wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:12 PM GMT

PDB ID	:	4V8I
Title	:	Crystal structure of YfiA bound to the 70S ribosome.
Authors	:	Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on	:	2011-12-12
Resolution	:	2.70 Å(reported)

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

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

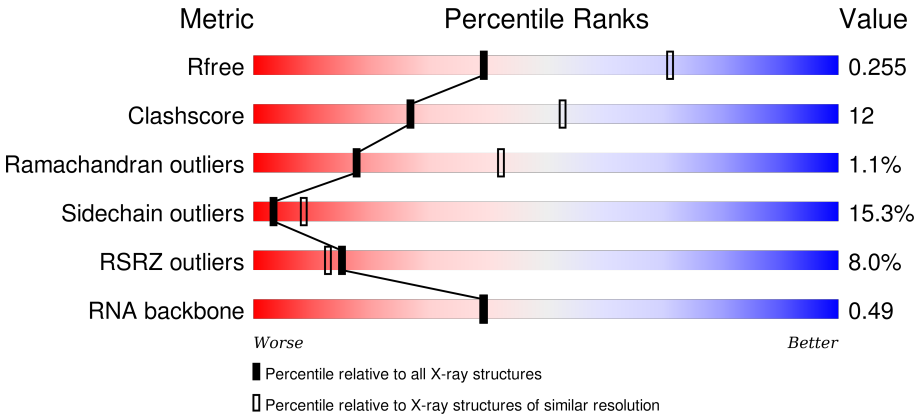
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	5% 39% 39% 15% 5% •
1	CA	1522	7% 35% 41% 18% • •
2	AB	256	11% 47% 36% 6% 11%
2	CB	256	31% 50% 36% 6% 8%

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Mol	Chain	Length	Quality of chain
3	AC	239	5% 63% 19% 14%
3	CC	239	23% 41% 36% 8% 14%
4	AD	209	17% 70% 23% 7%
4	CD	209	14% 61% 31% 8%
5	AE	162	56% 31% 9%
5	CE	162	9% 54% 32% 6% 9%
6	AF	101	4% 70% 23% 6%
6	CF	101	3% 70% 21% 7%
7	AG	156	4% 71% 24%
7	CG	156	28% 56% 37% 6%
8	AH	138	6% 64% 30% 6%
8	CH	138	10% 64% 29% 7%
9	AI	128	11% 52% 40% 5%
9	CI	128	36% 48% 41% 9%
10	AJ	105	19% 42% 40% 9% 9%
10	CJ	105	43% 54% 27% 10% 9%
11	AK	129	7% 67% 19% 12%
11	CK	129	12% 62% 23% 12%
12	AL	132	4% 65% 23% 8%
12	CL	132	15% 64% 25% 8%
13	AM	126	6% 50% 26% 13% 10%
13	CM	126	32% 47% 32% 10% 11%
14	AN	61	7% 52% 39% 7%
14	CN	61	31% 41% 38% 16%
15	AO	89	3% 63% 30%

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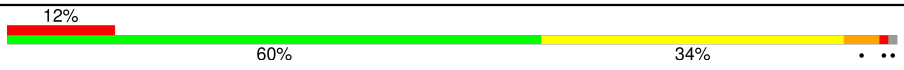
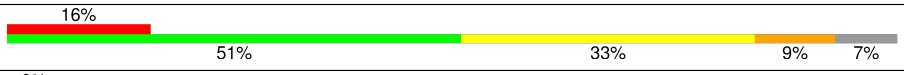
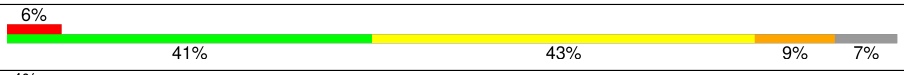
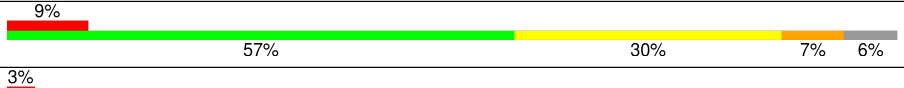
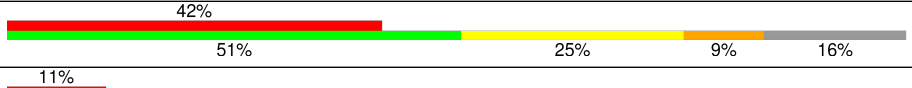
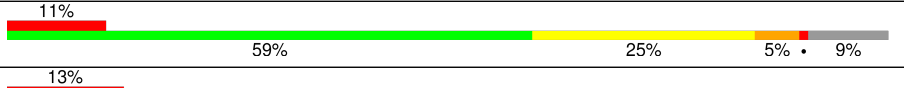
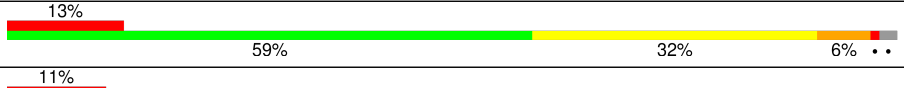
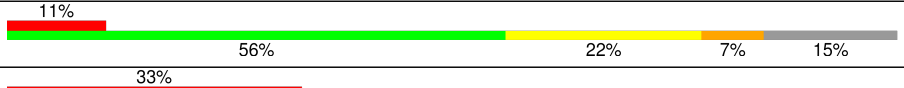
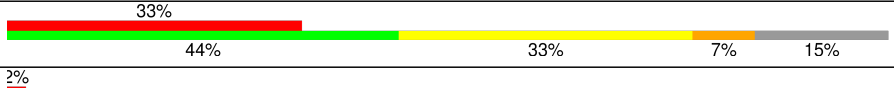
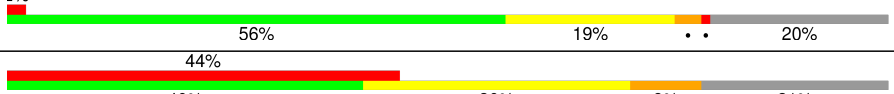
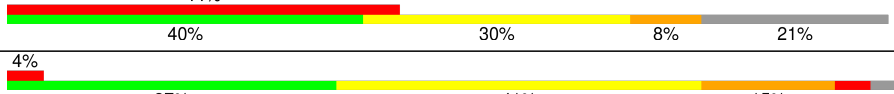
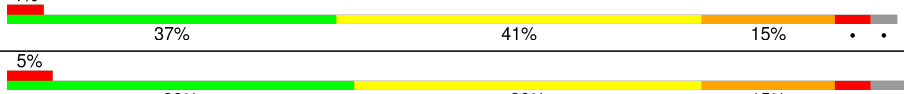
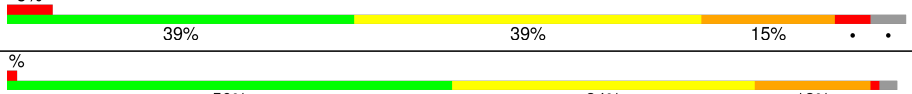
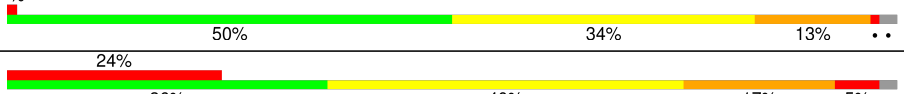
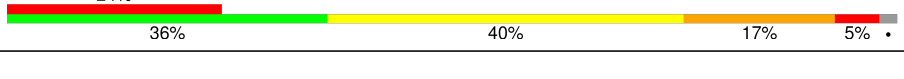
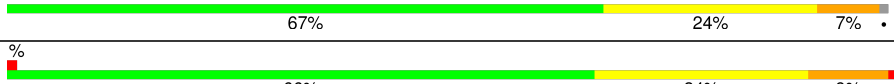
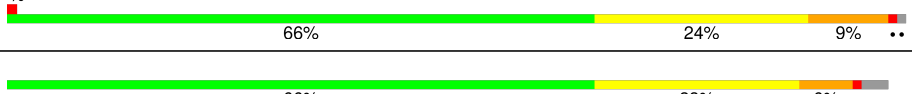
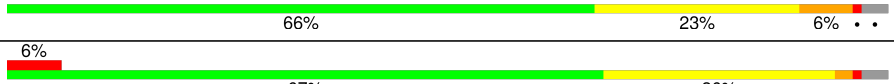
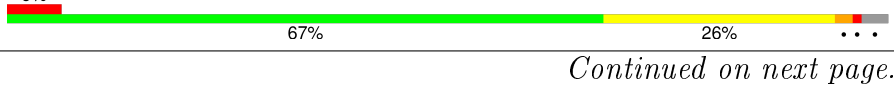
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AY	119	
22	CY	119	
23	BA	2915	
23	DA	2915	
24	BB	122	
24	DB	122	
25	BD	276	
25	DD	276	
26	BE	206	
26	DE	206	
27	BF	210	
27	DF	210	

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Mol	Chain	Length	Quality of chain
28	BG	182	3% 65% 29% 6%
28	DG	182	48% 61% 32% 5%
29	BH	180	2% 69% 24%
29	DH	180	32% 70% 23%
30	BI	148	9% 53% 36% 9%
30	DI	148	9% 52% 34% 12%
31	BN	140	64% 32%
31	DN	140	3% 65% 30% 5%
32	BO	122	77% 22%
32	DO	122	% 77% 20%
33	BP	150	% 65% 27% 5%
33	DP	150	12% 63% 26% 8%
34	BQ	141	68% 27%
34	DQ	141	6% 63% 32%
35	BR	118	65% 29% 5%
35	DR	118	64% 27% 8%
36	BS	112	% 56% 34% 7%
36	DS	112	24% 54% 35% 8%
37	BT	146	% 58% 26% 5% 10%
37	DT	146	% 59% 24% 5% 11%
38	BU	118	% 79% 16%
38	DU	118	3% 72% 23%
39	BV	101	% 70% 25% 5%
39	DV	101	9% 70% 22% 8%
40	BW	113	66% 25% 7%

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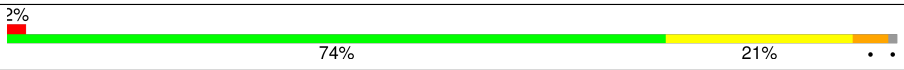
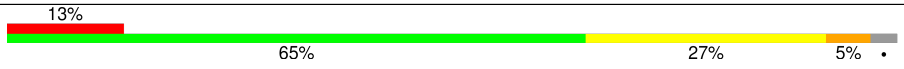
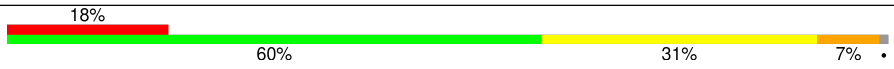
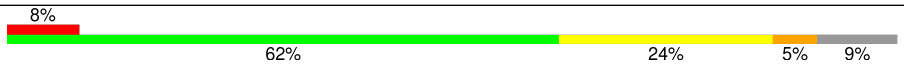
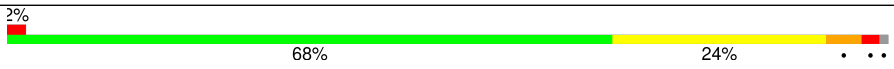
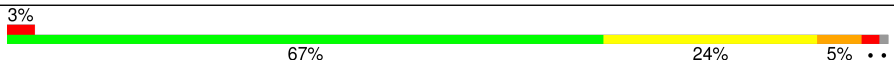
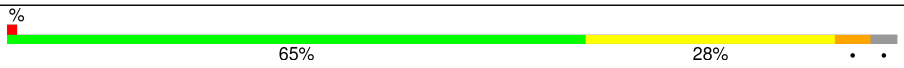
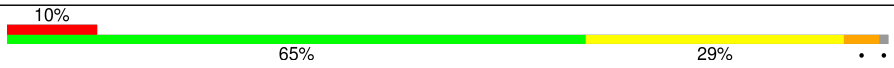
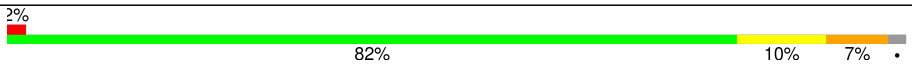
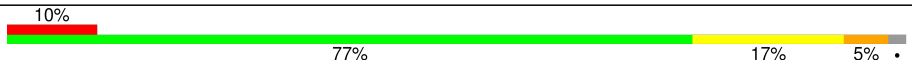
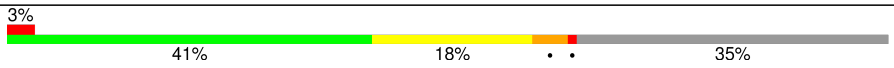
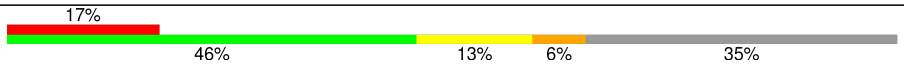
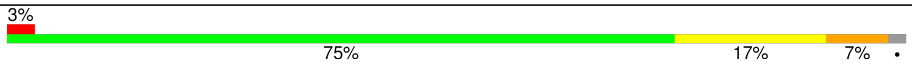
Mol	Chain	Length	Quality of chain
40	DW	113	
41	BX	96	
41	DX	96	
42	BY	110	
42	DY	110	
43	BZ	206	
43	DZ	206	
44	B0	85	
44	D0	85	
45	B1	98	
45	D1	98	
46	B2	72	
46	D2	72	
47	B3	60	
47	D3	60	
48	B4	71	
48	D4	71	
49	B5	60	
49	D5	60	
50	B6	54	
50	D6	54	
51	B7	49	
51	D7	49	
52	B8	65	
52	D8	65	

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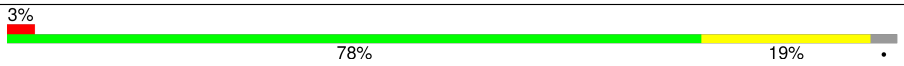
Mol	Chain	Length	Quality of chain
53	B9	37	
53	D9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	1619	-	-	-	X
54	MG	AA	1620	-	-	-	X
54	MG	AA	1626	-	-	-	X
54	MG	AA	1630	-	-	-	X
54	MG	AA	1634	-	-	-	X
54	MG	AA	1644	-	-	-	X
54	MG	AA	1649	-	-	-	X
54	MG	AA	1650	-	-	-	X
54	MG	AA	1651	-	-	-	X
54	MG	AA	1666	-	-	-	X
54	MG	AA	1679	-	-	-	X
54	MG	AA	1682	-	-	-	X
54	MG	AA	1691	-	-	-	X
54	MG	AA	1751	-	-	-	X
54	MG	AA	1752	-	-	-	X
54	MG	AA	1763	-	-	-	X
54	MG	AA	1765	-	-	-	X
54	MG	AA	1776	-	-	-	X
54	MG	AA	1784	-	-	-	X
54	MG	AA	1787	-	-	-	X
54	MG	AI	201	-	-	-	X
54	MG	AM	201	-	-	-	X
54	MG	B0	101	-	-	-	X
54	MG	B3	103	-	-	-	X
54	MG	B9	102	-	-	-	X
54	MG	BA	3008	-	-	-	X
54	MG	BA	3015	-	-	-	X
54	MG	BA	3018	-	-	-	X
54	MG	BA	3032	-	-	-	X
54	MG	BA	3033	-	-	-	X
54	MG	BA	3035	-	-	-	X
54	MG	BA	3053	-	-	-	X
54	MG	BA	3057	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3058	-	-	-	X
54	MG	BA	3060	-	-	-	X
54	MG	BA	3074	-	-	-	X
54	MG	BA	3080	-	-	-	X
54	MG	BA	3085	-	-	-	X
54	MG	BA	3086	-	-	-	X
54	MG	BA	3102	-	-	-	X
54	MG	BA	3103	-	-	-	X
54	MG	BA	3104	-	-	-	X
54	MG	BA	3148	-	-	-	X
54	MG	BA	3159	-	-	-	X
54	MG	BA	3162	-	-	-	X
54	MG	BA	3178	-	-	-	X
54	MG	BA	3179	-	-	-	X
54	MG	BA	3190	-	-	-	X
54	MG	BA	3191	-	-	-	X
54	MG	BA	3209	-	-	-	X
54	MG	BA	3230	-	-	-	X
54	MG	BA	3243	-	-	-	X
54	MG	BA	3248	-	-	-	X
54	MG	BA	3249	-	-	-	X
54	MG	BA	3279	-	-	-	X
54	MG	BA	3296	-	-	-	X
54	MG	BA	3335	-	-	-	X
54	MG	BA	3345	-	-	-	X
54	MG	BA	3358	-	-	-	X
54	MG	BA	3359	-	-	-	X
54	MG	BA	3360	-	-	-	X
54	MG	BA	3365	-	-	-	X
54	MG	BA	3371	-	-	-	X
54	MG	BA	3372	-	-	-	X
54	MG	BA	3377	-	-	-	X
54	MG	BA	3382	-	-	-	X
54	MG	BA	3386	-	-	-	X
54	MG	BA	3387	-	-	-	X
54	MG	BA	3388	-	-	-	X
54	MG	BA	3393	-	-	-	X
54	MG	BA	3398	-	-	-	X
54	MG	BA	3403	-	-	-	X
54	MG	BA	3406	-	-	-	X
54	MG	BA	3415	-	-	-	X
54	MG	BA	3418	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3421	-	-	-	X
54	MG	BA	3428	-	-	-	X
54	MG	BA	3430	-	-	-	X
54	MG	BA	3431	-	-	-	X
54	MG	BA	3433	-	-	-	X
54	MG	BA	3462	-	-	-	X
54	MG	BA	3481	-	-	-	X
54	MG	BA	3518	-	-	-	X
54	MG	BA	3520	-	-	-	X
54	MG	BA	3528	-	-	-	X
54	MG	BA	3533	-	-	-	X
54	MG	BA	3537	-	-	-	X
54	MG	BA	3543	-	-	-	X
54	MG	BA	3553	-	-	-	X
54	MG	BA	3568	-	-	-	X
54	MG	BA	3619	-	-	-	X
54	MG	BA	3620	-	-	-	X
54	MG	BA	3621	-	-	-	X
54	MG	BA	3624	-	-	-	X
54	MG	BA	3633	-	-	-	X
54	MG	BA	3643	-	-	-	X
54	MG	BA	3649	-	-	-	X
54	MG	BA	3654	-	-	-	X
54	MG	BE	301	-	-	-	X
54	MG	BE	302	-	-	-	X
54	MG	BE	303	-	-	-	X
54	MG	BE	304	-	-	-	X
54	MG	BF	302	-	-	-	X
54	MG	BF	305	-	-	-	X
54	MG	BR	203	-	-	-	X
54	MG	BU	201	-	-	-	X
54	MG	BU	203	-	-	-	X
54	MG	BV	201	-	-	-	X
54	MG	CA	1603	-	-	-	X
54	MG	CA	1615	-	-	-	X
54	MG	CA	1619	-	-	-	X
54	MG	CA	1620	-	-	-	X
54	MG	CA	1639	-	-	-	X
54	MG	CA	1645	-	-	-	X
54	MG	CA	1710	-	-	-	X
54	MG	CA	1739	-	-	-	X
54	MG	CA	1753	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	CA	1760	-	-	-	X
54	MG	CA	1768	-	-	-	X
54	MG	D7	101	-	-	-	X
54	MG	DA	3003	-	-	-	X
54	MG	DA	3008	-	-	-	X
54	MG	DA	3010	-	-	-	X
54	MG	DA	3012	-	-	-	X
54	MG	DA	3013	-	-	-	X
54	MG	DA	3019	-	-	-	X
54	MG	DA	3021	-	-	-	X
54	MG	DA	3025	-	-	-	X
54	MG	DA	3026	-	-	-	X
54	MG	DA	3034	-	-	-	X
54	MG	DA	3035	-	-	-	X
54	MG	DA	3042	-	-	-	X
54	MG	DA	3053	-	-	-	X
54	MG	DA	3054	-	-	-	X
54	MG	DA	3055	-	-	-	X
54	MG	DA	3062	-	-	-	X
54	MG	DA	3064	-	-	-	X
54	MG	DA	3072	-	-	-	X
54	MG	DA	3073	-	-	-	X
54	MG	DA	3086	-	-	-	X
54	MG	DA	3098	-	-	-	X
54	MG	DA	3100	-	-	-	X
54	MG	DA	3107	-	-	-	X
54	MG	DA	3115	-	-	-	X
54	MG	DA	3116	-	-	-	X
54	MG	DA	3129	-	-	-	X
54	MG	DA	3130	-	-	-	X
54	MG	DA	3131	-	-	-	X
54	MG	DA	3137	-	-	-	X
54	MG	DA	3150	-	-	-	X
54	MG	DA	3156	-	-	-	X
54	MG	DA	3162	-	-	-	X
54	MG	DA	3170	-	-	-	X
54	MG	DA	3175	-	-	-	X
54	MG	DA	3176	-	-	-	X
54	MG	DA	3179	-	-	-	X
54	MG	DA	3195	-	-	-	X
54	MG	DA	3199	-	-	-	X
54	MG	DA	3200	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3207	-	-	-	X
54	MG	DA	3210	-	-	-	X
54	MG	DA	3219	-	-	-	X
54	MG	DA	3221	-	-	-	X
54	MG	DA	3222	-	-	-	X
54	MG	DA	3245	-	-	-	X
54	MG	DA	3250	-	-	-	X
54	MG	DA	3257	-	-	-	X
54	MG	DA	3258	-	-	-	X
54	MG	DA	3259	-	-	-	X
54	MG	DA	3291	-	-	-	X
54	MG	DA	3295	-	-	-	X
54	MG	DA	3300	-	-	-	X
54	MG	DA	3307	-	-	-	X
54	MG	DA	3318	-	-	-	X
54	MG	DA	3366	-	-	-	X
54	MG	DA	3395	-	-	-	X
54	MG	DA	3398	-	-	-	X
54	MG	DA	3427	-	-	-	X
54	MG	DA	3428	-	-	-	X
54	MG	DA	3429	-	-	-	X
54	MG	DA	3430	-	-	-	X
54	MG	DA	3441	-	-	-	X
54	MG	DA	3455	-	-	-	X
54	MG	DA	3472	-	-	-	X
54	MG	DA	3484	-	-	-	X
54	MG	DA	3493	-	-	-	X
54	MG	DA	3496	-	-	-	X
54	MG	DA	3500	-	-	-	X
54	MG	DA	3513	-	-	-	X
54	MG	DA	3528	-	-	-	X
54	MG	DA	3549	-	-	-	X
54	MG	DA	3554	-	-	-	X
54	MG	DA	3569	-	-	-	X
54	MG	DA	3576	-	-	-	X
54	MG	DA	3577	-	-	-	X
54	MG	DA	3583	-	-	-	X
54	MG	DA	3587	-	-	-	X
54	MG	DD	304	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 287173 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1493	Total	C	N	O	P	0	0	0
			32102	14287	5955	10367	1493			
1	CA	1491	Total	C	N	O	P	0	0	0
			32056	14267	5945	10353	1491			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1817	1160	325	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1453	908	280	264	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1520	960	283	272	5			
4	CD	208	Total	C	N	O	S	0	0	0
			1537	968	287	276	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1106	700	204	198	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			781	495	137	146	3			
6	CF	99	Total	C	N	O	S	0	0	0
			776	492	135	146	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1167	727	224	210	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			
8	CH	138	Total	C	N	O	S	0	0	0
			1049	667	188	192	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	125	Total	C	N	O	0	0	0
			852	533	163	156			
9	CI	125	Total	C	N	O	0	0	0
			849	531	161	157			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	96	Total	C	N	O	0	0	0
			659	408	131	120			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O	0	0	0
			657	407	129	121			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			
12	CL	122	Total	C	N	O	S	0	0	0
			905	567	178	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			
13	CM	112	Total	C	N	O	S	0	0	0
			784	486	159	138	1			

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			478	303	99	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			474	300	98	72	4			

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			
16	CP	82	Total	C	N	O	S	0	0	0
			661	421	126	113	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			819	525	150	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			
19	CS	78	Total	C	N	O	S	0	0	0
			549	345	106	96	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			699	430	150	117	2			
20	CT	104	Total	C	N	O	S	0	0	0
			773	476	162	133	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total 199	C 122	N 48	O 29	0	0	0
21	CU	23	Total 180	C 112	N 41	O 27	0	0	0

- Molecule 22 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AY	95	Total 754	C 472	N 142	O 137	S 3	0	0	0
22	CY	94	Total 739	C 461	N 138	O 137	S 3	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	114	HIS	-	EXPRESSION TAG	UNP P0AD49
AY	115	HIS	-	EXPRESSION TAG	UNP P0AD49
AY	116	HIS	-	EXPRESSION TAG	UNP P0AD49
AY	117	HIS	-	EXPRESSION TAG	UNP P0AD49
AY	118	HIS	-	EXPRESSION TAG	UNP P0AD49
AY	119	HIS	-	EXPRESSION TAG	UNP P0AD49
CY	114	HIS	-	EXPRESSION TAG	UNP P0AD49
CY	115	HIS	-	EXPRESSION TAG	UNP P0AD49
CY	116	HIS	-	EXPRESSION TAG	UNP P0AD49
CY	117	HIS	-	EXPRESSION TAG	UNP P0AD49
CY	118	HIS	-	EXPRESSION TAG	UNP P0AD49
CY	119	HIS	-	EXPRESSION TAG	UNP P0AD49

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2827	Total 60898	C 27101	N 11400	O 19571	P 2826	0	0	0
23	DA	2798	Total 60264	C 26820	N 11274	O 19374	P 2796	0	0	0

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	203	Total	C	N	O	S	0	0	1
			1577	1004	298	273	2			
27	DF	203	Total	C	N	O	S	0	0	1
			1572	1003	298	269	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	146	Total	C	N	O	S	0	0	0
			1043	672	180	190	1			
30	DI	146	Total	C	N	O	S	0	0	0
			1043	672	180	190	1			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BS	110	Total	C	N	O	0	0	0
			865	544	172	149			
36	DS	110	Total	C	N	O	0	0	0
			873	550	174	149			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
37	DT	130	Total	C	N	O	S	0	0	0
			1058	663	212	182	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
39	DV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DW	111	Total	C	N	O	S	0	0	0
			877	552	171	152	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
41	DX	95	Total	C	N	O	S	0	0	0
			732	477	130	124	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
42	DY	107	Total	C	N	O	S	0	0	0
			781	502	145	128	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			
43	DZ	203	Total	C	N	O	S	0	0	0
			1528	973	268	284	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
44	D0	77	Total	C	N	O	S	0	0	0
			607	376	126	104	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
46	D2	71	Total	C	N	O	S	0	0	0
			584	361	118	103	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	B3	59	Total	C	N	O	0	0	0
			458	293	87	78			
47	D3	59	Total	C	N	O	0	0	0
			463	295	87	81			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
49	D5	59	Total	C	N	O	S	0	0	0
			451	283	89	74	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
50	D6	53	Total	C	N	O	S	0	0	0
			437	272	84	77	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
51	D7	48	Total	C	N	O	S	0	0	0
			402	248	97	55	2			

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

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

- Molecule 53 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AP	1	Total	Mg	0	0
			1	1		
54	BA	729	Total	Mg	0	0
			729	729		
54	CA	203	Total	Mg	0	0
			203	203		
54	DQ	4	Total	Mg	0	0
			4	4		
54	DF	5	Total	Mg	0	0
			5	5		
54	B8	1	Total	Mg	0	0
			1	1		
54	BE	6	Total	Mg	0	0
			6	6		
54	B1	1	Total	Mg	0	0
			1	1		
54	BP	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	DD	5	Total Mg 5 5	0	0
54	B5	1	Total Mg 1 1	0	0
54	BB	19	Total Mg 19 19	0	0
54	BT	3	Total Mg 3 3	0	0
54	D8	2	Total Mg 2 2	0	0
54	AE	1	Total Mg 1 1	0	0
54	B9	3	Total Mg 3 3	0	0
54	BF	6	Total Mg 6 6	0	0
54	DR	2	Total Mg 2 2	0	0
54	B2	2	Total Mg 2 2	0	0
54	AA	217	Total Mg 217 217	0	0
54	BQ	5	Total Mg 5 5	0	0
54	CQ	1	Total Mg 1 1	0	0
54	D7	2	Total Mg 2 2	0	0
54	B6	1	Total Mg 1 1	0	0
54	AM	2	Total Mg 2 2	0	0
54	BU	3	Total Mg 3 3	0	0
54	AD	2	Total Mg 2 2	0	0
54	BN	2	Total Mg 2 2	0	0
54	D0	1	Total Mg 1 1	0	0
54	BG	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	AI	1	Total Mg 1 1	0	0
54	BY	1	Total Mg 1 1	0	0
54	DE	3	Total Mg 3 3	0	0
54	B3	3	Total Mg 3 3	0	0
54	BR	5	Total Mg 5 5	0	0
54	D9	1	Total Mg 1 1	0	0
54	DA	637	Total Mg 637 637	0	0
54	DP	3	Total Mg 3 3	0	0
54	DW	1	Total Mg 1 1	0	0
54	B7	1	Total Mg 1 1	0	0
54	AL	1	Total Mg 1 1	0	0
54	BV	4	Total Mg 4 4	0	0
54	DO	3	Total Mg 3 3	0	0
54	BO	1	Total Mg 1 1	0	0
54	D1	1	Total Mg 1 1	0	0
54	BZ	2	Total Mg 2 2	0	0
54	BS	1	Total Mg 1 1	0	0
54	D5	2	Total Mg 2 2	0	0
54	BD	7	Total Mg 7 7	0	0
54	DT	2	Total Mg 2 2	0	0
54	B0	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	CE	1	Total Mg 1 1	0	0
54	BW	1	Total Mg 1 1	0	0
54	DB	10	Total Mg 10 10	0	0
54	AF	1	Total Mg 1 1	0	0
54	BH	1	Total Mg 1 1	0	0

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

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	443	Total O 443 443	0	0
56	AD	3	Total O 3 3	0	0
56	AE	2	Total O 2 2	0	0
56	AF	2	Total O 2 2	0	0
56	AG	2	Total O 2 2	0	0
56	AJ	1	Total O 1 1	0	0
56	AK	1	Total O 1 1	0	0
56	AL	3	Total O 3 3	0	0
56	AM	1	Total O 1 1	0	0
56	AO	1	Total O 1 1	0	0
56	AP	1	Total O 1 1	0	0
56	AQ	3	Total O 3 3	0	0
56	AY	1	Total O 1 1	0	0
56	BA	1988	Total O 1988 1988	0	0
56	BB	43	Total O 43 43	0	0
56	BD	21	Total O 21 21	0	0
56	BE	18	Total O 18 18	0	0
56	BF	18	Total O 18 18	0	0
56	BG	2	Total O 2 2	0	0
56	BH	2	Total O 2 2	0	0
56	BN	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	BO	3	Total O 3 3	0	0
56	BP	20	Total O 20 20	0	0
56	BQ	9	Total O 9 9	0	0
56	BR	8	Total O 8 8	0	0
56	BS	2	Total O 2 2	0	0
56	BT	5	Total O 5 5	0	0
56	BU	9	Total O 9 9	0	0
56	BV	13	Total O 13 13	0	0
56	BW	6	Total O 6 6	0	0
56	BX	2	Total O 2 2	0	0
56	BY	2	Total O 2 2	0	0
56	BZ	2	Total O 2 2	0	0
56	B0	4	Total O 4 4	0	0
56	B1	5	Total O 5 5	0	0
56	B3	4	Total O 4 4	0	0
56	B5	5	Total O 5 5	0	0
56	B6	2	Total O 2 2	0	0
56	B7	5	Total O 5 5	0	0
56	B8	11	Total O 11 11	0	0
56	B9	1	Total O 1 1	0	0
56	CA	400	Total O 400 400	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	CD	2	Total O 2 2	0	0
56	CE	4	Total O 4 4	0	0
56	CF	1	Total O 1 1	0	0
56	CK	1	Total O 1 1	0	0
56	CL	2	Total O 2 2	0	0
56	CP	3	Total O 3 3	0	0
56	CQ	3	Total O 3 3	0	0
56	CR	1	Total O 1 1	0	0
56	CT	2	Total O 2 2	0	0
56	CU	1	Total O 1 1	0	0
56	DA	1496	Total O 1496 1496	0	0
56	DB	33	Total O 33 33	0	0
56	DD	17	Total O 17 17	0	0
56	DE	12	Total O 12 12	0	0
56	DF	10	Total O 10 10	0	0
56	DN	2	Total O 2 2	0	0
56	DO	7	Total O 7 7	0	0
56	DP	11	Total O 11 11	0	0
56	DQ	2	Total O 2 2	0	0
56	DR	5	Total O 5 5	0	0
56	DT	3	Total O 3 3	0	0

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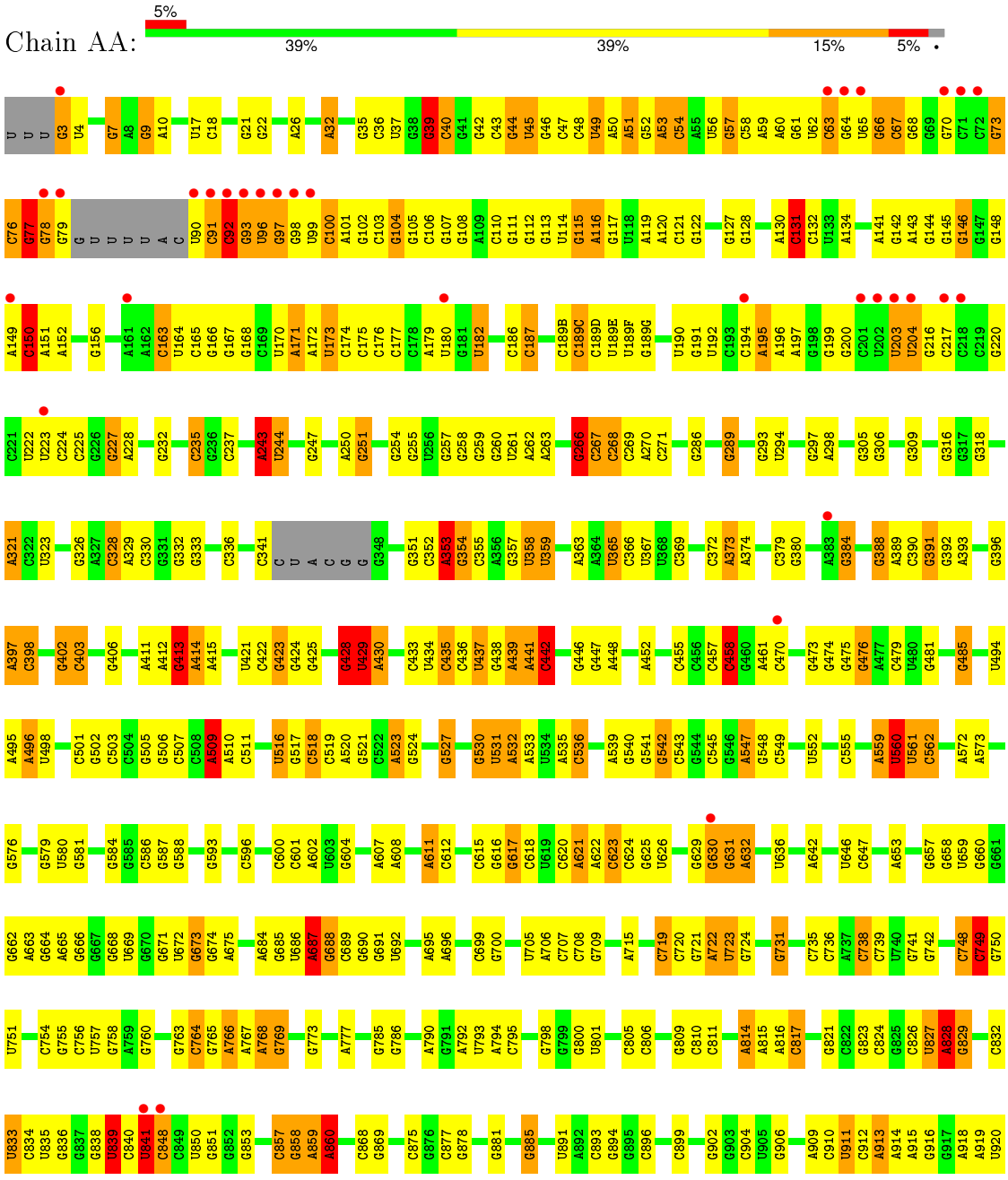
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DU	1	Total O 1 1	0	0
56	DV	1	Total O 1 1	0	0
56	DW	4	Total O 4 4	0	0
56	DX	2	Total O 2 2	0	0
56	DY	2	Total O 2 2	0	0
56	D0	2	Total O 2 2	0	0
56	D1	3	Total O 3 3	0	0
56	D2	1	Total O 1 1	0	0
56	D3	1	Total O 1 1	0	0
56	D5	3	Total O 3 3	0	0
56	D6	3	Total O 3 3	0	0
56	D7	3	Total O 3 3	0	0
56	D8	6	Total O 6 6	0	0
56	D9	1	Total O 1 1	0	0

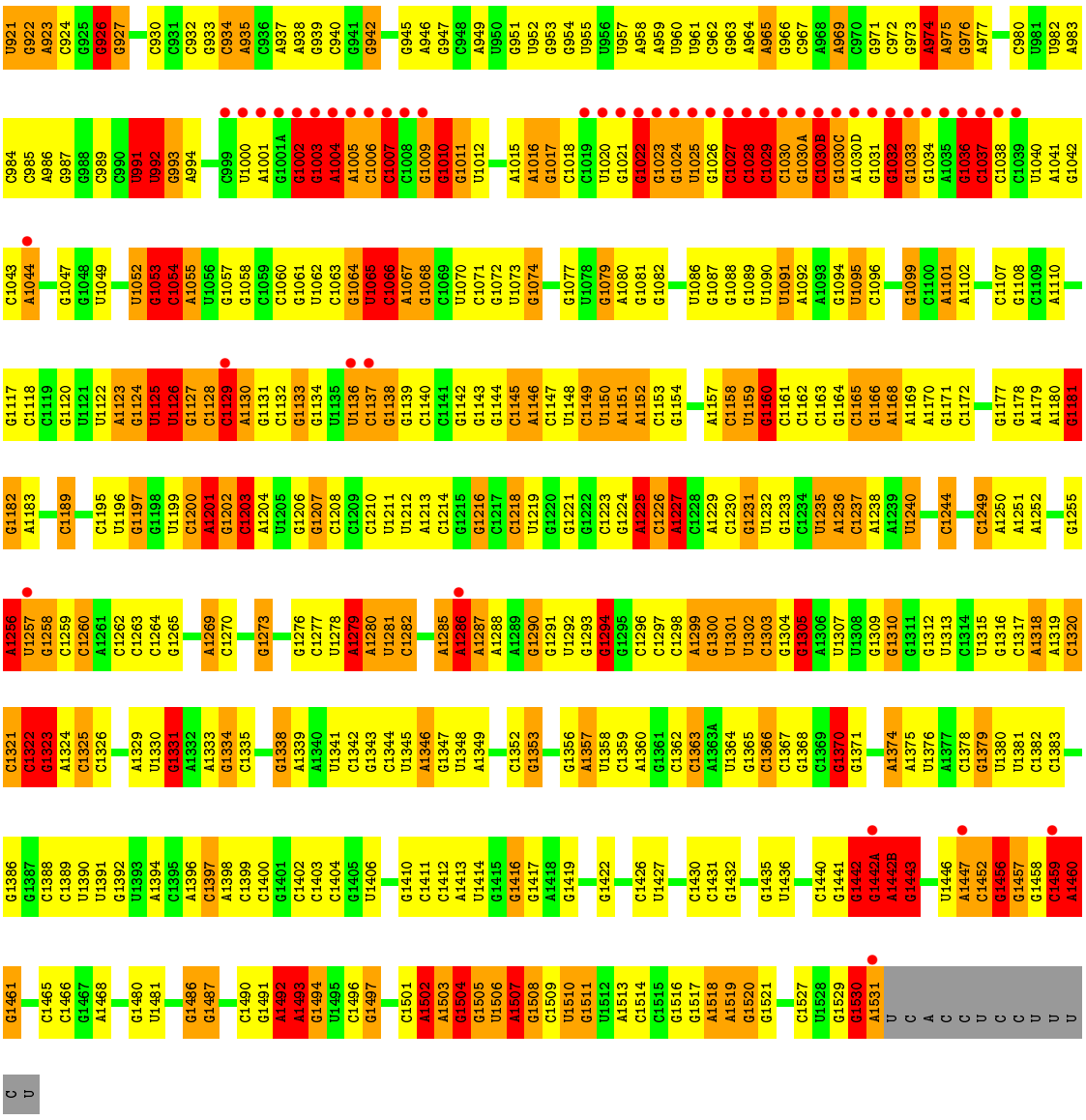
3 Residue-property plots (i)

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 Ribosomal RNA

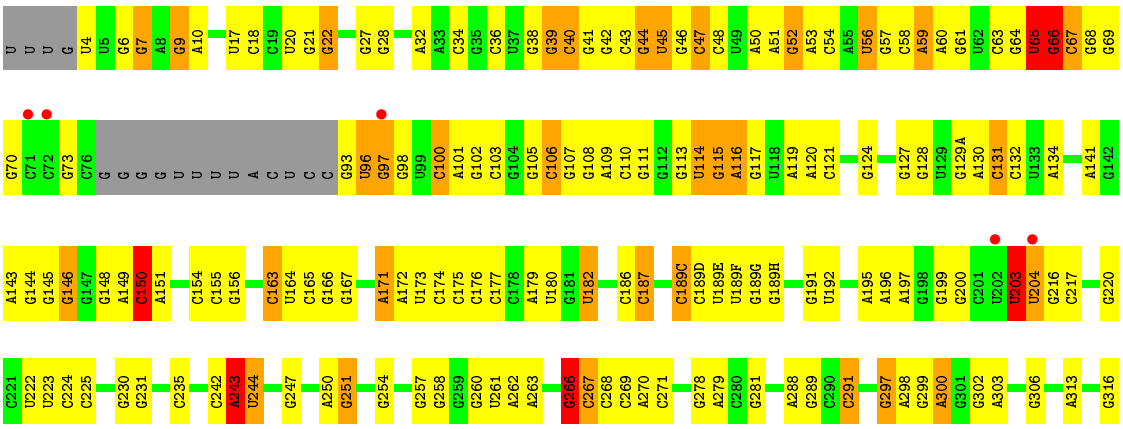
Chain AA:

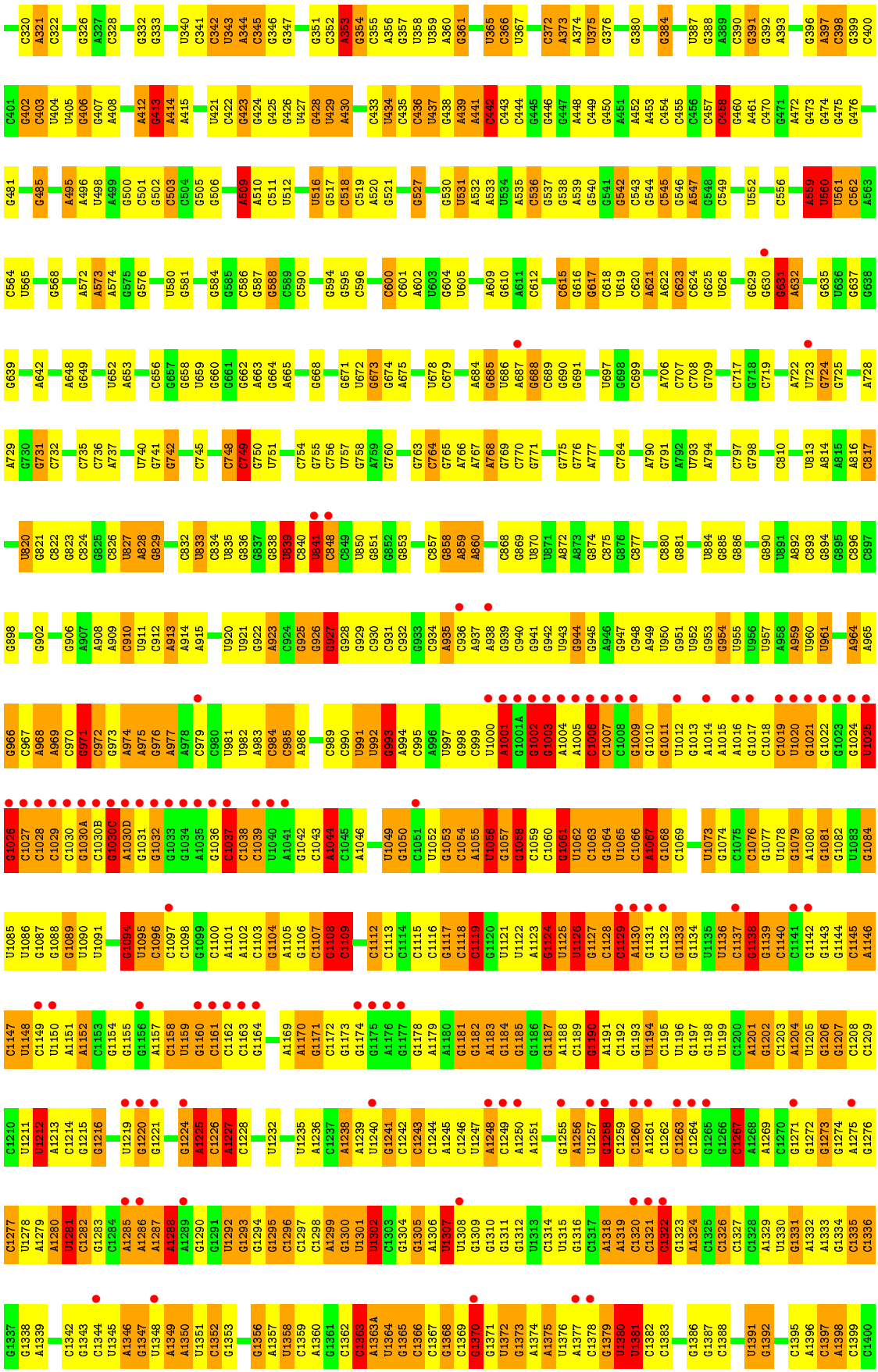


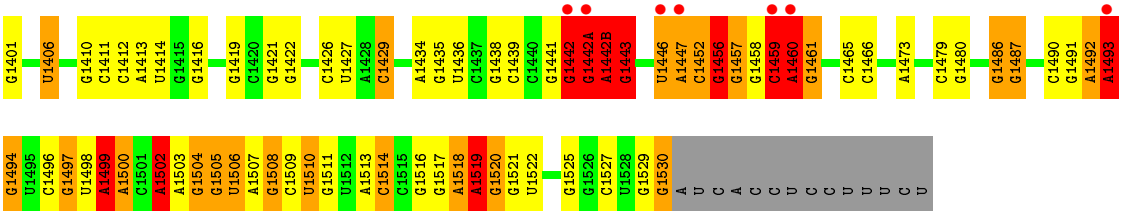


• Molecule 1: 16S Ribosomal RNA

Chain CA:

