	2	2	0	0
56	BH	4	4	4	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
57	CN	1	1	1	0	0

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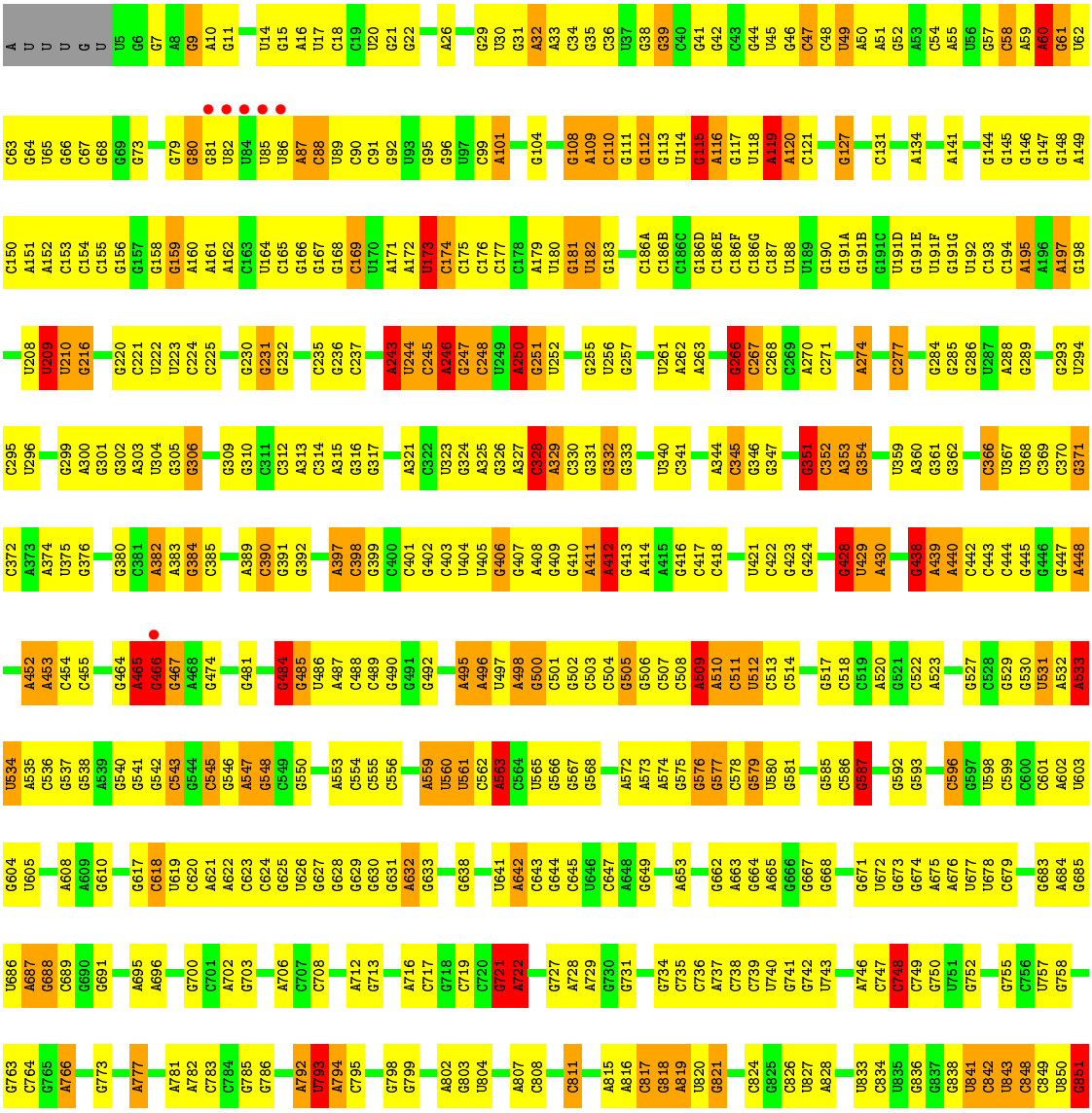
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
57	AD	1	1	1	0	0
			Total	Zn		
57	CD	1	1	1	0	0
			Total	Zn		
57	AN	1	1	1	0	0

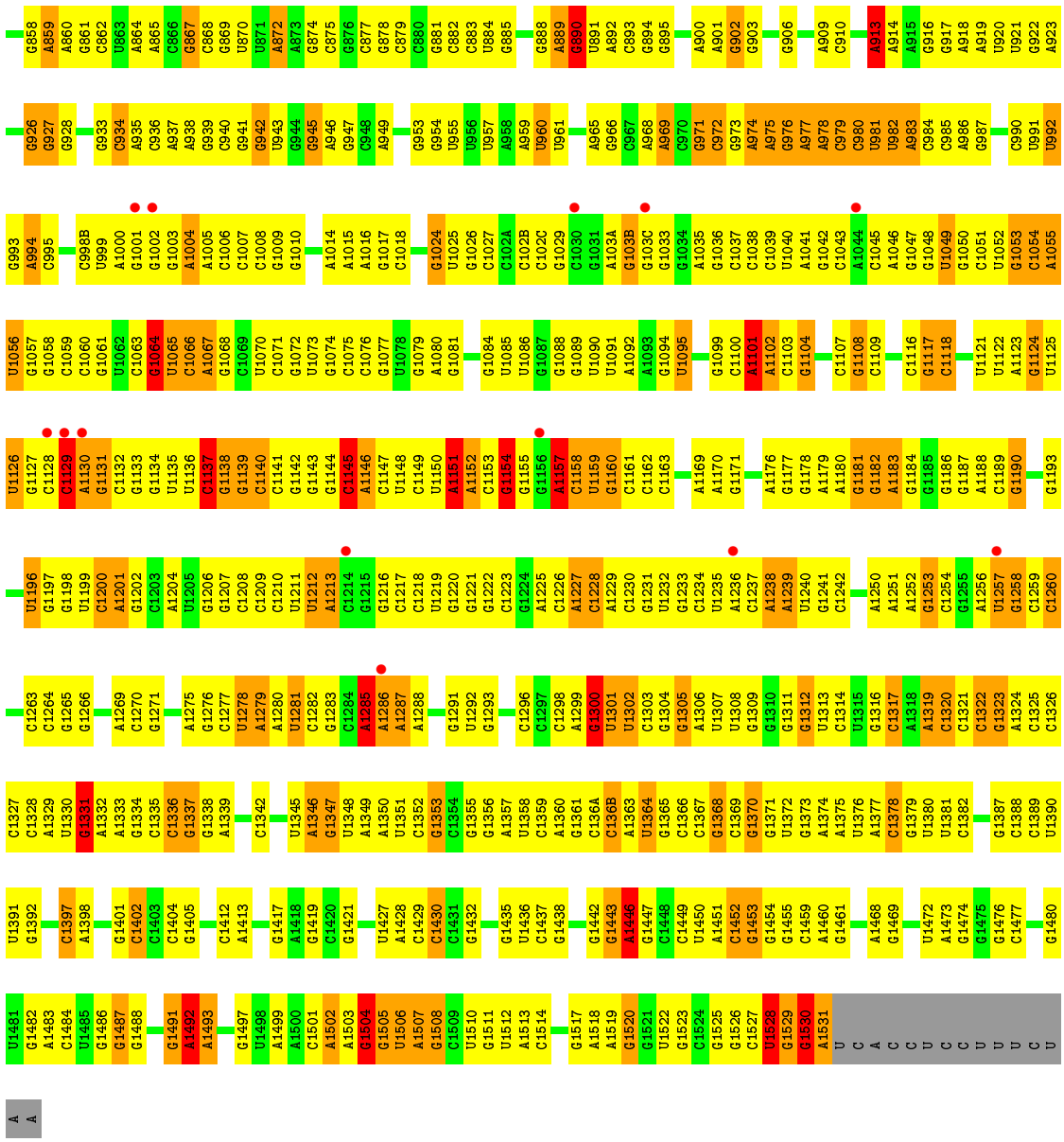
3 Residue-property plots (i)

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

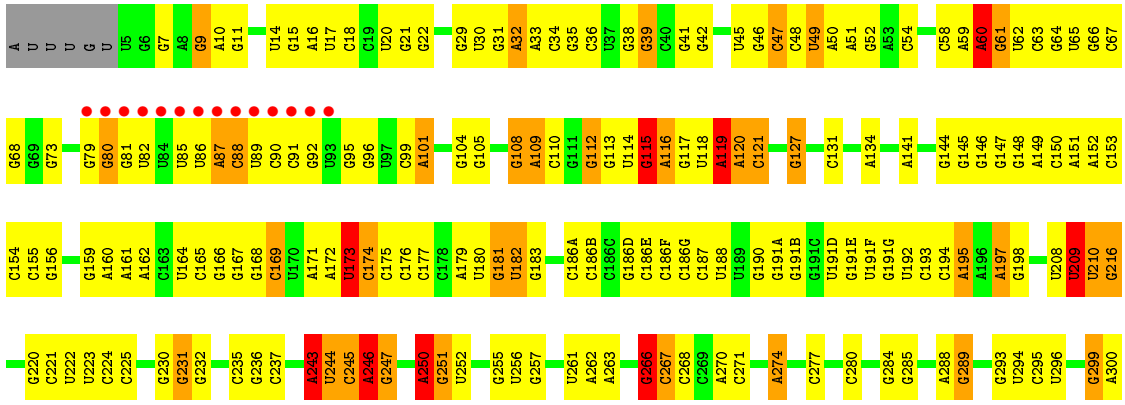
Chain AA:

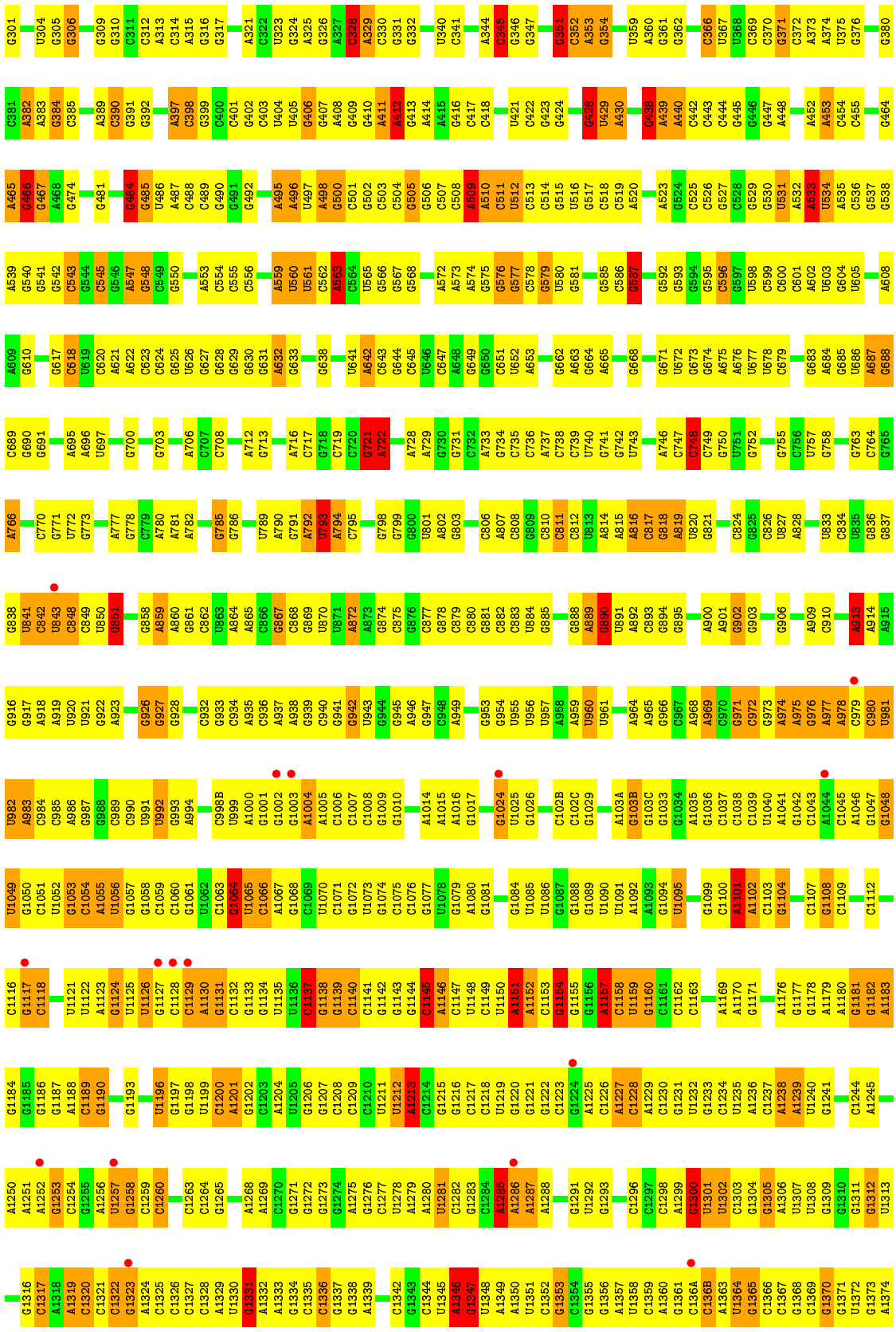


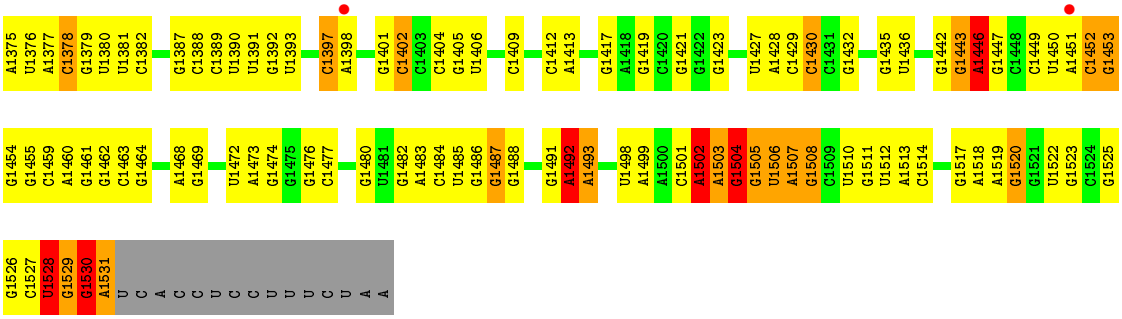


- Molecule 1: 16S RRNA

Chain CA:

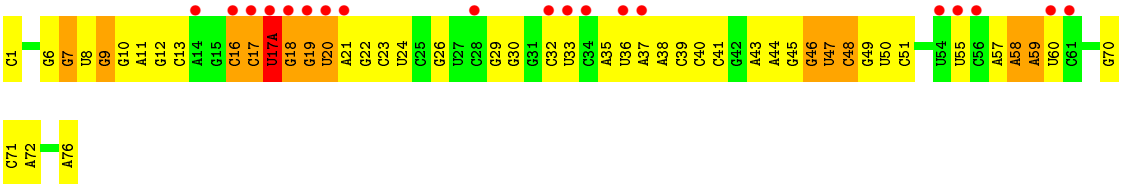






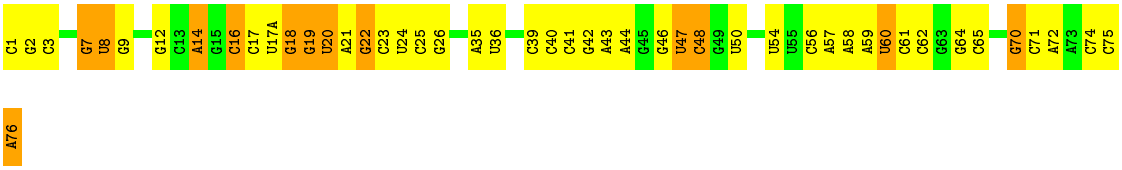
- Molecule 2: P AND E-SITE TRNA(FMET)

Chain AZ:



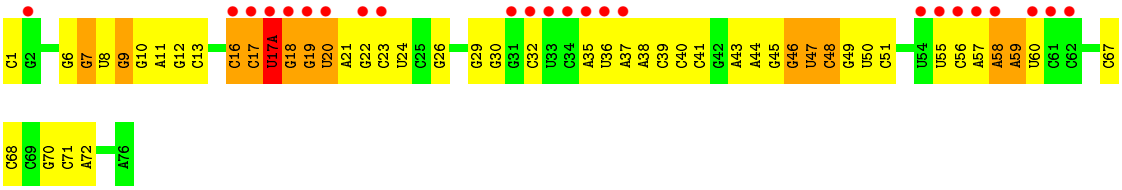
- Molecule 2: P AND E-SITE TRNA(FMET)

Chain AY:



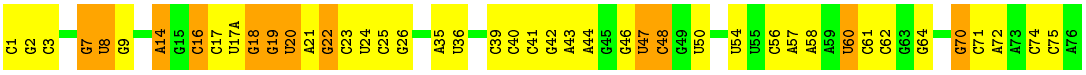
- Molecule 2: P AND E-SITE TRNA(FMET)

Chain CZ:



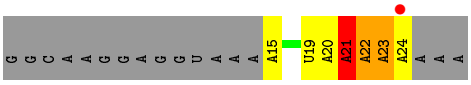
- Molecule 2: P AND E-SITE TRNA(FMET)

Chain CY:



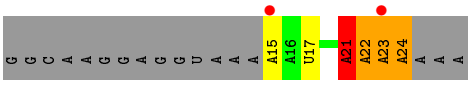
- Molecule 3: MRNA

Chain AV:



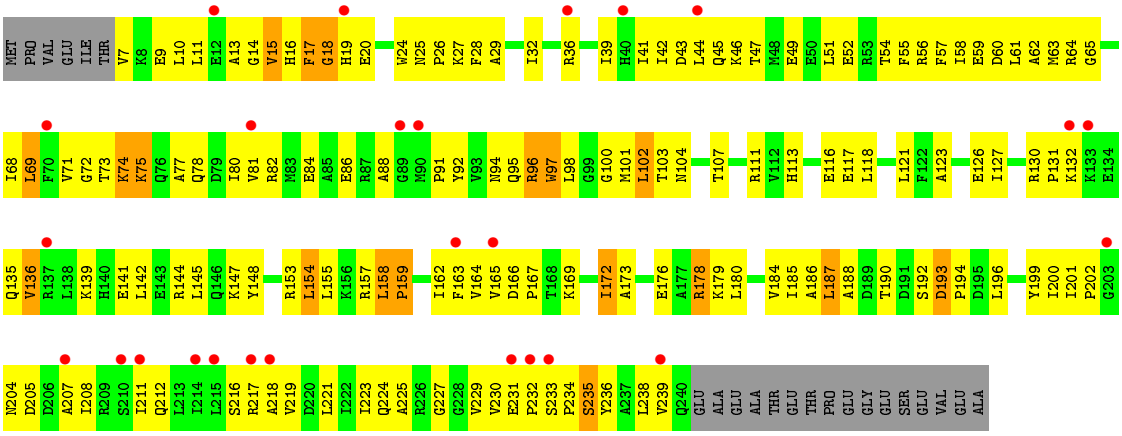
- Molecule 3: MRNA

Chain CV:



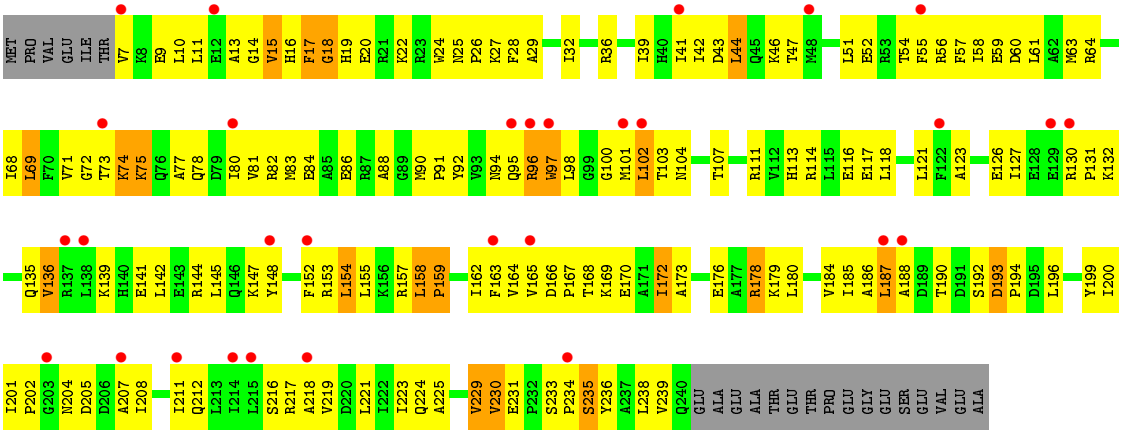
- Molecule 4: 30S ribosomal protein S2

Chain AB:



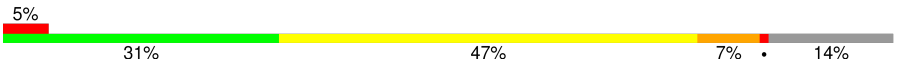
- Molecule 4: 30S ribosomal protein S2

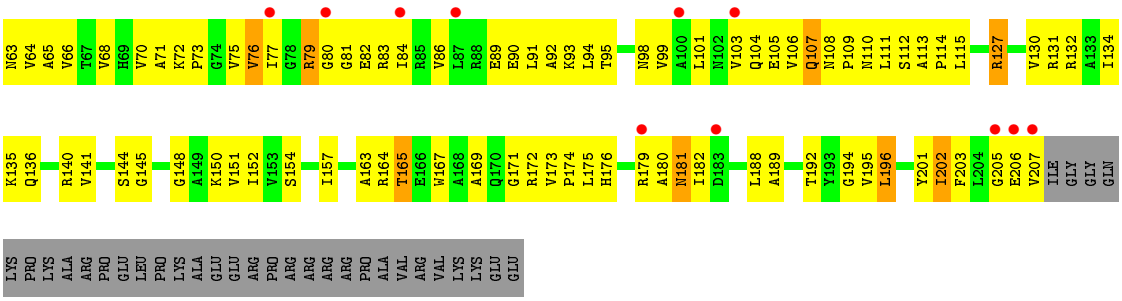
Chain CB:



- Molecule 5: 30S ribosomal protein S3

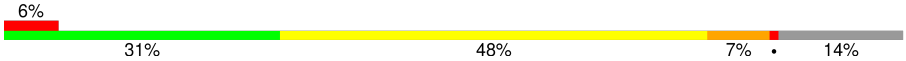
Chain AC:

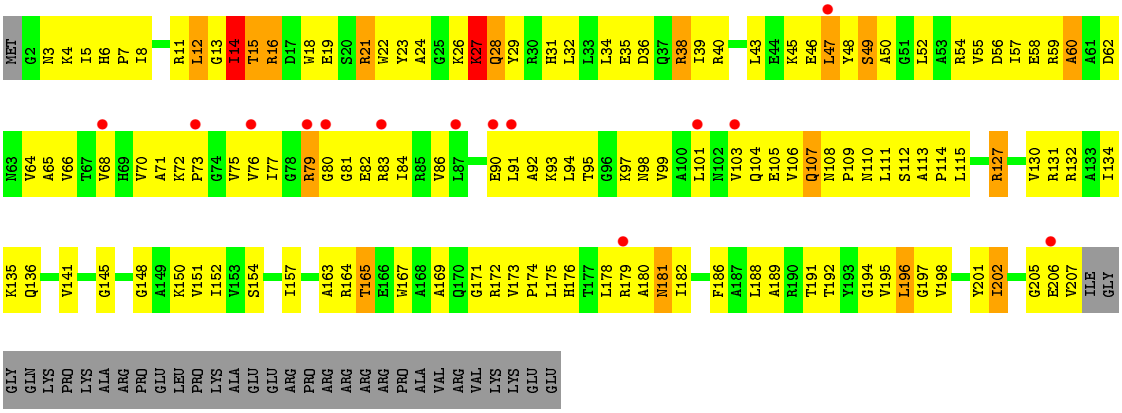




- Molecule 5: 30S ribosomal protein S3

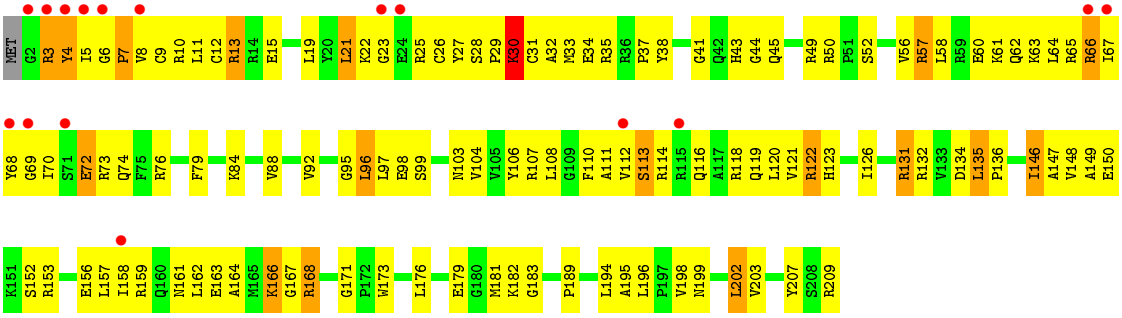
Chain CC:





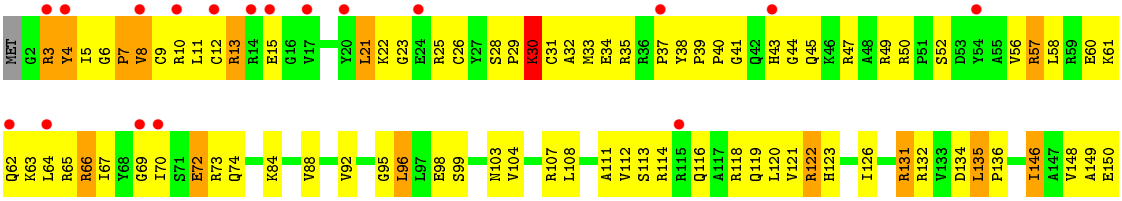
- Molecule 6: 30S ribosomal protein S4

Chain AD:



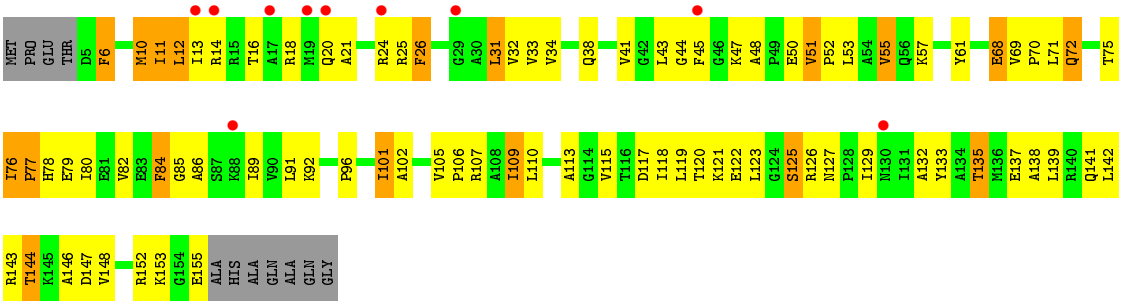
- Molecule 6: 30S ribosomal protein S4

Chain CD:



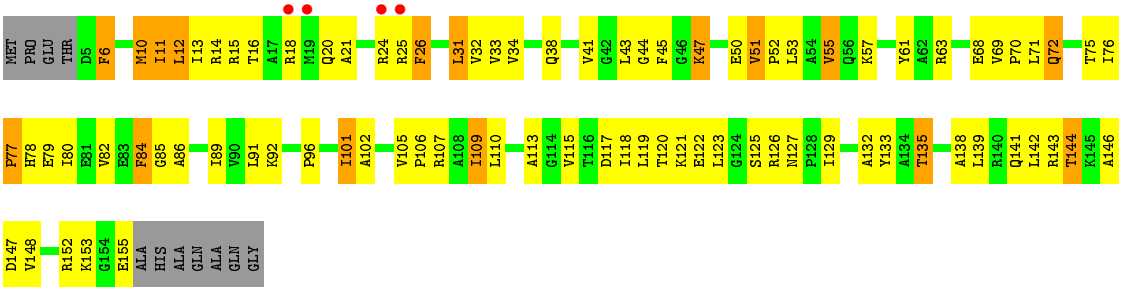
- Molecule 7: 30S ribosomal protein S5

Chain AE:



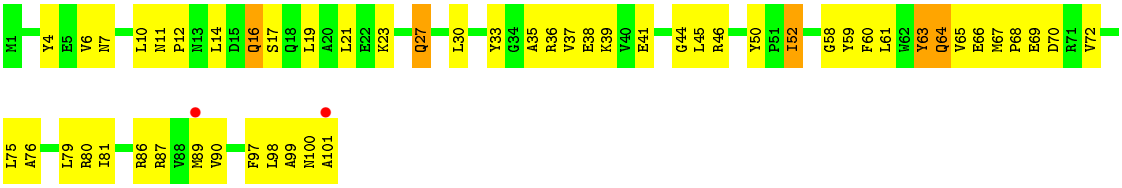
- Molecule 7: 30S ribosomal protein S5

Chain CE:



- Molecule 8: 30S ribosomal protein S6

Chain AF:

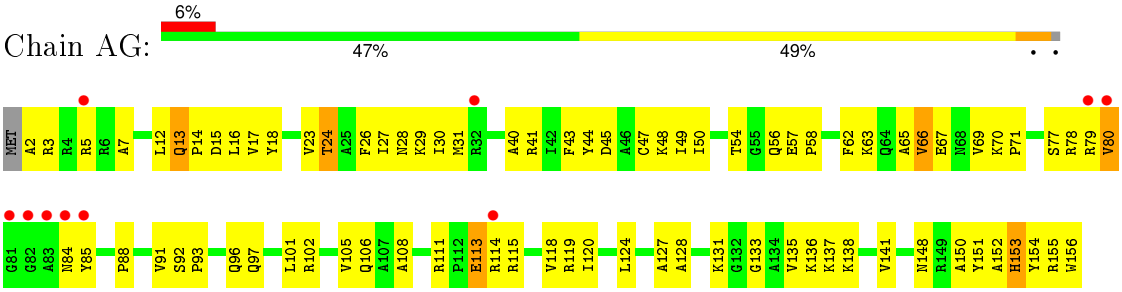


- Molecule 8: 30S ribosomal protein S6

Chain CF:

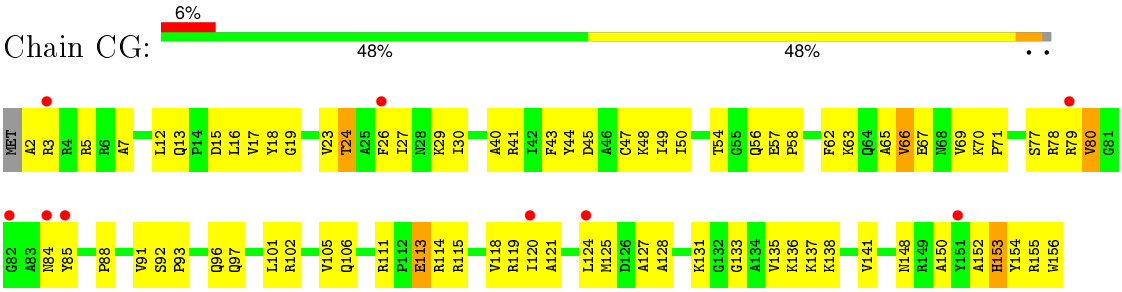
- Molecule 9: 30S ribosomal protein S7

Chain AG:



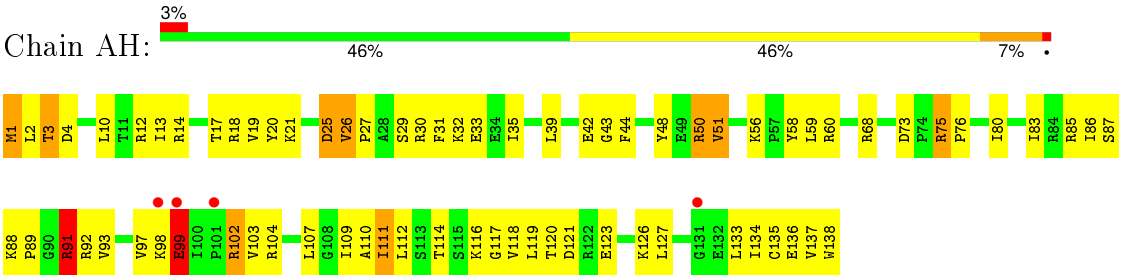
- Molecule 9: 30S ribosomal protein S7

Chain CG:



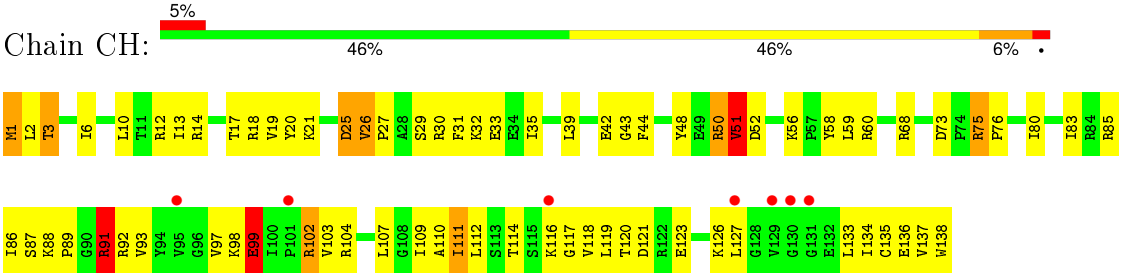
- Molecule 10: 30S ribosomal protein S8

Chain AH:



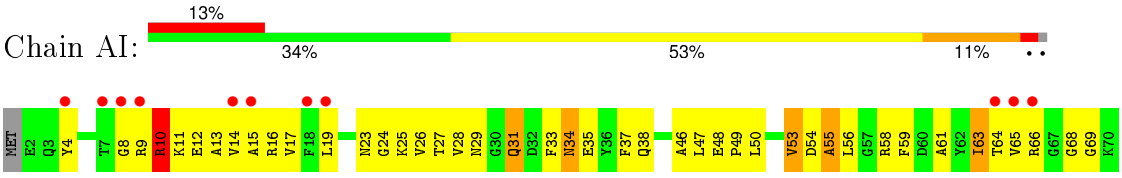
- Molecule 10: 30S ribosomal protein S8

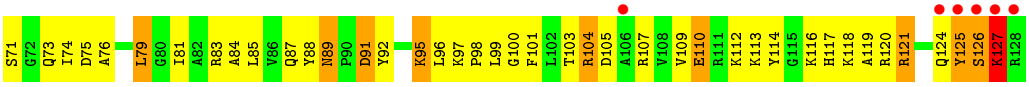
Chain CH:



- Molecule 11: 30S ribosomal protein S9

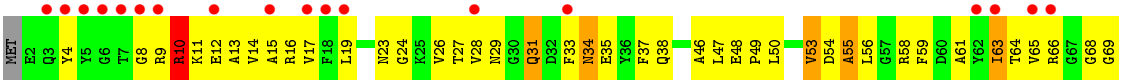
Chain AI:

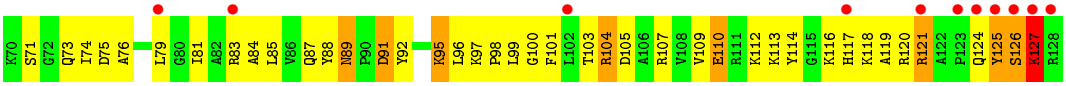




- Molecule 11: 30S ribosomal protein S9

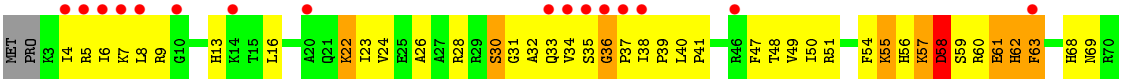
Chain CI:

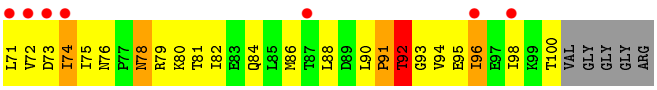




- Molecule 12: 30S ribosomal protein S10

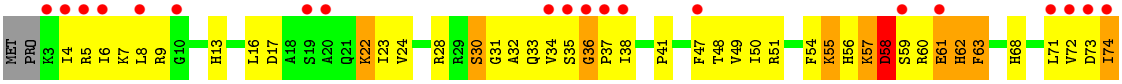
Chain AJ:

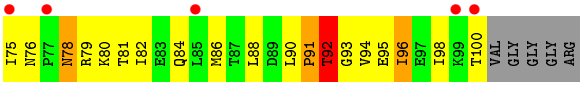




- Molecule 12: 30S ribosomal protein S10

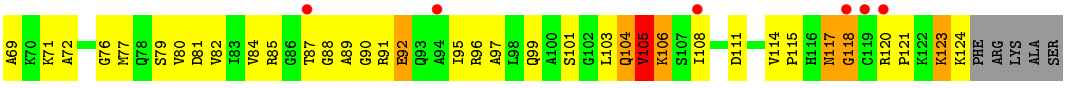
Chain CJ:





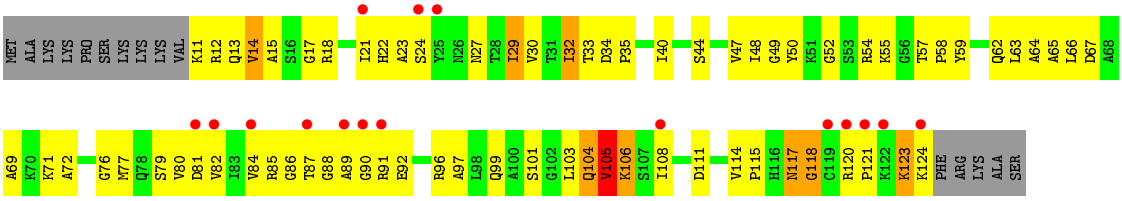
- Molecule 13: 30S ribosomal protein S11

Chain AK:



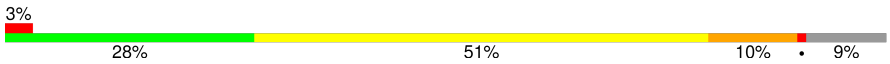
- Molecule 13: 30S ribosomal protein S11

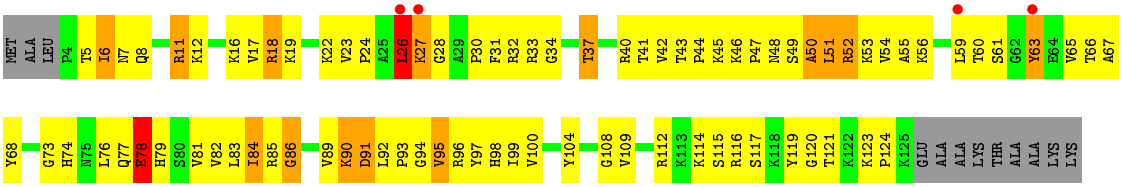
Chain CK:



- Molecule 14: 30S ribosomal protein S12

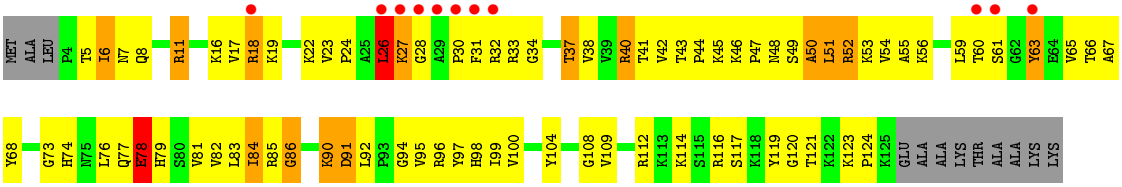
Chain AL:





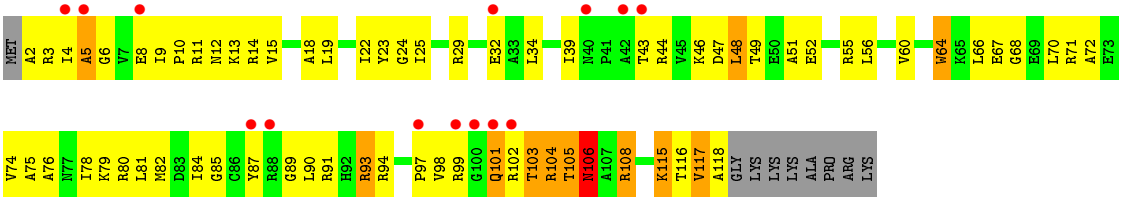
- Molecule 14: 30S ribosomal protein S12

Chain CL:



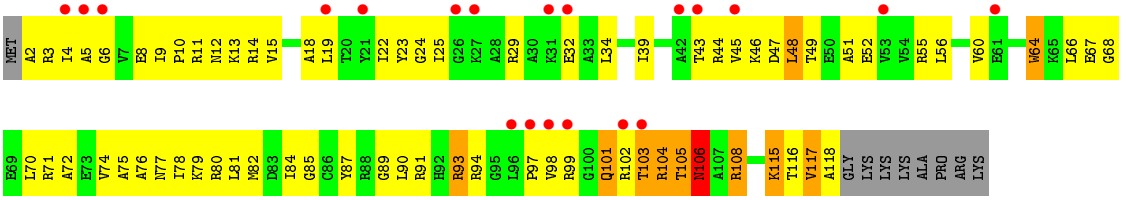
- Molecule 15: 30S ribosomal protein S13

Chain AM:



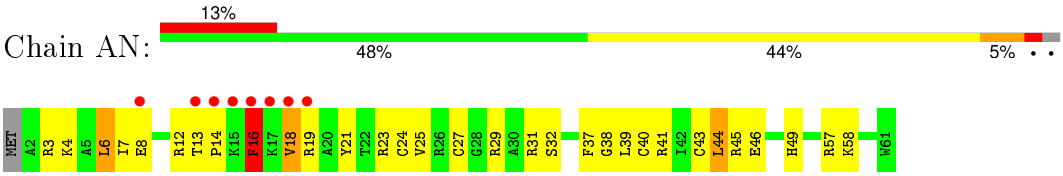
- Molecule 15: 30S ribosomal protein S13

Chain CM:



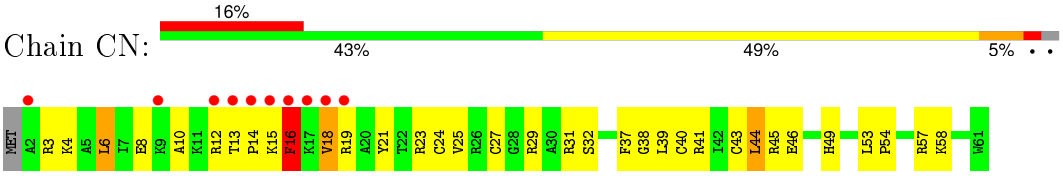
- Molecule 16: 30S ribosomal protein S14

Chain AN:



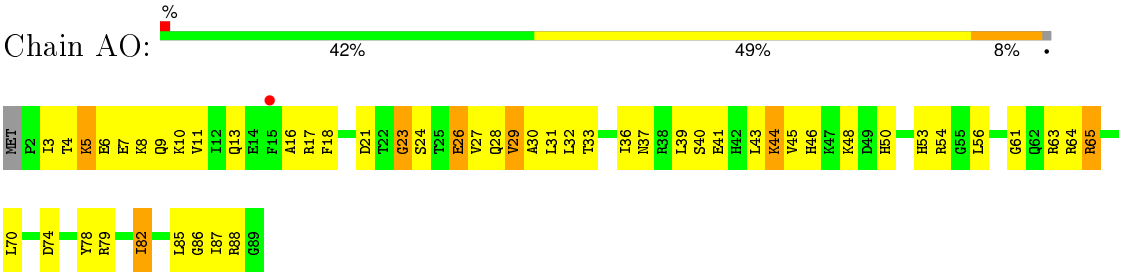
- Molecule 16: 30S ribosomal protein S14

Chain CN:



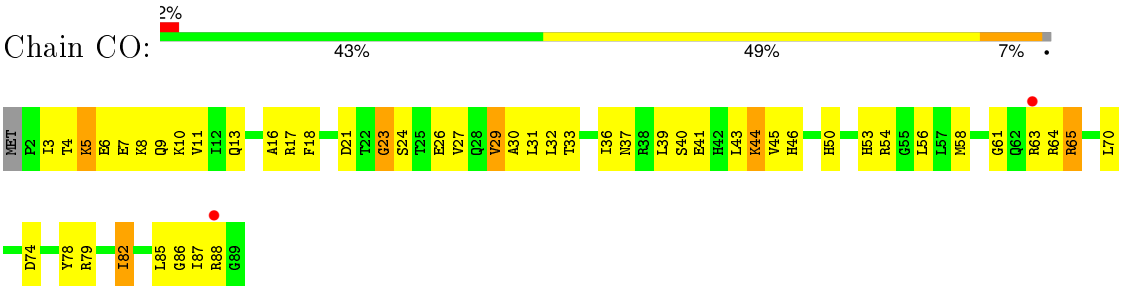
- Molecule 17: 30S ribosomal protein S15

Chain AO:



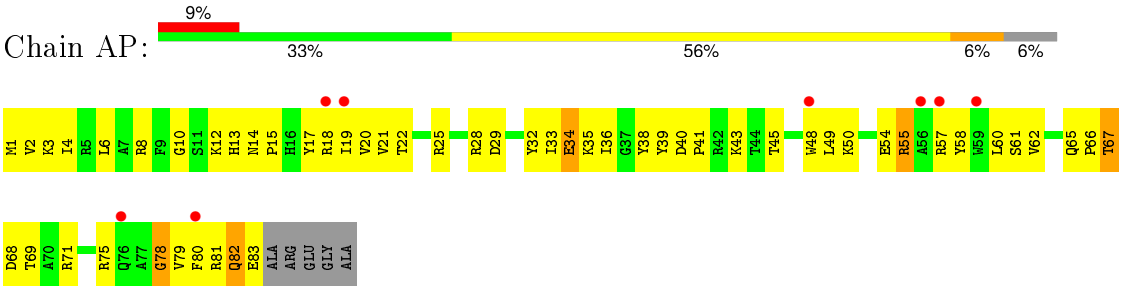
- Molecule 17: 30S ribosomal protein S15

Chain CO:



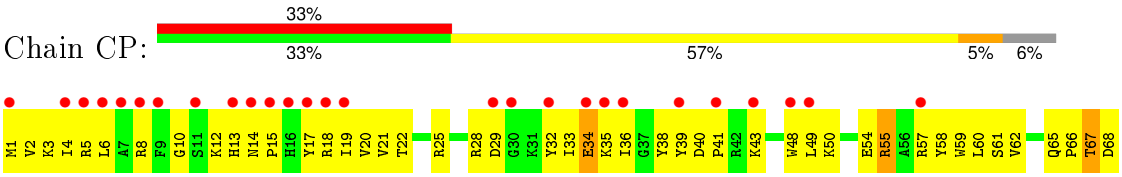
- Molecule 18: 30S ribosomal protein S16

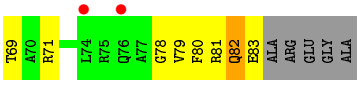
Chain AP:



- Molecule 18: 30S ribosomal protein S16

Chain CP:





- Molecule 19: 30S ribosomal protein S17

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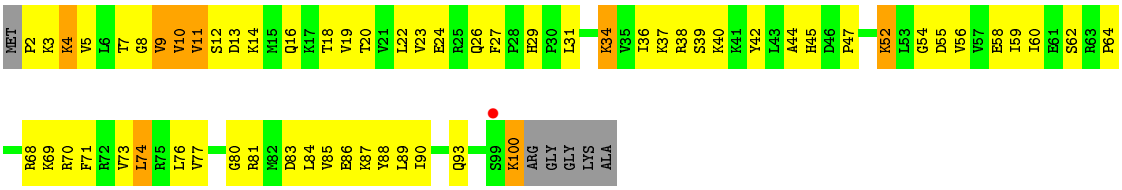

- Molecule 19: 30S ribosomal protein S17

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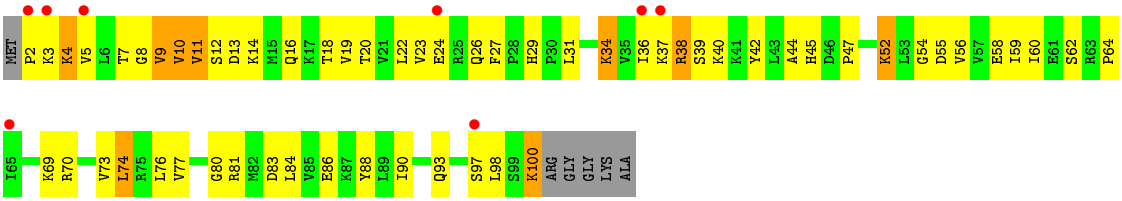

