



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:31 PM GMT

PDB ID : 4W2I  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with  
negamycin, mRNA and three deacylated tRNAs in the A, P and E sites  
Authors : Polikanov, Y.S.; Szal, T.; Jiang, F.; Gupta, P.; Matsuda, R.; Shiozuka, M.;  
Steitz, T.A.; Vazquez-Laslop, Nora; Mankin, A.S.  
Deposited on : 2014-09-12  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

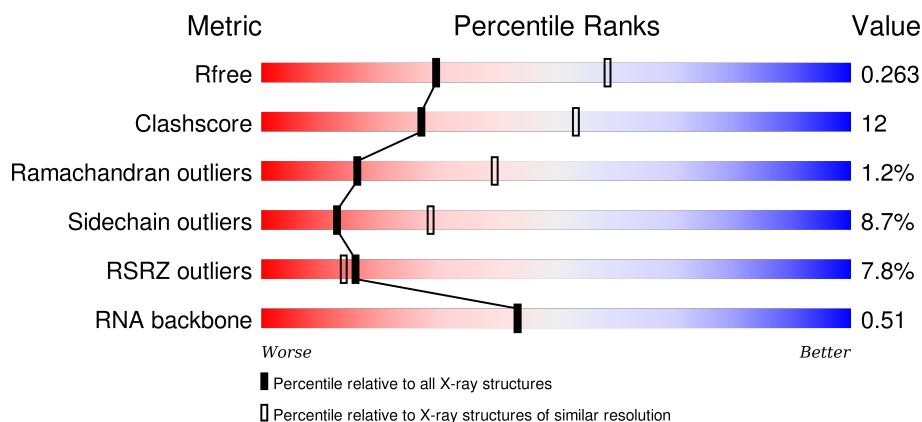
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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.








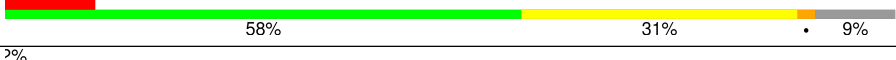

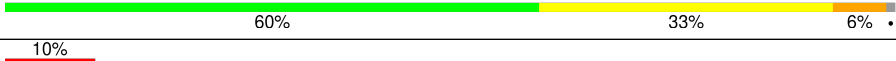

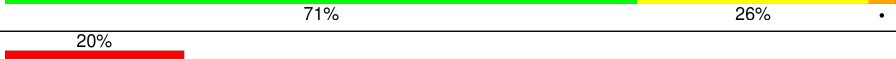
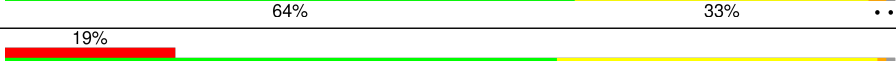
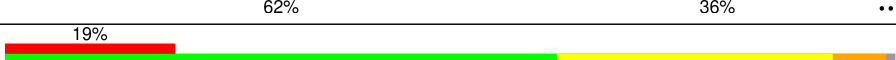


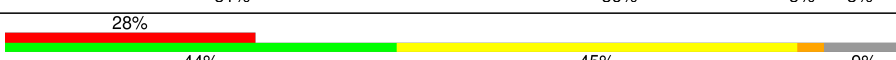
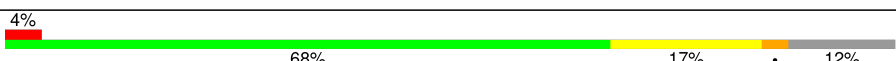
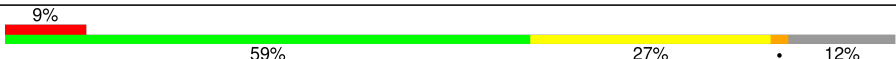
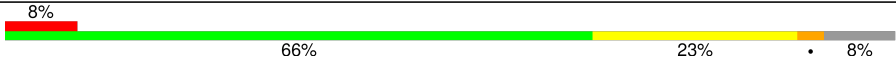



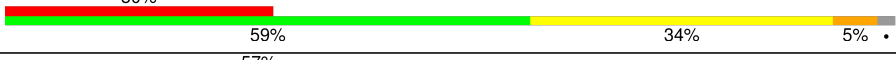

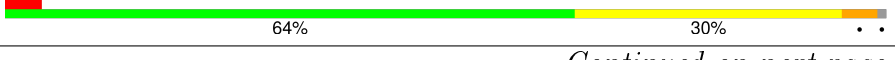

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1521	<div> <div>2%</div> <div>51% 36% 11% ..</div> </div>
1	CA	1521	<div> <div>2%</div> <div>46% 41% 11% .</div> </div>
2	AB	256	<div> <div>6%</div> <div>47% 36% 7% 10%</div> </div>
2	CB	256	<div> <div>18%</div> <div>44% 36% 10% 10%</div> </div>

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

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Mol	Chain	Length	Quality of chain
15	CO	89	
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	AV	24	
22	CV	24	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	77	
24	CX	77	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	

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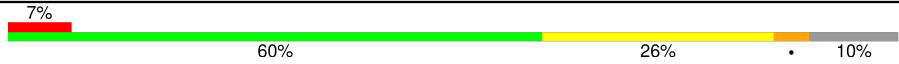

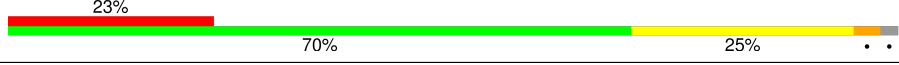

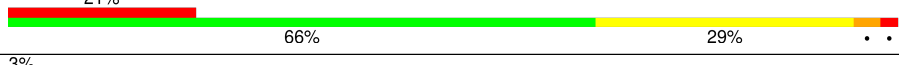
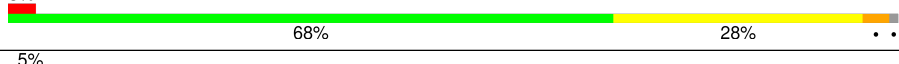
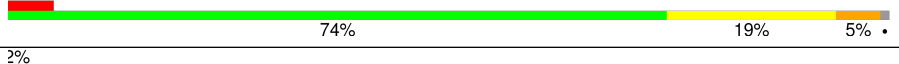

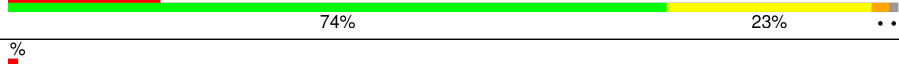


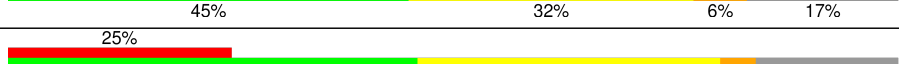
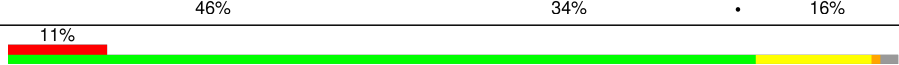
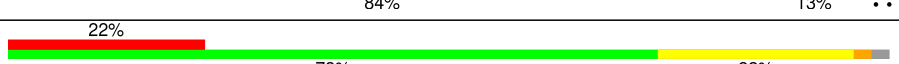

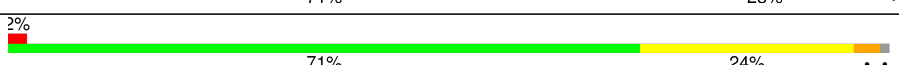
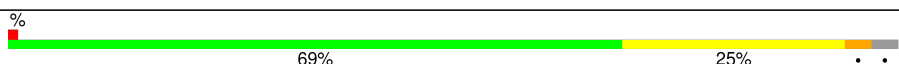
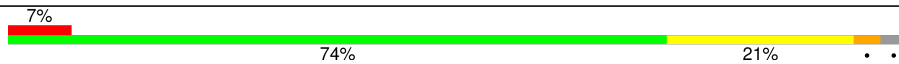
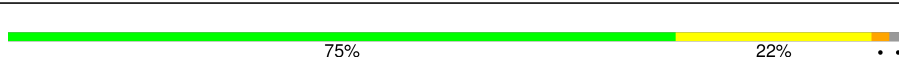


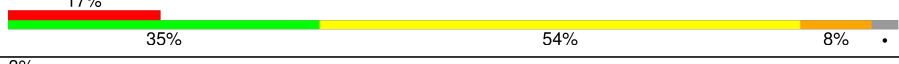
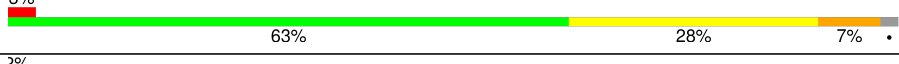




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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	