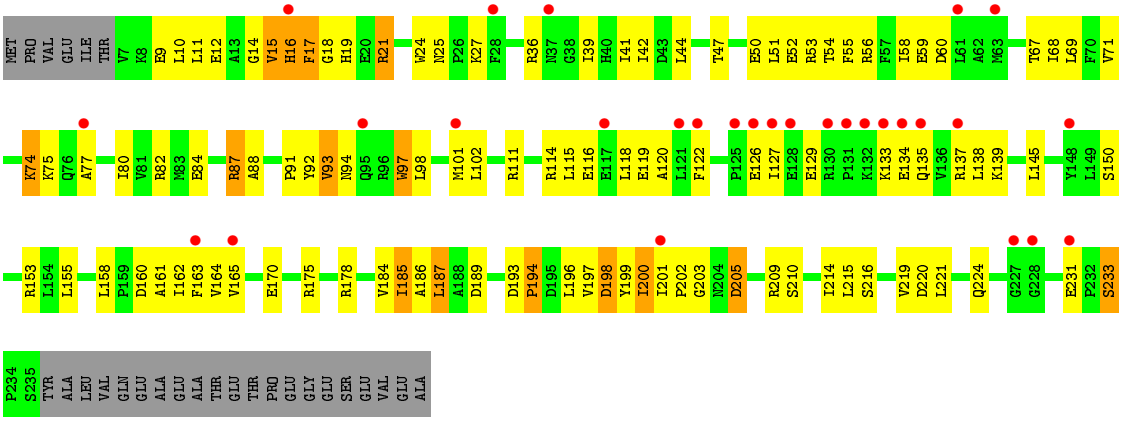






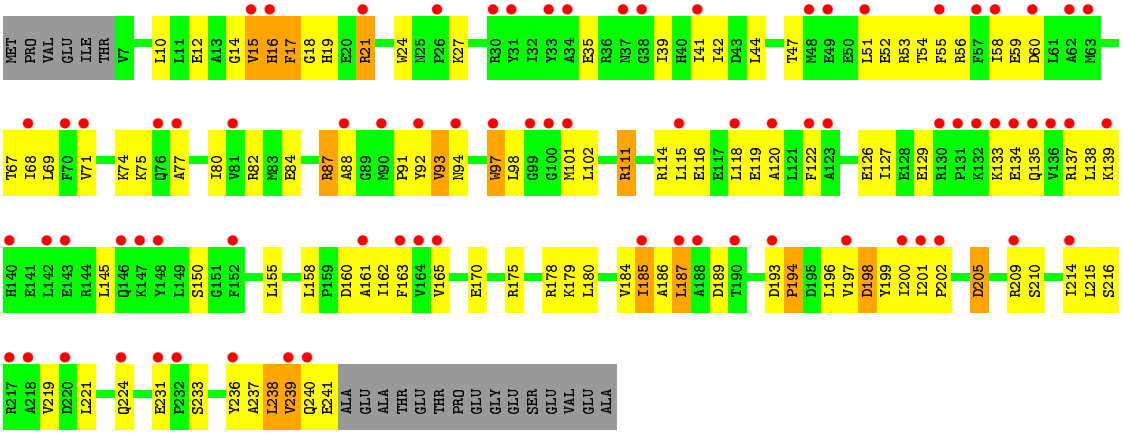
• Molecule 2: 30S Ribosomal Protein S2

Chain AB:



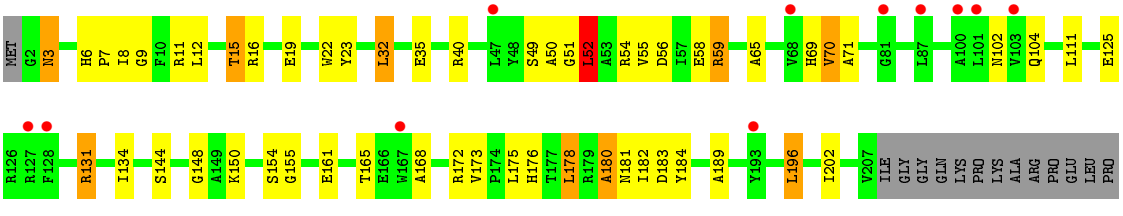
• Molecule 2: 30S Ribosomal Protein S2

Chain CB:

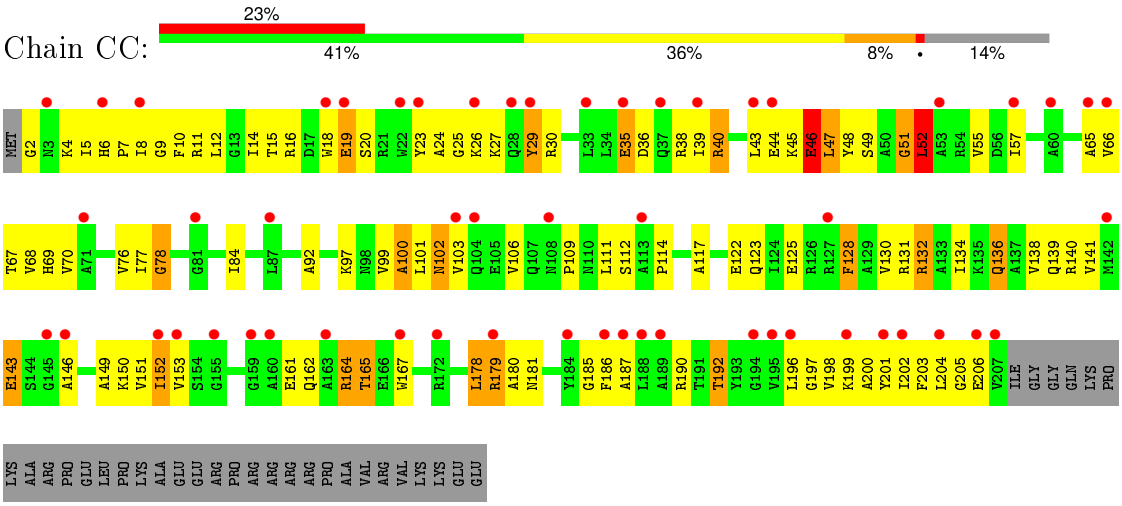


• Molecule 3: 30S Ribosomal Protein S3

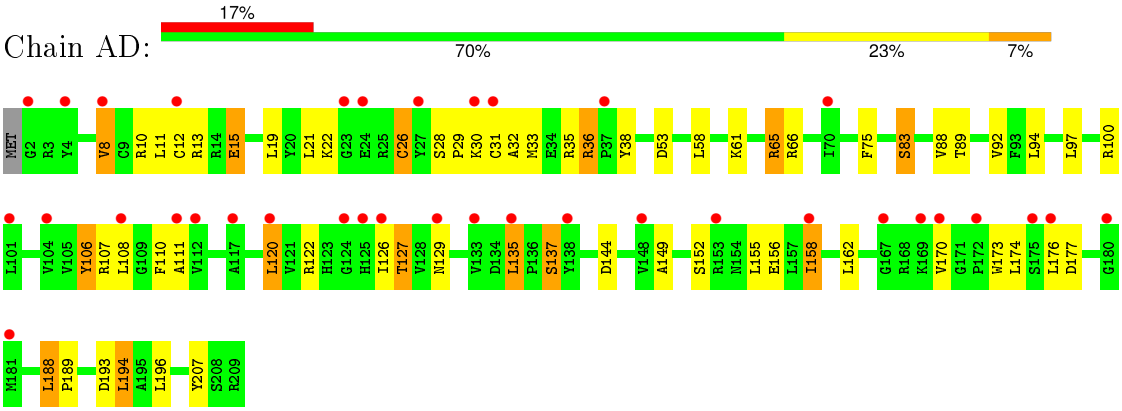
Chain AC:



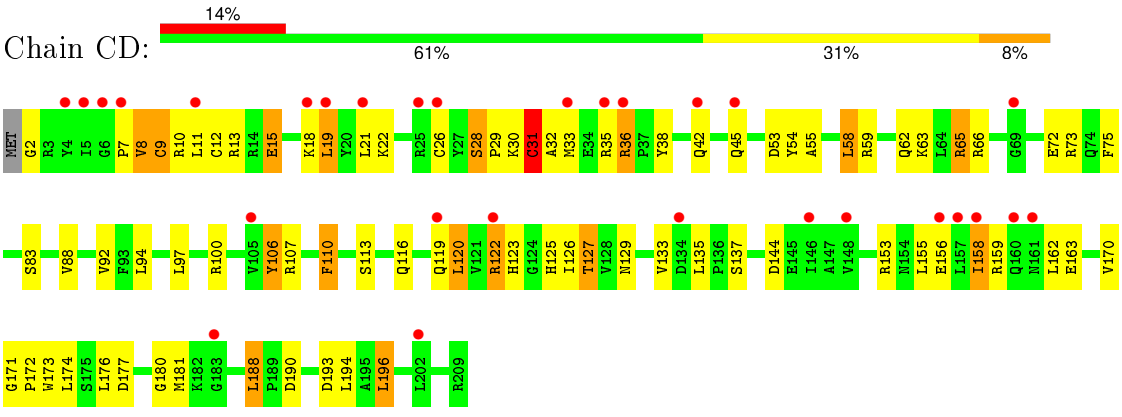
- Molecule 3: 30S Ribosomal Protein S3



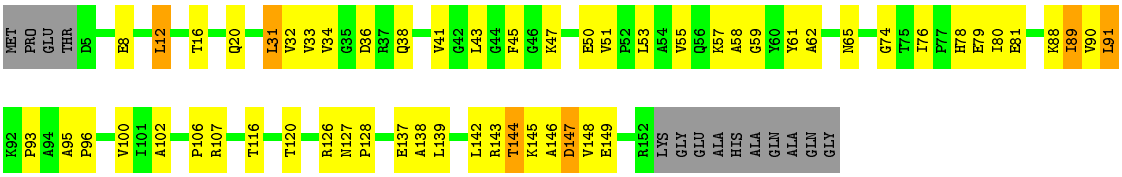
- Molecule 4: 30S Ribosomal Protein S4



- Molecule 4: 30S Ribosomal Protein S4

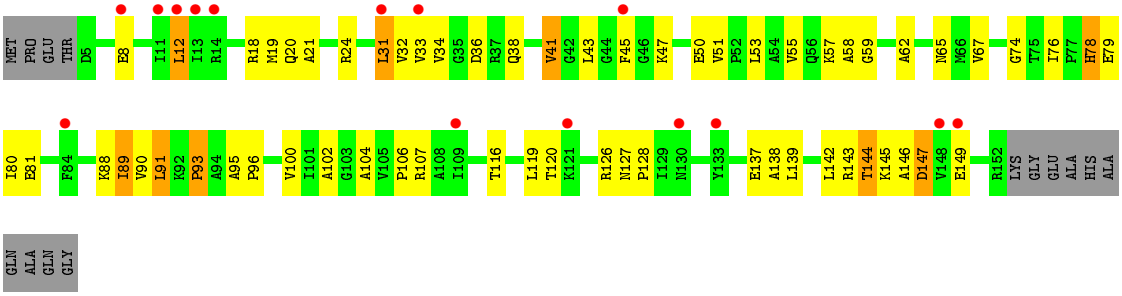


- Molecule 5: 30S Ribosomal Protein S5



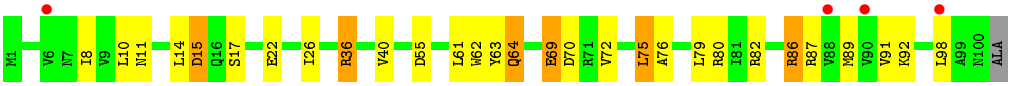
• Molecule 5: 30S Ribosomal Protein S5

Chain CE:



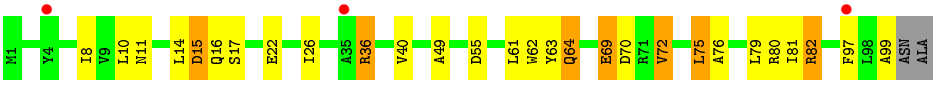
• Molecule 6: 30S Ribosomal Protein S6

Chain AF:



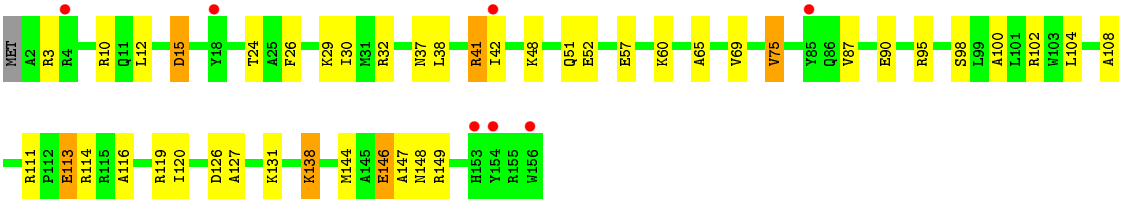
• Molecule 6: 30S Ribosomal Protein S6

Chain CF:



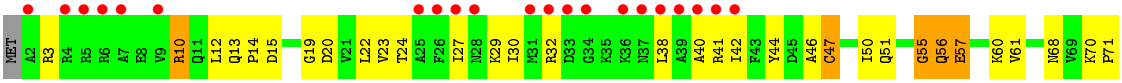
• Molecule 7: 30S Ribosomal Protein S7

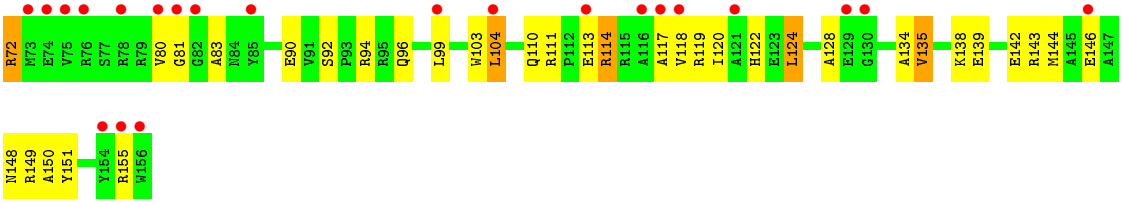
Chain AG:



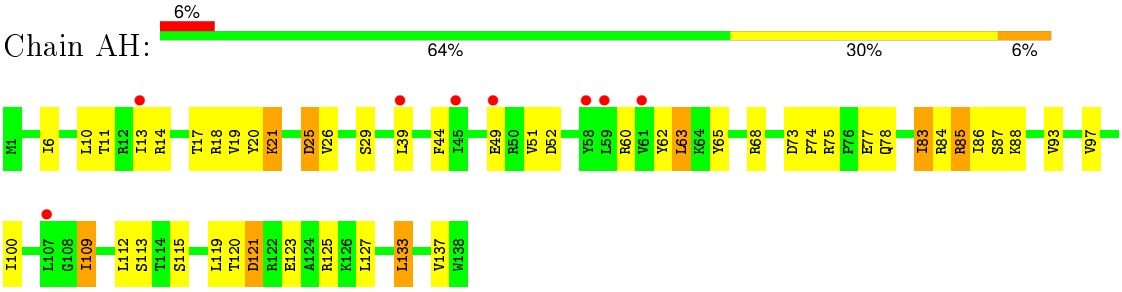
• Molecule 7: 30S Ribosomal Protein S7

Chain CG:

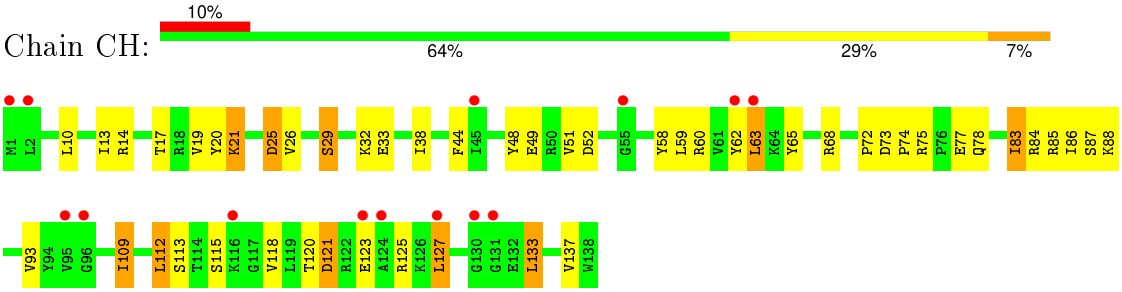




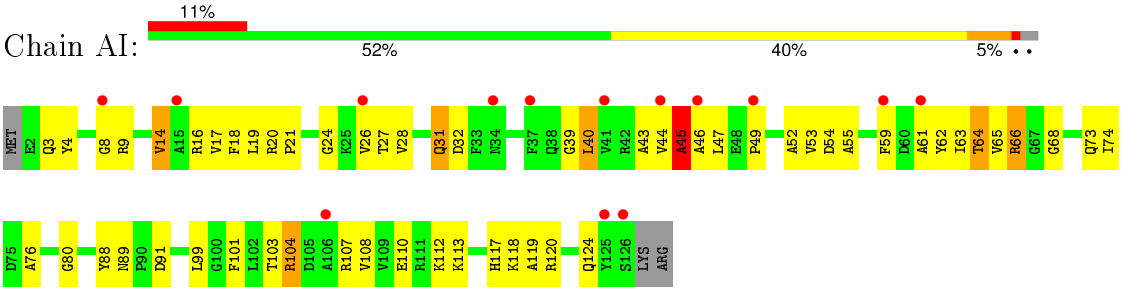
• Molecule 8: 30S Ribosomal Protein S8



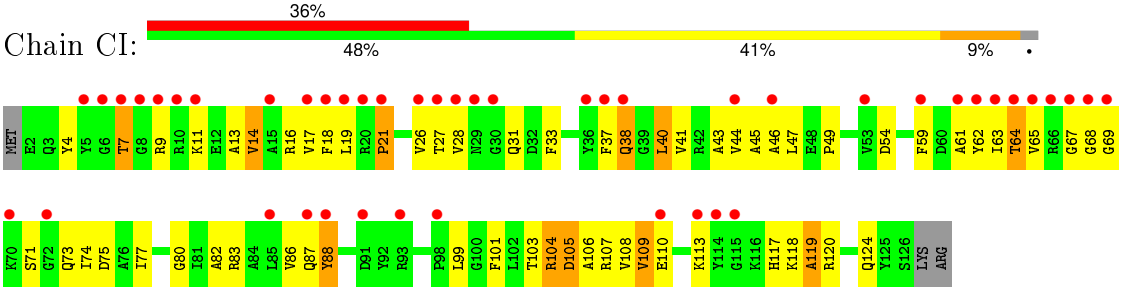
• Molecule 8: 30S Ribosomal Protein S8



• Molecule 9: 30S Ribosomal Protein S9

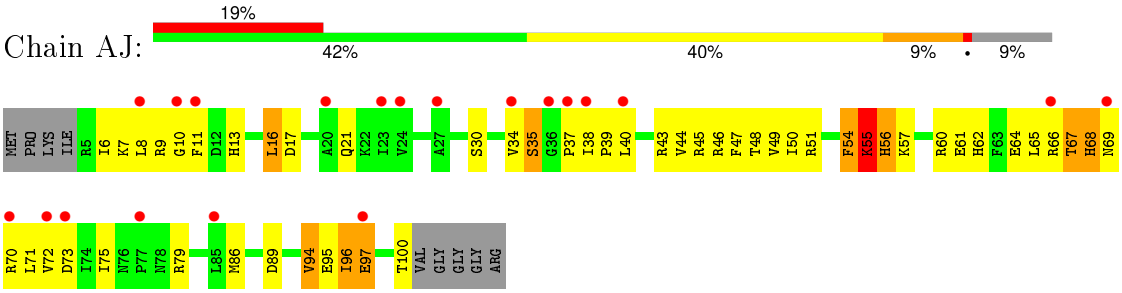


• Molecule 9: 30S Ribosomal Protein S9



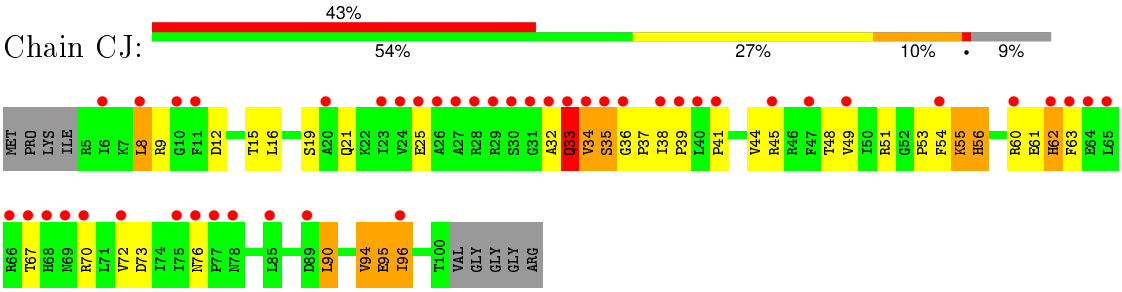
• Molecule 10: 30S Ribosomal Protein S10

Chain AJ:



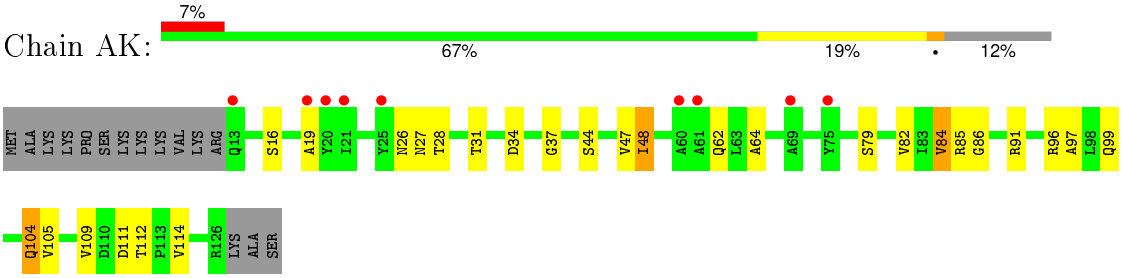
- Molecule 10: 30S Ribosomal Protein S10

Chain CJ:



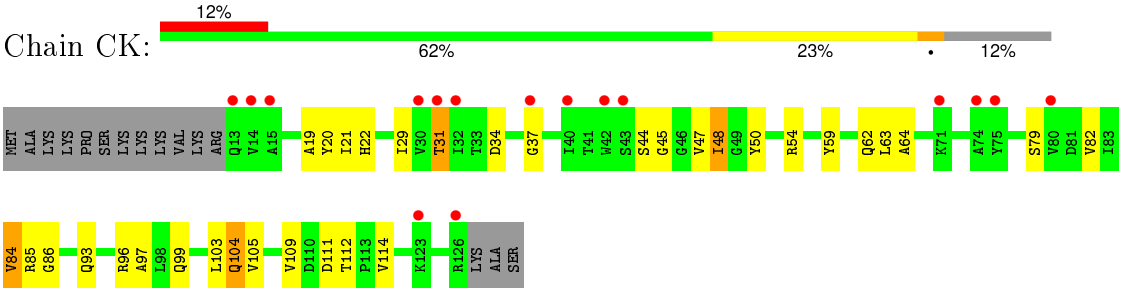
- Molecule 11: 30S Ribosomal Protein S11

Chain AK:



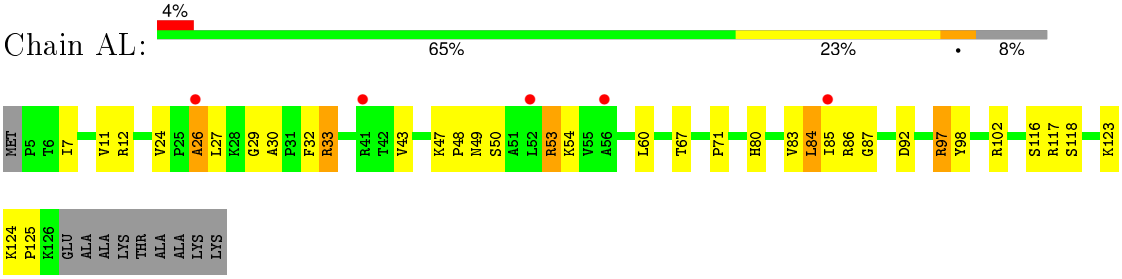
- Molecule 11: 30S Ribosomal Protein S11

Chain CK:



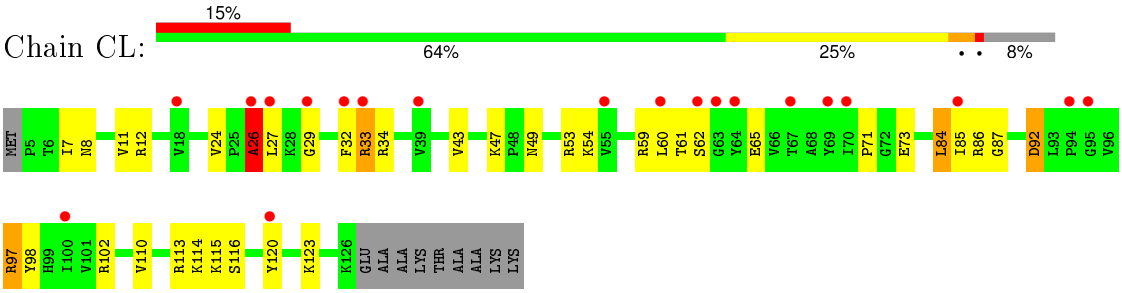
- Molecule 12: 30S Ribosomal Protein S12

Chain AL:



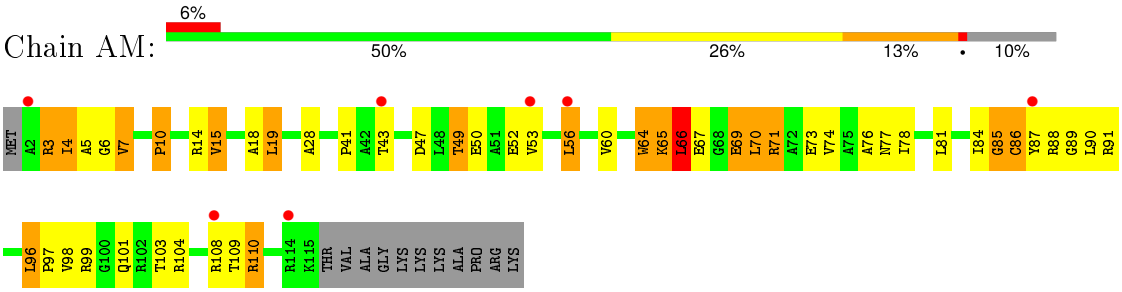
- Molecule 12: 30S Ribosomal Protein S12

Chain CL:



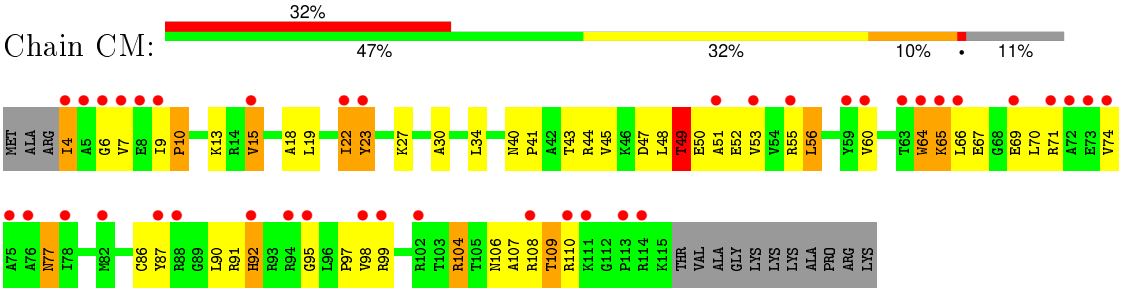
- Molecule 13: 30S Ribosomal Protein S13

Chain AM:



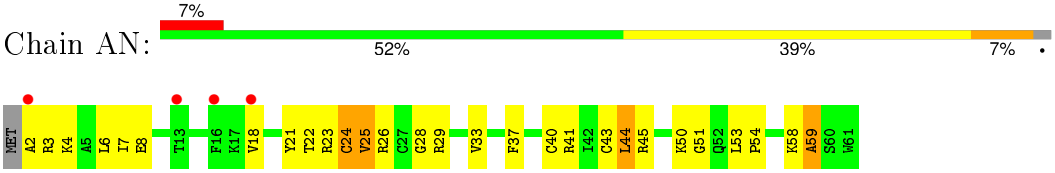
- Molecule 13: 30S Ribosomal Protein S13

Chain CM:



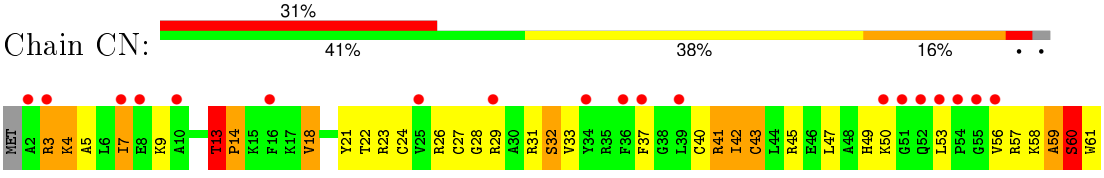
- Molecule 14: 30S Ribosomal Protein S14

Chain AN:



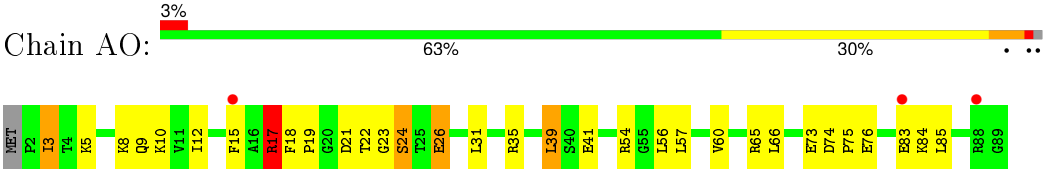
- Molecule 14: 30S Ribosomal Protein S14

Chain CN:



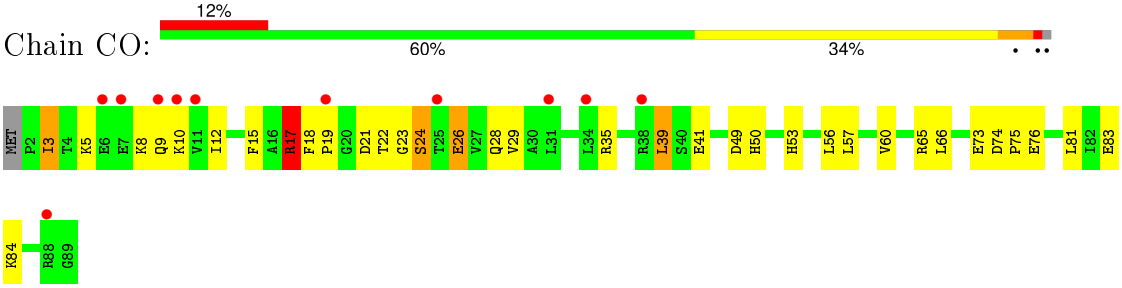
- Molecule 15: 30S Ribosomal Protein S15

Chain AO:



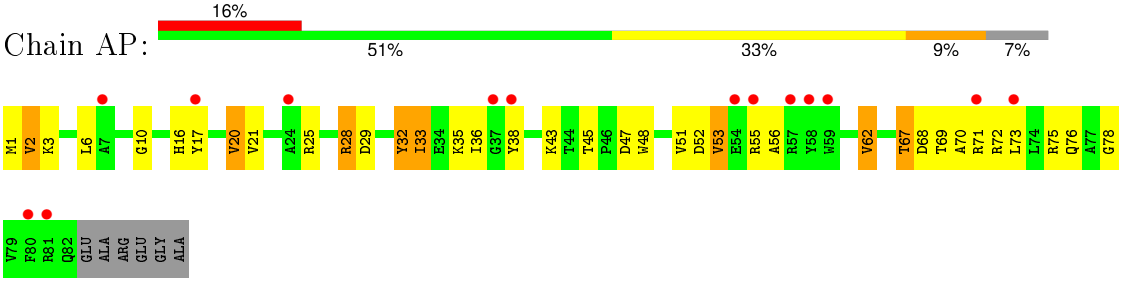
- Molecule 15: 30S Ribosomal Protein S15

Chain CO:



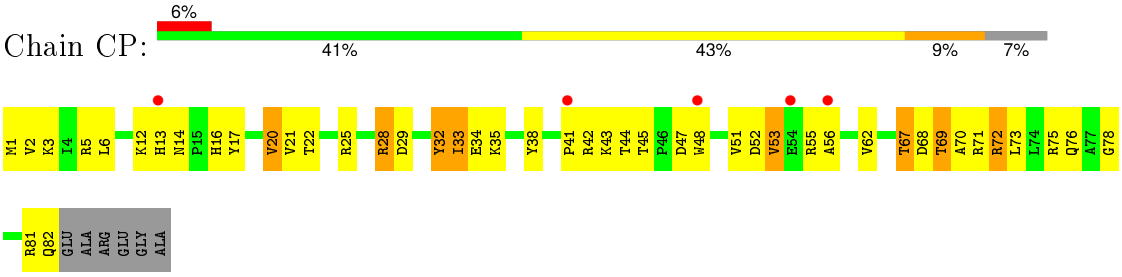
- Molecule 16: 30S Ribosomal Protein S16

Chain AP:



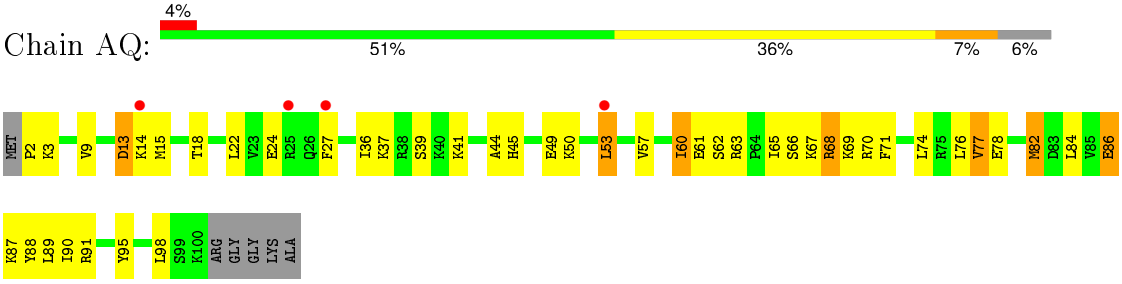
- Molecule 16: 30S Ribosomal Protein S16

Chain CP:



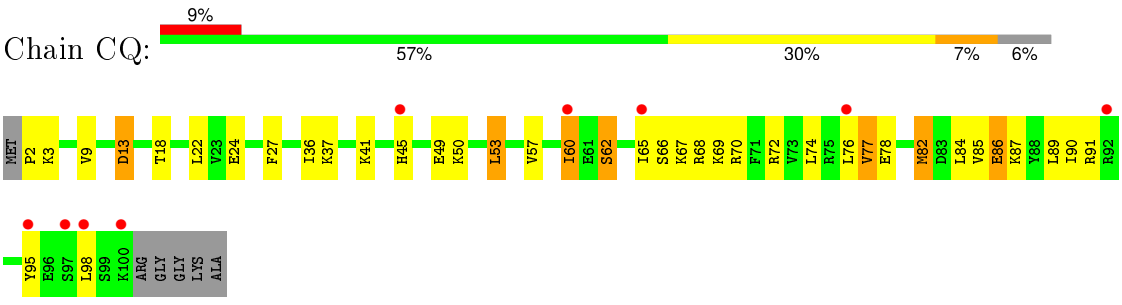
- Molecule 17: 30S Ribosomal Protein S17

Chain AQ:



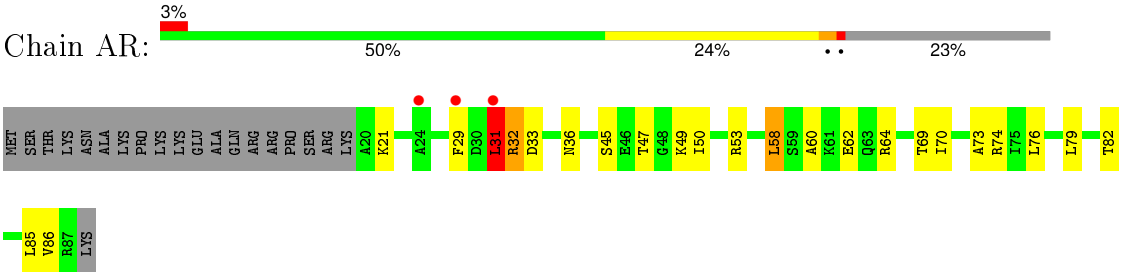
- Molecule 17: 30S Ribosomal Protein S17

Chain CQ:



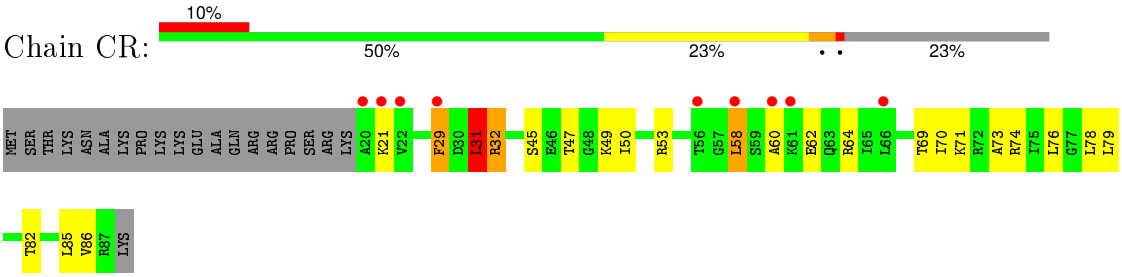
- Molecule 18: 30S Ribosomal Protein S18

Chain AR:



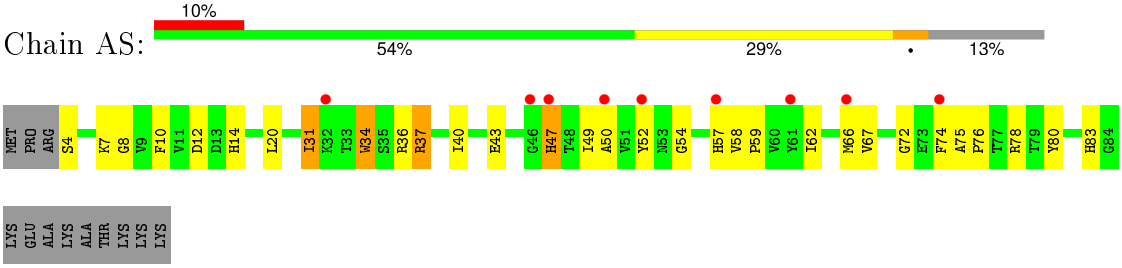
- Molecule 18: 30S Ribosomal Protein S18

Chain CR:



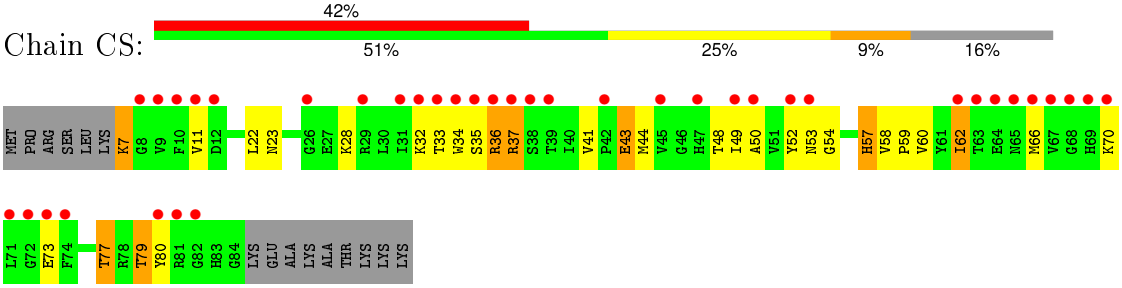
- Molecule 19: 30S Ribosomal Protein S19

Chain AS:



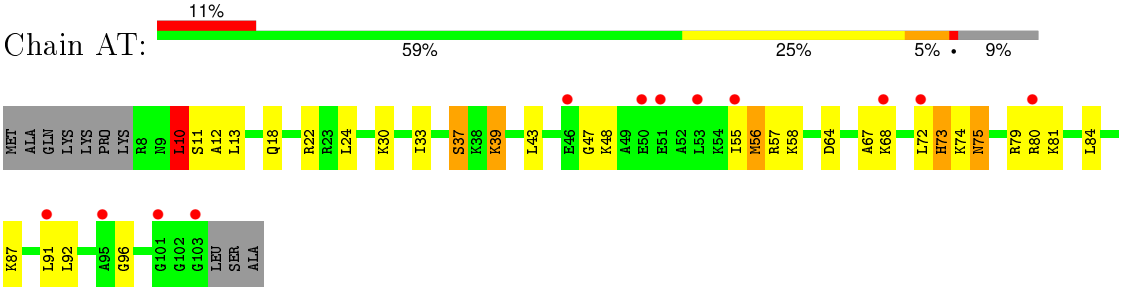
- Molecule 19: 30S Ribosomal Protein S19

Chain CS:



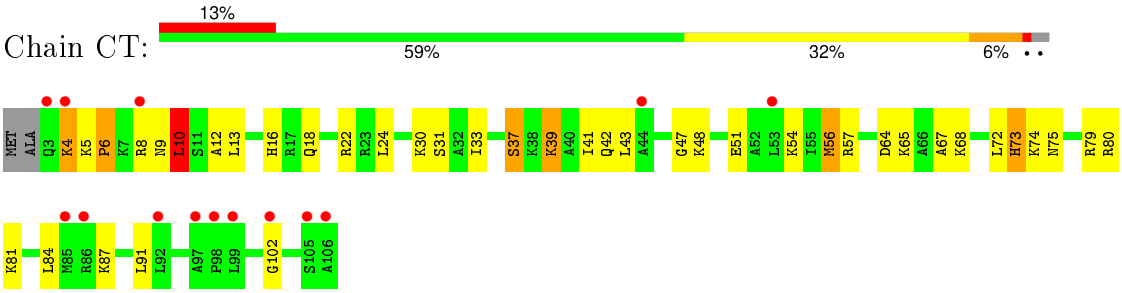
- Molecule 20: 30S Ribosomal Protein S20

Chain AT:



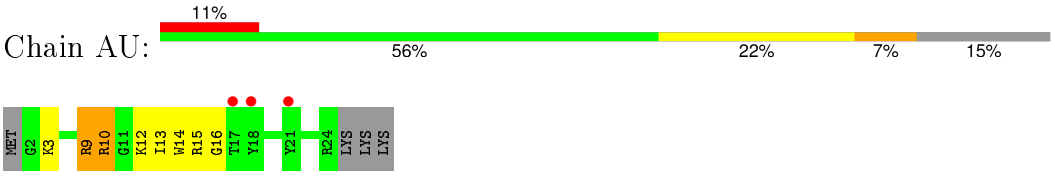
- Molecule 20: 30S Ribosomal Protein S20

Chain CT:



- Molecule 21: 30S Ribosomal Protein THX

Chain AU:

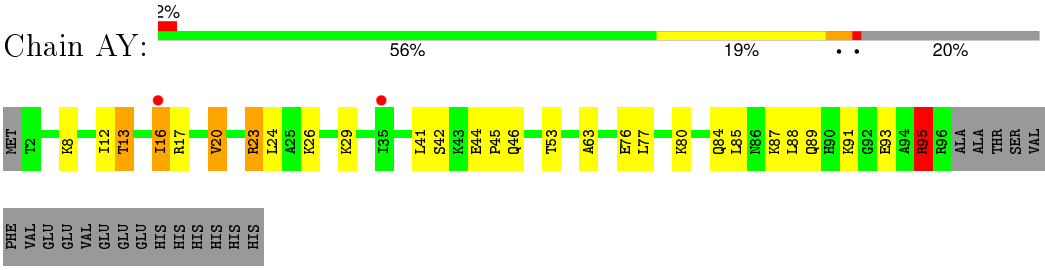


- Molecule 21: 30S Ribosomal Protein THX

Chain CU:

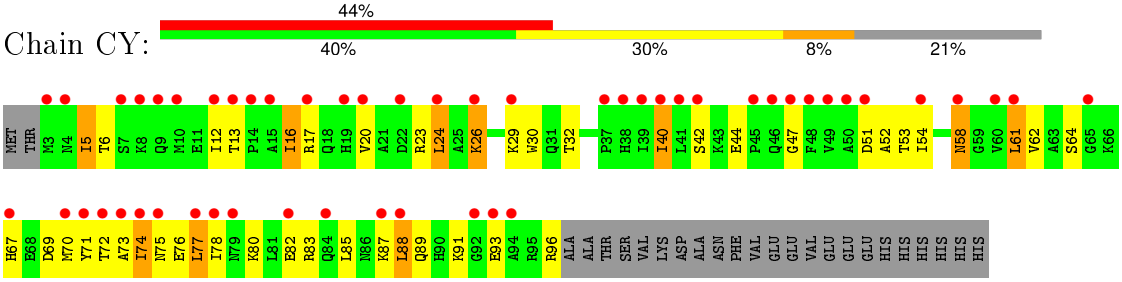
- Molecule 22: Ribosome-associated inhibitor A