- Molecule 20: 30S ribosomal protein S18

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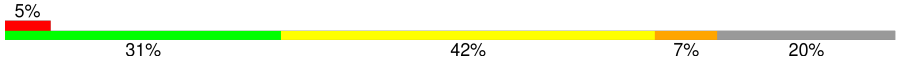

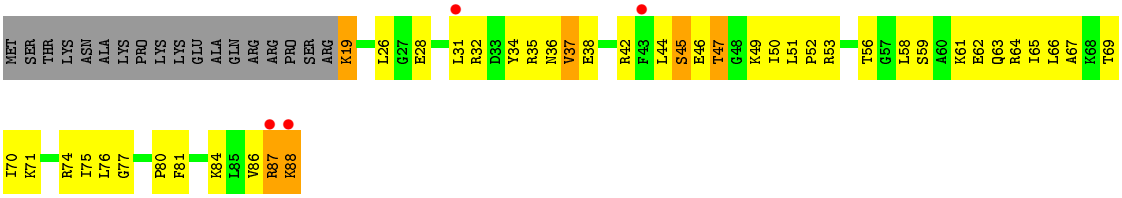

- Molecule 20: 30S ribosomal protein S18

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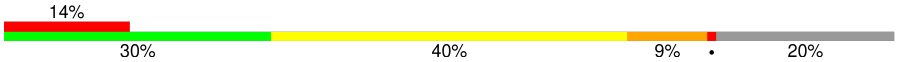

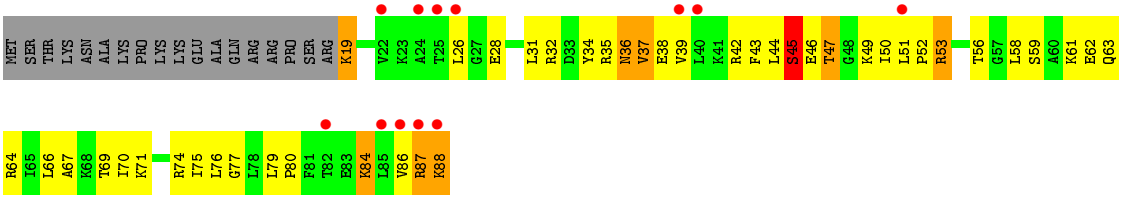

- Molecule 21: 30S ribosomal protein S19

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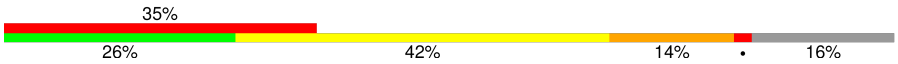

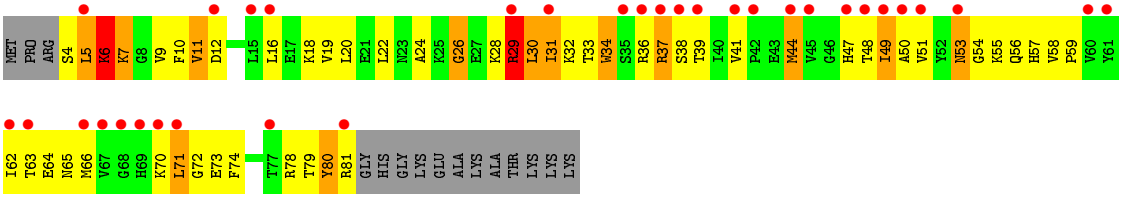

- Molecule 21: 30S ribosomal protein S19

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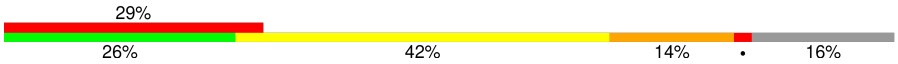

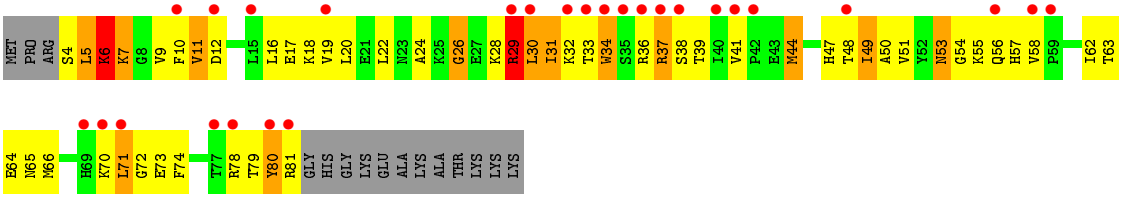

- Molecule 22: 30S ribosomal protein S20

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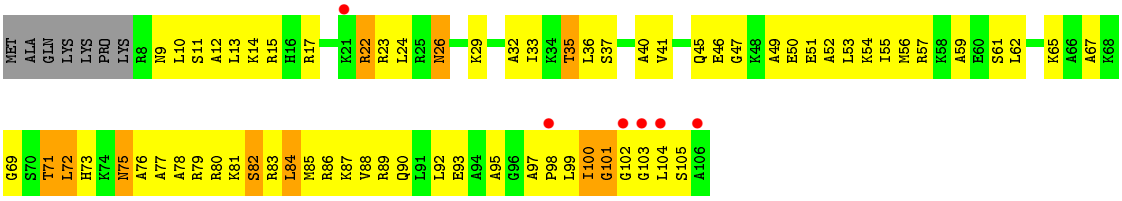

- Molecule 22: 30S ribosomal protein S20

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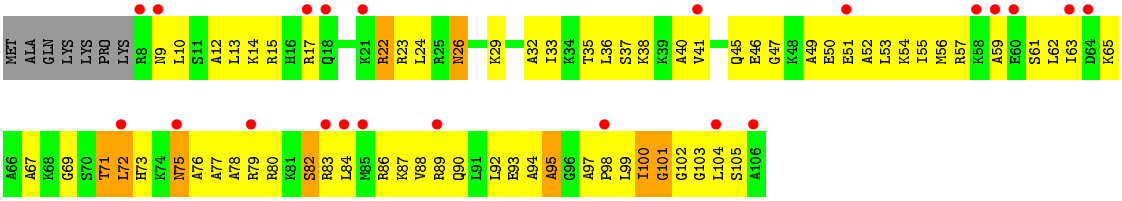
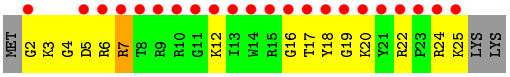


- Molecule 23: 30S ribosomal protein Thx

Chain AU:



- Molecule 23: 30S ribosomal protein Thx

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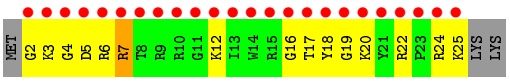
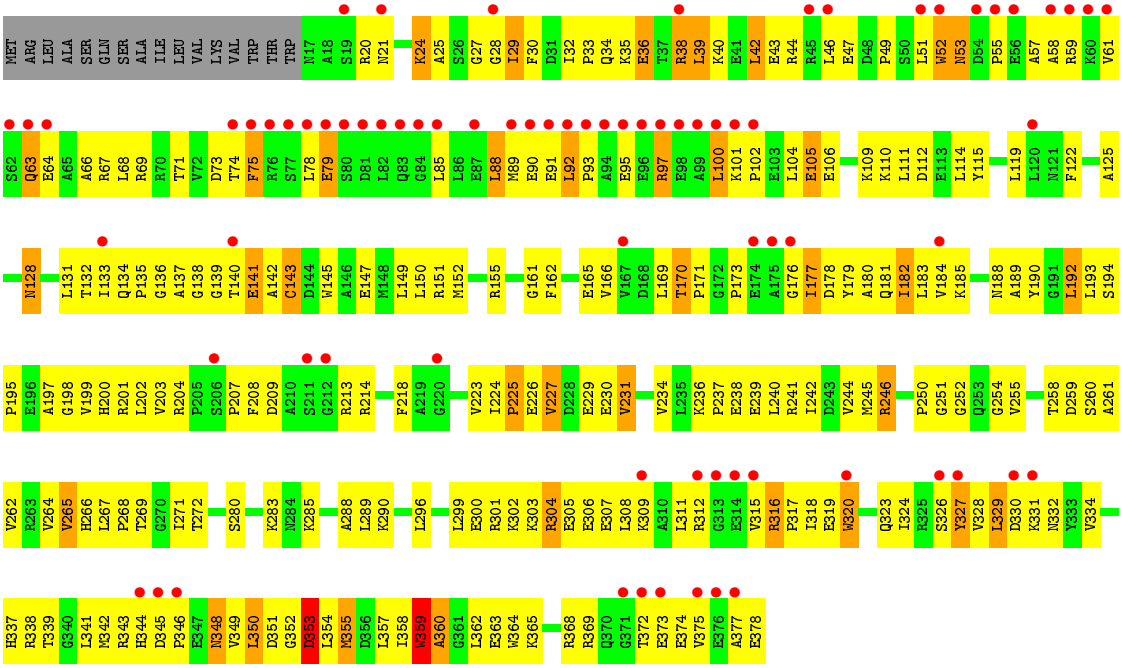


- Molecule 24: Bacterial peptide chain release factor 2 (RF-2)

Chain AX:



- Molecule 24: Bacterial peptide chain release factor 2 (RF-2)

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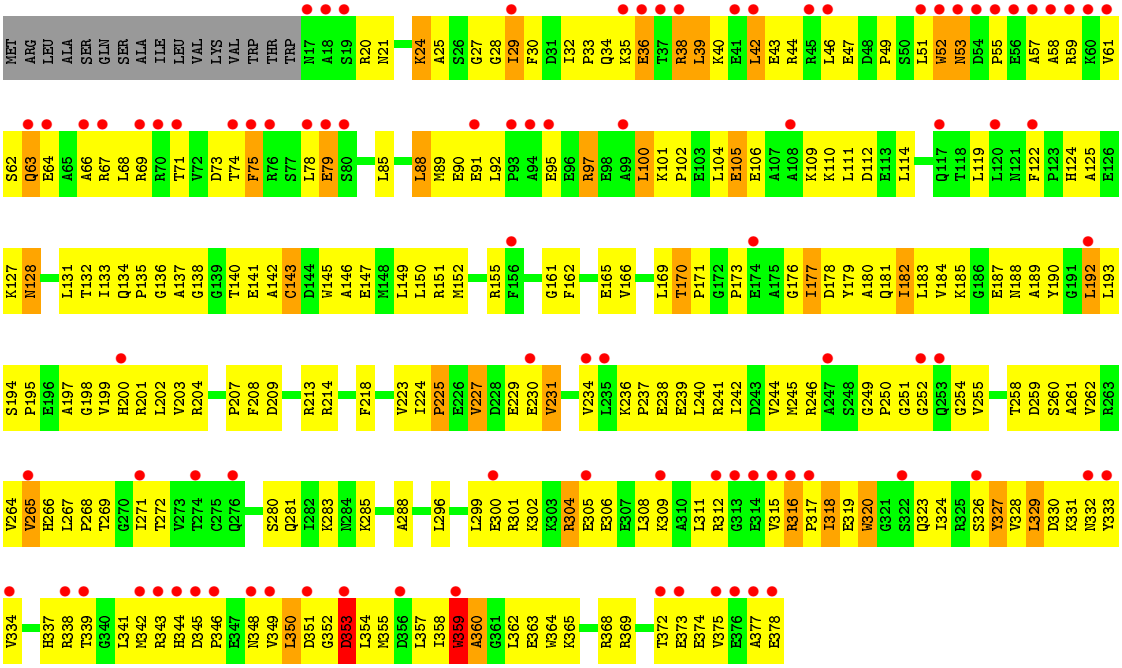
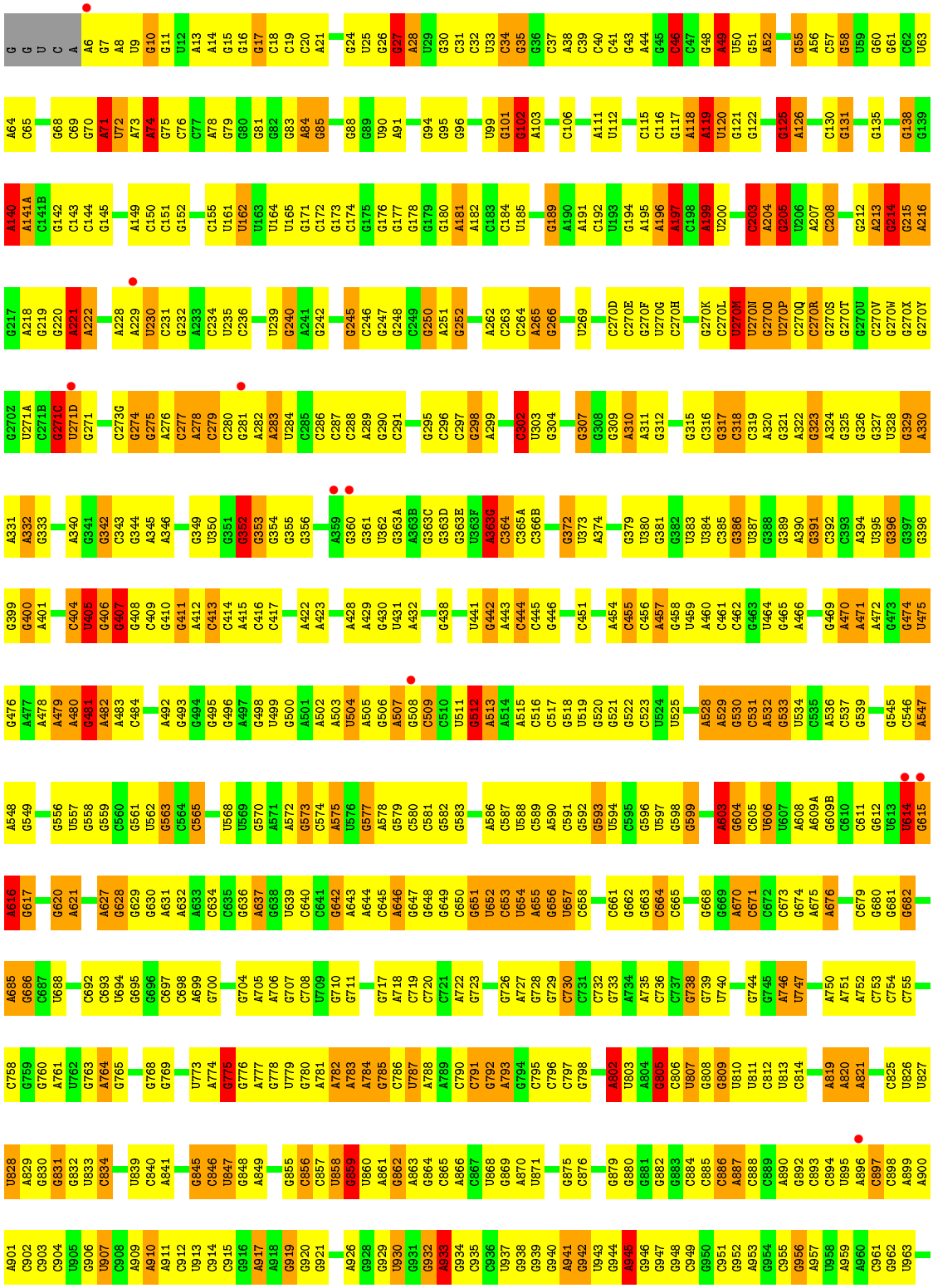
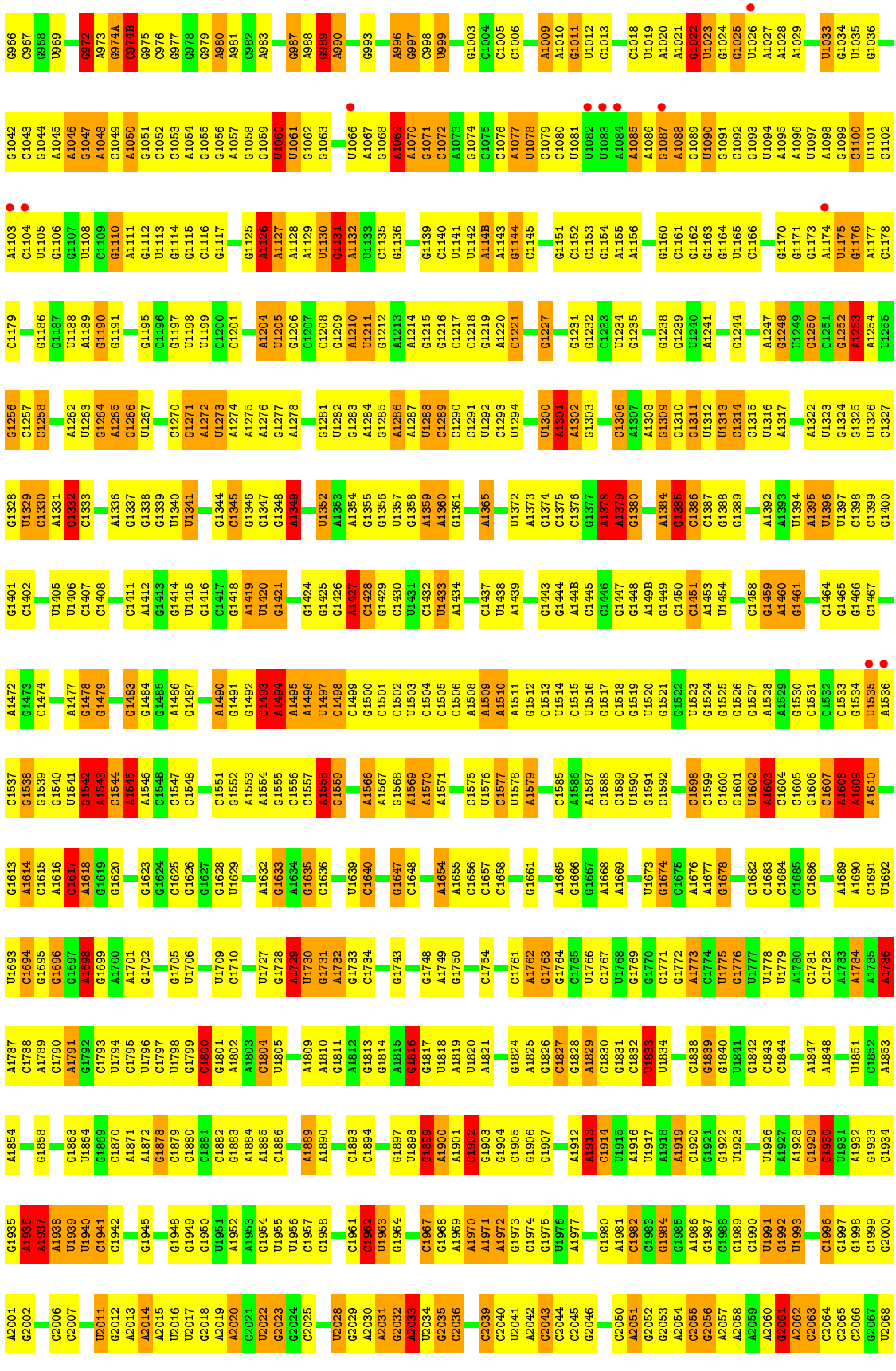


- Molecule 25: 23S RRNA

Chain BA: 3% 31% 48% 17%

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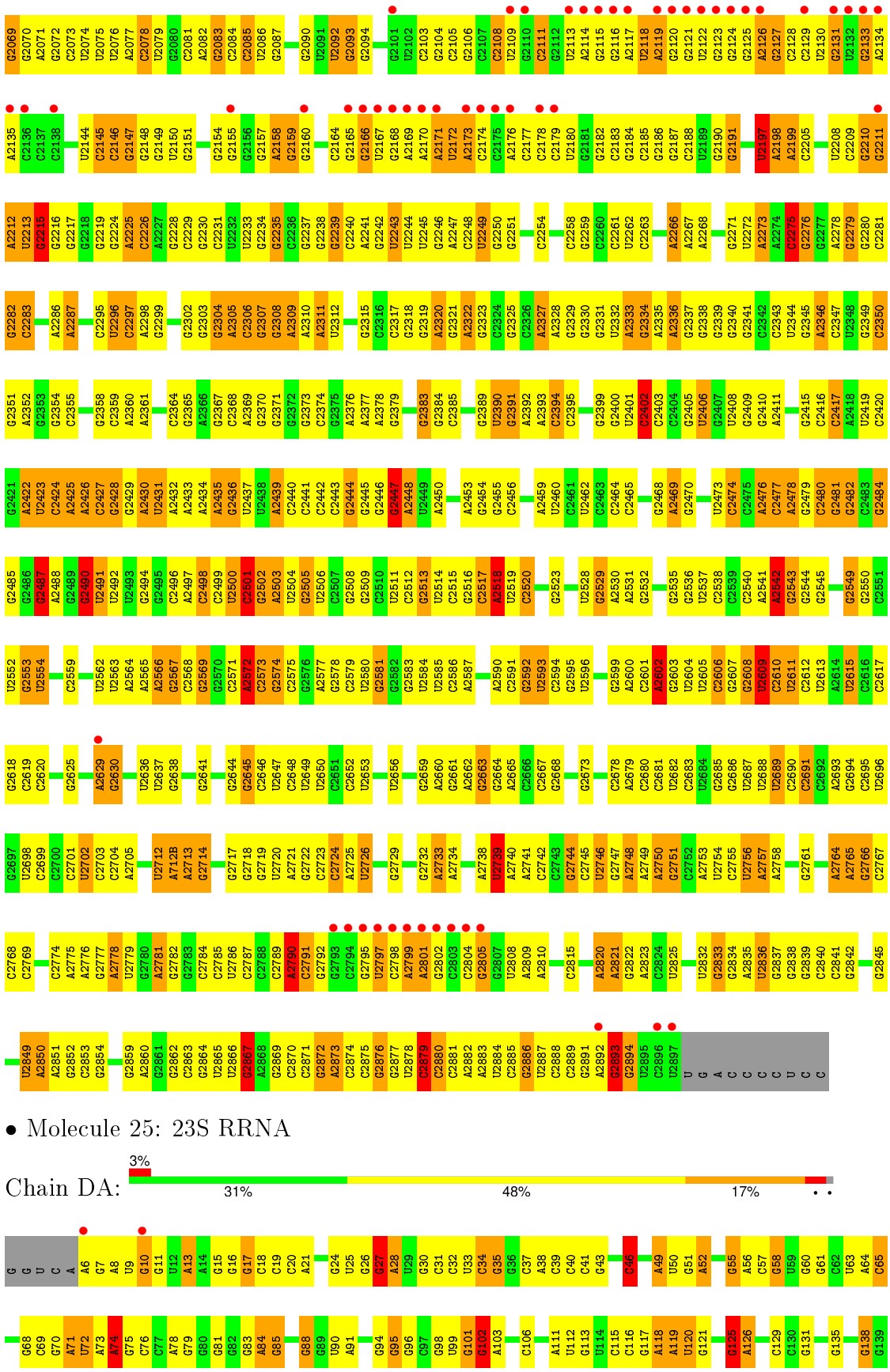

• Molecule 25: 23S RRNA

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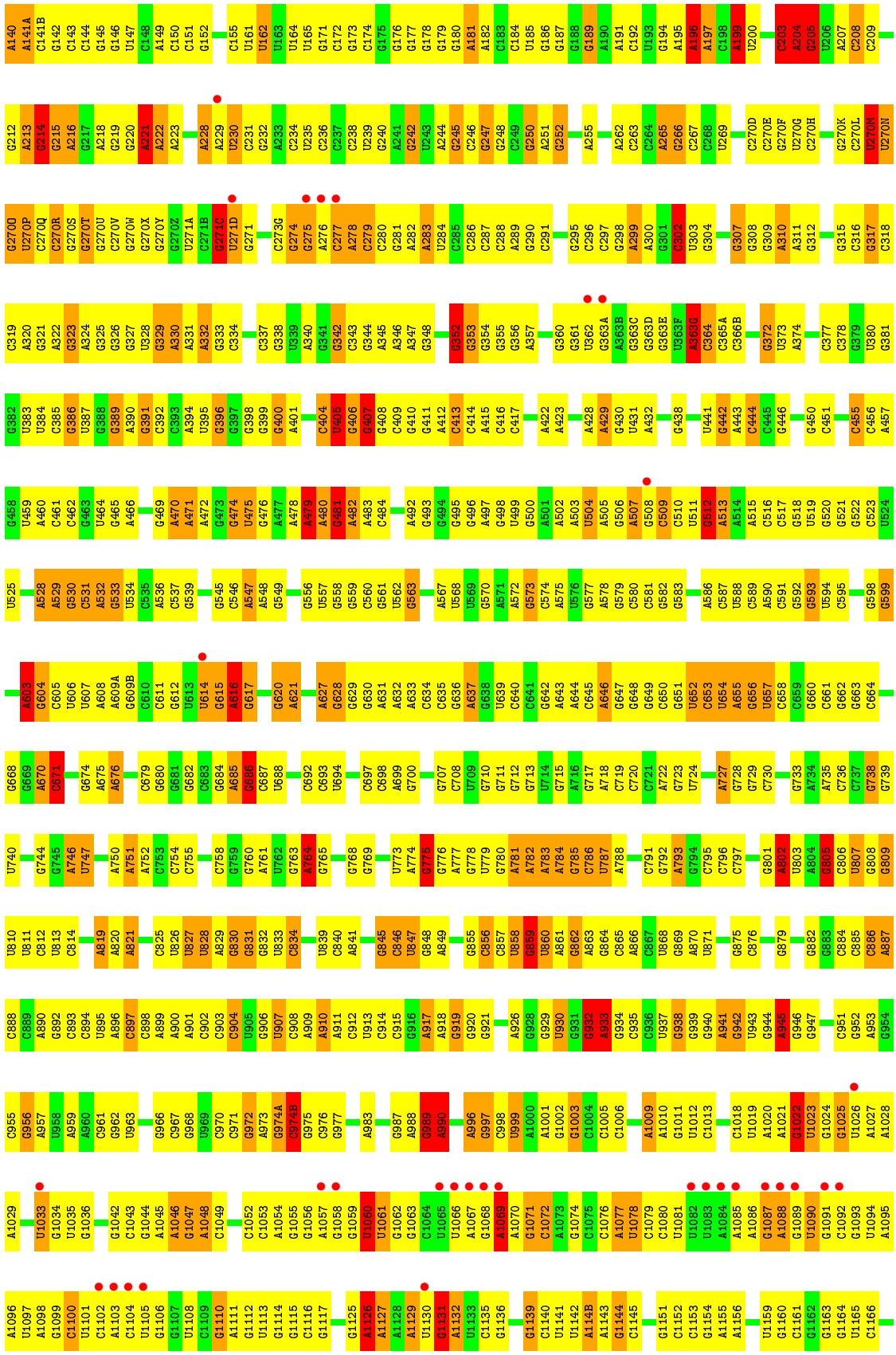
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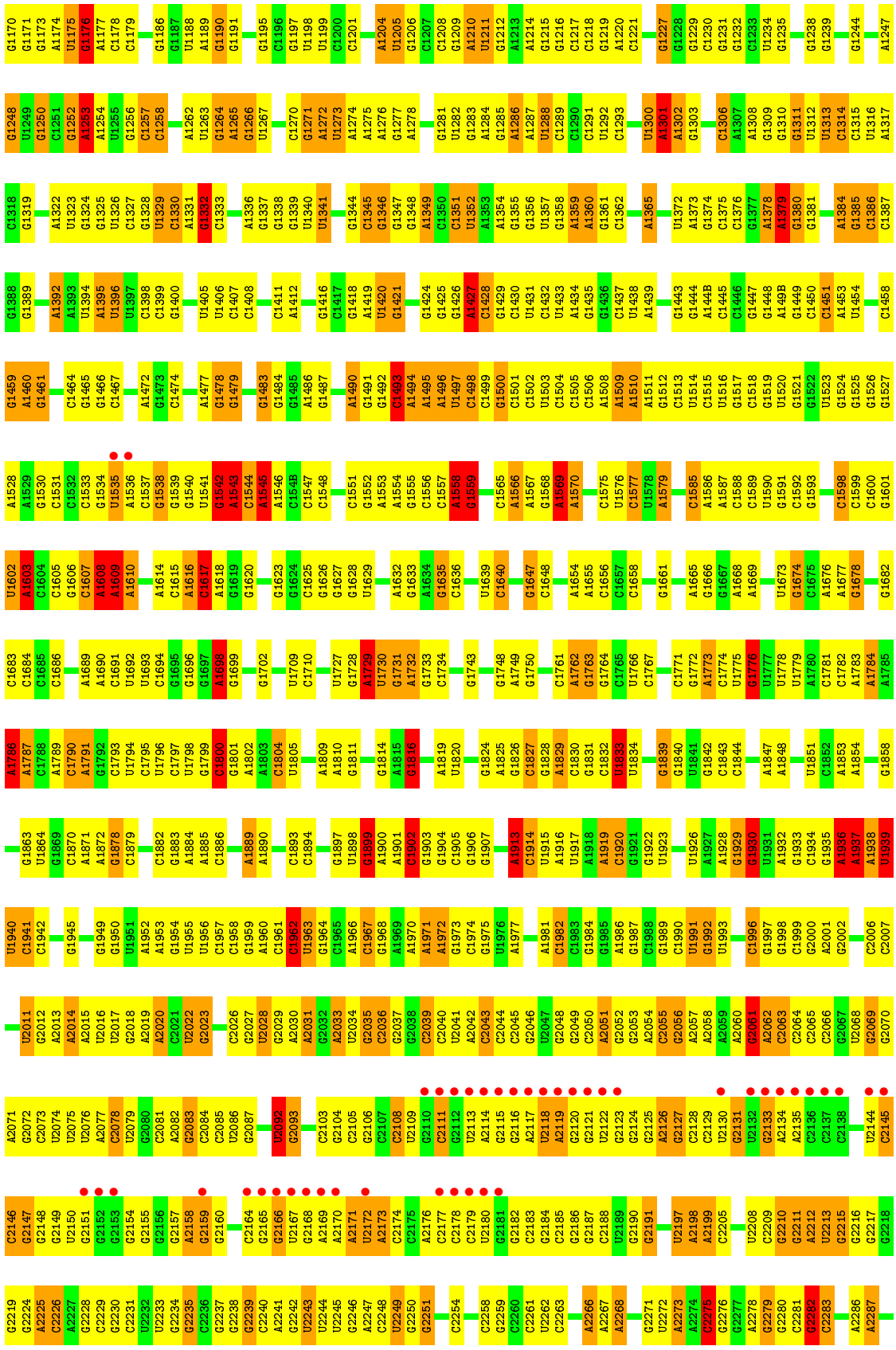
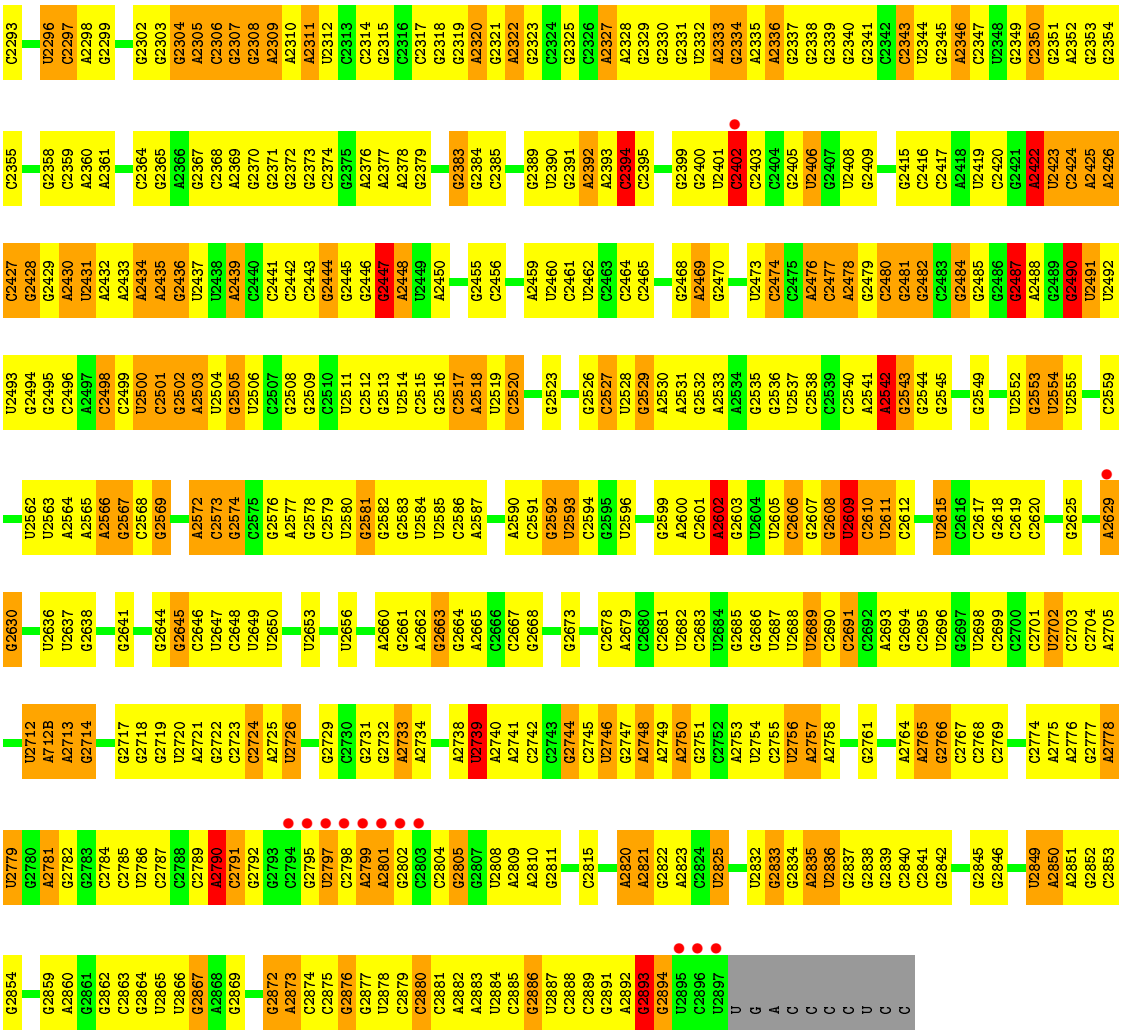
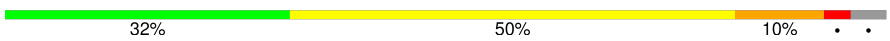
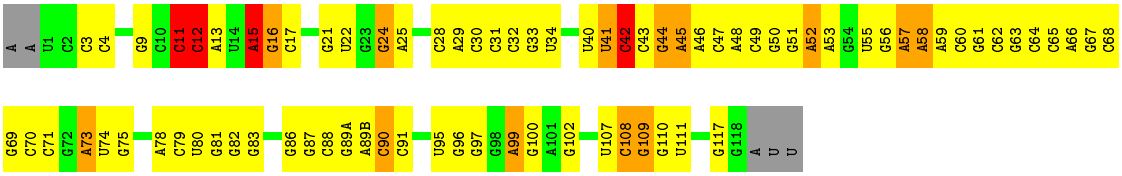




- Molecule 26: 5S RRNA

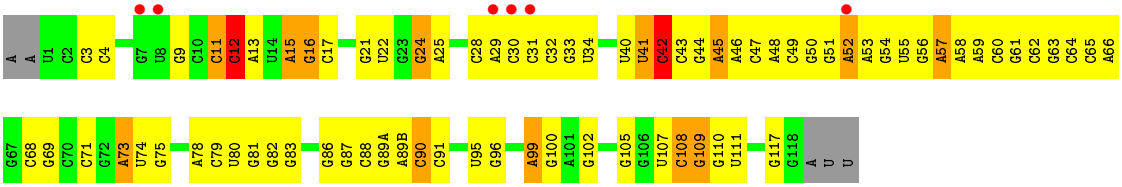
Chain BB:





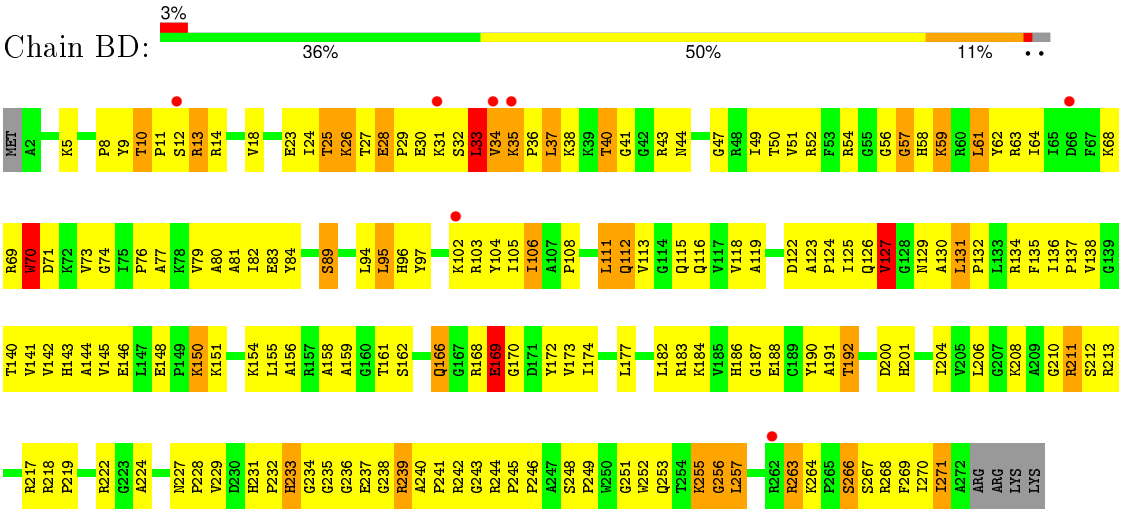
- Molecule 26: 5S RRNA

Chain DB:



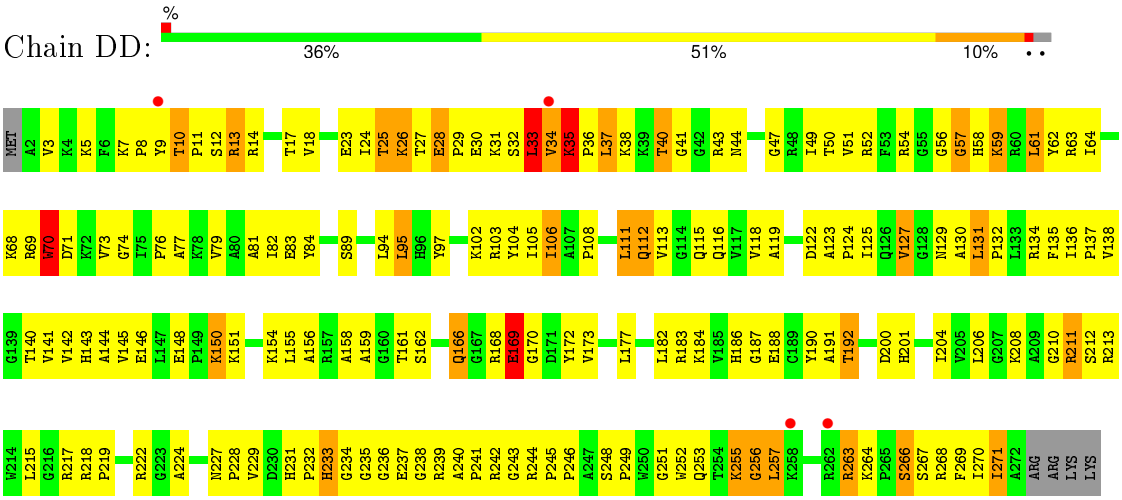
- Molecule 27: 50S ribosomal protein L2

Chain BD:



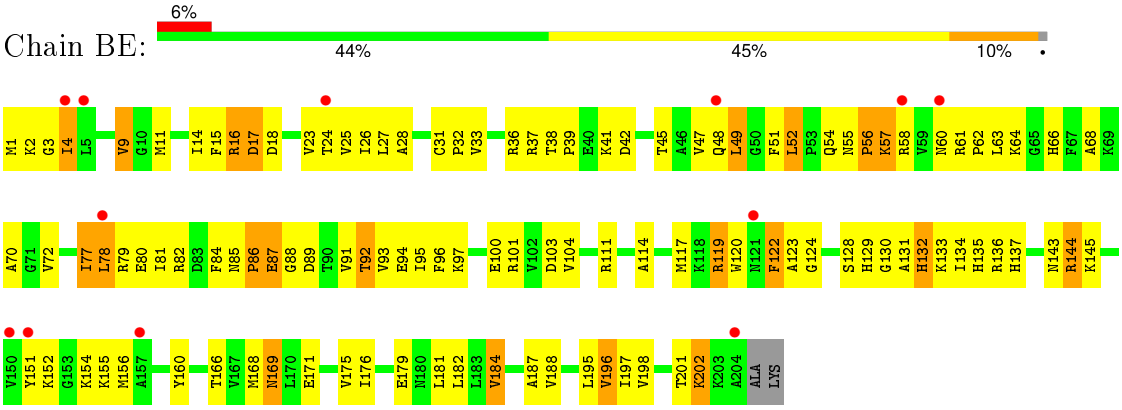
- Molecule 27: 50S ribosomal protein L2

Chain DD:



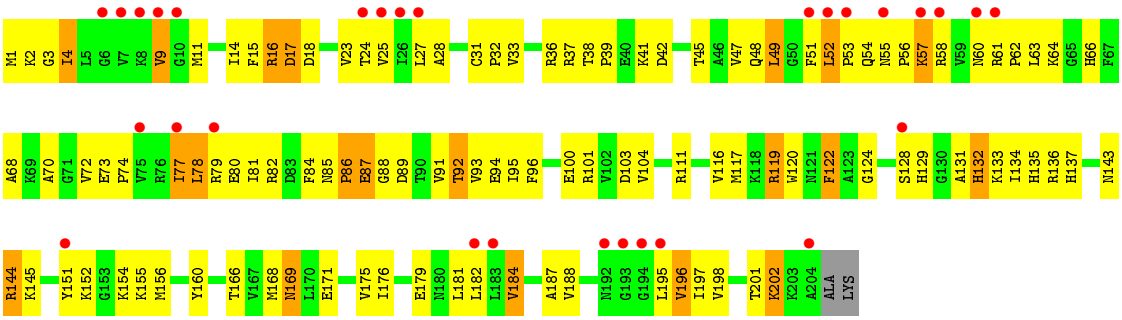
- Molecule 28: 50S ribosomal protein L3

Chain BE:



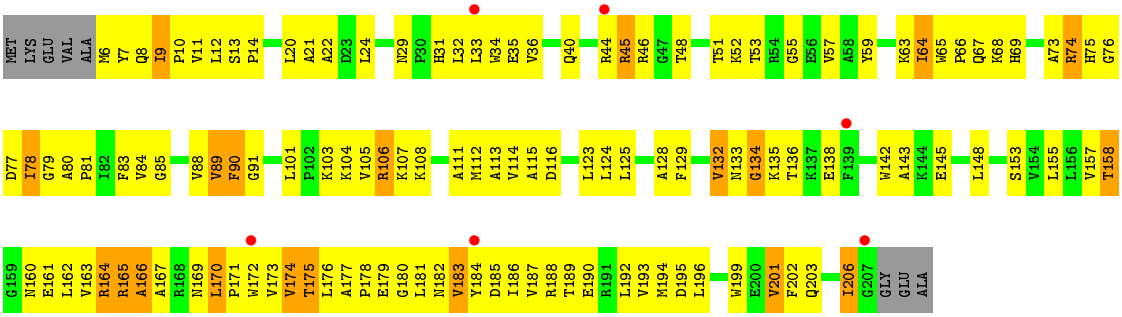
- Molecule 28: 50S ribosomal protein L3

Chain DE:



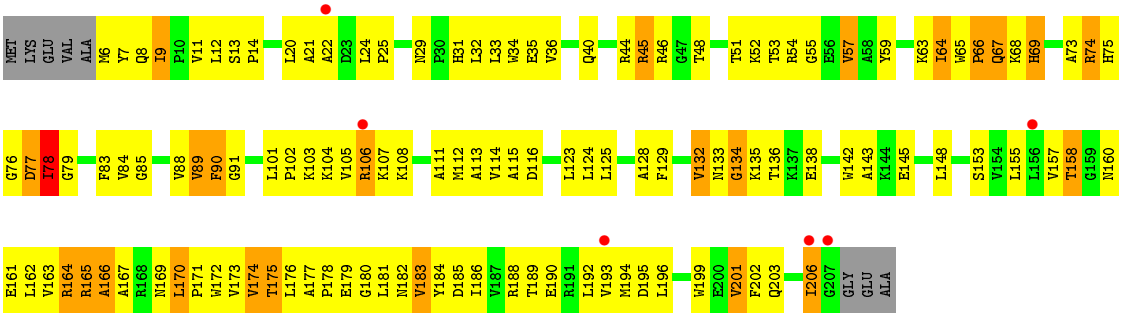
- Molecule 29: 50S ribosomal protein L4

Chain BF:



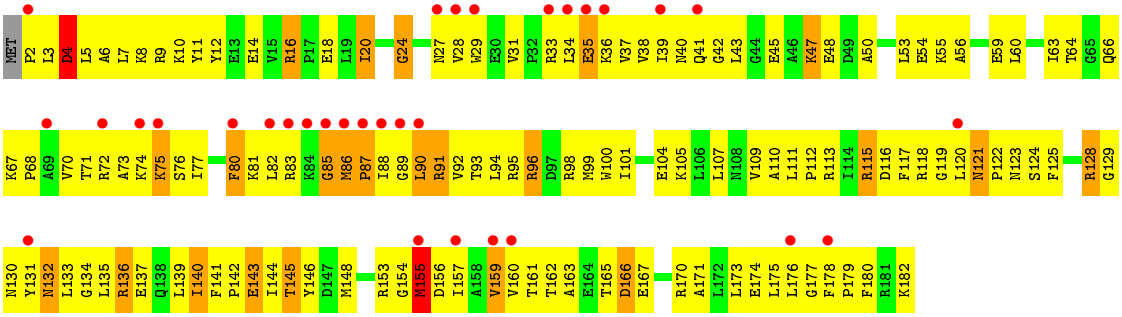
- Molecule 29: 50S ribosomal protein L4

Chain DF:



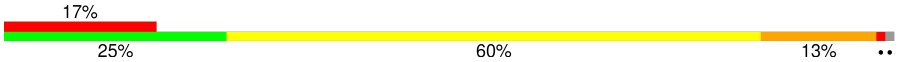
- Molecule 30: 50S ribosomal protein L5

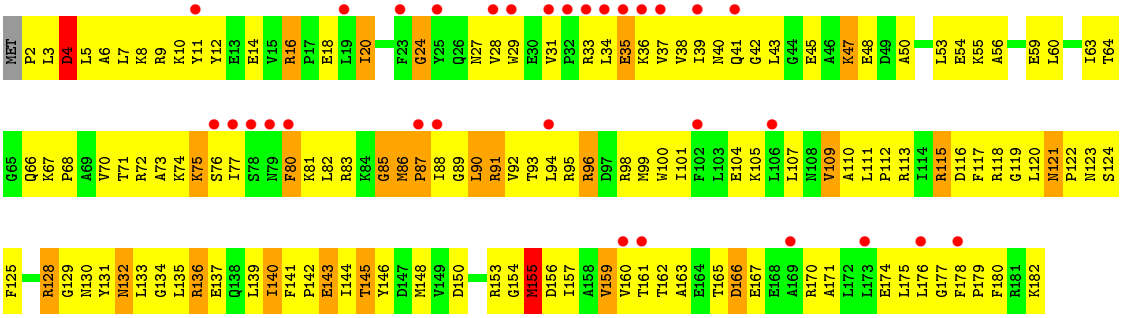
Chain BG:



- Molecule 30: 50S ribosomal protein L5

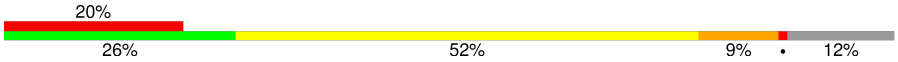
Chain DG:

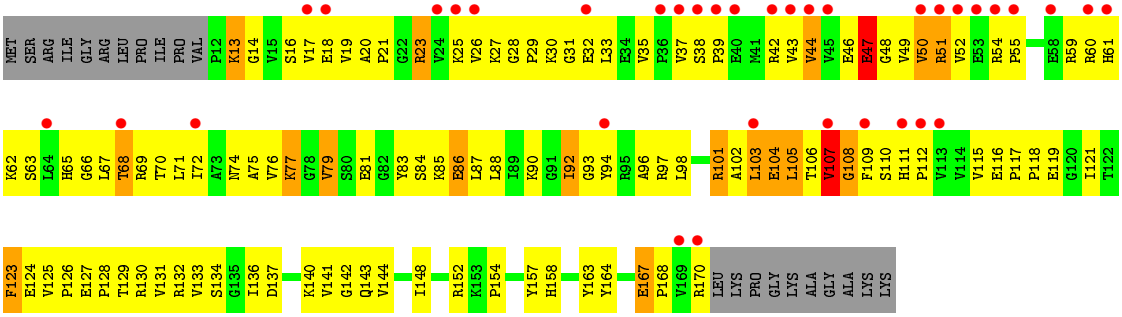




- Molecule 31: 50S ribosomal protein L6

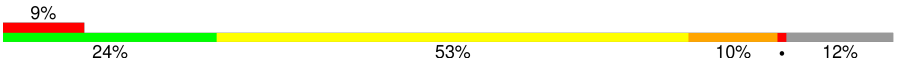
Chain BH:

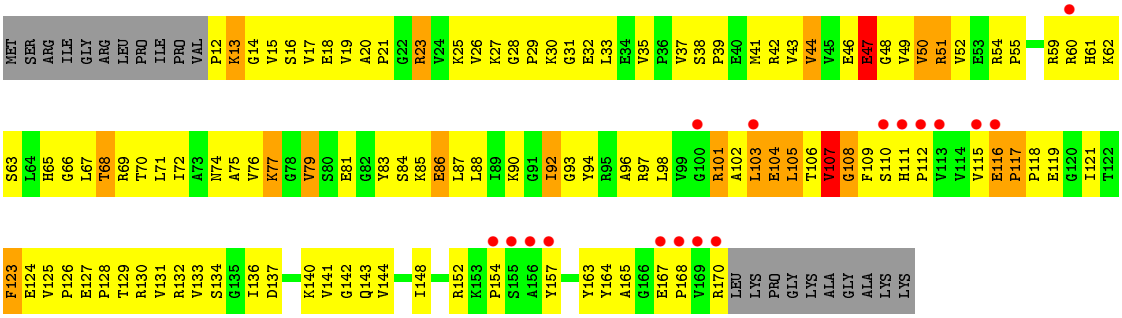




- Molecule 31: 50S ribosomal protein L6

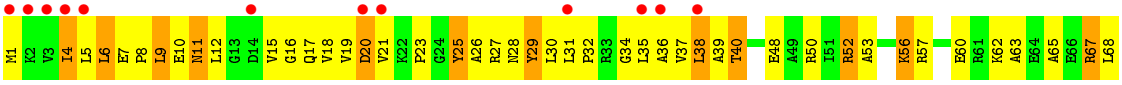
Chain DH:

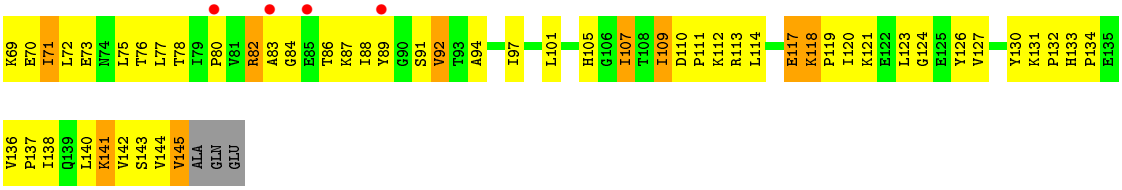




- Molecule 32: 50S ribosomal protein L9

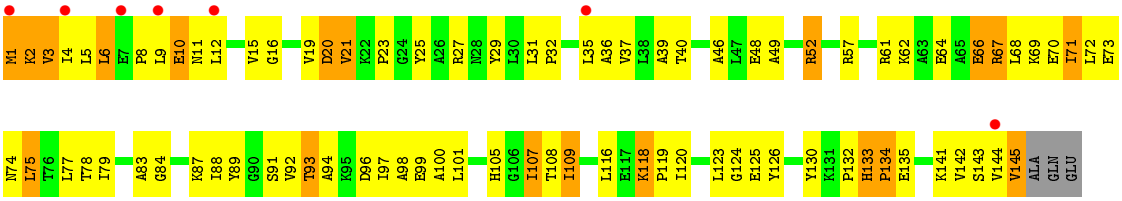
Chain BI:





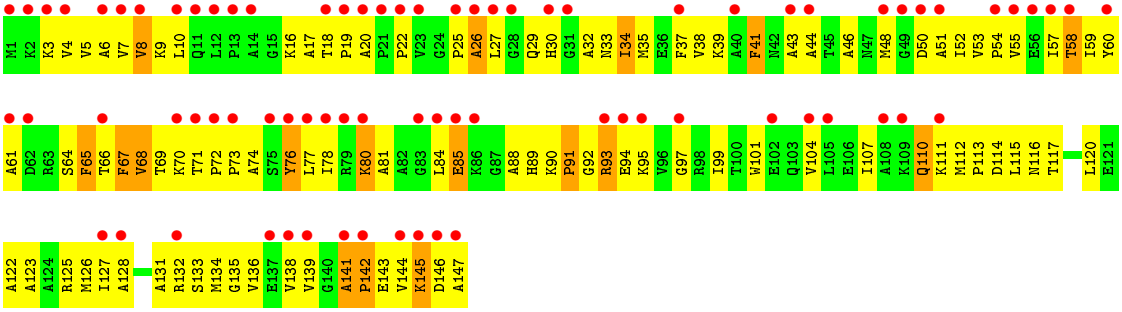
- Molecule 32: 50S ribosomal protein L9

Chain DI:



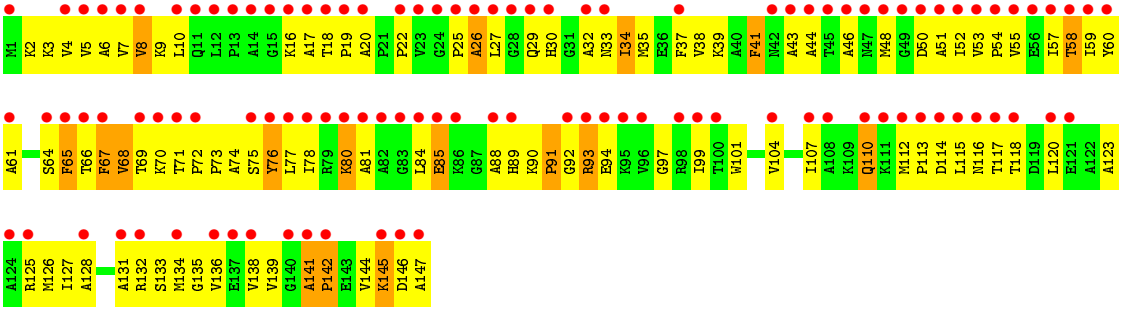
- Molecule 33: 50S ribosomal protein L11

Chain BK:



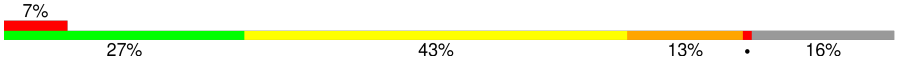
- Molecule 33: 50S ribosomal protein L11

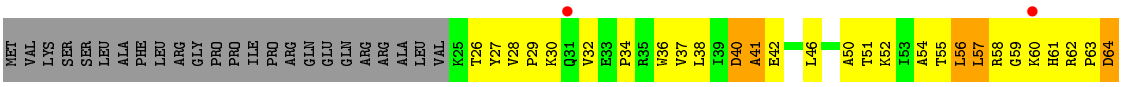
Chain DK:

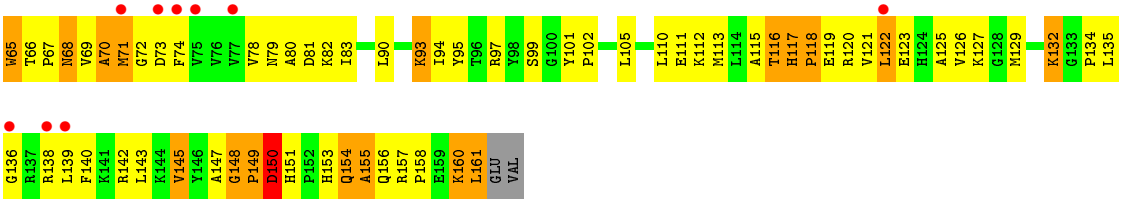


- Molecule 34: 50S ribosomal protein L13

Chain BN:

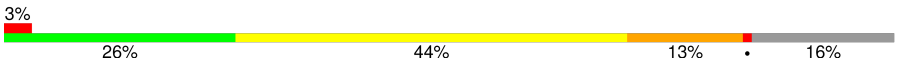


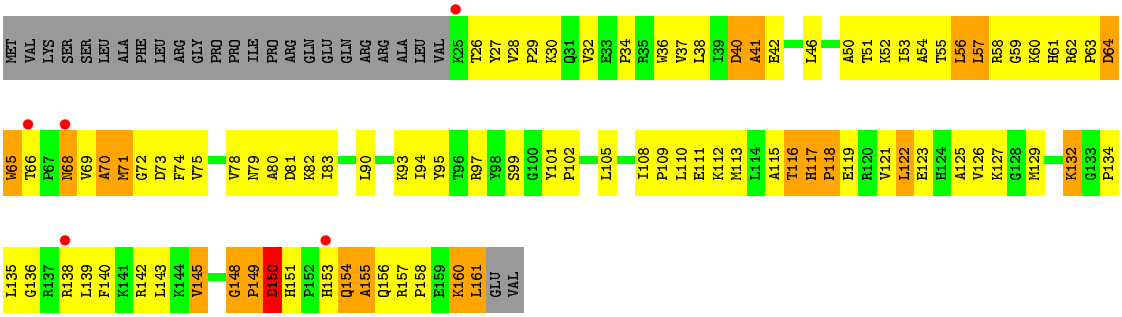




- Molecule 34: 50S ribosomal protein L13

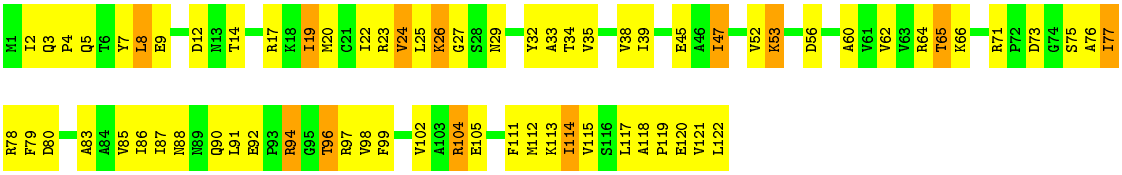
Chain DN:





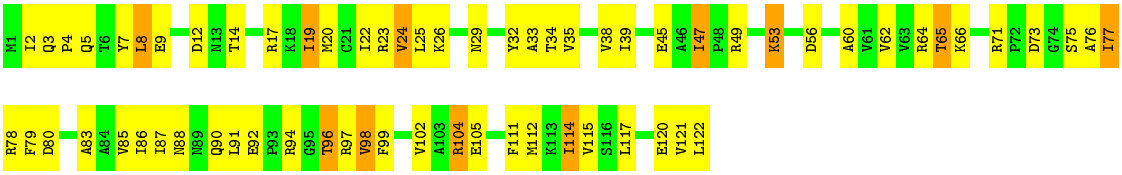
- Molecule 35: 50S ribosomal protein L14

Chain BO:



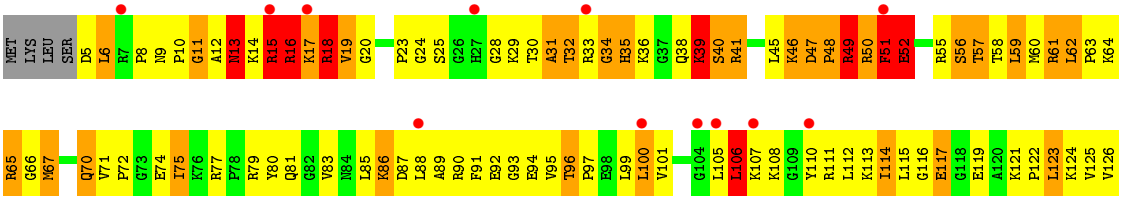
- Molecule 35: 50S ribosomal protein L14

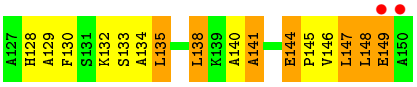
Chain DO:



- Molecule 36: 50S ribosomal protein L15

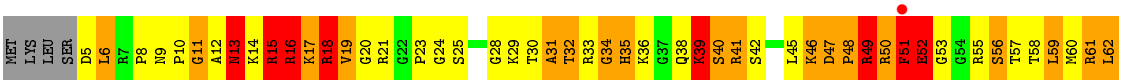
Chain BP:

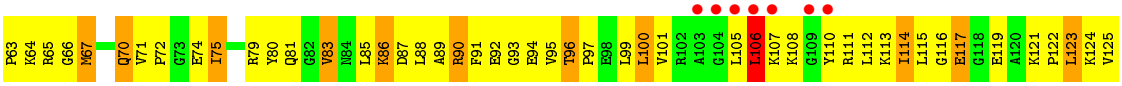


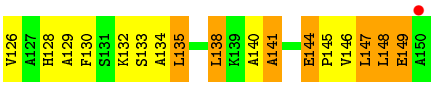


- Molecule 36: 50S ribosomal protein L15

Chain DP:

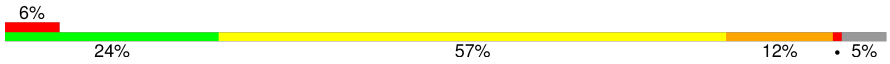


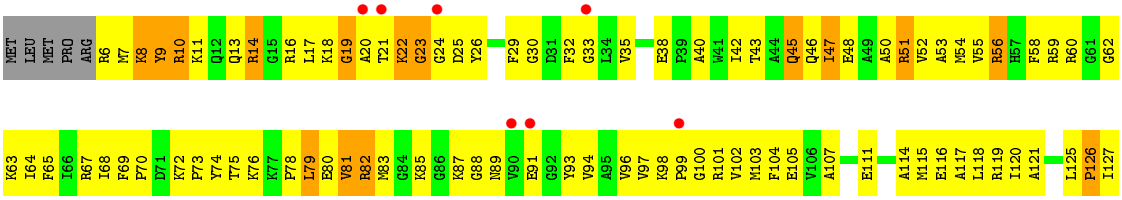


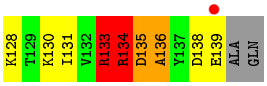


- Molecule 37: 50S ribosomal protein L16

Chain BQ:

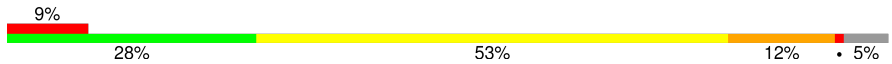


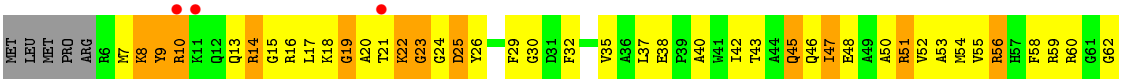


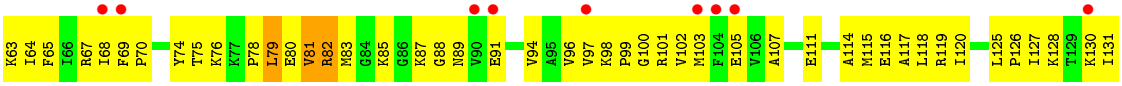


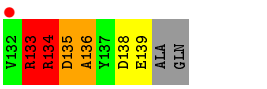
- Molecule 37: 50S ribosomal protein L16

Chain DQ:



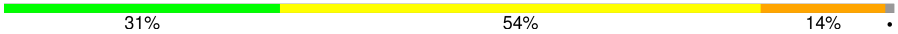






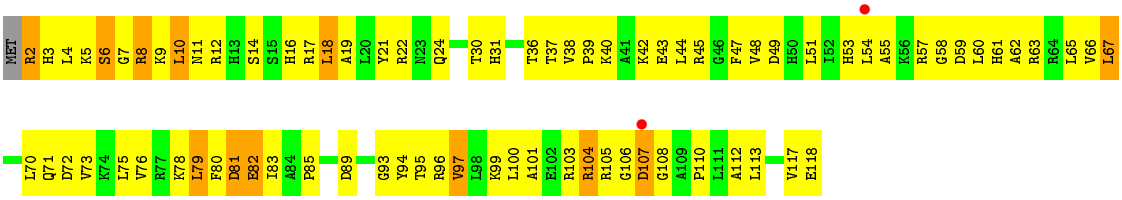
- Molecule 38: 50S ribosomal protein L17

Chain BR:



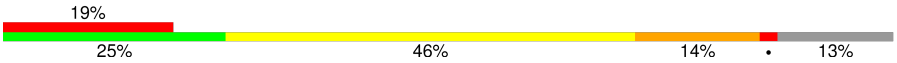
- Molecule 38: 50S ribosomal protein L17

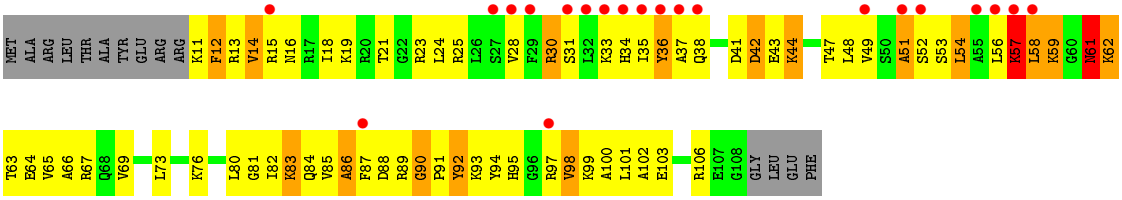
Chain DR:



- Molecule 39: 50S ribosomal protein L18

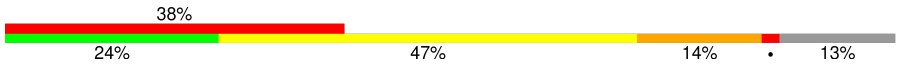
Chain BS:

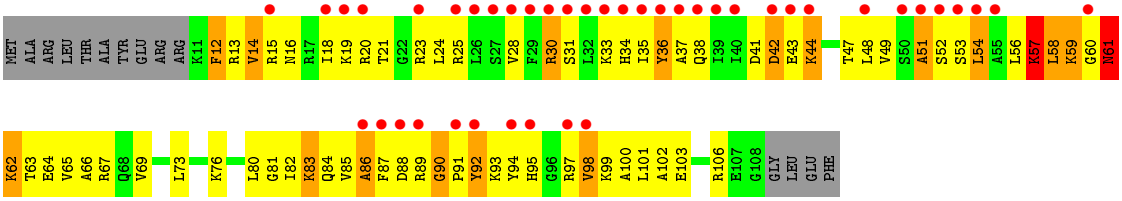




- Molecule 39: 50S ribosomal protein L18

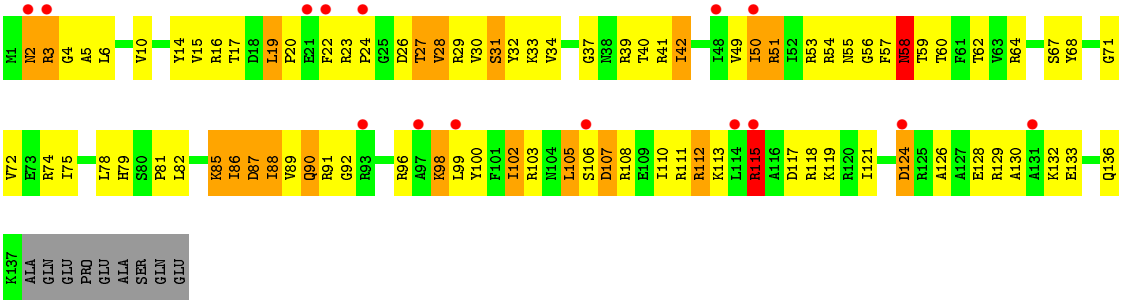
Chain DS:





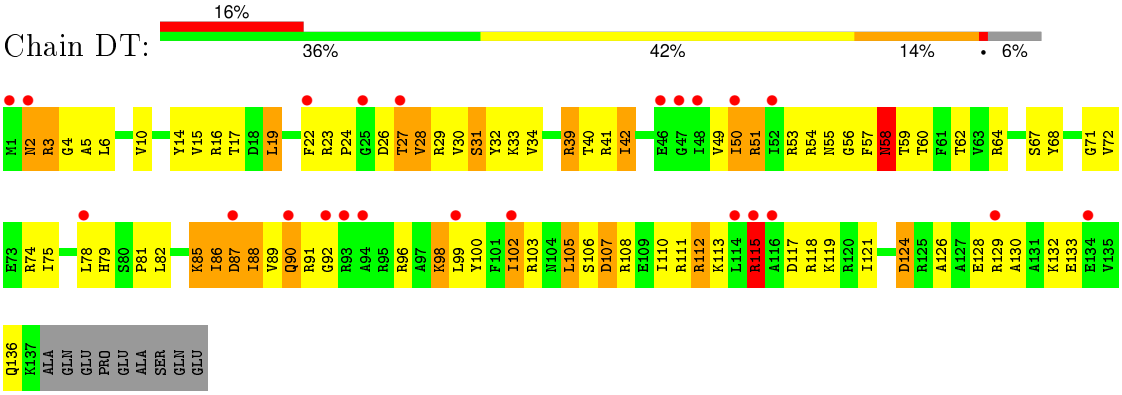
- Molecule 40: 50S ribosomal protein L19

Chain BT:



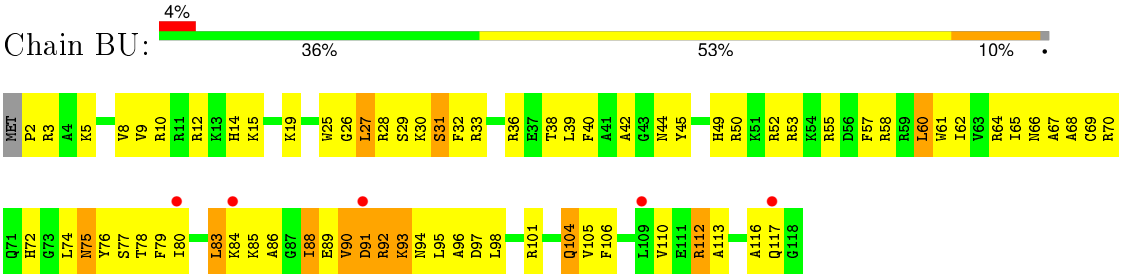
- Molecule 40: 50S ribosomal protein L19

Chain DT:



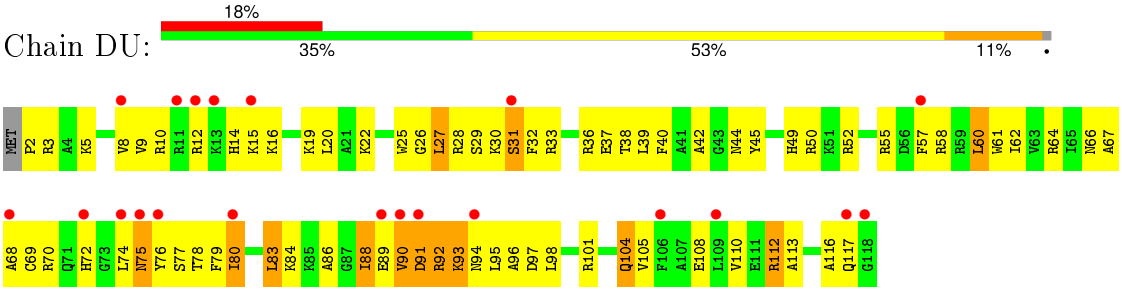
- Molecule 41: 50S ribosomal protein L20

Chain BU:



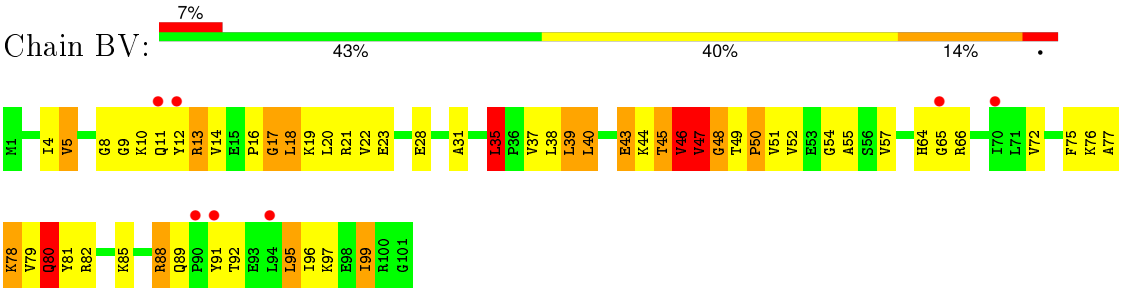
- Molecule 41: 50S ribosomal protein L20

Chain DU:



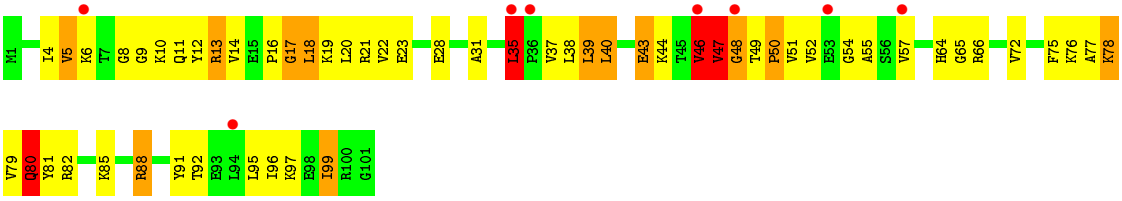
- Molecule 42: 50S ribosomal protein L21

Chain BV:



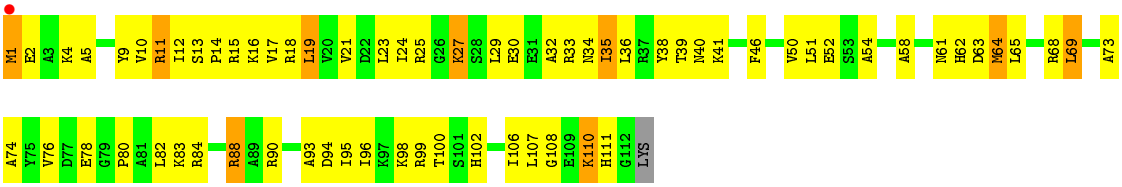
- Molecule 42: 50S ribosomal protein L21

Chain DV:



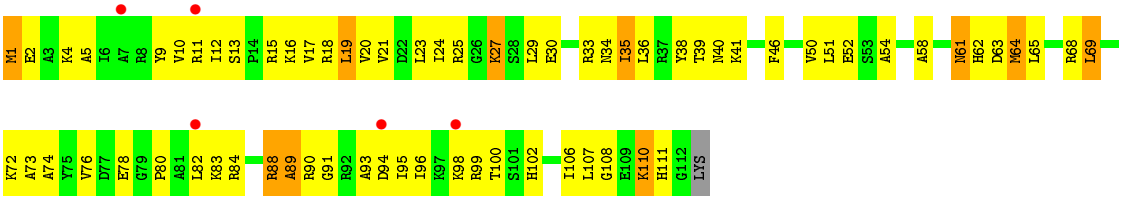
• Molecule 43: 50S ribosomal protein L22

Chain BW:



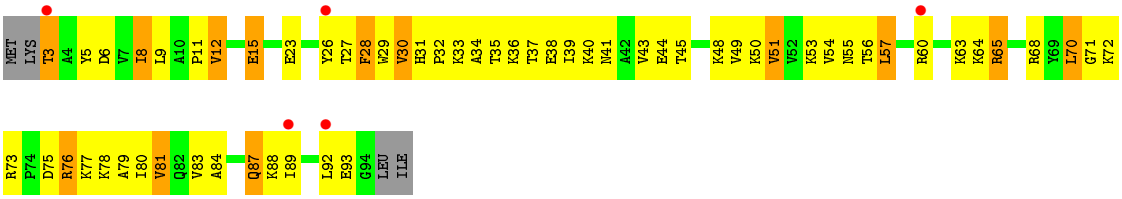
• Molecule 43: 50S ribosomal protein L22

Chain DW:



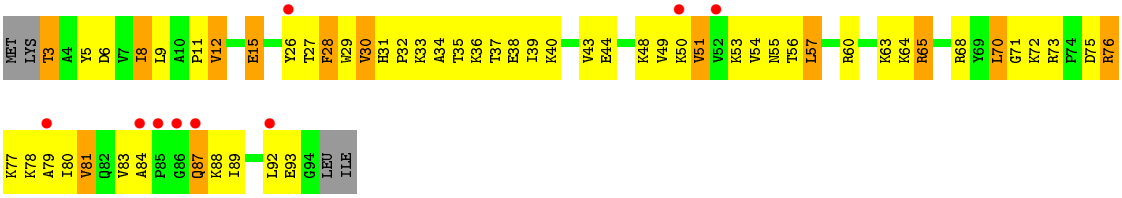
• Molecule 44: 50S ribosomal protein L23

Chain BX:



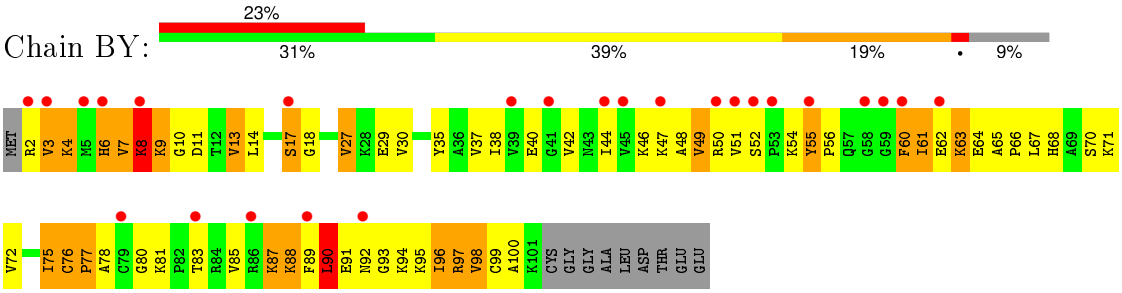
• Molecule 44: 50S ribosomal protein L23

Chain DX:



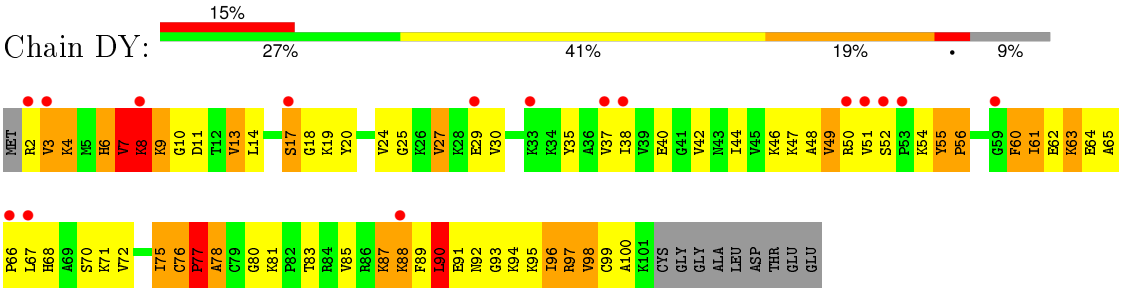
• Molecule 45: 50S ribosomal protein L24

Chain BY:



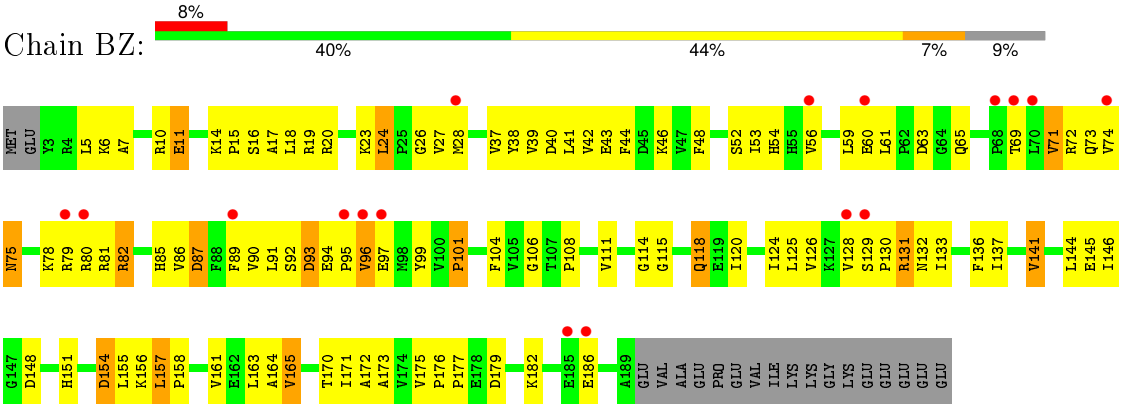
- Molecule 45: 50S ribosomal protein L24

Chain DY:



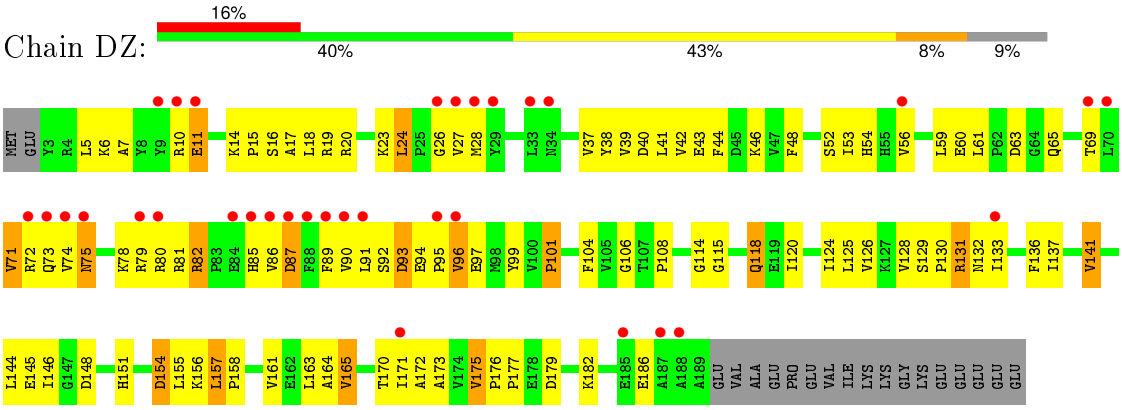
- Molecule 46: 50S ribosomal protein L25

Chain BZ:



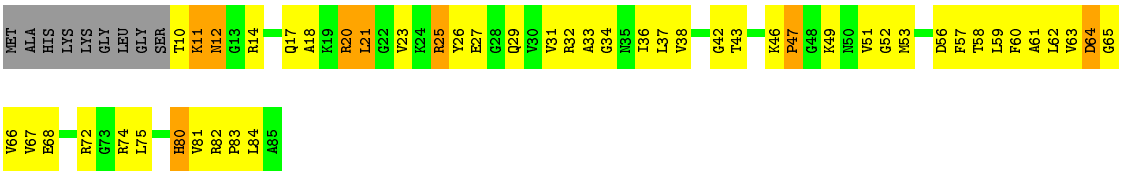
- Molecule 46: 50S ribosomal protein L25

Chain DZ:



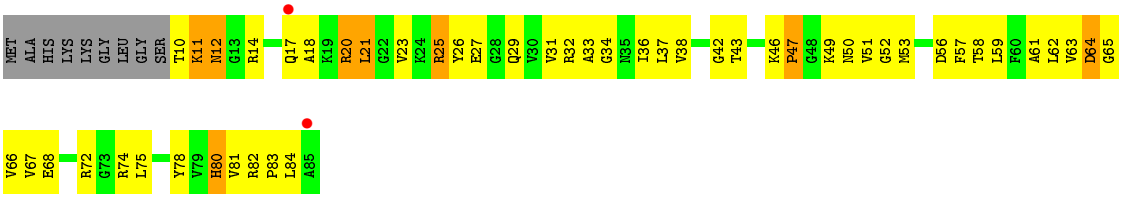
- Molecule 47: 50S ribosomal protein L27

Chain B0:



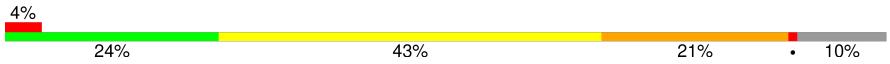
• Molecule 47: 50S ribosomal protein L27

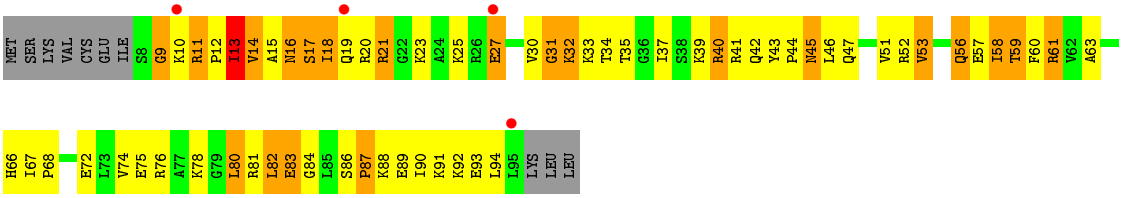
Chain D0:



• Molecule 48: 50S ribosomal protein L28

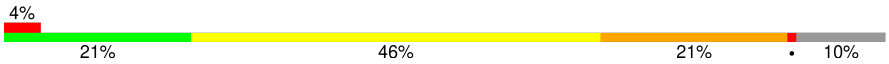
Chain B1:

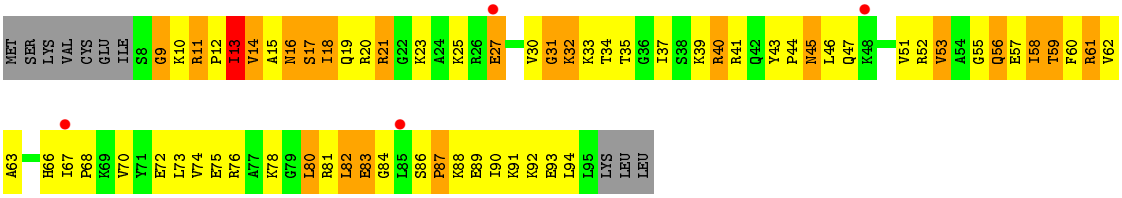




• Molecule 48: 50S ribosomal protein L28

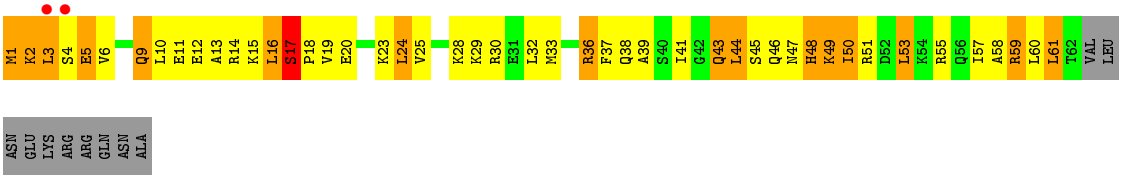
Chain D1:





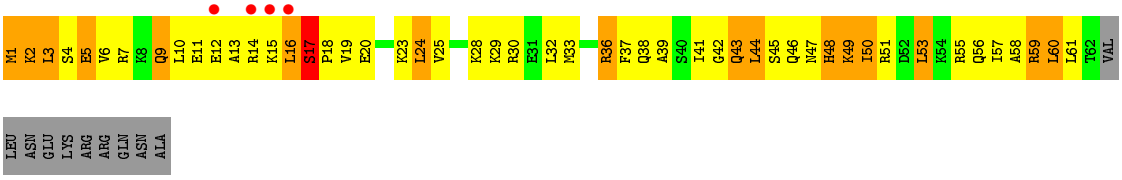
• Molecule 49: 50S ribosomal protein L29

Chain B2:



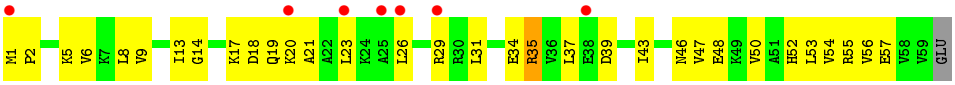
• Molecule 49: 50S ribosomal protein L29

Chain D2:



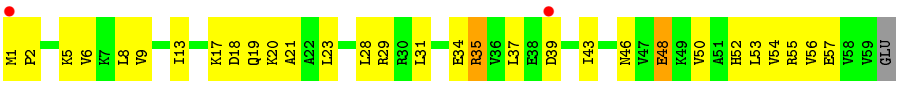
- Molecule 50: 50S ribosomal protein L30

Chain B3:



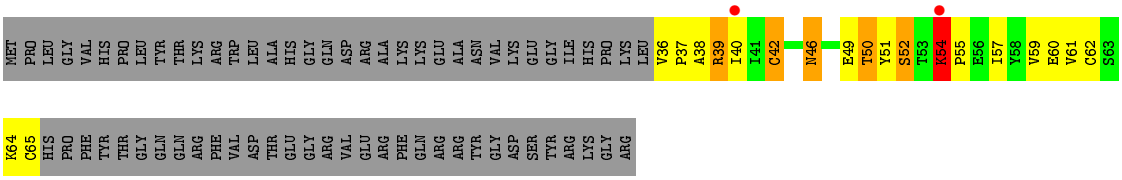
- Molecule 50: 50S ribosomal protein L30

Chain D3:



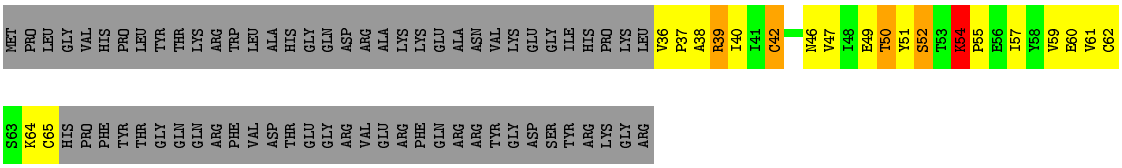
- Molecule 51: 50S ribosomal protein L31

Chain B4:



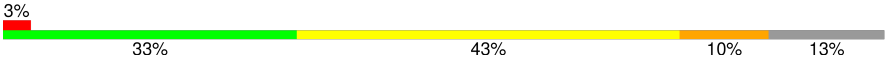
- Molecule 51: 50S ribosomal protein L31

Chain D4:



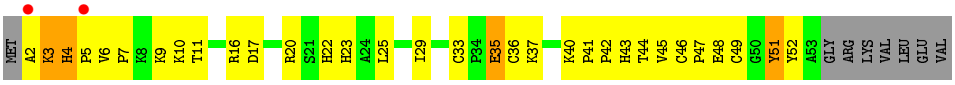
- Molecule 52: 50S ribosomal protein L32

Chain B5:



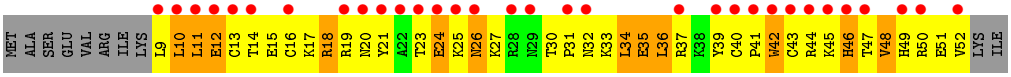
- Molecule 52: 50S ribosomal protein L32

Chain D5:



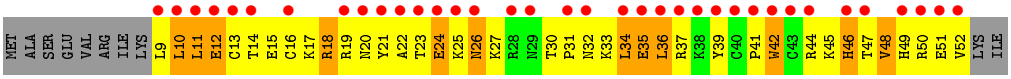
- Molecule 53: 50S ribosomal protein L33

Chain B6:



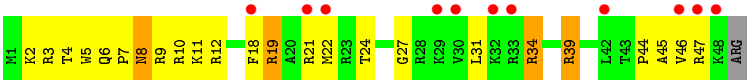
- Molecule 53: 50S ribosomal protein L33

Chain D6:



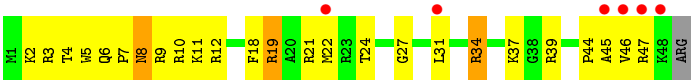
- Molecule 54: 50S ribosomal protein L34

Chain B7:



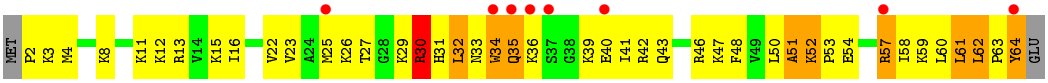
- Molecule 54: 50S ribosomal protein L34

Chain D7:



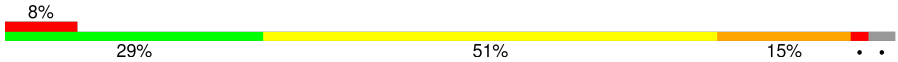
- Molecule 55: 50S ribosomal protein L35

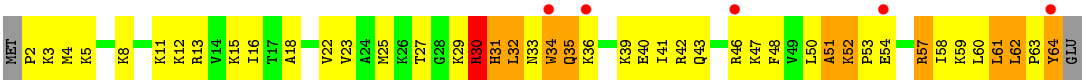
Chain B8:



- Molecule 55: 50S ribosomal protein L35

Chain D8:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	211.24Å 456.78Å 618.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 3.00 50.99 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.95-3.00) 97.2 (50.99-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.280 , 0.316 0.285 , 0.319	Depositor DCC
R_{free} test set	10486 reflections (0.92%)	DCC
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 1158087 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	301148	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% 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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.56	1/36194 (0.0%)	1.11	109/56493 (0.2%)
1	CA	0.55	1/36194 (0.0%)	1.10	110/56493 (0.2%)
2	AY	0.54	0/1832	1.03	2/2855 (0.1%)
2	AZ	0.46	0/1832	0.95	1/2855 (0.0%)
2	CY	0.54	0/1832	1.03	2/2855 (0.1%)
2	CZ	0.45	0/1832	0.94	1/2855 (0.0%)
3	AV	0.66	0/241	1.33	2/374 (0.5%)
3	CV	0.64	0/241	1.30	1/374 (0.3%)
4	AB	0.27	0/1935	0.46	0/2609
4	CB	0.27	0/1935	0.47	0/2609
5	AC	0.27	0/1636	0.46	0/2205
5	CC	0.28	0/1636	0.46	0/2205
6	AD	0.32	0/1733	0.50	0/2318
6	CD	0.30	0/1733	0.49	0/2318
7	AE	0.30	0/1171	0.50	0/1576
7	CE	0.29	0/1171	0.50	0/1576
8	AF	0.30	0/856	0.49	0/1154
8	CF	0.30	0/856	0.49	0/1154
9	AG	0.30	0/1276	0.47	0/1709
9	CG	0.28	0/1276	0.46	0/1709
10	AH	0.31	0/1136	0.52	0/1527
10	CH	0.29	0/1136	0.50	0/1527
11	AI	0.26	0/1029	0.45	0/1378
11	CI	0.26	0/1029	0.45	0/1378
12	AJ	0.29	0/807	0.49	0/1085
12	CJ	0.27	0/807	0.48	0/1085
13	AK	0.31	0/856	0.51	0/1157
13	CK	0.38	0/856	0.53	0/1157
14	AL	0.36	0/972	0.58	0/1301
14	CL	0.33	0/972	0.57	0/1301
15	AM	0.26	0/943	0.49	0/1265
15	CM	0.25	0/943	0.49	0/1265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	AN	0.28	0/501	0.47	0/664
16	CN	0.30	0/501	0.47	0/664
17	AO	0.33	0/745	0.48	0/992
17	CO	0.32	0/745	0.48	0/992
18	AP	0.33	0/716	0.50	0/963
18	CP	0.27	0/716	0.47	0/963
19	AQ	0.32	0/836	0.50	0/1117
19	CQ	0.30	0/836	0.48	0/1117
20	AR	0.32	0/579	0.49	0/768
20	CR	0.32	0/579	0.50	0/768
21	AS	0.25	0/642	0.46	0/865
21	CS	0.25	0/642	0.46	0/865
22	AT	0.30	0/764	0.48	0/1006
22	CT	0.27	0/764	0.47	0/1006
23	AU	0.24	0/212	0.47	0/277
23	CU	0.25	0/212	0.45	0/277
24	AX	0.30	0/2926	0.49	0/3953
24	CX	0.27	0/2926	0.48	0/3953
25	BA	0.65	0/69437	1.22	337/108401 (0.3%)
25	DA	0.66	2/69437 (0.0%)	1.22	323/108401 (0.3%)
26	BB	0.53	0/2853	1.12	10/4451 (0.2%)
26	DB	0.52	0/2853	1.11	8/4451 (0.2%)
27	BD	0.46	0/2154	0.67	1/2905 (0.0%)
27	DD	0.47	0/2154	0.67	1/2905 (0.0%)
28	BE	0.35	0/1596	0.58	0/2153
28	DE	0.34	0/1596	0.57	0/2153
29	BF	0.37	0/1621	0.57	0/2194
29	DF	0.38	0/1621	0.57	0/2194
30	BG	0.28	0/1500	0.50	0/2017
30	DG	0.27	0/1500	0.49	0/2017
31	BH	0.26	0/1245	0.48	0/1682
31	DH	0.28	0/1245	0.49	0/1682
32	BI	0.31	0/1147	0.53	0/1552
32	DI	0.32	0/1147	0.55	0/1552
33	BK	0.24	0/1108	0.45	0/1500
33	DK	0.24	0/1108	0.45	0/1500
34	BN	0.32	0/1123	0.55	0/1515
34	DN	0.33	0/1123	0.55	0/1515
35	BO	0.38	0/942	0.56	0/1268
35	DO	0.35	0/942	0.55	0/1268
36	BP	0.38	0/1131	0.71	1/1504 (0.1%)
36	DP	0.40	0/1131	0.72	2/1504 (0.1%)
37	BQ	0.38	0/1084	0.60	0/1449