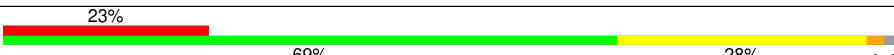
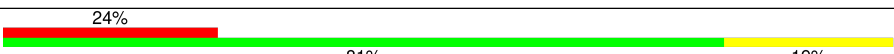
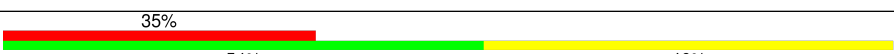
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Mol	Chain	Length	Quality of chain
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	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
56	MG	AA	3034	-	-	-	X
56	MG	AA	3052	-	-	-	X
56	MG	AA	3094	-	-	-	X
56	MG	AA	3127	-	-	-	X
56	MG	AA	3130	-	-	-	X
56	MG	AA	3172	-	-	-	X
56	MG	AE	3002	-	-	-	X
56	MG	AX	3002	-	-	-	X
56	MG	AX	3010	-	-	-	X
56	MG	B0	101	-	-	-	X
56	MG	B5	101	-	-	-	X
56	MG	B5	102	-	-	-	X
56	MG	B5	103	-	-	-	X
56	MG	B7	102	-	-	-	X
56	MG	BA	3007	-	-	-	X
56	MG	BA	3018	-	-	-	X
56	MG	BA	3022	-	-	-	X
56	MG	BA	3025	-	-	-	X
56	MG	BA	3026	-	-	-	X
56	MG	BA	3027	-	-	-	X
56	MG	BA	3028	-	-	-	X
56	MG	BA	3029	-	-	-	X
56	MG	BA	3061	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3089	-	-	-	X
56	MG	BA	3091	-	-	-	X
56	MG	BA	3094	-	-	-	X
56	MG	BA	3105	-	-	-	X
56	MG	BA	3106	-	-	-	X
56	MG	BA	3110	-	-	-	X
56	MG	BA	3116	-	-	-	X
56	MG	BA	3127	-	-	-	X
56	MG	BA	3131	-	-	-	X
56	MG	BA	3132	-	-	-	X
56	MG	BA	3136	-	-	-	X
56	MG	BA	3141	-	-	-	X
56	MG	BA	3143	-	-	-	X
56	MG	BA	3160	-	-	-	X
56	MG	BA	3164	-	-	-	X
56	MG	BA	3182	-	-	-	X
56	MG	BA	3188	-	-	-	X
56	MG	BA	3190	-	-	-	X
56	MG	BA	3194	-	-	-	X
56	MG	BA	3203	-	-	-	X
56	MG	BA	3209	-	-	-	X
56	MG	BA	3220	-	-	-	X
56	MG	BA	3237	-	-	-	X
56	MG	BA	3238	-	-	-	X
56	MG	BA	3244	-	-	-	X
56	MG	BA	3271	-	-	-	X
56	MG	BA	3327	-	-	-	X
56	MG	BA	3354	-	-	-	X
56	MG	BA	3399	-	-	-	X
56	MG	BA	3440	-	-	-	X
56	MG	BA	3460	-	-	-	X
56	MG	BA	3472	-	-	-	X
56	MG	BA	3479	-	-	-	X
56	MG	BA	3495	-	-	-	X
56	MG	BA	3541	-	-	-	X
56	MG	BA	3562	-	-	-	X
56	MG	BA	3615	-	-	-	X
56	MG	BA	3642	-	-	-	X
56	MG	BA	3649	-	-	-	X
56	MG	BA	3668	-	-	-	X
56	MG	BA	3672	-	-	-	X
56	MG	BA	3757	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3769	-	-	-	X
56	MG	BA	3773	-	-	-	X
56	MG	BA	3774	-	-	-	X
56	MG	BA	3776	-	-	-	X
56	MG	BA	3777	-	-	-	X
56	MG	BA	3782	-	-	-	X
56	MG	BA	3783	-	-	-	X
56	MG	BA	3785	-	-	-	X
56	MG	BD	304	-	-	-	X
56	MG	BD	305	-	-	-	X
56	MG	BD	307	-	-	-	X
56	MG	BD	308	-	-	-	X
56	MG	BD	309	-	-	-	X
56	MG	BD	311	-	-	-	X
56	MG	BE	304	-	-	-	X
56	MG	BF	301	-	-	-	X
56	MG	BF	302	-	-	-	X
56	MG	BF	304	-	-	-	X
56	MG	BF	305	-	-	-	X
56	MG	BF	306	-	-	-	X
56	MG	BF	308	-	-	-	X
56	MG	BF	309	-	-	-	X
56	MG	BN	3001	-	-	-	X
56	MG	BN	3004	-	-	-	X
56	MG	BN	3006	-	-	-	X
56	MG	BP	201	-	-	-	X
56	MG	BP	202	-	-	-	X
56	MG	BQ	3001	-	-	-	X
56	MG	BQ	3005	-	-	-	X
56	MG	BR	201	-	-	-	X
56	MG	BR	202	-	-	-	X
56	MG	BU	201	-	-	-	X
56	MG	BU	202	-	-	-	X
56	MG	BU	205	-	-	-	X
56	MG	BU	206	-	-	-	X
56	MG	BU	207	-	-	-	X
56	MG	BU	208	-	-	-	X
56	MG	BU	209	-	-	-	X
56	MG	BV	202	-	-	-	X
56	MG	BV	205	-	-	-	X
56	MG	BV	207	-	-	-	X
56	MG	BX	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	3032	-	-	-	X
56	MG	CA	3035	-	-	-	X
56	MG	CA	3048	-	-	-	X
56	MG	CA	3055	-	-	-	X
56	MG	CA	3092	-	-	-	X
56	MG	CA	3140	-	-	-	X
56	MG	D3	3001	-	-	-	X
56	MG	D7	101	-	-	-	X
56	MG	DA	3006	-	-	-	X
56	MG	DA	3015	-	-	-	X
56	MG	DA	3023	-	-	-	X
56	MG	DA	3024	-	-	-	X
56	MG	DA	3025	-	-	-	X
56	MG	DA	3037	-	-	-	X
56	MG	DA	3065	-	-	-	X
56	MG	DA	3071	-	-	-	X
56	MG	DA	3078	-	-	-	X
56	MG	DA	3086	-	-	-	X
56	MG	DA	3125	-	-	-	X
56	MG	DA	3156	-	-	-	X
56	MG	DA	3160	-	-	-	X
56	MG	DA	3168	-	-	-	X
56	MG	DA	3186	-	-	-	X
56	MG	DA	3233	-	-	-	X
56	MG	DA	3244	-	-	-	X
56	MG	DA	3251	-	-	-	X
56	MG	DA	3284	-	-	-	X
56	MG	DA	3316	-	-	-	X
56	MG	DA	3361	-	-	-	X
56	MG	DA	3415	-	-	-	X
56	MG	DA	3449	-	-	-	X
56	MG	DA	3471	-	-	-	X
56	MG	DA	3553	-	-	-	X
56	MG	DA	3556	-	-	-	X
56	MG	DA	3558	-	-	-	X
56	MG	DA	3617	-	-	-	X
56	MG	DA	3621	-	-	-	X
56	MG	DD	304	-	-	-	X
56	MG	DD	306	-	-	-	X
56	MG	DD	307	-	-	-	X
56	MG	DD	308	-	-	-	X
56	MG	DE	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DF	305	-	-	-	X
56	MG	DF	306	-	-	-	X
56	MG	DQ	3003	-	-	-	X
56	MG	DR	3001	-	-	-	X
56	MG	DU	3001	-	-	-	X
56	MG	DV	3001	-	-	-	X
56	MG	DV	3002	-	-	-	X
56	MG	DW	3002	-	-	-	X
57	NEG	AA	3216	-	-	X	X
57	NEG	AA	3219	-	-	-	X
57	NEG	AA	3221	-	-	-	X
57	NEG	AA	3222	-	-	-	X
57	NEG	AW	3004	-	-	-	X
57	NEG	CA	3170	-	-	-	X
57	NEG	CA	3173	-	-	-	X
57	NEG	CA	3174	-	-	-	X
57	NEG	CA	3175	-	-	-	X
57	NEG	CA	3177	-	-	-	X
57	NEG	CX	3004	-	-	-	X
59	ZN	B5	105	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297376 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	1496	Total	C	N	O	P	0	0	0
			32163	14314	5963	10390	1496			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
2	CB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	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
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	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
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- 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
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	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
			806	511	143	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	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
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			983	623	193	167				
9	CI	127	Total	C	N	O		0	0	0
			978	619	190	169				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	97	Total	C	N	O		0	0	0
			709	440	138	131				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			714	445	138	131	0	0	0

- 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		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

- 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		
			930	585	185	159	1	0	0
12	CL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	123	Total	C	N	O	S		
			958	592	198	166	2	0	0
13	CM	122	Total	C	N	O	S		
			950	586	197	165	2	0	0

- 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		
			492	312	104	72	4	0	0
14	CN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0

- 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		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

- 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
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	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
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	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
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

- Molecule 23 is a RNA chain called A/P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1588	713	285	515	73	2			
23	AY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1541	688	278	502	72	1			
23	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 24 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2822	Total	C	N	O	P	0	0	0
			60792	27054	11380	19537	2821			
25	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

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

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

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

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

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
29	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	DH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
33	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
35	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

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

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	110	Total	C	N	O		0	0	0
			877	553	175	149				
38	DS	110	Total	C	N	O		0	0	0
			870	549	173	148				

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
39	DT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

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

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
42	DW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
43	DX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
44	DY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
45	DZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
46	D0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	D1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

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

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	D3	59	Total	C	N	O	0	0	0
			464	296	90	78			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
51	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
52	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

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

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B4	1	Total	Mg	0	0
			1	1		
56	BA	785	Total	Mg	0	0
			785	785		
56	CA	172	Total	Mg	0	0
			172	172		
56	DQ	4	Total	Mg	0	0
			4	4		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	6	Total	Mg	0	0
			6	6		
56	CV	1	Total	Mg	0	0
			1	1		
56	B8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BE	8	Total 8	Mg 8	0	0
56	AW	4	Total 4	Mg 4	0	0
56	DU	3	Total 3	Mg 3	0	0
56	B1	1	Total 1	Mg 1	0	0
56	AN	3	Total 3	Mg 3	0	0
56	BP	4	Total 4	Mg 4	0	0
56	AX	11	Total 11	Mg 11	0	0
56	CN	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CY	1	Total 1	Mg 1	0	0
56	DD	9	Total 9	Mg 9	0	0
56	B5	5	Total 5	Mg 5	0	0
56	BB	18	Total 18	Mg 18	0	0
56	BT	1	Total 1	Mg 1	0	0
56	D8	1	Total 1	Mg 1	0	0
56	AE	2	Total 2	Mg 2	0	0
56	DG	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	11	Total 11	Mg 11	0	0
56	AV	3	Total 3	Mg 3	0	0
56	BX	2	Total 2	Mg 2	0	0

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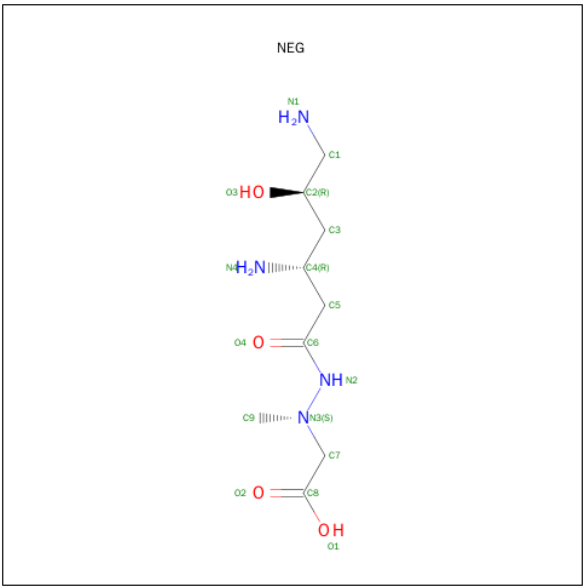
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56	B2	1	Total 1	Mg 1	0	0
56	AA	218	Total 218	Mg 218	0	0
56	BQ	5	Total 5	Mg 5	0	0
56	D7	1	Total 1	Mg 1	0	0
56	CX	2	Total 2	Mg 2	0	0
56	DV	3	Total 3	Mg 3	0	0
56	B6	1	Total 1	Mg 1	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	9	Total 9	Mg 9	0	0
56	DR	2	Total 2	Mg 2	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	6	Total 6	Mg 6	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	BG	2	Total 2	Mg 2	0	0
56	BY	1	Total 1	Mg 1	0	0
56	DE	4	Total 4	Mg 4	0	0
56	B3	2	Total 2	Mg 2	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	BR	3	Total 3	Mg 3	0	0
56	DA	623	Total 623	Mg 623	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CE	1	Total 1	Mg 1	0	0
56	DW	4	Total 4	Mg 4	0	0
56	D5	1	Total 1	Mg 1	0	0
56	B7	4	Total 4	Mg 4	0	0
56	CF	1	Total 1	Mg 1	0	0
56	BV	7	Total 7	Mg 7	0	0
56	DP	1	Total 1	Mg 1	0	0
56	DO	2	Total 2	Mg 2	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	DY	1	Total 1	Mg 1	0	0
56	CW	2	Total 2	Mg 2	0	0
56	CD	1	Total 1	Mg 1	0	0
56	BD	11	Total 11	Mg 11	0	0
56	B0	3	Total 3	Mg 3	0	0
56	AO	1	Total 1	Mg 1	0	0
56	BW	4	Total 4	Mg 4	0	0
56	AY	3	Total 3	Mg 3	0	0
56	CK	1	Total 1	Mg 1	0	0
56	AF	1	Total 1	Mg 1	0	0
56	DB	12	Total 12	Mg 12	0	0

- Molecule 57 is NEGAMYCIN (three-letter code: NEG) (formula: C<sub>9</sub>H<sub>20</sub>N<sub>4</sub>O<sub>4</sub>).