Chain AY:



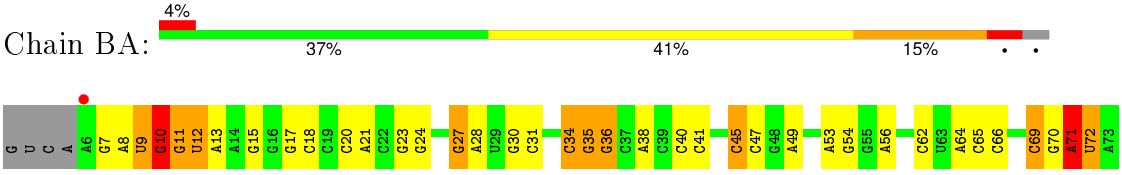
- Molecule 22: Ribosome-associated inhibitor A

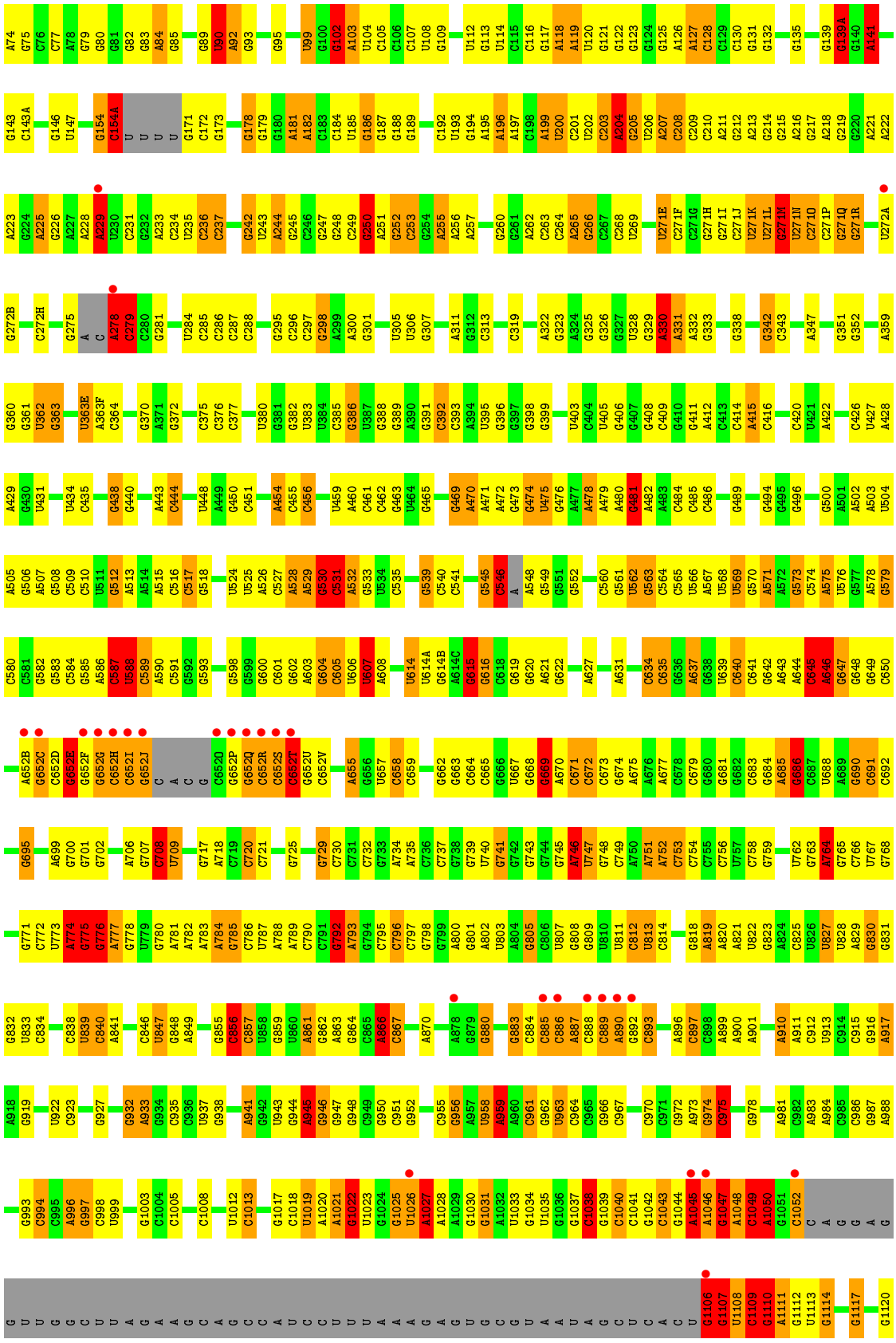
Chain CY:

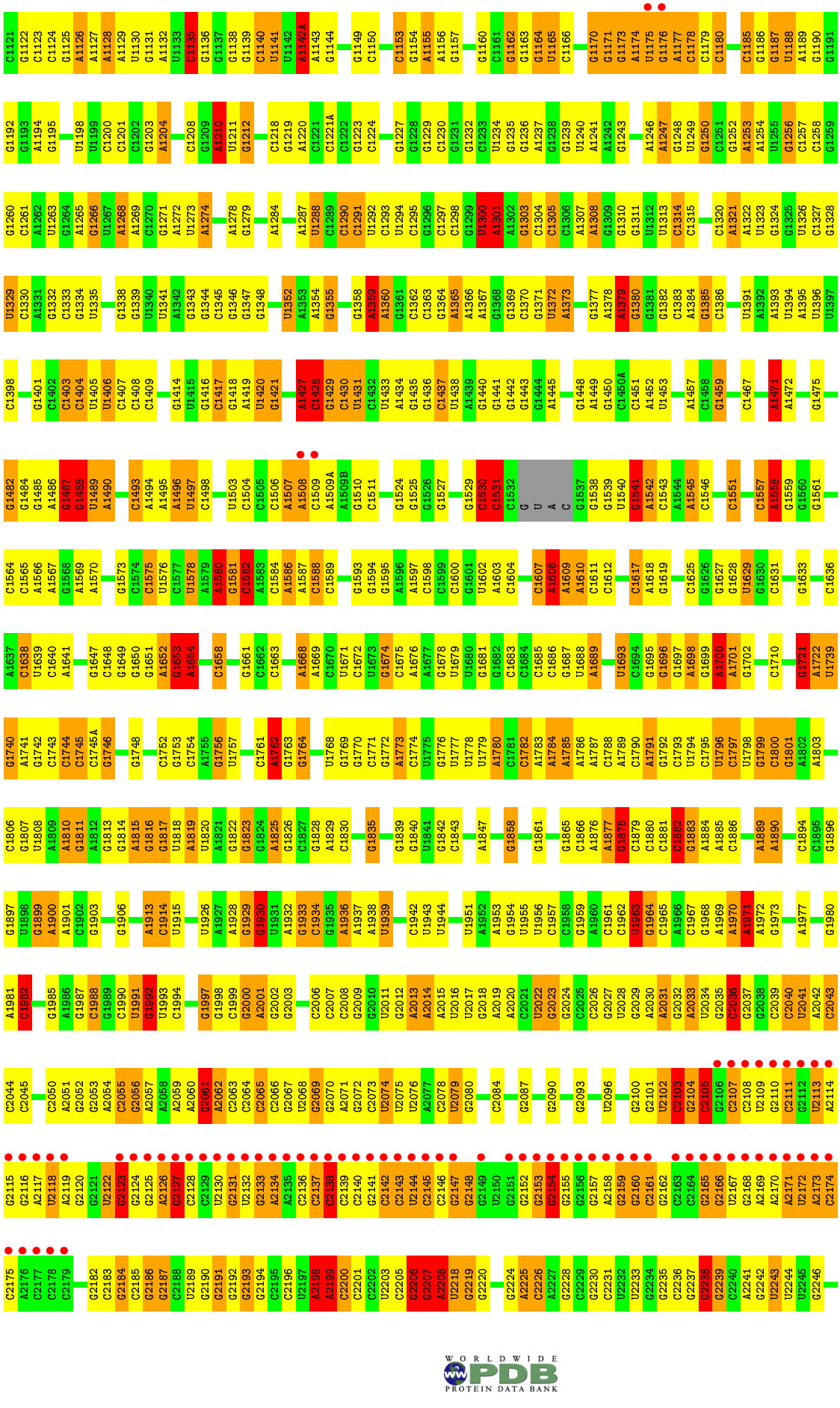


- Molecule 23: 23S Ribosomal RNA

Chain BA:



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G1192 G1193 A1194 G1195 U1198 U1199 C1200 C1201 C1202 G1203 A1204 C1208 G1209 A1210 U1211 G1212 C1218 G1219 A1220 C1221 C1221A C1222 G1223 C1224 G1227 G1228 G1229 C1230 G1231 G1232 C1233 U1234 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1242 G1243 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259
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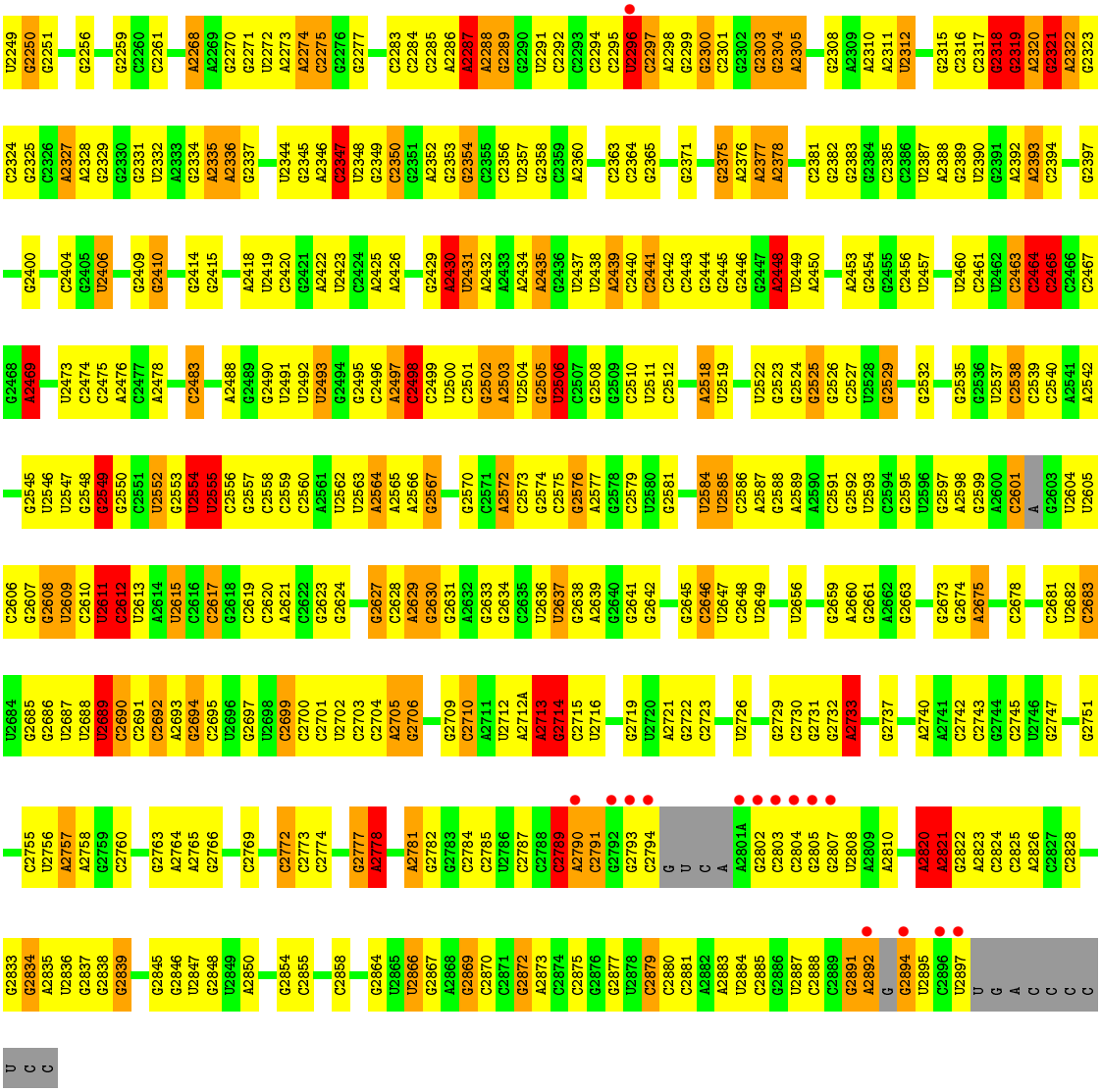
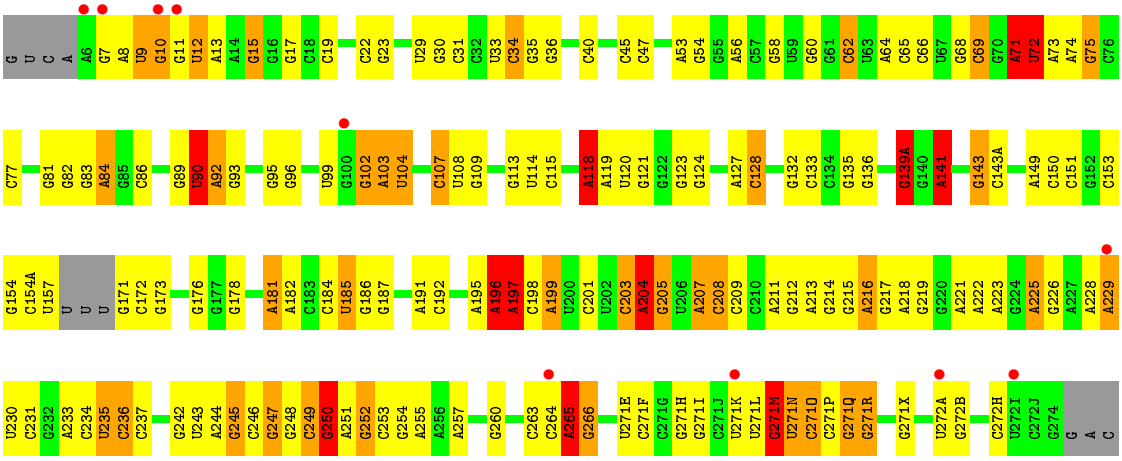
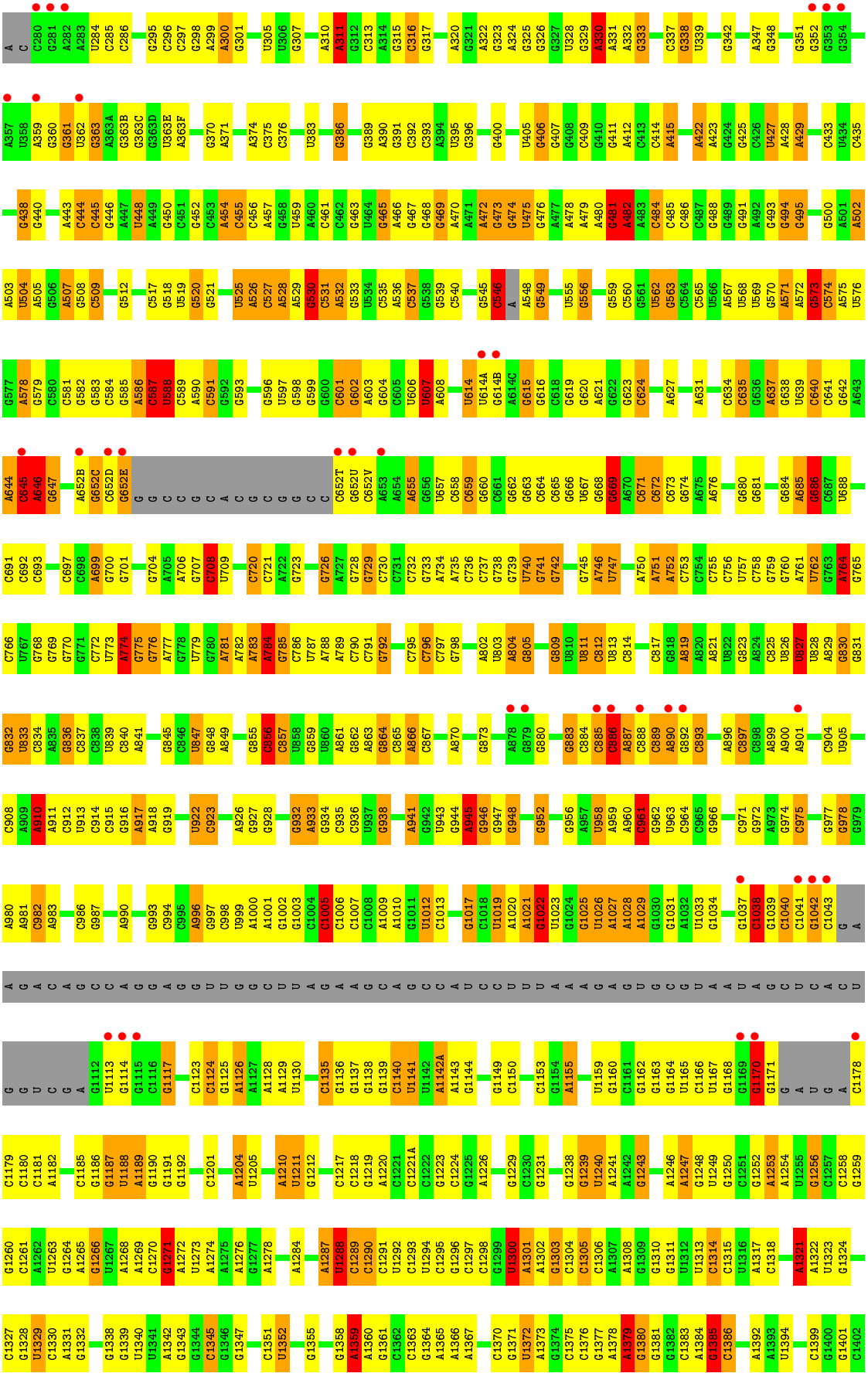
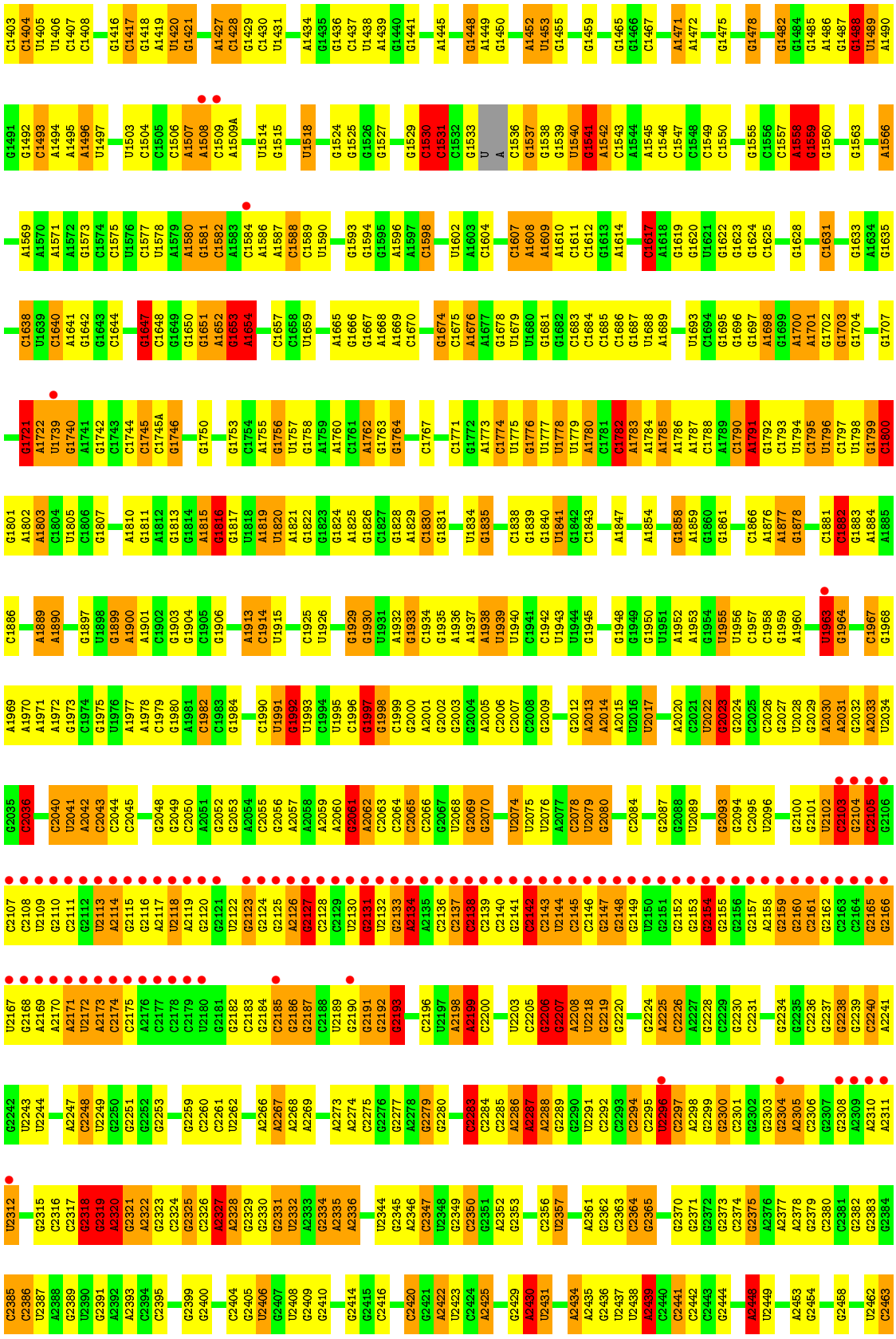


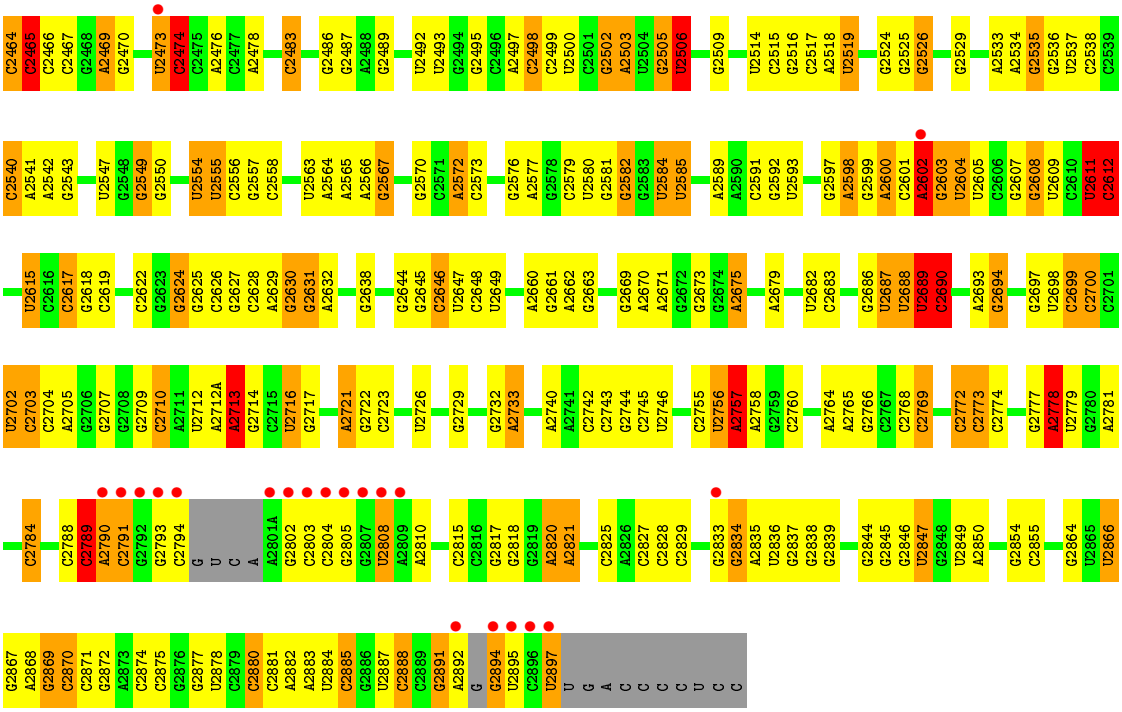
• Molecule 23: 23S Ribosomal RNA

Chain DA:



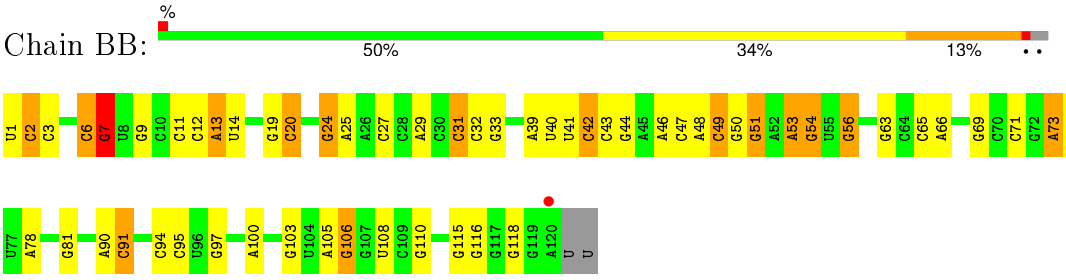






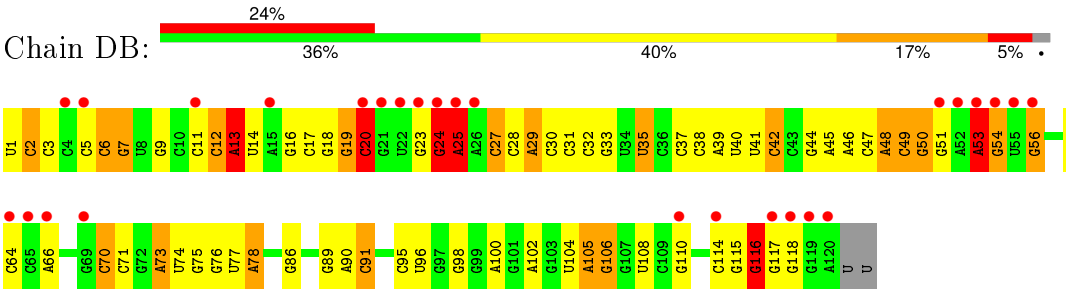
- Molecule 24: 5S Ribosomal RNA

Chain BB:



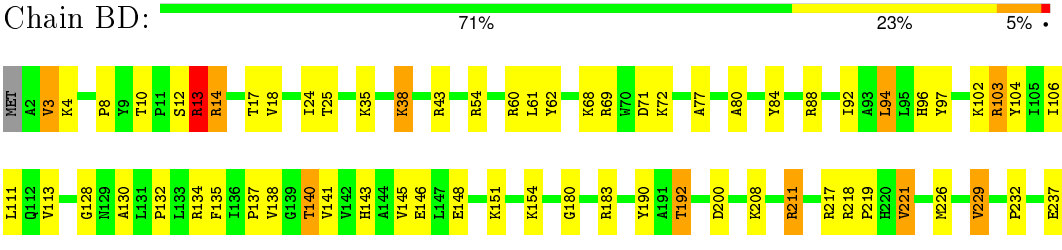
- Molecule 24: 5S Ribosomal RNA

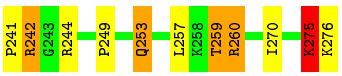
Chain DB:



- Molecule 25: 50S Ribosomal Protein L2

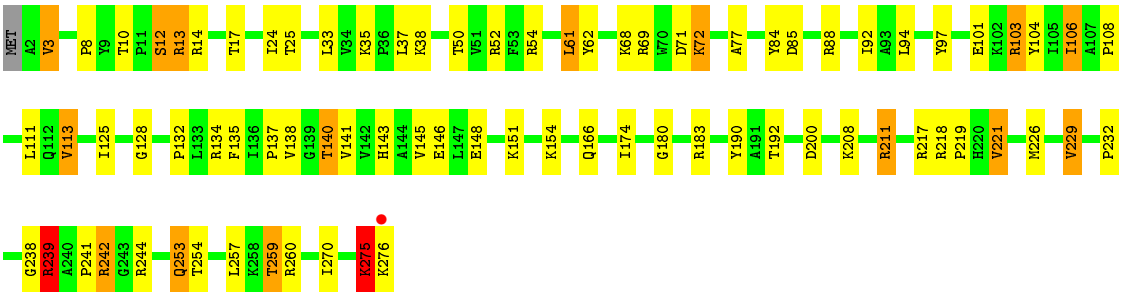
Chain BD:





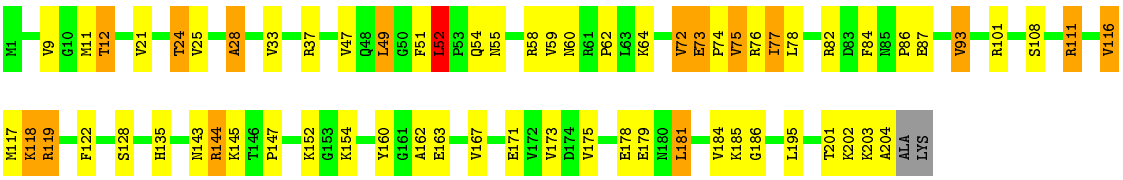
• Molecule 25: 50S Ribosomal Protein L2

Chain DD:



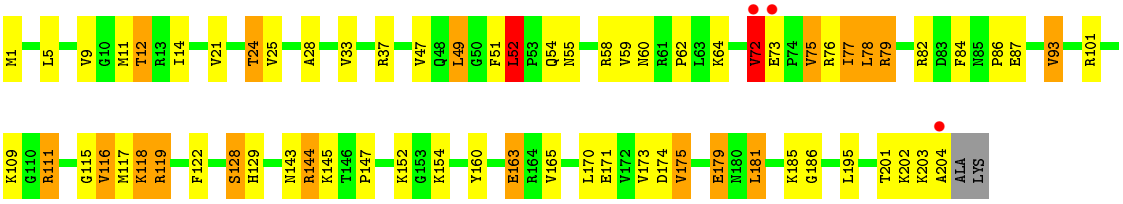
• Molecule 26: 50S Ribosomal Protein L3

Chain BE:



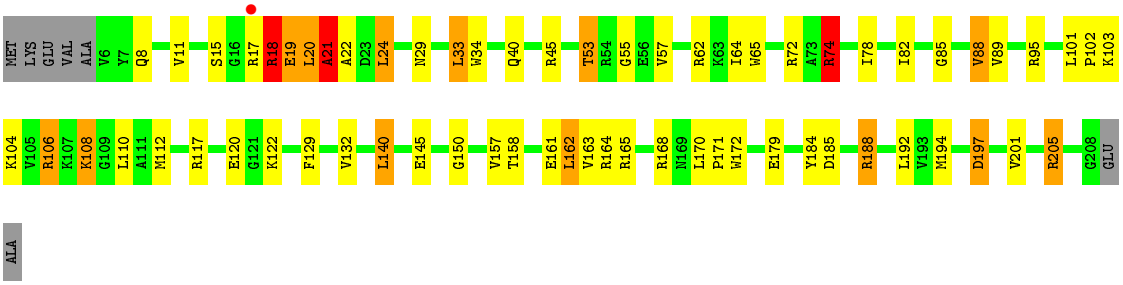
• Molecule 26: 50S Ribosomal Protein L3

Chain DE:



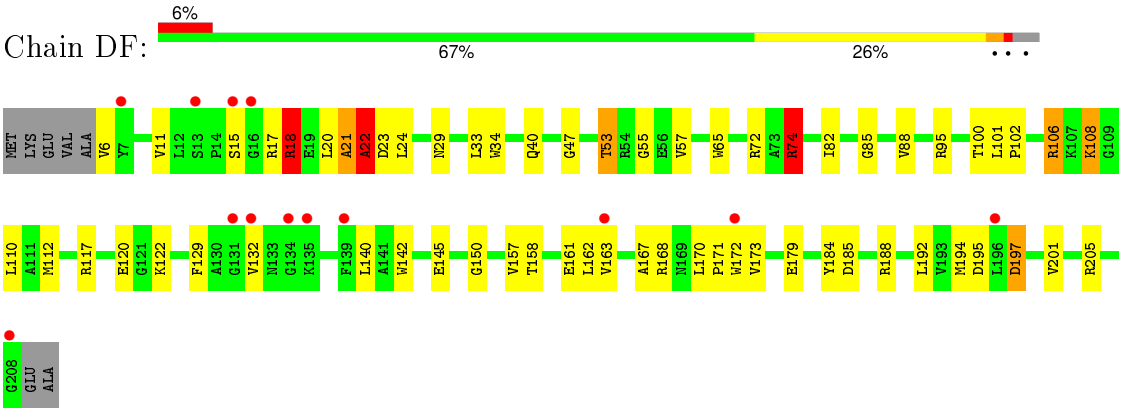
• Molecule 27: 50S Ribosomal Protein L4

Chain BF:



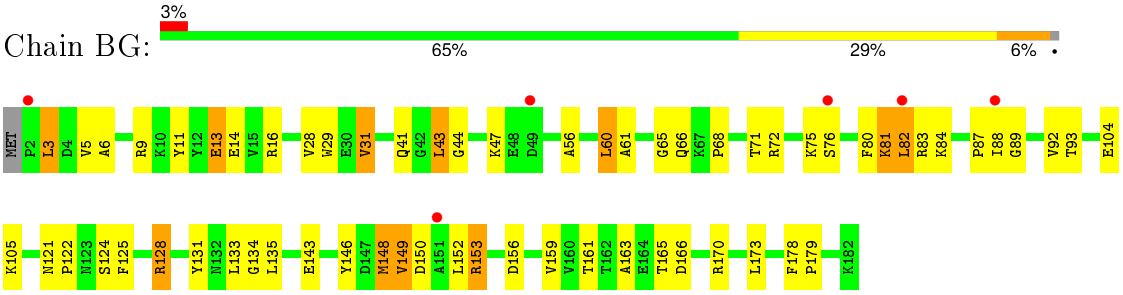
• Molecule 27: 50S Ribosomal Protein L4

Chain DF:



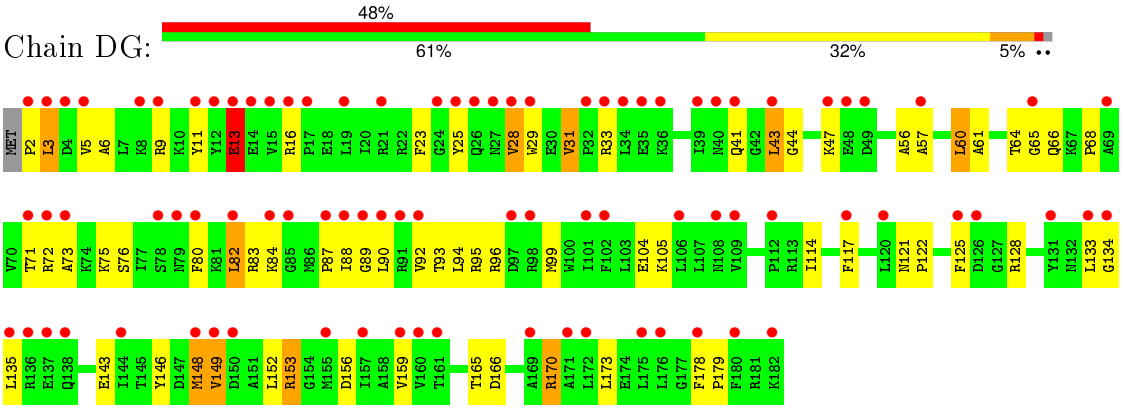
• Molecule 28: 50S Ribosomal Protein L5

Chain BG:



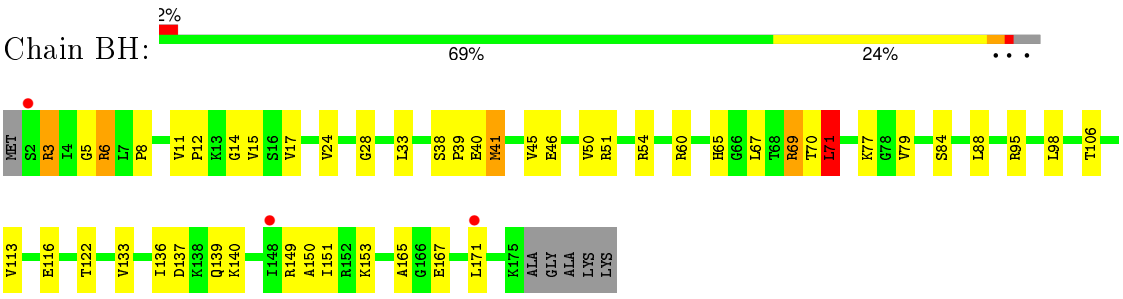
• Molecule 28: 50S Ribosomal Protein L5

Chain DG:



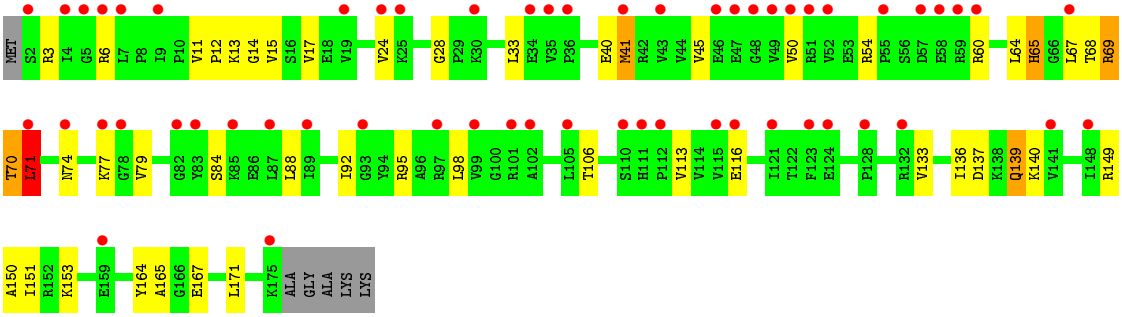
• Molecule 29: 50S Ribosomal Protein L6

Chain BH:



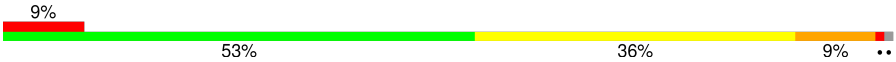
• Molecule 29: 50S Ribosomal Protein L6

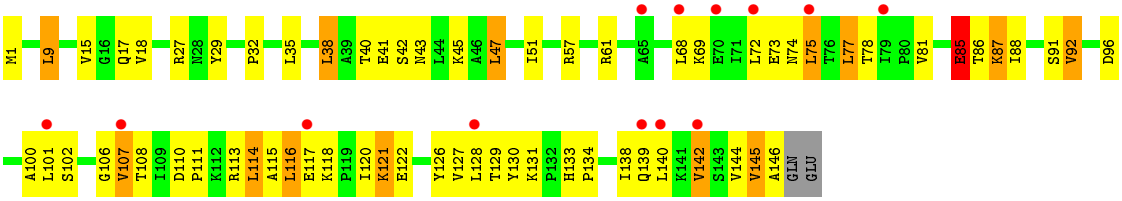
Chain DH:



- Molecule 30: 50S Ribosomal Protein L9

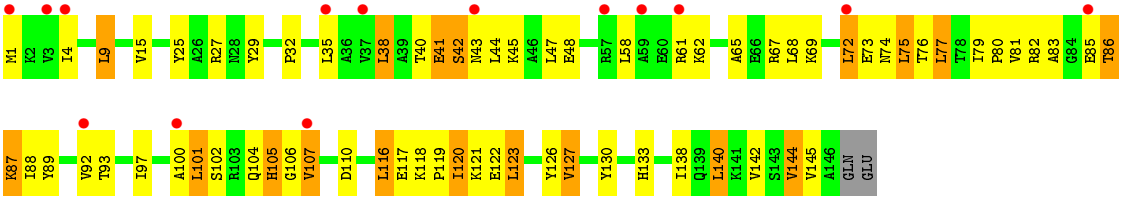
Chain BI:





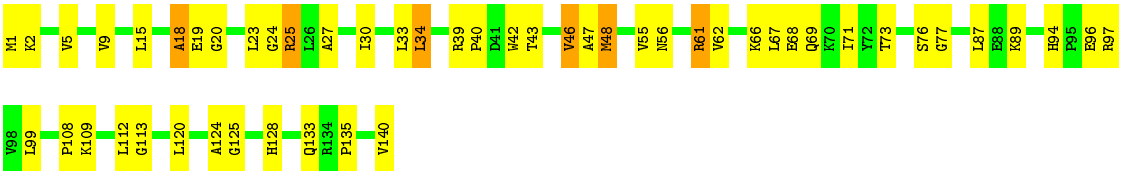
- Molecule 30: 50S Ribosomal Protein L9

Chain DI:



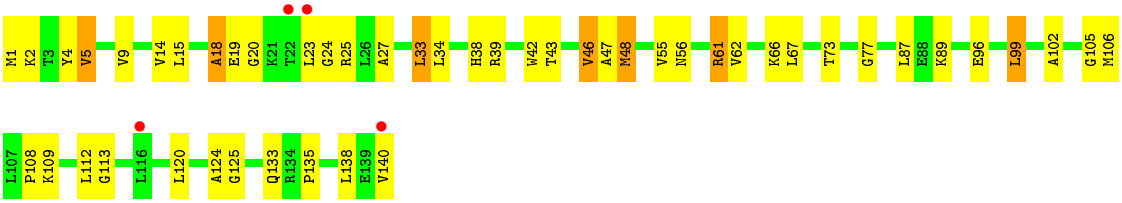
- Molecule 31: 50S Ribosomal Protein L13

Chain BN:



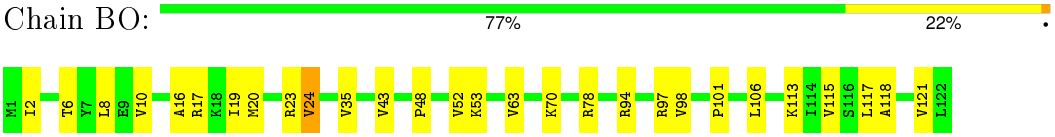
- Molecule 31: 50S Ribosomal Protein L13

Chain DN:



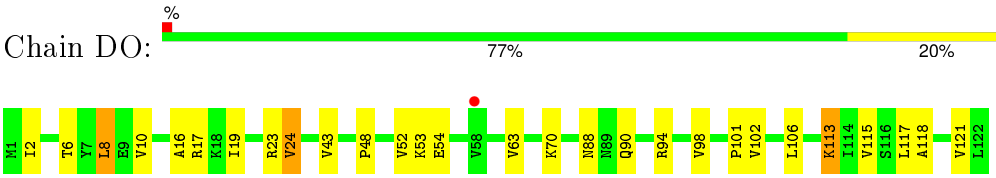
• Molecule 32: 50S Ribosomal Protein L14

Chain BO:



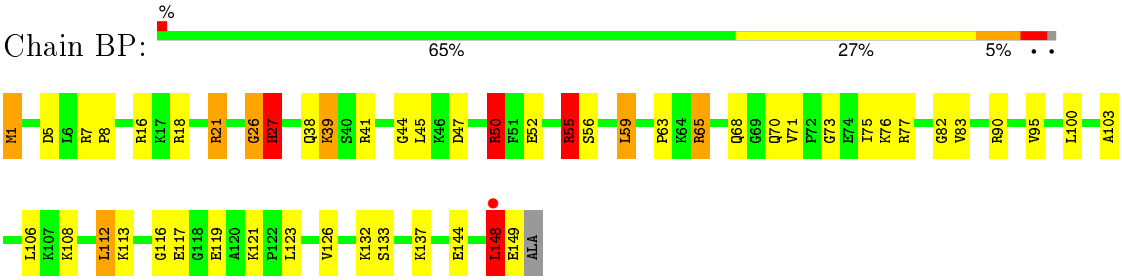
• Molecule 32: 50S Ribosomal Protein L14

Chain DO:



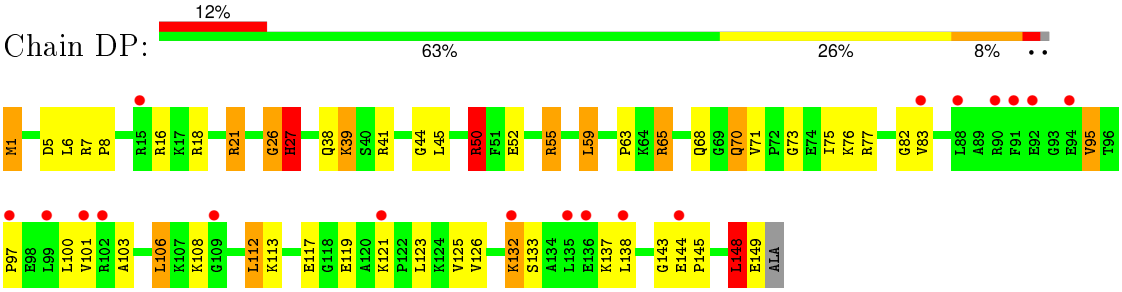
• Molecule 33: 50S Ribosomal Protein L15

Chain BP:



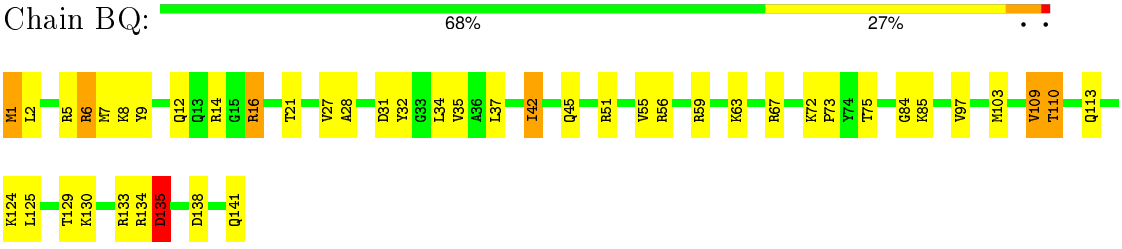
• Molecule 33: 50S Ribosomal Protein L15

Chain DP:



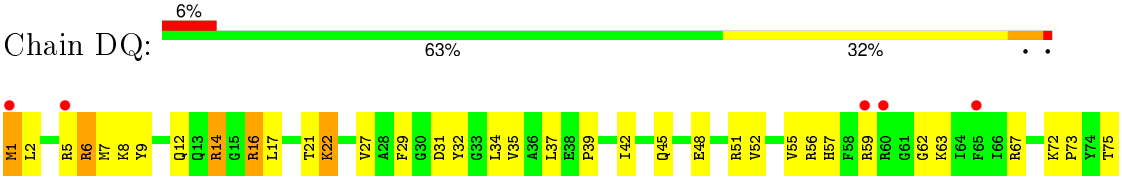
• Molecule 34: 50S Ribosomal Protein L16

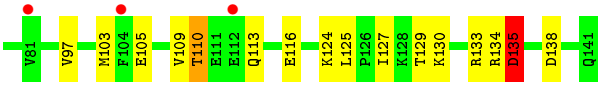
Chain BQ:



• Molecule 34: 50S Ribosomal Protein L16

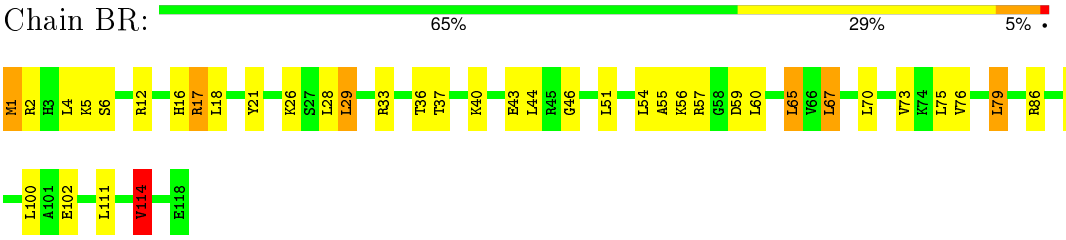
Chain DQ:





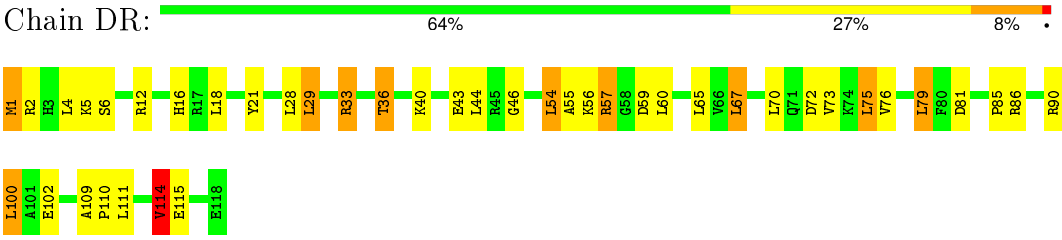
• Molecule 35: 50S Ribosomal Protein L17

Chain BR:



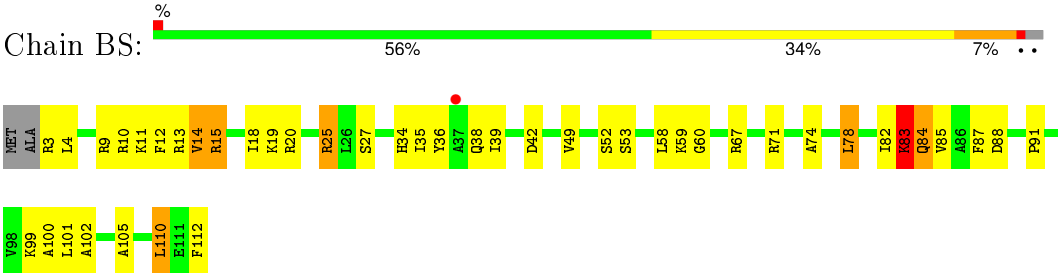
• Molecule 35: 50S Ribosomal Protein L17

Chain DR:



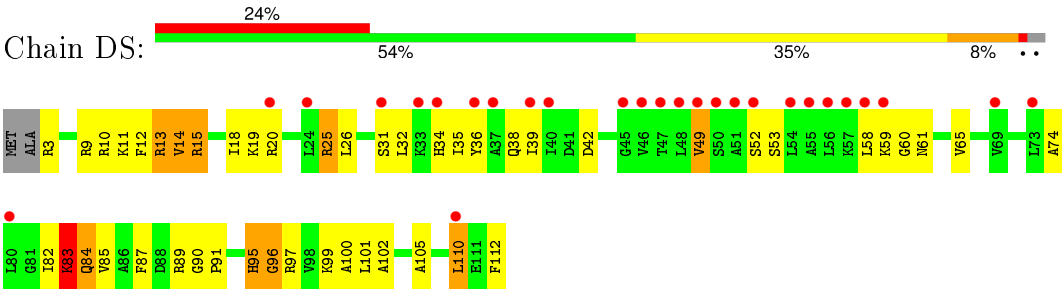
• Molecule 36: 50S Ribosomal Protein L18

Chain BS:



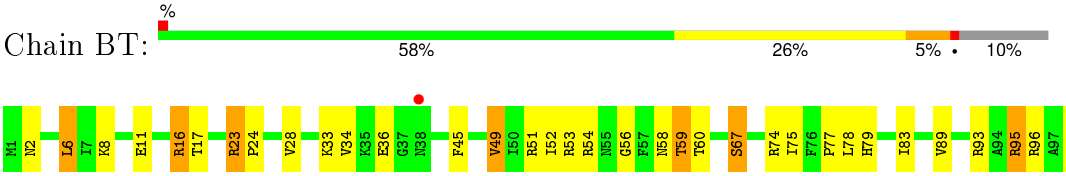
• Molecule 36: 50S Ribosomal Protein L18

Chain DS:



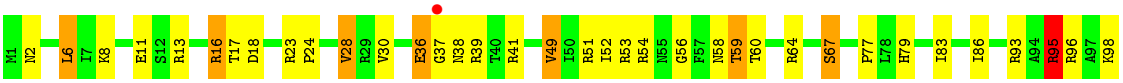
• Molecule 37: 50S Ribosomal Protein L19

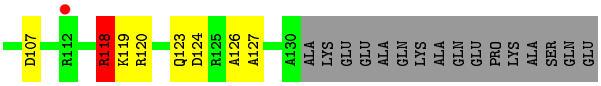
Chain BT:



• Molecule 37: 50S Ribosomal Protein L19

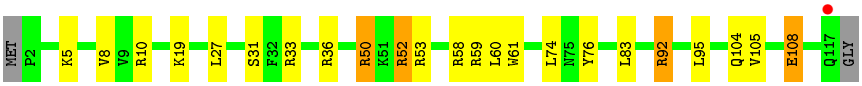
Chain DT:





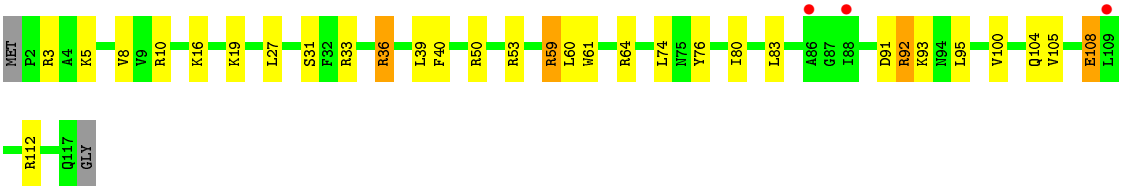
• Molecule 38: 50S Ribosomal Protein L20

Chain BU:



• Molecule 38: 50S Ribosomal Protein L20

Chain DU:

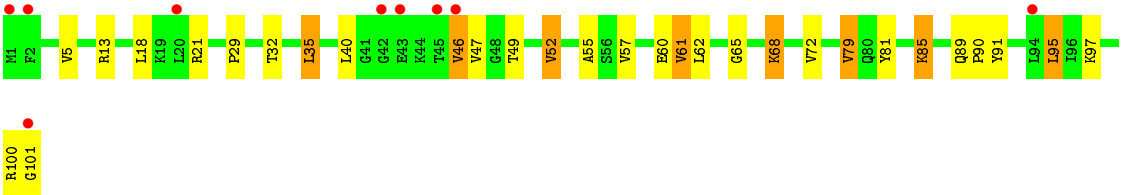


• Molecule 39: 50S Ribosomal Protein L21

Chain BV:

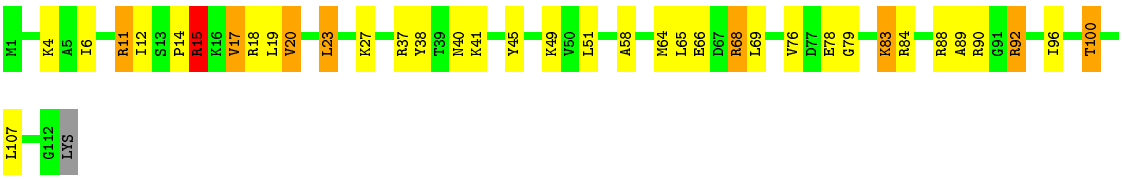
• Molecule 39: 50S Ribosomal Protein L21

Chain DV:



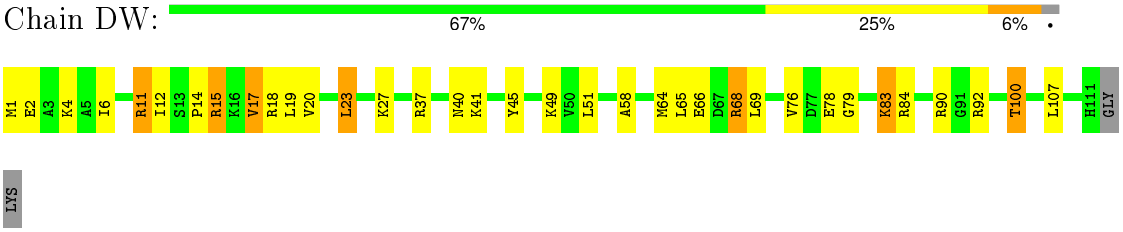
• Molecule 40: 50S Ribosomal Protein L22

Chain BW:



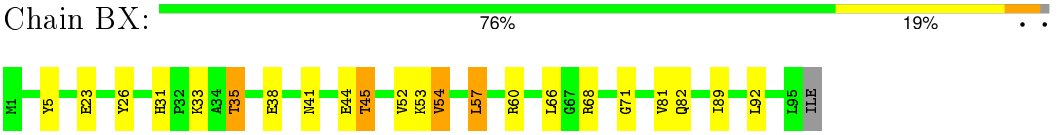
• Molecule 40: 50S Ribosomal Protein L22

Chain DW:



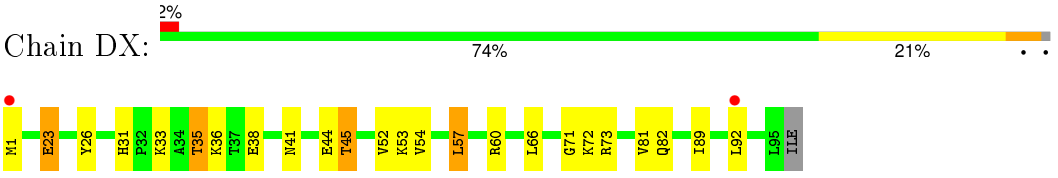
• Molecule 41: 50S Ribosomal Protein L23

Chain BX:



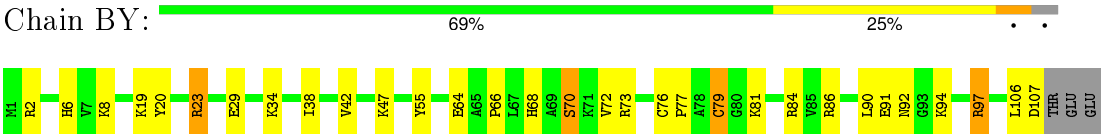
• Molecule 41: 50S Ribosomal Protein L23

Chain DX:



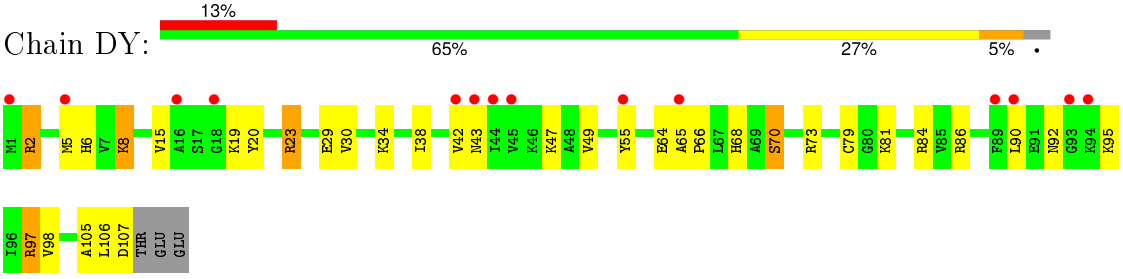
• Molecule 42: 50S Ribosomal Protein L24

Chain BY:



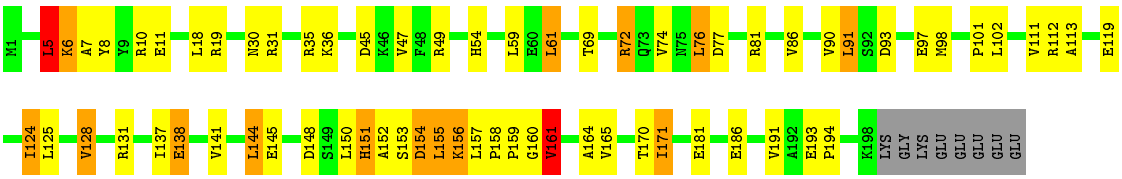
• Molecule 42: 50S Ribosomal Protein L24

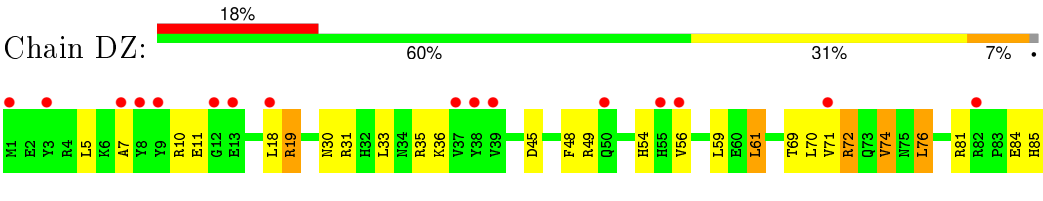
Chain DY:



• Molecule 43: 50S Ribosomal Protein L25

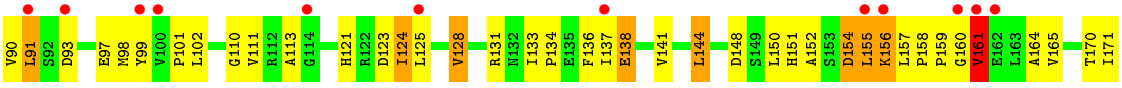
Chain BZ:

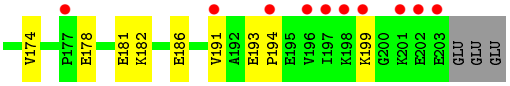




• Molecule 43: 50S Ribosomal Protein L25

Chain DZ:



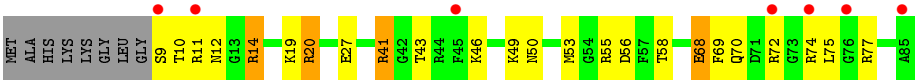


• Molecule 44: 50S Ribosomal Protein L27

Chain B0:

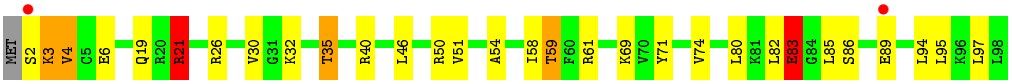
• Molecule 44: 50S Ribosomal Protein L27

Chain D0:



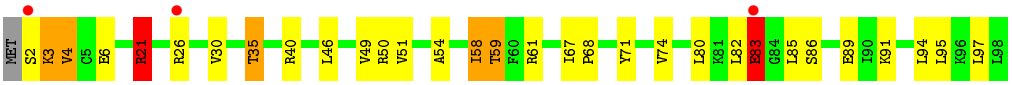
• Molecule 45: 50S Ribosomal Protein L28

Chain B1:



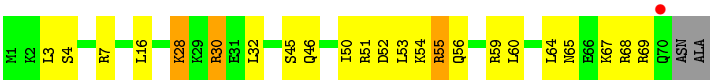
• Molecule 45: 50S Ribosomal Protein L28

Chain D1:



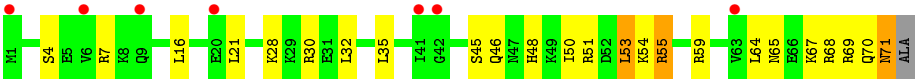
• Molecule 46: 50S Ribosomal Protein L29

Chain B2:



• Molecule 46: 50S Ribosomal Protein L29

Chain D2:

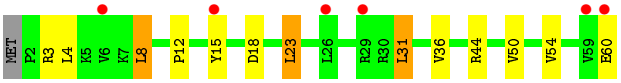


• Molecule 47: 50S Ribosomal Protein L30

Chain B3:

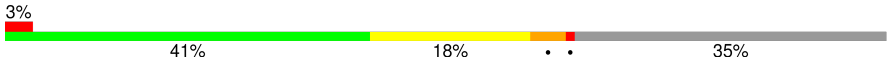
• Molecule 47: 50S Ribosomal Protein L30

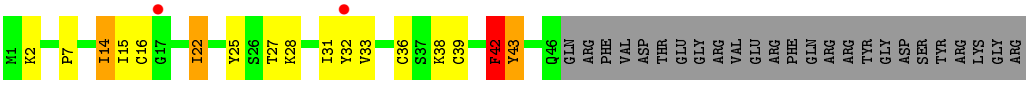
Chain D3:



• Molecule 48: 50S Ribosomal Protein L31

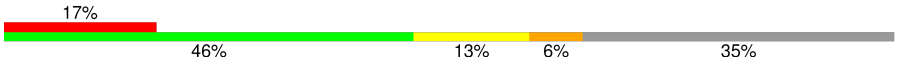
Chain B4:

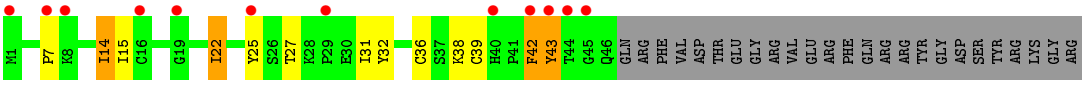




• Molecule 48: 50S Ribosomal Protein L31

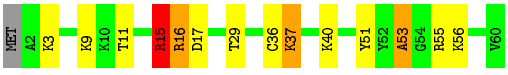
Chain D4:





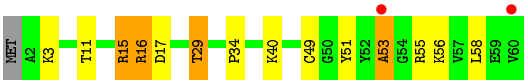
• Molecule 49: 50S Ribosomal Protein L32

Chain B5:



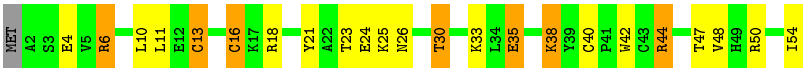
• Molecule 49: 50S Ribosomal Protein L32

Chain D5:



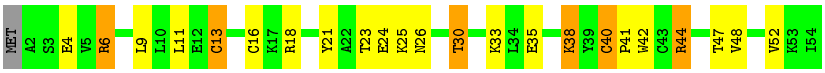
• Molecule 50: 50S Ribosomal Protein L33

Chain B6:



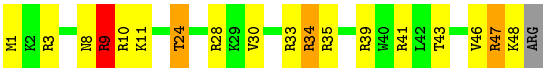
• Molecule 50: 50S Ribosomal Protein L33

Chain D6:



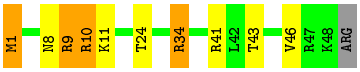
• Molecule 51: 50S Ribosomal Protein L34

Chain B7:



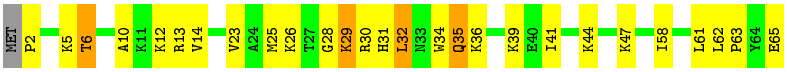
• Molecule 51: 50S Ribosomal Protein L34

Chain D7:



• Molecule 52: 50S Ribosomal Protein L35

Chain B8:

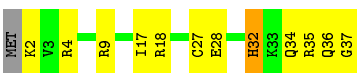


• Molecule 52: 50S Ribosomal Protein L35

Chain D8:

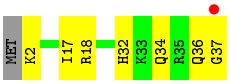
• Molecule 53: 50S ribosomal protein L36

Chain B9:



• Molecule 53: 50S ribosomal protein L36

Chain D9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.63Å 449.30Å 620.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 2.70 49.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.71-2.70) 98.4 (49.71-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.217 , 0.254 0.217 , 0.255	Depositor DCC
R_{free} test set	78243 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 1557851 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	287173	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AA	1.00	41/35935 (0.1%)	1.48	589/56084 (1.1%)
1	CA	0.97	39/35884 (0.1%)	1.44	557/56006 (1.0%)
2	AB	0.57	0/1811	0.74	0/2452
2	CB	0.62	0/1852	0.75	0/2510
3	AC	0.63	1/1474 (0.1%)	0.84	1/2003 (0.0%)
3	CC	0.67	0/1477	0.90	4/2006 (0.2%)
4	AD	0.73	2/1550 (0.1%)	0.87	1/2106 (0.0%)
4	CD	0.68	3/1567 (0.2%)	0.85	1/2125 (0.0%)
5	AE	0.60	0/1121	0.78	0/1517
5	CE	0.64	0/1122	0.81	0/1518
6	AF	0.61	0/794	0.79	0/1082
6	CF	0.58	0/789	0.78	0/1074
7	AG	0.59	0/1186	0.74	0/1603
7	CG	0.63	0/1183	0.74	0/1599
8	AH	0.52	0/1065	0.71	0/1445
8	CH	0.53	0/1069	0.69	0/1450
9	AI	0.60	0/867	0.85	0/1180
9	CI	0.70	0/864	0.84	0/1177
10	AJ	0.65	0/672	0.83	0/919
10	CJ	0.73	0/670	0.86	0/917
11	AK	0.59	0/843	0.74	0/1144
11	CK	0.60	0/843	0.75	0/1144
12	AL	0.67	0/925	0.83	0/1251
12	CL	0.65	0/921	0.87	2/1247 (0.2%)
13	AM	0.66	0/811	0.91	0/1103
13	CM	0.72	0/794	0.92	0/1081
14	AN	0.62	0/487	0.83	0/649
14	CN	0.68	0/483	0.91	1/645 (0.2%)
15	AO	0.59	0/735	0.84	2/981 (0.2%)
15	CO	0.57	0/735	0.79	1/981 (0.1%)
16	AP	0.60	0/667	0.83	0/905
16	CP	0.57	0/677	0.83	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.59	0/836	0.76	0/1117
17	CQ	0.62	0/832	0.77	0/1113
18	AR	0.51	0/519	0.82	1/699 (0.1%)
18	CR	0.52	0/519	0.81	0/699
19	AS	0.58	0/574	0.85	1/781 (0.1%)
19	CS	0.64	0/563	0.82	0/766
20	AT	0.59	0/701	0.86	2/930 (0.2%)
20	CT	0.60	0/776	0.83	2/1026 (0.2%)
21	AU	0.57	0/203	0.73	0/266
21	CU	0.71	0/184	0.85	0/244
22	AY	0.67	0/766	0.87	0/1034
22	CY	0.67	0/751	0.76	0/1017
23	BA	1.46	435/68200 (0.6%)	1.72	2119/106454 (2.0%)
23	DA	1.17	125/67486 (0.2%)	1.62	1697/105338 (1.6%)
24	BB	1.09	2/2878 (0.1%)	1.48	44/4490 (1.0%)
24	DB	1.27	9/2878 (0.3%)	1.51	51/4490 (1.1%)
25	BD	0.90	1/2186 (0.0%)	1.02	8/2944 (0.3%)
25	DD	0.79	0/2186	0.96	2/2944 (0.1%)
26	BE	0.89	0/1588	0.98	2/2145 (0.1%)
26	DE	0.79	1/1588 (0.1%)	0.96	1/2145 (0.0%)
27	BF	0.84	1/1612 (0.1%)	0.94	5/2184 (0.2%)
27	DF	0.71	0/1607	0.91	4/2178 (0.2%)
28	BG	0.55	0/1393	0.78	0/1892
28	DG	0.69	0/1393	0.80	0/1892
29	BH	0.68	0/1343	0.80	0/1820
29	DH	0.63	0/1343	0.75	0/1820
30	BI	0.63	0/1058	0.84	0/1449
30	DI	0.64	0/1058	0.90	1/1449 (0.1%)
31	BN	0.84	0/1139	0.96	4/1538 (0.3%)
31	DN	0.71	0/1139	0.89	1/1538 (0.1%)
32	BO	0.86	0/933	0.92	2/1257 (0.2%)
32	DO	0.77	0/933	0.91	1/1257 (0.1%)
33	BP	0.85	0/1148	1.02	7/1529 (0.5%)
33	DP	0.72	0/1148	0.97	5/1529 (0.3%)
34	BQ	0.85	0/1143	0.89	2/1527 (0.1%)
34	DQ	0.76	0/1143	0.90	2/1527 (0.1%)
35	BR	0.85	0/982	0.98	2/1312 (0.2%)
35	DR	0.71	0/982	0.92	1/1312 (0.1%)
36	BS	0.71	0/875	0.91	1/1168 (0.1%)
36	DS	0.78	0/883	0.89	1/1176 (0.1%)
37	BT	0.79	0/1077	0.98	2/1444 (0.1%)
37	DT	0.73	0/1072	0.97	4/1437 (0.3%)
38	BU	0.89	0/977	0.95	4/1301 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DU	0.78	0/977	0.83	0/1301
39	BV	0.85	0/782	0.92	0/1049
39	DV	0.77	0/786	0.89	0/1053
40	BW	0.97	2/891 (0.2%)	0.97	3/1197 (0.3%)
40	DW	0.85	0/887	0.91	1/1192 (0.1%)
41	BX	0.88	0/756	0.90	1/1016 (0.1%)
41	DX	0.78	0/746	0.88	1/1005 (0.1%)
42	BY	0.76	1/798 (0.1%)	1.04	4/1073 (0.4%)
42	DY	0.73	0/794	1.03	3/1067 (0.3%)
43	BZ	0.67	0/1555	0.85	4/2118 (0.2%)
43	DZ	0.71	0/1561	0.84	3/2131 (0.1%)
44	B0	0.78	0/602	0.94	3/804 (0.4%)
44	D0	0.76	0/615	0.90	0/820
45	B1	0.85	0/752	0.91	2/1003 (0.2%)
45	D1	0.76	0/752	0.92	2/1003 (0.2%)
46	B2	0.77	0/590	0.80	0/781
46	D2	0.73	0/586	0.78	0/779
47	B3	0.76	0/463	0.77	0/623
47	D3	0.74	0/468	0.75	0/628
48	B4	0.65	1/358 (0.3%)	0.82	1/487 (0.2%)
48	D4	0.73	0/358	0.80	0/487
49	B5	0.93	0/469	1.07	2/634 (0.3%)
49	D5	0.85	1/465 (0.2%)	0.99	1/630 (0.2%)
50	B6	0.89	1/456 (0.2%)	0.90	0/609
50	D6	0.81	0/444	0.86	0/595
51	B7	1.02	0/426	1.17	5/561 (0.9%)
51	D7	0.81	0/410	0.99	1/543 (0.2%)
52	B8	0.92	0/516	0.98	1/679 (0.1%)
52	D8	0.82	0/516	1.06	5/679 (0.7%)
53	B9	0.98	0/300	1.11	3/395 (0.8%)
53	D9	0.77	0/300	1.02	0/395
All	All	1.09	666/304847 (0.2%)	1.44	5184/456336 (1.1%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	CC	0	3
4	AD	0	1
4	CD	0	1
9	AI	0	3
9	CI	0	1
10	AJ	0	3
10	CJ	0	2
12	CL	0	2
13	AM	0	2
13	CM	0	1
14	CN	0	2
18	AR	0	1
18	CR	0	1
23	BA	0	4
23	DA	0	1
25	BD	0	1
25	DD	0	1
26	BE	0	1
26	DE	0	1
27	BF	0	3
27	DF	0	2
28	BG	0	1
28	DG	0	1
29	BH	0	1
29	DH	0	1
30	BI	0	1
31	BN	0	1
31	DN	0	1
33	BP	0	2
33	DP	0	2
36	BS	0	1
36	DS	0	1
37	BT	0	1
37	DT	0	1
41	BX	0	1
41	DX	0	1
43	BZ	0	1
43	DZ	0	1
45	B1	0	1
45	D1	0	1
48	B4	0	1
48	D4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	B5	0	1
49	D5	0	1
52	D8	0	1
All	All	0	68

The worst 5 of 666 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1459	C	N1-C2	18.78	1.58	1.40
1	CA	1459	C	N1-C2	17.97	1.58	1.40
1	CA	1442(A)	G	N9-C4	15.13	1.50	1.38
23	BA	1021	A	N9-C4	-14.91	1.28	1.37
23	BA	2287	A	N9-C4	-14.79	1.28	1.37

The worst 5 of 5184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1459	C	C6-N1-C2	-31.41	107.74	120.30
1	CA	1459	C	C6-N1-C2	-31.40	107.74	120.30
1	CA	1459	C	N3-C2-O2	-28.90	101.67	121.90
1	AA	1459	C	N3-C2-O2	-28.10	102.23	121.90
1	CA	1442(A)	G	N3-C4-C5	-25.05	116.07	128.60

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	14	GLY	Peptide
3	AC	180	ALA	Peptide
3	AC	50	ALA	Peptide
4	AD	29	PRO	Peptide
9	AI	39	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32102	0	16201	703	0
1	CA	32056	0	16179	905	0
2	AB	1777	0	1747	75	0
2	CB	1817	0	1785	78	0
3	AC	1450	0	1314	42	0
3	CC	1453	0	1320	78	0
4	AD	1520	0	1406	44	0
4	CD	1537	0	1430	89	0
5	AE	1105	0	1130	37	0
5	CE	1106	0	1132	39	0
6	AF	781	0	741	17	0
6	CF	776	0	733	20	0
7	AG	1167	0	1108	34	0
7	CG	1164	0	1106	47	0
8	AH	1045	0	1033	31	0
8	CH	1049	0	1037	33	0
9	AI	852	0	742	47	0
9	CI	849	0	735	56	0
10	AJ	659	0	552	40	0
10	CJ	657	0	547	38	0
11	AK	828	0	822	15	0
11	CK	828	0	822	23	0
12	AL	909	0	927	29	0
12	CL	905	0	916	29	0
13	AM	801	0	743	42	0
13	CM	784	0	730	40	0
14	AN	478	0	496	25	0
14	CN	474	0	485	35	0
15	AO	724	0	749	23	0
15	CO	724	0	749	28	0
16	AP	651	0	638	34	0
16	CP	661	0	653	47	0
17	AQ	823	0	891	29	0
17	CQ	819	0	880	27	0
18	AR	514	0	530	13	0
18	CR	514	0	530	18	0
19	AS	560	0	466	31	0
19	CS	549	0	468	25	0
20	AT	699	0	746	24	0
20	CT	773	0	836	32	0
21	AU	199	0	208	6	0
21	CU	180	0	173	9	0
22	AY	754	0	776	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CY	739	0	740	38	0
23	BA	60898	0	30697	759	0
23	DA	60264	0	30391	909	0
24	BB	2573	0	1306	27	0
24	DB	2573	0	1306	51	0
25	BD	2136	0	2218	55	0
25	DD	2136	0	2218	62	0
26	BE	1555	0	1607	41	0
26	DE	1555	0	1607	46	0
27	BF	1577	0	1612	44	0
27	DF	1572	0	1613	43	0
28	BG	1368	0	1324	37	0
28	DG	1368	0	1324	49	0
29	BH	1317	0	1376	23	0
29	DH	1317	0	1376	24	0
30	BI	1043	0	1054	39	0
30	DI	1043	0	1054	51	0
31	BN	1112	0	1180	25	0
31	DN	1112	0	1180	28	0
32	BO	923	0	981	12	0
32	DO	923	0	981	16	0
33	BP	1131	0	1201	39	0
33	DP	1131	0	1201	45	0
34	BQ	1122	0	1179	26	0
34	DQ	1122	0	1179	30	0
35	BR	968	0	1033	24	0
35	DR	968	0	1033	30	0
36	BS	865	0	905	38	0
36	DS	873	0	927	49	0
37	BT	1063	0	1103	29	0
37	DT	1058	0	1098	31	0
38	BU	959	0	1019	12	0
38	DU	959	0	1019	23	0
39	BV	771	0	830	14	1
39	DV	775	0	841	16	0
40	BW	881	0	935	22	0
40	DW	877	0	932	18	0
41	BX	742	0	799	14	0
41	DX	732	0	777	16	0
42	BY	785	0	828	16	0
42	DY	781	0	829	22	0
43	BZ	1522	0	1511	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DZ	1528	0	1476	59	0
44	B0	594	0	604	7	0
44	D0	607	0	622	18	0
45	B1	745	0	804	20	0
45	D1	745	0	804	22	0
46	B2	588	0	643	13	0
46	D2	584	0	623	16	0
47	B3	458	0	503	6	0
47	D3	463	0	507	8	0
48	B4	349	0	336	11	0
48	D4	349	0	336	12	0
49	B5	455	0	472	10	0
49	D5	451	0	461	11	0
50	B6	449	0	462	15	0
50	D6	437	0	440	16	0
51	B7	418	0	467	10	0
51	D7	402	0	434	5	0
52	B8	509	0	565	19	0
52	D8	509	0	565	26	0
53	B9	297	0	316	6	0
53	D9	297	0	316	6	0
54	AA	217	0	0	0	0
54	AD	2	0	0	0	0
54	AE	1	0	0	0	0
54	AF	1	0	0	0	0
54	AI	1	0	0	0	0
54	AL	1	0	0	0	0
54	AM	2	0	0	0	0
54	AP	1	0	0	0	0
54	B0	4	0	0	0	0
54	B1	1	0	0	0	0
54	B2	2	0	0	0	0
54	B3	3	0	0	0	0
54	B5	1	0	0	0	0
54	B6	1	0	0	0	0
54	B7	1	0	0	0	0
54	B8	1	0	0	0	0
54	B9	3	0	0	0	0
54	BA	729	0	0	0	0
54	BB	19	0	0	0	0
54	BD	7	0	0	0	0
54	BE	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	BF	6	0	0	0	0
54	BG	1	0	0	0	0
54	BH	1	0	0	0	0
54	BN	2	0	0	0	0
54	BO	1	0	0	0	0
54	BP	2	0	0	0	0
54	BQ	5	0	0	0	0
54	BR	5	0	0	0	0
54	BS	1	0	0	0	0
54	BT	3	0	0	0	0
54	BU	3	0	0	0	0
54	BV	4	0	0	0	0
54	BW	1	0	0	0	0
54	BY	1	0	0	0	0
54	BZ	2	0	0	0	0
54	CA	203	0	0	0	0
54	CE	1	0	0	0	0
54	CQ	1	0	0	0	0
54	D0	1	0	0	0	0
54	D1	1	0	0	0	0
54	D5	2	0	0	0	0
54	D7	2	0	0	0	0
54	D8	2	0	0	0	0
54	D9	1	0	0	0	0
54	DA	637	0	0	0	0
54	DB	10	0	0	0	0
54	DD	5	0	0	0	0
54	DE	3	0	0	0	0
54	DF	5	0	0	0	0
54	DO	3	0	0	0	0
54	DP	3	0	0	0	0
54	DQ	4	0	0	0	0
54	DR	2	0	0	0	0
54	DT	2	0	0	0	0
54	DW	1	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	B4	1	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B9	1	0	0	0	0
55	BY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
55	D4	1	0	0	0	0
55	D5	1	0	0	0	0
55	D6	1	0	0	0	0
55	D9	1	0	0	0	0
55	DY	1	0	0	0	0
56	AA	443	0	0	25	0
56	AD	3	0	0	2	0
56	AE	2	0	0	0	0
56	AF	2	0	0	0	0
56	AG	2	0	0	0	0
56	AJ	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	3	0	0	0	0
56	AM	1	0	0	0	0
56	AO	1	0	0	0	0
56	AP	1	0	0	0	0
56	AQ	3	0	0	0	0
56	AY	1	0	0	0	0
56	B0	4	0	0	0	0
56	B1	5	0	0	0	0
56	B3	4	0	0	0	0
56	B5	5	0	0	0	0
56	B6	2	0	0	0	0
56	B7	5	0	0	2	0
56	B8	11	0	0	0	0
56	B9	1	0	0	0	0
56	BA	1988	0	0	66	1
56	BB	43	0	0	1	0
56	BD	21	0	0	2	0
56	BE	18	0	0	1	0
56	BF	18	0	0	0	0
56	BG	2	0	0	0	0
56	BH	2	0	0	0	0
56	BN	7	0	0	0	0
56	BO	3	0	0	0	0
56	BP	20	0	0	0	0
56	BQ	9	0	0	0	0
56	BR	8	0	0	0	1
56	BS	2	0	0	0	0
56	BT	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BU	9	0	0	0	0
56	BV	13	0	0	1	1
56	BW	6	0	0	0	0
56	BX	2	0	0	0	0
56	BY	2	0	0	0	0
56	BZ	2	0	0	0	0
56	CA	400	0	0	32	0
56	CD	2	0	0	1	0
56	CE	4	0	0	0	0
56	CF	1	0	0	0	0
56	CK	1	0	0	0	0
56	CL	2	0	0	0	0
56	CP	3	0	0	0	0
56	CQ	3	0	0	0	0
56	CR	1	0	0	1	0
56	CT	2	0	0	0	0
56	CU	1	0	0	1	0
56	D0	2	0	0	0	0
56	D1	3	0	0	0	0
56	D2	1	0	0	0	0
56	D3	1	0	0	1	0
56	D5	3	0	0	0	0
56	D6	3	0	0	0	0
56	D7	3	0	0	0	0
56	D8	6	0	0	0	0
56	D9	1	0	0	0	0
56	DA	1496	0	0	107	0
56	DB	33	0	0	6	0
56	DD	17	0	0	2	0
56	DE	12	0	0	0	0
56	DF	10	0	0	0	0
56	DN	2	0	0	0	0
56	DO	7	0	0	0	0
56	DP	11	0	0	0	0
56	DQ	2	0	0	1	0
56	DR	5	0	0	0	0
56	DT	3	0	0	0	0
56	DU	1	0	0	0	0
56	DV	1	0	0	0	0
56	DW	4	0	0	0	0
56	DX	2	0	0	0	0
56	DY	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	287173	0	187292	5583	2

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 12.

The worst 5 of 5583 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)
23:BA:2296:U:O4	23:BA:2335:A:N6	1.59	1.34
23:DA:2296:U:O4	23:DA:2335:A:N6	1.59	1.33
1:CA:1164:G:H1	1:CA:1172:C:N4	1.45	1.15
23:BA:885:C:N4	23:BA:890:A:N6	1.97	1.13
1:AA:40:C:N4	1:AA:402:G:H1	1.47	1.12

All (2) 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)
56:BR:308:HOH:O	56:BV:310:HOH:O[4_445]	2.03	0.17
39:BV:101:GLY:O	56:BA:5729:HOH:O[4_545]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	227/256 (89%)	185 (82%)	40 (18%)	2 (1%)	21 49
2	CB	233/256 (91%)	187 (80%)	43 (18%)	3 (1%)	15 37
3	AC	204/239 (85%)	176 (86%)	28 (14%)	0	100 100
3	CC	204/239 (85%)	169 (83%)	31 (15%)	4 (2%)	9 24
4	AD	206/209 (99%)	186 (90%)	20 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	CD	206/209 (99%)	182 (88%)	23 (11%)	1 (0%)	34 63
5	AE	146/162 (90%)	128 (88%)	17 (12%)	1 (1%)	26 55
5	CE	146/162 (90%)	130 (89%)	15 (10%)	1 (1%)	26 55
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
6	CF	97/101 (96%)	95 (98%)	2 (2%)	0	100 100
7	AG	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	26 55
7	CG	153/156 (98%)	130 (85%)	22 (14%)	1 (1%)	26 55
8	AH	136/138 (99%)	129 (95%)	7 (5%)	0	100 100
8	CH	136/138 (99%)	128 (94%)	8 (6%)	0	100 100
9	AI	123/128 (96%)	108 (88%)	13 (11%)	2 (2%)	12 30
9	CI	123/128 (96%)	104 (85%)	14 (11%)	5 (4%)	3 7
10	AJ	94/105 (90%)	72 (77%)	15 (16%)	7 (7%)	1 1
10	CJ	94/105 (90%)	72 (77%)	18 (19%)	4 (4%)	3 7
11	AK	112/129 (87%)	103 (92%)	9 (8%)	0	100 100
11	CK	112/129 (87%)	104 (93%)	8 (7%)	0	100 100
12	AL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	24 51
12	CL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	24 51
13	AM	112/126 (89%)	86 (77%)	22 (20%)	4 (4%)	4 9
13	CM	110/126 (87%)	86 (78%)	18 (16%)	6 (6%)	2 4
14	AN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	11 29
14	CN	58/61 (95%)	49 (84%)	5 (9%)	4 (7%)	1 2
15	AO	86/89 (97%)	81 (94%)	5 (6%)	0	100 100
15	CO	86/89 (97%)	79 (92%)	7 (8%)	0	100 100
16	AP	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	15 37
16	CP	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	15 37
17	AQ	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	19 45
17	CQ	97/105 (92%)	89 (92%)	8 (8%)	0	100 100
18	AR	66/88 (75%)	55 (83%)	11 (17%)	0	100 100
18	CR	66/88 (75%)	56 (85%)	10 (15%)	0	100 100
19	AS	79/93 (85%)	67 (85%)	11 (14%)	1 (1%)	15 37
19	CS	76/93 (82%)	57 (75%)	18 (24%)	1 (1%)	15 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	AT	94/106 (89%)	77 (82%)	17 (18%)	0	100 100
20	CT	102/106 (96%)	79 (78%)	20 (20%)	3 (3%)	6 14
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
21	CU	21/27 (78%)	16 (76%)	5 (24%)	0	100 100
22	AY	93/119 (78%)	85 (91%)	7 (8%)	1 (1%)	17 42
22	CY	92/119 (77%)	87 (95%)	5 (5%)	0	100 100
25	BD	273/276 (99%)	262 (96%)	8 (3%)	3 (1%)	17 42
25	DD	273/276 (99%)	262 (96%)	8 (3%)	3 (1%)	17 42
26	BE	202/206 (98%)	191 (95%)	8 (4%)	3 (2%)	13 32
26	DE	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	13 32
27	BF	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	19 45
27	DF	201/210 (96%)	191 (95%)	8 (4%)	2 (1%)	19 45
28	BG	179/182 (98%)	149 (83%)	26 (14%)	4 (2%)	8 22
28	DG	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	17 42
29	BH	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	30 59
29	DH	172/180 (96%)	160 (93%)	9 (5%)	3 (2%)	11 29
30	BI	144/148 (97%)	116 (81%)	24 (17%)	4 (3%)	6 15
30	DI	144/148 (97%)	119 (83%)	22 (15%)	3 (2%)	9 23
31	BN	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	14 35
31	DN	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	14 35
32	BO	120/122 (98%)	118 (98%)	2 (2%)	0	100 100
32	DO	120/122 (98%)	118 (98%)	2 (2%)	0	100 100
33	BP	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	14 35
33	DP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	14 35
34	BQ	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	26 55
34	DQ	139/141 (99%)	131 (94%)	6 (4%)	2 (1%)	14 35
35	BR	116/118 (98%)	114 (98%)	2 (2%)	0	100 100
35	DR	116/118 (98%)	115 (99%)	1 (1%)	0	100 100
36	BS	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	21 49
36	DS	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	21 49
37	BT	129/146 (88%)	125 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
37	DT	128/146 (88%)	124 (97%)	3 (2%)	1 (1%)	24 51
38	BU	114/118 (97%)	114 (100%)	0	0	100 100
38	DU	114/118 (97%)	114 (100%)	0	0	100 100
39	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
39	DV	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
40	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
40	DW	109/113 (96%)	108 (99%)	1 (1%)	0	100 100
41	BX	93/96 (97%)	85 (91%)	8 (9%)	0	100 100
41	DX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	17 42
42	BY	105/110 (96%)	93 (89%)	12 (11%)	0	100 100
42	DY	105/110 (96%)	97 (92%)	8 (8%)	0	100 100
43	BZ	196/206 (95%)	178 (91%)	14 (7%)	4 (2%)	9 24
43	DZ	201/206 (98%)	181 (90%)	15 (8%)	5 (2%)	7 18
44	B0	74/85 (87%)	72 (97%)	2 (3%)	0	100 100
44	D0	75/85 (88%)	71 (95%)	4 (5%)	0	100 100
45	B1	95/98 (97%)	92 (97%)	1 (1%)	2 (2%)	9 23
45	D1	95/98 (97%)	92 (97%)	1 (1%)	2 (2%)	9 23
46	B2	68/72 (94%)	64 (94%)	4 (6%)	0	100 100
46	D2	69/72 (96%)	65 (94%)	4 (6%)	0	100 100
47	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
47	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
48	B4	44/71 (62%)	35 (80%)	8 (18%)	1 (2%)	8 20
48	D4	44/71 (62%)	34 (77%)	10 (23%)	0	100 100
49	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
49	D5	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
50	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
50	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
51	B7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	8 22
51	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	8 22
52	B8	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	12 30
52	D8	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	5 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	B9	34/37 (92%)	34 (100%)	0	0	100 100
53	D9	34/37 (92%)	34 (100%)	0	0	100 100
All	All	11568/12366 (94%)	10478 (91%)	965 (8%)	125 (1%)	17 42