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	DQ	0.36	0/1084	0.59	0/1449
38	BR	0.38	0/974	0.59	0/1302
38	DR	0.36	0/974	0.57	0/1302
39	BS	0.28	0/778	0.50	0/1036
39	DS	0.26	0/778	0.48	0/1036
40	BT	0.37	0/1157	0.53	0/1544
40	DT	0.32	0/1157	0.51	0/1544
41	BU	0.37	0/982	0.53	0/1306
41	DU	0.42	0/982	0.54	0/1306
42	BV	0.35	0/790	0.57	0/1057
42	DV	0.37	0/790	0.59	0/1057
43	BW	0.36	0/901	0.56	0/1209
43	DW	0.37	0/901	0.56	0/1209
44	BX	0.40	0/739	0.55	0/993
44	DX	0.42	0/739	0.56	0/993
45	BY	0.33	0/788	0.57	0/1051
45	DY	0.39	0/788	0.59	0/1051
46	BZ	0.28	0/1514	0.50	0/2056
46	DZ	0.28	0/1514	0.49	0/2056
47	B0	0.34	0/613	0.54	0/816
47	D0	0.32	0/613	0.54	0/816
48	B1	0.44	0/701	0.71	1/932 (0.1%)
48	D1	0.42	0/701	0.70	1/932 (0.1%)
49	B2	0.37	0/522	0.62	0/690
49	D2	0.40	0/522	0.63	0/690
50	B3	0.30	0/472	0.48	0/634
50	D3	0.31	0/472	0.49	0/634
51	B4	0.28	0/228	0.52	0/309
51	D4	0.26	0/228	0.52	0/309
52	B5	0.32	0/418	0.55	0/567
52	D5	0.33	0/418	0.58	0/567
53	B6	0.30	0/387	0.51	0/518
53	D6	0.29	0/387	0.50	0/518
54	B7	0.41	0/426	0.58	0/561
54	D7	0.44	0/426	0.64	0/561
55	B8	0.46	0/515	0.66	0/679
55	D8	0.42	0/515	0.65	0/679
All	All	0.55	4/324432 (0.0%)	1.04	913/484634 (0.2%)

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
27	BD	0	1
27	DD	0	1
36	BP	0	3
36	DP	0	3
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	DA	74	A	C3'-O3'	5.67	1.50	1.42
25	DA	2447	G	C3'-O3'	5.48	1.49	1.42
1	AA	1064	G	C3'-O3'	5.40	1.49	1.42
1	CA	115	G	C3'-O3'	5.06	1.49	1.42

The worst 5 of 913 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	1913	A	C1'-O4'-C4'	-12.89	99.59	109.90
25	DA	1559	G	C1'-O4'-C4'	-12.85	99.62	109.90
25	DA	945	A	C1'-O4'-C4'	-12.85	99.62	109.90
25	BA	1559	G	C1'-O4'-C4'	-12.81	99.65	109.90
25	DA	1786	A	C1'-O4'-C4'	-12.74	99.70	109.90

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BD	40	THR	Peptide
36	BP	51	PHE	Peptide
36	BP	52	GLU	Peptide
36	BP	9	ASN	Peptide
27	DD	40	THR	Peptide

5.2 Too-close contacts (i)

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32332	0	16318	1066	0
1	CA	32332	0	16318	1109	0
2	AY	1640	0	837	39	0
2	AZ	1640	0	837	49	0
2	CY	1640	0	837	33	0
2	CZ	1640	0	837	48	0
3	AV	214	0	110	6	0
3	CV	214	0	110	4	0
4	AB	1900	0	1951	159	0
4	CB	1900	0	1951	160	0
5	AC	1612	0	1677	125	0
5	CC	1612	0	1677	129	0
6	AD	1703	0	1763	112	0
6	CD	1703	0	1763	105	0
7	AE	1155	0	1213	91	0
7	CE	1155	0	1213	84	0
8	AF	843	0	857	49	0
8	CF	843	0	857	48	0
9	AG	1257	0	1296	81	0
9	CG	1257	0	1296	79	0
10	AH	1116	0	1177	77	0
10	CH	1116	0	1177	80	0
11	AI	1011	0	1043	104	0
11	CI	1011	0	1043	106	0
12	AJ	794	0	840	102	0
12	CJ	794	0	840	97	0
13	AK	842	0	859	72	0
13	CK	842	0	859	74	0
14	AL	956	0	1046	112	0
14	CL	956	0	1046	109	0
15	AM	933	0	992	97	0
15	CM	933	0	992	108	0
16	AN	492	0	531	36	0
16	CN	492	0	532	41	0
17	AO	734	0	771	50	0
17	CO	734	0	771	51	0
18	AP	700	0	720	52	0
18	CP	700	0	720	59	0
19	AQ	823	0	893	54	0
19	CQ	823	0	893	52	0
20	AR	574	0	644	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	CR	574	0	644	51	0
21	AS	629	0	652	77	0
21	CS	629	0	652	76	0
22	AT	762	0	859	68	0
22	CT	762	0	859	64	0
23	AU	208	0	221	12	0
23	CU	208	0	221	12	0
24	AX	2876	0	2867	244	0
24	CX	2876	0	2867	242	0
25	BA	61997	0	31250	2146	0
25	DA	61997	0	31250	2152	1
26	BB	2551	0	1295	95	0
26	DB	2551	0	1295	93	1
27	BD	2104	0	2182	225	0
27	DD	2104	0	2182	228	0
28	BE	1563	0	1629	138	0
28	DE	1563	0	1629	129	0
29	BF	1586	0	1632	141	0
29	DF	1586	0	1632	144	0
30	BG	1475	0	1537	154	0
30	DG	1475	0	1537	151	0
31	BH	1222	0	1282	112	0
31	DH	1222	0	1282	114	0
32	BI	1132	0	1220	104	0
32	DI	1132	0	1220	91	0
33	BK	1088	0	1138	107	0
33	DK	1088	0	1138	107	0
34	BN	1096	0	1168	96	0
34	DN	1096	0	1168	93	0
35	BO	932	0	994	64	0
35	DO	932	0	994	61	0
36	BP	1114	0	1187	226	0
36	DP	1114	0	1187	229	0
37	BQ	1064	0	1114	141	0
37	DQ	1064	0	1114	129	0
38	BR	960	0	1021	106	0
38	DR	960	0	1021	101	0
39	BS	770	0	832	96	0
39	DS	770	0	832	98	0
40	BT	1143	0	1211	100	0
40	DT	1143	0	1211	98	0
41	BU	964	0	1022	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	DU	964	0	1022	102	0
42	BV	779	0	852	77	0
42	DV	779	0	852	78	0
43	BW	890	0	951	68	0
43	DW	890	0	951	70	0
44	BX	725	0	778	69	0
44	DX	725	0	778	71	0
45	BY	775	0	870	106	0
45	DY	775	0	870	110	0
46	BZ	1482	0	1507	106	0
46	DZ	1482	0	1507	106	0
47	B0	605	0	628	45	0
47	D0	605	0	628	49	0
48	B1	694	0	764	92	0
48	D1	694	0	764	91	0
49	B2	520	0	575	76	0
49	D2	520	0	575	77	0
50	B3	467	0	523	29	0
50	D3	467	0	523	29	0
51	B4	225	0	225	19	0
51	D4	225	0	225	22	0
52	B5	404	0	420	54	0
52	D5	404	0	420	53	0
53	B6	380	0	391	55	0
53	D6	380	0	391	56	0
54	B7	418	0	467	36	0
54	D7	418	0	467	38	0
55	B8	507	0	576	68	0
55	D8	507	0	576	79	0
56	AA	428	0	0	0	0
56	AB	7	0	0	0	0
56	AC	4	0	0	0	0
56	AD	3	0	0	0	0
56	AE	8	0	0	0	0
56	AF	2	0	0	0	0
56	AG	2	0	0	0	0
56	AH	2	0	0	0	0
56	AI	1	0	0	0	0
56	AJ	1	0	0	0	0
56	AK	7	0	0	0	0
56	AL	4	0	0	0	0
56	AM	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AN	1	0	0	0	0
56	AO	2	0	0	0	0
56	AQ	1	0	0	0	0
56	AR	1	0	0	0	0
56	AT	2	0	0	0	0
56	AV	3	0	0	0	0
56	AX	14	0	0	0	0
56	AY	26	0	0	0	0
56	AZ	15	0	0	0	0
56	B0	3	0	0	0	0
56	B1	7	0	0	0	0
56	B2	3	0	0	0	0
56	B4	2	0	0	0	0
56	B5	2	0	0	0	0
56	B6	2	0	0	0	0
56	B8	4	0	0	0	0
56	BA	923	0	0	0	0
56	BB	35	0	0	0	0
56	BD	7	0	0	0	0
56	BE	6	0	0	0	0
56	BF	6	0	0	0	0
56	BG	2	0	0	0	0
56	BH	4	0	0	0	0
56	BI	6	0	0	0	0
56	BK	3	0	0	0	0
56	BN	4	0	0	0	0
56	BO	5	0	0	0	0
56	BP	2	0	0	0	0
56	BQ	6	0	0	0	0
56	BR	2	0	0	0	0
56	BS	3	0	0	0	0
56	BT	1	0	0	0	0
56	BU	1	0	0	0	0
56	BV	3	0	0	0	0
56	BW	2	0	0	0	0
56	BX	2	0	0	0	0
56	BY	3	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	222	0	0	0	0
56	CB	2	0	0	0	0
56	CC	1	0	0	0	0
56	CF	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CG	2	0	0	0	0
56	CH	2	0	0	0	0
56	CK	3	0	0	0	0
56	CL	1	0	0	0	0
56	CO	1	0	0	0	0
56	CQ	1	0	0	0	0
56	CS	1	0	0	0	0
56	CT	1	0	0	0	0
56	CY	14	0	0	0	0
56	CZ	14	0	0	0	0
56	D1	2	0	0	0	0
56	D6	1	0	0	0	0
56	D8	1	0	0	0	0
56	DA	491	0	0	0	0
56	DB	12	0	0	0	0
56	DD	9	0	0	0	0
56	DE	1	0	0	0	0
56	DF	1	0	0	0	0
56	DG	2	0	0	0	0
56	DI	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	2	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	2	0	0	0	0
56	DR	1	0	0	0	0
56	DT	1	0	0	0	0
56	DU	1	0	0	0	0
56	DY	1	0	0	0	0
57	AD	1	0	0	0	0
57	AN	1	0	0	0	0
57	CD	1	0	0	0	0
57	CN	1	0	0	0	0
All	All	301148	0	204431	14693	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 29.

The worst 5 of 14693 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)
55:B8:57:ARG:HB2	55:B8:57:ARG:HH11	1.11	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:B1:11:ARG:HB3	48:B1:12:PRO:HD2	1.14	1.13
48:D1:11:ARG:HB3	48:D1:12:PRO:HD2	1.18	1.12
36:BP:23:PRO:HD2	36:BP:33:ARG:NH2	1.67	1.09
25:BA:2630:G:H1'	25:BA:2894:G:H1'	1.35	1.09

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)
25:DA:1411:C:O3'	26:DB:53:A:O2'[1_655]	2.14	0.06

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
4	AB	232/256 (91%)	175 (75%)	47 (20%)	10 (4%)	3 19
4	CB	232/256 (91%)	174 (75%)	48 (21%)	10 (4%)	3 19
5	AC	204/239 (85%)	138 (68%)	51 (25%)	15 (7%)	1 6
5	CC	204/239 (85%)	138 (68%)	52 (26%)	14 (7%)	1 7
6	AD	206/209 (99%)	166 (81%)	30 (15%)	10 (5%)	3 16
6	CD	206/209 (99%)	169 (82%)	26 (13%)	11 (5%)	2 14
7	AE	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	4 21
7	CE	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	4 21
8	AF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	19 61
8	CF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	19 61
9	AG	153/156 (98%)	124 (81%)	28 (18%)	1 (1%)	26 70
9	CG	153/156 (98%)	125 (82%)	27 (18%)	1 (1%)	26 70
10	AH	136/138 (99%)	112 (82%)	18 (13%)	6 (4%)	3 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CH	136/138 (99%)	112 (82%)	18 (13%)	6 (4%)	3	18
11	AI	125/128 (98%)	93 (74%)	22 (18%)	10 (8%)	1	5
11	CI	125/128 (98%)	93 (74%)	23 (18%)	9 (7%)	1	7
12	AJ	96/105 (91%)	76 (79%)	14 (15%)	6 (6%)	2	9
12	CJ	96/105 (91%)	77 (80%)	13 (14%)	6 (6%)	2	9
13	AK	112/129 (87%)	94 (84%)	12 (11%)	6 (5%)	2	14
13	CK	112/129 (87%)	94 (84%)	12 (11%)	6 (5%)	2	14
14	AL	120/134 (90%)	87 (72%)	22 (18%)	11 (9%)	1	4
14	CL	120/134 (90%)	87 (72%)	22 (18%)	11 (9%)	1	4
15	AM	115/126 (91%)	91 (79%)	19 (16%)	5 (4%)	3	19
15	CM	115/126 (91%)	91 (79%)	20 (17%)	4 (4%)	4	24
16	AN	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	11	46
16	CN	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	11	46
17	AO	86/89 (97%)	70 (81%)	13 (15%)	3 (4%)	4	24
17	CO	86/89 (97%)	69 (80%)	14 (16%)	3 (4%)	4	24
18	AP	81/88 (92%)	59 (73%)	19 (24%)	3 (4%)	4	23
18	CP	81/88 (92%)	60 (74%)	18 (22%)	3 (4%)	4	23
19	AQ	97/105 (92%)	79 (81%)	16 (16%)	2 (2%)	9	40
19	CQ	97/105 (92%)	79 (81%)	16 (16%)	2 (2%)	9	40
20	AR	68/88 (77%)	45 (66%)	18 (26%)	5 (7%)	1	6
20	CR	68/88 (77%)	46 (68%)	17 (25%)	5 (7%)	1	6
21	AS	76/93 (82%)	50 (66%)	18 (24%)	8 (10%)	1	3
21	CS	76/93 (82%)	50 (66%)	18 (24%)	8 (10%)	1	3
22	AT	97/106 (92%)	72 (74%)	17 (18%)	8 (8%)	1	5
22	CT	97/106 (92%)	72 (74%)	18 (19%)	7 (7%)	1	7
23	AU	22/27 (82%)	12 (54%)	8 (36%)	2 (9%)	1	4
23	CU	22/27 (82%)	12 (54%)	8 (36%)	2 (9%)	1	4
24	AX	360/378 (95%)	288 (80%)	57 (16%)	15 (4%)	3	20
24	CX	360/378 (95%)	288 (80%)	58 (16%)	14 (4%)	4	21
27	BD	269/276 (98%)	208 (77%)	41 (15%)	20 (7%)	1	6
27	DD	269/276 (98%)	204 (76%)	46 (17%)	19 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	BE	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	4	21
28	DE	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	4	21
29	BF	200/210 (95%)	162 (81%)	28 (14%)	10 (5%)	3	15
29	DF	200/210 (95%)	162 (81%)	26 (13%)	12 (6%)	2	11
30	BG	179/182 (98%)	128 (72%)	39 (22%)	12 (7%)	1	8
30	DG	179/182 (98%)	127 (71%)	39 (22%)	13 (7%)	1	6
31	BH	157/180 (87%)	120 (76%)	30 (19%)	7 (4%)	3	18
31	DH	157/180 (87%)	121 (77%)	28 (18%)	8 (5%)	2	15
32	BI	143/148 (97%)	107 (75%)	29 (20%)	7 (5%)	3	16
32	DI	143/148 (97%)	121 (85%)	19 (13%)	3 (2%)	9	40
33	BK	145/147 (99%)	101 (70%)	35 (24%)	9 (6%)	2	10
33	DK	145/147 (99%)	101 (70%)	35 (24%)	9 (6%)	2	10
34	BN	135/163 (83%)	103 (76%)	17 (13%)	15 (11%)	0	2
34	DN	135/163 (83%)	101 (75%)	19 (14%)	15 (11%)	0	2
35	BO	120/122 (98%)	102 (85%)	14 (12%)	4 (3%)	5	26
35	DO	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	5	26
36	BP	144/150 (96%)	86 (60%)	35 (24%)	23 (16%)	0	1
36	DP	144/150 (96%)	88 (61%)	34 (24%)	22 (15%)	0	1
37	BQ	132/141 (94%)	96 (73%)	22 (17%)	14 (11%)	0	3
37	DQ	132/141 (94%)	93 (70%)	24 (18%)	15 (11%)	0	2
38	BR	115/118 (98%)	89 (77%)	19 (16%)	7 (6%)	2	11
38	DR	115/118 (98%)	91 (79%)	19 (16%)	5 (4%)	3	19
39	BS	96/112 (86%)	56 (58%)	29 (30%)	11 (12%)	0	2
39	DS	96/112 (86%)	56 (58%)	29 (30%)	11 (12%)	0	2
40	BT	135/146 (92%)	91 (67%)	30 (22%)	14 (10%)	1	3
40	DT	135/146 (92%)	91 (67%)	31 (23%)	13 (10%)	1	3
41	BU	115/118 (98%)	92 (80%)	19 (16%)	4 (4%)	4	24
41	DU	115/118 (98%)	91 (79%)	19 (16%)	5 (4%)	3	19
42	BV	99/101 (98%)	74 (75%)	15 (15%)	10 (10%)	1	3
42	DV	99/101 (98%)	74 (75%)	15 (15%)	10 (10%)	1	3
43	BW	110/113 (97%)	88 (80%)	18 (16%)	4 (4%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DW	110/113 (97%)	87 (79%)	18 (16%)	5 (4%)	3	18
44	BX	90/96 (94%)	73 (81%)	15 (17%)	2 (2%)	8	38
44	DX	90/96 (94%)	73 (81%)	15 (17%)	2 (2%)	8	38
45	BY	98/110 (89%)	64 (65%)	18 (18%)	16 (16%)	0	1
45	DY	98/110 (89%)	65 (66%)	17 (17%)	16 (16%)	0	1
46	BZ	185/206 (90%)	146 (79%)	31 (17%)	8 (4%)	3	19
46	DZ	185/206 (90%)	145 (78%)	32 (17%)	8 (4%)	3	19
47	B0	74/85 (87%)	61 (82%)	10 (14%)	3 (4%)	3	20
47	D0	74/85 (87%)	61 (82%)	10 (14%)	3 (4%)	3	20
48	B1	86/98 (88%)	59 (69%)	16 (19%)	11 (13%)	0	1
48	D1	86/98 (88%)	59 (69%)	16 (19%)	11 (13%)	0	1
49	B2	60/72 (83%)	43 (72%)	12 (20%)	5 (8%)	1	5
49	D2	60/72 (83%)	44 (73%)	11 (18%)	5 (8%)	1	5
50	B3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	4	24
50	D3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	4	24
51	B4	28/97 (29%)	18 (64%)	6 (21%)	4 (14%)	0	1
51	D4	28/97 (29%)	18 (64%)	6 (21%)	4 (14%)	0	1
52	B5	50/60 (83%)	40 (80%)	7 (14%)	3 (6%)	2	11
52	D5	50/60 (83%)	40 (80%)	7 (14%)	3 (6%)	2	11
53	B6	42/54 (78%)	27 (64%)	10 (24%)	5 (12%)	0	2
53	D6	42/54 (78%)	27 (64%)	10 (24%)	5 (12%)	0	2
54	B7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
54	D7	46/49 (94%)	42 (91%)	4 (9%)	0	100	100
55	B8	61/65 (94%)	42 (69%)	12 (20%)	7 (12%)	0	2
55	D8	61/65 (94%)	42 (69%)	12 (20%)	7 (12%)	0	2
All	All	12130/13206 (92%)	9225 (76%)	2153 (18%)	752 (6%)	2	10

5 of 752 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AC	45	LYS
5	AC	47	LEU
6	AD	5	ILE

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Mol	Chain	Res	Type
6	AD	44	GLY
7	AE	85	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AB	202/220 (92%)	186 (92%)	16 (8%)	15	48
4	CB	202/220 (92%)	185 (92%)	17 (8%)	14	45
5	AC	160/188 (85%)	138 (86%)	22 (14%)	4	20
5	CC	160/188 (85%)	138 (86%)	22 (14%)	4	20
6	AD	180/181 (99%)	160 (89%)	20 (11%)	8	29
6	CD	180/181 (99%)	161 (89%)	19 (11%)	8	31
7	AE	116/123 (94%)	99 (85%)	17 (15%)	4	18
7	CE	116/123 (94%)	99 (85%)	17 (15%)	4	18
8	AF	90/90 (100%)	80 (89%)	10 (11%)	8	29
8	CF	90/90 (100%)	81 (90%)	9 (10%)	9	34
9	AG	126/127 (99%)	119 (94%)	7 (6%)	26	65
9	CG	126/127 (99%)	119 (94%)	7 (6%)	26	65
10	AH	119/119 (100%)	106 (89%)	13 (11%)	8	30
10	CH	119/119 (100%)	106 (89%)	13 (11%)	8	30
11	AI	98/99 (99%)	85 (87%)	13 (13%)	5	21
11	CI	98/99 (99%)	86 (88%)	12 (12%)	6	25
12	AJ	88/92 (96%)	75 (85%)	13 (15%)	4	17
12	CJ	88/92 (96%)	75 (85%)	13 (15%)	4	17
13	AK	86/99 (87%)	74 (86%)	12 (14%)	4	19
13	CK	86/99 (87%)	74 (86%)	12 (14%)	4	19
14	AL	103/110 (94%)	91 (88%)	12 (12%)	7	27
14	CL	103/110 (94%)	91 (88%)	12 (12%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AM	94/101 (93%)	85 (90%)	9 (10%)	10	38
15	CM	94/101 (93%)	85 (90%)	9 (10%)	10	38
16	AN	49/50 (98%)	44 (90%)	5 (10%)	9	33
16	CN	49/50 (98%)	44 (90%)	5 (10%)	9	33
17	AO	79/80 (99%)	70 (89%)	9 (11%)	7	28
17	CO	79/80 (99%)	70 (89%)	9 (11%)	7	28
18	AP	72/74 (97%)	65 (90%)	7 (10%)	10	37
18	CP	72/74 (97%)	66 (92%)	6 (8%)	14	46
19	AQ	94/97 (97%)	86 (92%)	8 (8%)	13	45
19	CQ	94/97 (97%)	86 (92%)	8 (8%)	13	45
20	AR	61/77 (79%)	53 (87%)	8 (13%)	5	22
20	CR	61/77 (79%)	52 (85%)	9 (15%)	4	17
21	AS	69/80 (86%)	58 (84%)	11 (16%)	3	15
21	CS	69/80 (86%)	58 (84%)	11 (16%)	3	15
22	AT	76/82 (93%)	67 (88%)	9 (12%)	6	26
22	CT	76/82 (93%)	68 (90%)	8 (10%)	8	32
23	AU	19/22 (86%)	18 (95%)	1 (5%)	28	67
23	CU	19/22 (86%)	18 (95%)	1 (5%)	28	67
24	AX	305/319 (96%)	258 (85%)	47 (15%)	3	16
24	CX	305/319 (96%)	260 (85%)	45 (15%)	4	17
27	BD	213/218 (98%)	181 (85%)	32 (15%)	3	17
27	DD	213/218 (98%)	181 (85%)	32 (15%)	3	17
28	BE	165/166 (99%)	144 (87%)	21 (13%)	5	23
28	DE	165/166 (99%)	144 (87%)	21 (13%)	5	23
29	BF	161/166 (97%)	142 (88%)	19 (12%)	6	26
29	DF	161/166 (97%)	140 (87%)	21 (13%)	5	22
30	BG	155/156 (99%)	135 (87%)	20 (13%)	5	23
30	DG	155/156 (99%)	135 (87%)	20 (13%)	5	23
31	BH	132/148 (89%)	115 (87%)	17 (13%)	5	23
31	DH	132/148 (89%)	115 (87%)	17 (13%)	5	23
32	BI	122/124 (98%)	101 (83%)	21 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	DI	122/124 (98%)	103 (84%)	19 (16%)	3	16
33	BK	111/111 (100%)	95 (86%)	16 (14%)	4	18
33	DK	111/111 (100%)	95 (86%)	16 (14%)	4	18
34	BN	116/139 (84%)	98 (84%)	18 (16%)	3	16
34	DN	116/139 (84%)	98 (84%)	18 (16%)	3	16
35	BO	100/100 (100%)	86 (86%)	14 (14%)	4	19
35	DO	100/100 (100%)	85 (85%)	15 (15%)	3	17
36	BP	112/116 (97%)	80 (71%)	32 (29%)	0	2
36	DP	112/116 (97%)	79 (70%)	33 (30%)	0	2
37	BQ	105/111 (95%)	91 (87%)	14 (13%)	5	21
37	DQ	105/111 (95%)	91 (87%)	14 (13%)	5	21
38	BR	100/101 (99%)	90 (90%)	10 (10%)	9	34
38	DR	100/101 (99%)	91 (91%)	9 (9%)	12	41
39	BS	77/88 (88%)	66 (86%)	11 (14%)	4	19
39	DS	77/88 (88%)	66 (86%)	11 (14%)	4	19
40	BT	121/128 (94%)	101 (84%)	20 (16%)	3	13
40	DT	121/128 (94%)	101 (84%)	20 (16%)	3	13
41	BU	93/94 (99%)	82 (88%)	11 (12%)	6	26
41	DU	93/94 (99%)	83 (89%)	10 (11%)	8	30
42	BV	82/82 (100%)	68 (83%)	14 (17%)	2	12
42	DV	82/82 (100%)	69 (84%)	13 (16%)	3	15
43	BW	91/92 (99%)	80 (88%)	11 (12%)	6	25
43	DW	91/92 (99%)	80 (88%)	11 (12%)	6	25
44	BX	74/78 (95%)	58 (78%)	16 (22%)	1	6
44	DX	74/78 (95%)	59 (80%)	15 (20%)	1	7
45	BY	84/91 (92%)	72 (86%)	12 (14%)	4	19
45	DY	84/91 (92%)	70 (83%)	14 (17%)	3	13
46	BZ	162/179 (90%)	151 (93%)	11 (7%)	20	56
46	DZ	162/179 (90%)	150 (93%)	12 (7%)	17	52
47	B0	61/67 (91%)	53 (87%)	8 (13%)	5	22
47	D0	61/67 (91%)	53 (87%)	8 (13%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	B1	73/83 (88%)	58 (80%)	15 (20%)	1	7
48	D1	73/83 (88%)	57 (78%)	16 (22%)	1	6
49	B2	58/67 (87%)	45 (78%)	13 (22%)	1	5
49	D2	58/67 (87%)	45 (78%)	13 (22%)	1	5
50	B3	51/52 (98%)	49 (96%)	2 (4%)	39	77
50	D3	51/52 (98%)	49 (96%)	2 (4%)	39	77
51	B4	27/84 (32%)	21 (78%)	6 (22%)	1	5
51	D4	27/84 (32%)	22 (82%)	5 (18%)	2	10
52	B5	45/52 (86%)	41 (91%)	4 (9%)	12	42
52	D5	45/52 (86%)	42 (93%)	3 (7%)	20	57
53	B6	43/52 (83%)	34 (79%)	9 (21%)	1	7
53	D6	43/52 (83%)	34 (79%)	9 (21%)	1	7
54	B7	41/42 (98%)	35 (85%)	6 (15%)	4	18
54	D7	41/42 (98%)	35 (85%)	6 (15%)	4	18
55	B8	53/55 (96%)	47 (89%)	6 (11%)	7	28
55	D8	53/55 (96%)	47 (89%)	6 (11%)	7	28
All	All	10228/10944 (94%)	8877 (87%)	1351 (13%)	5	22

5 of 1351 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	B0	21	LEU
8	CF	27	GLN
44	DX	30	VAL
48	B1	76	ARG
4	CB	102	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 287 such sidechains are listed below:

Mol	Chain	Res	Type
50	B3	19	GLN
8	CF	73	ASN
46	DZ	75	ASN
52	B5	22	HIS
4	CB	204	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1525 (98%)	287 (19%)	107 (7%)
1	CA	1503/1525 (98%)	282 (18%)	106 (7%)
2	AY	76/77 (98%)	15 (19%)	6 (7%)
2	AZ	76/77 (98%)	15 (19%)	5 (6%)
2	CY	76/77 (98%)	14 (18%)	6 (7%)
2	CZ	76/77 (98%)	15 (19%)	5 (6%)
25	BA	2878/2894 (99%)	589 (20%)	178 (6%)
25	DA	2878/2894 (99%)	594 (20%)	173 (6%)
26	BB	118/124 (95%)	17 (14%)	6 (5%)
26	DB	118/124 (95%)	18 (15%)	6 (5%)
3	AV	10/27 (37%)	3 (30%)	3 (30%)
3	CV	10/27 (37%)	3 (30%)	3 (30%)
All	All	9322/9448 (98%)	1852 (19%)	604 (6%)

5 of 1852 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	22	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 604 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2427	C
1	CA	466	G
25	DA	2145	C
25	BA	2573	C
1	CA	48	C

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2392 ligands modelled in this entry, 2392 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	1504/1525 (98%)	-0.36	19 (1%)	79	53	35, 78, 175, 261	0
1	CA	1504/1525 (98%)	-0.10	32 (2%)	67	36	34, 99, 199, 271	0
2	AY	77/77 (100%)	-0.51	0	100	100	60, 90, 124, 194	0
2	AZ	77/77 (100%)	1.24	19 (24%)	1	1	146, 211, 242, 260	0
2	CY	77/77 (100%)	-0.34	0	100	100	59, 91, 127, 196	0
2	CZ	77/77 (100%)	1.84	24 (31%)	1	0	175, 231, 266, 276	0
3	AV	10/27 (37%)	0.22	1 (10%)	9	4	62, 77, 118, 184	0
3	CV	10/27 (37%)	0.83	2 (20%)	1	1	63, 104, 143, 196	0
4	AB	234/256 (91%)	0.41	26 (11%)	7	3	85, 126, 167, 194	0
4	CB	234/256 (91%)	0.54	30 (12%)	5	2	91, 127, 174, 204	0
5	AC	206/239 (86%)	0.04	11 (5%)	30	12	86, 121, 159, 183	0
5	CC	206/239 (86%)	0.27	14 (6%)	20	7	87, 126, 164, 178	0
6	AD	208/209 (99%)	0.15	16 (7%)	16	6	50, 79, 127, 164	0
6	CD	208/209 (99%)	0.53	21 (10%)	9	3	81, 115, 151, 184	0
7	AE	151/162 (93%)	0.04	10 (6%)	22	7	65, 90, 130, 192	0
7	CE	151/162 (93%)	0.11	4 (2%)	59	29	71, 100, 145, 173	0
8	AF	101/101 (100%)	-0.00	2 (1%)	68	39	69, 98, 137, 176	0
8	CF	101/101 (100%)	-0.09	1 (0%)	84	60	64, 94, 131, 149	0
9	AG	155/156 (99%)	0.05	10 (6%)	22	8	82, 113, 154, 172	0
9	CG	155/156 (99%)	0.18	9 (5%)	26	10	87, 125, 158, 181	0
10	AH	138/138 (100%)	0.08	4 (2%)	55	26	64, 90, 135, 146	0
10	CH	138/138 (100%)	0.26	7 (5%)	32	12	80, 107, 145, 171	0
11	AI	127/128 (99%)	0.80	17 (13%)	4	1	90, 134, 168, 182	0
11	CI	127/128 (99%)	1.41	29 (22%)	1	1	105, 140, 173, 227	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
12	AJ	98/105 (93%)	1.22	23 (23%) 1 1	87, 125, 166, 184	0
12	CJ	98/105 (93%)	1.46	25 (25%) 1 1	106, 144, 175, 186	0
13	AK	114/129 (88%)	0.10	7 (6%) 25 9	59, 88, 123, 160	0
13	CK	114/129 (88%)	0.44	16 (14%) 4 1	64, 91, 135, 175	0
14	AL	122/134 (91%)	0.01	4 (3%) 50 22	47, 67, 114, 144	0
14	CL	122/134 (91%)	0.29	11 (9%) 12 4	57, 89, 131, 185	0
15	AM	117/126 (92%)	0.46	14 (11%) 6 2	93, 122, 159, 171	0
15	CM	117/126 (92%)	0.90	20 (17%) 2 1	98, 143, 172, 188	0
16	AN	60/61 (98%)	0.72	8 (13%) 4 1	75, 109, 141, 193	0
16	CN	60/61 (98%)	0.97	10 (16%) 2 1	80, 113, 158, 175	0
17	AO	88/89 (98%)	0.15	1 (1%) 82 58	57, 90, 123, 145	0
17	CO	88/89 (98%)	0.09	2 (2%) 64 33	60, 91, 130, 145	0
18	AP	83/88 (94%)	0.62	8 (9%) 10 4	58, 75, 119, 184	0
18	CP	83/88 (94%)	1.48	29 (34%) 0 0	90, 123, 155, 202	0
19	AQ	99/105 (94%)	-0.04	1 (1%) 84 60	56, 79, 118, 142	0
19	CQ	99/105 (94%)	0.61	8 (8%) 15 5	76, 105, 140, 159	0
20	AR	70/88 (79%)	0.71	4 (5%) 27 10	68, 103, 147, 165	0
20	CR	70/88 (79%)	0.83	12 (17%) 2 1	64, 87, 139, 147	0
21	AS	78/93 (83%)	1.91	33 (42%) 0 0	98, 136, 170, 193	0
21	CS	78/93 (83%)	1.47	27 (34%) 0 0	114, 150, 184, 205	0
22	AT	99/106 (93%)	0.32	6 (6%) 25 9	51, 84, 138, 166	0
22	CT	99/106 (93%)	1.04	22 (22%) 1 1	87, 117, 160, 184	0
23	AU	24/27 (88%)	4.74	22 (91%) 0 0	93, 122, 162, 191	0
23	CU	24/27 (88%)	5.70	24 (100%) 0 0	100, 137, 178, 187	0
24	AX	362/378 (95%)	0.88	76 (20%) 1 1	61, 129, 207, 244	0
24	CX	362/378 (95%)	1.33	92 (25%) 1 1	94, 150, 244, 273	0
25	BA	2879/2894 (99%)	-0.34	76 (2%) 59 29	14, 64, 186, 278	0
25	DA	2879/2894 (99%)	-0.23	90 (3%) 52 24	10, 67, 204, 287	0
26	BB	119/124 (95%)	-0.29	0 100 100	69, 100, 144, 222	0
26	DB	119/124 (95%)	0.31	6 (5%) 32 13	87, 147, 205, 258	0
27	BD	271/276 (98%)	-0.03	7 (2%) 59 29	27, 51, 99, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	DD	271/276 (98%)	-0.07	4 (1%) 76 49	26, 51, 92, 146	0
28	BE	204/206 (99%)	0.09	12 (5%) 26 10	36, 69, 126, 159	0
28	DE	204/206 (99%)	0.51	29 (14%) 4 1	45, 85, 137, 186	0
29	BF	202/210 (96%)	-0.14	6 (2%) 54 25	38, 71, 131, 153	0
29	DF	202/210 (96%)	0.10	6 (2%) 54 25	34, 66, 124, 190	0
30	BG	181/182 (99%)	0.65	32 (17%) 2 1	88, 121, 164, 179	0
30	DG	181/182 (99%)	0.88	31 (17%) 2 1	113, 153, 182, 206	0
31	BH	159/180 (88%)	0.92	36 (22%) 1 1	97, 139, 185, 202	0
31	DH	159/180 (88%)	0.18	17 (10%) 8 3	79, 111, 154, 174	0
32	BI	145/148 (97%)	0.32	16 (11%) 7 3	54, 106, 147, 198	0
32	DI	145/148 (97%)	0.18	7 (4%) 34 14	58, 94, 129, 147	0
33	BK	147/147 (100%)	2.45	77 (52%) 0 0	177, 205, 225, 240	0
33	DK	147/147 (100%)	4.35	108 (73%) 0 0	207, 236, 257, 274	0
34	BN	137/163 (84%)	0.40	11 (8%) 15 5	55, 87, 131, 153	0
34	DN	137/163 (84%)	0.12	5 (3%) 46 20	59, 80, 130, 164	0
35	BO	122/122 (100%)	-0.38	0 100 100	32, 61, 101, 118	0
35	DO	122/122 (100%)	-0.38	0 100 100	47, 72, 108, 129	0
36	BP	146/150 (97%)	0.43	14 (9%) 10 4	35, 89, 148, 203	0
36	DP	146/150 (97%)	0.32	9 (6%) 24 9	21, 93, 146, 183	0
37	BQ	134/141 (95%)	0.29	8 (5%) 25 9	44, 79, 136, 188	0
37	DQ	134/141 (95%)	0.27	13 (9%) 10 4	56, 91, 148, 192	0
38	BR	117/118 (99%)	-0.14	0 100 100	31, 63, 114, 165	0
38	DR	117/118 (99%)	0.10	2 (1%) 73 45	48, 73, 130, 148	0
39	BS	98/112 (87%)	0.72	21 (21%) 1 1	66, 105, 140, 169	0
39	DS	98/112 (87%)	1.90	42 (42%) 0 0	106, 144, 177, 218	0
40	BT	137/146 (93%)	0.43	15 (10%) 7 3	41, 76, 136, 156	0
40	DT	137/146 (93%)	0.87	23 (16%) 2 1	66, 100, 155, 189	0
41	BU	117/118 (99%)	0.44	5 (4%) 39 16	45, 78, 124, 159	0
41	DU	117/118 (99%)	0.87	21 (17%) 2 1	39, 68, 120, 194	0
42	BV	101/101 (100%)	0.22	7 (6%) 20 7	63, 99, 144, 220	0
42	DV	101/101 (100%)	0.49	8 (7%) 15 5	46, 91, 143, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	BW	112/113 (99%)	-0.10	1 (0%) 85 64	39, 64, 111, 163	0
43	DW	112/113 (99%)	0.15	5 (4%) 37 15	31, 61, 119, 155	0
44	BX	92/96 (95%)	0.15	5 (5%) 29 11	50, 79, 122, 149	0
44	DX	92/96 (95%)	0.49	9 (9%) 10 4	38, 65, 114, 150	0
45	BY	100/110 (90%)	1.34	25 (25%) 1 1	75, 112, 179, 200	0
45	DY	100/110 (90%)	0.87	16 (16%) 3 1	53, 86, 160, 186	0
46	BZ	187/206 (90%)	0.37	17 (9%) 11 4	83, 119, 156, 196	0
46	DZ	187/206 (90%)	0.81	33 (17%) 2 1	107, 139, 176, 201	0
47	B0	76/85 (89%)	-0.07	0 100 100	56, 78, 115, 150	0
47	D0	76/85 (89%)	0.08	2 (2%) 59 29	73, 99, 139, 160	0
48	B1	88/98 (89%)	0.03	4 (4%) 37 15	31, 66, 119, 177	0
48	D1	88/98 (89%)	0.20	4 (4%) 37 15	34, 68, 143, 172	0
49	B2	62/72 (86%)	0.15	2 (3%) 51 23	55, 90, 131, 165	0
49	D2	62/72 (86%)	0.05	4 (6%) 22 8	37, 75, 147, 177	0
50	B3	59/60 (98%)	0.48	7 (11%) 6 2	65, 85, 145, 166	0
50	D3	59/60 (98%)	0.23	2 (3%) 49 21	57, 83, 129, 170	0
51	B4	30/97 (30%)	0.31	2 (6%) 21 7	101, 135, 178, 183	0
51	D4	30/97 (30%)	0.07	0 100 100	115, 149, 178, 183	0
52	B5	52/60 (86%)	0.20	2 (3%) 44 18	49, 79, 147, 166	0
52	D5	52/60 (86%)	-0.27	2 (3%) 44 18	42, 80, 147, 167	0
53	B6	44/54 (81%)	4.69	32 (72%) 0 0	106, 136, 175, 224	0
53	D6	44/54 (81%)	5.16	36 (81%) 0 0	111, 140, 175, 192	0
54	B7	48/49 (97%)	1.33	11 (22%) 1 1	38, 57, 119, 143	0
54	D7	48/49 (97%)	0.75	6 (12%) 5 2	31, 44, 96, 161	0
55	B8	63/65 (96%)	0.44	8 (12%) 5 2	42, 59, 117, 156	0
55	D8	63/65 (96%)	0.42	5 (7%) 15 5	48, 72, 133, 168	0
All	All	21662/22654 (95%)	0.22	1817 (8%) 14 5	10, 90, 190, 287	0

The worst 5 of 1817 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DF	207	GLY	21.0
53	B6	13	CYS	17.4

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Mol	Chain	Res	Type	RSRZ
11	CI	8	GLY	15.9
53	B6	23	THR	13.8
2	CZ	17(A)	U	13.2