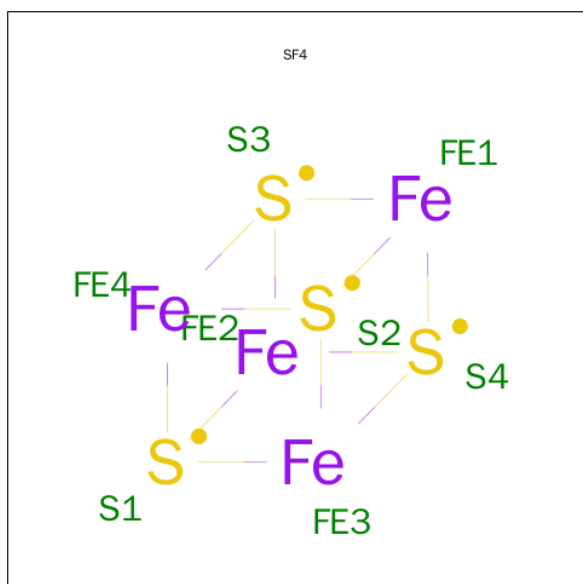
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57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AW	1	Total	C	N	O	0	0
			17	9	4	4		
57	AX	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CW	1	Total	C	N	O	0	0
			17	9	4	4		
57	CX	1	Total	C	N	O	0	0
			17	9	4	4		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AD	1	Total	Fe	S	0	0
			8	4	4		
58	CD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B5	1	Total	Zn	0	0
			1	1		

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

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	1	Total 1	K 1	0	0
60	CX	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	247	Total 247	O 247	0	0
61	AD	1	Total 1	O 1	0	0
61	AE	2	Total 2	O 2	0	0
61	AL	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AM	2	Total 2	O 2	0	0
61	AO	1	Total 1	O 1	0	0
61	AV	3	Total 3	O 3	0	0
61	AW	13	Total 13	O 13	0	0
61	AX	11	Total 11	O 11	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1396	Total 1396	O 1396	0	0
61	BB	34	Total 34	O 34	0	0
61	BD	12	Total 12	O 12	0	0
61	BE	11	Total 11	O 11	0	0
61	BF	5	Total 5	O 5	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BN	1	Total 1	O 1	0	0
61	BO	2	Total 2	O 2	0	0
61	BP	23	Total 23	O 23	0	0
61	BQ	3	Total 3	O 3	0	0
61	BR	1	Total 1	O 1	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	3	Total 3	O 3	0	0
61	BV	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BW	1	Total 1	O 1	0	0
61	BX	2	Total 2	O 2	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	8	Total 8	O 8	0	0
61	B3	1	Total 1	O 1	0	0
61	B5	6	Total 6	O 6	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	2	Total 2	O 2	0	0
61	B8	7	Total 7	O 7	0	0
61	CA	184	Total 184	O 184	0	0
61	CJ	2	Total 2	O 2	0	0
61	CP	1	Total 1	O 1	0	0
61	CV	2	Total 2	O 2	0	0
61	CW	3	Total 3	O 3	0	0
61	CX	6	Total 6	O 6	0	0
61	DA	960	Total 960	O 960	0	0
61	DB	8	Total 8	O 8	0	0
61	DD	16	Total 16	O 16	0	0
61	DE	9	Total 9	O 9	0	0
61	DF	5	Total 5	O 5	0	0
61	DN	3	Total 3	O 3	0	0

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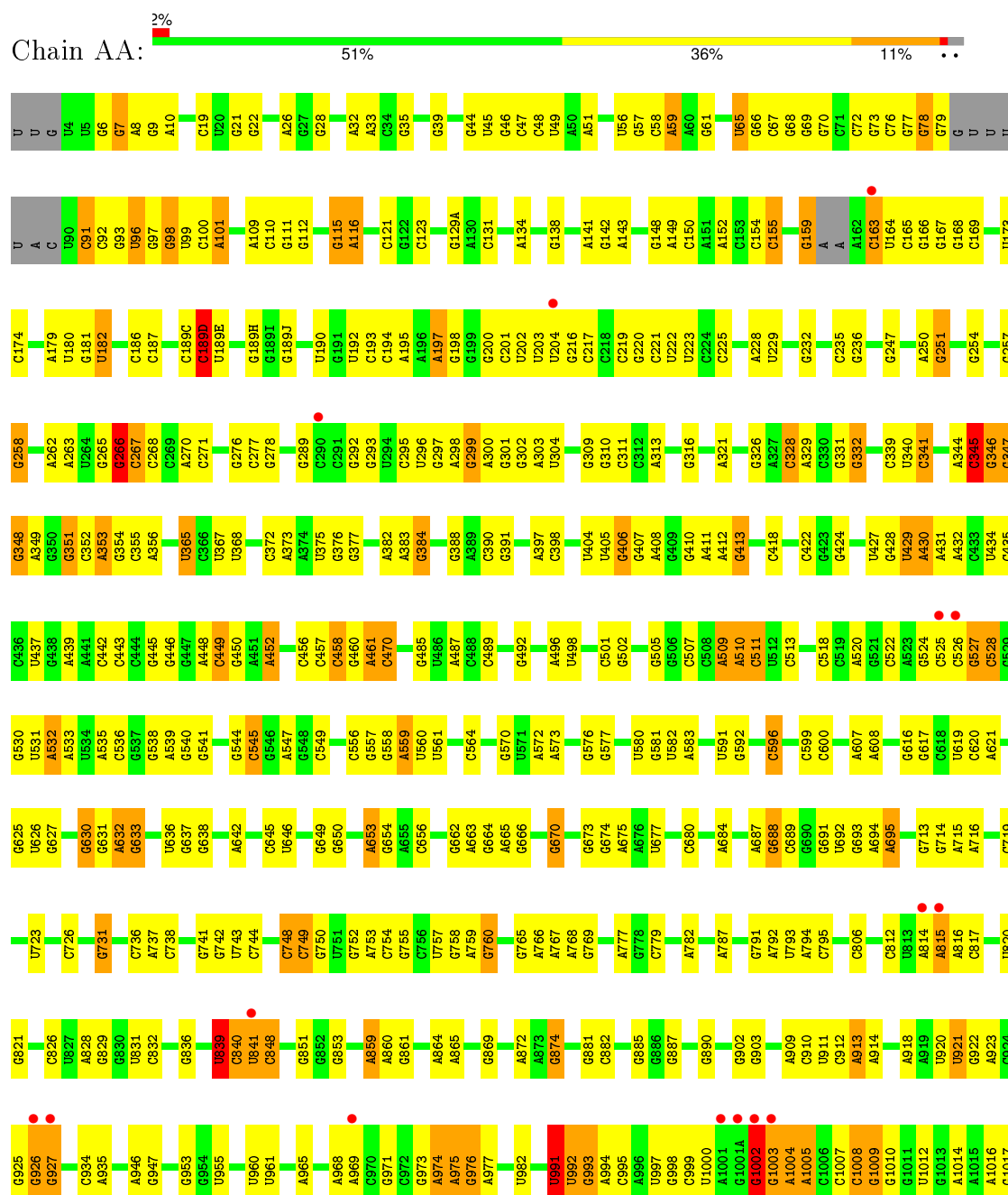
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DO	2	Total	O	0	0
			2	2		
61	DP	15	Total	O	0	0
			15	15		
61	DQ	1	Total	O	0	0
			1	1		
61	DR	1	Total	O	0	0
			1	1		
61	DU	1	Total	O	0	0
			1	1		
61	DW	1	Total	O	0	0
			1	1		
61	DX	1	Total	O	0	0
			1	1		
61	DY	2	Total	O	0	0
			2	2		
61	D0	8	Total	O	0	0
			8	8		
61	D1	4	Total	O	0	0
			4	4		
61	D7	2	Total	O	0	0
			2	2		
61	D8	1	Total	O	0	0
			1	1		