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	AJ	56	HIS
13	AM	84	ILE
27	BF	21	ALA
28	BG	82	LEU
30	BI	107	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	177/220 (80%)	148 (84%)	29 (16%)	3 7
2	CB	181/220 (82%)	151 (83%)	30 (17%)	3 7
3	AC	114/188 (61%)	97 (85%)	17 (15%)	4 9
3	CC	114/188 (61%)	86 (75%)	28 (25%)	1 2
4	AD	139/181 (77%)	119 (86%)	20 (14%)	4 10
4	CD	142/181 (78%)	120 (84%)	22 (16%)	3 8
5	AE	108/123 (88%)	95 (88%)	13 (12%)	6 14
5	CE	108/123 (88%)	94 (87%)	14 (13%)	5 12
6	AF	77/90 (86%)	66 (86%)	11 (14%)	4 10
6	CF	75/90 (83%)	65 (87%)	10 (13%)	5 11
7	AG	104/127 (82%)	91 (88%)	13 (12%)	6 13
7	CG	103/127 (81%)	83 (81%)	20 (19%)	2 4
8	AH	103/119 (87%)	87 (84%)	16 (16%)	3 8
8	CH	104/119 (87%)	88 (85%)	16 (15%)	3 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	AI	62/99 (63%)	53 (86%)	9 (14%)	4 10
9	CI	62/99 (63%)	53 (86%)	9 (14%)	4 10
10	AJ	52/92 (56%)	41 (79%)	11 (21%)	1 3
10	CJ	52/92 (56%)	40 (77%)	12 (23%)	1 2
11	AK	81/99 (82%)	73 (90%)	8 (10%)	10 22
11	CK	81/99 (82%)	73 (90%)	8 (10%)	10 22
12	AL	92/109 (84%)	83 (90%)	9 (10%)	10 23
12	CL	91/109 (84%)	85 (93%)	6 (7%)	21 45
13	AM	63/101 (62%)	46 (73%)	17 (27%)	0 2
13	CM	62/101 (61%)	45 (73%)	17 (27%)	0 1
14	AN	46/50 (92%)	38 (83%)	8 (17%)	2 6
14	CN	45/50 (90%)	33 (73%)	12 (27%)	0 2
15	AO	77/80 (96%)	64 (83%)	13 (17%)	2 6
15	CO	77/80 (96%)	64 (83%)	13 (17%)	2 6
16	AP	63/74 (85%)	50 (79%)	13 (21%)	1 4
16	CP	65/74 (88%)	51 (78%)	14 (22%)	1 3
17	AQ	94/97 (97%)	82 (87%)	12 (13%)	5 12
17	CQ	93/97 (96%)	81 (87%)	12 (13%)	5 12
18	AR	49/77 (64%)	40 (82%)	9 (18%)	2 5
18	CR	49/77 (64%)	40 (82%)	9 (18%)	2 5
19	AS	43/80 (54%)	37 (86%)	6 (14%)	4 10
19	CS	44/80 (55%)	32 (73%)	12 (27%)	0 1
20	AT	62/82 (76%)	53 (86%)	9 (14%)	4 10
20	CT	72/82 (88%)	61 (85%)	11 (15%)	3 8
21	AU	18/22 (82%)	15 (83%)	3 (17%)	3 7
21	CU	14/22 (64%)	11 (79%)	3 (21%)	1 3
22	AY	82/104 (79%)	70 (85%)	12 (15%)	4 9
22	CY	79/104 (76%)	63 (80%)	16 (20%)	1 4
25	BD	215/218 (99%)	191 (89%)	24 (11%)	7 17
25	DD	215/218 (99%)	190 (88%)	25 (12%)	7 16
26	BE	163/166 (98%)	140 (86%)	23 (14%)	4 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	DE	163/166 (98%)	139 (85%)	24 (15%)	4 9
27	BF	158/166 (95%)	134 (85%)	24 (15%)	3 9
27	DF	157/166 (95%)	135 (86%)	22 (14%)	4 10
28	BG	128/156 (82%)	107 (84%)	21 (16%)	3 7
28	DG	128/156 (82%)	107 (84%)	21 (16%)	3 7
29	BH	141/148 (95%)	125 (89%)	16 (11%)	7 16
29	DH	141/148 (95%)	128 (91%)	13 (9%)	11 25
30	BI	100/124 (81%)	73 (73%)	27 (27%)	0 2
30	DI	100/124 (81%)	75 (75%)	25 (25%)	1 2
31	BN	117/119 (98%)	99 (85%)	18 (15%)	3 8
31	DN	117/119 (98%)	99 (85%)	18 (15%)	3 8
32	BO	98/100 (98%)	89 (91%)	9 (9%)	11 25
32	DO	98/100 (98%)	91 (93%)	7 (7%)	18 41
33	BP	114/116 (98%)	94 (82%)	20 (18%)	2 6
33	DP	114/116 (98%)	95 (83%)	19 (17%)	3 7
34	BQ	111/111 (100%)	94 (85%)	17 (15%)	3 8
34	DQ	111/111 (100%)	95 (86%)	16 (14%)	4 10
35	BR	101/101 (100%)	81 (80%)	20 (20%)	1 4
35	DR	101/101 (100%)	81 (80%)	20 (20%)	1 4
36	BS	84/88 (96%)	70 (83%)	14 (17%)	3 7
36	DS	86/88 (98%)	70 (81%)	16 (19%)	2 5
37	BT	110/127 (87%)	90 (82%)	20 (18%)	2 5
37	DT	110/127 (87%)	93 (84%)	17 (16%)	3 8
38	BU	93/94 (99%)	80 (86%)	13 (14%)	4 10
38	DU	93/94 (99%)	81 (87%)	12 (13%)	5 12
39	BV	80/82 (98%)	65 (81%)	15 (19%)	2 5
39	DV	81/82 (99%)	65 (80%)	16 (20%)	1 4
40	BW	89/92 (97%)	77 (86%)	12 (14%)	5 11
40	DW	89/92 (97%)	78 (88%)	11 (12%)	6 13
41	BX	75/78 (96%)	66 (88%)	9 (12%)	6 14
41	DX	73/78 (94%)	66 (90%)	7 (10%)	10 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	BY	80/91 (88%)	66 (82%)	14 (18%)	2 6
42	DY	79/91 (87%)	64 (81%)	15 (19%)	2 5
43	BZ	159/179 (89%)	137 (86%)	22 (14%)	4 10
43	DZ	155/179 (87%)	136 (88%)	19 (12%)	6 14
44	B0	59/67 (88%)	52 (88%)	7 (12%)	6 15
44	D0	61/67 (91%)	51 (84%)	10 (16%)	3 7
45	B1	78/83 (94%)	65 (83%)	13 (17%)	3 7
45	D1	78/83 (94%)	66 (85%)	12 (15%)	3 8
46	B2	65/67 (97%)	57 (88%)	8 (12%)	6 14
46	D2	63/67 (94%)	55 (87%)	8 (13%)	5 13
47	B3	49/52 (94%)	44 (90%)	5 (10%)	9 21
47	D3	50/52 (96%)	44 (88%)	6 (12%)	6 14
48	B4	39/63 (62%)	34 (87%)	5 (13%)	5 12
48	D4	39/63 (62%)	35 (90%)	4 (10%)	9 20
49	B5	50/52 (96%)	43 (86%)	7 (14%)	4 10
49	D5	49/52 (94%)	44 (90%)	5 (10%)	9 21
50	B6	50/52 (96%)	40 (80%)	10 (20%)	1 4
50	D6	48/52 (92%)	37 (77%)	11 (23%)	1 3
51	B7	41/42 (98%)	35 (85%)	6 (15%)	4 9
51	D7	38/42 (90%)	32 (84%)	6 (16%)	3 8
52	B8	52/55 (94%)	45 (86%)	7 (14%)	5 11
52	D8	52/55 (94%)	45 (86%)	7 (14%)	5 11
53	B9	32/34 (94%)	30 (94%)	2 (6%)	22 48
53	D9	32/34 (94%)	31 (97%)	1 (3%)	47 78
All	All	8871/10274 (86%)	7518 (85%)	1353 (15%)	3 8

5 of 1353 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	B1	59	THR
5	CE	137	GLU
42	DY	6	HIS
48	B4	22	ILE
2	CB	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
4	CD	42	GLN
9	CI	3	GLN
33	DP	38	GLN
4	CD	45	GLN
7	CG	56	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1490/1522 (97%)	306 (20%)	32 (2%)
1	CA	1490/1522 (97%)	328 (22%)	34 (2%)
23	BA	2819/2915 (96%)	514 (18%)	72 (2%)
23	DA	2788/2915 (95%)	485 (17%)	64 (2%)
24	BB	119/122 (97%)	19 (15%)	0
24	DB	119/122 (97%)	21 (17%)	0
All	All	8825/9118 (96%)	1673 (18%)	202 (2%)

5 of 1673 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	G
1	AA	9	G
1	AA	32	A
1	AA	39	G

5 of 202 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2275	C
1	CA	428	G
23	DA	2172	U
23	BA	2406	U
23	BA	2789	C

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1945 ligands modelled in this entry, 1945 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1493/1522 (98%)	0.12	80 (5%) 29 28	37, 73, 129, 165	0
1	CA	1491/1522 (97%)	0.28	112 (7%) 17 15	40, 84, 135, 175	0
2	AB	229/256 (89%)	0.71	29 (12%) 5 4	76, 103, 123, 135	0
2	CB	235/256 (91%)	1.54	79 (33%) 0 0	80, 108, 127, 135	0
3	AC	206/239 (86%)	0.27	11 (5%) 30 28	62, 81, 98, 105	0
3	CC	206/239 (86%)	1.25	55 (26%) 1 1	85, 109, 122, 130	0
4	AD	208/209 (99%)	0.97	36 (17%) 2 1	64, 85, 105, 113	0
4	CD	208/209 (99%)	0.76	29 (13%) 4 3	68, 85, 103, 111	0
5	AE	148/162 (91%)	0.07	0 100 100	59, 73, 86, 101	0
5	CE	148/162 (91%)	0.56	15 (10%) 9 7	62, 77, 91, 105	0
6	AF	100/101 (99%)	0.04	4 (4%) 42 41	61, 72, 85, 100	0
6	CF	99/101 (98%)	0.20	3 (3%) 54 54	62, 74, 86, 95	0
7	AG	155/156 (99%)	-0.02	7 (4%) 37 36	64, 76, 91, 100	0
7	CG	155/156 (99%)	1.23	43 (27%) 1 1	86, 102, 111, 118	0
8	AH	138/138 (100%)	0.48	8 (5%) 26 25	61, 75, 83, 94	0
8	CH	138/138 (100%)	0.61	14 (10%) 9 7	64, 79, 87, 95	0
9	AI	125/128 (97%)	0.61	14 (11%) 7 5	64, 93, 106, 114	0
9	CI	125/128 (97%)	2.03	46 (36%) 0 0	89, 118, 126, 133	0
10	AJ	96/105 (91%)	1.27	20 (20%) 1 1	63, 96, 120, 124	0
10	CJ	96/105 (91%)	2.23	45 (46%) 0 0	95, 118, 135, 144	0
11	AK	114/129 (88%)	0.47	9 (7%) 15 13	50, 72, 91, 107	0
11	CK	114/129 (88%)	0.80	16 (14%) 4 3	54, 77, 95, 109	0
12	AL	122/132 (92%)	0.61	5 (4%) 41 41	54, 68, 82, 95	0
12	CL	122/132 (92%)	0.94	20 (16%) 2 2	55, 72, 85, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	114/126 (90%)	0.14	7 (6%) 25 23	68, 82, 97, 102	0
13	CM	112/126 (88%)	1.65	40 (35%) 0 0	94, 117, 126, 134	0
14	AN	60/61 (98%)	0.50	4 (6%) 21 19	68, 79, 92, 102	0
14	CN	60/61 (98%)	1.58	19 (31%) 1 0	99, 110, 121, 128	0
15	AO	88/89 (98%)	0.38	3 (3%) 49 49	52, 73, 90, 94	0
15	CO	88/89 (98%)	0.67	11 (12%) 5 4	58, 77, 91, 96	0
16	AP	82/88 (93%)	1.08	14 (17%) 2 1	68, 82, 100, 110	0
16	CP	82/88 (93%)	0.50	5 (6%) 25 23	66, 79, 94, 103	0
17	AQ	99/105 (94%)	0.42	4 (4%) 42 41	57, 74, 87, 92	0
17	CQ	99/105 (94%)	0.66	9 (9%) 11 9	60, 75, 85, 94	0
18	AR	68/88 (77%)	0.11	3 (4%) 38 37	62, 73, 92, 96	0
18	CR	68/88 (77%)	0.62	9 (13%) 4 4	65, 76, 92, 96	0
19	AS	81/93 (87%)	0.68	9 (11%) 7 5	74, 89, 105, 128	0
19	CS	78/93 (83%)	2.25	39 (50%) 0 0	100, 118, 130, 133	0
20	AT	96/106 (90%)	0.89	12 (12%) 5 4	66, 82, 100, 106	0
20	CT	104/106 (98%)	0.86	14 (13%) 4 3	64, 83, 103, 119	0
21	AU	23/27 (85%)	0.76	3 (13%) 5 4	71, 80, 83, 90	0
21	CU	23/27 (85%)	1.88	9 (39%) 0 0	97, 106, 115, 119	0
22	AY	95/119 (79%)	0.08	2 (2%) 67 68	51, 64, 81, 92	0
22	CY	94/119 (78%)	2.37	52 (55%) 0 0	76, 95, 113, 120	0
23	BA	2827/2915 (96%)	0.07	116 (4%) 41 41	24, 40, 120, 169	0
23	DA	2798/2915 (95%)	-0.17	158 (5%) 28 26	27, 46, 118, 170	0
24	BB	120/122 (98%)	-0.12	1 (0%) 87 88	39, 65, 76, 119	0
24	DB	120/122 (98%)	0.93	29 (24%) 1 1	50, 81, 97, 130	0
25	BD	275/276 (99%)	-0.08	0 100 100	24, 39, 51, 79	0
25	DD	275/276 (99%)	-0.23	1 (0%) 93 94	26, 43, 55, 84	0
26	BE	204/206 (99%)	-0.11	0 100 100	24, 44, 64, 81	0
26	DE	204/206 (99%)	-0.08	3 (1%) 76 76	27, 48, 69, 84	0
27	BF	203/210 (96%)	0.12	1 (0%) 91 93	25, 49, 82, 113	0
27	DF	203/210 (96%)	0.23	13 (6%) 23 21	28, 58, 84, 115	0
28	BG	181/182 (99%)	0.22	6 (3%) 50 50	64, 83, 108, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DG	181/182 (99%)	2.17	87 (48%) 0 0	78, 96, 116, 140	0
29	BH	174/180 (96%)	0.21	3 (1%) 73 74	49, 64, 80, 92	0
29	DH	174/180 (96%)	1.67	57 (32%) 0 0	61, 78, 92, 101	0
30	BI	146/148 (98%)	0.45	13 (8%) 12 9	46, 75, 91, 98	0
30	DI	146/148 (98%)	0.61	14 (9%) 10 8	49, 81, 99, 107	0
31	BN	140/140 (100%)	0.08	0 100 100	30, 44, 66, 83	0
31	DN	140/140 (100%)	-0.02	4 (2%) 55 55	35, 52, 73, 86	0
32	BO	122/122 (100%)	-0.13	0 100 100	34, 43, 62, 65	0
32	DO	122/122 (100%)	-0.31	1 (0%) 87 88	37, 47, 65, 68	0
33	BP	149/150 (99%)	0.20	1 (0%) 89 90	25, 51, 77, 96	0
33	DP	149/150 (99%)	0.51	18 (12%) 6 4	30, 60, 87, 99	0
34	BQ	141/141 (100%)	0.13	0 100 100	31, 47, 59, 74	0
34	DQ	141/141 (100%)	0.16	8 (5%) 27 26	39, 55, 69, 79	0
35	BR	118/118 (100%)	0.04	0 100 100	30, 39, 51, 62	0
35	DR	118/118 (100%)	-0.24	0 100 100	33, 42, 55, 67	0
36	BS	110/112 (98%)	0.18	1 (0%) 85 86	48, 62, 77, 85	0
36	DS	110/112 (98%)	1.51	27 (24%) 1 1	59, 74, 87, 93	0
37	BT	131/146 (89%)	-0.15	1 (0%) 87 88	38, 46, 76, 103	0
37	DT	130/146 (89%)	-0.22	2 (1%) 76 76	41, 50, 73, 105	0
38	BU	116/118 (98%)	0.13	1 (0%) 85 86	28, 38, 53, 70	0
38	DU	116/118 (98%)	-0.12	3 (2%) 59 59	33, 45, 61, 70	0
39	BV	101/101 (100%)	0.05	1 (0%) 84 85	27, 48, 67, 83	0
39	DV	101/101 (100%)	0.64	9 (8%) 12 9	32, 59, 76, 85	0
40	BW	112/113 (99%)	-0.14	0 100 100	28, 35, 52, 92	0
40	DW	111/113 (98%)	-0.33	0 100 100	32, 40, 58, 85	0
41	BX	95/96 (98%)	-0.01	0 100 100	33, 43, 65, 84	0
41	DX	95/96 (98%)	-0.01	2 (2%) 67 68	39, 50, 68, 89	0
42	BY	107/110 (97%)	-0.04	0 100 100	44, 55, 77, 88	0
42	DY	107/110 (97%)	0.74	14 (13%) 5 4	53, 63, 82, 91	0
43	BZ	198/206 (96%)	-0.03	0 100 100	48, 68, 91, 103	0
43	DZ	203/206 (98%)	1.01	38 (18%) 2 1	57, 78, 100, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	B0	76/85 (89%)	0.03	0 100 100	37, 44, 57, 75	0
44	D0	77/85 (90%)	0.45	7 (9%) 11 9	44, 52, 67, 101	0
45	B1	97/98 (98%)	0.14	2 (2%) 67 68	31, 44, 74, 82	0
45	D1	97/98 (98%)	-0.07	3 (3%) 52 52	33, 48, 78, 85	0
46	B2	70/72 (97%)	0.20	1 (1%) 78 77	42, 56, 67, 93	0
46	D2	71/72 (98%)	0.52	7 (9%) 9 7	51, 65, 76, 94	0
47	B3	59/60 (98%)	0.12	1 (1%) 73 74	33, 42, 66, 84	0
47	D3	59/60 (98%)	0.66	6 (10%) 9 6	39, 50, 76, 96	0
48	B4	46/71 (64%)	0.18	2 (4%) 39 38	73, 96, 111, 116	0
48	D4	46/71 (64%)	1.33	12 (26%) 1 1	89, 107, 118, 124	0
49	B5	59/60 (98%)	-0.08	0 100 100	23, 38, 56, 68	0
49	D5	59/60 (98%)	-0.10	2 (3%) 49 49	27, 43, 61, 73	0
50	B6	53/54 (98%)	-0.19	0 100 100	40, 46, 59, 66	0
50	D6	53/54 (98%)	-0.03	0 100 100	47, 52, 60, 70	0
51	B7	48/49 (97%)	0.02	0 100 100	26, 30, 51, 71	0
51	D7	48/49 (97%)	-0.15	0 100 100	28, 33, 54, 82	0
52	B8	64/65 (98%)	0.11	0 100 100	34, 38, 45, 57	0
52	D8	64/65 (98%)	0.10	1 (1%) 74 75	38, 44, 50, 60	0
53	B9	36/37 (97%)	0.16	0 100 100	38, 46, 57, 69	0
53	D9	36/37 (97%)	0.13	1 (2%) 56 57	45, 55, 66, 76	0
All	All	20617/21484 (95%)	0.29	1646 (7%) 15 13	23, 63, 117, 175	0

The worst 5 of 1646 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CA	1036	G	16.2
1	CA	1030(B)	C	13.2
23	DA	2139	C	12.7
9	CI	30	GLY	11.8
23	DA	2154	G	11.5