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3297	1/1	0.79	1.17	74.26	89,89,89,89	0
56	MG	DA	3335	1/1	0.97	0.64	56.96	3,3,3,3	0
56	MG	BA	3460	1/1	0.82	0.82	48.13	75,75,75,75	0
56	MG	BA	3722	1/1	0.94	0.76	38.22	66,66,66,66	0
56	MG	DA	3129	1/1	0.79	0.61	33.59	57,57,57,57	0
56	MG	DA	3101	1/1	0.69	0.65	32.95	64,64,64,64	0
56	MG	DA	3132	1/1	0.87	0.53	32.78	65,65,65,65	0
56	MG	BA	3436	1/1	0.73	0.52	31.32	47,47,47,47	0
56	MG	DA	3287	1/1	0.94	0.42	28.44	10,10,10,10	0
56	MG	BA	3597	1/1	0.78	0.73	22.28	48,48,48,48	0
56	MG	BA	3865	1/1	0.97	0.51	21.33	37,37,37,37	0
56	MG	DA	3207	1/1	0.92	0.57	19.73	50,50,50,50	0
56	MG	BA	3362	1/1	0.64	0.65	18.56	68,68,68,68	0
56	MG	DA	3423	1/1	0.90	0.56	18.40	28,28,28,28	0
56	MG	BA	3428	1/1	0.83	0.62	18.21	86,86,86,86	0
56	MG	BA	3075	1/1	0.98	0.42	18.14	29,29,29,29	0
56	MG	CA	1663	1/1	0.97	0.30	17.74	3,3,3,3	0
56	MG	BA	3471	1/1	0.75	0.37	17.59	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3283	1/1	0.82	0.39	16.64	63,63,63,63	0
56	MG	BA	3320	1/1	0.83	0.46	16.62	84,84,84,84	0
56	MG	BA	3143	1/1	0.89	0.55	16.43	64,64,64,64	0
56	MG	AA	1768	1/1	0.95	0.36	16.39	37,37,37,37	0
56	MG	CA	1736	1/1	0.88	0.37	16.26	3,3,3,3	0
56	MG	BA	3024	1/1	0.78	0.33	16.02	87,87,87,87	0
56	MG	BA	3673	1/1	0.93	0.28	15.64	19,19,19,19	0
56	MG	BA	3664	1/1	0.93	0.38	14.92	23,23,23,23	0
56	MG	BA	3538	1/1	0.95	0.47	14.39	30,30,30,30	0
56	MG	CA	1710	1/1	0.97	0.32	14.08	46,46,46,46	0
56	MG	BA	3131	1/1	0.92	0.60	13.79	72,72,72,72	0
56	MG	DA	3120	1/1	0.98	0.38	13.36	28,28,28,28	0
56	MG	BA	3426	1/1	0.89	0.28	13.29	20,20,20,20	0
56	MG	BA	3009	1/1	0.76	0.59	13.12	59,59,59,59	0
56	MG	BA	3521	1/1	0.92	0.30	12.99	45,45,45,45	0
56	MG	DA	3069	1/1	0.87	0.43	12.86	3,3,3,3	0
56	MG	BA	3168	1/1	0.87	0.42	12.81	52,52,52,52	0
56	MG	DA	3264	1/1	0.96	0.21	12.36	4,4,4,4	0
56	MG	BA	3042	1/1	0.91	0.45	12.17	74,74,74,74	0
56	MG	CA	1757	1/1	0.85	0.34	11.93	66,66,66,66	0
56	MG	BA	3662	1/1	0.89	0.33	11.85	35,35,35,35	0
56	MG	BA	3840	1/1	0.84	0.43	11.41	56,56,56,56	0
56	MG	BA	3709	1/1	0.74	0.29	11.36	70,70,70,70	0
56	MG	BA	3465	1/1	0.89	0.46	11.11	59,59,59,59	0
56	MG	BA	3867	1/1	0.94	0.34	10.91	50,50,50,50	0
56	MG	BA	3173	1/1	0.88	0.44	10.83	80,80,80,80	0
56	MG	CA	1655	1/1	0.90	0.32	10.58	38,38,38,38	0
56	MG	BA	3073	1/1	0.50	0.34	10.51	57,57,57,57	0
56	MG	DA	3315	1/1	0.82	0.33	10.46	62,62,62,62	0
56	MG	BF	303	1/1	0.72	0.92	10.43	50,50,50,50	0
56	MG	BA	3054	1/1	0.97	0.29	10.27	63,63,63,63	0
56	MG	BA	3904	1/1	0.89	0.41	10.22	53,53,53,53	0
56	MG	DA	3451	1/1	0.98	0.48	10.12	23,23,23,23	0
56	MG	AA	1979	1/1	0.92	0.38	9.69	58,58,58,58	0
56	MG	BA	3311	1/1	0.90	0.24	9.57	44,44,44,44	0
56	MG	BA	3148	1/1	0.96	0.35	9.55	35,35,35,35	0
56	MG	DA	3062	1/1	0.91	0.33	9.10	4,4,4,4	0
56	MG	BA	3467	1/1	0.99	0.38	9.07	21,21,21,21	0
56	MG	BA	3746	1/1	0.79	0.46	8.93	71,71,71,71	0
56	MG	DA	3047	1/1	0.92	0.28	8.75	3,3,3,3	0
56	MG	DD	5005	1/1	0.75	0.63	8.65	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3004	1/1	0.97	0.39	8.55	3,3,3,3	0
56	MG	DA	3051	1/1	0.86	0.27	8.08	3,3,3,3	0
56	MG	AA	1782	1/1	0.93	0.33	7.93	24,24,24,24	0
56	MG	AA	1725	1/1	0.85	0.47	7.80	56,56,56,56	0
56	MG	DA	3053	1/1	0.95	0.20	7.73	4,4,4,4	0
56	MG	DA	3418	1/1	0.98	0.26	7.68	3,3,3,3	0
56	MG	BA	3416	1/1	0.86	0.38	7.61	55,55,55,55	0
56	MG	DA	3444	1/1	0.95	0.38	7.60	3,3,3,3	0
56	MG	DA	3422	1/1	0.97	0.22	7.53	2,2,2,2	0
56	MG	DA	3488	1/1	0.96	0.26	7.20	3,3,3,3	0
56	MG	DA	3442	1/1	0.98	0.36	7.17	3,3,3,3	0
56	MG	BA	3077	1/1	0.60	0.22	7.17	59,59,59,59	0
56	MG	DA	3085	1/1	0.97	0.23	7.11	3,3,3,3	0
56	MG	DA	3092	1/1	0.98	0.29	7.06	4,4,4,4	0
56	MG	CA	1623	1/1	0.95	0.30	7.05	4,4,4,4	0
56	MG	AC	302	1/1	0.85	0.37	6.94	88,88,88,88	0
56	MG	BA	3549	1/1	0.92	0.29	6.88	27,27,27,27	0
56	MG	BA	3753	1/1	0.75	0.39	6.84	65,65,65,65	0
56	MG	BA	3590	1/1	0.85	0.22	6.80	32,32,32,32	0
56	MG	CA	1689	1/1	0.79	0.46	6.61	81,81,81,81	0
56	MG	CA	1712	1/1	0.80	0.26	6.58	39,39,39,39	0
56	MG	BA	3234	1/1	0.79	0.23	6.53	55,55,55,55	0
56	MG	AA	1975	1/1	0.92	0.31	6.26	66,66,66,66	0
56	MG	BA	3266	1/1	0.98	0.33	6.25	24,24,24,24	0
56	MG	DA	3468	1/1	0.92	0.44	5.97	3,3,3,3	0
56	MG	BA	3304	1/1	0.89	0.33	5.84	25,25,25,25	0
56	MG	AA	2009	1/1	0.94	0.28	5.82	47,47,47,47	0
56	MG	CA	1769	1/1	0.47	0.20	5.64	77,77,77,77	0
56	MG	DA	3424	1/1	0.86	0.38	5.47	14,14,14,14	0
56	MG	BA	3736	1/1	0.94	0.27	5.41	26,26,26,26	0
56	MG	CA	1697	1/1	0.93	0.25	5.32	52,52,52,52	0
56	MG	BA	3667	1/1	0.97	0.31	5.28	48,48,48,48	0
56	MG	DA	3204	1/1	0.77	0.33	5.19	43,43,43,43	0
56	MG	DA	3190	1/1	0.95	0.24	5.18	4,4,4,4	0
56	MG	BA	3214	1/1	0.95	0.36	5.15	19,19,19,19	0
56	MG	DA	3257	1/1	0.97	0.37	5.04	3,3,3,3	0
56	MG	BD	5002	1/1	0.94	0.32	5.04	82,82,82,82	0
56	MG	BA	3356	1/1	0.81	0.40	4.96	54,54,54,54	0
56	MG	AA	1772	1/1	0.91	0.31	4.93	40,40,40,40	0
56	MG	BA	3167	1/1	0.97	0.36	4.90	22,22,22,22	0
56	MG	BA	3270	1/1	0.89	0.44	4.80	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3332	1/1	0.87	0.28	4.78	33,33,33,33	0
56	MG	BA	3008	1/1	0.86	0.25	4.76	38,38,38,38	0
56	MG	AA	1793	1/1	0.73	0.32	4.75	82,82,82,82	0
56	MG	BA	3350	1/1	0.74	0.26	4.66	31,31,31,31	0
56	MG	BA	3872	1/1	0.85	0.24	4.64	54,54,54,54	0
56	MG	DA	3344	1/1	0.97	0.36	4.28	25,25,25,25	0
56	MG	AA	1613	1/1	0.97	0.24	4.23	45,45,45,45	0
56	MG	DA	3269	1/1	0.97	0.21	4.14	3,3,3,3	0
56	MG	AX	413	1/1	0.90	0.35	4.12	32,32,32,32	0
56	MG	DA	3445	1/1	0.94	0.22	4.11	4,4,4,4	0
56	MG	BA	3739	1/1	0.96	0.18	4.11	23,23,23,23	0
56	MG	CA	1639	1/1	0.93	0.28	4.10	3,3,3,3	0
56	MG	CA	1653	1/1	0.92	0.26	4.08	62,62,62,62	0
56	MG	AA	2017	1/1	0.94	0.26	4.06	47,47,47,47	0
56	MG	BO	205	1/1	0.72	0.32	4.01	86,86,86,86	0
56	MG	DA	3216	1/1	0.94	0.31	4.00	3,3,3,3	0
56	MG	DA	3134	1/1	0.98	0.42	3.98	21,21,21,21	0
56	MG	BA	3751	1/1	0.71	0.33	3.96	53,53,53,53	0
56	MG	BA	3236	1/1	0.96	0.15	3.94	35,35,35,35	0
56	MG	CA	1788	1/1	0.79	0.26	3.90	94,94,94,94	0
56	MG	BA	3611	1/1	0.99	0.24	3.82	8,8,8,8	0
56	MG	DA	3013	1/1	0.99	0.30	3.81	3,3,3,3	0
56	MG	BA	3832	1/1	0.95	0.27	3.71	28,28,28,28	0
56	MG	BA	3330	1/1	0.92	0.17	3.70	55,55,55,55	0
56	MG	DA	3028	1/1	0.92	0.29	3.70	4,4,4,4	0
56	MG	BA	3376	1/1	0.91	0.18	3.54	39,39,39,39	0
56	MG	BA	3879	1/1	0.92	0.31	3.31	46,46,46,46	0
56	MG	AY	123	1/1	0.79	0.28	3.24	42,42,42,42	0
56	MG	DA	3159	1/1	0.97	0.38	3.22	3,3,3,3	0
56	MG	BA	3898	1/1	0.93	0.36	3.21	38,38,38,38	0
56	MG	BF	302	1/1	0.91	0.24	3.20	59,59,59,59	0
56	MG	DA	3330	1/1	0.95	0.22	3.13	5,5,5,5	0
56	MG	BA	3627	1/1	0.92	0.12	3.11	22,22,22,22	0
56	MG	BA	3197	1/1	0.95	0.31	3.09	85,85,85,85	0
56	MG	BA	3132	1/1	0.93	0.21	3.08	40,40,40,40	0
56	MG	BA	3808	1/1	0.89	0.21	3.08	18,18,18,18	0
56	MG	BA	3267	1/1	0.88	0.28	3.05	21,21,21,21	0
56	MG	AA	1879	1/1	0.89	0.17	2.99	49,49,49,49	0
56	MG	BA	3595	1/1	0.91	0.21	2.95	62,62,62,62	0
56	MG	BA	3007	1/1	0.94	0.51	2.93	20,20,20,20	0
56	MG	DA	3180	1/1	0.93	0.32	2.91	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3447	1/1	0.89	0.32	2.91	15,15,15,15	0
56	MG	BA	3900	1/1	0.93	0.17	2.86	51,51,51,51	0
56	MG	DA	3417	1/1	0.93	0.23	2.85	4,4,4,4	0
56	MG	DA	3074	1/1	0.86	0.40	2.83	3,3,3,3	0
56	MG	AA	1686	1/1	0.95	0.18	2.81	43,43,43,43	0
56	MG	DA	3409	1/1	0.96	0.32	2.78	3,3,3,3	0
56	MG	BA	3294	1/1	0.98	0.23	2.74	4,4,4,4	0
56	MG	CA	1749	1/1	0.97	0.34	2.72	3,3,3,3	0
56	MG	AA	1838	1/1	0.91	0.26	2.66	18,18,18,18	0
56	MG	BA	3130	1/1	0.97	0.16	2.63	32,32,32,32	0
56	MG	BA	3361	1/1	0.96	0.25	2.57	16,16,16,16	0
56	MG	DA	3339	1/1	0.94	0.25	2.56	6,6,6,6	0
56	MG	BA	3218	1/1	0.95	0.35	2.56	25,25,25,25	0
56	MG	BA	3610	1/1	0.89	0.17	2.51	38,38,38,38	0
56	MG	AA	1713	1/1	0.95	0.23	2.50	39,39,39,39	0
56	MG	BA	3863	1/1	0.96	0.17	2.48	62,62,62,62	0
56	MG	DA	3131	1/1	0.84	0.30	2.48	31,31,31,31	0
56	MG	BA	3652	1/1	0.92	0.20	2.43	28,28,28,28	0
56	MG	BA	3349	1/1	0.85	0.17	2.43	46,46,46,46	0
56	MG	BA	3724	1/1	0.90	0.18	2.42	29,29,29,29	0
56	MG	DA	3149	1/1	0.89	0.28	2.35	3,3,3,3	0
56	MG	BA	3220	1/1	0.96	0.23	2.35	13,13,13,13	0
56	MG	AA	1920	1/1	0.89	0.25	2.28	26,26,26,26	0
56	MG	CA	1785	1/1	0.75	0.30	2.28	83,83,83,83	0
56	MG	BA	3633	1/1	0.97	0.23	2.28	36,36,36,36	0
56	MG	BA	3150	1/1	0.88	0.19	2.26	41,41,41,41	0
56	MG	AA	1752	1/1	0.72	0.23	2.26	66,66,66,66	0
56	MG	BA	3594	1/1	0.98	0.20	2.25	12,12,12,12	0
56	MG	BA	3368	1/1	0.96	0.23	2.24	63,63,63,63	0
56	MG	AA	1893	1/1	0.95	0.23	2.24	52,52,52,52	0
56	MG	AA	1874	1/1	0.95	0.22	2.19	44,44,44,44	0
56	MG	AA	1785	1/1	0.85	0.27	2.15	70,70,70,70	0
56	MG	BD	5001	1/1	0.95	0.34	2.14	61,61,61,61	0
56	MG	AA	1903	1/1	0.94	0.48	2.13	54,54,54,54	0
56	MG	DA	3470	1/1	0.96	0.23	2.12	4,4,4,4	0
56	MG	DA	3286	1/1	0.89	0.24	2.03	33,33,33,33	0
56	MG	AA	1674	1/1	0.87	0.15	2.03	52,52,52,52	0
56	MG	DA	3148	1/1	0.94	0.20	2.02	4,4,4,4	0
56	MG	BA	3407	1/1	0.86	0.42	1.98	56,56,56,56	0
56	MG	BA	3823	1/1	0.97	0.19	1.97	14,14,14,14	0
56	MG	DA	3081	1/1	0.97	0.16	1.86	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	CY	112	1/1	0.93	0.28	1.67	3,3,3,3	0
56	MG	CA	1762	1/1	0.71	0.28	1.67	69,69,69,69	0
56	MG	DA	3086	1/1	0.96	0.27	1.63	3,3,3,3	0
56	MG	B1	105	1/1	0.73	0.34	1.62	87,87,87,87	0
56	MG	BA	3836	1/1	0.92	0.22	1.60	20,20,20,20	0
56	MG	DA	3485	1/1	0.90	0.16	1.58	4,4,4,4	0
56	MG	DA	3058	1/1	0.96	0.20	1.54	3,3,3,3	0
56	MG	AA	1628	1/1	0.88	0.18	1.53	51,51,51,51	0
56	MG	BA	3704	1/1	0.62	0.17	1.46	88,88,88,88	0
56	MG	DA	3400	1/1	0.79	0.17	1.46	52,52,52,52	0
56	MG	AA	1941	1/1	0.95	0.24	1.44	42,42,42,42	0
56	MG	CA	1793	1/1	0.99	0.42	1.43	3,3,3,3	0
56	MG	BA	3334	1/1	0.79	0.12	1.41	77,77,77,77	0
56	MG	AA	1984	1/1	0.91	0.16	1.37	39,39,39,39	0
56	MG	BA	3555	1/1	0.94	0.20	1.35	7,7,7,7	0
56	MG	DA	3298	1/1	0.94	0.18	1.34	9,9,9,9	0
56	MG	BA	3126	1/1	0.89	0.12	1.21	46,46,46,46	0
56	MG	DA	3278	1/1	0.90	0.17	1.18	60,60,60,60	0
56	MG	BA	3579	1/1	0.61	0.14	1.14	69,69,69,69	0
56	MG	CA	1631	1/1	0.96	0.25	1.12	3,3,3,3	0
56	MG	DA	3234	1/1	0.95	0.18	1.11	3,3,3,3	0
56	MG	BA	3807	1/1	0.87	0.23	1.04	37,37,37,37	0
56	MG	DD	5004	1/1	0.93	0.26	1.04	42,42,42,42	0
56	MG	BA	3261	1/1	0.95	0.17	0.99	14,14,14,14	0
56	MG	BA	3679	1/1	0.96	0.23	0.95	5,5,5,5	0
56	MG	BA	3537	1/1	0.85	0.17	0.94	38,38,38,38	0
56	MG	BA	3276	1/1	0.92	0.25	0.93	52,52,52,52	0
56	MG	BA	3559	1/1	0.96	0.15	0.91	31,31,31,31	0
56	MG	BA	3322	1/1	0.95	0.20	0.88	40,40,40,40	0
56	MG	BA	3036	1/1	0.80	0.35	0.85	88,88,88,88	0
56	MG	DA	3176	1/1	0.95	0.28	0.80	4,4,4,4	0
56	MG	BA	3826	1/1	0.87	0.17	0.77	28,28,28,28	0
56	MG	BA	3777	1/1	0.95	0.16	0.76	32,32,32,32	0
56	MG	BA	3682	1/1	0.98	0.13	0.75	20,20,20,20	0
56	MG	AA	1659	1/1	0.87	0.16	0.72	49,49,49,49	0
56	MG	DA	3259	1/1	0.90	0.23	0.72	4,4,4,4	0
56	MG	AX	409	1/1	0.89	0.19	0.72	47,47,47,47	0
56	MG	CL	201	1/1	0.93	0.30	0.70	67,67,67,67	0
56	MG	CA	1799	1/1	0.92	0.13	0.69	5,5,5,5	0
56	MG	DA	3029	1/1	0.89	0.17	0.69	4,4,4,4	0
56	MG	BA	3095	1/1	0.80	0.13	0.64	40,40,40,40	0
56	MG	BA	3145	1/1	0.95	0.19	0.62	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3455	1/1	0.96	0.19	0.62	27,27,27,27	0
56	MG	CF	202	1/1	0.81	0.23	0.60	51,51,51,51	0
56	MG	BA	3499	1/1	0.92	0.12	0.54	57,57,57,57	0
56	MG	BA	3238	1/1	0.95	0.14	0.52	20,20,20,20	0
56	MG	AA	1704	1/1	0.91	0.17	0.52	48,48,48,48	0
56	MG	BA	3492	1/1	0.94	0.13	0.51	48,48,48,48	0
56	MG	AA	1900	1/1	0.97	0.45	0.49	39,39,39,39	0
56	MG	BA	3817	1/1	0.96	0.23	0.46	30,30,30,30	0
56	MG	CA	1775	1/1	0.79	0.38	0.44	91,91,91,91	0
56	MG	BA	3136	1/1	0.93	0.22	0.44	45,45,45,45	0
56	MG	CA	1783	1/1	0.66	0.23	0.44	65,65,65,65	0
56	MG	CZ	114	1/1	0.97	0.24	0.41	36,36,36,36	0
56	MG	BA	3451	1/1	0.99	0.15	0.38	13,13,13,13	0
56	MG	BA	3019	1/1	0.94	0.19	0.38	55,55,55,55	0
56	MG	AX	407	1/1	0.86	0.47	0.37	60,60,60,60	0
56	MG	AA	1829	1/1	0.97	0.28	0.36	43,43,43,43	0
56	MG	BA	3183	1/1	0.94	0.26	0.35	57,57,57,57	0
56	MG	DA	3141	1/1	0.99	0.14	0.34	4,4,4,4	0
56	MG	CA	1817	1/1	0.96	0.15	0.33	22,22,22,22	0
56	MG	BQ	204	1/1	0.92	0.17	0.32	80,80,80,80	0
56	MG	AA	1812	1/1	0.93	0.20	0.32	65,65,65,65	0
56	MG	BA	3716	1/1	0.88	0.14	0.26	24,24,24,24	0
56	MG	B8	104	1/1	0.81	0.28	0.26	49,49,49,49	0
56	MG	CA	1699	1/1	0.97	0.14	0.25	8,8,8,8	0
56	MG	CA	1737	1/1	0.87	0.15	0.23	35,35,35,35	0
56	MG	DD	5007	1/1	0.96	0.24	0.22	11,11,11,11	0
56	MG	DA	3151	1/1	0.98	0.18	0.19	4,4,4,4	0
56	MG	DA	3328	1/1	0.95	0.17	0.16	23,23,23,23	0
56	MG	BA	3785	1/1	0.90	0.21	0.15	25,25,25,25	0
56	MG	CA	1628	1/1	0.94	0.21	0.14	4,4,4,4	0
56	MG	DA	3215	1/1	0.94	0.16	0.12	4,4,4,4	0
56	MG	AA	1714	1/1	0.96	0.20	0.11	79,79,79,79	0
56	MG	BA	3295	1/1	0.76	0.20	0.09	22,22,22,22	0
56	MG	BB	219	1/1	0.82	0.20	0.09	41,41,41,41	0
56	MG	BA	3069	1/1	0.94	0.16	0.07	65,65,65,65	0
56	MG	DA	3059	1/1	0.97	0.21	0.05	3,3,3,3	0
56	MG	BA	3080	1/1	0.94	0.12	0.03	29,29,29,29	0
56	MG	CY	113	1/1	0.91	0.19	0.00	27,27,27,27	0
56	MG	DA	3068	1/1	0.95	0.18	-0.02	4,4,4,4	0
56	MG	AT	201	1/1	0.94	0.19	-0.08	57,57,57,57	0
56	MG	BA	3676	1/1	0.85	0.15	-0.10	44,44,44,44	0
56	MG	BA	3708	1/1	0.95	0.17	-0.11	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	2026	1/1	0.89	0.11	-0.14	26,26,26,26	0
56	MG	BA	3393	1/1	0.90	0.22	-0.15	61,61,61,61	0
56	MG	BA	3821	1/1	0.94	0.12	-0.19	22,22,22,22	0
56	MG	BA	3185	1/1	0.98	0.14	-0.23	8,8,8,8	0
56	MG	DA	3065	1/1	0.90	0.17	-0.23	45,45,45,45	0
56	MG	AA	2000	1/1	0.94	0.12	-0.23	46,46,46,46	0
56	MG	BA	3835	1/1	0.94	0.17	-0.30	8,8,8,8	0
56	MG	BA	3770	1/1	0.88	0.16	-0.31	30,30,30,30	0
56	MG	DA	3005	1/1	0.98	0.18	-0.31	3,3,3,3	0
56	MG	BA	3315	1/1	0.96	0.12	-0.33	28,28,28,28	0
56	MG	BA	3342	1/1	0.99	0.15	-0.40	20,20,20,20	0
56	MG	AC	304	1/1	0.91	0.21	-0.40	72,72,72,72	0
56	MG	CA	1786	1/1	0.95	0.27	-0.42	67,67,67,67	0
56	MG	AK	207	1/1	0.96	0.11	-0.43	65,65,65,65	0
56	MG	BA	3006	1/1	0.97	0.17	-0.44	11,11,11,11	0
56	MG	CA	1660	1/1	0.99	0.13	-0.44	5,5,5,5	0
56	MG	AN	102	1/1	0.93	0.23	-0.46	57,57,57,57	0
56	MG	BA	3513	1/1	0.86	0.14	-0.46	28,28,28,28	0
56	MG	BA	3317	1/1	0.94	0.14	-0.47	48,48,48,48	0
56	MG	BA	3417	1/1	0.98	0.16	-0.53	8,8,8,8	0
56	MG	BA	3293	1/1	0.97	0.16	-0.53	7,7,7,7	0
56	MG	BA	3404	1/1	0.88	0.14	-0.55	11,11,11,11	0
56	MG	BA	3018	1/1	0.91	0.16	-0.57	40,40,40,40	0
56	MG	CA	1760	1/1	0.96	0.16	-0.59	18,18,18,18	0
56	MG	BA	3841	1/1	0.92	0.14	-0.60	31,31,31,31	0
56	MG	AY	108	1/1	0.92	0.10	-0.62	59,59,59,59	0
56	MG	BA	3782	1/1	0.97	0.15	-0.62	21,21,21,21	0
56	MG	CA	1787	1/1	0.91	0.12	-0.63	57,57,57,57	0
56	MG	BA	3650	1/1	0.93	0.12	-0.63	5,5,5,5	0
56	MG	DA	3088	1/1	0.96	0.15	-0.65	4,4,4,4	0
56	MG	BA	3004	1/1	0.94	0.12	-0.65	27,27,27,27	0
56	MG	AK	202	1/1	0.86	0.16	-0.68	95,95,95,95	0
56	MG	AI	201	1/1	0.82	0.29	-0.72	59,59,59,59	0
56	MG	AA	1858	1/1	0.88	0.10	-0.72	72,72,72,72	0
56	MG	DA	3406	1/1	0.96	0.15	-0.74	5,5,5,5	0
56	MG	BA	3553	1/1	0.98	0.14	-0.76	12,12,12,12	0
56	MG	BD	5005	1/1	0.95	0.14	-0.76	10,10,10,10	0
56	MG	AA	1697	1/1	0.94	0.12	-0.78	48,48,48,48	0
56	MG	BA	3697	1/1	0.76	0.37	-0.78	72,72,72,72	0
56	MG	BA	3455	1/1	0.95	0.11	-0.78	26,26,26,26	0
56	MG	DA	3007	1/1	0.90	0.10	-0.88	25,25,25,25	0
56	MG	AV	5501	1/1	0.94	0.15	-0.89	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3017	1/1	0.96	0.09	-0.90	3,3,3,3	0
56	MG	DA	3342	1/1	0.97	0.14	-0.92	7,7,7,7	0
56	MG	AA	1947	1/1	0.67	0.12	-0.94	45,45,45,45	0
56	MG	CB	301	1/1	0.92	0.14	-0.95	39,39,39,39	0
57	ZN	CD	5001	1/1	0.98	0.24	-0.97	63,63,63,63	0
56	MG	AA	1650	1/1	0.93	0.14	-0.99	45,45,45,45	0
56	MG	AA	1688	1/1	0.89	0.08	-1.02	68,68,68,68	0
56	MG	BA	3497	1/1	0.86	0.10	-1.06	68,68,68,68	0
56	MG	AL	201	1/1	0.94	0.15	-1.06	28,28,28,28	0
56	MG	BA	3257	1/1	0.95	0.09	-1.07	28,28,28,28	0
56	MG	BA	3291	1/1	0.95	0.15	-1.11	9,9,9,9	0
57	ZN	AD	5001	1/1	0.96	0.24	-1.12	41,41,41,41	0
56	MG	BA	3639	1/1	0.95	0.18	-1.13	42,42,42,42	0
57	ZN	CN	101	1/1	0.95	0.16	-1.13	100,100,100,100	0
56	MG	AD	5002	1/1	0.93	0.12	-1.14	64,64,64,64	0
56	MG	DA	3391	1/1	0.87	0.11	-1.17	35,35,35,35	0
56	MG	BA	3112	1/1	0.92	0.13	-1.17	40,40,40,40	0
56	MG	DA	3123	1/1	0.98	0.13	-1.19	5,5,5,5	0
56	MG	BA	3616	1/1	0.98	0.08	-1.20	12,12,12,12	0
56	MG	BA	3583	1/1	0.79	0.09	-1.22	71,71,71,71	0
56	MG	CK	203	1/1	0.93	0.07	-1.24	85,85,85,85	0
56	MG	BA	3385	1/1	0.90	0.09	-1.25	63,63,63,63	0
56	MG	BA	3789	1/1	0.96	0.09	-1.29	36,36,36,36	0
56	MG	B4	101	1/1	0.85	0.10	-1.31	29,29,29,29	0
56	MG	AA	2015	1/1	0.88	0.11	-1.34	40,40,40,40	0
56	MG	BA	3809	1/1	0.97	0.12	-1.35	13,13,13,13	0
56	MG	DA	3034	1/1	0.98	0.11	-1.39	6,6,6,6	0
56	MG	DA	3066	1/1	0.93	0.13	-1.40	43,43,43,43	0
56	MG	DA	3133	1/1	0.97	0.09	-1.40	19,19,19,19	0
56	MG	BA	3668	1/1	0.90	0.15	-1.42	33,33,33,33	0
57	ZN	AN	101	1/1	0.97	0.11	-1.42	82,82,82,82	0
56	MG	BA	3307	1/1	0.87	0.14	-1.42	34,34,34,34	0
56	MG	BA	3051	1/1	0.93	0.09	-1.45	44,44,44,44	0
56	MG	BA	3703	1/1	0.84	0.08	-1.45	68,68,68,68	0
56	MG	DA	3285	1/1	0.90	0.13	-1.46	4,4,4,4	0
56	MG	BA	3299	1/1	0.95	0.13	-1.46	9,9,9,9	0
56	MG	BA	3586	1/1	0.96	0.11	-1.47	18,18,18,18	0
56	MG	AB	304	1/1	0.88	0.11	-1.49	73,73,73,73	0
56	MG	CA	1703	1/1	0.90	0.12	-1.49	29,29,29,29	0
56	MG	BA	3243	1/1	0.97	0.11	-1.51	26,26,26,26	0
56	MG	DA	3426	1/1	0.95	0.13	-1.54	5,5,5,5	0
56	MG	AA	1925	1/1	0.96	0.11	-1.55	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3212	1/1	0.97	0.12	-1.55	5,5,5,5	0
56	MG	BA	3372	1/1	0.90	0.05	-1.56	37,37,37,37	0
56	MG	DA	3107	1/1	0.81	0.09	-1.57	30,30,30,30	0
56	MG	BA	3700	1/1	0.86	0.14	-1.58	72,72,72,72	0
56	MG	BA	3869	1/1	0.91	0.13	-1.58	7,7,7,7	0
56	MG	BA	3319	1/1	0.94	0.08	-1.62	44,44,44,44	0
56	MG	BA	3151	1/1	0.85	0.09	-1.68	31,31,31,31	0
56	MG	BB	232	1/1	0.86	0.10	-1.69	58,58,58,58	0
56	MG	BE	301	1/1	0.83	0.09	-1.70	55,55,55,55	0
56	MG	AA	1719	1/1	0.91	0.13	-1.76	13,13,13,13	0
56	MG	CZ	101	1/1	0.94	0.07	-1.79	72,72,72,72	0
56	MG	AA	1969	1/1	0.66	0.09	-1.86	46,46,46,46	0
56	MG	BA	3383	1/1	0.91	0.12	-1.86	53,53,53,53	0
56	MG	AA	1703	1/1	0.95	0.12	-1.92	48,48,48,48	0
56	MG	CA	1744	1/1	0.89	0.10	-1.93	36,36,36,36	0
56	MG	BA	3473	1/1	0.92	0.13	-1.93	31,31,31,31	0
56	MG	BA	3612	1/1	0.85	0.10	-2.00	9,9,9,9	0
56	MG	BA	3493	1/1	0.94	0.07	-2.04	50,50,50,50	0
56	MG	AA	1927	1/1	0.98	0.15	-2.14	29,29,29,29	0
56	MG	BA	3308	1/1	0.95	0.13	-2.14	8,8,8,8	0
56	MG	DA	3414	1/1	0.94	0.13	-2.23	5,5,5,5	0
56	MG	BA	3366	1/1	0.89	0.07	-2.30	24,24,24,24	0
56	MG	DA	3340	1/1	0.96	0.11	-2.39	5,5,5,5	0
56	MG	BK	202	1/1	0.87	0.18	-2.42	83,83,83,83	0
56	MG	BQ	206	1/1	0.95	0.07	-2.51	13,13,13,13	0
56	MG	AA	1944	1/1	0.89	0.07	-2.57	48,48,48,48	0
56	MG	BA	3063	1/1	0.90	0.04	-2.58	86,86,86,86	0
56	MG	BA	3779	1/1	0.92	0.10	-2.67	22,22,22,22	0
56	MG	AA	1731	1/1	0.99	0.08	-2.76	17,17,17,17	0
56	MG	BA	3180	1/1	0.95	0.07	-2.81	36,36,36,36	0
56	MG	AA	1724	1/1	0.97	0.08	-2.82	35,35,35,35	0
56	MG	CA	1812	1/1	0.92	0.11	-2.84	36,36,36,36	0
56	MG	BA	3206	1/1	0.98	0.12	-2.91	35,35,35,35	0
56	MG	DA	3371	1/1	0.93	0.06	-3.00	56,56,56,56	0
56	MG	DA	3244	1/1	0.93	0.07	-3.03	5,5,5,5	0
56	MG	DA	3316	1/1	0.97	0.13	-3.05	4,4,4,4	0
56	MG	CA	1702	1/1	0.95	0.09	-3.17	24,24,24,24	0
56	MG	BA	3224	1/1	0.94	0.07	-3.38	32,32,32,32	0
56	MG	DA	3116	1/1	0.97	0.08	-3.66	3,3,3,3	0
56	MG	BA	3665	1/1	0.92	0.10	-3.69	24,24,24,24	0
56	MG	BB	223	1/1	0.96	0.08	-3.70	27,27,27,27	0
56	MG	DA	3032	1/1	0.97	0.07	-3.99	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3413	1/1	0.98	0.07	-4.01	43,43,43,43	0
56	MG	BA	3694	1/1	0.96	0.06	-4.52	77,77,77,77	0
56	MG	BA	3370	1/1	0.96	0.05	-5.10	46,46,46,46	0
56	MG	AJ	201	1/1	0.92	0.10	-5.34	49,49,49,49	0
56	MG	DA	3312	1/1	0.96	0.07	-5.62	46,46,46,46	0
56	MG	DA	3303	1/1	0.98	0.06	-5.87	10,10,10,10	0
56	MG	DA	3440	1/1	0.85	0.12	-6.01	4,4,4,4	0
56	MG	BA	3911	1/1	0.96	0.07	-6.34	22,22,22,22	0
56	MG	AA	1615	1/1	0.97	0.07	-8.68	4,4,4,4	0
56	MG	DA	3462	1/1	0.98	0.24	-	3,3,3,3	0
56	MG	DA	3109	1/1	0.96	0.27	-	3,3,3,3	0
56	MG	AA	1797	1/1	0.91	0.34	-	21,21,21,21	0
56	MG	BB	226	1/1	0.75	0.30	-	72,72,72,72	0
56	MG	CA	1698	1/1	0.96	0.19	-	37,37,37,37	0
56	MG	DA	3441	1/1	0.97	0.23	-	4,4,4,4	0
56	MG	AZ	103	1/1	0.74	0.09	-	66,66,66,66	0
56	MG	DA	3019	1/1	0.93	0.23	-	3,3,3,3	0
56	MG	DA	3379	1/1	0.97	0.34	-	3,3,3,3	0
56	MG	BA	3401	1/1	0.74	0.33	-	86,86,86,86	0
56	MG	BA	3351	1/1	0.96	0.15	-	22,22,22,22	0
56	MG	BA	3874	1/1	0.40	0.67	-	103,103,103,103	0
56	MG	AA	1919	1/1	0.09	0.15	-	88,88,88,88	0
56	MG	BA	3773	1/1	0.95	0.15	-	25,25,25,25	0
56	MG	BA	3783	1/1	0.94	0.14	-	27,27,27,27	0
56	MG	BA	3607	1/1	0.90	0.19	-	40,40,40,40	0
56	MG	BA	3124	1/1	0.86	0.25	-	56,56,56,56	0
56	MG	AZ	113	1/1	0.89	0.10	-	60,60,60,60	0
56	MG	DA	3171	1/1	0.93	0.16	-	3,3,3,3	0
56	MG	DA	3097	1/1	0.97	0.16	-	4,4,4,4	0
56	MG	DA	3399	1/1	0.98	0.35	-	58,58,58,58	0
56	MG	AA	1970	1/1	0.91	0.14	-	52,52,52,52	0
56	MG	DA	3270	1/1	0.98	0.22	-	4,4,4,4	0
56	MG	CA	1612	1/1	0.98	0.13	-	3,3,3,3	0
56	MG	BA	3410	1/1	0.83	0.15	-	67,67,67,67	0
56	MG	BB	210	1/1	0.88	0.33	-	72,72,72,72	0
56	MG	DA	3333	1/1	0.92	0.31	-	4,4,4,4	0
56	MG	CZ	110	1/1	0.84	0.18	-	68,68,68,68	0
56	MG	AA	1652	1/1	0.52	0.39	-	63,63,63,63	0
56	MG	BA	3064	1/1	0.95	0.17	-	57,57,57,57	0
56	MG	AA	2027	1/1	0.94	0.11	-	27,27,27,27	0
56	MG	AE	204	1/1	0.73	0.09	-	51,51,51,51	0
56	MG	DA	3071	1/1	0.94	0.25	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1761	1/1	0.92	0.15	-	39,39,39,39	0
56	MG	DA	3245	1/1	0.91	0.15	-	41,41,41,41	0
56	MG	BA	3419	1/1	0.90	0.25	-	50,50,50,50	0
56	MG	BA	3233	1/1	0.73	0.40	-	70,70,70,70	0
56	MG	AA	1856	1/1	0.88	0.48	-	49,49,49,49	0
56	MG	AA	1690	1/1	0.96	0.10	-	19,19,19,19	0
56	MG	BA	3029	1/1	0.89	0.30	-	59,59,59,59	0
56	MG	CA	1633	1/1	0.97	0.26	-	3,3,3,3	0
56	MG	BB	202	1/1	0.87	0.07	-	50,50,50,50	0
56	MG	AA	1989	1/1	0.70	0.66	-	81,81,81,81	0
56	MG	BA	3691	1/1	0.79	0.14	-	73,73,73,73	0
56	MG	BA	3923	1/1	0.73	0.29	-	57,57,57,57	0
56	MG	BA	3624	1/1	0.61	0.17	-	89,89,89,89	0
56	MG	BA	3463	1/1	0.96	0.14	-	38,38,38,38	0
56	MG	AA	1606	1/1	0.95	0.17	-	35,35,35,35	0
56	MG	CZ	113	1/1	0.96	0.45	-	3,3,3,3	0
56	MG	BE	305	1/1	0.94	0.12	-	22,22,22,22	0
56	MG	BA	3781	1/1	0.87	0.21	-	85,85,85,85	0
56	MG	BA	3853	1/1	0.97	0.29	-	25,25,25,25	0
56	MG	BA	3430	1/1	0.94	0.11	-	45,45,45,45	0
56	MG	AA	1685	1/1	0.92	0.15	-	28,28,28,28	0
56	MG	BA	3516	1/1	0.79	0.19	-	43,43,43,43	0
56	MG	BA	3861	1/1	0.82	0.18	-	65,65,65,65	0
56	MG	AA	2014	1/1	0.71	0.18	-	21,21,21,21	0
56	MG	DA	3067	1/1	0.91	0.13	-	17,17,17,17	0
56	MG	BA	3894	1/1	0.89	0.10	-	70,70,70,70	0
56	MG	CA	1804	1/1	0.99	0.25	-	4,4,4,4	0
56	MG	AA	1968	1/1	0.93	0.27	-	35,35,35,35	0
56	MG	AA	1904	1/1	0.88	0.45	-	77,77,77,77	0
56	MG	B1	101	1/1	0.99	0.28	-	31,31,31,31	0
56	MG	AA	1932	1/1	0.80	0.14	-	64,64,64,64	0
56	MG	BA	3086	1/1	0.98	0.14	-	23,23,23,23	0
56	MG	BA	3421	1/1	0.86	0.27	-	45,45,45,45	0
56	MG	BA	3052	1/1	0.94	0.18	-	71,71,71,71	0
56	MG	BA	3382	1/1	0.65	0.09	-	75,75,75,75	0
56	MG	AA	1991	1/1	0.92	0.10	-	84,84,84,84	0
56	MG	BA	3389	1/1	0.72	0.93	-	75,75,75,75	0
56	MG	AA	1935	1/1	0.75	0.10	-	53,53,53,53	0
56	MG	CA	1715	1/1	0.91	0.28	-	40,40,40,40	0
56	MG	BA	3910	1/1	0.95	0.30	-	40,40,40,40	0
56	MG	AA	1678	1/1	0.46	0.50	-	92,92,92,92	0
56	MG	BA	3908	1/1	0.93	0.18	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3305	1/1	0.97	0.09	-	18,18,18,18	0
56	MG	DA	3331	1/1	0.95	0.14	-	23,23,23,23	0
56	MG	DA	3350	1/1	0.92	0.15	-	63,63,63,63	0
56	MG	AA	1770	1/1	0.69	0.42	-	52,52,52,52	0
56	MG	BA	3591	1/1	0.95	0.18	-	29,29,29,29	0
56	MG	DA	3311	1/1	0.82	0.18	-	72,72,72,72	0
56	MG	BA	3645	1/1	0.98	0.15	-	30,30,30,30	0
56	MG	DA	3045	1/1	0.96	0.35	-	3,3,3,3	0
56	MG	AA	1807	1/1	0.90	0.12	-	36,36,36,36	0
56	MG	DA	3256	1/1	0.99	0.10	-	6,6,6,6	0
56	MG	AA	1990	1/1	0.93	0.12	-	63,63,63,63	0
56	MG	DA	3456	1/1	0.86	0.19	-	5,5,5,5	0
56	MG	AA	1638	1/1	0.66	0.45	-	72,72,72,72	0
56	MG	BA	3099	1/1	0.97	0.22	-	29,29,29,29	0
56	MG	AA	1967	1/1	0.95	0.09	-	28,28,28,28	0
56	MG	BA	3438	1/1	0.92	0.20	-	67,67,67,67	0
56	MG	CT	201	1/1	0.98	0.30	-	3,3,3,3	0
56	MG	AA	1744	1/1	0.86	0.28	-	74,74,74,74	0
56	MG	BA	3464	1/1	0.93	0.36	-	75,75,75,75	0
56	MG	BB	228	1/1	0.91	0.29	-	63,63,63,63	0
56	MG	AA	1953	1/1	0.66	0.14	-	87,87,87,87	0
56	MG	DA	3188	1/1	0.97	0.20	-	3,3,3,3	0
56	MG	BA	3244	1/1	0.93	0.38	-	31,31,31,31	0
56	MG	CA	1748	1/1	0.89	0.19	-	3,3,3,3	0
56	MG	BA	3727	1/1	0.88	0.28	-	44,44,44,44	0
56	MG	BA	3479	1/1	0.92	0.16	-	30,30,30,30	0
56	MG	BA	3088	1/1	0.88	0.34	-	63,63,63,63	0
56	MG	BA	3541	1/1	0.91	0.17	-	30,30,30,30	0
56	MG	DA	3348	1/1	0.86	0.11	-	60,60,60,60	0
56	MG	CA	1814	1/1	0.83	0.16	-	66,66,66,66	0
56	MG	BA	3053	1/1	0.89	0.29	-	78,78,78,78	0
56	MG	BQ	201	1/1	0.94	0.24	-	45,45,45,45	0
56	MG	BA	3918	1/1	0.84	0.55	-	63,63,63,63	0
56	MG	DD	5001	1/1	0.96	0.15	-	33,33,33,33	0
56	MG	BA	3805	1/1	0.92	0.20	-	40,40,40,40	0
56	MG	DA	3142	1/1	0.95	0.45	-	3,3,3,3	0
56	MG	BA	3712	1/1	0.79	0.42	-	77,77,77,77	0
56	MG	AY	112	1/1	0.93	0.20	-	38,38,38,38	0
56	MG	AA	1931	1/1	0.93	0.21	-	31,31,31,31	0
56	MG	DA	3474	1/1	0.95	0.22	-	3,3,3,3	0
56	MG	BA	3522	1/1	0.97	0.04	-	36,36,36,36	0
56	MG	AA	1777	1/1	0.93	0.27	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1720	1/1	0.93	0.18	-	36,36,36,36	0
56	MG	AY	125	1/1	0.94	0.52	-	36,36,36,36	0
56	MG	BA	3744	1/1	0.87	0.16	-	72,72,72,72	0
56	MG	BA	3387	1/1	0.89	0.11	-	56,56,56,56	0
56	MG	DA	3249	1/1	0.97	0.11	-	6,6,6,6	0
56	MG	BA	3653	1/1	0.59	0.51	-	61,61,61,61	0
56	MG	BA	3021	1/1	0.94	0.40	-	37,37,37,37	0
56	MG	BA	3677	1/1	0.92	0.14	-	30,30,30,30	0
56	MG	BA	3880	1/1	0.79	0.16	-	63,63,63,63	0
56	MG	DA	3341	1/1	0.98	0.36	-	3,3,3,3	0
56	MG	DA	3490	1/1	0.98	0.28	-	3,3,3,3	0
56	MG	BB	216	1/1	0.91	0.25	-	46,46,46,46	0
56	MG	DA	3208	1/1	0.95	0.27	-	4,4,4,4	0
56	MG	AA	1945	1/1	0.92	0.12	-	34,34,34,34	0
56	MG	DA	3429	1/1	0.95	0.47	-	3,3,3,3	0
56	MG	BA	3373	1/1	0.89	0.20	-	50,50,50,50	0
56	MG	DA	3317	1/1	0.96	0.33	-	43,43,43,43	0
56	MG	BQ	202	1/1	0.96	0.16	-	18,18,18,18	0
56	MG	BA	3121	1/1	0.92	0.07	-	61,61,61,61	0
56	MG	CA	1724	1/1	0.90	0.15	-	36,36,36,36	0
56	MG	DA	3010	1/1	0.95	0.17	-	3,3,3,3	0
56	MG	CA	1796	1/1	0.79	0.21	-	77,77,77,77	0
56	MG	BA	3324	1/1	0.91	0.29	-	50,50,50,50	0
56	MG	BA	3726	1/1	0.95	0.09	-	25,25,25,25	0
56	MG	BA	3379	1/1	0.83	0.27	-	115,115,115,115	0
56	MG	CA	1676	1/1	0.91	0.88	-	42,42,42,42	0
56	MG	BA	3316	1/1	0.95	0.07	-	35,35,35,35	0
56	MG	BA	3166	1/1	0.83	0.34	-	63,63,63,63	0
56	MG	DY	201	1/1	0.96	0.10	-	3,3,3,3	0
56	MG	AA	2004	1/1	0.90	0.14	-	51,51,51,51	0
56	MG	CA	1646	1/1	0.99	0.24	-	3,3,3,3	0
56	MG	BA	3641	1/1	0.90	0.34	-	63,63,63,63	0
56	MG	BA	3396	1/1	0.94	0.24	-	42,42,42,42	0
56	MG	DA	3290	1/1	0.80	0.36	-	64,64,64,64	0
56	MG	CA	1695	1/1	0.77	0.16	-	59,59,59,59	0
56	MG	BN	201	1/1	0.86	0.14	-	70,70,70,70	0
56	MG	BA	3437	1/1	0.36	0.37	-	117,117,117,117	0
56	MG	BA	3656	1/1	0.95	0.26	-	16,16,16,16	0
56	MG	BA	3445	1/1	0.49	0.27	-	63,63,63,63	0
56	MG	DA	3378	1/1	0.98	0.27	-	3,3,3,3	0
56	MG	AA	1980	1/1	0.94	0.12	-	38,38,38,38	0
56	MG	AA	1973	1/1	0.88	0.18	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3259	1/1	0.90	0.10	-	44,44,44,44	0
56	MG	DA	3398	1/1	0.81	0.41	-	55,55,55,55	0
56	MG	BA	3685	1/1	0.89	0.17	-	54,54,54,54	0
56	MG	BA	3798	1/1	0.89	0.11	-	54,54,54,54	0
56	MG	CA	1645	1/1	0.95	0.12	-	6,6,6,6	0
56	MG	BF	305	1/1	0.83	0.11	-	63,63,63,63	0
56	MG	DG	201	1/1	0.97	0.17	-	3,3,3,3	0
56	MG	BA	3705	1/1	0.87	0.21	-	42,42,42,42	0
56	MG	BA	3013	1/1	0.72	0.61	-	103,103,103,103	0
56	MG	BA	3016	1/1	0.95	0.09	-	50,50,50,50	0
56	MG	BA	3517	1/1	0.93	0.12	-	46,46,46,46	0
56	MG	DA	3172	1/1	0.92	0.26	-	3,3,3,3	0
56	MG	DA	3276	1/1	0.96	0.27	-	4,4,4,4	0