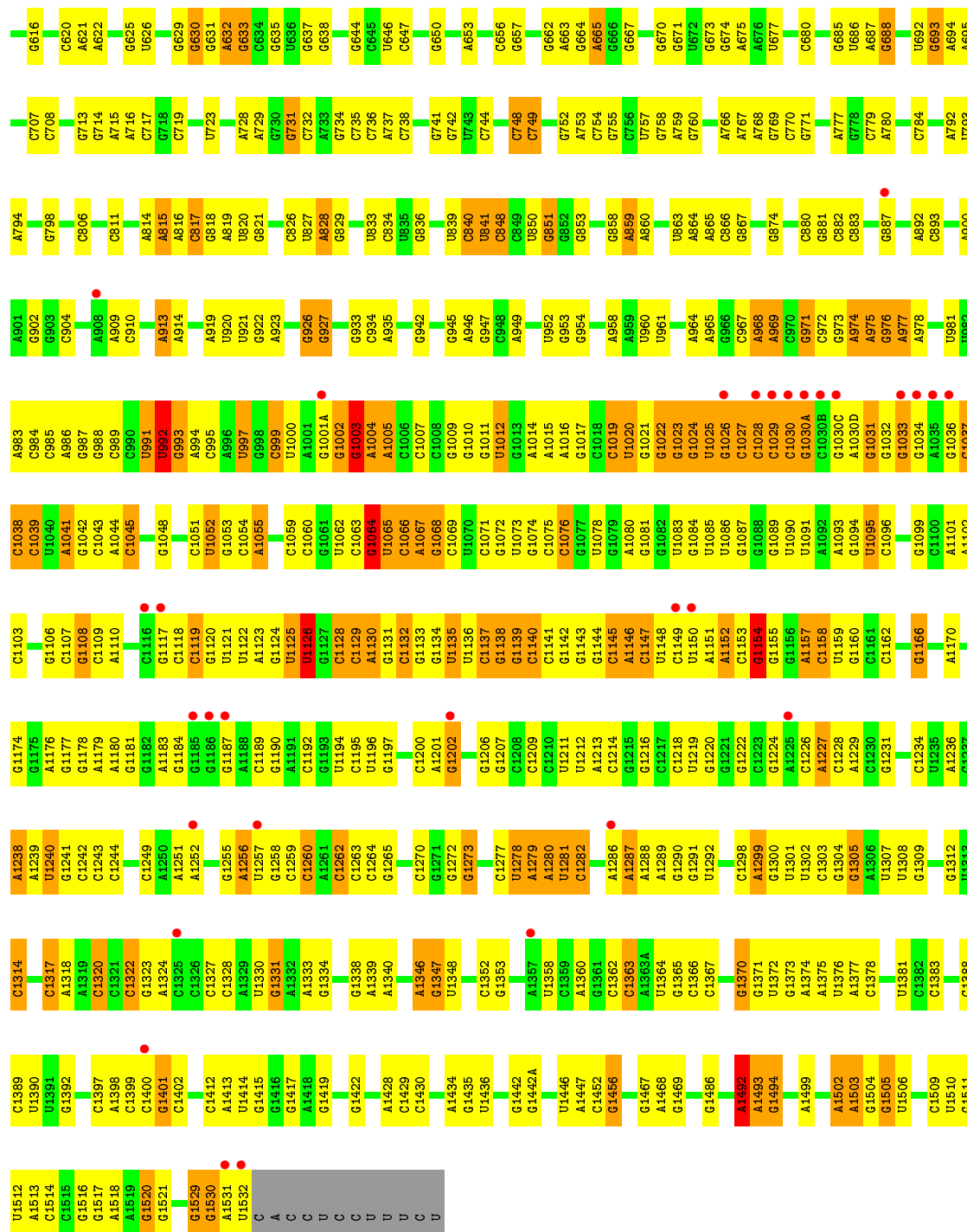
### 3 Residue-property plots

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

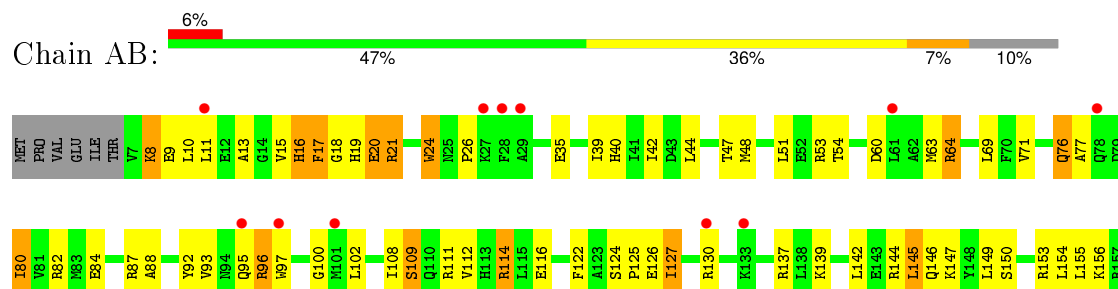
#### • Molecule 1: 16S Ribosomal RNA

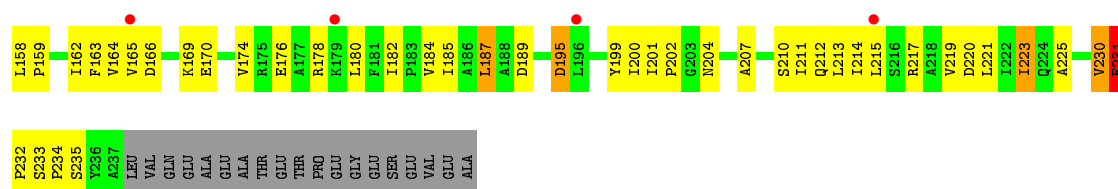




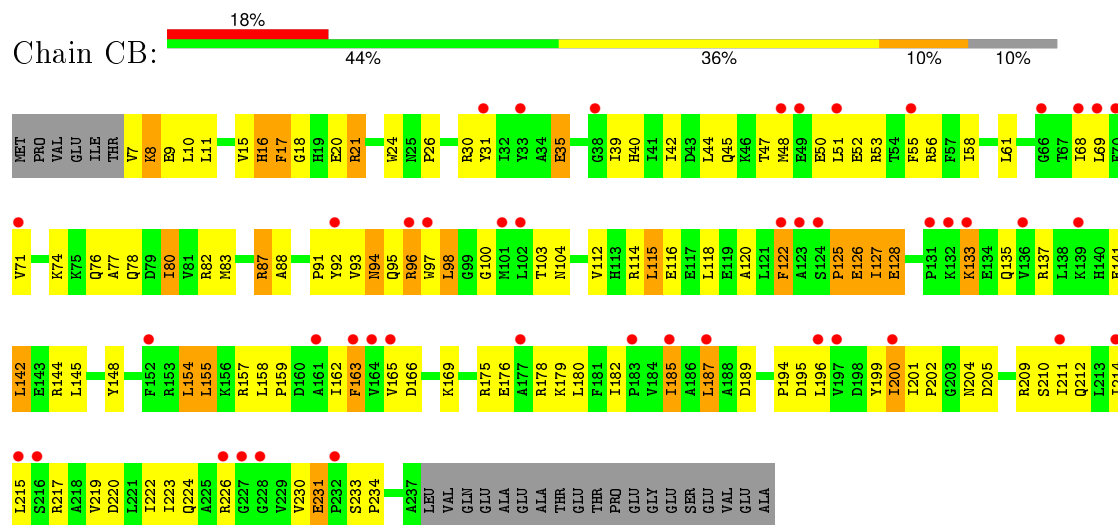


### • Molecule 2: 30S Ribosomal Protein S2

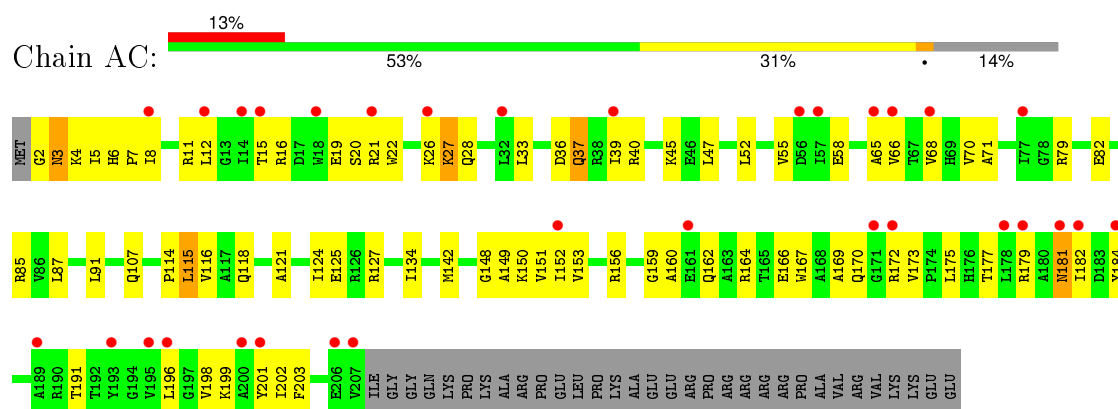




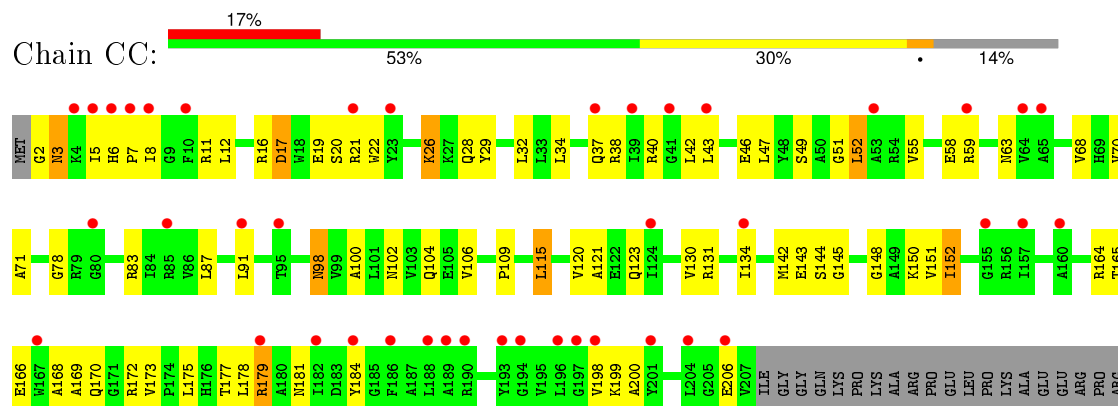
• Molecule 2: 30S Ribosomal Protein S2



• Molecule 3: 30S Ribosomal Protein S3

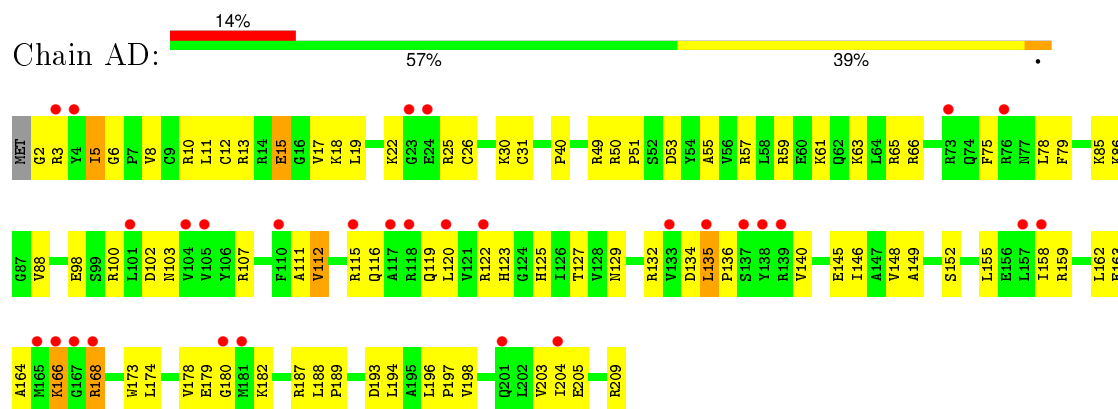


• Molecule 3: 30S Ribosomal Protein S3

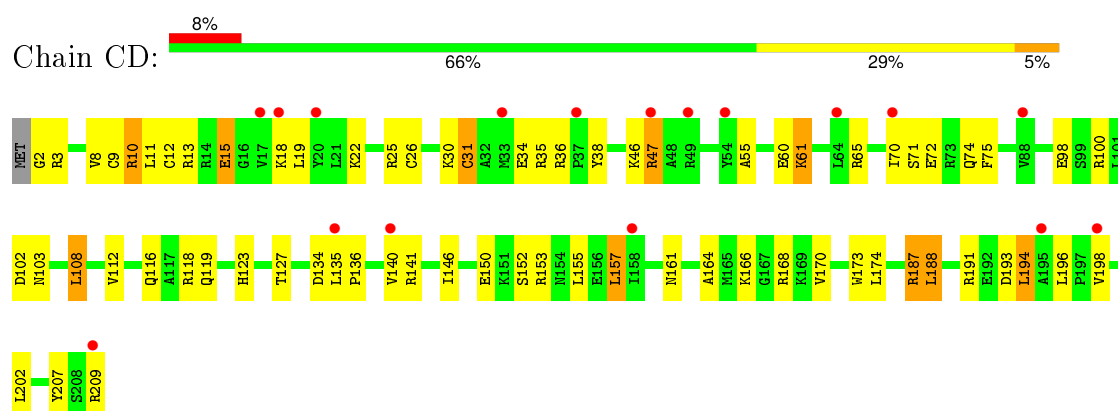


ARG  
ARG  
ARG  
PRO  
ALA  
VAL  
ARG  
VAL  
LYS  
LYS  
GLU  
GLU

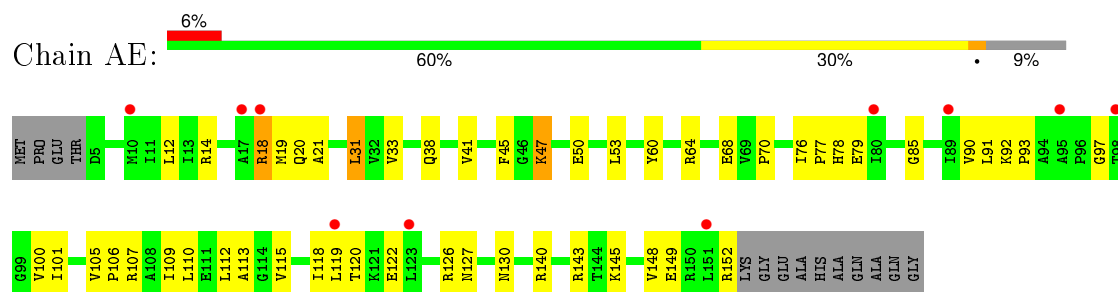
• Molecule 4: 30S Ribosomal Protein S4



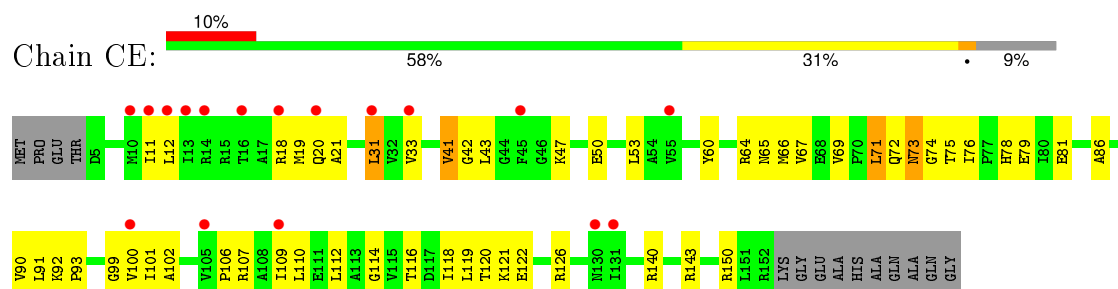
• Molecule 4: 30S Ribosomal Protein S4



• Molecule 5: 30S Ribosomal Protein S5

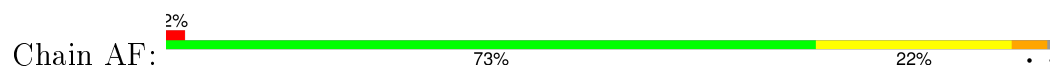


• Molecule 5: 30S Ribosomal Protein S5

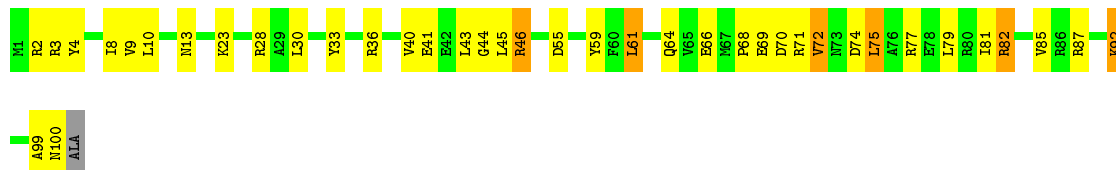