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1639	1/1	0.81	0.84	62.14	57,57,57,57	0
54	MG	BA	3620	1/1	0.96	0.42	42.28	40,40,40,40	0
54	MG	DA	3053	1/1	0.91	0.29	40.33	28,28,28,28	0
54	MG	AA	1619	1/1	0.89	0.57	39.12	45,45,45,45	0
54	MG	DA	3129	1/1	0.95	0.45	37.14	38,38,38,38	0
54	MG	BA	3462	1/1	0.83	0.44	37.03	36,36,36,36	0
54	MG	DA	3055	1/1	0.95	0.37	24.71	25,25,25,25	0
54	MG	DA	3583	1/1	0.87	0.46	23.32	35,35,35,35	0
54	MG	DA	3098	1/1	0.95	0.47	23.22	52,52,52,52	0
54	MG	CA	1753	1/1	0.90	0.36	22.30	74,74,74,74	0
54	MG	BA	3633	1/1	0.91	0.23	21.92	25,25,25,25	0
54	MG	DA	3175	1/1	0.78	0.35	21.85	31,31,31,31	0
54	MG	BA	3386	1/1	0.85	0.38	21.14	32,32,32,32	0
54	MG	DA	3307	1/1	0.91	0.49	20.84	79,79,79,79	0
54	MG	BA	3179	1/1	0.98	0.35	20.33	31,31,31,31	0
54	MG	BA	3191	1/1	0.97	0.28	17.79	43,43,43,43	0
54	MG	DA	3026	1/1	0.90	0.30	17.72	47,47,47,47	0
54	MG	BA	3359	1/1	0.96	0.32	17.46	19,19,19,19	0
54	MG	DA	3130	1/1	0.76	0.65	17.00	49,49,49,49	0
54	MG	DA	3086	1/1	0.77	0.29	17.00	54,54,54,54	0
54	MG	BA	3058	1/1	0.94	0.41	16.20	57,57,57,57	0
54	MG	DA	3150	1/1	0.99	0.33	15.62	29,29,29,29	0
54	MG	DA	3003	1/1	0.92	0.28	15.58	34,34,34,34	0
54	MG	DA	3577	1/1	0.78	0.34	15.57	57,57,57,57	0
54	MG	BA	3057	1/1	0.97	0.30	14.97	29,29,29,29	0
54	MG	DA	3013	1/1	0.80	0.27	14.55	60,60,60,60	0
54	MG	D7	101	1/1	0.88	0.66	14.55	41,41,41,41	0
54	MG	BF	302	1/1	0.98	0.46	13.62	31,31,31,31	0
54	MG	BE	301	1/1	0.89	0.46	13.36	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3116	1/1	0.96	0.33	13.30	26,26,26,26	0
54	MG	DA	3257	1/1	0.94	0.28	13.20	40,40,40,40	0
54	MG	DA	3025	1/1	0.95	0.33	12.24	35,35,35,35	0
54	MG	CA	1603	1/1	0.92	0.77	12.20	83,83,83,83	0
54	MG	BA	3085	1/1	0.95	0.23	12.14	23,23,23,23	0
54	MG	DA	3250	1/1	0.96	0.35	12.04	38,38,38,38	0
54	MG	BA	3398	1/1	0.94	0.27	11.97	30,30,30,30	0
54	MG	BV	201	1/1	0.95	0.33	11.93	30,30,30,30	0
54	MG	DA	3179	1/1	0.84	0.24	11.60	43,43,43,43	0
54	MG	BF	305	1/1	0.94	0.45	11.46	29,29,29,29	0
54	MG	AA	1763	1/1	0.95	0.26	11.38	73,73,73,73	0
54	MG	DA	3222	1/1	0.89	0.28	11.37	37,37,37,37	0
54	MG	DA	3176	1/1	0.90	0.29	11.32	37,37,37,37	0
54	MG	BA	3345	1/1	0.81	0.29	11.24	54,54,54,54	0
54	MG	AA	1784	1/1	0.91	0.30	10.78	63,63,63,63	0
54	MG	DA	3137	1/1	0.86	0.26	10.75	45,45,45,45	0
54	MG	DA	3064	1/1	0.94	0.30	10.64	36,36,36,36	0
54	MG	DA	3395	1/1	0.76	0.31	10.56	75,75,75,75	0
54	MG	BA	3074	1/1	0.75	0.32	10.44	32,32,32,32	0
54	MG	BA	3428	1/1	0.97	0.26	10.36	23,23,23,23	0
54	MG	BA	3018	1/1	0.89	0.29	10.25	52,52,52,52	0
54	MG	DA	3010	1/1	0.91	0.21	10.04	48,48,48,48	0
54	MG	DA	3170	1/1	0.95	0.27	9.95	31,31,31,31	0
54	MG	BA	3102	1/1	0.86	0.24	9.74	33,33,33,33	0
54	MG	DA	3472	1/1	0.89	0.20	9.72	73,73,73,73	0
54	MG	DA	3576	1/1	0.95	0.26	9.64	36,36,36,36	0
54	MG	BA	3643	1/1	0.91	0.34	9.59	28,28,28,28	0
54	MG	DA	3035	1/1	0.97	0.18	9.41	43,43,43,43	0
54	MG	BA	3358	1/1	0.97	0.33	9.09	22,22,22,22	0
54	MG	DA	3496	1/1	0.91	0.24	8.91	38,38,38,38	0
54	MG	DA	3318	1/1	0.72	0.25	8.84	75,75,75,75	0
54	MG	DA	3131	1/1	0.97	0.32	8.64	25,25,25,25	0
54	MG	DA	3398	1/1	0.93	0.23	8.61	53,53,53,53	0
54	MG	BA	3528	1/1	0.99	0.26	8.59	27,27,27,27	0
54	MG	AA	1620	1/1	0.94	0.37	8.41	61,61,61,61	0
54	MG	BA	3190	1/1	0.98	0.23	8.35	36,36,36,36	0
54	MG	DA	3366	1/1	0.97	0.23	8.28	41,41,41,41	0
54	MG	BA	3103	1/1	0.92	0.40	8.21	33,33,33,33	0
54	MG	CA	1620	1/1	0.84	0.40	8.19	74,74,74,74	0
54	MG	DA	3034	1/1	0.95	0.25	8.15	34,34,34,34	0
54	MG	DA	3107	1/1	0.98	0.23	8.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3033	1/1	0.94	0.25	8.01	31,31,31,31	0
54	MG	DA	3199	1/1	0.97	0.26	7.98	29,29,29,29	0
54	MG	BA	3433	1/1	0.94	0.29	7.62	31,31,31,31	0
54	MG	DA	3100	1/1	0.87	0.26	7.54	56,56,56,56	0
54	MG	BA	3520	1/1	0.96	0.22	7.39	29,29,29,29	0
54	MG	BA	3654	1/1	0.95	0.28	7.36	27,27,27,27	0
54	MG	DA	3115	1/1	0.97	0.28	7.35	33,33,33,33	0
54	MG	B0	101	1/1	0.94	0.30	7.34	40,40,40,40	0
54	MG	DA	3569	1/1	0.85	0.34	7.28	60,60,60,60	0
54	MG	AA	1650	1/1	0.90	0.27	7.21	74,74,74,74	0
54	MG	BA	3371	1/1	0.95	0.25	7.14	26,26,26,26	0
54	MG	BA	3619	1/1	0.86	0.35	7.11	75,75,75,75	0
54	MG	BA	3279	1/1	0.92	0.22	7.09	38,38,38,38	0
54	MG	AA	1679	1/1	0.88	0.29	7.06	58,58,58,58	0
54	MG	AA	1649	1/1	0.93	0.26	7.05	71,71,71,71	0
54	MG	DA	3258	1/1	0.94	0.23	7.03	35,35,35,35	0
54	MG	BA	3248	1/1	0.83	0.26	6.96	30,30,30,30	0
54	MG	DA	3021	1/1	0.97	0.20	6.89	32,32,32,32	0
54	MG	DA	3554	1/1	0.60	0.20	6.83	70,70,70,70	0
54	MG	AA	1751	1/1	0.99	0.26	6.76	54,54,54,54	0
54	MG	BA	3178	1/1	0.97	0.27	6.74	23,23,23,23	0
54	MG	BA	3624	1/1	0.93	0.27	6.68	36,36,36,36	0
54	MG	DA	3549	1/1	0.92	0.23	6.65	39,39,39,39	0
54	MG	BA	3008	1/1	0.98	0.24	6.62	20,20,20,20	0
54	MG	BA	3537	1/1	0.78	0.26	6.52	66,66,66,66	0
54	MG	DA	3500	1/1	0.88	0.21	6.50	56,56,56,56	0
54	MG	BA	3148	1/1	0.96	0.23	6.35	21,21,21,21	0
54	MG	DA	3156	1/1	0.95	0.23	6.35	34,34,34,34	0
54	MG	DA	3428	1/1	0.92	0.20	6.26	36,36,36,36	0
54	MG	BA	3209	1/1	0.97	0.24	6.20	19,19,19,19	0
54	MG	CA	1619	1/1	0.97	0.43	6.16	56,56,56,56	0
54	MG	BA	3060	1/1	0.98	0.24	6.11	49,49,49,49	0
54	MG	DA	3042	1/1	0.91	0.26	6.07	50,50,50,50	0
54	MG	BA	3406	1/1	0.98	0.21	6.02	25,25,25,25	0
54	MG	B3	103	1/1	0.97	0.27	6.01	38,38,38,38	0
54	MG	DA	3429	1/1	0.96	0.23	5.98	26,26,26,26	0
54	MG	DA	3200	1/1	0.96	0.17	5.83	34,34,34,34	0
54	MG	DA	3219	1/1	0.92	0.22	5.72	32,32,32,32	0
54	MG	BA	3621	1/1	0.86	0.21	5.68	35,35,35,35	0
54	MG	BA	3104	1/1	0.92	0.26	5.64	27,27,27,27	0
54	MG	AA	1626	1/1	0.95	0.23	5.58	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3295	1/1	0.80	0.19	5.52	58,58,58,58	0
54	MG	BA	3387	1/1	0.98	0.25	5.50	27,27,27,27	0
54	MG	BA	3543	1/1	0.98	0.21	5.46	29,29,29,29	0
54	MG	DA	3073	1/1	0.93	0.18	5.42	41,41,41,41	0
54	MG	CA	1710	1/1	0.93	0.21	5.36	55,55,55,55	0
54	MG	CA	1645	1/1	0.77	0.38	5.35	69,69,69,69	0
54	MG	BU	203	1/1	0.95	0.33	5.26	31,31,31,31	0
54	MG	DD	304	1/1	0.87	0.23	5.23	39,39,39,39	0
54	MG	DA	3528	1/1	0.98	0.22	5.20	36,36,36,36	0
54	MG	DA	3019	1/1	0.92	0.19	4.98	46,46,46,46	0
54	MG	AM	201	1/1	0.95	0.27	4.97	78,78,78,78	0
54	MG	AA	1776	1/1	0.93	0.25	4.79	68,68,68,68	0
54	MG	DA	3441	1/1	0.96	0.21	4.72	63,63,63,63	0
54	MG	CA	1739	1/1	0.84	0.27	4.69	76,76,76,76	0
54	MG	DA	3430	1/1	0.95	0.23	4.69	28,28,28,28	0
54	MG	BA	3388	1/1	0.98	0.25	4.62	20,20,20,20	0
54	MG	BA	3243	1/1	0.98	0.24	4.60	31,31,31,31	0
54	MG	AA	1630	1/1	0.85	0.29	4.60	76,76,76,76	0
54	MG	BA	3553	1/1	0.94	0.23	4.54	27,27,27,27	0
54	MG	DA	3291	1/1	0.95	0.18	4.44	64,64,64,64	0
54	MG	AA	1634	1/1	0.93	0.28	4.42	58,58,58,58	0
54	MG	CA	1760	1/1	0.92	0.32	4.21	93,93,93,93	0
54	MG	CA	1615	1/1	0.94	0.21	4.13	42,42,42,42	0
54	MG	BA	3481	1/1	0.94	0.21	4.11	22,22,22,22	0
54	MG	BA	3415	1/1	0.97	0.23	4.10	26,26,26,26	0
54	MG	DA	3008	1/1	0.97	0.22	4.09	44,44,44,44	0
54	MG	BA	3335	1/1	0.96	0.24	4.08	43,43,43,43	0
54	MG	BE	302	1/1	0.96	0.25	4.06	29,29,29,29	0
54	MG	BA	3080	1/1	0.95	0.22	4.05	42,42,42,42	0
54	MG	DA	3427	1/1	0.98	0.21	4.00	24,24,24,24	0
54	MG	BA	3230	1/1	0.95	0.24	3.90	29,29,29,29	0
54	MG	BA	3162	1/1	0.97	0.24	3.89	22,22,22,22	0
54	MG	DA	3210	1/1	0.97	0.18	3.89	47,47,47,47	0
54	MG	DA	3513	1/1	0.92	0.19	3.85	52,52,52,52	0
54	MG	DA	3162	1/1	0.92	0.17	3.76	33,33,33,33	0
54	MG	BA	3382	1/1	0.83	0.22	3.74	39,39,39,39	0
54	MG	BA	3430	1/1	0.97	0.22	3.74	27,27,27,27	0
54	MG	BA	3360	1/1	0.80	0.23	3.68	41,41,41,41	0
54	MG	AA	1752	1/1	0.96	0.24	3.66	102,102,102,102	0
54	MG	DA	3012	1/1	0.99	0.18	3.65	34,34,34,34	0
54	MG	BA	3518	1/1	0.98	0.28	3.62	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3587	1/1	0.98	0.18	3.57	49,49,49,49	0
54	MG	BA	3431	1/1	0.92	0.21	3.45	28,28,28,28	0
54	MG	DA	3484	1/1	0.85	0.26	3.45	34,34,34,34	0
54	MG	BA	3372	1/1	0.93	0.24	3.44	32,32,32,32	0
54	MG	BA	3649	1/1	0.98	0.21	3.40	30,30,30,30	0
54	MG	AA	1666	1/1	0.94	0.29	3.39	71,71,71,71	0
54	MG	DA	3221	1/1	0.93	0.21	3.34	27,27,27,27	0
54	MG	CA	1768	1/1	0.88	0.34	3.29	95,95,95,95	0
54	MG	BU	201	1/1	0.95	0.24	3.29	30,30,30,30	0
54	MG	BA	3249	1/1	0.98	0.24	3.12	20,20,20,20	0
54	MG	BE	304	1/1	0.94	0.27	3.07	53,53,53,53	0
54	MG	AA	1682	1/1	0.98	0.23	3.05	48,48,48,48	0
54	MG	BA	3015	1/1	0.93	0.21	2.96	32,32,32,32	0
54	MG	BA	3086	1/1	0.97	0.23	2.91	21,21,21,21	0
54	MG	BA	3159	1/1	0.97	0.20	2.91	44,44,44,44	0
54	MG	BA	3418	1/1	0.95	0.23	2.90	28,28,28,28	0
54	MG	B9	102	1/1	0.96	0.28	2.83	29,29,29,29	0
54	MG	BA	3365	1/1	0.97	0.20	2.82	33,33,33,33	0
54	MG	DA	3072	1/1	0.89	0.30	2.78	60,60,60,60	0
54	MG	AA	1765	1/1	0.83	0.21	2.72	57,57,57,57	0
54	MG	DA	3300	1/1	0.92	0.19	2.71	29,29,29,29	0
54	MG	BA	3296	1/1	0.88	0.19	2.66	40,40,40,40	0
54	MG	DA	3062	1/1	0.95	0.25	2.63	43,43,43,43	0
54	MG	BR	203	1/1	0.95	0.25	2.62	33,33,33,33	0
54	MG	AA	1644	1/1	0.86	0.16	2.62	58,58,58,58	0
54	MG	DA	3493	1/1	0.93	0.20	2.58	33,33,33,33	0
54	MG	BA	3533	1/1	0.89	0.19	2.58	24,24,24,24	0
54	MG	DA	3207	1/1	0.89	0.16	2.57	27,27,27,27	0
54	MG	DA	3259	1/1	0.97	0.16	2.57	39,39,39,39	0
54	MG	AA	1691	1/1	0.90	0.22	2.53	57,57,57,57	0
54	MG	BE	303	1/1	0.94	0.28	2.52	47,47,47,47	0
54	MG	BA	3568	1/1	0.92	0.19	2.51	35,35,35,35	0
54	MG	BA	3421	1/1	0.97	0.20	2.49	34,34,34,34	0
54	MG	BA	3053	1/1	0.88	0.21	2.44	33,33,33,33	0
54	MG	BA	3032	1/1	0.93	0.19	2.40	25,25,25,25	0
54	MG	BA	3393	1/1	0.97	0.20	2.37	29,29,29,29	0
54	MG	AA	1787	1/1	0.79	0.20	2.37	54,54,54,54	0
54	MG	DA	3054	1/1	0.92	0.21	2.35	46,46,46,46	0
54	MG	DA	3455	1/1	0.95	0.21	2.27	34,34,34,34	0
54	MG	BA	3377	1/1	0.81	0.19	2.24	44,44,44,44	0
54	MG	DA	3245	1/1	0.91	0.20	2.22	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1651	1/1	0.88	0.23	2.17	62,62,62,62	0
54	MG	DA	3195	1/1	0.97	0.17	2.08	33,33,33,33	0
54	MG	BA	3035	1/1	0.94	0.21	2.04	23,23,23,23	0
54	MG	AI	201	1/1	0.90	0.29	2.01	67,67,67,67	0
54	MG	BA	3403	1/1	0.97	0.19	2.01	35,35,35,35	0
54	MG	AA	1696	1/1	0.93	0.23	1.99	66,66,66,66	0
54	MG	CA	1611	1/1	0.94	0.18	1.92	56,56,56,56	0
54	MG	BA	3315	1/1	0.92	0.19	1.91	63,63,63,63	0
54	MG	BB	206	1/1	0.95	0.20	1.90	34,34,34,34	0
54	MG	BA	3037	1/1	0.92	0.17	1.89	33,33,33,33	0
54	MG	DA	3373	1/1	0.95	0.15	1.88	58,58,58,58	0
54	MG	BA	3389	1/1	0.97	0.22	1.86	30,30,30,30	0
54	MG	CA	1716	1/1	0.96	0.20	1.79	49,49,49,49	0
54	MG	B3	102	1/1	0.82	0.20	1.74	52,52,52,52	0
54	MG	DA	3473	1/1	0.99	0.23	1.68	34,34,34,34	0
54	MG	DA	3565	1/1	0.87	0.19	1.62	62,62,62,62	0
54	MG	BA	3267	1/1	0.86	0.18	1.60	56,56,56,56	0
54	MG	BA	3391	1/1	0.97	0.21	1.58	24,24,24,24	0
54	MG	BH	201	1/1	0.90	0.20	1.55	60,60,60,60	0
54	MG	BA	3636	1/1	0.93	0.19	1.55	25,25,25,25	0
54	MG	BA	3370	1/1	0.95	0.21	1.54	23,23,23,23	0
54	MG	BA	3357	1/1	0.98	0.19	1.50	40,40,40,40	0
54	MG	AA	1762	1/1	0.85	0.31	1.48	78,78,78,78	0
54	MG	DA	3246	1/1	0.95	0.17	1.44	41,41,41,41	0
54	MG	BD	302	1/1	0.96	0.26	1.43	37,37,37,37	0
54	MG	CA	1627	1/1	0.93	0.19	1.35	72,72,72,72	0
54	MG	BR	202	1/1	0.97	0.21	1.35	35,35,35,35	0
54	MG	DA	3393	1/1	0.76	0.19	1.31	52,52,52,52	0
54	MG	BA	3385	1/1	0.98	0.18	1.30	31,31,31,31	0
54	MG	CA	1621	1/1	0.95	0.23	1.30	87,87,87,87	0
54	MG	BA	3052	1/1	0.92	0.18	1.24	38,38,38,38	0
54	MG	DA	3097	1/1	0.94	0.18	1.21	30,30,30,30	0
54	MG	DA	3447	1/1	0.91	0.20	1.19	58,58,58,58	0
54	MG	DA	3402	1/1	0.76	0.17	1.19	53,53,53,53	0
54	MG	CA	1711	1/1	0.92	0.21	1.18	55,55,55,55	0
54	MG	AA	1657	1/1	0.97	0.24	1.17	51,51,51,51	0
54	MG	DA	3495	1/1	0.90	0.17	1.16	34,34,34,34	0
54	MG	DA	3348	1/1	0.81	0.14	1.13	87,87,87,87	0
54	MG	CA	1713	1/1	0.76	0.32	1.12	95,95,95,95	0
54	MG	DA	3178	1/1	0.92	0.15	1.12	42,42,42,42	0
54	MG	BA	3412	1/1	0.98	0.18	1.10	19,19,19,19	0
54	MG	AA	1631	1/1	0.95	0.17	1.10	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1661	1/1	0.91	0.16	1.09	55,55,55,55	0
54	MG	BA	3151	1/1	0.85	0.21	1.07	34,34,34,34	0
54	MG	AA	1616	1/1	0.90	0.17	1.07	55,55,55,55	0
54	MG	DA	3214	1/1	0.96	0.16	1.03	32,32,32,32	0
54	MG	DA	3166	1/1	0.86	0.16	1.03	56,56,56,56	0
54	MG	DA	3201	1/1	0.95	0.16	1.02	29,29,29,29	0
54	MG	DA	3068	1/1	0.94	0.16	1.00	38,38,38,38	0
54	MG	DA	3551	1/1	0.80	0.16	0.95	69,69,69,69	0
54	MG	BA	3339	1/1	0.96	0.16	0.91	34,34,34,34	0
54	MG	DA	3360	1/1	0.96	0.18	0.87	36,36,36,36	0
54	MG	BA	3227	1/1	0.92	0.24	0.86	55,55,55,55	0
54	MG	CA	1686	1/1	0.97	0.27	0.83	67,67,67,67	0
54	MG	CA	1783	1/1	0.89	0.27	0.82	73,73,73,73	0
54	MG	BA	3404	1/1	0.96	0.20	0.80	27,27,27,27	0
54	MG	BA	3069	1/1	0.97	0.16	0.79	42,42,42,42	0
54	MG	BA	3017	1/1	0.98	0.17	0.78	27,27,27,27	0
54	MG	DA	3421	1/1	0.97	0.15	0.77	44,44,44,44	0
54	MG	AA	1605	1/1	0.61	0.24	0.74	62,62,62,62	0
54	MG	BA	3698	1/1	0.99	0.22	0.70	24,24,24,24	0
54	MG	DA	3406	1/1	0.96	0.14	0.64	54,54,54,54	0
54	MG	BA	3505	1/1	0.91	0.17	0.64	38,38,38,38	0
54	MG	DA	3048	1/1	0.96	0.14	0.62	50,50,50,50	0
54	MG	BA	3541	1/1	0.94	0.19	0.61	21,21,21,21	0
54	MG	DA	3018	1/1	0.96	0.16	0.60	54,54,54,54	0
54	MG	DA	3059	1/1	0.89	0.16	0.55	43,43,43,43	0
54	MG	DA	3354	1/1	0.98	0.15	0.53	39,39,39,39	0
54	MG	CA	1743	1/1	0.96	0.16	0.49	65,65,65,65	0
54	MG	BA	3137	1/1	0.93	0.19	0.48	45,45,45,45	0
54	MG	DA	3184	1/1	0.92	0.14	0.48	33,33,33,33	0
54	MG	CA	1691	1/1	0.95	0.17	0.47	74,74,74,74	0
54	MG	BA	3258	1/1	0.97	0.21	0.45	18,18,18,18	0
54	MG	CA	1649	1/1	0.96	0.21	0.44	67,67,67,67	0
54	MG	DA	3292	1/1	0.69	0.18	0.42	59,59,59,59	0
54	MG	BA	3384	1/1	0.98	0.18	0.39	29,29,29,29	0
54	MG	AA	1773	1/1	0.97	0.19	0.39	52,52,52,52	0
54	MG	DA	3233	1/1	0.92	0.14	0.38	42,42,42,42	0
54	MG	CA	1779	1/1	0.82	0.18	0.35	116,116,116,116	0
54	MG	BA	3311	1/1	0.97	0.18	0.32	34,34,34,34	0
54	MG	DA	3390	1/1	0.87	0.19	0.29	73,73,73,73	0
55	ZN	AD	301	1/1	0.96	0.27	0.28	76,76,76,76	0
54	MG	DA	3041	1/1	0.96	0.14	0.27	34,34,34,34	0
54	MG	DA	3458	1/1	0.93	0.15	0.27	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3349	1/1	0.93	0.15	0.27	55,55,55,55	0
54	MG	BA	3632	1/1	0.97	0.18	0.25	29,29,29,29	0
54	MG	BA	3364	1/1	0.96	0.18	0.23	24,24,24,24	0
54	MG	DA	3532	1/1	0.96	0.13	0.21	58,58,58,58	0
54	MG	BE	305	1/1	0.91	0.20	0.20	35,35,35,35	0
54	MG	CA	1703	1/1	0.88	0.17	0.19	46,46,46,46	0
54	MG	BA	3628	1/1	0.97	0.16	0.18	46,46,46,46	0
54	MG	DA	3578	1/1	0.94	0.14	0.16	45,45,45,45	0
54	MG	DA	3401	1/1	0.95	0.15	0.16	56,56,56,56	0
54	MG	BA	3487	1/1	0.81	0.18	0.15	49,49,49,49	0
54	MG	DA	3491	1/1	0.96	0.16	0.15	42,42,42,42	0
54	MG	DA	3571	1/1	0.82	0.16	0.09	53,53,53,53	0
54	MG	BA	3095	1/1	0.97	0.18	0.04	39,39,39,39	0
54	MG	D9	102	1/1	0.95	0.17	0.01	51,51,51,51	0
55	ZN	CD	301	1/1	0.75	0.30	-0.03	93,93,93,93	0
54	MG	CA	1655	1/1	0.94	0.16	-0.03	66,66,66,66	0
54	MG	CA	1688	1/1	0.74	0.23	-0.06	110,110,110,110	0
54	MG	DA	3412	1/1	0.91	0.13	-0.10	75,75,75,75	0
54	MG	DA	3301	1/1	0.94	0.14	-0.12	31,31,31,31	0
54	MG	BA	3604	1/1	0.99	0.20	-0.15	43,43,43,43	0
54	MG	BA	3411	1/1	0.97	0.18	-0.22	24,24,24,24	0
54	MG	DA	3319	1/1	0.91	0.13	-0.26	53,53,53,53	0
54	MG	DA	3302	1/1	0.89	0.14	-0.26	51,51,51,51	0
54	MG	BA	3063	1/1	0.97	0.17	-0.26	31,31,31,31	0
54	MG	DA	3561	1/1	0.95	0.12	-0.26	65,65,65,65	0
54	MG	BB	202	1/1	0.92	0.17	-0.29	45,45,45,45	0
54	MG	AA	1717	1/1	0.93	0.19	-0.31	79,79,79,79	0
54	MG	BA	3029	1/1	0.89	0.18	-0.32	38,38,38,38	0
54	MG	BA	3476	1/1	0.96	0.14	-0.32	55,55,55,55	0
54	MG	BA	3443	1/1	0.96	0.17	-0.32	31,31,31,31	0
54	MG	BD	304	1/1	0.95	0.17	-0.35	19,19,19,19	0
54	MG	DA	3172	1/1	0.93	0.15	-0.37	30,30,30,30	0
54	MG	CA	1618	1/1	0.82	0.14	-0.37	61,61,61,61	0
54	MG	DA	3261	1/1	0.95	0.13	-0.38	37,37,37,37	0
54	MG	BA	3027	1/1	0.90	0.17	-0.40	32,32,32,32	0
54	MG	CA	1616	1/1	0.71	0.15	-0.40	71,71,71,71	0
55	ZN	B6	101	1/1	0.99	0.13	-0.40	42,42,42,42	0
54	MG	CA	1738	1/1	0.94	0.18	-0.44	52,52,52,52	0
54	MG	AA	1714	1/1	0.62	0.17	-0.44	58,58,58,58	0
54	MG	DQ	203	1/1	0.93	0.12	-0.46	62,62,62,62	0
54	MG	BA	3261	1/1	0.92	0.17	-0.48	21,21,21,21	0
54	MG	CA	1718	1/1	0.84	0.14	-0.49	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3290	1/1	0.97	0.12	-0.49	47,47,47,47	0
54	MG	BA	3157	1/1	0.96	0.16	-0.51	36,36,36,36	0
54	MG	DA	3183	1/1	0.97	0.14	-0.51	36,36,36,36	0
54	MG	DA	3572	1/1	0.86	0.13	-0.52	45,45,45,45	0
54	MG	DA	3114	1/1	0.95	0.13	-0.53	36,36,36,36	0
54	MG	CA	1679	1/1	0.99	0.15	-0.53	53,53,53,53	0
54	MG	BA	3084	1/1	0.91	0.17	-0.54	43,43,43,43	0
54	MG	DD	302	1/1	0.92	0.14	-0.56	32,32,32,32	0
54	MG	DO	201	1/1	0.72	0.13	-0.56	67,67,67,67	0
54	MG	AA	1774	1/1	0.94	0.14	-0.56	78,78,78,78	0
54	MG	BA	3275	1/1	0.97	0.15	-0.60	31,31,31,31	0
54	MG	DA	3420	1/1	0.93	0.12	-0.60	52,52,52,52	0
54	MG	CA	1664	1/1	0.12	0.15	-0.62	62,62,62,62	0
54	MG	DA	3011	1/1	0.93	0.16	-0.64	45,45,45,45	0
54	MG	DA	3017	1/1	0.97	0.11	-0.65	48,48,48,48	0
54	MG	BB	205	1/1	0.86	0.13	-0.65	48,48,48,48	0
54	MG	B6	102	1/1	0.78	0.17	-0.66	69,69,69,69	0
54	MG	DA	3186	1/1	0.95	0.13	-0.66	27,27,27,27	0
55	ZN	D6	101	1/1	0.98	0.13	-0.67	66,66,66,66	0
54	MG	DA	3432	1/1	0.80	0.12	-0.68	67,67,67,67	0
54	MG	DF	303	1/1	0.91	0.17	-0.71	56,56,56,56	0
54	MG	D8	102	1/1	0.94	0.15	-0.72	66,66,66,66	0
54	MG	DA	3603	1/1	0.95	0.14	-0.74	44,44,44,44	0
54	MG	DA	3051	1/1	0.90	0.14	-0.74	73,73,73,73	0
54	MG	DA	3289	1/1	0.86	0.13	-0.76	44,44,44,44	0
55	ZN	B5	102	1/1	0.99	0.14	-0.79	42,42,42,42	0
54	MG	DA	3057	1/1	0.96	0.14	-0.79	53,53,53,53	0
54	MG	CA	1665	1/1	0.92	0.16	-0.80	60,60,60,60	0
54	MG	BA	3405	1/1	0.98	0.16	-0.81	22,22,22,22	0
54	MG	BT	201	1/1	0.96	0.14	-0.81	49,49,49,49	0
54	MG	BA	3231	1/1	0.97	0.19	-0.82	35,35,35,35	0
54	MG	BA	3046	1/1	0.94	0.15	-0.83	35,35,35,35	0
54	MG	CA	1751	1/1	0.91	0.10	-0.84	89,89,89,89	0
54	MG	DA	3071	1/1	0.95	0.13	-0.85	39,39,39,39	0
54	MG	DA	3058	1/1	0.97	0.12	-0.85	38,38,38,38	0
54	MG	BA	3186	1/1	0.95	0.17	-0.85	30,30,30,30	0
54	MG	BA	3043	1/1	0.89	0.17	-0.86	30,30,30,30	0
54	MG	DA	3403	1/1	0.87	0.12	-0.87	56,56,56,56	0
55	ZN	BY	201	1/1	0.99	0.12	-0.88	54,54,54,54	0
54	MG	BA	3424	1/1	0.95	0.14	-0.88	25,25,25,25	0
54	MG	DA	3052	1/1	0.96	0.14	-0.88	35,35,35,35	0
54	MG	DA	3082	1/1	0.97	0.12	-0.91	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3106	1/1	0.95	0.12	-0.93	48,48,48,48	0
54	MG	DA	3204	1/1	0.96	0.14	-0.95	32,32,32,32	0
55	ZN	D4	101	1/1	0.73	0.09	-0.96	173,173,173,173	0
55	ZN	D5	101	1/1	0.97	0.10	-0.96	53,53,53,53	0
54	MG	DA	3335	1/1	0.82	0.13	-0.96	68,68,68,68	0
54	MG	BG	201	1/1	0.89	0.13	-0.97	56,56,56,56	0
54	MG	DA	3075	1/1	0.90	0.13	-0.98	48,48,48,48	0
54	MG	DA	3328	1/1	0.84	0.12	-1.03	52,52,52,52	0
54	MG	AA	1743	1/1	0.95	0.15	-1.03	58,58,58,58	0
54	MG	DA	3275	1/1	0.84	0.13	-1.03	69,69,69,69	0
54	MG	BA	3454	1/1	0.92	0.12	-1.04	55,55,55,55	0
54	MG	BO	201	1/1	0.94	0.15	-1.06	53,53,53,53	0
54	MG	BA	3408	1/1	0.90	0.16	-1.07	24,24,24,24	0
55	ZN	D9	101	1/1	0.98	0.09	-1.11	68,68,68,68	0
54	MG	CA	1747	1/1	0.94	0.15	-1.11	63,63,63,63	0
55	ZN	B4	101	1/1	0.86	0.07	-1.12	117,117,117,117	0
54	MG	AA	1606	1/1	0.89	0.12	-1.14	63,63,63,63	0
54	MG	CA	1741	1/1	0.27	0.12	-1.14	117,117,117,117	0
54	MG	AA	1712	1/1	0.98	0.15	-1.17	43,43,43,43	0
54	MG	AD	303	1/1	0.92	0.13	-1.18	84,84,84,84	0
54	MG	BA	3313	1/1	0.98	0.16	-1.19	23,23,23,23	0
54	MG	BA	3082	1/1	0.98	0.16	-1.25	26,26,26,26	0
54	MG	BA	3662	1/1	0.92	0.15	-1.28	26,26,26,26	0
54	MG	BB	210	1/1	0.89	0.15	-1.33	62,62,62,62	0
54	MG	AA	1789	1/1	0.88	0.11	-1.36	78,78,78,78	0
54	MG	CA	1722	1/1	0.98	0.13	-1.37	58,58,58,58	0
55	ZN	CN	101	1/1	0.96	0.08	-1.37	108,108,108,108	0
54	MG	DA	3336	1/1	0.97	0.13	-1.38	53,53,53,53	0
54	MG	DA	3151	1/1	0.94	0.13	-1.39	31,31,31,31	0
54	MG	DA	3357	1/1	0.93	0.13	-1.41	45,45,45,45	0
54	MG	DA	3344	1/1	0.94	0.10	-1.44	56,56,56,56	0
54	MG	DA	3228	1/1	0.98	0.13	-1.46	60,60,60,60	0
54	MG	DB	201	1/1	0.91	0.11	-1.48	67,67,67,67	0
54	MG	D1	101	1/1	0.84	0.09	-1.53	59,59,59,59	0
54	MG	DA	3343	1/1	0.95	0.11	-1.56	54,54,54,54	0
54	MG	DA	3440	1/1	0.98	0.12	-1.59	65,65,65,65	0
54	MG	BA	3564	1/1	0.69	0.12	-1.60	67,67,67,67	0
54	MG	BA	3263	1/1	0.90	0.11	-1.60	63,63,63,63	0
54	MG	DA	3443	1/1	0.91	0.07	-1.62	51,51,51,51	0
54	MG	BA	3301	1/1	0.89	0.11	-1.63	61,61,61,61	0
54	MG	BA	3283	1/1	0.95	0.16	-1.66	36,36,36,36	0
55	ZN	DY	201	1/1	0.97	0.05	-1.68	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DE	302	1/1	0.96	0.14	-1.80	37,37,37,37	0
54	MG	BA	3048	1/1	0.93	0.13	-1.81	35,35,35,35	0
54	MG	CA	1643	1/1	0.67	0.12	-1.85	76,76,76,76	0
54	MG	BA	3409	1/1	0.97	0.14	-1.87	26,26,26,26	0
54	MG	DA	3005	1/1	0.96	0.12	-1.88	53,53,53,53	0
54	MG	DA	3415	1/1	0.89	0.12	-1.90	53,53,53,53	0
54	MG	BA	3549	1/1	0.94	0.15	-1.94	22,22,22,22	0
54	MG	DA	3304	1/1	0.95	0.10	-1.94	39,39,39,39	0
54	MG	DA	3252	1/1	0.93	0.13	-1.95	45,45,45,45	0
54	MG	DA	3212	1/1	0.94	0.09	-1.97	32,32,32,32	0
54	MG	AA	1708	1/1	0.96	0.13	-1.98	61,61,61,61	0
54	MG	DA	3471	1/1	0.92	0.14	-2.00	41,41,41,41	0
54	MG	BA	3224	1/1	0.95	0.17	-2.01	28,28,28,28	0
54	MG	BA	3450	1/1	0.98	0.13	-2.06	24,24,24,24	0
54	MG	DA	3056	1/1	0.93	0.11	-2.08	31,31,31,31	0
54	MG	DA	3266	1/1	0.90	0.12	-2.08	40,40,40,40	0
54	MG	BA	3416	1/1	0.97	0.16	-2.18	22,22,22,22	0
54	MG	BQ	203	1/1	0.96	0.14	-2.18	38,38,38,38	0
54	MG	BA	3010	1/1	0.99	0.14	-2.19	27,27,27,27	0
54	MG	DA	3240	1/1	0.76	0.11	-2.21	56,56,56,56	0
54	MG	BA	3608	1/1	0.93	0.13	-2.21	21,21,21,21	0
54	MG	AA	1632	1/1	0.90	0.11	-2.22	64,64,64,64	0
54	MG	BA	3464	1/1	0.97	0.14	-2.24	28,28,28,28	0
54	MG	BA	3650	1/1	0.94	0.14	-2.25	53,53,53,53	0
54	MG	BF	303	1/1	0.96	0.12	-2.29	43,43,43,43	0
55	ZN	B9	101	1/1	0.99	0.10	-2.29	49,49,49,49	0
54	MG	CA	1744	1/1	0.94	0.08	-2.33	69,69,69,69	0
54	MG	DA	3433	1/1	0.97	0.11	-2.36	34,34,34,34	0
54	MG	BA	3244	1/1	0.87	0.13	-2.37	49,49,49,49	0
54	MG	CA	1755	1/1	0.88	0.13	-2.38	79,79,79,79	0
54	MG	DA	3248	1/1	0.97	0.10	-2.42	59,59,59,59	0
54	MG	BA	3627	1/1	0.91	0.13	-2.47	40,40,40,40	0
54	MG	CA	1662	1/1	0.96	0.09	-2.51	54,54,54,54	0
54	MG	AA	1745	1/1	0.92	0.10	-2.51	63,63,63,63	0
54	MG	BA	3041	1/1	0.99	0.13	-2.54	29,29,29,29	0
54	MG	BA	3216	1/1	0.95	0.12	-2.55	64,64,64,64	0
54	MG	BA	3020	1/1	0.79	0.09	-2.56	69,69,69,69	0
54	MG	DA	3434	1/1	0.95	0.08	-2.57	60,60,60,60	0
54	MG	DA	3313	1/1	0.97	0.12	-2.58	34,34,34,34	0
54	MG	BA	3354	1/1	0.98	0.13	-2.58	24,24,24,24	0
54	MG	BA	3455	1/1	0.95	0.09	-2.59	41,41,41,41	0
54	MG	BA	3254	1/1	0.96	0.12	-2.60	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3036	1/1	0.97	0.12	-2.61	41,41,41,41	0
54	MG	DA	3288	1/1	0.94	0.12	-2.62	51,51,51,51	0
54	MG	DA	3350	1/1	0.94	0.08	-2.68	40,40,40,40	0
54	MG	CA	1712	1/1	0.94	0.08	-2.69	55,55,55,55	0
54	MG	DA	3380	1/1	0.93	0.09	-2.71	47,47,47,47	0
54	MG	BA	3045	1/1	0.97	0.19	-2.71	35,35,35,35	0
54	MG	BA	3177	1/1	0.97	0.13	-2.73	41,41,41,41	0
55	ZN	AN	101	1/1	0.99	0.11	-2.74	118,118,118,118	0
54	MG	AA	1728	1/1	0.98	0.07	-2.78	68,68,68,68	0
54	MG	BA	3232	1/1	0.99	0.16	-2.82	24,24,24,24	0
54	MG	DA	3269	1/1	0.95	0.10	-2.82	36,36,36,36	0
54	MG	DE	301	1/1	0.96	0.10	-2.82	29,29,29,29	0
54	MG	BA	3381	1/1	0.95	0.12	-2.88	41,41,41,41	0
54	MG	BA	3508	1/1	0.99	0.10	-3.01	33,33,33,33	0
54	MG	BA	3466	1/1	0.94	0.07	-3.05	78,78,78,78	0
54	MG	AA	1808	1/1	0.93	0.12	-3.06	43,43,43,43	0
54	MG	BA	3602	1/1	0.97	0.06	-3.06	43,43,43,43	0
54	MG	BA	3328	1/1	0.81	0.13	-3.07	49,49,49,49	0
54	MG	CA	1663	1/1	0.90	0.14	-3.07	75,75,75,75	0
54	MG	DA	3180	1/1	0.96	0.11	-3.08	29,29,29,29	0
54	MG	DA	3588	1/1	0.94	0.11	-3.12	38,38,38,38	0
54	MG	BA	3310	1/1	0.96	0.13	-3.15	19,19,19,19	0
54	MG	AA	1742	1/1	0.92	0.12	-3.19	78,78,78,78	0
54	MG	BA	3379	1/1	0.91	0.12	-3.20	30,30,30,30	0
54	MG	BA	3098	1/1	0.93	0.13	-3.22	39,39,39,39	0
54	MG	BD	303	1/1	0.95	0.12	-3.31	33,33,33,33	0
54	MG	AA	1739	1/1	0.94	0.11	-3.31	72,72,72,72	0
54	MG	BA	3557	1/1	0.80	0.14	-3.36	25,25,25,25	0
54	MG	BA	3395	1/1	0.85	0.11	-3.40	37,37,37,37	0
54	MG	BA	3349	1/1	0.98	0.15	-3.40	30,30,30,30	0
54	MG	DB	207	1/1	0.81	0.08	-3.41	82,82,82,82	0
54	MG	BA	3056	1/1	0.91	0.13	-3.46	32,32,32,32	0
54	MG	DA	3022	1/1	0.93	0.10	-3.49	37,37,37,37	0
54	MG	DA	3069	1/1	0.95	0.10	-3.49	67,67,67,67	0
54	MG	DA	3405	1/1	0.85	0.13	-3.54	56,56,56,56	0
54	MG	BD	305	1/1	0.98	0.07	-3.55	46,46,46,46	0
54	MG	DA	3255	1/1	0.80	0.08	-3.57	51,51,51,51	0
54	MG	DA	3016	1/1	0.94	0.09	-3.58	64,64,64,64	0
54	MG	CA	1608	1/1	0.94	0.12	-3.58	54,54,54,54	0
54	MG	DA	3174	1/1	0.96	0.11	-3.58	24,24,24,24	0
54	MG	BA	3396	1/1	0.98	0.15	-3.61	39,39,39,39	0
54	MG	BA	3329	1/1	0.89	0.14	-3.61	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3060	1/1	0.90	0.09	-3.66	57,57,57,57	0
54	MG	BA	3185	1/1	0.89	0.10	-3.67	44,44,44,44	0
54	MG	DA	3274	1/1	0.86	0.09	-3.67	51,51,51,51	0
54	MG	DA	3609	1/1	0.97	0.10	-3.71	42,42,42,42	0
54	MG	DA	3394	1/1	0.89	0.11	-3.74	59,59,59,59	0
54	MG	BA	3380	1/1	0.96	0.11	-3.82	37,37,37,37	0
54	MG	AA	1788	1/1	0.74	0.11	-3.82	76,76,76,76	0
54	MG	BA	3127	1/1	0.97	0.11	-3.83	30,30,30,30	0
54	MG	AA	1720	1/1	0.96	0.10	-3.84	74,74,74,74	0
54	MG	CA	1656	1/1	0.97	0.07	-3.85	66,66,66,66	0
54	MG	DA	3279	1/1	0.92	0.07	-3.93	66,66,66,66	0
54	MG	BB	204	1/1	0.94	0.10	-3.96	47,47,47,47	0
54	MG	DA	3600	1/1	0.95	0.07	-3.98	33,33,33,33	0
54	MG	BA	3667	1/1	0.97	0.12	-4.01	22,22,22,22	0
54	MG	DA	3334	1/1	0.94	0.10	-4.04	45,45,45,45	0
54	MG	DA	3243	1/1	0.97	0.11	-4.04	32,32,32,32	0
54	MG	DA	3339	1/1	0.96	0.08	-4.13	53,53,53,53	0
54	MG	BA	3245	1/1	0.97	0.10	-4.21	29,29,29,29	0
54	MG	AA	1754	1/1	0.90	0.09	-4.22	49,49,49,49	0
54	MG	BA	3402	1/1	0.99	0.14	-4.23	31,31,31,31	0
54	MG	BA	3083	1/1	0.94	0.10	-4.27	32,32,32,32	0
54	MG	DA	3604	1/1	0.93	0.07	-4.38	72,72,72,72	0
54	MG	DA	3512	1/1	0.93	0.08	-4.49	43,43,43,43	0
54	MG	DA	3315	1/1	0.83	0.07	-4.51	49,49,49,49	0
54	MG	BA	3562	1/1	0.89	0.08	-4.62	34,34,34,34	0
54	MG	DA	3330	1/1	0.85	0.11	-4.71	56,56,56,56	0
54	MG	DA	3268	1/1	0.81	0.09	-4.74	54,54,54,54	0
54	MG	BA	3182	1/1	0.96	0.10	-4.92	30,30,30,30	0
54	MG	BA	3674	1/1	0.92	0.10	-4.93	62,62,62,62	0
54	MG	BA	3181	1/1	0.97	0.07	-5.00	41,41,41,41	0
54	MG	BR	205	1/1	0.94	0.12	-5.01	45,45,45,45	0
54	MG	DA	3217	1/1	0.92	0.07	-5.16	54,54,54,54	0
54	MG	BA	3356	1/1	0.95	0.09	-5.20	55,55,55,55	0
54	MG	BA	3312	1/1	0.98	0.12	-5.29	32,32,32,32	0
54	MG	BA	3293	1/1	0.96	0.11	-5.30	36,36,36,36	0
54	MG	BA	3116	1/1	0.92	0.10	-5.35	50,50,50,50	0
54	MG	BA	3506	1/1	0.96	0.07	-5.40	33,33,33,33	0
54	MG	BA	3149	1/1	0.95	0.13	-5.41	24,24,24,24	0
54	MG	DA	3181	1/1	0.95	0.09	-5.41	50,50,50,50	0
54	MG	DA	3160	1/1	0.95	0.04	-5.43	42,42,42,42	0
54	MG	BA	3132	1/1	0.95	0.11	-5.50	45,45,45,45	0
54	MG	CA	1698	1/1	0.96	0.10	-5.58	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3080	1/1	0.97	0.09	-5.63	48,48,48,48	0
54	MG	DA	3267	1/1	0.92	0.07	-5.65	34,34,34,34	0
54	MG	BA	3166	1/1	0.98	0.09	-5.73	53,53,53,53	0
54	MG	AA	1737	1/1	0.97	0.12	-5.88	41,41,41,41	0
54	MG	BA	3644	1/1	0.95	0.15	-6.00	35,35,35,35	0
54	MG	CA	1693	1/1	0.98	0.07	-6.08	73,73,73,73	0
54	MG	DA	3213	1/1	0.94	0.10	-6.31	33,33,33,33	0
54	MG	BA	3700	1/1	0.98	0.08	-6.40	41,41,41,41	0
54	MG	DA	3155	1/1	0.89	0.10	-6.61	53,53,53,53	0
54	MG	BA	3180	1/1	0.97	0.09	-6.65	42,42,42,42	0
54	MG	BA	3407	1/1	0.99	0.13	-6.66	24,24,24,24	0
54	MG	BA	3337	1/1	0.95	0.07	-6.73	27,27,27,27	0
54	MG	BA	3155	1/1	0.91	0.13	-6.77	37,37,37,37	0
54	MG	BA	3426	1/1	0.96	0.09	-6.87	28,28,28,28	0
54	MG	DA	3271	1/1	0.95	0.05	-6.89	42,42,42,42	0
54	MG	AA	1722	1/1	0.97	0.05	-6.90	48,48,48,48	0
54	MG	BA	3175	1/1	0.95	0.07	-7.02	31,31,31,31	0
54	MG	BA	3023	1/1	0.94	0.11	-7.46	43,43,43,43	0
54	MG	BA	3212	1/1	0.97	0.07	-7.51	52,52,52,52	0
54	MG	CA	1697	1/1	0.83	0.06	-7.56	95,95,95,95	0
54	MG	BA	3214	1/1	0.94	0.07	-7.77	39,39,39,39	0
54	MG	BA	3573	1/1	0.95	0.10	-7.90	54,54,54,54	0
54	MG	DA	3215	1/1	0.95	0.09	-7.93	30,30,30,30	0
54	MG	BA	3062	1/1	0.97	0.11	-7.98	32,32,32,32	0
54	MG	AA	1705	1/1	0.95	0.08	-8.35	46,46,46,46	0
54	MG	DA	3590	1/1	0.97	0.07	-8.49	59,59,59,59	0
54	MG	BA	3242	1/1	0.87	0.08	-8.76	45,45,45,45	0
54	MG	BA	3486	1/1	0.92	0.14	-9.05	25,25,25,25	0
54	MG	BA	3170	1/1	0.95	0.10	-9.57	38,38,38,38	0
54	MG	BA	3493	1/1	0.96	0.11	-9.81	65,65,65,65	0
54	MG	DA	3203	1/1	0.98	0.06	-9.91	36,36,36,36	0
54	MG	DA	3202	1/1	0.96	0.05	-10.14	29,29,29,29	0
54	MG	BA	3542	1/1	0.94	0.07	-10.72	33,33,33,33	0
54	MG	BA	3237	1/1	0.93	0.06	-11.15	41,41,41,41	0
54	MG	BA	3238	1/1	0.87	0.10	-11.51	39,39,39,39	0
54	MG	BA	3115	1/1	0.98	0.08	-12.93	35,35,35,35	0
54	MG	BA	3326	1/1	0.90	0.07	-20.78	46,46,46,46	0
54	MG	BA	3176	1/1	0.99	0.10	-23.28	27,27,27,27	0
54	MG	BA	3259	1/1	0.96	0.13	-25.17	20,20,20,20	0
54	MG	BB	213	1/1	0.86	0.11	-	46,46,46,46	0
54	MG	AA	1613	1/1	0.85	0.34	-	77,77,77,77	0
54	MG	DR	201	1/1	0.95	0.31	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3007	1/1	0.96	0.25	-	59,59,59,59	0
54	MG	DA	3102	1/1	0.96	0.23	-	48,48,48,48	0
54	MG	CA	1749	1/1	0.95	0.16	-	69,69,69,69	0
54	MG	AA	1719	1/1	0.94	0.16	-	66,66,66,66	0
54	MG	DA	3459	1/1	0.95	0.09	-	90,90,90,90	0
54	MG	DA	3593	1/1	0.92	0.15	-	58,58,58,58	0
54	MG	BA	3228	1/1	0.94	0.26	-	44,44,44,44	0
54	MG	AA	1735	1/1	0.98	0.44	-	62,62,62,62	0
54	MG	DA	3352	1/1	0.84	0.15	-	82,82,82,82	0
54	MG	DP	201	1/1	0.81	0.20	-	78,78,78,78	0
54	MG	BZ	302	1/1	0.96	0.13	-	45,45,45,45	0
54	MG	CA	1617	1/1	0.91	0.29	-	63,63,63,63	0
54	MG	BA	3435	1/1	0.96	0.05	-	40,40,40,40	0
54	MG	BA	3504	1/1	0.93	0.16	-	53,53,53,53	0
54	MG	DA	3384	1/1	0.86	0.35	-	49,49,49,49	0
54	MG	BA	3483	1/1	0.94	0.22	-	31,31,31,31	0
54	MG	BA	3563	1/1	0.94	0.12	-	59,59,59,59	0
54	MG	DA	3099	1/1	0.95	0.25	-	54,54,54,54	0
54	MG	BA	3429	1/1	0.94	0.13	-	59,59,59,59	0
54	MG	BA	3287	1/1	0.85	0.27	-	44,44,44,44	0
54	MG	DA	3573	1/1	0.82	0.54	-	68,68,68,68	0
54	MG	DA	3276	1/1	0.93	0.16	-	76,76,76,76	0
54	MG	BA	3658	1/1	0.90	0.09	-	61,61,61,61	0
54	MG	BB	201	1/1	0.76	0.22	-	67,67,67,67	0
54	MG	DA	3153	1/1	0.97	0.10	-	32,32,32,32	0
54	MG	BT	203	1/1	0.98	0.06	-	51,51,51,51	0
54	MG	BA	3704	1/1	0.83	0.18	-	70,70,70,70	0
54	MG	DA	3312	1/1	0.84	0.12	-	52,52,52,52	0
54	MG	BA	3206	1/1	0.91	0.14	-	67,67,67,67	0
54	MG	BA	3246	1/1	0.96	0.15	-	46,46,46,46	0
54	MG	DA	3422	1/1	0.94	0.07	-	71,71,71,71	0
54	MG	BA	3663	1/1	0.97	0.06	-	53,53,53,53	0
54	MG	CA	1658	1/1	0.97	0.10	-	64,64,64,64	0
54	MG	BA	3716	1/1	0.80	0.17	-	54,54,54,54	0
54	MG	BA	3436	1/1	0.78	0.17	-	41,41,41,41	0
54	MG	CA	1758	1/1	0.53	0.24	-	64,64,64,64	0
54	MG	DA	3135	1/1	0.89	0.17	-	59,59,59,59	0
54	MG	AA	1677	1/1	0.96	0.05	-	50,50,50,50	0
54	MG	DA	3236	1/1	0.84	0.09	-	40,40,40,40	0
54	MG	BA	3109	1/1	0.95	0.12	-	37,37,37,37	0
54	MG	BA	3480	1/1	0.94	0.10	-	58,58,58,58	0
54	MG	AA	1807	1/1	0.88	0.11	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3294	1/1	0.91	0.10	-	67,67,67,67	0
54	MG	BA	3088	1/1	0.92	0.15	-	42,42,42,42	0
54	MG	BA	3200	1/1	0.97	0.16	-	24,24,24,24	0
54	MG	DA	3136	1/1	0.81	0.71	-	62,62,62,62	0