56	MG	DO	201	1/1	0.99	0.30	-	3,3,3,3	0
56	MG	CH	201	1/1	0.90	0.41	-	58,58,58,58	0
56	MG	BA	3776	1/1	0.82	0.23	-	43,43,43,43	0
56	MG	BA	3915	1/1	0.95	0.29	-	41,41,41,41	0
56	MG	BA	3107	1/1	0.90	0.13	-	49,49,49,49	0
56	MG	DA	3325	1/1	0.97	0.28	-	3,3,3,3	0
56	MG	AA	1746	1/1	0.98	0.17	-	39,39,39,39	0
56	MG	AA	2020	1/1	0.87	0.13	-	74,74,74,74	0
56	MG	BA	3435	1/1	0.94	0.12	-	32,32,32,32	0
56	MG	AA	1965	1/1	0.94	0.34	-	54,54,54,54	0
56	MG	BA	3260	1/1	0.48	0.26	-	75,75,75,75	0
56	MG	AA	1825	1/1	0.93	0.17	-	31,31,31,31	0
56	MG	D1	102	1/1	0.93	0.23	-	53,53,53,53	0
56	MG	AA	1660	1/1	0.91	0.12	-	77,77,77,77	0
56	MG	BA	3391	1/1	0.95	0.14	-	51,51,51,51	0
56	MG	DA	3454	1/1	0.94	0.14	-	45,45,45,45	0
56	MG	CA	1638	1/1	0.96	0.30	-	3,3,3,3	0
56	MG	CA	1798	1/1	0.97	0.35	-	3,3,3,3	0
56	MG	BA	3399	1/1	0.74	0.10	-	73,73,73,73	0
56	MG	CF	204	1/1	0.97	0.31	-	3,3,3,3	0
56	MG	AA	1801	1/1	0.96	0.07	-	55,55,55,55	0
56	MG	AA	1647	1/1	0.83	0.28	-	64,64,64,64	0
56	MG	CA	1759	1/1	0.94	0.27	-	48,48,48,48	0
56	MG	DD	5009	1/1	0.93	0.37	-	29,29,29,29	0
56	MG	AA	1679	1/1	0.87	0.41	-	51,51,51,51	0
56	MG	DA	3261	1/1	0.98	0.30	-	3,3,3,3	0
56	MG	CA	1664	1/1	0.98	0.18	-	3,3,3,3	0
56	MG	BA	3120	1/1	0.92	0.37	-	53,53,53,53	0
56	MG	BA	3108	1/1	0.89	0.15	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3510	1/1	0.81	0.26	-	61,61,61,61	0
56	MG	BA	3713	1/1	0.95	0.18	-	33,33,33,33	0
56	MG	BA	3015	1/1	0.95	0.20	-	60,60,60,60	0
56	MG	BA	3619	1/1	0.89	0.21	-	42,42,42,42	0
56	MG	BA	3742	1/1	0.74	0.15	-	70,70,70,70	0
56	MG	CY	105	1/1	0.84	0.17	-	52,52,52,52	0
56	MG	AA	1809	1/1	0.94	0.23	-	90,90,90,90	0
56	MG	BA	3328	1/1	0.95	0.12	-	38,38,38,38	0
56	MG	BA	3084	1/1	0.85	0.46	-	62,62,62,62	0
56	MG	BA	3081	1/1	0.99	0.19	-	31,31,31,31	0
56	MG	BA	3138	1/1	0.91	0.22	-	27,27,27,27	0
56	MG	AY	118	1/1	0.78	0.12	-	83,83,83,83	0
56	MG	BA	3274	1/1	0.97	0.14	-	21,21,21,21	0
56	MG	BA	3660	1/1	0.98	0.26	-	12,12,12,12	0
56	MG	BA	3544	1/1	0.91	0.40	-	72,72,72,72	0
56	MG	AA	1765	1/1	0.97	0.30	-	11,11,11,11	0
56	MG	DA	3361	1/1	0.92	0.64	-	78,78,78,78	0
56	MG	DA	3380	1/1	0.81	0.24	-	64,64,64,64	0
56	MG	AA	1978	1/1	0.80	0.17	-	35,35,35,35	0
56	MG	BA	3589	1/1	0.95	0.10	-	29,29,29,29	0
56	MG	DA	3475	1/1	0.95	0.18	-	3,3,3,3	0
56	MG	CA	1609	1/1	0.97	0.33	-	3,3,3,3	0
56	MG	BB	201	1/1	0.69	0.40	-	59,59,59,59	0
56	MG	BA	3551	1/1	0.98	0.17	-	19,19,19,19	0
56	MG	DA	3377	1/1	0.93	0.09	-	43,43,43,43	0
56	MG	BA	3427	1/1	0.90	0.13	-	34,34,34,34	0
56	MG	BA	3198	1/1	0.68	0.45	-	76,76,76,76	0
56	MG	CA	1752	1/1	0.98	0.37	-	3,3,3,3	0
56	MG	BA	3195	1/1	0.87	0.22	-	47,47,47,47	0
56	MG	AA	1895	1/1	0.96	0.09	-	52,52,52,52	0
56	MG	AA	1673	1/1	0.95	0.17	-	64,64,64,64	0
56	MG	BA	3070	1/1	0.92	0.24	-	37,37,37,37	0
56	MG	CA	1667	1/1	0.84	0.12	-	58,58,58,58	0
56	MG	CA	1706	1/1	0.85	0.27	-	62,62,62,62	0
56	MG	AA	1709	1/1	0.85	0.16	-	54,54,54,54	0
56	MG	BA	3820	1/1	0.94	0.24	-	59,59,59,59	0
56	MG	BA	3043	1/1	0.79	0.15	-	58,58,58,58	0
56	MG	BA	3599	1/1	0.90	0.53	-	50,50,50,50	0
56	MG	DA	3425	1/1	0.92	0.16	-	5,5,5,5	0
56	MG	CA	1683	1/1	0.88	0.27	-	61,61,61,61	0
56	MG	BA	3348	1/1	0.94	0.17	-	37,37,37,37	0
56	MG	DA	3359	1/1	0.83	0.11	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	CA	1620	1/1	0.99	0.18	-	4,4,4,4	0
56	MG	BA	3882	1/1	0.98	0.24	-	42,42,42,42	0
56	MG	DA	3073	1/1	0.96	0.12	-	6,6,6,6	0
56	MG	AA	1918	1/1	0.87	0.07	-	58,58,58,58	0
56	MG	AA	1602	1/1	0.85	0.51	-	74,74,74,74	0
56	MG	BA	3885	1/1	0.95	0.12	-	67,67,67,67	0
56	MG	BA	3488	1/1	0.95	0.15	-	52,52,52,52	0
56	MG	AT	202	1/1	0.90	0.10	-	58,58,58,58	0
56	MG	AA	2001	1/1	0.97	0.14	-	29,29,29,29	0
56	MG	AA	1943	1/1	0.95	0.14	-	56,56,56,56	0
56	MG	BA	3897	1/1	0.88	0.23	-	48,48,48,48	0
56	MG	AX	408	1/1	0.85	0.10	-	57,57,57,57	0
56	MG	BA	3604	1/1	0.83	0.49	-	50,50,50,50	0
56	MG	DA	3369	1/1	0.90	0.22	-	43,43,43,43	0
56	MG	CA	1688	1/1	0.96	0.32	-	54,54,54,54	0
56	MG	BA	3409	1/1	0.79	0.11	-	58,58,58,58	0
56	MG	BA	3560	1/1	0.82	0.28	-	52,52,52,52	0
56	MG	AA	1616	1/1	0.89	0.29	-	47,47,47,47	0
56	MG	DA	3221	1/1	0.95	0.35	-	52,52,52,52	0
56	MG	BA	3511	1/1	0.78	0.11	-	43,43,43,43	0
56	MG	AA	1778	1/1	0.94	0.33	-	37,37,37,37	0
56	MG	AA	1614	1/1	0.90	0.38	-	49,49,49,49	0
56	MG	AA	1655	1/1	0.84	0.15	-	61,61,61,61	0
56	MG	BA	3912	1/1	0.95	0.10	-	26,26,26,26	0
56	MG	DA	3402	1/1	0.96	0.15	-	32,32,32,32	0
56	MG	AA	1834	1/1	0.92	0.14	-	43,43,43,43	0
56	MG	DA	3268	1/1	0.95	0.17	-	4,4,4,4	0
56	MG	BA	3027	1/1	0.81	0.32	-	86,86,86,86	0
56	MG	DA	3121	1/1	0.78	0.21	-	41,41,41,41	0
56	MG	AA	1802	1/1	0.93	0.22	-	39,39,39,39	0
56	MG	AA	1897	1/1	0.77	0.39	-	62,62,62,62	0
56	MG	AA	1818	1/1	0.81	0.79	-	74,74,74,74	0
56	MG	DB	208	1/1	0.87	0.20	-	3,3,3,3	0
56	MG	BA	3701	1/1	0.89	0.12	-	58,58,58,58	0
56	MG	DA	3023	1/1	0.93	0.25	-	3,3,3,3	0
56	MG	BA	3580	1/1	0.86	0.20	-	54,54,54,54	0
56	MG	BA	3082	1/1	0.91	0.15	-	56,56,56,56	0
56	MG	BA	3502	1/1	0.85	0.18	-	61,61,61,61	0
56	MG	CA	1606	1/1	0.99	0.32	-	3,3,3,3	0
56	MG	BA	3279	1/1	0.86	0.20	-	39,39,39,39	0
56	MG	BA	3683	1/1	0.77	0.32	-	63,63,63,63	0
56	MG	DA	3466	1/1	0.92	0.27	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3471	1/1	0.96	0.16	-	4,4,4,4	0
56	MG	DD	5003	1/1	0.88	0.27	-	65,65,65,65	0
56	MG	AA	1745	1/1	0.92	0.06	-	75,75,75,75	0
56	MG	CA	1684	1/1	0.82	0.22	-	74,74,74,74	0
56	MG	AA	1627	1/1	0.98	0.13	-	29,29,29,29	0
56	MG	BA	3483	1/1	0.83	0.43	-	47,47,47,47	0
56	MG	BH	203	1/1	0.87	0.10	-	56,56,56,56	0
56	MG	AZ	101	1/1	0.85	0.15	-	63,63,63,63	0
56	MG	AA	1629	1/1	0.97	0.12	-	32,32,32,32	0
56	MG	BA	3403	1/1	0.76	0.23	-	98,98,98,98	0
56	MG	BA	3343	1/1	0.71	0.65	-	70,70,70,70	0
56	MG	CA	1771	1/1	0.86	0.23	-	80,80,80,80	0
56	MG	AA	1981	1/1	0.95	0.16	-	52,52,52,52	0
56	MG	DA	3436	1/1	0.96	0.18	-	4,4,4,4	0
56	MG	BA	3248	1/1	0.87	0.27	-	43,43,43,43	0
56	MG	DA	3327	1/1	0.97	0.34	-	4,4,4,4	0
56	MG	DA	3055	1/1	0.94	0.30	-	3,3,3,3	0
56	MG	BA	3702	1/1	0.88	0.13	-	83,83,83,83	0
56	MG	BA	3256	1/1	0.89	0.60	-	60,60,60,60	0
56	MG	BA	3232	1/1	0.91	0.12	-	58,58,58,58	0
56	MG	DA	3428	1/1	0.82	0.38	-	3,3,3,3	0
56	MG	DA	3396	1/1	0.79	0.19	-	66,66,66,66	0
56	MG	BB	205	1/1	0.38	0.43	-	100,100,100,100	0
56	MG	AA	1924	1/1	0.94	0.25	-	58,58,58,58	0
56	MG	BA	3023	1/1	0.90	0.15	-	44,44,44,44	0
56	MG	BR	201	1/1	0.90	0.15	-	34,34,34,34	0
56	MG	AX	412	1/1	0.94	0.20	-	56,56,56,56	0
56	MG	BA	3602	1/1	0.94	0.32	-	43,43,43,43	0
56	MG	BA	3765	1/1	0.87	0.41	-	60,60,60,60	0
56	MG	DA	3349	1/1	0.98	0.14	-	29,29,29,29	0
56	MG	DA	3299	1/1	0.93	0.18	-	50,50,50,50	0
56	MG	BA	3297	1/1	0.91	0.17	-	45,45,45,45	0
56	MG	BA	3429	1/1	0.95	0.26	-	51,51,51,51	0
56	MG	BA	3472	1/1	0.90	0.14	-	10,10,10,10	0
56	MG	BA	3593	1/1	0.78	0.47	-	64,64,64,64	0
56	MG	BA	3336	1/1	0.93	0.10	-	45,45,45,45	0
56	MG	BA	3357	1/1	0.89	0.16	-	31,31,31,31	0
56	MG	BA	3169	1/1	0.89	0.19	-	67,67,67,67	0
56	MG	DA	3016	1/1	0.96	0.18	-	3,3,3,3	0
56	MG	CA	1708	1/1	0.94	0.15	-	36,36,36,36	0
56	MG	DA	3193	1/1	0.96	0.14	-	7,7,7,7	0
56	MG	DA	3367	1/1	0.90	0.10	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3264	1/1	0.83	0.24	-	60,60,60,60	0
56	MG	DA	3227	1/1	0.98	0.30	-	3,3,3,3	0
56	MG	AA	1619	1/1	0.70	0.47	-	62,62,62,62	0
56	MG	BA	3298	1/1	0.92	0.31	-	30,30,30,30	0
56	MG	DA	3491	1/1	0.98	0.33	-	3,3,3,3	0
56	MG	AA	1835	1/1	0.98	0.20	-	37,37,37,37	0
56	MG	AA	2006	1/1	0.92	0.21	-	53,53,53,53	0
56	MG	DA	3002	1/1	0.93	0.31	-	3,3,3,3	0
56	MG	AA	1632	1/1	0.91	0.12	-	35,35,35,35	0
56	MG	CA	1756	1/1	0.97	0.20	-	3,3,3,3	0
56	MG	BA	3193	1/1	0.66	0.53	-	83,83,83,83	0
56	MG	DA	3203	1/1	0.95	0.26	-	15,15,15,15	0
56	MG	BA	3659	1/1	0.91	0.26	-	43,43,43,43	0
56	MG	B8	103	1/1	0.94	0.14	-	61,61,61,61	0
56	MG	BA	3543	1/1	0.80	0.26	-	38,38,38,38	0
56	MG	BB	235	1/1	0.57	0.13	-	59,59,59,59	0
56	MG	CA	1764	1/1	0.96	0.29	-	3,3,3,3	0
56	MG	BA	3870	1/1	0.87	0.29	-	47,47,47,47	0
56	MG	AA	1913	1/1	0.93	0.10	-	54,54,54,54	0
56	MG	AA	1670	1/1	0.82	0.31	-	67,67,67,67	0
56	MG	BA	3470	1/1	0.68	0.35	-	77,77,77,77	0
56	MG	AL	204	1/1	0.95	0.07	-	43,43,43,43	0
56	MG	DA	3260	1/1	0.94	0.30	-	3,3,3,3	0
56	MG	BA	3572	1/1	0.89	0.15	-	34,34,34,34	0
56	MG	CA	1647	1/1	0.97	0.24	-	3,3,3,3	0
56	MG	BA	3284	1/1	0.97	0.17	-	15,15,15,15	0
56	MG	AA	1621	1/1	0.97	0.14	-	25,25,25,25	0
56	MG	DA	3224	1/1	0.96	0.13	-	5,5,5,5	0
56	MG	DA	3337	1/1	0.93	0.19	-	4,4,4,4	0
56	MG	BA	3457	1/1	0.97	0.25	-	11,11,11,11	0
56	MG	CA	1807	1/1	0.97	0.31	-	3,3,3,3	0
56	MG	BD	5007	1/1	0.68	0.21	-	55,55,55,55	0
56	MG	BA	3819	1/1	0.87	0.50	-	34,34,34,34	0
56	MG	AB	303	1/1	0.92	0.14	-	40,40,40,40	0
56	MG	AA	1992	1/1	0.81	0.17	-	77,77,77,77	0
56	MG	BQ	205	1/1	0.76	0.25	-	57,57,57,57	0
56	MG	AA	1691	1/1	0.80	0.15	-	37,37,37,37	0
56	MG	CA	1654	1/1	0.93	0.19	-	28,28,28,28	0
56	MG	CA	1601	1/1	0.91	0.29	-	3,3,3,3	0
56	MG	CA	1634	1/1	0.97	0.09	-	6,6,6,6	0
56	MG	BA	3059	1/1	0.90	0.10	-	74,74,74,74	0
56	MG	BA	3582	1/1	0.98	0.07	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3482	1/1	0.90	0.20	-	4,4,4,4	0
56	MG	AA	1892	1/1	0.93	0.22	-	30,30,30,30	0
56	MG	AA	1642	1/1	0.96	0.16	-	57,57,57,57	0
56	MG	DA	3206	1/1	0.95	0.14	-	5,5,5,5	0
56	MG	DA	3147	1/1	0.96	0.36	-	3,3,3,3	0
56	MG	BA	3155	1/1	0.97	0.42	-	46,46,46,46	0
56	MG	BA	3453	1/1	0.87	0.29	-	57,57,57,57	0
56	MG	BA	3635	1/1	0.97	0.12	-	37,37,37,37	0
56	MG	BA	3890	1/1	0.98	0.20	-	25,25,25,25	0
56	MG	CZ	106	1/1	0.42	0.15	-	82,82,82,82	0
56	MG	DA	3320	1/1	0.37	0.72	-	82,82,82,82	0
56	MG	BA	3333	1/1	0.96	0.11	-	55,55,55,55	0
56	MG	BA	3434	1/1	0.88	0.25	-	68,68,68,68	0
56	MG	CA	1743	1/1	0.77	0.09	-	52,52,52,52	0
56	MG	DA	3218	1/1	0.96	0.16	-	4,4,4,4	0
56	MG	CA	1789	1/1	0.92	0.31	-	43,43,43,43	0
56	MG	AX	404	1/1	0.78	0.39	-	92,92,92,92	0
56	MG	AZ	111	1/1	0.91	0.16	-	71,71,71,71	0
56	MG	CA	1773	1/1	0.85	0.12	-	66,66,66,66	0
56	MG	BU	201	1/1	0.67	0.40	-	83,83,83,83	0
56	MG	AA	1798	1/1	0.92	0.11	-	25,25,25,25	0
56	MG	CA	1626	1/1	0.87	0.56	-	3,3,3,3	0
56	MG	BA	3480	1/1	0.83	0.18	-	43,43,43,43	0
56	MG	DA	3211	1/1	0.91	0.28	-	4,4,4,4	0
56	MG	CY	101	1/1	0.96	0.22	-	3,3,3,3	0
56	MG	BA	3535	1/1	0.68	0.28	-	62,62,62,62	0
56	MG	DA	3266	1/1	0.99	0.25	-	3,3,3,3	0
56	MG	DA	3433	1/1	0.98	0.24	-	3,3,3,3	0
56	MG	BA	3824	1/1	0.96	0.13	-	17,17,17,17	0
56	MG	BA	3251	1/1	0.90	0.10	-	41,41,41,41	0
56	MG	BA	3441	1/1	0.76	0.57	-	70,70,70,70	0
56	MG	DA	3427	1/1	0.96	0.55	-	3,3,3,3	0
56	MG	AK	201	1/1	0.85	0.61	-	76,76,76,76	0
56	MG	BA	3122	1/1	0.81	0.12	-	56,56,56,56	0
56	MG	AA	1810	1/1	0.90	0.57	-	64,64,64,64	0
56	MG	BA	3253	1/1	0.90	0.34	-	71,71,71,71	0
56	MG	BA	3862	1/1	0.83	0.10	-	85,85,85,85	0
56	MG	BA	3339	1/1	0.90	0.19	-	66,66,66,66	0
56	MG	BA	3412	1/1	0.72	0.19	-	64,64,64,64	0
56	MG	DT	201	1/1	0.98	0.36	-	3,3,3,3	0
56	MG	AY	103	1/1	0.72	0.09	-	87,87,87,87	0
56	MG	AA	1933	1/1	0.89	0.13	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AD	5003	1/1	0.89	0.07	-	42,42,42,42	0
56	MG	BA	3563	1/1	0.93	0.14	-	57,57,57,57	0
56	MG	AA	1956	1/1	0.81	0.21	-	58,58,58,58	0
56	MG	BA	3201	1/1	0.91	0.24	-	67,67,67,67	0
56	MG	BA	3178	1/1	0.84	0.20	-	51,51,51,51	0
56	MG	DA	3363	1/1	0.97	0.41	-	3,3,3,3	0
56	MG	CA	1741	1/1	0.84	0.27	-	50,50,50,50	0
56	MG	B1	106	1/1	0.91	0.24	-	56,56,56,56	0
56	MG	AA	1645	1/1	0.81	0.26	-	42,42,42,42	0
56	MG	CA	1746	1/1	0.93	0.17	-	57,57,57,57	0
56	MG	AA	1832	1/1	0.97	0.27	-	33,33,33,33	0
56	MG	BA	3040	1/1	0.96	0.31	-	97,97,97,97	0
56	MG	BA	3140	1/1	0.90	0.20	-	33,33,33,33	0
56	MG	BA	3184	1/1	0.88	0.15	-	45,45,45,45	0
56	MG	DA	3014	1/1	0.98	0.38	-	3,3,3,3	0
56	MG	DA	3072	1/1	0.94	0.20	-	3,3,3,3	0
56	MG	AZ	107	1/1	0.88	0.07	-	78,78,78,78	0
56	MG	DA	3046	1/1	0.96	0.25	-	4,4,4,4	0
56	MG	DA	3196	1/1	0.95	0.22	-	4,4,4,4	0
56	MG	CY	106	1/1	0.88	0.34	-	66,66,66,66	0
56	MG	BA	3418	1/1	0.94	0.49	-	54,54,54,54	0
56	MG	AA	1942	1/1	0.88	0.19	-	34,34,34,34	0
56	MG	BA	3504	1/1	0.97	0.10	-	34,34,34,34	0
56	MG	B6	101	1/1	0.94	0.10	-	44,44,44,44	0
56	MG	BA	3816	1/1	0.96	0.21	-	38,38,38,38	0
56	MG	BA	3487	1/1	0.95	0.20	-	26,26,26,26	0
56	MG	AO	102	1/1	0.87	0.40	-	48,48,48,48	0
56	MG	CA	1661	1/1	0.95	0.25	-	3,3,3,3	0
56	MG	DA	3102	1/1	0.87	0.31	-	74,74,74,74	0
56	MG	CA	1727	1/1	0.95	0.11	-	53,53,53,53	0
56	MG	DA	3146	1/1	0.96	0.31	-	3,3,3,3	0
56	MG	AY	121	1/1	0.88	0.12	-	41,41,41,41	0
56	MG	CA	1675	1/1	0.93	0.31	-	65,65,65,65	0
56	MG	CA	1713	1/1	0.64	0.57	-	80,80,80,80	0
56	MG	CA	1610	1/1	0.92	0.17	-	4,4,4,4	0
56	MG	BA	3314	1/1	0.96	0.25	-	22,22,22,22	0
56	MG	CA	1619	1/1	0.95	0.27	-	4,4,4,4	0
56	MG	DA	3389	1/1	0.85	0.17	-	70,70,70,70	0
56	MG	BA	3035	1/1	0.90	0.27	-	51,51,51,51	0
56	MG	AA	1786	1/1	0.82	0.18	-	61,61,61,61	0
56	MG	BA	3162	1/1	0.88	0.24	-	58,58,58,58	0
56	MG	CY	114	1/1	0.89	0.36	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3337	1/1	0.89	0.24	-	69,69,69,69	0
56	MG	BA	3500	1/1	0.93	0.11	-	21,21,21,21	0
56	MG	BA	3767	1/1	0.97	0.17	-	31,31,31,31	0
56	MG	AA	1643	1/1	0.82	0.34	-	50,50,50,50	0
56	MG	BA	3719	1/1	0.91	0.17	-	37,37,37,37	0
56	MG	AB	305	1/1	0.89	0.16	-	56,56,56,56	0
56	MG	BA	3326	1/1	0.93	0.08	-	45,45,45,45	0
56	MG	DA	3265	1/1	0.98	0.17	-	3,3,3,3	0
56	MG	BA	3689	1/1	0.90	0.30	-	80,80,80,80	0
56	MG	AB	307	1/1	0.89	0.08	-	45,45,45,45	0
56	MG	AA	1623	1/1	0.80	0.43	-	74,74,74,74	0
56	MG	DA	3163	1/1	0.97	0.24	-	3,3,3,3	0
56	MG	BA	3512	1/1	0.90	0.09	-	62,62,62,62	0
56	MG	BA	3252	1/1	0.53	0.10	-	80,80,80,80	0
56	MG	BA	3229	1/1	0.81	0.27	-	47,47,47,47	0
56	MG	BA	3892	1/1	0.93	0.15	-	46,46,46,46	0
56	MG	DA	3435	1/1	0.96	0.17	-	4,4,4,4	0
56	MG	AA	1750	1/1	0.72	0.15	-	97,97,97,97	0
56	MG	DA	3397	1/1	0.95	0.22	-	24,24,24,24	0
56	MG	AA	1995	1/1	0.89	0.11	-	44,44,44,44	0
56	MG	DA	3421	1/1	0.90	0.14	-	35,35,35,35	0
56	MG	BA	3507	1/1	0.88	0.16	-	82,82,82,82	0
56	MG	BF	304	1/1	0.85	0.36	-	65,65,65,65	0
56	MG	AB	302	1/1	0.88	0.10	-	50,50,50,50	0
56	MG	AA	1890	1/1	0.94	0.18	-	21,21,21,21	0
56	MG	DA	3295	1/1	0.86	0.16	-	33,33,33,33	0
56	MG	BA	3039	1/1	0.85	0.43	-	67,67,67,67	0
56	MG	BA	3446	1/1	0.90	0.38	-	58,58,58,58	0
56	MG	BA	3128	1/1	0.91	0.23	-	60,60,60,60	0
56	MG	AA	1754	1/1	0.83	0.28	-	70,70,70,70	0
56	MG	AA	1658	1/1	0.91	0.13	-	29,29,29,29	0
56	MG	DA	3449	1/1	0.87	0.13	-	53,53,53,53	0
56	MG	BA	3678	1/1	0.88	0.40	-	37,37,37,37	0
56	MG	BA	3049	1/1	0.83	0.24	-	56,56,56,56	0
56	MG	BA	3514	1/1	0.90	0.33	-	53,53,53,53	0
56	MG	DA	3099	1/1	0.94	0.26	-	3,3,3,3	0
56	MG	CA	1704	1/1	0.87	0.34	-	63,63,63,63	0
56	MG	DA	3217	1/1	0.80	0.07	-	58,58,58,58	0
56	MG	CA	1652	1/1	0.88	0.59	-	44,44,44,44	0
56	MG	DA	3452	1/1	0.93	0.22	-	38,38,38,38	0
56	MG	AA	1639	1/1	0.73	0.16	-	59,59,59,59	0
56	MG	BA	3477	1/1	0.79	0.12	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	CA	1802	1/1	0.95	0.28	-	3,3,3,3	0
56	MG	AA	1706	1/1	0.95	0.12	-	36,36,36,36	0
56	MG	CA	1806	1/1	0.98	0.34	-	3,3,3,3	0
56	MG	DA	3232	1/1	0.94	0.06	-	37,37,37,37	0
56	MG	AA	1737	1/1	0.97	0.26	-	36,36,36,36	0
56	MG	AA	1851	1/1	0.91	0.35	-	69,69,69,69	0
56	MG	B0	101	1/1	0.81	0.63	-	63,63,63,63	0
56	MG	CA	1725	1/1	0.96	0.04	-	54,54,54,54	0
56	MG	AA	1609	1/1	0.80	0.14	-	58,58,58,58	0
56	MG	DA	3210	1/1	0.59	0.38	-	3,3,3,3	0
56	MG	DA	3453	1/1	0.96	0.46	-	3,3,3,3	0
56	MG	BA	3026	1/1	0.89	0.20	-	33,33,33,33	0
56	MG	DA	3353	1/1	0.91	0.06	-	61,61,61,61	0
56	MG	B1	107	1/1	0.88	0.15	-	56,56,56,56	0
56	MG	BA	3814	1/1	0.95	0.33	-	47,47,47,47	0
56	MG	AA	1663	1/1	0.96	0.06	-	33,33,33,33	0
56	MG	DA	3281	1/1	0.82	0.27	-	63,63,63,63	0
56	MG	CK	201	1/1	0.81	0.37	-	70,70,70,70	0
56	MG	AA	2012	1/1	0.83	0.27	-	55,55,55,55	0
56	MG	BA	3887	1/1	0.91	0.20	-	66,66,66,66	0
56	MG	BA	3643	1/1	0.54	0.39	-	68,68,68,68	0
56	MG	BA	3732	1/1	0.91	0.57	-	68,68,68,68	0
56	MG	CA	1672	1/1	0.97	0.32	-	3,3,3,3	0
56	MG	BA	3526	1/1	0.94	0.20	-	49,49,49,49	0
56	MG	DR	201	1/1	0.95	0.28	-	3,3,3,3	0
56	MG	AA	1824	1/1	0.95	0.47	-	34,34,34,34	0
56	MG	AA	1665	1/1	0.91	0.10	-	38,38,38,38	0
56	MG	AA	1618	1/1	0.93	0.16	-	50,50,50,50	0
56	MG	DA	3309	1/1	0.96	0.22	-	4,4,4,4	0
56	MG	BA	3830	1/1	0.96	0.12	-	12,12,12,12	0
56	MG	DA	3118	1/1	0.94	0.32	-	6,6,6,6	0
56	MG	BA	3666	1/1	0.87	0.14	-	46,46,46,46	0
56	MG	AA	1949	1/1	0.54	0.30	-	90,90,90,90	0
56	MG	DA	3345	1/1	0.97	0.61	-	3,3,3,3	0
56	MG	BA	3378	1/1	0.97	0.11	-	32,32,32,32	0
56	MG	BA	3447	1/1	0.94	0.46	-	31,31,31,31	0
56	MG	DA	3483	1/1	0.97	0.19	-	4,4,4,4	0
56	MG	BW	202	1/1	0.92	0.21	-	38,38,38,38	0
56	MG	DA	3385	1/1	0.93	0.22	-	51,51,51,51	0
56	MG	BA	3037	1/1	0.86	0.41	-	61,61,61,61	0
56	MG	AA	1972	1/1	0.96	0.11	-	43,43,43,43	0
56	MG	BA	3125	1/1	0.90	0.07	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3657	1/1	0.88	0.48	-	56,56,56,56	0
56	MG	BA	3686	1/1	0.91	0.57	-	49,49,49,49	0
56	MG	CA	1780	1/1	0.95	0.08	-	51,51,51,51	0
56	MG	AA	1601	1/1	0.90	0.25	-	37,37,37,37	0
56	MG	DA	3087	1/1	0.92	0.23	-	3,3,3,3	0
56	MG	AR	101	1/1	0.97	0.07	-	32,32,32,32	0
56	MG	AA	1987	1/1	0.91	0.07	-	40,40,40,40	0
56	MG	DA	3382	1/1	0.96	0.07	-	42,42,42,42	0
56	MG	BA	3621	1/1	0.94	0.18	-	50,50,50,50	0
56	MG	AA	1939	1/1	0.91	0.36	-	47,47,47,47	0
56	MG	BA	3263	1/1	0.78	0.55	-	47,47,47,47	0
56	MG	AA	1635	1/1	0.95	0.11	-	52,52,52,52	0
56	MG	BA	3687	1/1	0.88	0.24	-	59,59,59,59	0
56	MG	DA	3090	1/1	0.97	0.28	-	3,3,3,3	0
56	MG	BA	3714	1/1	0.86	0.28	-	60,60,60,60	0
56	MG	AA	1795	1/1	0.95	0.16	-	64,64,64,64	0
56	MG	BB	218	1/1	0.84	0.11	-	78,78,78,78	0
56	MG	BA	3762	1/1	0.92	0.21	-	28,28,28,28	0
56	MG	BA	3170	1/1	0.69	0.34	-	80,80,80,80	0
56	MG	AA	1738	1/1	0.89	0.21	-	47,47,47,47	0
56	MG	CA	1670	1/1	0.82	0.23	-	43,43,43,43	0
56	MG	CZ	108	1/1	0.86	0.14	-	69,69,69,69	0
56	MG	BA	3030	1/1	0.94	0.22	-	36,36,36,36	0
56	MG	AA	1727	1/1	0.87	0.32	-	59,59,59,59	0
56	MG	AA	1915	1/1	0.31	0.20	-	109,109,109,109	0
56	MG	DA	3293	1/1	0.88	0.32	-	61,61,61,61	0
56	MG	BA	3625	1/1	0.88	0.20	-	43,43,43,43	0
56	MG	DA	3394	1/1	0.92	0.17	-	53,53,53,53	0
56	MG	BA	3913	1/1	0.86	0.23	-	45,45,45,45	0
56	MG	DA	3124	1/1	0.96	0.15	-	14,14,14,14	0
56	MG	AA	1894	1/1	0.94	0.28	-	35,35,35,35	0
56	MG	AB	306	1/1	0.80	0.28	-	56,56,56,56	0
56	MG	CZ	105	1/1	0.81	0.05	-	74,74,74,74	0
56	MG	BA	3883	1/1	0.95	0.14	-	67,67,67,67	0
56	MG	BA	3282	1/1	0.97	0.13	-	34,34,34,34	0
56	MG	BA	3877	1/1	0.86	0.27	-	76,76,76,76	0
56	MG	AA	1781	1/1	0.98	0.21	-	28,28,28,28	0
56	MG	CA	1792	1/1	0.95	0.54	-	3,3,3,3	0
56	MG	DA	3430	1/1	0.98	0.14	-	6,6,6,6	0
56	MG	DA	3262	1/1	0.94	0.35	-	3,3,3,3	0
56	MG	DA	3478	1/1	0.98	0.36	-	3,3,3,3	0
56	MG	BX	101	1/1	0.80	0.26	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3916	1/1	0.92	0.19	-	59,59,59,59	0
56	MG	DA	3292	1/1	0.82	0.33	-	74,74,74,74	0
56	MG	BA	3327	1/1	0.92	0.18	-	64,64,64,64	0
56	MG	BA	3587	1/1	0.94	0.15	-	40,40,40,40	0
56	MG	CA	1644	1/1	0.91	0.24	-	3,3,3,3	0
56	MG	AA	1702	1/1	0.95	0.33	-	48,48,48,48	0
56	MG	CY	110	1/1	0.83	0.25	-	90,90,90,90	0
56	MG	AA	1934	1/1	0.87	0.36	-	65,65,65,65	0
56	MG	CA	1720	1/1	0.94	0.11	-	27,27,27,27	0
56	MG	DA	3162	1/1	0.95	0.21	-	3,3,3,3	0
56	MG	DA	3050	1/1	0.87	0.35	-	3,3,3,3	0
56	MG	AA	1865	1/1	0.86	0.13	-	73,73,73,73	0
56	MG	CC	301	1/1	0.98	0.25	-	3,3,3,3	0
56	MG	DN	201	1/1	0.94	0.60	-	3,3,3,3	0
56	MG	AA	1929	1/1	0.76	0.22	-	71,71,71,71	0
56	MG	AA	1836	1/1	0.87	0.29	-	53,53,53,53	0
56	MG	AA	1867	1/1	0.78	0.12	-	51,51,51,51	0
56	MG	DB	206	1/1	0.93	0.13	-	4,4,4,4	0
56	MG	BA	3684	1/1	0.83	0.18	-	50,50,50,50	0
56	MG	DA	3035	1/1	0.94	0.45	-	3,3,3,3	0
56	MG	AA	1996	1/1	0.88	0.28	-	56,56,56,56	0
56	MG	BA	3637	1/1	0.69	0.29	-	61,61,61,61	0
56	MG	AA	1662	1/1	0.91	0.46	-	45,45,45,45	0
56	MG	BA	3640	1/1	0.90	0.14	-	24,24,24,24	0
56	MG	AH	202	1/1	0.87	0.27	-	51,51,51,51	0
56	MG	BA	3672	1/1	0.96	0.06	-	18,18,18,18	0
56	MG	DA	3294	1/1	0.84	0.63	-	63,63,63,63	0
56	MG	BB	206	1/1	0.93	0.13	-	51,51,51,51	0
56	MG	BA	3571	1/1	0.90	0.28	-	39,39,39,39	0
56	MG	BE	304	1/1	0.80	0.19	-	79,79,79,79	0
56	MG	AA	1811	1/1	0.98	0.22	-	37,37,37,37	0
56	MG	CA	1641	1/1	0.96	0.33	-	3,3,3,3	0
56	MG	DA	3347	1/1	0.93	0.10	-	35,35,35,35	0
56	MG	AA	1862	1/1	0.97	0.12	-	41,41,41,41	0
56	MG	BA	3374	1/1	0.67	0.44	-	85,85,85,85	0
56	MG	BA	3363	1/1	0.93	0.22	-	42,42,42,42	0
56	MG	CA	1621	1/1	0.93	0.26	-	3,3,3,3	0
56	MG	AA	1624	1/1	0.93	0.14	-	43,43,43,43	0
56	MG	BT	201	1/1	0.55	0.70	-	81,81,81,81	0
56	MG	AY	126	1/1	0.89	0.42	-	68,68,68,68	0
56	MG	AA	1982	1/1	0.91	0.30	-	51,51,51,51	0
56	MG	BA	3636	1/1	0.93	0.14	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1821	1/1	0.49	0.28	-	90,90,90,90	0
56	MG	BA	3089	1/1	0.90	0.32	-	69,69,69,69	0
56	MG	AA	1742	1/1	0.91	0.11	-	67,67,67,67	0
56	MG	AZ	102	1/1	0.68	0.13	-	71,71,71,71	0
56	MG	CA	1690	1/1	0.87	0.21	-	54,54,54,54	0
56	MG	CA	1671	1/1	0.88	0.14	-	63,63,63,63	0
56	MG	BA	3758	1/1	0.58	0.53	-	94,94,94,94	0
56	MG	CA	1677	1/1	0.81	0.24	-	103,103,103,103	0
56	MG	DD	5006	1/1	0.86	0.32	-	47,47,47,47	0
56	MG	BA	3211	1/1	0.93	0.16	-	80,80,80,80	0
56	MG	AA	1784	1/1	0.99	0.28	-	25,25,25,25	0
56	MG	DA	3362	1/1	0.93	0.13	-	82,82,82,82	0
56	MG	AA	1871	1/1	0.92	0.29	-	68,68,68,68	0
56	MG	CA	1635	1/1	0.91	0.17	-	4,4,4,4	0
56	MG	BA	3842	1/1	0.95	0.19	-	16,16,16,16	0
56	MG	BA	3661	1/1	0.64	0.39	-	71,71,71,71	0
56	MG	DA	3365	1/1	0.99	0.29	-	3,3,3,3	0
56	MG	BA	3654	1/1	0.98	0.20	-	12,12,12,12	0
56	MG	BA	3134	1/1	0.90	0.18	-	23,23,23,23	0
56	MG	AA	1751	1/1	0.88	0.17	-	61,61,61,61	0
56	MG	AA	1843	1/1	0.96	0.13	-	41,41,41,41	0
56	MG	DA	3153	1/1	0.87	0.22	-	5,5,5,5	0
56	MG	AA	1872	1/1	0.87	0.33	-	59,59,59,59	0
56	MG	CA	1735	1/1	0.90	0.19	-	31,31,31,31	0
56	MG	CA	1809	1/1	0.94	0.32	-	3,3,3,3	0
56	MG	BA	3630	1/1	0.74	0.18	-	47,47,47,47	0
56	MG	BA	3748	1/1	0.94	0.23	-	35,35,35,35	0
56	MG	DA	3145	1/1	0.96	0.23	-	4,4,4,4	0
56	MG	BA	3034	1/1	0.93	0.14	-	43,43,43,43	0
56	MG	BA	3215	1/1	0.95	0.14	-	27,27,27,27	0
56	MG	BA	3302	1/1	0.97	0.31	-	47,47,47,47	0
56	MG	CA	1666	1/1	0.94	0.22	-	3,3,3,3	0
56	MG	BA	3190	1/1	0.90	0.26	-	77,77,77,77	0
56	MG	AE	205	1/1	0.84	0.12	-	65,65,65,65	0
56	MG	DA	3108	1/1	0.89	0.35	-	59,59,59,59	0
56	MG	BA	3292	1/1	0.92	0.80	-	36,36,36,36	0
56	MG	AA	1951	1/1	0.60	0.35	-	59,59,59,59	0
56	MG	BA	3221	1/1	0.88	0.45	-	33,33,33,33	0
56	MG	CA	1722	1/1	0.83	0.20	-	49,49,49,49	0
56	MG	BB	222	1/1	0.86	0.20	-	39,39,39,39	0
56	MG	AA	1696	1/1	0.82	0.36	-	59,59,59,59	0
56	MG	CA	1691	1/1	0.91	0.16	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AY	115	1/1	0.82	0.13	-	65,65,65,65	0
56	MG	BB	208	1/1	0.91	0.19	-	63,63,63,63	0
56	MG	DA	3026	1/1	0.93	0.43	-	3,3,3,3	0
56	MG	BV	202	1/1	0.89	0.64	-	38,38,38,38	0
56	MG	AA	1819	1/1	0.68	0.28	-	76,76,76,76	0
56	MG	AF	202	1/1	0.85	0.09	-	41,41,41,41	0
56	MG	BA	3886	1/1	0.91	0.17	-	69,69,69,69	0
56	MG	BA	3181	1/1	0.85	0.20	-	23,23,23,23	0
56	MG	AA	1794	1/1	0.89	0.12	-	19,19,19,19	0
56	MG	DA	3271	1/1	0.99	0.21	-	3,3,3,3	0
56	MG	BA	3529	1/1	0.84	0.42	-	64,64,64,64	0
56	MG	AA	1823	1/1	0.83	0.24	-	47,47,47,47	0
56	MG	BA	3119	1/1	0.78	0.25	-	54,54,54,54	0
56	MG	DA	3226	1/1	0.94	0.11	-	4,4,4,4	0
56	MG	BB	215	1/1	0.82	0.11	-	103,103,103,103	0
56	MG	DF	301	1/1	0.94	0.45	-	3,3,3,3	0
56	MG	DA	3460	1/1	0.97	0.07	-	6,6,6,6	0
56	MG	BA	3681	1/1	0.91	0.87	-	59,59,59,59	0
56	MG	AA	1986	1/1	0.92	0.27	-	52,52,52,52	0
56	MG	BB	230	1/1	0.60	0.37	-	50,50,50,50	0
56	MG	AE	208	1/1	0.96	0.11	-	42,42,42,42	0
56	MG	DA	3443	1/1	0.94	0.30	-	3,3,3,3	0
56	MG	BA	3554	1/1	0.97	0.28	-	7,7,7,7	0
56	MG	BP	201	1/1	0.81	0.47	-	68,68,68,68	0
56	MG	AA	2003	1/1	0.86	0.16	-	54,54,54,54	0
56	MG	CA	1622	1/1	0.99	0.23	-	3,3,3,3	0
56	MG	DA	3077	1/1	0.96	0.12	-	5,5,5,5	0
56	MG	AB	301	1/1	0.90	0.12	-	62,62,62,62	0
56	MG	AA	1716	1/1	0.96	0.12	-	24,24,24,24	0
56	MG	AA	1677	1/1	0.95	0.10	-	74,74,74,74	0
56	MG	AA	1700	1/1	0.88	0.34	-	45,45,45,45	0
56	MG	DA	3463	1/1	0.98	0.13	-	4,4,4,4	0
56	MG	AA	1661	1/1	0.76	0.13	-	66,66,66,66	0
56	MG	BA	3189	1/1	0.73	0.28	-	96,96,96,96	0
56	MG	BA	3058	1/1	0.84	0.08	-	67,67,67,67	0
56	MG	BA	3596	1/1	0.94	0.12	-	13,13,13,13	0
56	MG	DA	3119	1/1	0.90	0.23	-	58,58,58,58	0
56	MG	BA	3153	1/1	0.96	0.29	-	41,41,41,41	0
56	MG	CA	1745	1/1	0.95	0.14	-	36,36,36,36	0
56	MG	BE	303	1/1	0.86	0.10	-	53,53,53,53	0
56	MG	DA	3310	1/1	0.90	0.17	-	57,57,57,57	0
56	MG	AX	406	1/1	0.94	0.19	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3721	1/1	0.98	0.26	-	34,34,34,34	0
56	MG	BA	3527	1/1	0.91	0.12	-	38,38,38,38	0
56	MG	BA	3096	1/1	0.96	0.08	-	60,60,60,60	0
56	MG	DA	3273	1/1	0.98	0.26	-	3,3,3,3	0
56	MG	DA	3183	1/1	0.94	0.28	-	3,3,3,3	0
56	MG	BA	3895	1/1	0.93	0.21	-	51,51,51,51	0
56	MG	DA	3319	1/1	0.93	0.17	-	43,43,43,43	0
56	MG	AA	1868	1/1	0.86	0.25	-	38,38,38,38	0
56	MG	BA	3585	1/1	0.92	0.17	-	35,35,35,35	0
56	MG	DA	3255	1/1	0.98	0.23	-	12,12,12,12	0
56	MG	DA	3214	1/1	0.97	0.30	-	4,4,4,4	0
56	MG	BI	206	1/1	0.97	0.26	-	67,67,67,67	0
56	MG	CF	205	1/1	0.91	0.15	-	57,57,57,57	0
56	MG	CA	1730	1/1	0.97	0.24	-	4,4,4,4	0
56	MG	BA	3505	1/1	0.59	0.15	-	92,92,92,92	0
56	MG	BA	3301	1/1	0.90	0.21	-	31,31,31,31	0
56	MG	AA	1983	1/1	0.83	0.43	-	67,67,67,67	0
56	MG	AC	301	1/1	0.85	0.19	-	75,75,75,75	0
56	MG	BA	3546	1/1	0.90	0.28	-	40,40,40,40	0
56	MG	BA	3212	1/1	0.92	0.07	-	29,29,29,29	0
56	MG	CA	1642	1/1	0.98	0.42	-	3,3,3,3	0
56	MG	BA	3917	1/1	0.87	0.16	-	51,51,51,51	0
56	MG	DA	3243	1/1	0.97	0.20	-	4,4,4,4	0
56	MG	BA	3699	1/1	0.92	0.05	-	79,79,79,79	0
56	MG	BA	3577	1/1	0.91	0.16	-	60,60,60,60	0
56	MG	AA	1667	1/1	0.76	0.25	-	70,70,70,70	0
56	MG	BA	3310	1/1	0.90	0.68	-	73,73,73,73	0
56	MG	DA	3201	1/1	0.97	0.15	-	6,6,6,6	0
56	MG	DA	3075	1/1	0.97	0.12	-	4,4,4,4	0
56	MG	CA	1673	1/1	0.91	0.15	-	49,49,49,49	0
56	MG	AY	117	1/1	0.92	0.15	-	68,68,68,68	0
56	MG	BA	3289	1/1	0.97	0.17	-	31,31,31,31	0
56	MG	BA	3532	1/1	0.90	0.30	-	55,55,55,55	0
56	MG	AA	1930	1/1	0.96	0.07	-	59,59,59,59	0
56	MG	BA	3462	1/1	0.87	0.17	-	35,35,35,35	0
56	MG	BA	3306	1/1	0.62	0.43	-	52,52,52,52	0
56	MG	BA	3397	1/1	0.78	0.09	-	52,52,52,52	0
56	MG	BA	3741	1/1	0.90	0.11	-	52,52,52,52	0
56	MG	AZ	105	1/1	0.89	0.13	-	78,78,78,78	0
56	MG	AA	1808	1/1	0.93	0.14	-	46,46,46,46	0
56	MG	BA	3242	1/1	0.97	0.18	-	23,23,23,23	0
56	MG	DA	3126	1/1	0.96	0.61	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1963	1/1	0.93	0.21	-	56,56,56,56	0
56	MG	AA	1799	1/1	0.91	0.10	-	31,31,31,31	0
56	MG	BA	3241	1/1	0.95	0.18	-	48,48,48,48	0
56	MG	AY	124	1/1	0.81	0.43	-	51,51,51,51	0
56	MG	BA	3290	1/1	0.95	0.16	-	15,15,15,15	0
56	MG	BA	3605	1/1	0.96	0.29	-	12,12,12,12	0
56	MG	AA	1648	1/1	0.87	0.40	-	87,87,87,87	0
56	MG	BA	3405	1/1	0.91	0.20	-	44,44,44,44	0
56	MG	AA	1666	1/1	0.90	0.13	-	61,61,61,61	0
56	MG	BA	3833	1/1	0.95	0.16	-	9,9,9,9	0
56	MG	BA	3871	1/1	0.86	0.79	-	65,65,65,65	0
56	MG	AE	203	1/1	0.84	0.29	-	72,72,72,72	0
56	MG	BA	3847	1/1	0.76	0.44	-	62,62,62,62	0
56	MG	BA	3439	1/1	0.96	0.17	-	18,18,18,18	0
56	MG	BB	227	1/1	0.77	0.31	-	54,54,54,54	0
56	MG	BA	3171	1/1	0.70	0.72	-	77,77,77,77	0
56	MG	DA	3302	1/1	0.98	0.11	-	44,44,44,44	0
56	MG	AA	1887	1/1	0.91	0.14	-	31,31,31,31	0
56	MG	DA	3006	1/1	0.94	0.46	-	3,3,3,3	0
56	MG	AH	201	1/1	0.93	0.20	-	27,27,27,27	0
56	MG	BA	3258	1/1	0.86	0.15	-	50,50,50,50	0
56	MG	AA	1852	1/1	0.89	0.16	-	18,18,18,18	0
56	MG	AA	1610	1/1	0.84	0.23	-	65,65,65,65	0
56	MG	AZ	108	1/1	0.91	0.08	-	60,60,60,60	0
56	MG	AA	1889	1/1	0.87	0.41	-	30,30,30,30	0
56	MG	CA	1643	1/1	0.96	0.17	-	3,3,3,3	0
56	MG	BA	3104	1/1	0.91	0.12	-	67,67,67,67	0
56	MG	AD	5004	1/1	0.96	0.19	-	48,48,48,48	0
56	MG	CZ	107	1/1	0.94	0.13	-	57,57,57,57	0
56	MG	CA	1774	1/1	0.95	0.48	-	82,82,82,82	0
56	MG	BA	3715	1/1	0.92	0.18	-	28,28,28,28	0