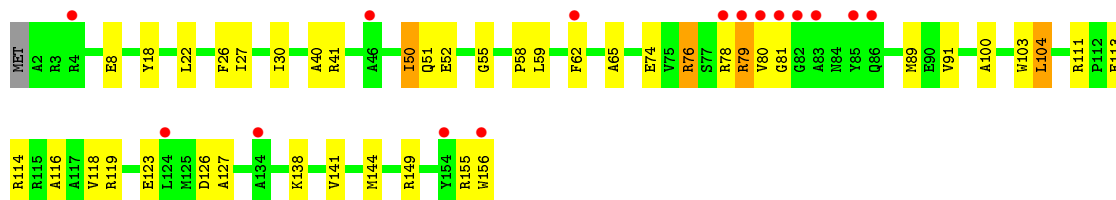
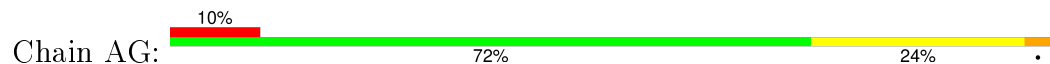
- Molecule 6: 30S Ribosomal Protein S6



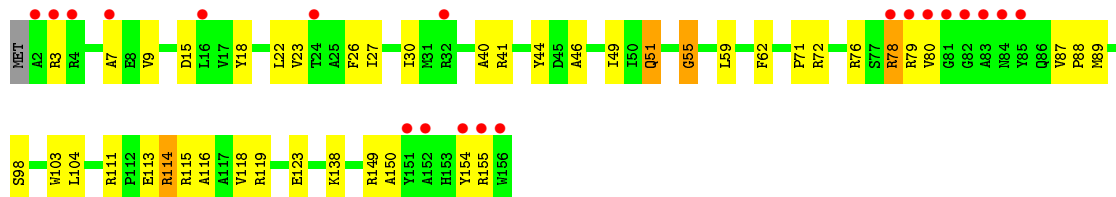
- Molecule 6: 30S Ribosomal Protein S6



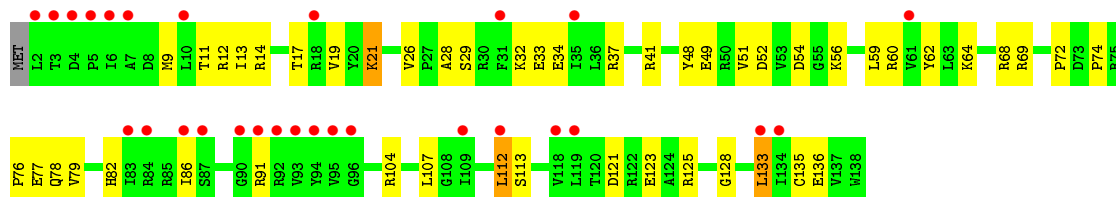
- Molecule 7: 30S Ribosomal Protein S7



- Molecule 7: 30S Ribosomal Protein S7

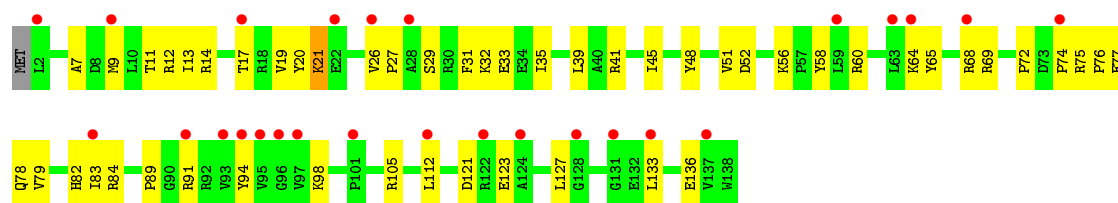


- Molecule 8: 30S Ribosomal Protein S8

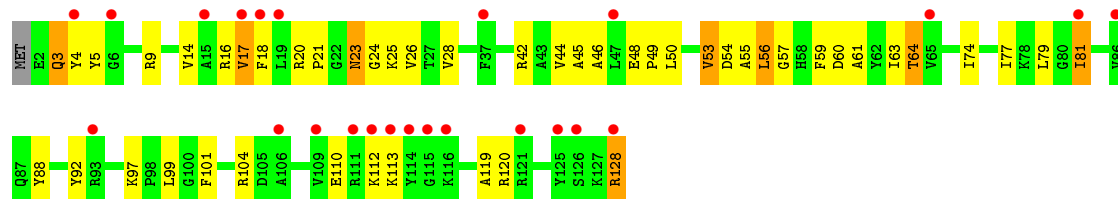


- Molecule 8: 30S Ribosomal Protein S8

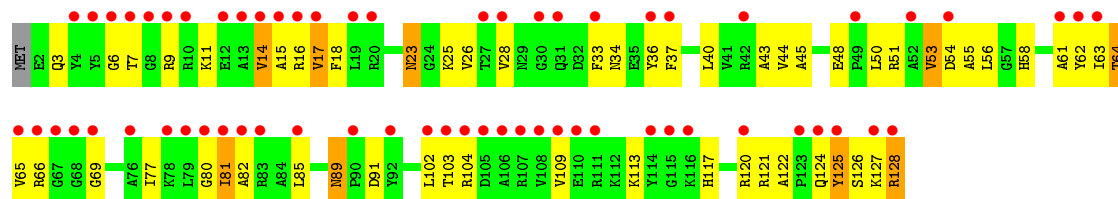




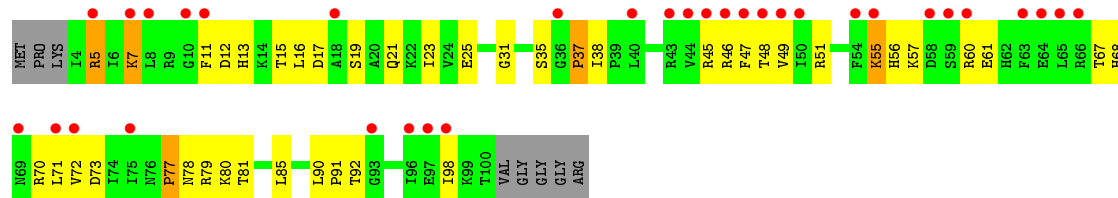
• Molecule 9: 30S Ribosomal Protein S9



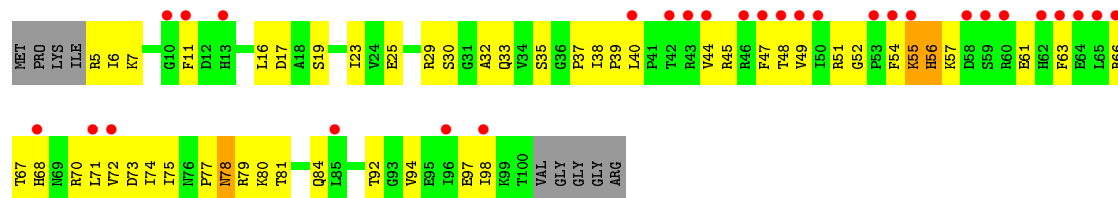
• Molecule 9: 30S Ribosomal Protein S9



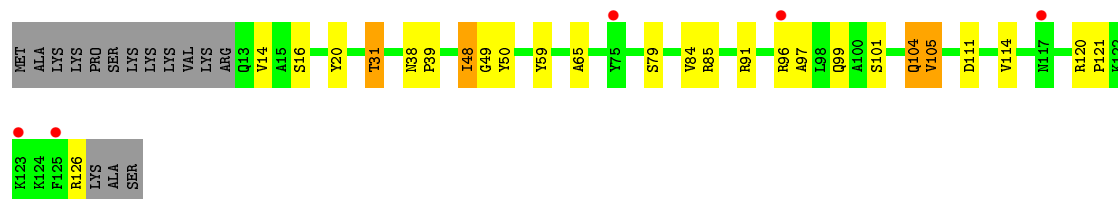
• Molecule 10: 30S Ribosomal Protein S10



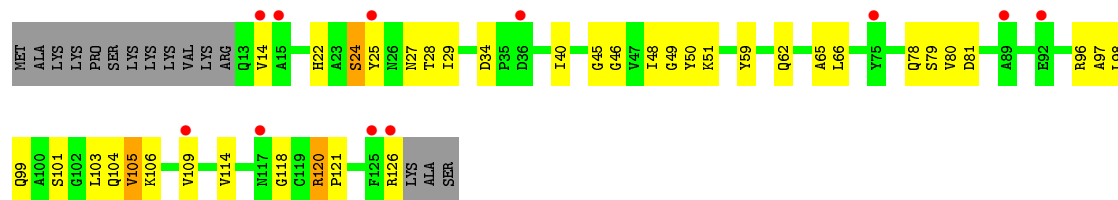
• Molecule 10: 30S Ribosomal Protein S10



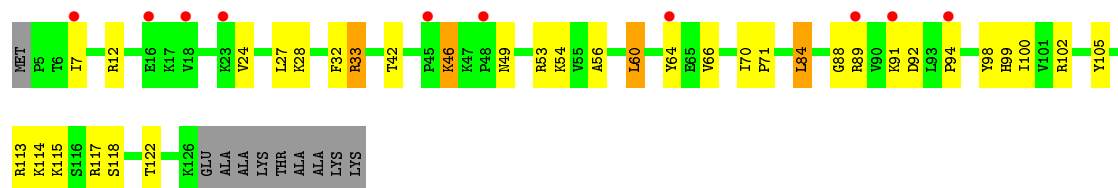
• Molecule 11: 30S Ribosomal Protein S11



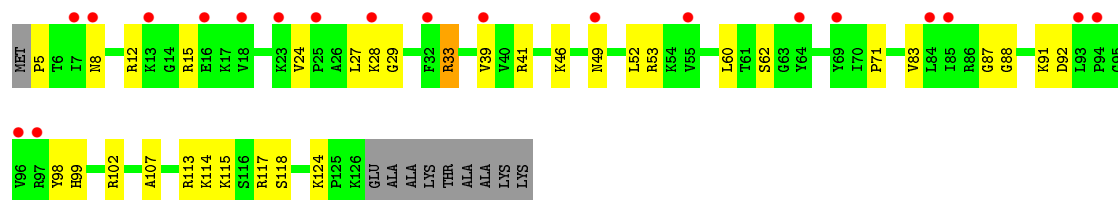
- Molecule 11: 30S Ribosomal Protein S11