54	MG	DA	3141	1/1	0.62	0.36	-	70,70,70,70	0
54	MG	AA	1723	1/1	0.95	0.11	-	82,82,82,82	0
54	MG	BB	219	1/1	0.93	0.17	-	54,54,54,54	0
54	MG	BA	3390	1/1	0.93	0.25	-	33,33,33,33	0
54	MG	DA	3410	1/1	0.69	0.20	-	80,80,80,80	0
54	MG	B9	104	1/1	0.94	0.10	-	52,52,52,52	0
54	MG	CA	1782	1/1	0.87	0.21	-	63,63,63,63	0
54	MG	BA	3123	1/1	0.97	0.21	-	48,48,48,48	0
54	MG	DA	3103	1/1	0.95	0.33	-	48,48,48,48	0
54	MG	BA	3666	1/1	0.94	0.14	-	78,78,78,78	0
54	MG	DB	204	1/1	0.97	0.18	-	65,65,65,65	0
54	MG	BA	3211	1/1	0.97	0.15	-	49,49,49,49	0
54	MG	DA	3539	1/1	0.93	0.16	-	54,54,54,54	0
54	MG	DA	3502	1/1	0.84	0.08	-	78,78,78,78	0
54	MG	CA	1794	1/1	0.93	0.12	-	57,57,57,57	0
54	MG	DA	3594	1/1	0.89	0.09	-	62,62,62,62	0
54	MG	BA	3229	1/1	0.94	0.14	-	61,61,61,61	0
54	MG	BA	3047	1/1	0.94	0.13	-	30,30,30,30	0
54	MG	DA	3359	1/1	0.87	0.39	-	69,69,69,69	0
54	MG	BA	3350	1/1	0.97	0.14	-	28,28,28,28	0
54	MG	DA	3253	1/1	0.91	0.12	-	58,58,58,58	0
54	MG	CA	1776	1/1	0.82	0.23	-	76,76,76,76	0
54	MG	BA	3635	1/1	0.95	0.07	-	72,72,72,72	0
54	MG	AA	1790	1/1	0.96	0.20	-	63,63,63,63	0
54	MG	AA	1792	1/1	0.96	0.09	-	51,51,51,51	0
54	MG	BA	3589	1/1	0.93	0.15	-	41,41,41,41	0
54	MG	CA	1742	1/1	0.84	0.12	-	99,99,99,99	0
54	MG	DA	3522	1/1	0.95	0.13	-	59,59,59,59	0
54	MG	AA	1601	1/1	0.96	0.40	-	52,52,52,52	0
54	MG	AA	1716	1/1	0.88	0.06	-	62,62,62,62	0
54	MG	BA	3465	1/1	0.91	0.15	-	24,24,24,24	0
54	MG	BA	3026	1/1	0.88	0.21	-	50,50,50,50	0
54	MG	DA	3570	1/1	0.92	0.14	-	63,63,63,63	0
54	MG	DW	201	1/1	0.95	0.06	-	63,63,63,63	0
54	MG	DA	3413	1/1	0.96	0.06	-	78,78,78,78	0
54	MG	DA	3117	1/1	0.89	0.17	-	69,69,69,69	0
54	MG	DA	3575	1/1	0.90	0.21	-	98,98,98,98	0
54	MG	BA	3576	1/1	0.89	0.10	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3668	1/1	0.96	0.08	-	60,60,60,60	0
54	MG	CA	1674	1/1	0.80	0.12	-	80,80,80,80	0
54	MG	DA	3439	1/1	0.94	0.34	-	57,57,57,57	0
54	MG	DA	3283	1/1	0.84	0.14	-	51,51,51,51	0
54	MG	BA	3468	1/1	0.95	0.15	-	63,63,63,63	0
54	MG	BA	3699	1/1	0.94	0.12	-	43,43,43,43	0
54	MG	BA	3011	1/1	0.92	0.30	-	47,47,47,47	0
54	MG	BA	3348	1/1	0.95	0.09	-	44,44,44,44	0
54	MG	BA	3130	1/1	0.82	0.13	-	79,79,79,79	0
54	MG	AA	1733	1/1	0.94	0.12	-	59,59,59,59	0
54	MG	BA	3005	1/1	0.93	0.12	-	56,56,56,56	0
54	MG	DA	3314	1/1	0.91	0.16	-	31,31,31,31	0
54	MG	BA	3447	1/1	0.79	0.09	-	53,53,53,53	0
54	MG	BA	3199	1/1	0.98	0.05	-	46,46,46,46	0
54	MG	DA	3090	1/1	0.89	0.14	-	45,45,45,45	0
54	MG	AA	1704	1/1	0.94	0.07	-	75,75,75,75	0
54	MG	CA	1651	1/1	0.94	0.10	-	55,55,55,55	0
54	MG	DA	3519	1/1	0.90	0.17	-	61,61,61,61	0
54	MG	BA	3590	1/1	0.68	0.35	-	77,77,77,77	0
54	MG	DF	304	1/1	0.97	0.07	-	41,41,41,41	0
54	MG	BT	202	1/1	0.91	0.28	-	52,52,52,52	0
54	MG	DA	3534	1/1	0.94	0.25	-	53,53,53,53	0
54	MG	DA	3251	1/1	0.95	0.20	-	41,41,41,41	0
54	MG	BA	3366	1/1	0.97	0.20	-	36,36,36,36	0
54	MG	BA	3491	1/1	0.81	0.11	-	72,72,72,72	0
54	MG	CA	1706	1/1	0.92	0.21	-	76,76,76,76	0
54	MG	BA	3323	1/1	0.97	0.12	-	57,57,57,57	0
54	MG	DA	3001	1/1	0.93	0.12	-	38,38,38,38	0
54	MG	BQ	201	1/1	0.69	0.37	-	61,61,61,61	0
54	MG	BA	3314	1/1	0.84	0.16	-	39,39,39,39	0
54	MG	AA	1636	1/1	0.92	0.10	-	49,49,49,49	0
54	MG	BA	3292	1/1	0.96	0.09	-	36,36,36,36	0
54	MG	BA	3437	1/1	0.98	0.17	-	28,28,28,28	0
54	MG	AA	1686	1/1	0.61	0.32	-	68,68,68,68	0
54	MG	DA	3520	1/1	0.89	0.13	-	74,74,74,74	0
54	MG	BA	3555	1/1	0.98	0.13	-	23,23,23,23	0
54	MG	BA	3501	1/1	0.78	0.15	-	51,51,51,51	0
54	MG	DA	3436	1/1	0.87	0.13	-	77,77,77,77	0
54	MG	BA	3055	1/1	0.93	0.27	-	44,44,44,44	0
54	MG	DA	3542	1/1	0.93	0.23	-	65,65,65,65	0
54	MG	BA	3580	1/1	0.94	0.17	-	49,49,49,49	0
54	MG	CA	1677	1/1	0.75	0.20	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1747	1/1	0.98	0.07	-	60,60,60,60	0
54	MG	DA	3396	1/1	0.98	0.14	-	48,48,48,48	0
54	MG	AA	1628	1/1	0.93	0.34	-	81,81,81,81	0
54	MG	AA	1635	1/1	0.63	0.11	-	77,77,77,77	0
54	MG	DA	3544	1/1	0.96	0.15	-	67,67,67,67	0
54	MG	BA	3714	1/1	0.87	0.14	-	47,47,47,47	0
54	MG	CA	1659	1/1	0.88	0.13	-	89,89,89,89	0
54	MG	DA	3244	1/1	0.85	0.19	-	32,32,32,32	0
54	MG	CA	1759	1/1	0.79	0.09	-	95,95,95,95	0
54	MG	BA	3691	1/1	0.95	0.11	-	57,57,57,57	0
54	MG	BA	3256	1/1	0.92	0.14	-	38,38,38,38	0
54	MG	BA	3319	1/1	0.98	0.17	-	26,26,26,26	0
54	MG	DA	3168	1/1	0.87	0.17	-	41,41,41,41	0
54	MG	DA	3431	1/1	0.99	0.15	-	27,27,27,27	0
54	MG	CA	1740	1/1	0.98	0.35	-	72,72,72,72	0
54	MG	CA	1791	1/1	0.71	0.15	-	72,72,72,72	0
54	MG	CA	1680	1/1	0.90	0.04	-	92,92,92,92	0
54	MG	BA	3597	1/1	0.95	0.14	-	36,36,36,36	0
54	MG	BA	3107	1/1	0.93	0.23	-	47,47,47,47	0
54	MG	DA	3297	1/1	0.89	0.13	-	49,49,49,49	0
54	MG	DA	3310	1/1	0.94	0.30	-	47,47,47,47	0
54	MG	BA	3324	1/1	0.93	0.13	-	48,48,48,48	0
54	MG	DE	303	1/1	0.97	0.31	-	31,31,31,31	0
54	MG	DA	3375	1/1	0.85	0.05	-	60,60,60,60	0
54	MG	AA	1668	1/1	0.93	0.07	-	52,52,52,52	0
54	MG	BA	3492	1/1	0.94	0.11	-	57,57,57,57	0
54	MG	DA	3190	1/1	0.91	0.14	-	43,43,43,43	0
54	MG	DA	3438	1/1	0.95	0.09	-	54,54,54,54	0
54	MG	BA	3234	1/1	0.92	0.10	-	61,61,61,61	0
54	MG	CA	1775	1/1	0.91	0.11	-	78,78,78,78	0
54	MG	BB	212	1/1	0.97	0.08	-	49,49,49,49	0
54	MG	DA	3424	1/1	0.91	0.19	-	49,49,49,49	0
54	MG	CA	1788	1/1	0.94	0.11	-	51,51,51,51	0
54	MG	BA	3442	1/1	0.97	0.26	-	24,24,24,24	0
54	MG	BA	3195	1/1	0.96	0.10	-	46,46,46,46	0
54	MG	BA	3527	1/1	0.93	0.15	-	51,51,51,51	0
54	MG	AA	1665	1/1	0.92	0.20	-	66,66,66,66	0
54	MG	DA	3636	1/1	0.84	0.19	-	66,66,66,66	0
54	MG	BA	3108	1/1	0.94	0.14	-	51,51,51,51	0
54	MG	CA	1778	1/1	0.77	0.10	-	83,83,83,83	0
54	MG	BA	3152	1/1	0.80	0.17	-	48,48,48,48	0
54	MG	DA	3567	1/1	0.95	0.15	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BD	307	1/1	0.83	0.22	-	65,65,65,65	0
54	MG	BA	3456	1/1	0.97	0.13	-	37,37,37,37	0
54	MG	BQ	205	1/1	0.90	0.15	-	42,42,42,42	0
54	MG	CA	1767	1/1	0.89	0.10	-	86,86,86,86	0
54	MG	CA	1670	1/1	0.93	0.23	-	80,80,80,80	0
54	MG	BA	3220	1/1	0.90	0.32	-	62,62,62,62	0
54	MG	DA	3091	1/1	0.95	0.98	-	38,38,38,38	0
54	MG	BA	3299	1/1	0.94	0.17	-	44,44,44,44	0
54	MG	BA	3252	1/1	0.88	0.13	-	52,52,52,52	0
54	MG	DA	3385	1/1	0.97	0.15	-	59,59,59,59	0
54	MG	AA	1730	1/1	0.84	0.18	-	70,70,70,70	0
54	MG	DA	3198	1/1	0.87	0.39	-	52,52,52,52	0
54	MG	BA	3327	1/1	0.89	0.07	-	69,69,69,69	0
54	MG	BA	3425	1/1	0.95	0.16	-	38,38,38,38	0
54	MG	CA	1785	1/1	0.75	0.17	-	84,84,84,84	0
54	MG	BS	201	1/1	0.97	0.13	-	63,63,63,63	0
54	MG	BD	306	1/1	0.93	0.19	-	30,30,30,30	0
54	MG	B7	101	1/1	0.87	0.08	-	45,45,45,45	0
54	MG	AA	1815	1/1	0.95	0.09	-	72,72,72,72	0
54	MG	DA	3376	1/1	0.94	0.13	-	73,73,73,73	0
54	MG	DA	3414	1/1	0.80	0.10	-	66,66,66,66	0
54	MG	BA	3222	1/1	0.88	0.08	-	34,34,34,34	0
54	MG	DA	3388	1/1	0.93	0.35	-	73,73,73,73	0
54	MG	BA	3140	1/1	0.94	0.17	-	44,44,44,44	0
54	MG	DA	3536	1/1	0.89	0.06	-	76,76,76,76	0
54	MG	DA	3543	1/1	0.80	0.13	-	54,54,54,54	0
54	MG	DA	3325	1/1	0.92	0.11	-	72,72,72,72	0
54	MG	DA	3614	1/1	0.62	0.86	-	92,92,92,92	0
54	MG	BA	3394	1/1	0.98	0.11	-	27,27,27,27	0
54	MG	BA	3660	1/1	0.97	0.05	-	39,39,39,39	0
54	MG	CA	1704	1/1	0.97	0.13	-	71,71,71,71	0
54	MG	AA	1803	1/1	0.95	0.08	-	81,81,81,81	0
54	MG	BA	3131	1/1	0.98	0.14	-	28,28,28,28	0
54	MG	DA	3535	1/1	0.90	0.38	-	67,67,67,67	0
54	MG	BA	3392	1/1	0.97	0.29	-	29,29,29,29	0
54	MG	AA	1647	1/1	0.95	0.30	-	73,73,73,73	0
54	MG	CA	1756	1/1	0.88	0.09	-	77,77,77,77	0
54	MG	BA	3236	1/1	0.95	0.15	-	27,27,27,27	0
54	MG	AA	1801	1/1	0.85	0.08	-	87,87,87,87	0
54	MG	BA	3050	1/1	0.98	0.26	-	54,54,54,54	0
54	MG	CA	1632	1/1	0.85	0.31	-	57,57,57,57	0
54	MG	BA	3670	1/1	0.86	0.16	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3087	1/1	0.95	0.23	-	36,36,36,36	0
54	MG	BA	3548	1/1	0.98	0.13	-	32,32,32,32	0
54	MG	DA	3630	1/1	0.96	0.05	-	76,76,76,76	0
54	MG	BA	3135	1/1	0.94	0.10	-	50,50,50,50	0
54	MG	AA	1758	1/1	0.94	0.13	-	48,48,48,48	0
54	MG	CA	1708	1/1	0.99	0.06	-	73,73,73,73	0
54	MG	BA	3438	1/1	0.98	0.14	-	31,31,31,31	0
54	MG	BA	3298	1/1	0.95	0.23	-	43,43,43,43	0
54	MG	BQ	204	1/1	0.93	0.12	-	46,46,46,46	0
54	MG	DA	3036	1/1	0.85	0.25	-	62,62,62,62	0
54	MG	BA	3579	1/1	0.70	0.26	-	57,57,57,57	0
54	MG	DA	3161	1/1	0.96	0.15	-	47,47,47,47	0
54	MG	BA	3007	1/1	0.87	0.15	-	41,41,41,41	0
54	MG	CA	1745	1/1	0.98	0.28	-	52,52,52,52	0
54	MG	CA	1702	1/1	0.90	0.12	-	55,55,55,55	0
54	MG	B8	101	1/1	0.94	0.30	-	45,45,45,45	0
54	MG	DA	3462	1/1	0.85	0.15	-	63,63,63,63	0
54	MG	AA	1798	1/1	0.91	0.11	-	67,67,67,67	0
54	MG	BA	3603	1/1	0.91	0.27	-	39,39,39,39	0
54	MG	DA	3031	1/1	0.91	0.36	-	46,46,46,46	0
54	MG	CA	1765	1/1	0.92	0.10	-	87,87,87,87	0
54	MG	BA	3068	1/1	0.91	0.09	-	40,40,40,40	0
54	MG	DA	3270	1/1	0.96	0.17	-	24,24,24,24	0
54	MG	DA	3382	1/1	0.93	0.07	-	57,57,57,57	0
54	MG	BQ	202	1/1	0.97	0.22	-	47,47,47,47	0
54	MG	DA	3182	1/1	0.79	0.16	-	45,45,45,45	0
54	MG	CA	1629	1/1	0.78	0.32	-	81,81,81,81	0
54	MG	BA	3250	1/1	0.98	0.12	-	39,39,39,39	0
54	MG	DA	3490	1/1	0.94	0.09	-	60,60,60,60	0
54	MG	DA	3468	1/1	0.98	0.06	-	66,66,66,66	0
54	MG	DA	3238	1/1	0.97	0.08	-	44,44,44,44	0
54	MG	DA	3545	1/1	0.92	0.07	-	53,53,53,53	0
54	MG	AA	1678	1/1	0.92	0.43	-	75,75,75,75	0
54	MG	BA	3606	1/1	0.87	0.10	-	63,63,63,63	0
54	MG	BA	3496	1/1	0.88	0.30	-	56,56,56,56	0
54	MG	AA	1767	1/1	0.57	0.18	-	70,70,70,70	0
54	MG	BA	3586	1/1	0.96	0.19	-	39,39,39,39	0
54	MG	DA	3232	1/1	0.95	0.09	-	45,45,45,45	0
54	MG	BA	3126	1/1	0.97	0.17	-	30,30,30,30	0
54	MG	AA	1661	1/1	0.97	0.18	-	62,62,62,62	0
54	MG	DA	3306	1/1	0.94	0.11	-	68,68,68,68	0
54	MG	AA	1757	1/1	0.82	0.22	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1741	1/1	0.94	0.18	-	58,58,58,58	0
54	MG	BA	3561	1/1	0.85	0.16	-	46,46,46,46	0
54	MG	DA	3127	1/1	0.97	0.25	-	24,24,24,24	0
54	MG	AA	1689	1/1	0.94	0.17	-	56,56,56,56	0
54	MG	DA	3038	1/1	0.80	0.21	-	85,85,85,85	0
54	MG	BA	3479	1/1	0.93	0.09	-	77,77,77,77	0
54	MG	BA	3724	1/1	0.92	0.11	-	97,97,97,97	0
54	MG	DA	3595	1/1	0.93	0.18	-	90,90,90,90	0
54	MG	BA	3306	1/1	0.94	0.13	-	61,61,61,61	0
54	MG	DB	209	1/1	0.96	0.14	-	67,67,67,67	0
54	MG	AA	1641	1/1	0.93	0.18	-	62,62,62,62	0
54	MG	BN	201	1/1	0.90	0.12	-	57,57,57,57	0
54	MG	BA	3547	1/1	0.92	0.20	-	33,33,33,33	0
54	MG	BA	3558	1/1	0.98	0.13	-	60,60,60,60	0
54	MG	BA	3536	1/1	0.85	0.20	-	54,54,54,54	0
54	MG	AA	1643	1/1	0.95	0.15	-	56,56,56,56	0
54	MG	DA	3308	1/1	0.95	0.17	-	70,70,70,70	0
54	MG	CA	1769	1/1	0.96	0.10	-	58,58,58,58	0
54	MG	DA	3351	1/1	0.87	0.14	-	68,68,68,68	0
54	MG	AA	1759	1/1	0.92	0.21	-	74,74,74,74	0
54	MG	AA	1629	1/1	0.95	0.51	-	59,59,59,59	0
54	MG	DA	3149	1/1	0.83	0.42	-	46,46,46,46	0
54	MG	BA	3171	1/1	0.93	0.12	-	49,49,49,49	0
54	MG	DA	3399	1/1	0.87	0.17	-	80,80,80,80	0
54	MG	BA	3578	1/1	0.94	0.10	-	49,49,49,49	0
54	MG	BA	3551	1/1	0.96	0.10	-	60,60,60,60	0
54	MG	BA	3721	1/1	0.92	0.41	-	53,53,53,53	0
54	MG	BA	3110	1/1	0.95	0.14	-	60,60,60,60	0
54	MG	DA	3020	1/1	0.86	0.08	-	66,66,66,66	0
54	MG	CA	1604	1/1	0.67	0.49	-	70,70,70,70	0
54	MG	DA	3029	1/1	0.99	0.14	-	37,37,37,37	0
54	MG	CA	1799	1/1	0.93	0.10	-	99,99,99,99	0
54	MG	CA	1650	1/1	0.81	0.33	-	65,65,65,65	0
54	MG	BA	3449	1/1	0.85	0.14	-	40,40,40,40	0
54	MG	AA	1618	1/1	0.92	0.57	-	57,57,57,57	0
54	MG	BA	3203	1/1	0.96	0.23	-	39,39,39,39	0
54	MG	AA	1778	1/1	0.97	0.10	-	74,74,74,74	0
54	MG	AA	1615	1/1	0.88	0.16	-	76,76,76,76	0
54	MG	BA	3695	1/1	0.95	0.12	-	52,52,52,52	0
54	MG	DA	3541	1/1	0.90	0.14	-	46,46,46,46	0
54	MG	BA	3523	1/1	0.96	0.14	-	43,43,43,43	0
54	MG	CA	1642	1/1	0.91	0.61	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3224	1/1	0.93	0.11	-	60,60,60,60	0
54	MG	DA	3529	1/1	0.95	0.14	-	65,65,65,65	0
54	MG	DA	3311	1/1	0.94	0.13	-	31,31,31,31	0
54	MG	BA	3690	1/1	0.82	0.09	-	42,42,42,42	0
54	MG	DA	3110	1/1	0.89	0.19	-	56,56,56,56	0
54	MG	BA	3318	1/1	0.94	0.08	-	64,64,64,64	0
54	MG	AA	1608	1/1	0.77	0.21	-	66,66,66,66	0
54	MG	BA	3194	1/1	0.97	0.19	-	52,52,52,52	0
54	MG	BA	3560	1/1	0.77	0.28	-	93,93,93,93	0
54	MG	AA	1674	1/1	0.58	0.12	-	75,75,75,75	0
54	MG	BA	3587	1/1	0.87	0.07	-	60,60,60,60	0
54	MG	CA	1622	1/1	0.87	0.14	-	65,65,65,65	0
54	MG	BA	3270	1/1	0.92	0.11	-	51,51,51,51	0
54	MG	AA	1756	1/1	0.80	0.10	-	107,107,107,107	0
54	MG	BA	3678	1/1	0.98	0.29	-	47,47,47,47	0
54	MG	BA	3685	1/1	0.81	0.30	-	69,69,69,69	0
54	MG	CA	1671	1/1	0.68	0.07	-	78,78,78,78	0
54	MG	CA	1644	1/1	0.89	0.12	-	63,63,63,63	0
54	MG	DA	3448	1/1	0.96	0.28	-	53,53,53,53	0
54	MG	BA	3516	1/1	0.96	0.07	-	54,54,54,54	0
54	MG	AA	1755	1/1	0.85	0.38	-	76,76,76,76	0
54	MG	DA	3327	1/1	0.92	0.08	-	66,66,66,66	0
54	MG	CA	1660	1/1	0.71	0.23	-	65,65,65,65	0
54	MG	CA	1638	1/1	0.96	0.60	-	65,65,65,65	0
54	MG	BA	3705	1/1	0.91	0.10	-	57,57,57,57	0
54	MG	DA	3467	1/1	0.82	0.11	-	85,85,85,85	0
54	MG	BA	3611	1/1	0.96	0.06	-	32,32,32,32	0
54	MG	BA	3613	1/1	0.99	0.10	-	50,50,50,50	0
54	MG	CA	1792	1/1	0.94	0.14	-	65,65,65,65	0
54	MG	DA	3140	1/1	0.83	0.40	-	60,60,60,60	0
54	MG	DA	3627	1/1	0.93	0.12	-	58,58,58,58	0
54	MG	AA	1797	1/1	0.88	0.10	-	106,106,106,106	0
54	MG	DA	3065	1/1	0.83	0.25	-	74,74,74,74	0
54	MG	AA	1725	1/1	0.94	0.13	-	62,62,62,62	0
54	MG	BA	3490	1/1	0.92	0.23	-	74,74,74,74	0
54	MG	DA	3225	1/1	0.98	0.11	-	53,53,53,53	0
54	MG	BA	3024	1/1	0.94	0.26	-	44,44,44,44	0
54	MG	CA	1772	1/1	0.97	0.09	-	61,61,61,61	0
54	MG	BA	3346	1/1	0.97	0.09	-	43,43,43,43	0
54	MG	DA	3345	1/1	0.96	0.15	-	56,56,56,56	0
54	MG	CA	1696	1/1	0.93	0.07	-	71,71,71,71	0
54	MG	DA	3465	1/1	0.90	0.07	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1800	1/1	0.88	0.05	-	76,76,76,76	0
54	MG	CA	1725	1/1	0.95	0.20	-	91,91,91,91	0
54	MG	BA	3274	1/1	0.96	0.13	-	48,48,48,48	0
54	MG	BA	3638	1/1	0.82	0.15	-	82,82,82,82	0
54	MG	DA	3634	1/1	0.92	0.20	-	75,75,75,75	0
54	MG	BA	3172	1/1	0.80	0.13	-	65,65,65,65	0
54	MG	BA	3696	1/1	0.96	0.06	-	38,38,38,38	0
54	MG	DA	3474	1/1	0.89	0.19	-	41,41,41,41	0
54	MG	BA	3189	1/1	0.97	0.06	-	71,71,71,71	0
54	MG	BA	3679	1/1	0.75	0.09	-	80,80,80,80	0
54	MG	DA	3305	1/1	0.93	0.15	-	66,66,66,66	0
54	MG	DA	3049	1/1	0.93	0.10	-	49,49,49,49	0
54	MG	BA	3484	1/1	0.98	0.08	-	41,41,41,41	0
54	MG	BA	3044	1/1	0.92	0.25	-	53,53,53,53	0
54	MG	DA	3404	1/1	0.87	0.28	-	62,62,62,62	0
54	MG	DA	3625	1/1	0.93	0.12	-	76,76,76,76	0
54	MG	DB	205	1/1	0.75	0.23	-	92,92,92,92	0
54	MG	B2	102	1/1	0.87	0.19	-	60,60,60,60	0
54	MG	DA	3241	1/1	0.94	0.19	-	47,47,47,47	0
54	MG	BA	3325	1/1	0.97	0.23	-	28,28,28,28	0
54	MG	DA	3197	1/1	0.94	0.09	-	28,28,28,28	0
54	MG	CA	1601	1/1	0.92	0.19	-	55,55,55,55	0
54	MG	B9	103	1/1	0.89	0.18	-	52,52,52,52	0
54	MG	BA	3073	1/1	0.85	0.10	-	74,74,74,74	0
54	MG	DA	3558	1/1	0.65	0.25	-	70,70,70,70	0
54	MG	DA	3514	1/1	0.94	0.29	-	92,92,92,92	0
54	MG	DA	3227	1/1	0.93	0.07	-	39,39,39,39	0
54	MG	DA	3517	1/1	0.94	0.15	-	52,52,52,52	0
54	MG	DA	3249	1/1	0.86	0.14	-	47,47,47,47	0
54	MG	DA	3165	1/1	0.96	0.13	-	36,36,36,36	0
54	MG	BA	3160	1/1	0.91	0.12	-	32,32,32,32	0
54	MG	AA	1731	1/1	0.92	0.17	-	72,72,72,72	0
54	MG	DQ	201	1/1	0.96	0.12	-	52,52,52,52	0
54	MG	BA	3128	1/1	0.79	0.23	-	63,63,63,63	0
54	MG	BA	3013	1/1	0.91	0.28	-	24,24,24,24	0
54	MG	DA	3355	1/1	0.93	0.10	-	67,67,67,67	0
54	MG	AA	1693	1/1	0.88	0.17	-	72,72,72,72	0
54	MG	CA	1633	1/1	0.97	0.18	-	50,50,50,50	0
54	MG	BA	3291	1/1	0.92	0.07	-	68,68,68,68	0
54	MG	BA	3665	1/1	0.95	0.06	-	72,72,72,72	0
54	MG	BA	3522	1/1	0.92	0.24	-	53,53,53,53	0
54	MG	AA	1799	1/1	0.95	0.15	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3331	1/1	0.91	0.11	-	47,47,47,47	0
54	MG	BF	304	1/1	0.88	0.09	-	47,47,47,47	0
54	MG	DA	3146	1/1	0.97	0.25	-	55,55,55,55	0
54	MG	BA	3347	1/1	0.93	0.23	-	44,44,44,44	0
54	MG	DA	3085	1/1	0.93	0.08	-	60,60,60,60	0
54	MG	BA	3105	1/1	0.89	0.29	-	44,44,44,44	0
54	MG	BA	3021	1/1	0.95	0.23	-	67,67,67,67	0
54	MG	DA	3605	1/1	0.87	0.17	-	49,49,49,49	0
54	MG	DA	3451	1/1	0.85	0.10	-	60,60,60,60	0
54	MG	BA	3478	1/1	0.91	0.14	-	50,50,50,50	0
54	MG	DA	3619	1/1	0.81	0.15	-	57,57,57,57	0
54	MG	AA	1683	1/1	0.95	0.21	-	69,69,69,69	0
54	MG	DA	3128	1/1	0.95	0.32	-	47,47,47,47	0
54	MG	BA	3028	1/1	0.96	0.16	-	34,34,34,34	0
54	MG	AA	1687	1/1	0.94	0.22	-	79,79,79,79	0
54	MG	CA	1684	1/1	0.95	0.27	-	82,82,82,82	0
54	MG	DA	3101	1/1	0.84	0.14	-	60,60,60,60	0
54	MG	CA	1602	1/1	0.93	0.23	-	70,70,70,70	0
54	MG	BA	3014	1/1	0.90	0.19	-	61,61,61,61	0
54	MG	DA	3139	1/1	0.91	0.32	-	53,53,53,53	0
54	MG	DA	3142	1/1	0.96	0.11	-	48,48,48,48	0
54	MG	BA	3729	1/1	0.97	0.25	-	42,42,42,42	0
54	MG	DA	3187	1/1	0.98	0.14	-	44,44,44,44	0
54	MG	DA	3613	1/1	0.96	0.15	-	45,45,45,45	0
54	MG	BA	3139	1/1	0.98	0.17	-	55,55,55,55	0
54	MG	DA	3145	1/1	0.79	0.13	-	60,60,60,60	0
54	MG	CQ	201	1/1	0.86	0.11	-	76,76,76,76	0
54	MG	BA	3351	1/1	0.95	0.11	-	49,49,49,49	0
54	MG	CA	1730	1/1	0.83	0.16	-	65,65,65,65	0
54	MG	BA	3378	1/1	0.99	0.12	-	24,24,24,24	0
54	MG	BA	3368	1/1	0.99	0.08	-	27,27,27,27	0
54	MG	DA	3504	1/1	0.97	0.12	-	52,52,52,52	0
54	MG	BA	3281	1/1	0.86	0.12	-	43,43,43,43	0
54	MG	BA	3655	1/1	0.61	0.35	-	68,68,68,68	0
54	MG	BA	3353	1/1	0.94	0.11	-	51,51,51,51	0
54	MG	AA	1806	1/1	0.94	0.15	-	60,60,60,60	0
54	MG	DA	3626	1/1	0.89	0.10	-	75,75,75,75	0
54	MG	BA	3120	1/1	0.84	0.10	-	54,54,54,54	0
54	MG	DA	3523	1/1	0.87	0.15	-	73,73,73,73	0
54	MG	AA	1607	1/1	0.94	0.11	-	57,57,57,57	0
54	MG	CA	1673	1/1	0.94	0.20	-	73,73,73,73	0
54	MG	DA	3477	1/1	0.76	0.09	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1737	1/1	0.91	0.23	-	75,75,75,75	0
54	MG	DA	3125	1/1	0.97	0.24	-	59,59,59,59	0
54	MG	AD	302	1/1	0.90	0.42	-	73,73,73,73	0
54	MG	BA	3530	1/1	0.92	0.06	-	95,95,95,95	0
54	MG	CA	1676	1/1	0.98	0.06	-	64,64,64,64	0
54	MG	BA	3071	1/1	0.87	0.22	-	46,46,46,46	0
54	MG	DA	3516	1/1	0.94	0.08	-	56,56,56,56	0
54	MG	BA	3475	1/1	0.95	0.07	-	45,45,45,45	0
54	MG	DA	3444	1/1	0.95	0.12	-	73,73,73,73	0
54	MG	DA	3030	1/1	0.93	0.43	-	63,63,63,63	0
54	MG	CA	1735	1/1	0.86	0.12	-	85,85,85,85	0
54	MG	BA	3469	1/1	0.92	0.16	-	65,65,65,65	0
54	MG	DA	3498	1/1	0.94	0.24	-	39,39,39,39	0
54	MG	DA	3046	1/1	0.94	0.27	-	58,58,58,58	0
54	MG	DA	3589	1/1	0.95	0.07	-	42,42,42,42	0
54	MG	BA	3514	1/1	0.90	0.10	-	29,29,29,29	0
54	MG	BA	3072	1/1	0.77	0.21	-	48,48,48,48	0
54	MG	CA	1675	1/1	0.87	0.18	-	75,75,75,75	0
54	MG	BA	3489	1/1	0.98	0.04	-	57,57,57,57	0
54	MG	DA	3579	1/1	0.80	0.18	-	52,52,52,52	0
54	MG	DA	3374	1/1	0.87	0.09	-	73,73,73,73	0
54	MG	AA	1697	1/1	0.96	0.16	-	50,50,50,50	0
54	MG	CA	1750	1/1	0.73	0.14	-	88,88,88,88	0
54	MG	BA	3271	1/1	0.94	0.09	-	66,66,66,66	0
54	MG	BB	209	1/1	0.97	0.15	-	45,45,45,45	0
54	MG	BA	3122	1/1	0.96	0.13	-	46,46,46,46	0
54	MG	BA	3001	1/1	0.94	0.13	-	45,45,45,45	0
54	MG	DA	3157	1/1	0.90	0.17	-	33,33,33,33	0
54	MG	DA	3568	1/1	0.95	0.16	-	62,62,62,62	0
54	MG	DO	202	1/1	0.85	0.08	-	60,60,60,60	0
54	MG	AA	1652	1/1	0.84	0.19	-	63,63,63,63	0
54	MG	BA	3079	1/1	0.97	0.18	-	45,45,45,45	0
54	MG	AA	1715	1/1	0.93	0.16	-	61,61,61,61	0
54	MG	BA	3715	1/1	0.89	0.16	-	88,88,88,88	0
54	MG	AL	201	1/1	0.95	0.07	-	65,65,65,65	0
54	MG	BA	3401	1/1	0.97	0.28	-	34,34,34,34	0
54	MG	DA	3239	1/1	0.98	0.12	-	46,46,46,46	0
54	MG	CA	1641	1/1	0.92	0.21	-	62,62,62,62	0
54	MG	DA	3446	1/1	0.87	0.10	-	68,68,68,68	0
54	MG	BA	3600	1/1	0.70	0.24	-	58,58,58,58	0
54	MG	DA	3470	1/1	0.94	0.12	-	50,50,50,50	0
54	MG	BA	3334	1/1	0.72	0.17	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3119	1/1	0.97	0.08	-	57,57,57,57	0
54	MG	AA	1814	1/1	0.98	0.13	-	66,66,66,66	0
54	MG	DA	3509	1/1	0.87	0.16	-	70,70,70,70	0
54	MG	BA	3168	1/1	0.87	0.15	-	68,68,68,68	0
54	MG	BD	301	1/1	0.95	0.17	-	51,51,51,51	0
54	MG	AA	1667	1/1	0.86	0.17	-	84,84,84,84	0
54	MG	BA	3198	1/1	0.99	0.20	-	35,35,35,35	0
54	MG	BA	3512	1/1	0.75	0.21	-	71,71,71,71	0
54	MG	BA	3657	1/1	0.93	0.20	-	91,91,91,91	0
54	MG	DA	3096	1/1	0.66	0.21	-	61,61,61,61	0
54	MG	DA	3494	1/1	0.76	0.26	-	64,64,64,64	0
54	MG	BA	3290	1/1	0.93	0.13	-	27,27,27,27	0
54	MG	DA	3381	1/1	0.95	0.10	-	55,55,55,55	0
54	MG	BA	3269	1/1	0.95	0.11	-	51,51,51,51	0
54	MG	AP	101	1/1	0.96	0.10	-	81,81,81,81	0
54	MG	DA	3423	1/1	0.95	0.08	-	37,37,37,37	0
54	MG	DA	3231	1/1	0.94	0.10	-	51,51,51,51	0
54	MG	BA	3459	1/1	0.96	0.24	-	57,57,57,57	0
54	MG	BA	3002	1/1	0.93	0.10	-	60,60,60,60	0
54	MG	CA	1715	1/1	0.77	0.20	-	85,85,85,85	0
54	MG	AA	1700	1/1	0.92	0.29	-	69,69,69,69	0
54	MG	AA	1771	1/1	0.96	0.06	-	67,67,67,67	0
54	MG	DA	3466	1/1	0.74	0.17	-	65,65,65,65	0
54	MG	BA	3217	1/1	0.92	0.08	-	60,60,60,60	0
54	MG	BA	3463	1/1	0.93	0.14	-	38,38,38,38	0
54	MG	DA	3566	1/1	0.90	0.19	-	70,70,70,70	0
54	MG	BA	3147	1/1	0.94	0.23	-	33,33,33,33	0
54	MG	BA	3233	1/1	0.95	0.07	-	53,53,53,53	0
54	MG	DA	3557	1/1	0.96	0.38	-	55,55,55,55	0
54	MG	BA	3022	1/1	0.95	0.24	-	38,38,38,38	0
54	MG	BA	3701	1/1	0.86	0.15	-	34,34,34,34	0
54	MG	BA	3223	1/1	0.96	0.15	-	24,24,24,24	0
54	MG	DA	3104	1/1	0.96	0.46	-	51,51,51,51	0
54	MG	DA	3418	1/1	0.87	0.09	-	48,48,48,48	0
54	MG	BA	3114	1/1	0.97	0.08	-	39,39,39,39	0
54	MG	BA	3262	1/1	0.97	0.04	-	51,51,51,51	0
54	MG	BA	3467	1/1	0.86	0.13	-	63,63,63,63	0
54	MG	CA	1801	1/1	0.89	0.09	-	88,88,88,88	0
54	MG	BA	3006	1/1	0.86	0.11	-	67,67,67,67	0
54	MG	CA	1762	1/1	0.95	0.12	-	86,86,86,86	0
54	MG	BA	3717	1/1	0.84	0.14	-	45,45,45,45	0
54	MG	BA	3445	1/1	0.95	0.06	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3063	1/1	0.87	0.25	-	47,47,47,47	0
54	MG	DA	3596	1/1	0.87	0.38	-	60,60,60,60	0
54	MG	AA	1800	1/1	0.95	0.18	-	70,70,70,70	0
54	MG	DA	3265	1/1	0.98	0.16	-	34,34,34,34	0
54	MG	DA	3014	1/1	0.54	0.50	-	73,73,73,73	0
54	MG	BA	3584	1/1	0.94	0.15	-	48,48,48,48	0
54	MG	BA	3340	1/1	0.93	0.09	-	38,38,38,38	0
54	MG	BA	3235	1/1	0.93	0.15	-	45,45,45,45	0
54	MG	BA	3383	1/1	0.95	0.13	-	26,26,26,26	0
54	MG	CA	1723	1/1	0.95	0.14	-	66,66,66,66	0
54	MG	CA	1687	1/1	0.97	0.18	-	68,68,68,68	0
54	MG	BA	3637	1/1	0.90	0.15	-	81,81,81,81	0
54	MG	DA	3602	1/1	0.85	0.09	-	53,53,53,53	0
54	MG	DA	3622	1/1	0.78	0.10	-	80,80,80,80	0
54	MG	DA	3435	1/1	0.72	0.09	-	77,77,77,77	0
54	MG	AA	1718	1/1	0.93	0.11	-	59,59,59,59	0
54	MG	BA	3219	1/1	0.91	0.17	-	67,67,67,67	0
54	MG	DA	3515	1/1	0.95	0.13	-	54,54,54,54	0
54	MG	BA	3075	1/1	0.91	0.19	-	36,36,36,36	0
54	MG	AA	1795	1/1	0.95	0.08	-	87,87,87,87	0
54	MG	AA	1669	1/1	0.87	0.12	-	80,80,80,80	0
54	MG	BA	3712	1/1	0.94	0.14	-	49,49,49,49	0
54	MG	BA	3521	1/1	0.96	0.17	-	35,35,35,35	0
54	MG	BA	3681	1/1	0.97	0.22	-	31,31,31,31	0
54	MG	AA	1612	1/1	0.97	0.15	-	61,61,61,61	0
54	MG	DA	3040	1/1	0.77	0.15	-	58,58,58,58	0
54	MG	DA	3548	1/1	0.97	0.11	-	54,54,54,54	0
54	MG	BY	202	1/1	0.95	0.15	-	49,49,49,49	0
54	MG	AA	1642	1/1	0.97	0.14	-	53,53,53,53	0
54	MG	DA	3612	1/1	0.98	0.36	-	49,49,49,49	0
54	MG	BA	3040	1/1	0.91	0.14	-	52,52,52,52	0
54	MG	BA	3722	1/1	0.92	0.12	-	71,71,71,71	0
54	MG	DA	3032	1/1	0.84	0.34	-	59,59,59,59	0
54	MG	BA	3515	1/1	0.98	0.10	-	35,35,35,35	0
54	MG	BA	3146	1/1	0.94	0.23	-	34,34,34,34	0
54	MG	DA	3591	1/1	0.92	0.25	-	39,39,39,39	0
54	MG	BA	3446	1/1	0.96	0.14	-	42,42,42,42	0
54	MG	BA	3472	1/1	0.98	0.07	-	34,34,34,34	0
54	MG	DA	3309	1/1	0.89	0.21	-	45,45,45,45	0
54	MG	BA	3012	1/1	0.97	0.17	-	37,37,37,37	0
54	MG	DA	3487	1/1	0.98	0.27	-	65,65,65,65	0
54	MG	AA	1699	1/1	0.89	0.17	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BB	203	1/1	0.93	0.24	-	48,48,48,48	0
54	MG	DA	3083	1/1	0.89	0.11	-	50,50,50,50	0
54	MG	CA	1763	1/1	0.79	0.08	-	66,66,66,66	0
54	MG	DA	3285	1/1	0.93	0.22	-	68,68,68,68	0
54	MG	DA	3171	1/1	0.95	0.10	-	28,28,28,28	0
54	MG	BA	3651	1/1	0.94	0.29	-	34,34,34,34	0
54	MG	CA	1736	1/1	0.84	0.19	-	94,94,94,94	0
54	MG	BA	3289	1/1	0.92	0.24	-	58,58,58,58	0
54	MG	DA	3601	1/1	0.98	0.15	-	32,32,32,32	0
54	MG	CA	1728	1/1	0.94	0.05	-	79,79,79,79	0
54	MG	BA	3591	1/1	0.90	0.24	-	104,104,104,104	0
54	MG	DA	3262	1/1	0.91	0.19	-	55,55,55,55	0
54	MG	DA	3216	1/1	0.90	0.10	-	43,43,43,43	0
54	MG	CA	1699	1/1	0.94	0.29	-	73,73,73,73	0
54	MG	BA	3307	1/1	0.90	0.15	-	46,46,46,46	0
54	MG	DA	3321	1/1	0.84	0.20	-	74,74,74,74	0
54	MG	BA	3585	1/1	0.94	0.09	-	65,65,65,65	0
54	MG	BA	3183	1/1	0.94	0.12	-	37,37,37,37	0
54	MG	DA	3537	1/1	0.94	0.18	-	49,49,49,49	0
54	MG	DA	3237	1/1	0.88	0.10	-	51,51,51,51	0
54	MG	DA	3111	1/1	0.95	0.19	-	44,44,44,44	0
54	MG	BA	3534	1/1	0.91	0.09	-	69,69,69,69	0
54	MG	BA	3164	1/1	0.97	0.17	-	39,39,39,39	0
54	MG	BA	3025	1/1	0.92	0.19	-	34,34,34,34	0
54	MG	BA	3647	1/1	0.94	0.13	-	59,59,59,59	0
54	MG	BA	3112	1/1	0.93	0.19	-	52,52,52,52	0
54	MG	BB	214	1/1	0.98	0.14	-	38,38,38,38	0
54	MG	BA	3051	1/1	0.98	0.13	-	33,33,33,33	0
54	MG	CA	1795	1/1	0.93	0.06	-	66,66,66,66	0
54	MG	AA	1724	1/1	0.89	0.12	-	93,93,93,93	0
54	MG	DA	3617	1/1	0.83	0.08	-	74,74,74,74	0
54	MG	BA	3138	1/1	0.97	0.06	-	64,64,64,64	0
54	MG	AA	1673	1/1	0.96	0.05	-	76,76,76,76	0
54	MG	BA	3038	1/1	0.93	0.19	-	34,34,34,34	0
54	MG	BA	3009	1/1	0.97	0.22	-	23,23,23,23	0
54	MG	DA	3479	1/1	0.77	0.16	-	66,66,66,66	0
54	MG	CA	1771	1/1	0.89	0.21	-	71,71,71,71	0
54	MG	CA	1701	1/1	0.94	0.05	-	74,74,74,74	0
54	MG	CA	1606	1/1	0.77	0.36	-	83,83,83,83	0
54	MG	DA	3061	1/1	0.94	0.08	-	45,45,45,45	0
54	MG	DA	3124	1/1	0.69	0.21	-	69,69,69,69	0
54	MG	DD	301	1/1	0.92	0.07	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3303	1/1	0.96	0.14	-	46,46,46,46	0
54	MG	DD	305	1/1	0.93	0.16	-	56,56,56,56	0
54	MG	BA	3432	1/1	0.85	0.20	-	68,68,68,68	0
54	MG	DA	3378	1/1	0.97	0.11	-	65,65,65,65	0
54	MG	AA	1746	1/1	0.97	0.14	-	63,63,63,63	0
54	MG	DA	3284	1/1	0.83	0.19	-	70,70,70,70	0
54	MG	AA	1698	1/1	0.85	0.20	-	78,78,78,78	0
54	MG	CA	1789	1/1	0.91	0.12	-	66,66,66,66	0
54	MG	DA	3606	1/1	0.70	0.32	-	82,82,82,82	0
54	MG	DA	3377	1/1	0.97	0.07	-	74,74,74,74	0
54	MG	DA	3416	1/1	0.82	0.17	-	64,64,64,64	0
54	MG	BA	3367	1/1	0.97	0.22	-	34,34,34,34	0
54	MG	BA	3295	1/1	0.96	0.20	-	52,52,52,52	0
54	MG	BA	3545	1/1	0.72	0.10	-	63,63,63,63	0
54	MG	BA	3067	1/1	0.85	0.56	-	55,55,55,55	0
54	MG	DA	3211	1/1	0.86	0.08	-	38,38,38,38	0
54	MG	AA	1794	1/1	0.58	0.20	-	111,111,111,111	0
54	MG	BA	3042	1/1	0.88	0.18	-	27,27,27,27	0
54	MG	BA	3559	1/1	0.88	0.27	-	56,56,56,56	0
54	MG	AA	1817	1/1	0.93	0.33	-	78,78,78,78	0
54	MG	DA	3371	1/1	0.86	0.28	-	76,76,76,76	0
54	MG	BA	3693	1/1	0.95	0.09	-	36,36,36,36	0
54	MG	AA	1753	1/1	0.94	0.11	-	71,71,71,71	0
54	MG	D5	103	1/1	0.72	0.17	-	61,61,61,61	0
54	MG	CA	1719	1/1	0.79	0.11	-	90,90,90,90	0
54	MG	BA	3117	1/1	0.80	0.21	-	67,67,67,67	0
54	MG	DA	3356	1/1	0.92	0.34	-	44,44,44,44	0
54	MG	AA	1653	1/1	0.97	0.20	-	64,64,64,64	0
54	MG	DA	3453	1/1	0.86	0.09	-	49,49,49,49	0
54	MG	BA	3550	1/1	0.94	0.12	-	50,50,50,50	0
54	MG	BA	3451	1/1	0.94	0.07	-	49,49,49,49	0
54	MG	AA	1655	1/1	0.98	0.07	-	64,64,64,64	0
54	MG	AA	1614	1/1	0.93	0.20	-	42,42,42,42	0
54	MG	DA	3169	1/1	0.98	0.14	-	32,32,32,32	0
54	MG	AA	1681	1/1	0.92	0.08	-	44,44,44,44	0
54	MG	DA	3286	1/1	0.85	0.13	-	69,69,69,69	0
54	MG	BA	3684	1/1	0.95	0.16	-	64,64,64,64	0
54	MG	BA	3061	1/1	0.90	0.16	-	44,44,44,44	0
54	MG	BA	3221	1/1	0.97	0.17	-	51,51,51,51	0
54	MG	BA	3582	1/1	0.90	0.27	-	66,66,66,66	0
54	MG	BA	3575	1/1	0.98	0.17	-	59,59,59,59	0
54	MG	DA	3043	1/1	0.96	0.06	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3153	1/1	0.95	0.14	-	36,36,36,36	0
54	MG	DA	3152	1/1	0.90	0.21	-	52,52,52,52	0
54	MG	BA	3470	1/1	0.95	0.11	-	33,33,33,33	0
54	MG	CA	1777	1/1	0.81	0.12	-	130,130,130,130	0
54	MG	CA	1714	1/1	0.96	0.19	-	67,67,67,67	0
54	MG	BA	3305	1/1	0.90	0.09	-	67,67,67,67	0
54	MG	BA	3273	1/1	0.95	0.15	-	60,60,60,60	0
54	MG	BA	3526	1/1	0.90	0.22	-	55,55,55,55	0
54	MG	BF	306	1/1	0.93	0.12	-	61,61,61,61	0
54	MG	AA	1732	1/1	0.96	0.38	-	68,68,68,68	0
54	MG	B3	101	1/1	0.78	0.19	-	54,54,54,54	0
54	MG	DA	3452	1/1	0.93	0.22	-	45,45,45,45	0
54	MG	BA	3065	1/1	0.96	0.17	-	36,36,36,36	0
54	MG	BA	3689	1/1	0.88	0.17	-	55,55,55,55	0
54	MG	AA	1645	1/1	0.94	0.09	-	54,54,54,54	0
54	MG	CA	1682	1/1	0.93	0.20	-	60,60,60,60	0
54	MG	DA	3581	1/1	0.88	0.16	-	46,46,46,46	0
54	MG	DA	3367	1/1	0.92	0.06	-	67,67,67,67	0
54	MG	BA	3414	1/1	0.97	0.19	-	23,23,23,23	0
54	MG	DA	3028	1/1	0.87	0.12	-	62,62,62,62	0
54	MG	AA	1659	1/1	0.95	0.21	-	75,75,75,75	0
54	MG	CA	1729	1/1	0.49	0.23	-	84,84,84,84	0
54	MG	BA	3297	1/1	0.92	0.12	-	52,52,52,52	0
54	MG	DA	3273	1/1	0.96	0.05	-	93,93,93,93	0
54	MG	AA	1796	1/1	0.93	0.31	-	100,100,100,100	0
54	MG	BA	3513	1/1	0.91	0.12	-	46,46,46,46	0
54	MG	BA	3510	1/1	0.87	0.07	-	77,77,77,77	0
54	MG	DA	3189	1/1	0.99	0.14	-	36,36,36,36	0
54	MG	BA	3163	1/1	0.90	0.31	-	30,30,30,30	0
54	MG	DA	3555	1/1	0.95	0.44	-	63,63,63,63	0
54	MG	D7	102	1/1	0.87	0.18	-	65,65,65,65	0
54	MG	BA	3614	1/1	0.95	0.34	-	47,47,47,47	0
54	MG	BA	3629	1/1	0.93	0.24	-	34,34,34,34	0
54	MG	BA	3165	1/1	0.73	0.33	-	41,41,41,41	0
54	MG	BA	3355	1/1	0.96	0.10	-	51,51,51,51	0
54	MG	BA	3460	1/1	0.95	0.10	-	51,51,51,51	0
54	MG	DA	3317	1/1	0.91	0.20	-	55,55,55,55	0
54	MG	BA	3457	1/1	0.85	0.08	-	53,53,53,53	0
54	MG	DA	3531	1/1	0.95	0.04	-	51,51,51,51	0
54	MG	CA	1681	1/1	0.68	0.21	-	83,83,83,83	0
54	MG	DA	3147	1/1	0.94	0.11	-	52,52,52,52	0
54	MG	CA	1652	1/1	0.92	0.18	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3497	1/1	0.99	0.16	-	29,29,29,29	0
54	MG	BA	3134	1/1	0.87	0.08	-	50,50,50,50	0
54	MG	BA	3554	1/1	0.92	0.13	-	41,41,41,41	0
54	MG	DA	3084	1/1	0.78	0.23	-	45,45,45,45	0
54	MG	BA	3677	1/1	0.94	0.11	-	72,72,72,72	0
54	MG	DA	3133	1/1	0.95	0.39	-	50,50,50,50	0
54	MG	BA	3552	1/1	0.98	0.13	-	26,26,26,26	0
54	MG	BA	3639	1/1	0.90	0.13	-	56,56,56,56	0
54	MG	BA	3502	1/1	0.96	0.17	-	34,34,34,34	0
54	MG	CA	1803	1/1	0.85	0.17	-	55,55,55,55	0
54	MG	AA	1664	1/1	0.93	0.12	-	74,74,74,74	0
54	MG	DA	3368	1/1	0.96	0.07	-	56,56,56,56	0
54	MG	AA	1779	1/1	0.81	0.17	-	68,68,68,68	0
54	MG	BA	3440	1/1	0.95	0.07	-	50,50,50,50	0
54	MG	BA	3169	1/1	0.83	0.16	-	60,60,60,60	0
54	MG	CA	1761	1/1	0.71	0.13	-	92,92,92,92	0
54	MG	BA	3363	1/1	0.94	0.22	-	48,48,48,48	0
54	MG	DA	3489	1/1	0.94	0.16	-	48,48,48,48	0
54	MG	DA	3506	1/1	0.96	0.16	-	57,57,57,57	0
54	MG	DA	3009	1/1	0.98	0.17	-	27,27,27,27	0
54	MG	AA	1662	1/1	0.97	0.08	-	64,64,64,64	0
54	MG	DP	203	1/1	0.94	0.12	-	61,61,61,61	0
54	MG	CA	1717	1/1	0.94	0.08	-	85,85,85,85	0
54	MG	BA	3003	1/1	0.86	0.40	-	68,68,68,68	0
54	MG	AA	1617	1/1	0.95	0.35	-	58,58,58,58	0
54	MG	BA	3535	1/1	0.80	0.10	-	58,58,58,58	0
54	MG	DA	3629	1/1	0.87	0.10	-	80,80,80,80	0
54	MG	BA	3100	1/1	0.96	0.20	-	41,41,41,41	0
54	MG	AA	1764	1/1	0.76	0.27	-	70,70,70,70	0
54	MG	DA	3411	1/1	0.82	0.14	-	89,89,89,89	0
54	MG	AA	1721	1/1	0.86	0.12	-	77,77,77,77	0
54	MG	AE	201	1/1	0.95	0.24	-	62,62,62,62	0
54	MG	DA	3437	1/1	0.97	0.19	-	54,54,54,54	0
54	MG	CA	1648	1/1	0.96	0.09	-	72,72,72,72	0
54	MG	DA	3346	1/1	0.78	0.12	-	57,57,57,57	0
54	MG	BA	3300	1/1	0.92	0.15	-	54,54,54,54	0
54	MG	CA	1752	1/1	0.91	0.11	-	91,91,91,91	0
54	MG	DB	202	1/1	0.98	0.20	-	67,67,67,67	0
54	MG	DR	202	1/1	0.98	0.17	-	45,45,45,45	0