56	MG	DA	3228	1/1	0.94	0.12	-	4,4,4,4	0
56	MG	DA	3284	1/1	0.97	0.07	-	8,8,8,8	0
56	MG	AA	1998	1/1	0.73	0.20	-	57,57,57,57	0
56	MG	BA	3567	1/1	0.89	0.36	-	23,23,23,23	0
56	MG	DA	3393	1/1	0.98	0.06	-	47,47,47,47	0
56	MG	CA	1732	1/1	0.91	0.35	-	63,63,63,63	0
56	MG	AA	1789	1/1	0.78	0.18	-	77,77,77,77	0
56	MG	BB	225	1/1	0.88	0.16	-	48,48,48,48	0
56	MG	CZ	112	1/1	0.89	0.15	-	63,63,63,63	0
56	MG	DA	3084	1/1	0.96	0.34	-	3,3,3,3	0
56	MG	AA	1909	1/1	0.97	0.12	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3300	1/1	0.79	0.41	-	78,78,78,78	0
56	MG	BA	3002	1/1	0.88	0.32	-	47,47,47,47	0
56	MG	BA	3531	1/1	0.97	0.13	-	12,12,12,12	0
56	MG	BA	3164	1/1	0.95	0.80	-	35,35,35,35	0
56	MG	AA	1780	1/1	0.97	0.17	-	24,24,24,24	0
56	MG	BA	3191	1/1	0.97	0.11	-	26,26,26,26	0
56	MG	DA	3352	1/1	0.98	0.30	-	3,3,3,3	0
56	MG	BA	3629	1/1	0.94	0.19	-	50,50,50,50	0
56	MG	BA	3730	1/1	0.80	0.51	-	86,86,86,86	0
56	MG	AA	1758	1/1	0.91	0.20	-	22,22,22,22	0
56	MG	BK	201	1/1	0.90	0.30	-	60,60,60,60	0
56	MG	BA	3032	1/1	0.90	0.09	-	30,30,30,30	0
56	MG	BA	3048	1/1	0.56	0.87	-	58,58,58,58	0
56	MG	DA	3368	1/1	0.96	0.22	-	3,3,3,3	0
56	MG	AA	1722	1/1	0.93	0.08	-	34,34,34,34	0
56	MG	BA	3613	1/1	0.95	0.10	-	32,32,32,32	0
56	MG	BG	202	1/1	0.86	0.14	-	63,63,63,63	0
56	MG	BA	3481	1/1	0.84	0.81	-	65,65,65,65	0
56	MG	BA	3072	1/1	0.80	0.31	-	61,61,61,61	0
56	MG	BY	202	1/1	0.82	0.17	-	42,42,42,42	0
56	MG	BA	3432	1/1	0.87	0.10	-	52,52,52,52	0
56	MG	DA	3112	1/1	0.97	0.09	-	26,26,26,26	0
56	MG	AA	1649	1/1	0.93	0.15	-	37,37,37,37	0
56	MG	CA	1629	1/1	0.99	0.20	-	4,4,4,4	0
56	MG	AA	1922	1/1	0.92	0.45	-	46,46,46,46	0
56	MG	DA	3388	1/1	0.81	0.12	-	19,19,19,19	0
56	MG	BA	3688	1/1	0.79	0.13	-	74,74,74,74	0
56	MG	CA	1821	1/1	0.91	0.21	-	29,29,29,29	0
56	MG	AA	1816	1/1	0.91	0.31	-	55,55,55,55	0
56	MG	BA	3390	1/1	0.87	0.10	-	67,67,67,67	0
56	MG	BA	3787	1/1	0.93	0.22	-	47,47,47,47	0
56	MG	CB	302	1/1	0.97	0.14	-	3,3,3,3	0
56	MG	DA	3420	1/1	0.95	0.19	-	4,4,4,4	0
56	MG	AA	1672	1/1	0.86	0.35	-	69,69,69,69	0
56	MG	AA	1684	1/1	0.43	0.46	-	61,61,61,61	0
56	MG	DA	3122	1/1	0.98	0.25	-	4,4,4,4	0
56	MG	DA	3027	1/1	0.96	0.15	-	6,6,6,6	0
56	MG	AA	1792	1/1	0.92	0.21	-	63,63,63,63	0
56	MG	DA	3070	1/1	0.99	0.27	-	4,4,4,4	0
56	MG	BA	3194	1/1	0.93	0.12	-	36,36,36,36	0
56	MG	DU	201	1/1	0.94	0.38	-	3,3,3,3	0
56	MG	AA	1775	1/1	0.96	0.16	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3240	1/1	0.83	0.55	-	40,40,40,40	0
56	MG	DA	3458	1/1	0.98	0.17	-	6,6,6,6	0
56	MG	BA	3558	1/1	0.95	0.19	-	10,10,10,10	0
56	MG	BA	3901	1/1	0.86	0.38	-	62,62,62,62	0
56	MG	BA	3801	1/1	0.75	0.19	-	51,51,51,51	0
56	MG	DA	3305	1/1	0.94	0.14	-	23,23,23,23	0
56	MG	AL	202	1/1	0.93	0.09	-	34,34,34,34	0
56	MG	DA	3012	1/1	0.95	0.24	-	3,3,3,3	0
56	MG	AA	1937	1/1	0.87	0.28	-	61,61,61,61	0
56	MG	DA	3110	1/1	0.91	0.06	-	48,48,48,48	0
56	MG	DA	3164	1/1	0.93	0.15	-	4,4,4,4	0
56	MG	AA	1888	1/1	0.90	0.41	-	39,39,39,39	0
56	MG	BA	3740	1/1	0.93	0.29	-	53,53,53,53	0
56	MG	BA	3615	1/1	0.81	0.15	-	56,56,56,56	0
56	MG	BA	3359	1/1	0.92	0.78	-	70,70,70,70	0
56	MG	DA	3048	1/1	0.90	0.24	-	4,4,4,4	0
56	MG	DA	3030	1/1	0.97	0.15	-	4,4,4,4	0
56	MG	AA	1842	1/1	0.88	0.50	-	75,75,75,75	0
56	MG	AA	1634	1/1	0.92	0.13	-	43,43,43,43	0
56	MG	BA	3127	1/1	0.94	0.11	-	22,22,22,22	0
56	MG	DA	3338	1/1	0.93	0.27	-	3,3,3,3	0
56	MG	CA	1790	1/1	0.88	0.31	-	57,57,57,57	0
56	MG	BA	3388	1/1	0.95	0.09	-	61,61,61,61	0
56	MG	DA	3280	1/1	0.96	0.31	-	34,34,34,34	0
56	MG	AG	201	1/1	0.91	0.17	-	72,72,72,72	0
56	MG	BA	3061	1/1	0.46	0.10	-	76,76,76,76	0
56	MG	BA	3398	1/1	0.88	0.09	-	56,56,56,56	0
56	MG	CA	1779	1/1	0.80	0.49	-	76,76,76,76	0
56	MG	BA	3146	1/1	0.77	0.17	-	33,33,33,33	0
56	MG	CA	1731	1/1	0.94	0.22	-	3,3,3,3	0
56	MG	BZ	301	1/1	0.71	0.16	-	81,81,81,81	0
56	MG	BA	3829	1/1	0.95	0.15	-	40,40,40,40	0
56	MG	BO	202	1/1	0.93	0.09	-	54,54,54,54	0
56	MG	BA	3411	1/1	0.92	0.14	-	51,51,51,51	0
56	MG	CA	1656	1/1	0.93	0.23	-	5,5,5,5	0
56	MG	AA	1641	1/1	0.91	0.13	-	27,27,27,27	0
56	MG	AA	1622	1/1	0.69	0.33	-	72,72,72,72	0
56	MG	BA	3103	1/1	0.87	0.60	-	78,78,78,78	0
56	MG	DA	3407	1/1	0.99	0.30	-	3,3,3,3	0
56	MG	DA	3439	1/1	0.98	0.26	-	4,4,4,4	0
56	MG	DA	3098	1/1	0.93	0.30	-	3,3,3,3	0
56	MG	AY	114	1/1	0.90	0.23	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3364	1/1	0.81	0.46	-	40,40,40,40	0
56	MG	BA	3780	1/1	0.93	0.27	-	32,32,32,32	0
56	MG	AA	1884	1/1	0.94	0.16	-	26,26,26,26	0
56	MG	BA	3044	1/1	0.90	0.23	-	49,49,49,49	0
56	MG	DA	3128	1/1	0.95	0.17	-	12,12,12,12	0
56	MG	AA	1605	1/1	0.28	0.42	-	88,88,88,88	0
56	MG	BA	3768	1/1	0.87	0.15	-	31,31,31,31	0
56	MG	AA	1848	1/1	0.91	0.28	-	56,56,56,56	0
56	MG	DA	3060	1/1	0.96	0.17	-	4,4,4,4	0
56	MG	DA	3373	1/1	0.66	0.26	-	92,92,92,92	0
56	MG	BA	3574	1/1	0.88	0.29	-	74,74,74,74	0
56	MG	BA	3268	1/1	0.89	0.21	-	45,45,45,45	0
56	MG	BB	224	1/1	0.83	0.18	-	65,65,65,65	0
56	MG	BA	3338	1/1	0.92	0.45	-	56,56,56,56	0
56	MG	BA	3539	1/1	0.97	0.17	-	12,12,12,12	0
56	MG	BA	3101	1/1	0.87	0.26	-	47,47,47,47	0
56	MG	BA	3494	1/1	0.91	0.10	-	44,44,44,44	0
56	MG	DA	3476	1/1	0.96	0.23	-	3,3,3,3	0
56	MG	BA	3778	1/1	0.85	0.19	-	63,63,63,63	0
56	MG	AA	1946	1/1	0.94	0.12	-	59,59,59,59	0
56	MG	BA	3845	1/1	0.90	0.55	-	68,68,68,68	0
56	MG	BA	3542	1/1	0.88	0.17	-	27,27,27,27	0
56	MG	AX	411	1/1	0.72	0.49	-	75,75,75,75	0
56	MG	CZ	103	1/1	0.88	0.10	-	42,42,42,42	0
56	MG	CA	1668	1/1	0.91	0.35	-	3,3,3,3	0
56	MG	DA	3177	1/1	0.97	0.42	-	3,3,3,3	0
56	MG	AA	1739	1/1	0.83	0.25	-	55,55,55,55	0
56	MG	DA	3103	1/1	0.89	0.29	-	62,62,62,62	0
56	MG	CA	1701	1/1	0.99	0.14	-	13,13,13,13	0
56	MG	BA	3046	1/1	0.94	0.15	-	38,38,38,38	0
56	MG	BA	3810	1/1	0.95	0.27	-	12,12,12,12	0
56	MG	BA	3618	1/1	0.96	0.09	-	19,19,19,19	0
56	MG	DA	3024	1/1	0.96	0.16	-	3,3,3,3	0
56	MG	AA	1620	1/1	0.95	0.19	-	56,56,56,56	0
56	MG	BA	3588	1/1	0.90	0.09	-	24,24,24,24	0
56	MG	AA	1839	1/1	0.96	0.08	-	18,18,18,18	0
56	MG	DA	3416	1/1	0.98	0.21	-	3,3,3,3	0
56	MG	DA	3049	1/1	0.93	0.13	-	5,5,5,5	0
56	MG	CA	1810	1/1	0.93	0.63	-	59,59,59,59	0
56	MG	CA	1795	1/1	0.91	0.13	-	54,54,54,54	0
56	MG	AA	1878	1/1	0.72	0.24	-	67,67,67,67	0
56	MG	CA	1754	1/1	0.92	0.24	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3617	1/1	0.83	0.24	-	66,66,66,66	0
56	MG	BB	213	1/1	0.87	0.21	-	53,53,53,53	0
56	MG	BA	3634	1/1	0.94	0.73	-	33,33,33,33	0
56	MG	AA	1675	1/1	0.85	0.17	-	58,58,58,58	0
56	MG	BA	3144	1/1	0.96	0.35	-	45,45,45,45	0
56	MG	CA	1822	1/1	0.94	0.38	-	3,3,3,3	0
56	MG	AA	1928	1/1	0.93	0.13	-	52,52,52,52	0
56	MG	BA	3851	1/1	0.98	0.21	-	17,17,17,17	0
56	MG	CA	1679	1/1	0.22	0.88	-	90,90,90,90	0
56	MG	BB	229	1/1	0.92	0.23	-	33,33,33,33	0
56	MG	CA	1819	1/1	0.91	0.11	-	36,36,36,36	0
56	MG	B4	102	1/1	0.97	0.18	-	31,31,31,31	0
56	MG	BA	3422	1/1	0.72	0.36	-	59,59,59,59	0
56	MG	BA	3791	1/1	0.89	0.66	-	63,63,63,63	0
56	MG	DA	3346	1/1	0.88	0.33	-	56,56,56,56	0
56	MG	BA	3859	1/1	0.79	0.34	-	80,80,80,80	0
56	MG	BA	3309	1/1	0.91	0.23	-	17,17,17,17	0
56	MG	BY	201	1/1	0.91	0.15	-	68,68,68,68	0
56	MG	DA	3219	1/1	0.93	0.44	-	3,3,3,3	0
56	MG	BA	3920	1/1	0.90	0.20	-	54,54,54,54	0
56	MG	BA	3503	1/1	0.96	0.06	-	41,41,41,41	0
56	MG	DA	3106	1/1	0.90	0.21	-	46,46,46,46	0
56	MG	AA	1800	1/1	0.89	0.15	-	54,54,54,54	0
56	MG	DA	3223	1/1	0.97	0.28	-	4,4,4,4	0
56	MG	DA	3307	1/1	0.92	0.14	-	39,39,39,39	0
56	MG	CA	1761	1/1	0.97	0.11	-	30,30,30,30	0
56	MG	BA	3097	1/1	0.93	0.14	-	54,54,54,54	0
56	MG	AA	1651	1/1	0.34	0.33	-	106,106,106,106	0
56	MG	CA	1674	1/1	0.94	0.38	-	57,57,57,57	0
56	MG	BA	3747	1/1	0.74	0.43	-	64,64,64,64	0
56	MG	CA	1608	1/1	0.98	0.24	-	3,3,3,3	0
56	MG	DA	3386	1/1	0.95	0.21	-	3,3,3,3	0
56	MG	DB	204	1/1	0.97	0.27	-	3,3,3,3	0
56	MG	DA	3018	1/1	0.98	0.22	-	3,3,3,3	0
56	MG	BA	3321	1/1	0.92	0.15	-	40,40,40,40	0
56	MG	BI	203	1/1	0.85	0.15	-	53,53,53,53	0
56	MG	BA	3106	1/1	0.92	0.08	-	68,68,68,68	0
56	MG	BA	3033	1/1	0.93	0.19	-	38,38,38,38	0
56	MG	BA	3022	1/1	0.87	0.19	-	61,61,61,61	0
56	MG	CA	1784	1/1	0.97	0.30	-	3,3,3,3	0
56	MG	BA	3888	1/1	0.91	0.18	-	53,53,53,53	0
56	MG	AA	1906	1/1	0.81	0.16	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1917	1/1	0.96	0.07	-	52,52,52,52	0
56	MG	AA	1630	1/1	0.82	0.34	-	65,65,65,65	0
56	MG	CA	1714	1/1	0.88	0.34	-	62,62,62,62	0
56	MG	AE	207	1/1	0.94	0.09	-	38,38,38,38	0
56	MG	AA	1776	1/1	0.93	0.16	-	30,30,30,30	0
56	MG	BA	3525	1/1	0.74	0.10	-	77,77,77,77	0
56	MG	BA	3815	1/1	0.92	0.28	-	28,28,28,28	0
56	MG	AA	1718	1/1	0.97	0.17	-	79,79,79,79	0
56	MG	BA	3811	1/1	0.96	0.24	-	52,52,52,52	0
56	MG	BA	3792	1/1	0.75	0.31	-	85,85,85,85	0
56	MG	BA	3670	1/1	0.90	0.28	-	37,37,37,37	0
56	MG	BA	3074	1/1	0.98	0.09	-	26,26,26,26	0
56	MG	AA	1755	1/1	0.96	0.13	-	47,47,47,47	0
56	MG	DA	3288	1/1	0.94	0.20	-	33,33,33,33	0
56	MG	BA	3864	1/1	0.72	0.29	-	78,78,78,78	0
56	MG	BA	3711	1/1	0.90	0.24	-	70,70,70,70	0
56	MG	AA	1962	1/1	0.94	0.54	-	48,48,48,48	0
56	MG	BA	3111	1/1	0.93	0.23	-	35,35,35,35	0
56	MG	BA	3647	1/1	0.93	0.17	-	48,48,48,48	0
56	MG	CY	111	1/1	0.76	0.48	-	60,60,60,60	0
56	MG	CA	1648	1/1	0.89	0.15	-	33,33,33,33	0
56	MG	AK	203	1/1	0.93	0.12	-	49,49,49,49	0
56	MG	AY	107	1/1	0.89	0.08	-	67,67,67,67	0
56	MG	BA	3889	1/1	0.89	0.19	-	44,44,44,44	0
56	MG	DA	3095	1/1	0.95	0.22	-	3,3,3,3	0
56	MG	CA	1723	1/1	0.88	0.42	-	67,67,67,67	0
56	MG	BH	201	1/1	0.96	0.07	-	54,54,54,54	0
56	MG	CA	1717	1/1	0.97	0.16	-	21,21,21,21	0
56	MG	BA	3530	1/1	0.95	0.15	-	60,60,60,60	0
56	MG	AA	1950	1/1	0.66	0.15	-	73,73,73,73	0
56	MG	AA	1974	1/1	0.89	0.41	-	48,48,48,48	0
56	MG	BA	3323	1/1	0.87	0.25	-	57,57,57,57	0
56	MG	DA	3450	1/1	0.98	0.27	-	12,12,12,12	0
56	MG	BA	3598	1/1	0.69	0.47	-	73,73,73,73	0
56	MG	CA	1747	1/1	0.98	0.44	-	3,3,3,3	0
56	MG	BA	3856	1/1	0.90	0.09	-	36,36,36,36	0
56	MG	DA	3374	1/1	0.96	0.29	-	3,3,3,3	0
56	MG	BA	3763	1/1	0.91	0.15	-	52,52,52,52	0
56	MG	BA	3852	1/1	0.95	0.16	-	35,35,35,35	0
56	MG	DA	3313	1/1	0.73	0.39	-	69,69,69,69	0
56	MG	BA	3628	1/1	0.72	0.15	-	71,71,71,71	0
56	MG	CA	1808	1/1	0.93	0.48	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3729	1/1	0.98	0.28	-	38,38,38,38	0
56	MG	DA	3289	1/1	0.96	0.23	-	59,59,59,59	0
56	MG	BA	3157	1/1	0.86	0.39	-	55,55,55,55	0
56	MG	BA	3231	1/1	0.76	0.24	-	63,63,63,63	0
56	MG	BA	3377	1/1	0.85	0.14	-	73,73,73,73	0
56	MG	AA	1787	1/1	0.93	0.17	-	54,54,54,54	0
56	MG	AA	1783	1/1	0.96	0.44	-	28,28,28,28	0
56	MG	DA	3154	1/1	0.88	0.17	-	3,3,3,3	0
56	MG	AA	2010	1/1	0.94	0.19	-	33,33,33,33	0
56	MG	DA	3489	1/1	0.98	0.19	-	4,4,4,4	0
56	MG	D1	101	1/1	0.95	0.32	-	3,3,3,3	0
56	MG	BI	201	1/1	0.50	0.14	-	78,78,78,78	0
56	MG	BA	3137	1/1	0.97	0.11	-	19,19,19,19	0
56	MG	DA	3140	1/1	0.98	0.18	-	3,3,3,3	0
56	MG	AA	1740	1/1	0.97	0.23	-	30,30,30,30	0
56	MG	CA	1611	1/1	0.96	0.29	-	3,3,3,3	0
56	MG	CG	202	1/1	0.71	0.24	-	82,82,82,82	0
56	MG	AA	1607	1/1	0.87	0.21	-	62,62,62,62	0
56	MG	AA	1936	1/1	0.80	0.21	-	97,97,97,97	0
56	MG	AA	1748	1/1	0.87	0.09	-	41,41,41,41	0
56	MG	AA	1640	1/1	0.94	0.18	-	36,36,36,36	0
56	MG	BA	3347	1/1	0.91	0.07	-	43,43,43,43	0
56	MG	AX	405	1/1	0.68	0.08	-	74,74,74,74	0
56	MG	BA	3461	1/1	0.77	0.21	-	69,69,69,69	0
56	MG	CH	202	1/1	0.78	0.14	-	59,59,59,59	0
56	MG	BA	3565	1/1	0.81	0.21	-	50,50,50,50	0
56	MG	DA	3136	1/1	0.98	0.18	-	8,8,8,8	0
56	MG	DA	3308	1/1	0.86	0.13	-	46,46,46,46	0
56	MG	AA	1840	1/1	0.99	0.24	-	26,26,26,26	0
56	MG	CQ	201	1/1	0.91	0.35	-	3,3,3,3	0
56	MG	BA	3738	1/1	0.76	0.94	-	57,57,57,57	0
56	MG	BA	3825	1/1	0.88	0.29	-	45,45,45,45	0
56	MG	BA	3680	1/1	0.71	0.16	-	60,60,60,60	0
56	MG	DA	3252	1/1	0.95	0.38	-	23,23,23,23	0
56	MG	BA	3222	1/1	0.74	0.34	-	39,39,39,39	0
56	MG	BA	3518	1/1	0.82	0.29	-	58,58,58,58	0
56	MG	CK	202	1/1	0.76	0.21	-	91,91,91,91	0
56	MG	AF	201	1/1	0.84	0.11	-	87,87,87,87	0
56	MG	BA	3760	1/1	0.91	0.36	-	49,49,49,49	0
56	MG	BA	3614	1/1	0.76	0.21	-	56,56,56,56	0
56	MG	BA	3402	1/1	0.94	0.09	-	49,49,49,49	0
56	MG	BA	3506	1/1	0.68	0.25	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1911	1/1	0.87	0.11	-	63,63,63,63	0
56	MG	BA	3287	1/1	0.92	0.23	-	27,27,27,27	0
56	MG	DA	3390	1/1	0.85	0.13	-	73,73,73,73	0
56	MG	AY	102	1/1	0.92	0.17	-	58,58,58,58	0
56	MG	AA	1948	1/1	0.85	0.12	-	56,56,56,56	0
56	MG	DA	3078	1/1	0.95	0.30	-	4,4,4,4	0
56	MG	BA	3367	1/1	0.56	0.32	-	53,53,53,53	0
56	MG	CA	1603	1/1	0.97	0.21	-	4,4,4,4	0
56	MG	BA	3547	1/1	0.96	0.22	-	16,16,16,16	0
56	MG	AA	2008	1/1	0.94	0.25	-	49,49,49,49	0
56	MG	AA	1687	1/1	0.92	0.12	-	47,47,47,47	0
56	MG	BA	3922	1/1	0.88	0.11	-	56,56,56,56	0
56	MG	DA	3200	1/1	0.91	0.44	-	3,3,3,3	0
56	MG	BA	3564	1/1	0.93	0.17	-	54,54,54,54	0
56	MG	AM	203	1/1	0.92	0.30	-	47,47,47,47	0
56	MG	BA	3281	1/1	0.91	0.18	-	61,61,61,61	0
56	MG	CA	1681	1/1	0.91	0.26	-	3,3,3,3	0
56	MG	BA	3142	1/1	0.98	0.16	-	24,24,24,24	0
56	MG	BA	3891	1/1	0.76	0.32	-	58,58,58,58	0
56	MG	B2	102	1/1	0.80	0.52	-	62,62,62,62	0
56	MG	AA	1612	1/1	0.83	0.42	-	68,68,68,68	0
56	MG	CA	1659	1/1	0.94	0.22	-	3,3,3,3	0
56	MG	AA	1710	1/1	0.92	0.23	-	40,40,40,40	0
56	MG	BA	3296	1/1	0.69	0.43	-	68,68,68,68	0
56	MG	BA	3875	1/1	0.94	0.10	-	27,27,27,27	0
56	MG	DA	3387	1/1	0.86	0.12	-	77,77,77,77	0
56	MG	DA	3165	1/1	0.94	0.23	-	4,4,4,4	0
56	MG	BA	3163	1/1	0.81	0.30	-	91,91,91,91	0
56	MG	AA	1847	1/1	0.85	0.18	-	30,30,30,30	0
56	MG	AA	1964	1/1	0.66	0.40	-	79,79,79,79	0
56	MG	BA	3028	1/1	0.91	0.34	-	39,39,39,39	0
56	MG	BA	3524	1/1	0.74	0.08	-	44,44,44,44	0
56	MG	AA	1877	1/1	0.98	0.19	-	24,24,24,24	0
56	MG	BA	3649	1/1	0.96	0.33	-	30,30,30,30	0
56	MG	BA	3449	1/1	0.80	0.76	-	73,73,73,73	0
56	MG	BA	3876	1/1	0.73	0.45	-	88,88,88,88	0
56	MG	BA	3420	1/1	0.93	0.25	-	19,19,19,19	0
56	MG	BA	3139	1/1	0.92	0.35	-	59,59,59,59	0
56	MG	BA	3902	1/1	0.92	0.21	-	66,66,66,66	0
56	MG	CA	1719	1/1	0.91	0.22	-	60,60,60,60	0
56	MG	DA	3412	1/1	0.98	0.25	-	3,3,3,3	0
56	MG	BA	3485	1/1	0.87	0.15	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1955	1/1	0.79	0.49	-	82,82,82,82	0
56	MG	BA	3466	1/1	0.86	0.30	-	67,67,67,67	0
56	MG	AA	1653	1/1	0.49	0.43	-	95,95,95,95	0
56	MG	BA	3696	1/1	0.93	0.32	-	69,69,69,69	0
56	MG	CA	1693	1/1	0.97	0.18	-	58,58,58,58	0
56	MG	AA	2007	1/1	0.93	0.24	-	23,23,23,23	0
56	MG	AA	1896	1/1	0.96	0.14	-	26,26,26,26	0
56	MG	AA	1844	1/1	0.90	0.63	-	101,101,101,101	0
56	MG	DQ	202	1/1	0.93	0.31	-	3,3,3,3	0
56	MG	BA	3100	1/1	0.80	0.17	-	57,57,57,57	0
56	MG	DA	3025	1/1	0.98	0.26	-	3,3,3,3	0
56	MG	AA	1891	1/1	0.94	0.14	-	61,61,61,61	0
56	MG	AA	1769	1/1	0.72	0.67	-	87,87,87,87	0
56	MG	AA	1757	1/1	0.92	0.13	-	60,60,60,60	0
56	MG	BA	3271	1/1	0.96	0.19	-	57,57,57,57	0
56	MG	BA	3345	1/1	0.86	0.18	-	42,42,42,42	0
56	MG	AZ	112	1/1	0.91	0.10	-	46,46,46,46	0
56	MG	AA	1676	1/1	0.92	0.09	-	66,66,66,66	0
56	MG	DA	3209	1/1	0.98	0.33	-	3,3,3,3	0
56	MG	DA	3329	1/1	0.97	0.17	-	10,10,10,10	0
56	MG	DA	3357	1/1	0.98	0.22	-	3,3,3,3	0
56	MG	CZ	102	1/1	0.92	0.07	-	51,51,51,51	0
56	MG	BA	3288	1/1	0.92	0.19	-	43,43,43,43	0
56	MG	DA	3351	1/1	0.97	0.26	-	40,40,40,40	0
56	MG	DA	3279	1/1	0.92	0.40	-	30,30,30,30	0
56	MG	BA	3620	1/1	0.87	0.23	-	53,53,53,53	0
56	MG	CA	1624	1/1	0.95	0.23	-	3,3,3,3	0
56	MG	AA	1985	1/1	0.86	0.17	-	52,52,52,52	0
56	MG	BY	203	1/1	0.95	0.18	-	58,58,58,58	0
56	MG	AZ	115	1/1	0.90	0.09	-	39,39,39,39	0
56	MG	BA	3262	1/1	0.94	0.25	-	7,7,7,7	0
56	MG	AZ	106	1/1	0.58	0.46	-	93,93,93,93	0
56	MG	AX	402	1/1	0.89	0.08	-	42,42,42,42	0
56	MG	DA	3113	1/1	0.77	0.23	-	85,85,85,85	0
56	MG	BA	3209	1/1	0.80	0.30	-	54,54,54,54	0
56	MG	AA	1882	1/1	0.81	0.32	-	53,53,53,53	0
56	MG	BA	3056	1/1	0.94	0.21	-	66,66,66,66	0
56	MG	BB	212	1/1	0.65	0.17	-	82,82,82,82	0
56	MG	DA	3267	1/1	0.97	0.17	-	3,3,3,3	0
56	MG	DA	3274	1/1	0.95	0.44	-	3,3,3,3	0
56	MG	BA	3312	1/1	0.95	0.17	-	36,36,36,36	0
56	MG	BA	3255	1/1	0.86	0.15	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3839	1/1	0.73	0.38	-	60,60,60,60	0
56	MG	AA	1866	1/1	0.94	0.10	-	26,26,26,26	0
56	MG	DA	3251	1/1	0.80	0.28	-	51,51,51,51	0
56	MG	CA	1739	1/1	0.96	0.35	-	3,3,3,3	0
56	MG	BA	3519	1/1	0.85	0.15	-	82,82,82,82	0
56	MG	BA	3752	1/1	0.85	0.78	-	71,71,71,71	0
56	MG	BA	3501	1/1	0.86	0.12	-	58,58,58,58	0
56	MG	DA	3003	1/1	0.94	0.21	-	4,4,4,4	0
56	MG	AA	1826	1/1	0.92	0.12	-	46,46,46,46	0
56	MG	AA	2024	1/1	0.87	0.23	-	53,53,53,53	0
56	MG	DA	3241	1/1	0.89	0.14	-	73,73,73,73	0
56	MG	BA	3010	1/1	0.83	0.97	-	72,72,72,72	0
56	MG	AA	1910	1/1	0.89	0.08	-	88,88,88,88	0
56	MG	CA	1627	1/1	0.97	0.29	-	3,3,3,3	0
56	MG	BD	5006	1/1	0.89	0.14	-	11,11,11,11	0
56	MG	BA	3114	1/1	0.78	0.15	-	63,63,63,63	0
56	MG	DA	3408	1/1	0.96	0.27	-	4,4,4,4	0
56	MG	CA	1640	1/1	0.80	0.22	-	4,4,4,4	0
56	MG	BA	3094	1/1	0.94	0.09	-	76,76,76,76	0
56	MG	DA	3383	1/1	0.81	1.03	-	71,71,71,71	0
56	MG	BP	202	1/1	0.95	0.12	-	24,24,24,24	0
56	MG	BA	3903	1/1	0.94	0.16	-	71,71,71,71	0
56	MG	BA	3899	1/1	0.40	1.00	-	73,73,73,73	0
56	MG	AA	1790	1/1	0.34	0.15	-	97,97,97,97	0
56	MG	CA	1782	1/1	0.98	0.17	-	3,3,3,3	0
56	MG	BO	201	1/1	0.79	0.26	-	62,62,62,62	0
56	MG	DA	3459	1/1	0.98	0.40	-	4,4,4,4	0
56	MG	DA	3015	1/1	0.96	0.08	-	6,6,6,6	0
56	MG	BA	3331	1/1	0.82	0.06	-	74,74,74,74	0
56	MG	CA	1751	1/1	0.95	0.27	-	3,3,3,3	0
56	MG	BA	3386	1/1	0.92	0.14	-	79,79,79,79	0
56	MG	DA	3392	1/1	0.94	0.18	-	38,38,38,38	0
56	MG	CA	1753	1/1	0.95	0.19	-	3,3,3,3	0
56	MG	BA	3775	1/1	0.93	0.09	-	36,36,36,36	0
56	MG	CA	1625	1/1	0.96	0.33	-	3,3,3,3	0
56	MG	BA	3448	1/1	0.92	0.25	-	21,21,21,21	0
56	MG	BA	3250	1/1	0.76	0.22	-	81,81,81,81	0
56	MG	DA	3189	1/1	0.90	0.16	-	5,5,5,5	0
56	MG	B8	102	1/1	0.94	0.16	-	57,57,57,57	0
56	MG	BA	3545	1/1	0.93	0.12	-	23,23,23,23	0
56	MG	DA	3343	1/1	0.99	0.34	-	3,3,3,3	0
56	MG	BA	3318	1/1	0.97	0.07	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3487	1/1	0.97	0.30	-	3,3,3,3	0
56	MG	BA	3496	1/1	0.68	0.23	-	63,63,63,63	0
56	MG	DA	3364	1/1	0.97	0.20	-	3,3,3,3	0
56	MG	DA	3175	1/1	0.96	0.27	-	3,3,3,3	0
56	MG	BA	3091	1/1	0.91	0.17	-	37,37,37,37	0
56	MG	BA	3490	1/1	0.88	0.24	-	75,75,75,75	0
56	MG	DA	3178	1/1	0.94	0.20	-	4,4,4,4	0
56	MG	B1	104	1/1	0.95	0.12	-	38,38,38,38	0
56	MG	AA	1692	1/1	0.89	0.49	-	79,79,79,79	0
56	MG	BA	3165	1/1	0.92	0.28	-	21,21,21,21	0
56	MG	BA	3031	1/1	0.73	0.39	-	74,74,74,74	0
56	MG	CA	1694	1/1	0.77	0.12	-	60,60,60,60	0
56	MG	BA	3152	1/1	0.86	0.39	-	49,49,49,49	0
56	MG	AA	1759	1/1	0.97	0.26	-	15,15,15,15	0
56	MG	BA	3380	1/1	0.95	0.07	-	43,43,43,43	0
56	MG	DA	3235	1/1	0.87	0.10	-	24,24,24,24	0
56	MG	BA	3828	1/1	0.87	0.23	-	46,46,46,46	0
56	MG	AY	113	1/1	0.72	0.85	-	89,89,89,89	0
56	MG	BA	3914	1/1	0.77	0.16	-	47,47,47,47	0
56	MG	BA	3213	1/1	0.94	0.27	-	43,43,43,43	0
56	MG	AA	1736	1/1	0.95	0.13	-	63,63,63,63	0
56	MG	BA	3247	1/1	0.87	0.34	-	42,42,42,42	0
56	MG	AX	401	1/1	0.91	0.12	-	74,74,74,74	0
56	MG	CA	1682	1/1	0.85	0.18	-	52,52,52,52	0
56	MG	BA	3187	1/1	0.91	0.25	-	54,54,54,54	0
56	MG	DA	3150	1/1	0.95	0.15	-	4,4,4,4	0
56	MG	DA	3115	1/1	0.91	0.23	-	62,62,62,62	0
56	MG	AA	1633	1/1	0.83	0.19	-	77,77,77,77	0
56	MG	BA	3001	1/1	0.96	0.19	-	38,38,38,38	0
56	MG	AA	1708	1/1	0.86	0.33	-	33,33,33,33	0
56	MG	BA	3237	1/1	0.95	0.11	-	28,28,28,28	0
56	MG	AA	1864	1/1	0.78	0.12	-	71,71,71,71	0
56	MG	DA	3082	1/1	0.94	0.36	-	3,3,3,3	0
56	MG	B6	102	1/1	0.89	0.09	-	57,57,57,57	0
56	MG	BA	3850	1/1	0.81	0.31	-	54,54,54,54	0
56	MG	DA	3254	1/1	0.94	0.15	-	42,42,42,42	0
56	MG	AA	2002	1/1	0.89	0.15	-	47,47,47,47	0
56	MG	DA	3041	1/1	0.89	0.07	-	52,52,52,52	0
56	MG	BA	3893	1/1	0.95	0.05	-	62,62,62,62	0
56	MG	BA	3896	1/1	0.89	0.18	-	58,58,58,58	0
56	MG	AA	1854	1/1	0.87	0.13	-	39,39,39,39	0
56	MG	DA	3135	1/1	0.96	0.18	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BN	203	1/1	0.80	0.31	-	72,72,72,72	0
56	MG	BA	3118	1/1	0.98	0.09	-	23,23,23,23	0
56	MG	DA	3434	1/1	0.96	0.18	-	3,3,3,3	0
56	MG	DA	3054	1/1	0.94	0.12	-	5,5,5,5	0
56	MG	BA	3788	1/1	0.90	0.19	-	69,69,69,69	0
56	MG	DA	3480	1/1	0.97	0.27	-	3,3,3,3	0
56	MG	CY	107	1/1	0.76	0.27	-	60,60,60,60	0
56	MG	DA	3160	1/1	0.98	0.33	-	3,3,3,3	0
56	MG	DA	3152	1/1	0.95	0.12	-	5,5,5,5	0
56	MG	AA	2016	1/1	0.93	0.28	-	43,43,43,43	0
56	MG	DA	3238	1/1	0.86	0.14	-	62,62,62,62	0
56	MG	BA	3020	1/1	0.63	0.38	-	73,73,73,73	0
56	MG	DA	3137	1/1	0.97	0.64	-	3,3,3,3	0
56	MG	BA	3609	1/1	0.74	0.38	-	39,39,39,39	0
56	MG	AA	1608	1/1	0.95	0.11	-	43,43,43,43	0
56	MG	AA	1923	1/1	0.76	0.35	-	79,79,79,79	0
56	MG	BA	3369	1/1	0.91	0.07	-	60,60,60,60	0
56	MG	BA	3745	1/1	0.73	0.72	-	70,70,70,70	0
56	MG	AA	1938	1/1	0.48	0.36	-	58,58,58,58	0
56	MG	DA	3213	1/1	0.97	0.12	-	4,4,4,4	0
56	MG	AA	1846	1/1	0.80	0.38	-	68,68,68,68	0
56	MG	CS	101	1/1	0.98	0.26	-	3,3,3,3	0
56	MG	DA	3438	1/1	0.97	0.21	-	6,6,6,6	0
56	MG	BA	3576	1/1	0.91	0.14	-	43,43,43,43	0
56	MG	DA	3263	1/1	0.97	0.27	-	4,4,4,4	0
56	MG	CA	1781	1/1	0.69	0.21	-	59,59,59,59	0
56	MG	AY	116	1/1	0.96	0.31	-	40,40,40,40	0
56	MG	CY	109	1/1	0.95	0.23	-	3,3,3,3	0
56	MG	AA	1733	1/1	0.96	0.13	-	38,38,38,38	0
56	MG	BA	3057	1/1	0.71	0.16	-	80,80,80,80	0
56	MG	BA	3313	1/1	0.97	0.07	-	33,33,33,33	0
56	MG	DA	3375	1/1	0.87	0.13	-	88,88,88,88	0
56	MG	BB	233	1/1	0.89	0.10	-	48,48,48,48	0
56	MG	BA	3199	1/1	0.79	0.26	-	65,65,65,65	0
56	MG	DA	3021	1/1	0.94	0.20	-	4,4,4,4	0
56	MG	AA	1626	1/1	0.98	0.26	-	20,20,20,20	0
56	MG	BA	3570	1/1	0.89	0.20	-	62,62,62,62	0
56	MG	DA	3448	1/1	0.96	0.12	-	21,21,21,21	0
56	MG	BA	3489	1/1	0.95	0.10	-	32,32,32,32	0
56	MG	BA	3655	1/1	0.90	0.18	-	38,38,38,38	0
56	MG	BA	3228	1/1	0.89	0.17	-	31,31,31,31	0
56	MG	DA	3185	1/1	0.96	0.24	-	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3358	1/1	0.98	0.18	-	17,17,17,17	0
56	MG	BB	209	1/1	0.94	0.14	-	63,63,63,63	0
56	MG	AA	1831	1/1	0.96	0.15	-	68,68,68,68	0
56	MG	BA	3200	1/1	0.87	0.72	-	76,76,76,76	0
56	MG	BA	3346	1/1	0.85	0.32	-	65,65,65,65	0
56	MG	BA	3592	1/1	0.93	0.20	-	47,47,47,47	0
56	MG	CA	1616	1/1	0.97	0.08	-	5,5,5,5	0
56	MG	BA	3757	1/1	0.74	0.43	-	76,76,76,76	0
56	MG	DA	3197	1/1	0.99	0.18	-	3,3,3,3	0
56	MG	AA	1644	1/1	0.97	0.17	-	54,54,54,54	0
56	MG	BA	3766	1/1	0.95	0.21	-	31,31,31,31	0
56	MG	AA	1617	1/1	0.89	0.15	-	48,48,48,48	0
56	MG	AY	122	1/1	0.89	0.16	-	58,58,58,58	0
56	MG	B5	102	1/1	0.89	0.10	-	49,49,49,49	0
56	MG	CF	203	1/1	0.84	0.28	-	51,51,51,51	0
56	MG	DA	3376	1/1	0.80	0.10	-	75,75,75,75	0
56	MG	BA	3223	1/1	0.95	0.12	-	36,36,36,36	0
56	MG	BA	3482	1/1	0.84	0.28	-	63,63,63,63	0
56	MG	DA	3381	1/1	0.91	0.23	-	3,3,3,3	0
56	MG	BA	3123	1/1	0.86	0.07	-	55,55,55,55	0
56	MG	BB	207	1/1	0.60	0.30	-	84,84,84,84	0
56	MG	BA	3698	1/1	0.72	0.19	-	94,94,94,94	0
56	MG	DA	3096	1/1	0.95	0.32	-	3,3,3,3	0
56	MG	CA	1801	1/1	0.92	0.24	-	3,3,3,3	0
56	MG	AA	1773	1/1	0.80	0.33	-	46,46,46,46	0
56	MG	BA	3790	1/1	0.77	0.23	-	86,86,86,86	0
56	MG	DA	3199	1/1	0.81	0.28	-	59,59,59,59	0
56	MG	BA	3415	1/1	0.90	0.18	-	65,65,65,65	0
56	MG	BA	3469	1/1	0.90	0.20	-	46,46,46,46	0
56	MG	DA	3446	1/1	0.97	0.35	-	3,3,3,3	0
56	MG	BA	3837	1/1	0.86	0.48	-	71,71,71,71	0
56	MG	DA	3038	1/1	0.94	0.20	-	4,4,4,4	0
56	MG	B0	103	1/1	0.95	0.12	-	30,30,30,30	0
56	MG	BB	231	1/1	0.93	0.22	-	54,54,54,54	0
56	MG	BA	3866	1/1	0.88	0.19	-	25,25,25,25	0
56	MG	DA	3354	1/1	0.92	0.09	-	43,43,43,43	0
56	MG	AA	1863	1/1	0.82	0.11	-	57,57,57,57	0
56	MG	AA	1729	1/1	0.89	0.34	-	60,60,60,60	0
56	MG	CA	1618	1/1	0.94	0.25	-	4,4,4,4	0
56	MG	BA	3265	1/1	0.77	0.24	-	42,42,42,42	0
56	MG	BA	3556	1/1	0.86	0.30	-	45,45,45,45	0
56	MG	AA	1817	1/1	0.93	0.24	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3651	1/1	0.81	0.32	-	37,37,37,37	0
56	MG	BA	3092	1/1	0.86	0.41	-	73,73,73,73	0
56	MG	BA	3756	1/1	0.88	0.38	-	49,49,49,49	0
56	MG	BA	3921	1/1	0.93	0.19	-	53,53,53,53	0
56	MG	BA	3047	1/1	0.93	0.19	-	54,54,54,54	0
56	MG	CA	1604	1/1	0.97	0.27	-	3,3,3,3	0
56	MG	AA	1693	1/1	0.86	0.21	-	79,79,79,79	0
56	MG	BA	3105	1/1	0.95	0.56	-	30,30,30,30	0
56	MG	DA	3304	1/1	0.63	0.33	-	76,76,76,76	0
56	MG	AA	2028	1/1	0.96	0.18	-	65,65,65,65	0
56	MG	BA	3038	1/1	0.87	0.14	-	41,41,41,41	0
56	MG	BR	202	1/1	0.96	0.26	-	89,89,89,89	0
56	MG	BA	3135	1/1	0.88	0.24	-	43,43,43,43	0
56	MG	BA	3720	1/1	0.92	0.16	-	28,28,28,28	0
56	MG	AX	403	1/1	0.89	0.10	-	68,68,68,68	0
56	MG	CA	1811	1/1	0.72	0.37	-	79,79,79,79	0
56	MG	AA	1861	1/1	0.96	0.05	-	47,47,47,47	0
56	MG	BV	201	1/1	0.90	0.13	-	53,53,53,53	0
56	MG	AA	1756	1/1	0.94	0.25	-	41,41,41,41	0
56	MG	DA	3431	1/1	0.97	0.23	-	3,3,3,3	0
56	MG	BS	203	1/1	0.89	0.20	-	52,52,52,52	0
56	MG	B2	101	1/1	0.57	0.36	-	76,76,76,76	0
56	MG	BI	202	1/1	0.95	0.05	-	53,53,53,53	0
56	MG	BA	3050	1/1	0.83	0.14	-	44,44,44,44	0
56	MG	BA	3273	1/1	0.73	0.61	-	74,74,74,74	0
56	MG	DA	3138	1/1	0.91	0.41	-	3,3,3,3	0
56	MG	CA	1651	1/1	0.95	0.22	-	28,28,28,28	0
56	MG	CA	1818	1/1	0.87	0.43	-	59,59,59,59	0
56	MG	BA	3690	1/1	0.81	0.31	-	80,80,80,80	0
56	MG	AA	1886	1/1	0.92	0.21	-	50,50,50,50	0
56	MG	DB	202	1/1	0.95	0.30	-	3,3,3,3	0
56	MG	CA	1636	1/1	0.98	0.36	-	3,3,3,3	0
56	MG	DA	3167	1/1	0.96	0.11	-	6,6,6,6	0
56	MG	BA	3012	1/1	0.97	0.32	-	75,75,75,75	0
56	MG	CF	201	1/1	0.94	0.14	-	40,40,40,40	0
56	MG	DA	3225	1/1	0.95	0.18	-	4,4,4,4	0
56	MG	DA	3334	1/1	0.89	0.49	-	3,3,3,3	0
56	MG	BA	3834	1/1	0.99	0.34	-	12,12,12,12	0
56	MG	BA	3623	1/1	0.35	0.22	-	103,103,103,103	0
56	MG	BA	3154	1/1	0.82	0.17	-	41,41,41,41	0
56	MG	DA	3037	1/1	0.96	0.27	-	4,4,4,4	0
56	MG	DA	3157	1/1	0.95	0.35	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3846	1/1	0.93	0.16	-	55,55,55,55	0
56	MG	BA	3205	1/1	0.84	0.56	-	55,55,55,55	0
56	MG	BA	3600	1/1	0.66	0.44	-	47,47,47,47	0
56	MG	DA	3464	1/1	0.98	0.31	-	3,3,3,3	0
56	MG	BA	3731	1/1	0.81	0.29	-	53,53,53,53	0
56	MG	BQ	203	1/1	0.87	0.19	-	46,46,46,46	0
56	MG	BA	3365	1/1	0.90	0.37	-	53,53,53,53	0
56	MG	AX	414	1/1	0.75	0.36	-	97,97,97,97	0
56	MG	AA	1907	1/1	0.90	0.26	-	76,76,76,76	0
56	MG	BA	3919	1/1	0.90	0.27	-	49,49,49,49	0
56	MG	AA	1717	1/1	0.89	0.23	-	75,75,75,75	0
56	MG	BA	3459	1/1	0.96	0.18	-	18,18,18,18	0
56	MG	BA	3498	1/1	0.94	0.34	-	45,45,45,45	0
56	MG	BA	3093	1/1	0.37	0.61	-	80,80,80,80	0
56	MG	CA	1777	1/1	0.98	0.22	-	4,4,4,4	0
56	MG	AA	1637	1/1	0.90	0.08	-	54,54,54,54	0
56	MG	BA	3750	1/1	0.95	0.16	-	45,45,45,45	0
56	MG	BA	3669	1/1	0.94	0.34	-	52,52,52,52	0
56	MG	BA	3041	1/1	0.89	0.37	-	98,98,98,98	0
56	MG	DP	201	1/1	0.94	0.35	-	3,3,3,3	0
56	MG	BA	3495	1/1	0.91	0.09	-	48,48,48,48	0
56	MG	DA	3139	1/1	0.92	0.39	-	3,3,3,3	0
56	MG	AA	1822	1/1	0.88	0.20	-	40,40,40,40	0
56	MG	CA	1721	1/1	0.90	0.32	-	49,49,49,49	0
56	MG	AA	1603	1/1	0.88	0.30	-	91,91,91,91	0
56	MG	AA	1766	1/1	0.86	0.37	-	33,33,33,33	0
56	MG	DA	3432	1/1	0.91	0.32	-	3,3,3,3	0
56	MG	AY	101	1/1	0.75	0.44	-	68,68,68,68	0
56	MG	DA	3091	1/1	0.96	0.49	-	3,3,3,3	0
56	MG	DA	3182	1/1	0.90	0.25	-	3,3,3,3	0
56	MG	AA	1876	1/1	0.86	0.20	-	69,69,69,69	0
56	MG	AA	1883	1/1	0.96	0.20	-	42,42,42,42	0
56	MG	CA	1740	1/1	0.93	0.37	-	41,41,41,41	0
56	MG	BA	3710	1/1	0.91	0.19	-	52,52,52,52	0
56	MG	DA	3246	1/1	0.92	0.25	-	3,3,3,3	0
56	MG	DB	203	1/1	0.93	0.26	-	3,3,3,3	0
56	MG	AA	1833	1/1	0.81	0.13	-	60,60,60,60	0
56	MG	DA	3356	1/1	0.85	0.08	-	56,56,56,56	0
56	MG	DA	3275	1/1	0.99	0.29	-	4,4,4,4	0
56	MG	DA	3247	1/1	0.92	0.27	-	3,3,3,3	0
56	MG	DA	3105	1/1	0.84	0.21	-	55,55,55,55	0
56	MG	AA	1712	1/1	0.92	0.22	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3277	1/1	0.98	0.34	-	3,3,3,3	0
56	MG	AA	1747	1/1	0.97	0.10	-	41,41,41,41	0
56	MG	BA	3179	1/1	0.93	0.12	-	32,32,32,32	0
56	MG	DA	3404	1/1	0.98	0.14	-	5,5,5,5	0
56	MG	AA	1705	1/1	0.96	0.39	-	50,50,50,50	0
56	MG	B5	101	1/1	0.84	0.28	-	63,63,63,63	0
56	MG	DB	209	1/1	0.96	0.34	-	3,3,3,3	0
56	MG	BA	3838	1/1	0.93	0.13	-	29,29,29,29	0