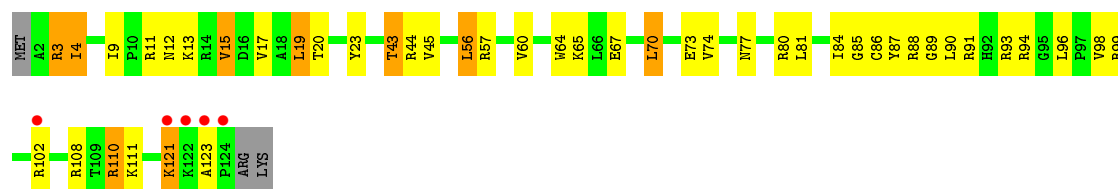
- Molecule 12: 30S Ribosomal Protein S12



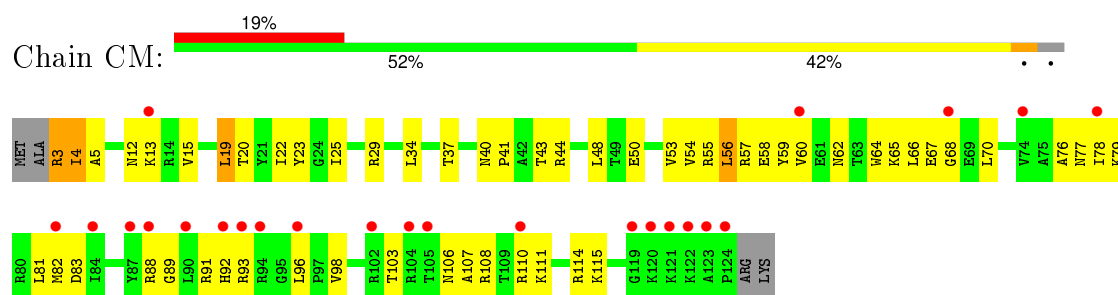
- Molecule 12: 30S Ribosomal Protein S12



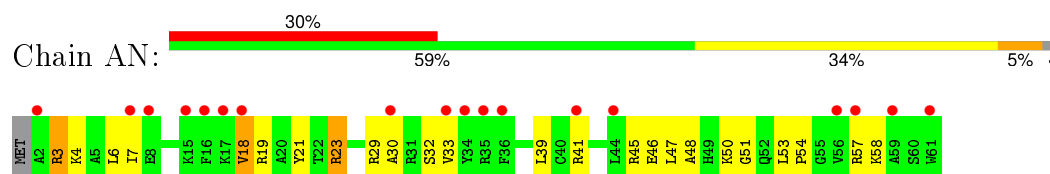
- Molecule 13: 30S Ribosomal Protein S13



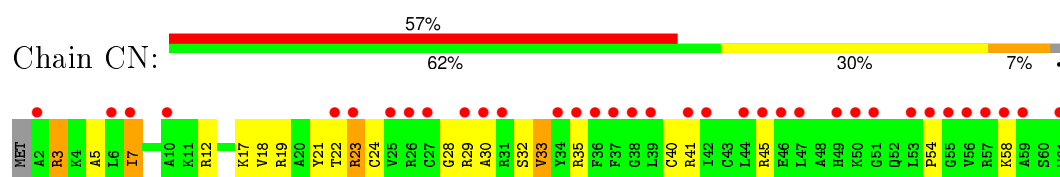
- Molecule 13: 30S Ribosomal Protein S13



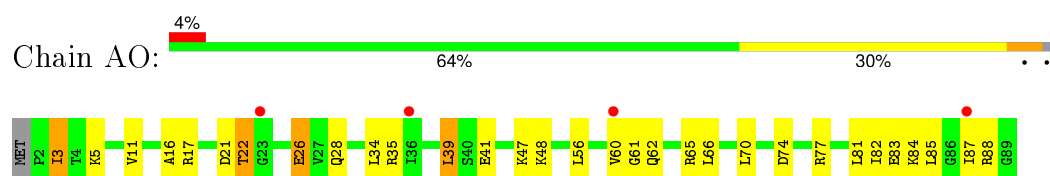
• Molecule 14: 30S Ribosomal Protein S14



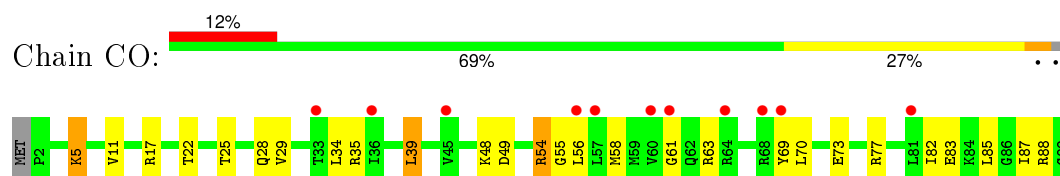
• Molecule 14: 30S Ribosomal Protein S14



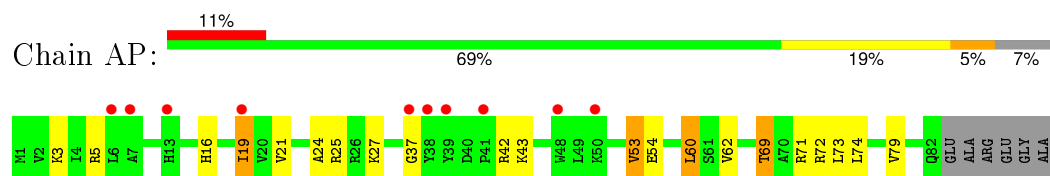
• Molecule 15: 30S Ribosomal Protein S15



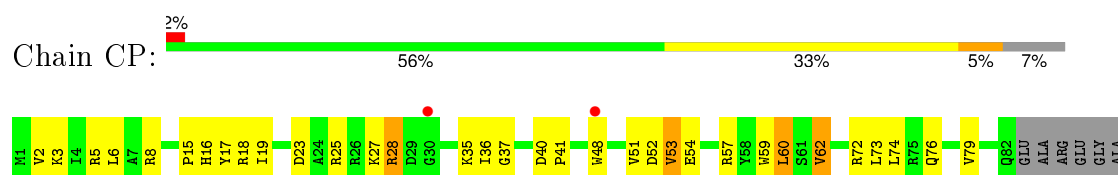
• Molecule 15: 30S Ribosomal Protein S15



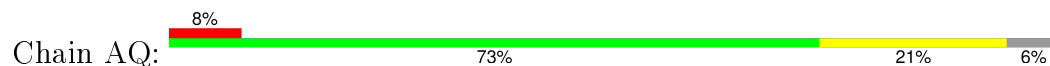
• Molecule 16: 30S Ribosomal Protein S16



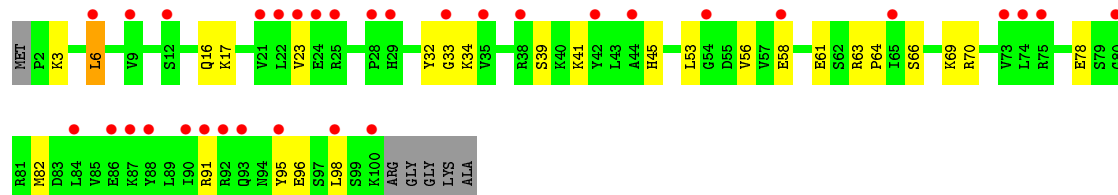
• Molecule 16: 30S Ribosomal Protein S16



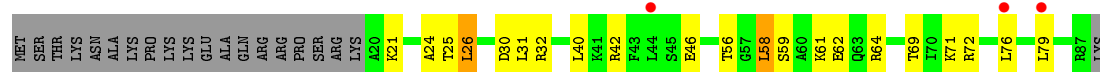
- Molecule 17: 30S Ribosomal Protein S17



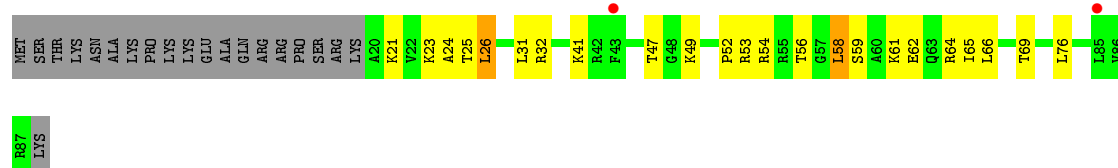
- Molecule 17: 30S Ribosomal Protein S17



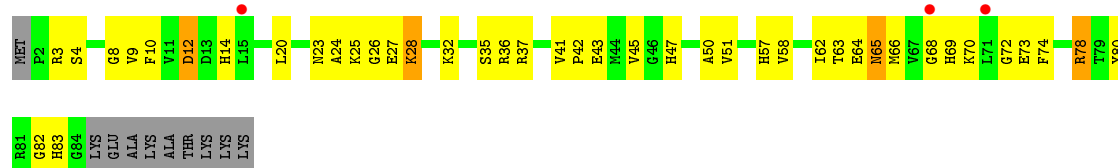
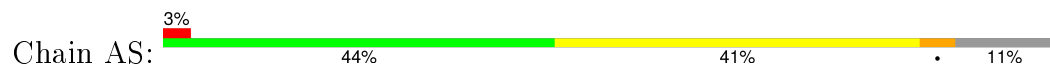
- Molecule 18: 30S Ribosomal Protein S18



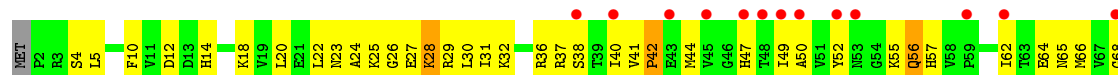
- Molecule 18: 30S Ribosomal Protein S18

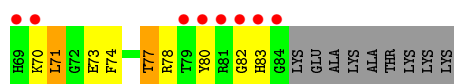


- Molecule 19: 30S Ribosomal Protein S19

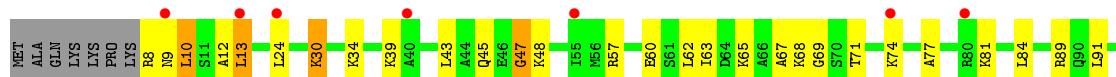


- Molecule 19: 30S Ribosomal Protein S19

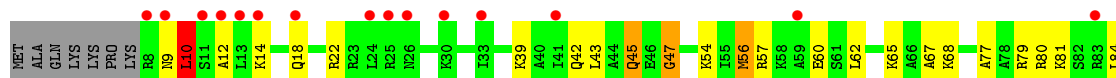




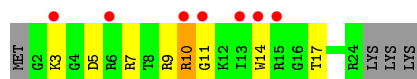
- Molecule 20: 30S Ribosomal Protein S20



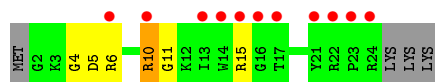
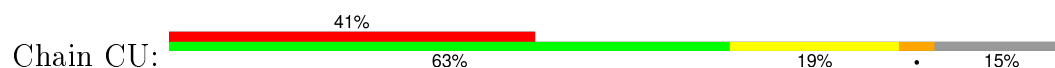
- Molecule 20: 30S Ribosomal Protein S20



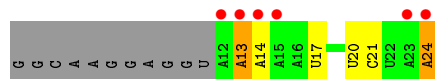
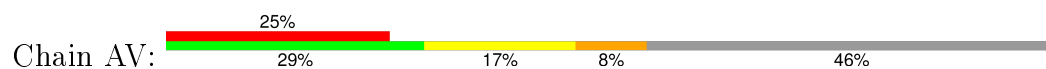
- Molecule 21: 30S Ribosomal Protein THX