54	MG	BA	3727	1/1	0.96	0.17	-	94,94,94,94	0
54	MG	BA	3336	1/1	0.85	0.16	-	71,71,71,71	0
54	MG	BA	3499	1/1	0.86	0.19	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DB	206	1/1	0.23	1.96	-	115,115,115,115	0
54	MG	AA	1702	1/1	0.97	0.06	-	67,67,67,67	0
54	MG	AA	1793	1/1	0.81	0.23	-	78,78,78,78	0
54	MG	BA	3441	1/1	0.97	0.14	-	58,58,58,58	0
54	MG	BB	207	1/1	0.96	0.17	-	49,49,49,49	0
54	MG	DA	3081	1/1	0.93	0.13	-	60,60,60,60	0
54	MG	DA	3078	1/1	0.98	0.31	-	41,41,41,41	0
54	MG	BA	3204	1/1	0.97	0.20	-	47,47,47,47	0
54	MG	DA	3134	1/1	0.85	0.22	-	71,71,71,71	0
54	MG	DA	3369	1/1	0.86	0.11	-	85,85,85,85	0
54	MG	BA	3659	1/1	0.85	0.07	-	61,61,61,61	0
54	MG	BA	3709	1/1	0.88	0.12	-	47,47,47,47	0
54	MG	DA	3167	1/1	0.93	0.11	-	30,30,30,30	0
54	MG	DA	3050	1/1	0.83	0.17	-	52,52,52,52	0
54	MG	CA	1787	1/1	0.86	0.20	-	84,84,84,84	0
54	MG	DT	202	1/1	0.93	0.06	-	62,62,62,62	0
54	MG	BA	3277	1/1	0.87	0.21	-	32,32,32,32	0
54	MG	AA	1786	1/1	0.85	0.13	-	89,89,89,89	0
54	MG	CA	1636	1/1	0.95	0.19	-	58,58,58,58	0
54	MG	BA	3495	1/1	0.92	0.12	-	57,57,57,57	0
54	MG	DA	3592	1/1	0.72	0.12	-	72,72,72,72	0
54	MG	BA	3111	1/1	0.77	0.74	-	67,67,67,67	0
54	MG	DA	3138	1/1	0.96	0.36	-	49,49,49,49	0
54	MG	CA	1612	1/1	0.77	0.77	-	84,84,84,84	0
54	MG	DA	3616	1/1	0.89	0.09	-	63,63,63,63	0
54	MG	BA	3427	1/1	0.94	0.13	-	28,28,28,28	0
54	MG	BA	3419	1/1	0.94	0.15	-	29,29,29,29	0
54	MG	BA	3034	1/1	0.85	0.20	-	40,40,40,40	0
54	MG	BR	204	1/1	0.56	0.20	-	49,49,49,49	0
54	MG	DA	3511	1/1	0.98	0.07	-	44,44,44,44	0
54	MG	AA	1769	1/1	0.82	0.11	-	69,69,69,69	0
54	MG	CA	1631	1/1	0.83	0.10	-	87,87,87,87	0
54	MG	CA	1672	1/1	0.94	0.09	-	74,74,74,74	0
54	MG	DA	3469	1/1	0.93	0.16	-	56,56,56,56	0
54	MG	BA	3710	1/1	0.91	0.08	-	63,63,63,63	0
54	MG	BA	3174	1/1	0.91	0.24	-	73,73,73,73	0
54	MG	DA	3177	1/1	0.99	0.19	-	32,32,32,32	0
54	MG	DA	3158	1/1	0.97	0.20	-	49,49,49,49	0
54	MG	CA	1657	1/1	0.55	0.15	-	85,85,85,85	0
54	MG	BA	3434	1/1	0.96	0.10	-	56,56,56,56	0
54	MG	DA	3525	1/1	0.92	0.21	-	57,57,57,57	0
54	MG	DA	3478	1/1	0.69	0.29	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1780	1/1	0.95	0.11	-	74,74,74,74	0
54	MG	BA	3646	1/1	0.87	0.17	-	38,38,38,38	0
54	MG	BA	3593	1/1	0.96	0.29	-	34,34,34,34	0
54	MG	DA	3044	1/1	0.94	0.41	-	55,55,55,55	0
54	MG	BA	3049	1/1	0.98	0.21	-	26,26,26,26	0
54	MG	CA	1754	1/1	0.95	0.12	-	77,77,77,77	0
54	MG	DA	3242	1/1	0.98	0.12	-	36,36,36,36	0
54	MG	BA	3240	1/1	0.91	0.14	-	66,66,66,66	0
54	MG	DA	3108	1/1	0.73	0.38	-	70,70,70,70	0
54	MG	BA	3077	1/1	0.89	0.21	-	43,43,43,43	0
54	MG	AA	1713	1/1	0.95	0.18	-	61,61,61,61	0
54	MG	D0	101	1/1	0.67	0.16	-	78,78,78,78	0
54	MG	AA	1791	1/1	0.87	0.16	-	68,68,68,68	0
54	MG	DA	3461	1/1	0.94	0.08	-	76,76,76,76	0
54	MG	BR	201	1/1	0.95	0.43	-	39,39,39,39	0
54	MG	BA	3320	1/1	0.97	0.15	-	42,42,42,42	0
54	MG	AA	1770	1/1	0.92	0.08	-	80,80,80,80	0
54	MG	BA	3196	1/1	0.92	0.19	-	52,52,52,52	0
54	MG	BA	3251	1/1	0.85	0.13	-	24,24,24,24	0
54	MG	DA	3492	1/1	0.96	0.17	-	59,59,59,59	0
54	MG	BA	3362	1/1	0.94	0.14	-	30,30,30,30	0
54	MG	DA	3599	1/1	0.97	0.07	-	45,45,45,45	0
54	MG	BA	3294	1/1	0.96	0.08	-	32,32,32,32	0
54	MG	BA	3569	1/1	0.83	0.12	-	67,67,67,67	0
54	MG	BA	3121	1/1	0.97	0.34	-	26,26,26,26	0
54	MG	BA	3452	1/1	0.95	0.11	-	54,54,54,54	0
54	MG	DA	3633	1/1	0.98	0.19	-	49,49,49,49	0
54	MG	BA	3247	1/1	0.97	0.12	-	45,45,45,45	0
54	MG	BA	3601	1/1	0.98	0.16	-	43,43,43,43	0
54	MG	BA	3097	1/1	0.91	0.14	-	40,40,40,40	0
54	MG	BA	3532	1/1	0.89	0.19	-	31,31,31,31	0
54	MG	DA	3159	1/1	0.62	0.15	-	66,66,66,66	0
54	MG	DA	3481	1/1	0.94	0.16	-	51,51,51,51	0
54	MG	AA	1685	1/1	0.92	0.38	-	57,57,57,57	0
54	MG	BA	3598	1/1	0.97	0.18	-	34,34,34,34	0
54	MG	BA	3054	1/1	0.96	0.13	-	31,31,31,31	0
54	MG	DA	3121	1/1	0.91	0.20	-	62,62,62,62	0
54	MG	AA	1610	1/1	0.91	0.09	-	64,64,64,64	0
54	MG	DA	3632	1/1	0.67	0.14	-	72,72,72,72	0
54	MG	DA	3087	1/1	0.92	0.36	-	52,52,52,52	0
54	MG	BA	3352	1/1	0.93	0.09	-	37,37,37,37	0
54	MG	BA	3016	1/1	0.89	0.15	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3324	1/1	0.87	0.24	-	86,86,86,86	0
54	MG	DA	3370	1/1	0.87	0.19	-	87,87,87,87	0
54	MG	DA	3417	1/1	0.95	0.10	-	59,59,59,59	0
54	MG	DA	3419	1/1	0.91	0.10	-	51,51,51,51	0
54	MG	DA	3299	1/1	0.95	0.08	-	33,33,33,33	0
54	MG	BA	3031	1/1	0.84	0.14	-	66,66,66,66	0
54	MG	DA	3223	1/1	0.94	0.08	-	39,39,39,39	0
54	MG	DA	3045	1/1	0.94	0.19	-	48,48,48,48	0
54	MG	BA	3066	1/1	0.92	0.10	-	41,41,41,41	0
54	MG	BA	3333	1/1	0.91	0.05	-	54,54,54,54	0
54	MG	DA	3112	1/1	0.94	0.20	-	48,48,48,48	0
54	MG	AA	1711	1/1	0.98	0.11	-	35,35,35,35	0
54	MG	BA	3509	1/1	0.82	0.14	-	77,77,77,77	0
54	MG	DQ	202	1/1	0.98	0.31	-	39,39,39,39	0
54	MG	AA	1633	1/1	0.76	0.21	-	69,69,69,69	0
54	MG	AA	1772	1/1	0.81	0.14	-	71,71,71,71	0
54	MG	DA	3234	1/1	0.96	0.20	-	52,52,52,52	0
54	MG	BA	3477	1/1	0.61	0.18	-	101,101,101,101	0
54	MG	BA	3725	1/1	0.87	0.14	-	57,57,57,57	0
54	MG	B1	101	1/1	0.95	0.22	-	40,40,40,40	0
54	MG	BA	3278	1/1	0.95	0.20	-	39,39,39,39	0
54	MG	DA	3533	1/1	0.88	0.07	-	79,79,79,79	0
54	MG	DA	3256	1/1	0.96	0.22	-	57,57,57,57	0
54	MG	DA	3326	1/1	0.84	0.17	-	69,69,69,69	0
54	MG	DA	3093	1/1	0.85	0.24	-	55,55,55,55	0
54	MG	DA	3552	1/1	0.98	0.08	-	56,56,56,56	0
54	MG	BA	3090	1/1	0.95	0.32	-	30,30,30,30	0
54	MG	DA	3480	1/1	0.88	0.06	-	57,57,57,57	0
54	MG	DA	3298	1/1	0.85	0.11	-	51,51,51,51	0
54	MG	BA	3265	1/1	0.90	0.05	-	69,69,69,69	0
54	MG	AA	1603	1/1	0.78	0.11	-	62,62,62,62	0
54	MG	BA	3167	1/1	0.91	0.12	-	45,45,45,45	0
54	MG	BA	3625	1/1	0.92	0.22	-	52,52,52,52	0
54	MG	DA	3123	1/1	0.96	0.12	-	48,48,48,48	0
54	MG	CA	1625	1/1	0.92	0.21	-	69,69,69,69	0
54	MG	BA	3205	1/1	0.82	0.12	-	67,67,67,67	0
54	MG	CA	1683	1/1	0.96	0.06	-	71,71,71,71	0
54	MG	BA	3400	1/1	0.96	0.07	-	39,39,39,39	0
54	MG	BA	3458	1/1	0.89	0.11	-	45,45,45,45	0
54	MG	BA	3610	1/1	0.94	0.13	-	36,36,36,36	0
54	MG	CA	1757	1/1	0.89	0.16	-	75,75,75,75	0
54	MG	DA	3148	1/1	0.90	0.11	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1720	1/1	0.92	0.17	-	84,84,84,84	0
54	MG	DA	3620	1/1	0.90	0.06	-	65,65,65,65	0
54	MG	BA	3192	1/1	0.88	0.21	-	62,62,62,62	0
54	MG	BA	3634	1/1	0.95	0.05	-	63,63,63,63	0
54	MG	DA	3333	1/1	0.92	0.14	-	54,54,54,54	0
54	MG	BA	3707	1/1	0.94	0.09	-	49,49,49,49	0
54	MG	DA	3316	1/1	0.75	0.12	-	87,87,87,87	0
54	MG	BA	3142	1/1	0.91	0.29	-	36,36,36,36	0
54	MG	BA	3498	1/1	0.99	0.14	-	45,45,45,45	0
54	MG	BV	203	1/1	0.96	0.10	-	56,56,56,56	0
54	MG	BA	3488	1/1	0.98	0.11	-	20,20,20,20	0
54	MG	CA	1689	1/1	0.89	0.04	-	90,90,90,90	0
54	MG	BA	3531	1/1	0.94	0.20	-	25,25,25,25	0
54	MG	CA	1694	1/1	0.88	0.10	-	69,69,69,69	0
54	MG	BA	3133	1/1	0.95	0.20	-	30,30,30,30	0
54	MG	DA	3407	1/1	0.97	0.15	-	51,51,51,51	0
54	MG	BA	3266	1/1	0.93	0.18	-	66,66,66,66	0
54	MG	BZ	301	1/1	0.90	0.28	-	61,61,61,61	0
54	MG	BA	3113	1/1	0.88	0.24	-	48,48,48,48	0
54	MG	AA	1775	1/1	0.98	0.11	-	63,63,63,63	0
54	MG	DA	3386	1/1	0.96	0.18	-	64,64,64,64	0
54	MG	BA	3076	1/1	0.83	0.40	-	58,58,58,58	0
54	MG	BA	3188	1/1	0.93	0.15	-	47,47,47,47	0
54	MG	AA	1805	1/1	0.95	0.11	-	82,82,82,82	0
54	MG	DA	3004	1/1	0.85	0.24	-	64,64,64,64	0
54	MG	DA	3293	1/1	0.92	0.11	-	85,85,85,85	0
54	MG	BA	3546	1/1	0.93	0.12	-	46,46,46,46	0
54	MG	DA	3486	1/1	0.77	0.28	-	44,44,44,44	0
54	MG	DA	3547	1/1	0.52	0.44	-	89,89,89,89	0
54	MG	DA	3550	1/1	0.90	0.19	-	51,51,51,51	0
54	MG	BA	3239	1/1	0.91	0.08	-	63,63,63,63	0
54	MG	DT	201	1/1	0.93	0.07	-	52,52,52,52	0
54	MG	BA	3059	1/1	0.73	0.20	-	54,54,54,54	0
54	MG	CA	1773	1/1	0.88	0.14	-	89,89,89,89	0
54	MG	AA	1703	1/1	0.89	0.28	-	64,64,64,64	0
54	MG	AA	1637	1/1	0.96	0.34	-	64,64,64,64	0
54	MG	AA	1670	1/1	0.95	0.18	-	56,56,56,56	0
54	MG	DA	3120	1/1	0.97	0.17	-	47,47,47,47	0
54	MG	CA	1798	1/1	0.93	0.28	-	67,67,67,67	0
54	MG	DA	3597	1/1	0.93	0.18	-	73,73,73,73	0
54	MG	AA	1812	1/1	0.94	0.24	-	82,82,82,82	0
54	MG	B5	101	1/1	0.90	0.16	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3426	1/1	0.98	0.13	-	55,55,55,55	0
54	MG	DA	3372	1/1	0.94	0.13	-	79,79,79,79	0
54	MG	BA	3241	1/1	0.98	0.18	-	56,56,56,56	0
54	MG	DA	3024	1/1	0.88	0.24	-	64,64,64,64	0
54	MG	BA	3574	1/1	0.92	0.19	-	41,41,41,41	0
54	MG	BA	3344	1/1	0.94	0.15	-	41,41,41,41	0
54	MG	AA	1709	1/1	0.94	0.14	-	57,57,57,57	0
54	MG	BA	3207	1/1	0.94	0.08	-	57,57,57,57	0
54	MG	BA	3461	1/1	0.94	0.09	-	62,62,62,62	0
54	MG	DA	3077	1/1	0.88	0.19	-	42,42,42,42	0
54	MG	BA	3675	1/1	0.94	0.09	-	48,48,48,48	0
54	MG	AA	1611	1/1	0.78	0.15	-	75,75,75,75	0
54	MG	AA	1804	1/1	0.91	0.19	-	64,64,64,64	0
54	MG	D8	101	1/1	0.90	0.26	-	52,52,52,52	0
54	MG	BA	3260	1/1	0.83	0.33	-	31,31,31,31	0
54	MG	BA	3572	1/1	0.95	0.08	-	44,44,44,44	0
54	MG	BB	208	1/1	0.96	0.14	-	33,33,33,33	0
54	MG	AA	1625	1/1	0.97	0.31	-	42,42,42,42	0
54	MG	DA	3296	1/1	0.94	0.27	-	61,61,61,61	0
54	MG	BA	3669	1/1	0.76	0.14	-	44,44,44,44	0
54	MG	D5	102	1/1	0.97	0.11	-	44,44,44,44	0
54	MG	BA	3309	1/1	0.83	0.15	-	69,69,69,69	0
54	MG	DA	3226	1/1	0.83	0.16	-	41,41,41,41	0
54	MG	AA	1783	1/1	0.92	0.20	-	71,71,71,71	0
54	MG	BA	3583	1/1	0.81	0.09	-	63,63,63,63	0
54	MG	DA	3527	1/1	0.98	0.15	-	38,38,38,38	0
54	MG	AA	1777	1/1	0.83	0.13	-	100,100,100,100	0
54	MG	AA	1734	1/1	0.90	0.10	-	50,50,50,50	0
54	MG	BA	3369	1/1	0.94	0.11	-	27,27,27,27	0
54	MG	AA	1785	1/1	0.90	0.16	-	61,61,61,61	0
54	MG	BA	3645	1/1	0.96	0.18	-	59,59,59,59	0
54	MG	BA	3517	1/1	0.57	0.17	-	91,91,91,91	0
54	MG	BA	3529	1/1	0.88	0.26	-	52,52,52,52	0
54	MG	CA	1607	1/1	0.55	0.99	-	96,96,96,96	0
54	MG	BA	3630	1/1	0.96	0.12	-	57,57,57,57	0
54	MG	BA	3129	1/1	0.86	0.07	-	69,69,69,69	0
54	MG	DA	3126	1/1	0.88	0.17	-	56,56,56,56	0
54	MG	DA	3501	1/1	0.92	0.13	-	85,85,85,85	0
54	MG	DA	3584	1/1	0.97	0.08	-	37,37,37,37	0
54	MG	BA	3652	1/1	0.94	0.13	-	51,51,51,51	0
54	MG	BA	3268	1/1	0.96	0.07	-	52,52,52,52	0
54	MG	BA	3595	1/1	0.92	0.09	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3322	1/1	0.91	0.20	-	61,61,61,61	0
54	MG	DA	3559	1/1	0.82	0.41	-	76,76,76,76	0
54	MG	CA	1700	1/1	0.92	0.12	-	56,56,56,56	0
54	MG	AA	1744	1/1	0.96	0.14	-	74,74,74,74	0
54	MG	BA	3125	1/1	0.97	0.16	-	39,39,39,39	0
54	MG	DA	3118	1/1	0.83	0.15	-	75,75,75,75	0
54	MG	AM	202	1/1	0.90	0.14	-	59,59,59,59	0
54	MG	DA	3278	1/1	0.92	0.06	-	71,71,71,71	0
54	MG	DA	3188	1/1	0.91	0.15	-	51,51,51,51	0
54	MG	DA	3206	1/1	0.91	0.12	-	34,34,34,34	0
54	MG	DA	3067	1/1	0.92	0.26	-	58,58,58,58	0
54	MG	BA	3648	1/1	0.92	0.20	-	42,42,42,42	0
54	MG	DA	3192	1/1	0.95	0.09	-	37,37,37,37	0
54	MG	BA	3673	1/1	0.88	0.27	-	69,69,69,69	0
54	MG	CA	1774	1/1	0.93	0.22	-	73,73,73,73	0
54	MG	DA	3524	1/1	0.92	0.09	-	61,61,61,61	0
54	MG	DA	3538	1/1	0.93	0.16	-	60,60,60,60	0
54	MG	BA	3631	1/1	0.96	0.25	-	35,35,35,35	0
54	MG	BA	3687	1/1	0.95	0.09	-	53,53,53,53	0
54	MG	BA	3664	1/1	0.89	0.08	-	56,56,56,56	0
54	MG	BA	3150	1/1	0.91	0.10	-	70,70,70,70	0
54	MG	BA	3143	1/1	0.93	0.17	-	23,23,23,23	0
54	MG	DA	3586	1/1	0.78	0.21	-	142,142,142,142	0
54	MG	BA	3417	1/1	0.95	0.13	-	25,25,25,25	0
54	MG	DA	3383	1/1	0.92	0.14	-	59,59,59,59	0
54	MG	BA	3343	1/1	0.83	0.17	-	48,48,48,48	0
54	MG	DA	3340	1/1	0.84	0.17	-	72,72,72,72	0
54	MG	DA	3610	1/1	0.96	0.10	-	79,79,79,79	0
54	MG	BA	3096	1/1	0.97	0.22	-	36,36,36,36	0
54	MG	DA	3260	1/1	0.96	0.12	-	57,57,57,57	0
54	MG	DA	3122	1/1	0.72	0.25	-	58,58,58,58	0
54	MG	BA	3374	1/1	0.97	0.20	-	27,27,27,27	0
54	MG	BA	3202	1/1	0.92	0.13	-	67,67,67,67	0
54	MG	DA	3562	1/1	0.92	0.17	-	65,65,65,65	0
54	MG	CA	1748	1/1	0.97	0.19	-	57,57,57,57	0
54	MG	DA	3132	1/1	0.93	0.11	-	54,54,54,54	0
54	MG	AA	1658	1/1	0.75	0.25	-	73,73,73,73	0
54	MG	CA	1705	1/1	0.81	0.16	-	72,72,72,72	0
54	MG	AA	1688	1/1	0.92	0.20	-	62,62,62,62	0
54	MG	AA	1646	1/1	0.77	0.26	-	87,87,87,87	0
54	MG	DA	3106	1/1	0.91	0.26	-	55,55,55,55	0
54	MG	BA	3565	1/1	0.95	0.20	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1734	1/1	0.94	0.15	-	79,79,79,79	0
54	MG	CA	1793	1/1	0.74	0.20	-	89,89,89,89	0
54	MG	DA	3488	1/1	0.97	0.16	-	46,46,46,46	0
54	MG	BA	3124	1/1	0.97	0.17	-	24,24,24,24	0
54	MG	DA	3457	1/1	0.96	0.14	-	59,59,59,59	0
54	MG	DA	3194	1/1	0.93	0.20	-	22,22,22,22	0
54	MG	DA	3037	1/1	0.92	0.17	-	52,52,52,52	0
54	MG	BA	3692	1/1	0.89	0.13	-	38,38,38,38	0
54	MG	DA	3163	1/1	0.84	0.14	-	39,39,39,39	0
54	MG	DA	3445	1/1	0.92	0.13	-	45,45,45,45	0
54	MG	CA	1646	1/1	0.74	0.11	-	71,71,71,71	0
54	MG	DA	3229	1/1	0.94	0.16	-	76,76,76,76	0
54	MG	BW	201	1/1	0.93	0.15	-	44,44,44,44	0
54	MG	BA	3423	1/1	0.87	0.09	-	46,46,46,46	0
54	MG	DA	3482	1/1	0.92	0.14	-	69,69,69,69	0
54	MG	DA	3218	1/1	0.92	0.09	-	57,57,57,57	0
54	MG	DA	3499	1/1	0.98	0.07	-	55,55,55,55	0
54	MG	BA	3208	1/1	0.92	0.26	-	57,57,57,57	0
54	MG	BN	202	1/1	0.91	0.12	-	57,57,57,57	0
54	MG	CA	1605	1/1	0.89	0.15	-	63,63,63,63	0
54	MG	BA	3511	1/1	0.76	0.09	-	72,72,72,72	0
54	MG	DA	3503	1/1	0.80	0.12	-	59,59,59,59	0
54	MG	DA	3089	1/1	0.86	0.29	-	50,50,50,50	0
54	MG	B0	104	1/1	0.95	0.06	-	49,49,49,49	0
54	MG	CA	1623	1/1	0.94	0.12	-	60,60,60,60	0
54	MG	DA	3510	1/1	0.95	0.15	-	46,46,46,46	0
54	MG	BA	3706	1/1	0.95	0.10	-	44,44,44,44	0
54	MG	BA	3609	1/1	0.96	0.04	-	37,37,37,37	0
54	MG	DA	3392	1/1	0.92	0.09	-	43,43,43,43	0
54	MG	DA	3553	1/1	0.92	0.11	-	64,64,64,64	0
54	MG	DA	3191	1/1	0.90	0.18	-	56,56,56,56	0
54	MG	BA	3688	1/1	0.82	0.12	-	72,72,72,72	0
54	MG	AA	1695	1/1	0.84	0.14	-	57,57,57,57	0
54	MG	DA	3070	1/1	0.95	0.26	-	51,51,51,51	0
54	MG	DA	3164	1/1	0.73	0.15	-	64,64,64,64	0
54	MG	BA	3728	1/1	0.98	0.07	-	47,47,47,47	0
54	MG	DA	3144	1/1	0.87	0.23	-	54,54,54,54	0
54	MG	AA	1740	1/1	0.91	0.26	-	70,70,70,70	0
54	MG	DA	3580	1/1	0.96	0.18	-	39,39,39,39	0
54	MG	BA	3703	1/1	0.96	0.06	-	26,26,26,26	0
54	MG	AA	1726	1/1	0.97	0.22	-	75,75,75,75	0
54	MG	DA	3076	1/1	0.89	0.37	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3105	1/1	0.94	0.20	-	54,54,54,54	0
54	MG	BA	3713	1/1	0.96	0.10	-	35,35,35,35	0
54	MG	BA	3671	1/1	0.92	0.31	-	50,50,50,50	0
54	MG	BA	3264	1/1	0.49	0.10	-	86,86,86,86	0
54	MG	DQ	204	1/1	0.91	0.14	-	67,67,67,67	0
54	MG	DA	3281	1/1	0.89	0.25	-	85,85,85,85	0
54	MG	CA	1668	1/1	0.91	0.26	-	65,65,65,65	0
54	MG	BV	202	1/1	0.91	0.33	-	83,83,83,83	0
54	MG	BA	3494	1/1	0.95	0.14	-	52,52,52,52	0
54	MG	DA	3628	1/1	0.87	0.10	-	59,59,59,59	0
54	MG	AA	1760	1/1	0.92	0.27	-	74,74,74,74	0
54	MG	CA	1666	1/1	0.88	0.12	-	71,71,71,71	0
54	MG	BA	3285	1/1	0.79	0.30	-	96,96,96,96	0
54	MG	BA	3556	1/1	0.98	0.20	-	52,52,52,52	0
54	MG	AA	1738	1/1	0.95	0.04	-	62,62,62,62	0
54	MG	BA	3193	1/1	0.97	0.14	-	46,46,46,46	0
54	MG	BA	3594	1/1	0.85	0.17	-	56,56,56,56	0
54	MG	AA	1672	1/1	0.95	0.13	-	50,50,50,50	0
54	MG	BA	3607	1/1	0.96	0.07	-	76,76,76,76	0
54	MG	DA	3585	1/1	0.95	0.29	-	36,36,36,36	0
54	MG	BA	3030	1/1	0.90	0.26	-	44,44,44,44	0
54	MG	CA	1802	1/1	0.98	0.08	-	60,60,60,60	0
54	MG	DA	3143	1/1	0.85	0.26	-	62,62,62,62	0
54	MG	CA	1764	1/1	0.84	0.13	-	90,90,90,90	0
54	MG	BA	3210	1/1	0.86	0.16	-	58,58,58,58	0
54	MG	DA	3006	1/1	0.94	0.17	-	42,42,42,42	0
54	MG	DA	3563	1/1	0.94	0.41	-	57,57,57,57	0
54	MG	AA	1648	1/1	0.98	0.19	-	73,73,73,73	0
54	MG	DA	3220	1/1	0.90	0.10	-	48,48,48,48	0
54	MG	DA	3364	1/1	0.90	0.10	-	54,54,54,54	0
54	MG	DA	3193	1/1	0.94	0.08	-	66,66,66,66	0
54	MG	DA	3033	1/1	0.93	0.19	-	48,48,48,48	0
54	MG	BP	202	1/1	0.88	0.28	-	54,54,54,54	0
54	MG	BA	3694	1/1	0.94	0.19	-	21,21,21,21	0
54	MG	BA	3004	1/1	0.98	0.20	-	53,53,53,53	0
54	MG	BA	3723	1/1	0.73	0.12	-	70,70,70,70	0
54	MG	BA	3303	1/1	0.96	0.15	-	40,40,40,40	0
54	MG	BA	3099	1/1	0.90	0.27	-	47,47,47,47	0
54	MG	BA	3622	1/1	0.97	0.09	-	31,31,31,31	0
54	MG	BA	3039	1/1	0.96	0.14	-	58,58,58,58	0
54	MG	BA	3540	1/1	0.92	0.07	-	64,64,64,64	0
54	MG	BA	3616	1/1	0.96	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
54	MG	AA	1802	1/1	0.95	0.37	-	64,64,64,64	0
54	MG	CA	1614	1/1	0.92	0.16	-	70,70,70,70	0
54	MG	DA	3408	1/1	0.92	0.08	-	54,54,54,54	0
54	MG	DA	3023	1/1	0.94	0.30	-	68,68,68,68	0
54	MG	DA	3391	1/1	0.91	0.10	-	62,62,62,62	0
54	MG	DF	302	1/1	0.90	0.18	-	63,63,63,63	0
54	MG	DA	3323	1/1	0.95	0.13	-	69,69,69,69	0
54	MG	CA	1695	1/1	0.92	0.33	-	76,76,76,76	0
54	MG	DA	3442	1/1	0.93	0.19	-	59,59,59,59	0
54	MG	BA	3282	1/1	0.98	0.18	-	29,29,29,29	0
54	MG	BA	3686	1/1	0.92	0.07	-	43,43,43,43	0
54	MG	AA	1663	1/1	0.96	0.09	-	62,62,62,62	0
54	MG	DA	3230	1/1	0.99	0.09	-	31,31,31,31	0
54	MG	BA	3697	1/1	0.98	0.18	-	27,27,27,27	0
54	MG	BA	3145	1/1	0.91	0.17	-	33,33,33,33	0
54	MG	BA	3070	1/1	0.93	0.33	-	39,39,39,39	0
54	MG	AA	1748	1/1	0.98	0.14	-	57,57,57,57	0
54	MG	DA	3608	1/1	0.92	0.10	-	74,74,74,74	0
54	MG	CA	1790	1/1	0.93	0.14	-	48,48,48,48	0
54	MG	CA	1733	1/1	0.91	0.11	-	89,89,89,89	0
54	MG	AA	1810	1/1	0.95	0.15	-	67,67,67,67	0
54	MG	DA	3263	1/1	0.91	0.10	-	54,54,54,54	0
54	MG	BA	3642	1/1	0.90	0.14	-	46,46,46,46	0
54	MG	BA	3064	1/1	0.90	0.31	-	54,54,54,54	0
54	MG	BA	3507	1/1	0.90	0.14	-	67,67,67,67	0
54	MG	DA	3353	1/1	0.92	0.06	-	79,79,79,79	0
54	MG	DA	3400	1/1	0.95	0.17	-	41,41,41,41	0
54	MG	DA	3095	1/1	0.93	0.18	-	65,65,65,65	0
54	MG	BA	3284	1/1	0.92	0.21	-	37,37,37,37	0
54	MG	DA	3623	1/1	0.92	0.16	-	42,42,42,42	0
54	MG	DA	3341	1/1	0.69	0.14	-	60,60,60,60	0
54	MG	CA	1678	1/1	0.97	0.09	-	55,55,55,55	0
54	MG	BA	3682	1/1	0.91	0.17	-	55,55,55,55	0
54	MG	BA	3448	1/1	0.94	0.20	-	46,46,46,46	0
54	MG	BA	3615	1/1	0.92	0.38	-	60,60,60,60	0
54	MG	DA	3387	1/1	0.86	0.08	-	72,72,72,72	0
54	MG	BA	3081	1/1	0.98	0.14	-	38,38,38,38	0
54	MG	DA	3450	1/1	0.89	0.12	-	70,70,70,70	0
54	MG	CA	1727	1/1	0.98	0.26	-	63,63,63,63	0
54	MG	DA	3618	1/1	0.64	0.37	-	93,93,93,93	0
54	MG	BA	3184	1/1	0.89	0.22	-	37,37,37,37	0
54	MG	AA	1604	1/1	0.90	0.55	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3611	1/1	0.94	0.17	-	57,57,57,57	0
54	MG	CA	1766	1/1	0.86	0.16	-	65,65,65,65	0
54	MG	BA	3413	1/1	0.99	0.14	-	24,24,24,24	0
54	MG	DA	3631	1/1	0.98	0.06	-	54,54,54,54	0
54	MG	CA	1797	1/1	0.79	0.21	-	68,68,68,68	0
54	MG	DA	3088	1/1	0.87	0.20	-	39,39,39,39	0
54	MG	BA	3525	1/1	0.96	0.13	-	47,47,47,47	0
54	MG	DA	3337	1/1	0.68	0.24	-	65,65,65,65	0
54	MG	DA	3363	1/1	0.91	0.14	-	51,51,51,51	0
54	MG	BA	3322	1/1	0.75	0.28	-	54,54,54,54	0
54	MG	DA	3526	1/1	0.94	0.13	-	42,42,42,42	0
54	MG	AA	1761	1/1	0.92	0.06	-	65,65,65,65	0
54	MG	BA	3361	1/1	0.88	0.21	-	30,30,30,30	0
54	MG	AF	201	1/1	0.92	0.16	-	53,53,53,53	0
54	MG	BA	3288	1/1	0.97	0.17	-	44,44,44,44	0
54	MG	BA	3439	1/1	0.98	0.08	-	30,30,30,30	0
54	MG	BA	3444	1/1	0.92	0.14	-	50,50,50,50	0
54	MG	DA	3338	1/1	0.84	0.23	-	67,67,67,67	0
54	MG	BA	3156	1/1	0.95	0.15	-	28,28,28,28	0
54	MG	DA	3556	1/1	0.88	0.05	-	87,87,87,87	0
54	MG	BA	3672	1/1	0.75	0.31	-	69,69,69,69	0
54	MG	CA	1784	1/1	0.93	0.12	-	53,53,53,53	0
54	MG	BA	3154	1/1	0.96	0.12	-	47,47,47,47	0
54	MG	AA	1729	1/1	0.91	0.10	-	55,55,55,55	0
54	MG	CA	1690	1/1	0.84	0.14	-	75,75,75,75	0
54	MG	DA	3379	1/1	0.96	0.11	-	69,69,69,69	0
54	MG	BA	3161	1/1	0.96	0.18	-	20,20,20,20	0
54	MG	BA	3317	1/1	0.87	0.16	-	69,69,69,69	0
54	MG	AA	1602	1/1	0.95	0.19	-	70,70,70,70	0
54	MG	DA	3331	1/1	0.94	0.12	-	48,48,48,48	0
54	MG	B0	102	1/1	0.96	0.15	-	50,50,50,50	0
54	MG	DA	3475	1/1	0.95	0.16	-	60,60,60,60	0
54	MG	BA	3473	1/1	0.95	0.14	-	54,54,54,54	0
54	MG	DA	3546	1/1	0.94	0.07	-	64,64,64,64	0
54	MG	BA	3726	1/1	0.61	0.16	-	73,73,73,73	0
54	MG	BA	3719	1/1	0.92	0.10	-	83,83,83,83	0
54	MG	DA	3397	1/1	0.96	0.15	-	59,59,59,59	0
54	MG	BF	301	1/1	0.92	0.15	-	40,40,40,40	0
54	MG	BA	3376	1/1	0.93	0.19	-	37,37,37,37	0
54	MG	DA	3358	1/1	0.94	0.07	-	59,59,59,59	0
54	MG	BB	215	1/1	0.97	0.11	-	57,57,57,57	0
54	MG	BA	3567	1/1	0.91	0.16	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3612	1/1	0.90	0.26	-	58,58,58,58	0
54	MG	BA	3397	1/1	0.94	0.14	-	36,36,36,36	0
54	MG	DA	3521	1/1	0.93	0.14	-	43,43,43,43	0
54	MG	AA	1627	1/1	0.94	0.19	-	58,58,58,58	0
54	MG	CA	1669	1/1	0.85	0.20	-	71,71,71,71	0
54	MG	DA	3409	1/1	0.89	0.10	-	53,53,53,53	0
54	MG	BA	3623	1/1	0.87	0.18	-	85,85,85,85	0
54	MG	AA	1766	1/1	0.95	0.12	-	57,57,57,57	0
54	MG	AA	1684	1/1	0.93	0.10	-	43,43,43,43	0
54	MG	BA	3656	1/1	0.84	0.21	-	50,50,50,50	0
54	MG	CA	1732	1/1	0.95	0.23	-	63,63,63,63	0
54	MG	CA	1653	1/1	0.85	0.15	-	85,85,85,85	0
54	MG	DA	3264	1/1	0.90	0.11	-	91,91,91,91	0
54	MG	BA	3605	1/1	0.00	0.57	-	89,89,89,89	0
54	MG	BA	3618	1/1	0.91	0.09	-	67,67,67,67	0
54	MG	CA	1721	1/1	0.96	0.10	-	53,53,53,53	0
54	MG	BA	3308	1/1	0.93	0.06	-	51,51,51,51	0
54	MG	DA	3635	1/1	0.83	0.19	-	54,54,54,54	0
54	MG	AA	1639	1/1	0.89	0.36	-	64,64,64,64	0
54	MG	DA	3463	1/1	0.86	0.15	-	67,67,67,67	0
54	MG	BA	3136	1/1	0.89	0.17	-	24,24,24,24	0
54	MG	CA	1709	1/1	0.89	0.18	-	76,76,76,76	0
54	MG	AA	1782	1/1	0.94	0.14	-	59,59,59,59	0
54	MG	DA	3254	1/1	0.98	0.24	-	39,39,39,39	0
54	MG	DA	3365	1/1	0.89	0.20	-	51,51,51,51	0
54	MG	DA	3361	1/1	0.97	0.24	-	40,40,40,40	0
54	MG	DA	3329	1/1	0.93	0.19	-	34,34,34,34	0
54	MG	BB	218	1/1	0.96	0.09	-	69,69,69,69	0
54	MG	DA	3483	1/1	0.96	0.08	-	63,63,63,63	0
54	MG	BA	3093	1/1	0.98	0.13	-	28,28,28,28	0
54	MG	AA	1680	1/1	0.91	0.34	-	54,54,54,54	0
54	MG	DA	3027	1/1	0.86	0.19	-	47,47,47,47	0
54	MG	BA	3280	1/1	0.89	0.12	-	57,57,57,57	0
54	MG	BA	3503	1/1	0.96	0.23	-	23,23,23,23	0
54	MG	BA	3592	1/1	0.91	0.14	-	62,62,62,62	0
54	MG	DA	3074	1/1	0.94	0.17	-	46,46,46,46	0
54	MG	DA	3208	1/1	0.95	0.12	-	31,31,31,31	0
54	MG	BA	3092	1/1	0.93	0.18	-	40,40,40,40	0
54	MG	AA	1624	1/1	0.91	0.15	-	49,49,49,49	0
54	MG	DA	3564	1/1	0.97	0.11	-	61,61,61,61	0
54	MG	BA	3019	1/1	0.98	0.14	-	23,23,23,23	0
54	MG	BA	3524	1/1	0.97	0.08	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1692	1/1	0.92	0.40	-	66,66,66,66	0
54	MG	DB	203	1/1	0.92	0.11	-	61,61,61,61	0
54	MG	AA	1701	1/1	0.94	0.06	-	68,68,68,68	0
54	MG	DA	3574	1/1	0.88	0.18	-	77,77,77,77	0
54	MG	DA	3425	1/1	0.93	0.25	-	42,42,42,42	0
54	MG	DA	3624	1/1	0.92	0.24	-	56,56,56,56	0
54	MG	BA	3676	1/1	0.96	0.20	-	46,46,46,46	0
54	MG	BA	3213	1/1	0.92	0.18	-	28,28,28,28	0
54	MG	AA	1813	1/1	0.73	0.17	-	86,86,86,86	0
54	MG	DA	3092	1/1	0.76	0.17	-	54,54,54,54	0
54	MG	BA	3321	1/1	0.94	0.10	-	77,77,77,77	0
54	MG	DA	3621	1/1	0.98	0.13	-	41,41,41,41	0
54	MG	BA	3286	1/1	0.85	0.18	-	42,42,42,42	0
54	MG	DA	3280	1/1	0.92	0.19	-	52,52,52,52	0
54	MG	AA	1809	1/1	0.94	0.37	-	79,79,79,79	0
54	MG	BA	3255	1/1	0.96	0.10	-	25,25,25,25	0
54	MG	CA	1647	1/1	0.78	0.11	-	103,103,103,103	0
54	MG	DA	3185	1/1	0.84	0.22	-	47,47,47,47	0
54	MG	DD	303	1/1	0.81	0.14	-	53,53,53,53	0
54	MG	CA	1628	1/1	0.93	0.22	-	71,71,71,71	0
54	MG	B0	103	1/1	0.85	0.15	-	71,71,71,71	0
54	MG	CA	1610	1/1	0.90	0.27	-	67,67,67,67	0
54	MG	BA	3187	1/1	0.91	0.27	-	69,69,69,69	0
54	MG	BA	3588	1/1	0.93	0.10	-	55,55,55,55	0
54	MG	DA	3507	1/1	0.87	0.15	-	90,90,90,90	0
54	MG	DA	3113	1/1	0.94	0.18	-	56,56,56,56	0
54	MG	DA	3530	1/1	0.86	0.10	-	66,66,66,66	0
54	MG	BA	3641	1/1	0.92	0.15	-	47,47,47,47	0
54	MG	BA	3158	1/1	0.95	0.23	-	22,22,22,22	0
54	MG	CA	1637	1/1	0.86	0.14	-	98,98,98,98	0
54	MG	DA	3505	1/1	0.88	0.17	-	66,66,66,66	0
54	MG	BA	3091	1/1	0.92	0.24	-	34,34,34,34	0
54	MG	BA	3617	1/1	0.80	0.24	-	44,44,44,44	0
54	MG	BA	3276	1/1	0.86	0.11	-	47,47,47,47	0
54	MG	DA	3282	1/1	0.95	0.07	-	64,64,64,64	0
54	MG	AA	1727	1/1	0.94	0.18	-	82,82,82,82	0
54	MG	DA	3456	1/1	0.90	0.12	-	45,45,45,45	0
54	MG	BA	3570	1/1	0.92	0.12	-	50,50,50,50	0
54	MG	BA	3482	1/1	0.98	0.20	-	21,21,21,21	0
54	MG	BA	3626	1/1	0.88	0.15	-	68,68,68,68	0
54	MG	DA	3464	1/1	0.90	0.09	-	35,35,35,35	0
54	MG	DA	3047	1/1	0.96	0.20	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3226	1/1	0.88	0.14	-	49,49,49,49	0
54	MG	CA	1724	1/1	0.91	0.15	-	60,60,60,60	0
54	MG	DA	3272	1/1	0.82	0.10	-	69,69,69,69	0
54	MG	BA	3197	1/1	0.92	0.15	-	58,58,58,58	0
54	MG	DA	3476	1/1	0.73	0.09	-	95,95,95,95	0
54	MG	BA	3257	1/1	0.95	0.19	-	21,21,21,21	0
54	MG	CA	1685	1/1	0.98	0.27	-	62,62,62,62	0
54	MG	AA	1622	1/1	0.88	0.17	-	60,60,60,60	0
54	MG	CA	1640	1/1	0.85	0.20	-	63,63,63,63	0
54	MG	AA	1811	1/1	0.95	0.08	-	65,65,65,65	0
54	MG	AA	1690	1/1	0.90	0.10	-	60,60,60,60	0
54	MG	BA	3661	1/1	0.86	0.17	-	40,40,40,40	0
54	MG	CA	1796	1/1	0.80	0.14	-	85,85,85,85	0
54	MG	DA	3615	1/1	0.99	0.07	-	67,67,67,67	0
54	MG	BA	3078	1/1	0.96	0.23	-	45,45,45,45	0
54	MG	AA	1816	1/1	0.83	0.18	-	75,75,75,75	0
54	MG	DA	3247	1/1	0.75	0.26	-	73,73,73,73	0
54	MG	BA	3341	1/1	0.94	0.16	-	44,44,44,44	0
54	MG	BA	3471	1/1	0.95	0.10	-	50,50,50,50	0
54	MG	BA	3474	1/1	0.95	0.17	-	63,63,63,63	0
54	MG	DA	3002	1/1	0.97	0.11	-	45,45,45,45	0
54	MG	BA	3316	1/1	0.96	0.06	-	43,43,43,43	0
54	MG	DA	3485	1/1	0.95	0.14	-	33,33,33,33	0
54	MG	DA	3389	1/1	0.92	0.08	-	82,82,82,82	0
54	MG	BA	3253	1/1	0.90	0.12	-	39,39,39,39	0
54	MG	DA	3332	1/1	0.98	0.15	-	28,28,28,28	0
54	MG	DA	3607	1/1	0.97	0.09	-	65,65,65,65	0
54	MG	DA	3347	1/1	0.69	0.23	-	87,87,87,87	0
54	MG	BA	3173	1/1	0.94	0.15	-	63,63,63,63	0
54	MG	AA	1623	1/1	0.78	0.18	-	85,85,85,85	0
54	MG	DA	3362	1/1	0.91	0.22	-	53,53,53,53	0
54	MG	BA	3338	1/1	0.98	0.08	-	49,49,49,49	0
54	MG	DF	305	1/1	0.97	0.14	-	74,74,74,74	0
54	MG	AA	1621	1/1	0.92	0.64	-	63,63,63,63	0
54	MG	BA	3653	1/1	0.82	0.12	-	58,58,58,58	0
54	MG	BU	202	1/1	0.95	0.25	-	34,34,34,34	0
54	MG	CA	1634	1/1	0.92	0.10	-	40,40,40,40	0
54	MG	CA	1626	1/1	0.89	0.70	-	86,86,86,86	0
54	MG	BA	3399	1/1	0.97	0.14	-	42,42,42,42	0
54	MG	BA	3144	1/1	0.86	0.23	-	51,51,51,51	0
54	MG	AA	1781	1/1	0.95	0.10	-	71,71,71,71	0
54	MG	DA	3277	1/1	0.85	0.10	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BV	204	1/1	0.91	0.09	-	67,67,67,67	0
54	MG	AA	1654	1/1	0.87	0.09	-	77,77,77,77	0
54	MG	BB	216	1/1	0.94	0.31	-	59,59,59,59	0
54	MG	DA	3497	1/1	0.80	0.21	-	40,40,40,40	0
54	MG	DA	3235	1/1	0.93	0.16	-	58,58,58,58	0
54	MG	BA	3702	1/1	0.86	0.09	-	66,66,66,66	0
54	MG	CA	1726	1/1	0.96	0.10	-	77,77,77,77	0
54	MG	BP	201	1/1	0.96	0.16	-	44,44,44,44	0
54	MG	BA	3711	1/1	0.89	0.13	-	52,52,52,52	0
54	MG	AA	1780	1/1	0.88	0.17	-	72,72,72,72	0
54	MG	BA	3218	1/1	0.94	0.12	-	56,56,56,56	0
54	MG	BA	3330	1/1	0.95	0.20	-	45,45,45,45	0
54	MG	BA	3500	1/1	0.93	0.18	-	68,68,68,68	0
54	MG	AA	1609	1/1	0.95	0.16	-	66,66,66,66	0
54	MG	BA	3272	1/1	0.89	0.08	-	40,40,40,40	0
54	MG	AA	1710	1/1	0.97	0.22	-	52,52,52,52	0
54	MG	BA	3094	1/1	0.96	0.29	-	33,33,33,33	0
54	MG	DA	3173	1/1	0.92	0.12	-	34,34,34,34	0
54	MG	DB	210	1/1	0.69	0.18	-	82,82,82,82	0
54	MG	CA	1692	1/1	0.94	0.10	-	64,64,64,64	0
54	MG	BA	3519	1/1	0.94	0.12	-	26,26,26,26	0
54	MG	CA	1786	1/1	0.86	0.30	-	83,83,83,83	0
54	MG	BA	3539	1/1	0.94	0.05	-	58,58,58,58	0
54	MG	CA	1731	1/1	0.90	0.22	-	62,62,62,62	0
54	MG	AA	1656	1/1	0.95	0.14	-	69,69,69,69	0
54	MG	BA	3544	1/1	0.96	0.13	-	60,60,60,60	0
54	MG	DA	3508	1/1	0.85	0.24	-	73,73,73,73	0
54	MG	BA	3201	1/1	0.90	0.16	-	57,57,57,57	0
54	MG	BA	3718	1/1	0.93	0.11	-	49,49,49,49	0
54	MG	BA	3342	1/1	0.95	0.04	-	43,43,43,43	0
54	MG	CA	1654	1/1	0.82	0.21	-	63,63,63,63	0
54	MG	B2	101	1/1	0.95	0.19	-	46,46,46,46	0
54	MG	BA	3118	1/1	0.88	0.16	-	59,59,59,59	0
54	MG	CA	1613	1/1	0.81	0.26	-	68,68,68,68	0
54	MG	DA	3582	1/1	0.91	0.06	-	83,83,83,83	0
54	MG	AA	1660	1/1	0.94	0.30	-	62,62,62,62	0
54	MG	BA	3485	1/1	0.92	0.26	-	31,31,31,31	0
54	MG	BA	3304	1/1	0.99	0.15	-	33,33,33,33	0
54	MG	BA	3453	1/1	0.75	0.15	-	65,65,65,65	0
54	MG	DA	3109	1/1	0.92	0.45	-	57,57,57,57	0
54	MG	AA	1750	1/1	0.96	0.18	-	55,55,55,55	0
54	MG	BA	3089	1/1	0.96	0.13	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3577	1/1	0.72	0.11	-	59,59,59,59	0
54	MG	BA	3302	1/1	0.93	0.22	-	47,47,47,47	0
54	MG	AA	1749	1/1	0.90	0.15	-	58,58,58,58	0
54	MG	AA	1671	1/1	0.98	0.09	-	64,64,64,64	0
54	MG	CA	1609	1/1	0.91	0.56	-	77,77,77,77	0
54	MG	BA	3683	1/1	0.92	0.23	-	95,95,95,95	0
54	MG	CA	1770	1/1	0.93	0.09	-	71,71,71,71	0
54	MG	AA	1675	1/1	0.43	0.16	-	106,106,106,106	0
54	MG	BA	3599	1/1	0.94	0.17	-	63,63,63,63	0
54	MG	BA	3720	1/1	0.92	0.09	-	64,64,64,64	0
54	MG	DB	208	1/1	0.56	0.18	-	96,96,96,96	0
54	MG	DA	3154	1/1	0.97	0.15	-	47,47,47,47	0
54	MG	BA	3566	1/1	0.95	0.20	-	48,48,48,48	0
54	MG	AA	1694	1/1	0.96	0.09	-	76,76,76,76	0
54	MG	BA	3215	1/1	0.95	0.12	-	41,41,41,41	0
54	MG	BA	3375	1/1	0.80	0.14	-	61,61,61,61	0
54	MG	DA	3066	1/1	0.93	0.22	-	51,51,51,51	0
54	MG	BA	3680	1/1	0.95	0.12	-	37,37,37,37	0
54	MG	BA	3373	1/1	0.98	0.19	-	46,46,46,46	0
54	MG	DA	3287	1/1	0.96	0.15	-	52,52,52,52	0
54	MG	CA	1667	1/1	0.97	0.35	-	66,66,66,66	0
54	MG	DA	3320	1/1	0.93	0.06	-	54,54,54,54	0
54	MG	BA	3596	1/1	0.87	0.23	-	59,59,59,59	0
54	MG	DA	3119	1/1	0.92	0.18	-	38,38,38,38	0
54	MG	AA	1706	1/1	0.88	0.15	-	59,59,59,59	0
54	MG	BA	3581	1/1	0.95	0.12	-	42,42,42,42	0
54	MG	BB	217	1/1	0.98	0.09	-	66,66,66,66	0
54	MG	DA	3209	1/1	0.91	0.13	-	45,45,45,45	0
54	MG	CA	1630	1/1	0.53	0.44	-	78,78,78,78	0
54	MG	BE	306	1/1	0.96	0.23	-	24,24,24,24	0
54	MG	BB	211	1/1	0.77	0.10	-	61,61,61,61	0
54	MG	CE	201	1/1	0.94	0.10	-	78,78,78,78	0
54	MG	AA	1676	1/1	0.88	0.17	-	86,86,86,86	0
54	MG	DA	3094	1/1	0.72	0.33	-	54,54,54,54	0
54	MG	DA	3637	1/1	0.97	0.13	-	63,63,63,63	0
54	MG	DO	203	1/1	0.97	0.12	-	75,75,75,75	0
54	MG	BA	3225	1/1	0.97	0.19	-	19,19,19,19	0
54	MG	DA	3454	1/1	0.90	0.20	-	42,42,42,42	0
54	MG	DA	3560	1/1	0.99	0.12	-	57,57,57,57	0
54	MG	AA	1638	1/1	0.96	0.19	-	64,64,64,64	0
54	MG	CA	1624	1/1	0.75	0.19	-	65,65,65,65	0
54	MG	AA	1640	1/1	0.97	0.13	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3039	1/1	0.88	0.21	-	57,57,57,57	0
54	MG	DA	3015	1/1	0.90	0.12	-	56,56,56,56	0
54	MG	CA	1781	1/1	0.78	0.15	-	100,100,100,100	0
54	MG	DA	3079	1/1	0.89	0.26	-	54,54,54,54	0
54	MG	DA	3598	1/1	0.86	0.16	-	64,64,64,64	0
54	MG	DA	3460	1/1	0.95	0.16	-	32,32,32,32	0
54	MG	BA	3708	1/1	0.96	0.18	-	49,49,49,49	0
54	MG	DA	3342	1/1	0.93	0.14	-	40,40,40,40	0
54	MG	BA	3420	1/1	0.95	0.15	-	23,23,23,23	0
54	MG	CA	1635	1/1	0.83	0.44	-	63,63,63,63	0
54	MG	AA	1736	1/1	0.96	0.29	-	67,67,67,67	0
54	MG	AA	1707	1/1	0.92	0.20	-	79,79,79,79	0
54	MG	BA	3332	1/1	0.95	0.13	-	37,37,37,37	0
54	MG	CA	1707	1/1	0.86	0.41	-	73,73,73,73	0
54	MG	CA	1746	1/1	0.65	0.23	-	113,113,113,113	0
54	MG	BA	3538	1/1	0.94	0.10	-	55,55,55,55	0
54	MG	DF	301	1/1	0.90	0.20	-	51,51,51,51	0
54	MG	BA	3101	1/1	0.94	0.21	-	37,37,37,37	0
54	MG	DA	3196	1/1	0.85	0.32	-	37,37,37,37	0
54	MG	BA	3410	1/1	0.98	0.28	-	56,56,56,56	0
54	MG	DA	3518	1/1	0.96	0.17	-	53,53,53,53	0
54	MG	DA	3540	1/1	0.93	0.10	-	48,48,48,48	0
54	MG	DA	3449	1/1	0.91	0.09	-	57,57,57,57	0
54	MG	BA	3571	1/1	0.97	0.16	-	74,74,74,74	0
54	MG	BA	3422	1/1	0.96	0.11	-	33,33,33,33	0
54	MG	AA	1768	1/1	0.95	0.32	-	79,79,79,79	0
54	MG	BA	3640	1/1	0.82	0.17	-	55,55,55,55	0
54	MG	BA	3141	1/1	0.90	0.12	-	67,67,67,67	0
54	MG	DP	202	1/1	0.90	0.11	-	53,53,53,53	0
54	MG	DA	3205	1/1	0.79	0.12	-	44,44,44,44	0

6.5 Other polymers

There are no such residues in this entry.