56	MG	BA	3172	1/1	0.81	0.16	-	54,54,54,54	0
56	MG	DA	3326	1/1	0.89	0.17	-	4,4,4,4	0
56	MG	DA	3158	1/1	0.96	0.32	-	3,3,3,3	0
56	MG	BA	3764	1/1	0.97	0.15	-	45,45,45,45	0
56	MG	BB	234	1/1	0.95	0.11	-	23,23,23,23	0
56	MG	CA	1768	1/1	0.91	0.22	-	46,46,46,46	0
56	MG	DA	3230	1/1	0.80	0.13	-	58,58,58,58	0
56	MG	CA	1718	1/1	0.82	0.21	-	41,41,41,41	0
56	MG	DA	3052	1/1	0.93	0.31	-	3,3,3,3	0
56	MG	DA	3192	1/1	0.95	0.39	-	3,3,3,3	0
56	MG	BA	3534	1/1	0.81	0.30	-	61,61,61,61	0
56	MG	DA	3282	1/1	0.84	0.49	-	72,72,72,72	0
56	MG	AA	1898	1/1	0.95	0.11	-	27,27,27,27	0
56	MG	DA	3403	1/1	0.81	0.22	-	64,64,64,64	0
56	MG	DA	3360	1/1	0.87	0.28	-	56,56,56,56	0
56	MG	CA	1709	1/1	0.91	0.13	-	55,55,55,55	0
56	MG	BA	3375	1/1	0.74	0.19	-	76,76,76,76	0
56	MG	BA	3761	1/1	0.88	0.15	-	29,29,29,29	0
56	MG	AO	101	1/1	0.97	0.21	-	33,33,33,33	0
56	MG	AY	120	1/1	0.85	0.10	-	40,40,40,40	0
56	MG	DA	3022	1/1	0.93	0.21	-	3,3,3,3	0
56	MG	BA	3045	1/1	0.86	0.56	-	56,56,56,56	0
56	MG	BA	3857	1/1	0.95	0.23	-	71,71,71,71	0
56	MG	AA	1762	1/1	0.90	0.12	-	43,43,43,43	0
56	MG	CA	1765	1/1	0.93	0.35	-	3,3,3,3	0
56	MG	BB	211	1/1	0.70	0.17	-	81,81,81,81	0
56	MG	AA	1959	1/1	0.96	0.11	-	54,54,54,54	0
56	MG	BH	204	1/1	0.84	0.14	-	77,77,77,77	0
56	MG	CA	1763	1/1	0.74	1.37	-	77,77,77,77	0
56	MG	BB	214	1/1	0.84	0.27	-	55,55,55,55	0
56	MG	BA	3249	1/1	0.95	0.29	-	58,58,58,58	0
56	MG	BA	3303	1/1	0.98	0.26	-	12,12,12,12	0
56	MG	DD	5002	1/1	0.92	0.14	-	33,33,33,33	0
56	MG	BA	3278	1/1	0.73	0.28	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3523	1/1	0.91	0.08	-	62,62,62,62	0
56	MG	DA	3195	1/1	0.91	0.36	-	3,3,3,3	0
56	MG	BA	3400	1/1	0.55	0.09	-	101,101,101,101	0
56	MG	BA	3458	1/1	0.86	0.34	-	50,50,50,50	0
56	MG	BA	3528	1/1	0.84	0.27	-	60,60,60,60	0
56	MG	BN	202	1/1	0.81	0.20	-	46,46,46,46	0
56	MG	CA	1632	1/1	0.95	0.41	-	3,3,3,3	0
56	MG	CY	102	1/1	0.92	0.33	-	3,3,3,3	0
56	MG	DA	3191	1/1	0.92	0.27	-	4,4,4,4	0
56	MG	CA	1738	1/1	0.47	0.31	-	64,64,64,64	0
56	MG	DA	3144	1/1	0.95	0.25	-	4,4,4,4	0
56	MG	AA	2021	1/1	0.85	0.10	-	43,43,43,43	0
56	MG	BA	3116	1/1	0.82	0.31	-	44,44,44,44	0
56	MG	DA	3166	1/1	0.97	0.28	-	3,3,3,3	0
56	MG	BA	3806	1/1	0.91	0.44	-	29,29,29,29	0
56	MG	BA	3174	1/1	0.95	0.17	-	83,83,83,83	0
56	MG	BA	3227	1/1	0.89	0.16	-	46,46,46,46	0
56	MG	BH	202	1/1	0.87	0.16	-	56,56,56,56	0
56	MG	DA	3314	1/1	0.72	0.36	-	70,70,70,70	0
56	MG	AE	201	1/1	0.94	0.08	-	52,52,52,52	0
56	MG	BX	102	1/1	0.94	0.19	-	25,25,25,25	0
56	MG	AM	201	1/1	0.81	0.53	-	86,86,86,86	0
56	MG	CG	201	1/1	0.85	0.12	-	70,70,70,70	0
56	MG	CA	1815	1/1	0.78	0.27	-	63,63,63,63	0
56	MG	BA	3226	1/1	0.96	0.18	-	43,43,43,43	0
56	MG	CA	1805	1/1	0.97	0.23	-	3,3,3,3	0
56	MG	AY	106	1/1	0.95	0.10	-	58,58,58,58	0
56	MG	AA	1997	1/1	0.91	0.23	-	56,56,56,56	0
56	MG	BA	3371	1/1	0.92	0.16	-	53,53,53,53	0
56	MG	DA	3411	1/1	0.96	0.21	-	3,3,3,3	0
56	MG	AX	410	1/1	0.87	0.11	-	73,73,73,73	0
56	MG	BA	3454	1/1	0.55	0.32	-	63,63,63,63	0
56	MG	CA	1696	1/1	0.66	0.29	-	60,60,60,60	0
56	MG	BA	3076	1/1	0.82	0.46	-	51,51,51,51	0
56	MG	BA	3474	1/1	0.72	0.48	-	73,73,73,73	0
56	MG	CA	1726	1/1	0.92	0.09	-	37,37,37,37	0
56	MG	CA	1657	1/1	0.96	0.24	-	3,3,3,3	0
56	MG	BA	3671	1/1	0.98	0.11	-	57,57,57,57	0
56	MG	AA	1771	1/1	0.83	0.26	-	45,45,45,45	0
56	MG	BA	3341	1/1	0.86	0.28	-	70,70,70,70	0
56	MG	CA	1650	1/1	0.97	0.55	-	73,73,73,73	0
56	MG	BA	3208	1/1	0.90	0.09	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3561	1/1	0.89	0.29	-	75,75,75,75	0
56	MG	DI	201	1/1	0.84	0.12	-	38,38,38,38	0
56	MG	DA	3187	1/1	0.95	0.30	-	3,3,3,3	0
56	MG	BA	3827	1/1	0.92	0.21	-	48,48,48,48	0
56	MG	AA	1711	1/1	0.81	0.40	-	58,58,58,58	0
56	MG	DA	3237	1/1	0.88	0.20	-	51,51,51,51	0
56	MG	AA	1828	1/1	0.86	0.29	-	69,69,69,69	0
56	MG	AA	1669	1/1	0.94	0.17	-	58,58,58,58	0
56	MG	BA	3245	1/1	0.92	0.24	-	39,39,39,39	0
56	MG	DA	3229	1/1	0.95	0.21	-	3,3,3,3	0
56	MG	BA	3754	1/1	0.93	0.41	-	44,44,44,44	0
56	MG	CA	1662	1/1	0.97	0.19	-	4,4,4,4	0
56	MG	AA	1814	1/1	0.89	0.19	-	47,47,47,47	0
56	MG	BA	3536	1/1	0.84	0.32	-	70,70,70,70	0
56	MG	CO	101	1/1	0.90	0.22	-	33,33,33,33	0
56	MG	BW	201	1/1	0.63	0.41	-	80,80,80,80	0
56	MG	DA	3093	1/1	0.96	0.36	-	3,3,3,3	0
56	MG	AA	1735	1/1	0.91	0.10	-	44,44,44,44	0
56	MG	BA	3217	1/1	0.97	0.17	-	12,12,12,12	0
56	MG	BO	204	1/1	0.89	0.31	-	50,50,50,50	0
56	MG	BA	3246	1/1	0.91	0.33	-	60,60,60,60	0
56	MG	AA	1763	1/1	0.86	0.13	-	41,41,41,41	0
56	MG	DA	3242	1/1	0.93	0.34	-	3,3,3,3	0
56	MG	DA	3205	1/1	0.98	0.23	-	38,38,38,38	0
56	MG	CA	1700	1/1	0.97	0.09	-	12,12,12,12	0
56	MG	DA	3253	1/1	0.95	0.24	-	3,3,3,3	0
56	MG	BA	3141	1/1	0.95	0.14	-	68,68,68,68	0
56	MG	BA	3907	1/1	0.97	0.34	-	27,27,27,27	0
56	MG	BB	221	1/1	0.90	0.44	-	65,65,65,65	0
56	MG	AE	206	1/1	0.92	0.05	-	57,57,57,57	0
56	MG	DA	3222	1/1	0.93	0.20	-	41,41,41,41	0
56	MG	AM	202	1/1	0.93	0.07	-	58,58,58,58	0
56	MG	BA	3408	1/1	0.91	0.25	-	50,50,50,50	0
56	MG	DA	3057	1/1	0.99	0.29	-	3,3,3,3	0
56	MG	DA	3061	1/1	0.95	0.24	-	4,4,4,4	0
56	MG	CZ	109	1/1	0.81	0.10	-	95,95,95,95	0
56	MG	DA	3169	1/1	0.92	0.33	-	3,3,3,3	0
56	MG	B8	101	1/1	0.88	0.29	-	30,30,30,30	0
56	MG	BA	3381	1/1	0.86	0.20	-	48,48,48,48	0
56	MG	BV	203	1/1	0.95	0.04	-	52,52,52,52	0
56	MG	CA	1637	1/1	0.99	0.15	-	4,4,4,4	0
56	MG	DA	3240	1/1	0.93	0.19	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1726	1/1	0.94	0.22	-	53,53,53,53	0
56	MG	CA	1686	1/1	0.75	0.26	-	48,48,48,48	0
56	MG	DA	3355	1/1	0.91	0.08	-	56,56,56,56	0
56	MG	AA	1611	1/1	0.86	0.29	-	48,48,48,48	0
56	MG	DA	3143	1/1	0.95	0.28	-	3,3,3,3	0
56	MG	DA	3198	1/1	0.95	0.36	-	4,4,4,4	0
56	MG	AE	202	1/1	0.93	0.15	-	64,64,64,64	0
56	MG	BA	3083	1/1	0.88	0.28	-	71,71,71,71	0
56	MG	DA	3401	1/1	0.93	0.21	-	39,39,39,39	0
56	MG	AA	2019	1/1	0.94	0.32	-	70,70,70,70	0
56	MG	AA	1853	1/1	0.79	0.15	-	24,24,24,24	0
56	MG	DA	3063	1/1	0.97	0.31	-	3,3,3,3	0
56	MG	AA	1837	1/1	0.96	0.13	-	17,17,17,17	0
56	MG	CA	1800	1/1	0.95	0.41	-	3,3,3,3	0
56	MG	BA	3491	1/1	0.97	0.23	-	38,38,38,38	0
56	MG	BA	3160	1/1	0.87	0.17	-	54,54,54,54	0
56	MG	BA	3113	1/1	0.72	0.24	-	85,85,85,85	0
56	MG	BA	3772	1/1	0.95	0.10	-	48,48,48,48	0
56	MG	BA	3203	1/1	0.94	0.15	-	39,39,39,39	0
56	MG	AA	1695	1/1	0.91	0.18	-	52,52,52,52	0
56	MG	BA	3352	1/1	0.90	0.11	-	17,17,17,17	0
56	MG	BA	3638	1/1	0.86	0.21	-	48,48,48,48	0
56	MG	DA	3130	1/1	0.90	0.32	-	3,3,3,3	0
56	MG	DG	202	1/1	0.87	0.15	-	59,59,59,59	0
56	MG	DA	3079	1/1	0.96	0.39	-	3,3,3,3	0
56	MG	CA	1816	1/1	0.94	0.59	-	61,61,61,61	0
56	MG	DA	3220	1/1	0.96	0.27	-	21,21,21,21	0
56	MG	CZ	104	1/1	0.92	0.24	-	3,3,3,3	0
56	MG	AA	1701	1/1	0.97	0.10	-	29,29,29,29	0
56	MG	BA	3515	1/1	0.94	0.10	-	68,68,68,68	0
56	MG	DA	3437	1/1	0.91	0.53	-	3,3,3,3	0
56	MG	AA	1916	1/1	0.87	0.09	-	63,63,63,63	0
56	MG	BF	301	1/1	0.72	0.13	-	63,63,63,63	0
56	MG	DA	3114	1/1	0.72	0.30	-	83,83,83,83	0
56	MG	AA	1860	1/1	0.82	0.23	-	58,58,58,58	0
56	MG	BA	3803	1/1	0.97	0.14	-	32,32,32,32	0
56	MG	BA	3606	1/1	0.90	0.59	-	52,52,52,52	0
56	MG	DE	301	1/1	0.95	0.09	-	5,5,5,5	0
56	MG	BA	3906	1/1	0.84	0.24	-	67,67,67,67	0
56	MG	AA	1926	1/1	0.98	0.07	-	30,30,30,30	0
56	MG	DA	3323	1/1	0.88	0.50	-	3,3,3,3	0
56	MG	CA	1733	1/1	0.95	0.28	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1707	1/1	0.90	0.11	-	37,37,37,37	0
56	MG	BA	3129	1/1	0.96	0.19	-	48,48,48,48	0
56	MG	BA	3844	1/1	0.95	0.15	-	36,36,36,36	0
56	MG	BA	3117	1/1	0.53	0.54	-	63,63,63,63	0
56	MG	BA	3769	1/1	0.91	0.10	-	28,28,28,28	0
56	MG	AA	1680	1/1	0.91	0.46	-	51,51,51,51	0
56	MG	BA	3440	1/1	0.95	0.35	-	73,73,73,73	0
56	MG	AA	1805	1/1	0.98	0.05	-	22,22,22,22	0
56	MG	BA	3818	1/1	0.87	0.55	-	71,71,71,71	0
56	MG	BA	3475	1/1	0.93	0.09	-	22,22,22,22	0
56	MG	DA	3301	1/1	0.97	0.21	-	42,42,42,42	0
56	MG	BA	3601	1/1	0.91	0.18	-	30,30,30,30	0
56	MG	DA	3336	1/1	0.91	0.15	-	25,25,25,25	0
56	MG	AA	1721	1/1	0.94	0.11	-	44,44,44,44	0
56	MG	AA	1671	1/1	0.95	0.17	-	59,59,59,59	0
56	MG	DA	3473	1/1	0.96	0.17	-	3,3,3,3	0
56	MG	DA	3181	1/1	0.94	0.28	-	3,3,3,3	0
56	MG	BA	3098	1/1	0.97	0.09	-	27,27,27,27	0
56	MG	BA	3066	1/1	0.93	0.11	-	67,67,67,67	0
56	MG	BA	3693	1/1	0.86	0.14	-	62,62,62,62	0
56	MG	AA	1732	1/1	0.88	0.17	-	21,21,21,21	0
56	MG	BA	3692	1/1	0.83	0.39	-	52,52,52,52	0
56	MG	DA	3174	1/1	0.98	0.20	-	3,3,3,3	0
56	MG	BB	204	1/1	0.90	0.11	-	51,51,51,51	0
56	MG	BA	3774	1/1	0.96	0.24	-	42,42,42,42	0
56	MG	CA	1742	1/1	0.82	0.19	-	54,54,54,54	0
56	MG	AZ	104	1/1	0.90	0.11	-	61,61,61,61	0
56	MG	BA	3196	1/1	0.81	0.37	-	50,50,50,50	0
56	MG	AA	1604	1/1	0.97	0.21	-	43,43,43,43	0
56	MG	BA	3285	1/1	0.93	0.17	-	48,48,48,48	0
56	MG	BA	3854	1/1	0.97	0.45	-	60,60,60,60	0
56	MG	BA	3158	1/1	0.95	0.11	-	42,42,42,42	0
56	MG	AA	1767	1/1	0.86	0.11	-	45,45,45,45	0
56	MG	BA	3182	1/1	0.95	0.15	-	20,20,20,20	0
56	MG	BA	3216	1/1	0.94	0.21	-	54,54,54,54	0
56	MG	AV	5500	1/1	0.89	0.32	-	71,71,71,71	0
56	MG	DA	3173	1/1	0.98	0.21	-	3,3,3,3	0
56	MG	BI	204	1/1	0.95	0.22	-	32,32,32,32	0
56	MG	AA	1694	1/1	0.93	0.15	-	52,52,52,52	0
56	MG	BA	3071	1/1	0.91	0.23	-	35,35,35,35	0
56	MG	AA	1977	1/1	0.94	0.28	-	64,64,64,64	0
56	MG	AQ	201	1/1	0.96	0.08	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3127	1/1	0.95	0.35	-	3,3,3,3	0
56	MG	AY	110	1/1	0.88	0.15	-	31,31,31,31	0
56	MG	BA	3329	1/1	0.65	0.14	-	79,79,79,79	0
56	MG	CA	1766	1/1	0.91	0.09	-	64,64,64,64	0
56	MG	DA	3089	1/1	0.96	0.14	-	4,4,4,4	0
56	MG	DA	3258	1/1	0.99	0.10	-	6,6,6,6	0
56	MG	DA	3202	1/1	0.96	0.44	-	3,3,3,3	0
56	MG	AA	1899	1/1	0.70	0.35	-	59,59,59,59	0
56	MG	D8	101	1/1	0.91	0.35	-	3,3,3,3	0
56	MG	BA	3734	1/1	0.92	0.27	-	59,59,59,59	0
56	MG	BA	3017	1/1	0.93	0.12	-	52,52,52,52	0
56	MG	BA	3509	1/1	0.81	0.18	-	34,34,34,34	0
56	MG	AL	203	1/1	0.93	0.08	-	43,43,43,43	0
56	MG	AA	1901	1/1	0.94	0.25	-	88,88,88,88	0
56	MG	AA	1966	1/1	0.89	0.14	-	29,29,29,29	0
56	MG	BA	3802	1/1	0.87	0.17	-	47,47,47,47	0
56	MG	BA	3003	1/1	0.88	0.10	-	36,36,36,36	0
56	MG	AA	1857	1/1	0.95	0.17	-	43,43,43,43	0
56	MG	CA	1605	1/1	0.99	0.33	-	3,3,3,3	0
56	MG	BA	3025	1/1	0.91	0.22	-	58,58,58,58	0
56	MG	AY	111	1/1	0.86	0.18	-	60,60,60,60	0
56	MG	BA	3566	1/1	0.94	0.13	-	43,43,43,43	0
56	MG	BA	3822	1/1	0.96	0.32	-	34,34,34,34	0
56	MG	AA	1815	1/1	0.92	0.25	-	43,43,43,43	0
56	MG	BA	3239	1/1	0.64	0.48	-	69,69,69,69	0
56	MG	BA	3442	1/1	0.86	0.16	-	46,46,46,46	0
56	MG	CA	1711	1/1	0.77	0.82	-	57,57,57,57	0
56	MG	BA	3186	1/1	0.94	0.11	-	67,67,67,67	0
56	MG	AY	119	1/1	0.95	0.09	-	50,50,50,50	0
56	MG	AA	1715	1/1	0.79	0.25	-	50,50,50,50	0
56	MG	DA	3064	1/1	0.98	0.33	-	4,4,4,4	0
56	MG	BF	306	1/1	0.86	0.17	-	47,47,47,47	0
56	MG	BA	3060	1/1	0.88	0.07	-	83,83,83,83	0
56	MG	BA	3793	1/1	0.89	0.14	-	54,54,54,54	0
56	MG	BA	3394	1/1	0.92	0.18	-	41,41,41,41	0
56	MG	BA	3384	1/1	0.83	0.18	-	60,60,60,60	0
56	MG	BA	3188	1/1	0.94	0.10	-	53,53,53,53	0
56	MG	DA	3011	1/1	0.97	0.22	-	3,3,3,3	0
56	MG	BA	3737	1/1	0.90	0.15	-	50,50,50,50	0
56	MG	DA	3020	1/1	0.99	0.32	-	3,3,3,3	0
56	MG	AA	1954	1/1	0.94	0.28	-	74,74,74,74	0
56	MG	AA	2022	1/1	0.90	0.10	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1753	1/1	0.90	0.21	-	62,62,62,62	0
56	MG	BA	3784	1/1	0.91	0.22	-	33,33,33,33	0
56	MG	BK	203	1/1	0.97	0.14	-	72,72,72,72	0
56	MG	DA	3231	1/1	0.83	0.18	-	72,72,72,72	0
56	MG	AA	1796	1/1	0.97	0.17	-	60,60,60,60	0
56	MG	BB	220	1/1	0.66	0.58	-	84,84,84,84	0
56	MG	AA	1881	1/1	0.75	0.48	-	98,98,98,98	0
56	MG	BA	3843	1/1	0.88	0.20	-	60,60,60,60	0
56	MG	B1	103	1/1	0.97	0.09	-	37,37,37,37	0
56	MG	DA	3179	1/1	0.99	0.47	-	3,3,3,3	0
56	MG	CA	1665	1/1	0.97	0.29	-	3,3,3,3	0
56	MG	AA	1849	1/1	0.97	0.13	-	10,10,10,10	0
56	MG	DA	3484	1/1	0.98	0.39	-	3,3,3,3	0
56	MG	BA	3848	1/1	0.93	0.18	-	61,61,61,61	0
56	MG	BA	3608	1/1	0.93	0.28	-	40,40,40,40	0
56	MG	BA	3868	1/1	0.92	0.13	-	11,11,11,11	0
56	MG	DA	3236	1/1	0.93	0.08	-	53,53,53,53	0
56	MG	DA	3125	1/1	0.91	0.19	-	28,28,28,28	0
56	MG	AA	2018	1/1	0.98	0.25	-	23,23,23,23	0
56	MG	DA	3008	1/1	0.95	0.23	-	4,4,4,4	0
56	MG	BA	3540	1/1	0.70	0.26	-	65,65,65,65	0
56	MG	AA	1699	1/1	0.81	0.38	-	61,61,61,61	0
56	MG	BA	3646	1/1	0.87	0.15	-	47,47,47,47	0
56	MG	DA	3036	1/1	0.95	0.19	-	5,5,5,5	0
56	MG	AA	1734	1/1	0.94	0.14	-	27,27,27,27	0
56	MG	BA	3468	1/1	0.97	0.40	-	22,22,22,22	0
56	MG	AA	1813	1/1	0.79	0.30	-	67,67,67,67	0
56	MG	DA	3410	1/1	0.97	0.18	-	3,3,3,3	0
56	MG	BA	3804	1/1	0.94	0.16	-	44,44,44,44	0
56	MG	AA	1636	1/1	0.78	0.11	-	67,67,67,67	0
56	MG	BA	3219	1/1	0.95	0.16	-	17,17,17,17	0
56	MG	BA	3065	1/1	0.82	0.13	-	78,78,78,78	0
56	MG	AA	2023	1/1	0.87	0.10	-	33,33,33,33	0
56	MG	BA	3584	1/1	0.95	0.28	-	54,54,54,54	0
56	MG	BA	3102	1/1	0.82	0.22	-	89,89,89,89	0
56	MG	BA	3325	1/1	0.93	0.40	-	66,66,66,66	0
56	MG	CA	1734	1/1	0.96	0.10	-	29,29,29,29	0
56	MG	BA	3813	1/1	0.97	0.10	-	15,15,15,15	0
56	MG	AA	1912	1/1	0.92	0.14	-	62,62,62,62	0
56	MG	BA	3581	1/1	0.76	0.12	-	69,69,69,69	0
56	MG	AA	1803	1/1	0.94	0.16	-	55,55,55,55	0
56	MG	DA	3472	1/1	0.98	0.28	-	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	CA	1614	1/1	0.98	0.25	-	3,3,3,3	0
56	MG	BA	3354	1/1	0.95	0.34	-	59,59,59,59	0
56	MG	AA	1730	1/1	0.82	0.25	-	72,72,72,72	0
56	MG	AA	2013	1/1	0.94	0.32	-	40,40,40,40	0
56	MG	BB	203	1/1	0.90	0.05	-	51,51,51,51	0
56	MG	BA	3632	1/1	0.97	0.23	-	51,51,51,51	0
56	MG	AZ	110	1/1	0.91	0.19	-	69,69,69,69	0
56	MG	AA	1988	1/1	0.90	0.10	-	65,65,65,65	0
56	MG	AA	1999	1/1	0.96	0.11	-	47,47,47,47	0
56	MG	AA	1804	1/1	0.94	0.35	-	56,56,56,56	0
56	MG	DA	3250	1/1	0.95	0.24	-	3,3,3,3	0
56	MG	BA	3444	1/1	0.92	0.29	-	42,42,42,42	0
56	MG	BA	3133	1/1	0.76	0.34	-	53,53,53,53	0
56	MG	AA	1914	1/1	0.91	0.14	-	70,70,70,70	0
56	MG	BA	3340	1/1	0.67	0.58	-	73,73,73,73	0
56	MG	DB	201	1/1	0.96	0.28	-	3,3,3,3	0
56	MG	BA	3881	1/1	0.85	0.41	-	68,68,68,68	0
56	MG	AA	1859	1/1	0.88	0.12	-	76,76,76,76	0
56	MG	DA	3415	1/1	0.97	0.23	-	4,4,4,4	0
56	MG	AA	1961	1/1	0.97	0.37	-	61,61,61,61	0
56	MG	DA	3324	1/1	0.95	0.51	-	3,3,3,3	0
56	MG	BA	3159	1/1	0.91	0.20	-	61,61,61,61	0
56	MG	B0	102	1/1	0.93	0.15	-	37,37,37,37	0
56	MG	BA	3272	1/1	0.89	0.20	-	54,54,54,54	0
56	MG	BA	3204	1/1	0.94	0.09	-	34,34,34,34	0
56	MG	DB	207	1/1	0.99	0.18	-	4,4,4,4	0
56	MG	CA	1716	1/1	0.91	0.17	-	58,58,58,58	0
56	MG	AA	1741	1/1	0.89	0.15	-	60,60,60,60	0
56	MG	AA	2005	1/1	0.88	0.20	-	49,49,49,49	0
56	MG	BA	3718	1/1	0.93	0.41	-	51,51,51,51	0
56	MG	BS	201	1/1	0.93	0.16	-	46,46,46,46	0
56	MG	DA	3296	1/1	0.96	0.59	-	46,46,46,46	0
56	MG	CA	1680	1/1	0.85	0.19	-	34,34,34,34	0
56	MG	BA	3707	1/1	0.86	0.50	-	77,77,77,77	0
56	MG	BA	3626	1/1	0.88	0.17	-	62,62,62,62	0
56	MG	BA	3087	1/1	0.95	0.31	-	24,24,24,24	0
56	MG	BN	204	1/1	0.95	0.11	-	43,43,43,43	0
56	MG	CY	108	1/1	0.81	0.19	-	60,60,60,60	0
56	MG	AA	1656	1/1	0.86	0.15	-	47,47,47,47	0
56	MG	DQ	201	1/1	0.91	0.25	-	4,4,4,4	0
56	MG	BA	3799	1/1	0.97	0.11	-	29,29,29,29	0
56	MG	CA	1803	1/1	0.96	0.26	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3849	1/1	0.89	0.35	-	52,52,52,52	0
56	MG	DA	3479	1/1	0.96	0.23	-	3,3,3,3	0
56	MG	AA	1682	1/1	0.92	0.17	-	40,40,40,40	0
56	MG	AA	1827	1/1	0.83	0.26	-	44,44,44,44	0
56	MG	DA	3366	1/1	0.89	0.14	-	86,86,86,86	0
56	MG	BA	3149	1/1	0.83	0.19	-	29,29,29,29	0
56	MG	AA	1873	1/1	0.83	0.40	-	77,77,77,77	0
56	MG	BA	3755	1/1	0.96	0.19	-	58,58,58,58	0
56	MG	AA	1728	1/1	0.93	0.39	-	46,46,46,46	0
56	MG	AA	1779	1/1	0.87	0.69	-	34,34,34,34	0
56	MG	CZ	111	1/1	0.94	0.33	-	3,3,3,3	0
56	MG	DA	3457	1/1	0.89	0.20	-	4,4,4,4	0
56	MG	AA	1875	1/1	0.62	0.55	-	83,83,83,83	0
56	MG	BA	3578	1/1	0.92	0.09	-	48,48,48,48	0
56	MG	AA	1993	1/1	0.97	0.21	-	46,46,46,46	0
56	MG	BA	3674	1/1	0.96	0.15	-	12,12,12,12	0
56	MG	DA	3370	1/1	0.75	0.22	-	71,71,71,71	0
56	MG	DA	3044	1/1	0.95	0.19	-	3,3,3,3	0
56	MG	BA	3794	1/1	0.69	0.12	-	65,65,65,65	0
56	MG	BA	3452	1/1	0.94	0.14	-	44,44,44,44	0
56	MG	BA	3395	1/1	0.89	0.14	-	22,22,22,22	0
56	MG	DA	3372	1/1	0.97	0.28	-	3,3,3,3	0
56	MG	B2	103	1/1	0.95	0.37	-	36,36,36,36	0
56	MG	BA	3079	1/1	0.94	0.29	-	51,51,51,51	0
56	MG	AA	1631	1/1	0.94	0.20	-	39,39,39,39	0
56	MG	BA	3796	1/1	0.97	0.14	-	30,30,30,30	0
56	MG	BA	3005	1/1	0.82	0.26	-	51,51,51,51	0
56	MG	BA	3424	1/1	0.90	0.37	-	55,55,55,55	0
56	MG	BA	3658	1/1	0.95	0.12	-	36,36,36,36	0
56	MG	BA	3392	1/1	0.88	0.13	-	52,52,52,52	0
56	MG	BA	3575	1/1	0.93	0.12	-	53,53,53,53	0
56	MG	CA	1770	1/1	0.93	0.12	-	54,54,54,54	0
56	MG	DA	3083	1/1	0.96	0.21	-	3,3,3,3	0
56	MG	AA	1668	1/1	0.88	0.08	-	46,46,46,46	0
56	MG	DA	3272	1/1	0.98	0.28	-	3,3,3,3	0
56	MG	AA	1681	1/1	0.95	0.11	-	27,27,27,27	0
56	MG	AA	1880	1/1	0.94	0.11	-	40,40,40,40	0
56	MG	DA	3283	1/1	0.82	0.82	-	70,70,70,70	0
56	MG	CA	1772	1/1	0.88	0.26	-	3,3,3,3	0
56	MG	BA	3360	1/1	0.85	0.25	-	65,65,65,65	0
56	MG	BA	3909	1/1	0.88	0.21	-	39,39,39,39	0
56	MG	DD	5008	1/1	0.93	0.13	-	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AY	109	1/1	0.91	0.17	-	47,47,47,47	0
56	MG	BA	3192	1/1	0.85	0.29	-	50,50,50,50	0
56	MG	BA	3090	1/1	0.96	0.08	-	43,43,43,43	0
56	MG	AZ	114	1/1	0.95	0.09	-	60,60,60,60	0
56	MG	BA	3443	1/1	0.81	0.18	-	71,71,71,71	0
56	MG	DB	212	1/1	0.97	0.23	-	3,3,3,3	0
56	MG	DA	3040	1/1	0.95	0.23	-	3,3,3,3	0
56	MG	CA	1602	1/1	0.94	0.09	-	5,5,5,5	0
56	MG	DA	3009	1/1	0.98	0.26	-	3,3,3,3	0
56	MG	BA	3878	1/1	0.88	0.17	-	44,44,44,44	0
56	MG	AA	1683	1/1	0.94	0.16	-	74,74,74,74	0
56	MG	BO	203	1/1	0.94	0.23	-	55,55,55,55	0
56	MG	AA	1646	1/1	0.84	0.19	-	38,38,38,38	0
56	MG	BA	3156	1/1	0.69	0.49	-	53,53,53,53	0
56	MG	B1	102	1/1	0.97	0.08	-	9,9,9,9	0
56	MG	BA	3431	1/1	0.65	0.17	-	63,63,63,63	0
56	MG	BA	3520	1/1	0.89	0.19	-	61,61,61,61	0
56	MG	AA	1952	1/1	0.89	0.13	-	83,83,83,83	0
56	MG	BA	3147	1/1	0.80	0.48	-	52,52,52,52	0
56	MG	BA	3175	1/1	0.89	0.32	-	69,69,69,69	0
56	MG	BA	3433	1/1	0.90	0.24	-	67,67,67,67	0
56	MG	AA	1664	1/1	0.71	0.19	-	73,73,73,73	0
56	MG	DA	3477	1/1	0.96	0.25	-	3,3,3,3	0
56	MG	BA	3067	1/1	0.96	0.07	-	48,48,48,48	0
56	MG	AK	205	1/1	0.93	0.39	-	61,61,61,61	0
56	MG	CA	1797	1/1	0.94	0.50	-	28,28,28,28	0
56	MG	DA	3039	1/1	0.91	0.20	-	4,4,4,4	0
56	MG	CA	1687	1/1	0.89	0.29	-	46,46,46,46	0
56	MG	DA	3384	1/1	0.94	0.34	-	3,3,3,3	0
56	MG	AA	1791	1/1	0.95	0.08	-	81,81,81,81	0
56	MG	DA	3306	1/1	0.95	0.25	-	3,3,3,3	0
56	MG	CA	1615	1/1	0.93	0.25	-	3,3,3,3	0
56	MG	AZ	109	1/1	0.91	0.16	-	79,79,79,79	0
56	MG	CA	1813	1/1	0.90	0.13	-	64,64,64,64	0
56	MG	BA	3569	1/1	0.94	0.28	-	40,40,40,40	0
56	MG	BA	3478	1/1	0.93	0.17	-	52,52,52,52	0
56	MG	BA	3800	1/1	0.67	0.40	-	74,74,74,74	0
56	MG	BA	3286	1/1	0.97	0.23	-	17,17,17,17	0
56	MG	BA	3210	1/1	0.79	0.14	-	69,69,69,69	0
56	MG	BA	3831	1/1	0.95	0.22	-	34,34,34,34	0
56	MG	AA	1806	1/1	0.98	0.32	-	27,27,27,27	0
56	MG	DB	211	1/1	0.94	0.26	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	BA	3735	1/1	0.97	0.12	-	29,29,29,29	0
56	MG	CA	1617	1/1	0.97	0.11	-	4,4,4,4	0
56	MG	CA	1705	1/1	0.76	0.86	-	60,60,60,60	0
56	MG	CA	1776	1/1	0.97	0.23	-	3,3,3,3	0
56	MG	AY	105	1/1	0.98	0.08	-	39,39,39,39	0
56	MG	DA	3318	1/1	0.70	0.32	-	45,45,45,45	0
56	MG	AA	1869	1/1	0.95	0.16	-	47,47,47,47	0
56	MG	BA	3728	1/1	0.95	0.17	-	34,34,34,34	0
56	MG	BA	3277	1/1	0.88	0.18	-	57,57,57,57	0
56	MG	DA	3321	1/1	0.98	0.29	-	4,4,4,4	0
56	MG	DA	3043	1/1	0.98	0.20	-	3,3,3,3	0
56	MG	BA	3797	1/1	0.95	0.12	-	52,52,52,52	0
56	MG	BG	201	1/1	0.91	0.37	-	64,64,64,64	0
56	MG	BA	3786	1/1	0.94	0.37	-	18,18,18,18	0
56	MG	BA	3085	1/1	0.92	0.24	-	29,29,29,29	0
56	MG	BA	3406	1/1	0.94	0.29	-	23,23,23,23	0
56	MG	BE	302	1/1	0.73	0.40	-	67,67,67,67	0
56	MG	AA	1976	1/1	0.93	0.17	-	70,70,70,70	0
56	MG	CA	1685	1/1	0.72	0.48	-	68,68,68,68	0
56	MG	CA	1750	1/1	0.96	0.18	-	4,4,4,4	0
56	MG	DA	3094	1/1	0.96	0.36	-	3,3,3,3	0
56	MG	DA	3184	1/1	0.95	0.24	-	3,3,3,3	0
56	MG	AA	1971	1/1	0.92	0.42	-	57,57,57,57	0
56	MG	BA	3344	1/1	0.94	0.37	-	47,47,47,47	0
56	MG	DA	3170	1/1	0.94	0.33	-	3,3,3,3	0
56	MG	BA	3743	1/1	0.89	0.27	-	64,64,64,64	0
56	MG	CA	1791	1/1	0.87	0.41	-	54,54,54,54	0
56	MG	DA	3467	1/1	0.90	0.18	-	3,3,3,3	0
56	MG	AA	1698	1/1	0.80	0.25	-	53,53,53,53	0
56	MG	CY	104	1/1	0.77	0.09	-	78,78,78,78	0
56	MG	DA	3186	1/1	0.96	0.11	-	4,4,4,4	0
56	MG	BE	306	1/1	0.77	0.13	-	71,71,71,71	0
56	MG	CA	1767	1/1	0.81	0.10	-	64,64,64,64	0
56	MG	AA	2011	1/1	0.88	0.31	-	75,75,75,75	0
56	MG	CA	1678	1/1	0.85	0.18	-	49,49,49,49	0
56	MG	BA	3717	1/1	0.92	0.13	-	67,67,67,67	0
56	MG	BA	3423	1/1	0.90	0.16	-	21,21,21,21	0
56	MG	BA	3011	1/1	0.76	0.21	-	47,47,47,47	0
56	MG	BA	3663	1/1	0.92	0.32	-	50,50,50,50	0
56	MG	DA	3111	1/1	0.97	0.25	-	3,3,3,3	0
56	MG	AA	1957	1/1	0.84	0.07	-	61,61,61,61	0
56	MG	AA	2025	1/1	0.87	0.57	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1788	1/1	0.89	0.46	-	66,66,66,66	0
56	MG	DA	3405	1/1	0.93	0.11	-	4,4,4,4	0
56	MG	DA	3161	1/1	0.97	0.34	-	3,3,3,3	0
56	MG	BA	3269	1/1	0.93	0.11	-	31,31,31,31	0
56	MG	CA	1607	1/1	0.97	0.23	-	3,3,3,3	0
56	MG	BA	3603	1/1	0.85	0.24	-	47,47,47,47	0
56	MG	BA	3176	1/1	0.59	0.43	-	66,66,66,66	0
56	MG	DA	3033	1/1	0.90	0.17	-	4,4,4,4	0
56	MG	AK	204	1/1	0.87	0.11	-	82,82,82,82	0
56	MG	BA	3548	1/1	0.84	0.14	-	36,36,36,36	0
56	MG	CA	1649	1/1	0.92	0.09	-	35,35,35,35	0
56	MG	BA	3335	1/1	0.94	0.15	-	52,52,52,52	0
56	MG	CA	1758	1/1	0.69	0.17	-	78,78,78,78	0
56	MG	DA	3291	1/1	0.88	0.22	-	44,44,44,44	0
56	MG	AK	206	1/1	0.75	0.29	-	69,69,69,69	0
56	MG	AA	1921	1/1	0.96	0.17	-	60,60,60,60	0
56	MG	BA	3280	1/1	0.93	0.18	-	29,29,29,29	0
56	MG	BB	217	1/1	0.82	0.39	-	74,74,74,74	0
56	MG	BA	3275	1/1	0.82	0.32	-	46,46,46,46	0
56	MG	DA	3001	1/1	0.96	0.17	-	55,55,55,55	0
56	MG	DA	3465	1/1	0.96	0.20	-	3,3,3,3	0
56	MG	AA	1994	1/1	0.92	0.30	-	52,52,52,52	0
56	MG	BA	3230	1/1	0.84	0.12	-	60,60,60,60	0
56	MG	BA	3860	1/1	0.92	0.08	-	62,62,62,62	0
56	MG	AA	1905	1/1	0.93	0.23	-	50,50,50,50	0
56	MG	BA	3723	1/1	0.90	0.13	-	7,7,7,7	0
56	MG	DA	3395	1/1	0.96	0.23	-	41,41,41,41	0
56	MG	AG	202	1/1	0.93	0.11	-	56,56,56,56	0
56	MG	BA	3414	1/1	0.98	0.10	-	23,23,23,23	0
56	MG	BA	3759	1/1	0.83	0.24	-	47,47,47,47	0
56	MG	BA	3207	1/1	0.80	0.12	-	73,73,73,73	0
56	MG	AC	303	1/1	0.95	0.07	-	56,56,56,56	0
56	MG	AA	1743	1/1	0.84	0.11	-	63,63,63,63	0
56	MG	AA	1830	1/1	0.96	0.12	-	55,55,55,55	0
56	MG	CA	1669	1/1	0.77	0.57	-	79,79,79,79	0
56	MG	DA	3239	1/1	0.84	0.10	-	78,78,78,78	0
56	MG	DA	3080	1/1	0.94	0.23	-	3,3,3,3	0
56	MG	DA	3486	1/1	0.92	0.48	-	3,3,3,3	0
56	MG	BA	3225	1/1	0.95	0.12	-	27,27,27,27	0
56	MG	DB	210	1/1	0.82	0.20	-	3,3,3,3	0
56	MG	BA	3068	1/1	0.65	0.20	-	50,50,50,50	0
56	MG	AA	1845	1/1	0.96	0.10	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3031	1/1	0.93	0.48	-	3,3,3,3	0
56	MG	BA	3573	1/1	0.96	0.16	-	62,62,62,62	0
56	MG	CA	1658	1/1	0.97	0.27	-	3,3,3,3	0
56	MG	DA	3248	1/1	0.95	0.13	-	3,3,3,3	0
56	MG	BA	3631	1/1	0.96	0.27	-	67,67,67,67	0
56	MG	BA	3062	1/1	0.92	0.12	-	56,56,56,56	0
56	MG	AA	1774	1/1	0.90	0.14	-	39,39,39,39	0
56	MG	BA	3300	1/1	0.79	0.39	-	61,61,61,61	0
56	MG	BA	3550	1/1	0.77	0.32	-	42,42,42,42	0
56	MG	DA	3076	1/1	0.96	0.17	-	3,3,3,3	0
56	MG	BA	3353	1/1	0.95	0.23	-	37,37,37,37	0
56	MG	AA	1689	1/1	0.88	0.12	-	55,55,55,55	0
56	MG	CA	1630	1/1	0.94	0.56	-	3,3,3,3	0
56	MG	BA	3706	1/1	0.96	0.20	-	45,45,45,45	0
56	MG	BA	3450	1/1	0.98	0.15	-	24,24,24,24	0
56	MG	BA	3110	1/1	0.94	0.08	-	65,65,65,65	0
56	MG	BA	3533	1/1	0.95	0.12	-	2,2,2,2	0
56	MG	BA	3202	1/1	0.86	0.53	-	57,57,57,57	0
56	MG	AA	1960	1/1	0.90	0.29	-	53,53,53,53	0
56	MG	AA	1654	1/1	0.94	0.15	-	75,75,75,75	0
56	MG	DA	3322	1/1	0.95	0.30	-	3,3,3,3	0
56	MG	DA	3104	1/1	0.90	0.42	-	21,21,21,21	0
56	MG	AA	1760	1/1	0.92	0.10	-	8,8,8,8	0
56	MG	AA	1841	1/1	0.97	0.23	-	8,8,8,8	0
56	MG	DA	3168	1/1	0.95	0.20	-	4,4,4,4	0
56	MG	BA	3733	1/1	0.93	0.30	-	38,38,38,38	0
56	MG	AA	1870	1/1	0.92	0.24	-	85,85,85,85	0
56	MG	AA	1820	1/1	0.89	0.14	-	46,46,46,46	0
56	MG	BA	3161	1/1	0.89	0.40	-	103,103,103,103	0
56	MG	DA	3469	1/1	0.96	0.39	-	3,3,3,3	0
56	MG	BA	3858	1/1	0.92	0.24	-	60,60,60,60	0
56	MG	BA	3749	1/1	0.85	0.52	-	53,53,53,53	0
56	MG	DA	3194	1/1	0.95	0.21	-	3,3,3,3	0
56	MG	DA	3233	1/1	0.97	0.11	-	43,43,43,43	0
56	MG	BA	3812	1/1	0.87	0.16	-	40,40,40,40	0
56	MG	BA	3508	1/1	0.93	0.14	-	33,33,33,33	0
56	MG	DA	3419	1/1	0.95	0.32	-	3,3,3,3	0
56	MG	BA	3622	1/1	0.92	0.09	-	60,60,60,60	0
56	MG	CA	1729	1/1	0.86	0.35	-	36,36,36,36	0
56	MG	BA	3235	1/1	0.92	0.09	-	47,47,47,47	0
56	MG	DA	3155	1/1	0.95	0.18	-	4,4,4,4	0
56	MG	BA	3484	1/1	0.95	0.19	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	AA	1958	1/1	0.57	0.68	-	87,87,87,87	0
56	MG	BA	3905	1/1	0.86	0.25	-	65,65,65,65	0
56	MG	BA	3855	1/1	0.95	0.14	-	49,49,49,49	0
56	MG	DB	205	1/1	0.95	0.28	-	3,3,3,3	0
56	MG	AA	1940	1/1	0.85	0.39	-	53,53,53,53	0
56	MG	AA	1855	1/1	0.95	0.23	-	21,21,21,21	0
56	MG	DA	3413	1/1	0.90	0.18	-	3,3,3,3	0
56	MG	BA	3425	1/1	0.86	0.29	-	48,48,48,48	0
56	MG	BA	3795	1/1	0.67	0.35	-	84,84,84,84	0
56	MG	BA	3644	1/1	0.96	0.24	-	26,26,26,26	0
56	MG	CA	1755	1/1	0.95	0.24	-	4,4,4,4	0
56	MG	AA	1902	1/1	0.75	0.51	-	61,61,61,61	0
56	MG	CA	1794	1/1	0.88	0.17	-	35,35,35,35	0
56	MG	AA	1908	1/1	0.92	0.28	-	85,85,85,85	0
56	MG	BA	3476	1/1	0.97	0.08	-	18,18,18,18	0
56	MG	CA	1778	1/1	0.98	0.15	-	3,3,3,3	0
56	MG	DO	202	1/1	0.92	0.11	-	4,4,4,4	0
56	MG	BA	3725	1/1	0.85	0.12	-	23,23,23,23	0
56	MG	BA	3562	1/1	0.95	0.13	-	28,28,28,28	0
56	MG	BA	3568	1/1	0.93	0.16	-	33,33,33,33	0
56	MG	BA	3456	1/1	0.94	0.12	-	24,24,24,24	0
56	MG	BA	3771	1/1	0.82	0.50	-	72,72,72,72	0
56	MG	AA	1723	1/1	0.78	0.31	-	76,76,76,76	0
56	MG	BI	205	1/1	0.84	0.11	-	45,45,45,45	0
56	MG	DA	3481	1/1	0.87	0.21	-	4,4,4,4	0
56	MG	AA	1657	1/1	0.91	0.11	-	45,45,45,45	0
56	MG	CA	1692	1/1	0.94	0.14	-	34,34,34,34	0
56	MG	AV	5502	1/1	0.62	0.58	-	89,89,89,89	0
56	MG	BA	3014	1/1	0.77	0.37	-	65,65,65,65	0
56	MG	BA	3109	1/1	0.76	0.18	-	70,70,70,70	0
56	MG	BA	3078	1/1	0.85	0.18	-	51,51,51,51	0
56	MG	BA	3873	1/1	0.86	0.41	-	44,44,44,44	0
56	MG	CA	1707	1/1	0.95	0.14	-	36,36,36,36	0
56	MG	BD	5004	1/1	0.93	0.16	-	50,50,50,50	0
56	MG	AA	1850	1/1	0.95	0.11	-	38,38,38,38	0
56	MG	AA	1885	1/1	0.67	0.33	-	58,58,58,58	0
56	MG	DA	3117	1/1	0.96	0.11	-	28,28,28,28	0
56	MG	AA	1625	1/1	0.98	0.20	-	44,44,44,44	0
56	MG	BS	202	1/1	0.87	0.07	-	42,42,42,42	0
56	MG	BA	3557	1/1	0.94	0.20	-	29,29,29,29	0
56	MG	DA	3358	1/1	0.93	0.19	-	54,54,54,54	0
56	MG	BA	3648	1/1	0.80	0.21	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
56	MG	DA	3461	1/1	0.96	0.19	-	4,4,4,4	0
56	MG	CY	103	1/1	0.95	0.16	-	31,31,31,31	0
56	MG	BD	5003	1/1	0.74	0.16	-	57,57,57,57	0
56	MG	BA	3355	1/1	0.94	0.10	-	33,33,33,33	0
56	MG	DA	3156	1/1	0.96	0.39	-	3,3,3,3	0
56	MG	BA	3675	1/1	0.95	0.23	-	43,43,43,43	0
56	MG	CA	1728	1/1	0.91	0.30	-	57,57,57,57	0
56	MG	DA	3042	1/1	0.94	0.04	-	69,69,69,69	0
56	MG	BA	3552	1/1	0.98	0.07	-	15,15,15,15	0
56	MG	BA	3055	1/1	0.76	0.20	-	73,73,73,73	0
56	MG	BA	3695	1/1	0.94	0.15	-	70,70,70,70	0
56	MG	DA	3100	1/1	0.94	0.19	-	4,4,4,4	0
56	MG	BA	3884	1/1	0.58	0.24	-	80,80,80,80	0
56	MG	DA	3056	1/1	0.96	0.28	-	63,63,63,63	0
56	MG	BA	3642	1/1	0.86	0.14	-	67,67,67,67	0
56	MG	BA	3486	1/1	0.87	0.12	-	36,36,36,36	0
56	MG	CA	1613	1/1	0.95	0.21	-	3,3,3,3	0
56	MG	BA	3332	1/1	0.62	0.15	-	90,90,90,90	0
56	MG	BA	3177	1/1	0.95	0.10	-	40,40,40,40	0
56	MG	AA	1764	1/1	0.76	0.42	-	72,72,72,72	0
56	MG	AA	1749	1/1	0.91	0.12	-	68,68,68,68	0
56	MG	AY	104	1/1	0.95	0.10	-	64,64,64,64	0
56	MG	BA	3254	1/1	0.85	0.23	-	79,79,79,79	0
56	MG	CA	1820	1/1	0.95	0.24	-	43,43,43,43	0
56	MG	D6	101	1/1	0.95	0.11	-	43,43,43,43	0
56	MG	BA	3115	1/1	0.96	0.08	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.