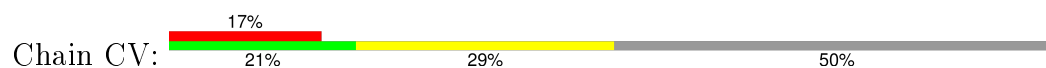
- Molecule 21: 30S Ribosomal Protein THX



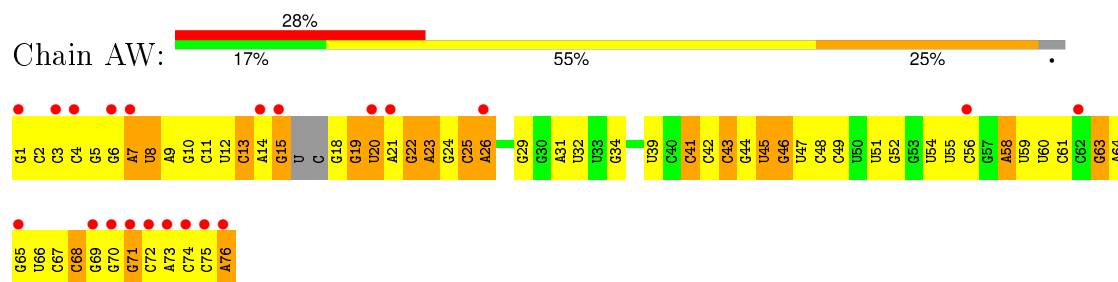
- Molecule 22: mRNA



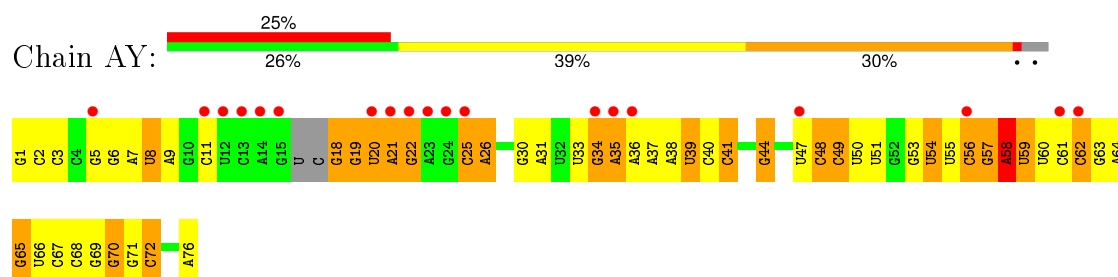
- Molecule 22: mRNA



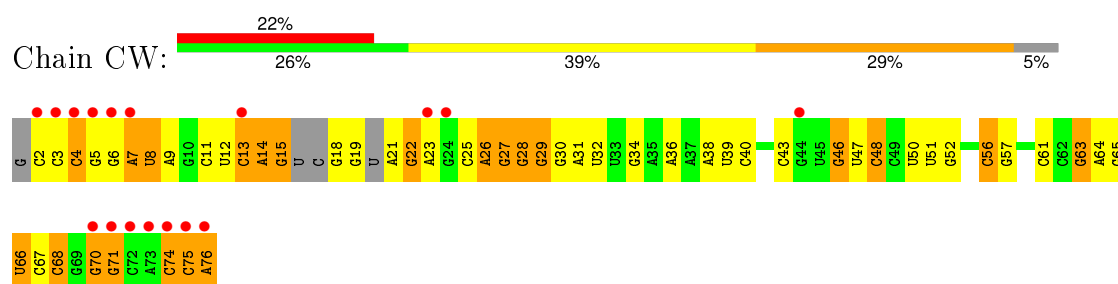
- Molecule 23: A/P-site tRNA



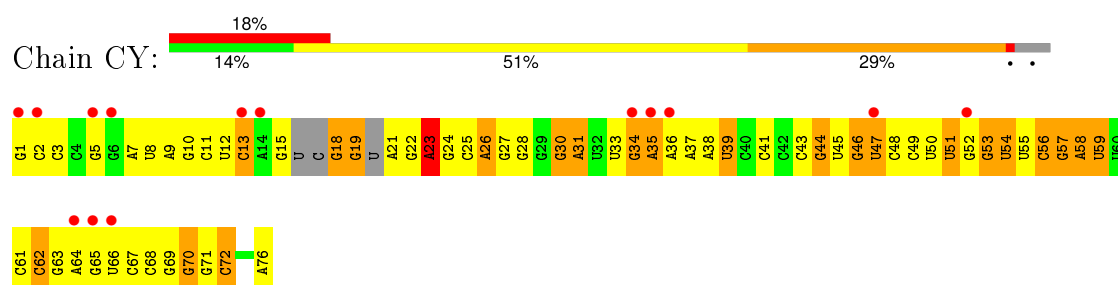
- Molecule 23: A/P-site tRNA



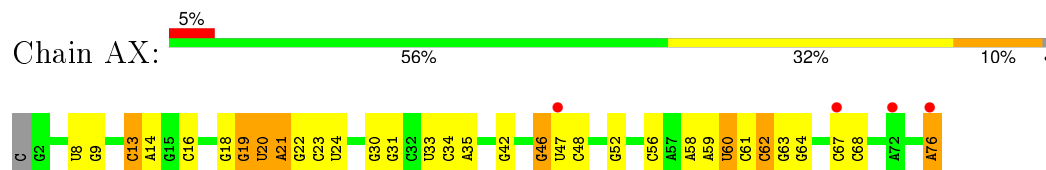
- Molecule 23: A/P-site tRNA



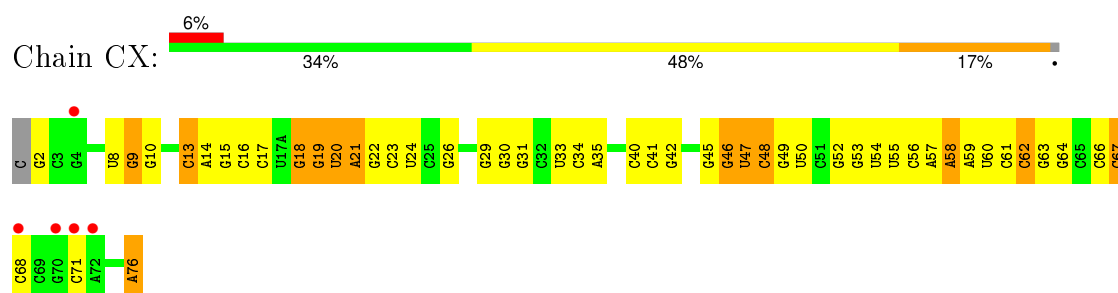
- Molecule 23: A/P-site tRNA



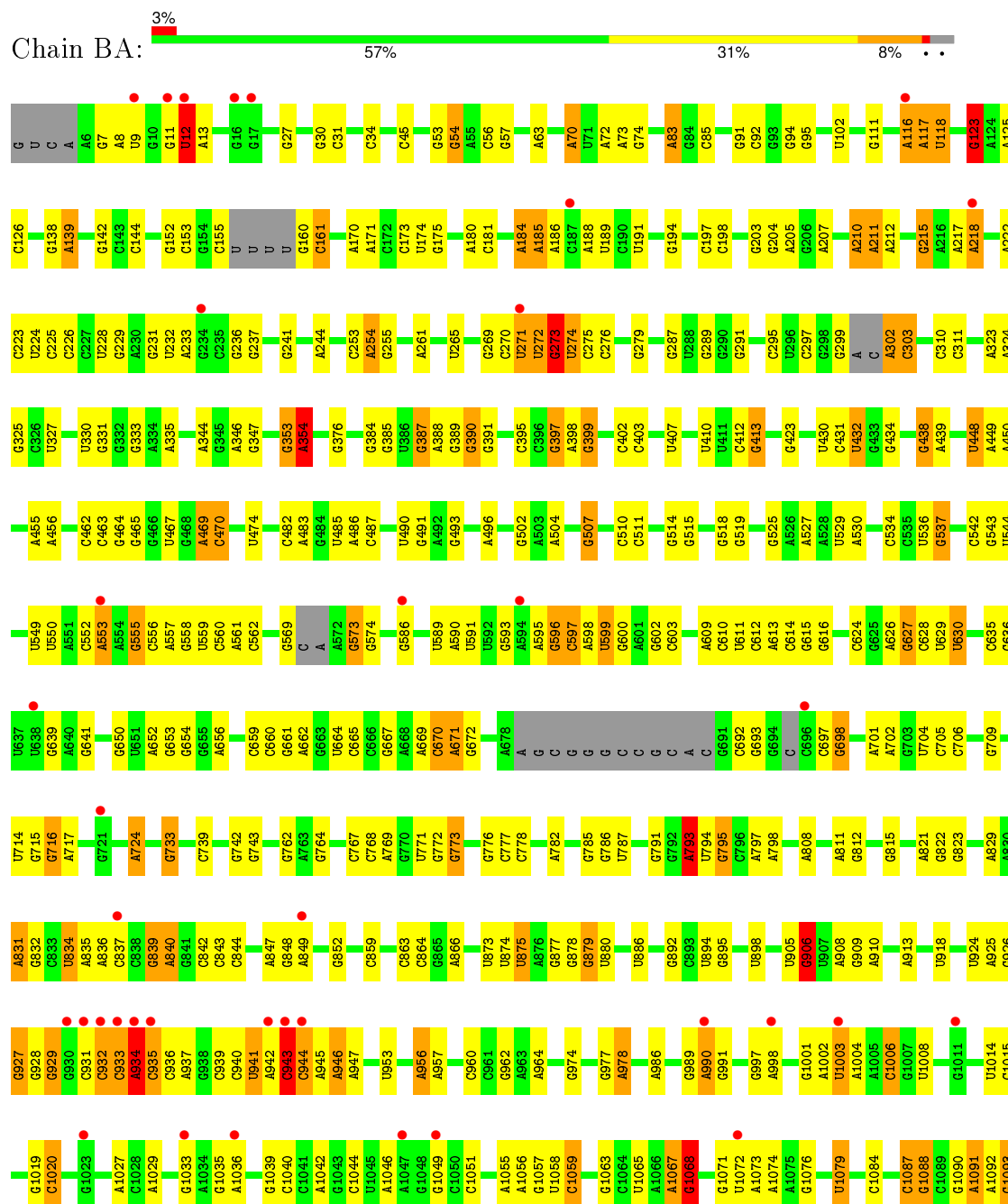
- Molecule 24: E-site tRNA



- Molecule 24: E-site tRNA

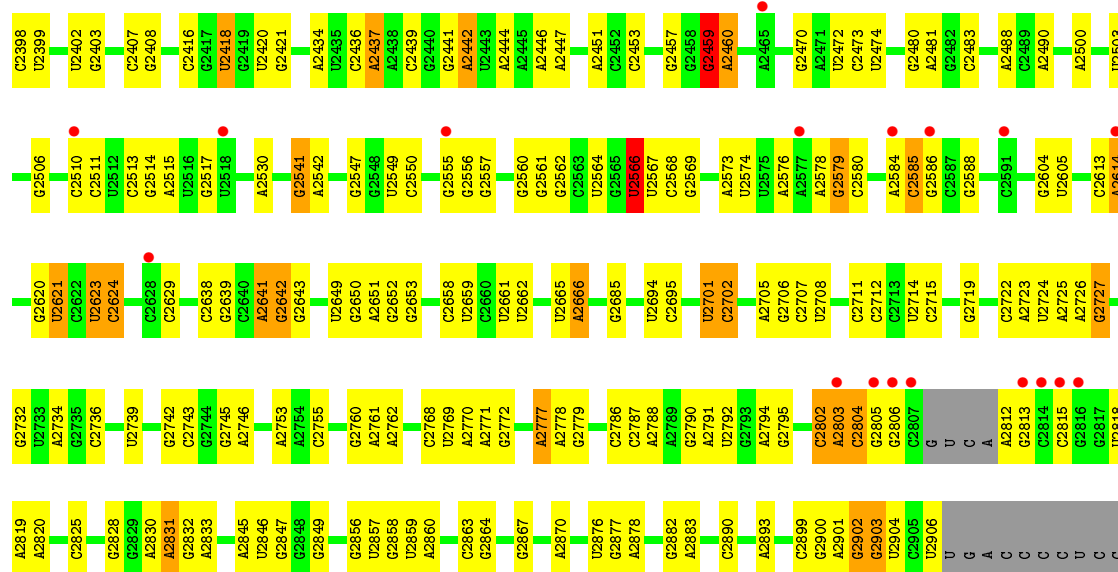


• Molecule 25: 23S Ribosomal RNA

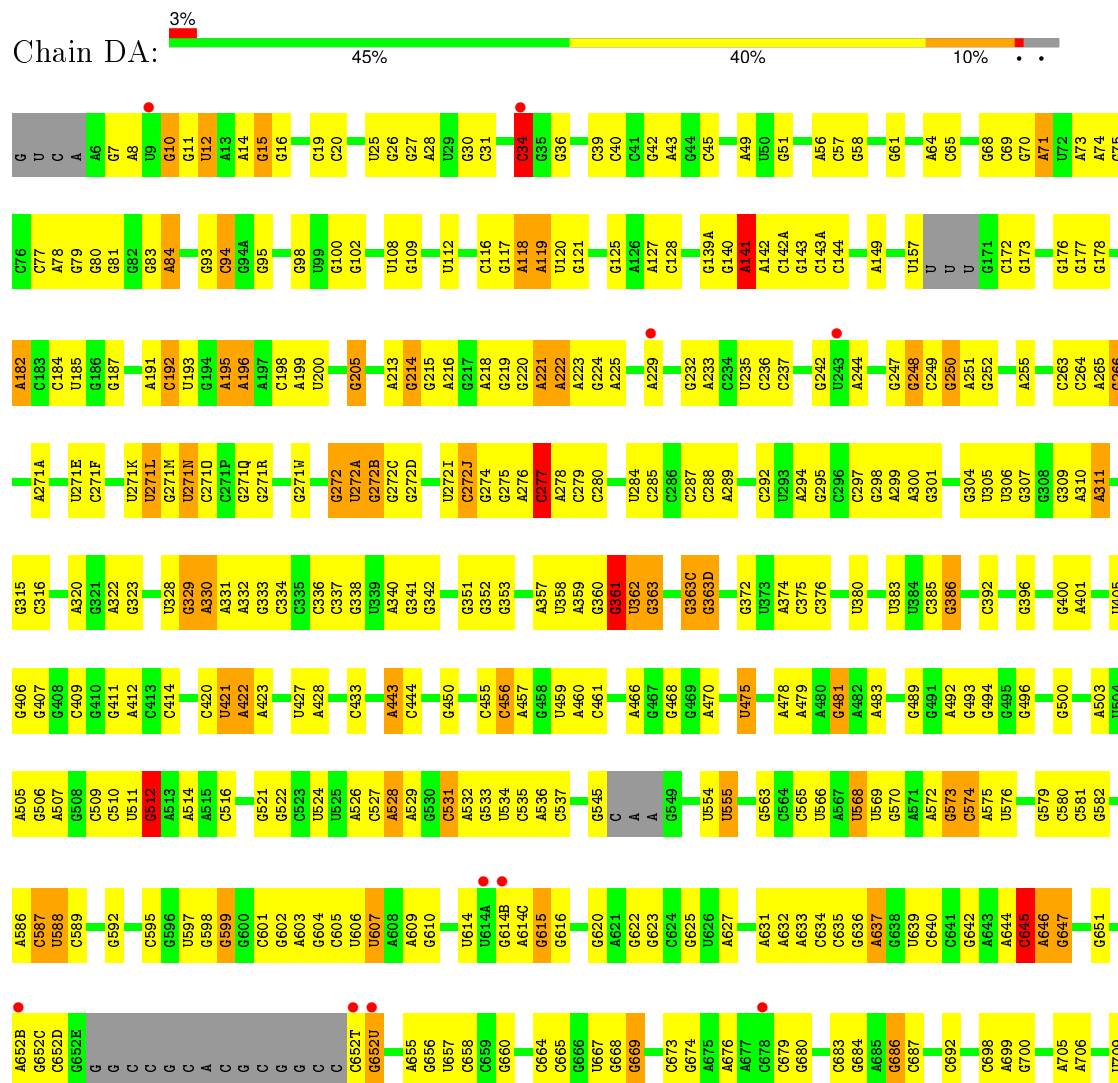




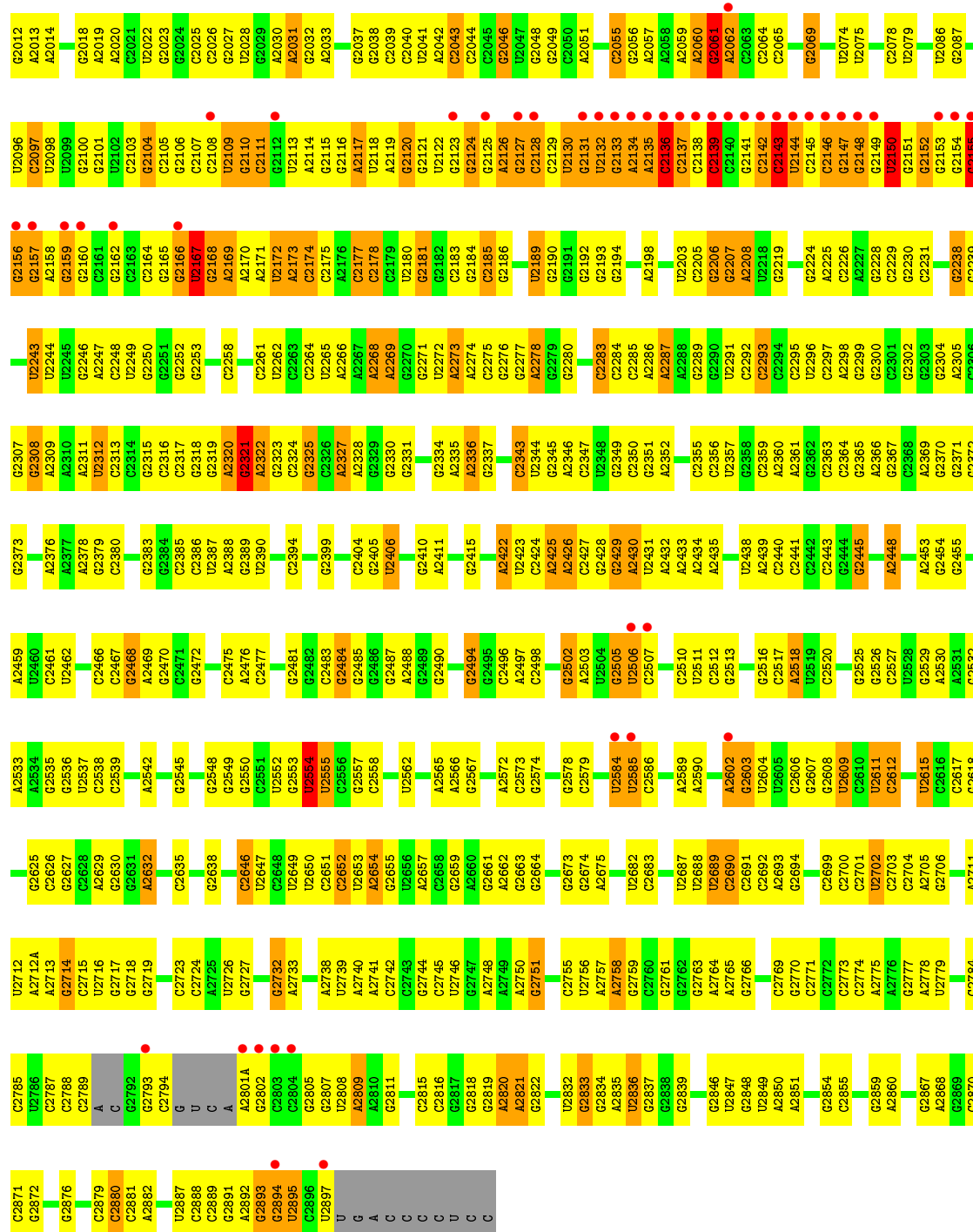




• Molecule 25: 23S Ribosomal RNA

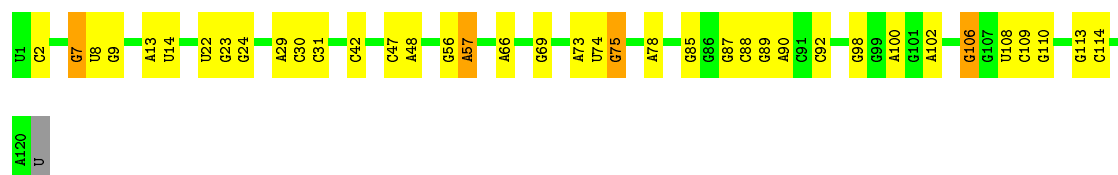


C1914	G1593	G1702	G1815	C1914	G1416	G1325	C1224	U1142	U1014	G946	C881	C806	G710
U1915	G1594	G1703	G1816	C1504	C1417	G1326	G1225	A1142A	G1015	G947	G882	U807	G711
U1917	G1595	U1709	G1817	A1508	A1418	U1327	A1226	A1143	U1019	G948	C883	G808	G717
G1922	G1596	C1710	G1822	C1509	A1419	U1328	G1235	C1147	A1020	C949	C884	G809	G717
U1923	A1597	C1711	G1823	C1509A	U1420	U1329	G1236	A1148	A1021	G950	C885	U810	C720
C1924	C1598	C1712	G1824	A1509B	G1421	C1330	G1237	G1149	G1022	C951	C886	U811	G726
A1927	A1608	G1713	A1825	G1510	G1422	A1331	G1238	C1150	U1023	G952	A887	C812	G726
A1928	A1609	U1710	A1826	C1511	A1427	G1337	G1239	G1151	G1025	G953	C888	U813	G726
G1929	A1610	G1721	G1827	U1512	C1428	U1338	U1239	C1152	A1026	C955	A890	C817	G729
G1930	A1614	A1722	G1828	U1514	G1429	G1338	U1240	C1153	U1027	C956	G892	G730	G730
U1931	A1618	G1740	A1830	U1514	C1430	U1341	A1241	A1155	A1028	U957	C893	G818	C731
U1932	A1618	U1741	U1833	G1519	U1431	U1344	G1242	A1156	A1029	U958	C894	A819	A734
G1933	G1626	A1742	U1834	G1520	A1434	G1344	G1244	A1157	A1030	A959	U955	A820	A734
A1937	G1627	C1745A	G1835	C1530	C1437	U1352	A1247	C1158	G1031	A960	A896	A821	G739
A1938	U1628	G1746	C1837	C1531	A1445	A1353	G1250	U1159	A1032	G962	C898	C825	U740
U1939	U1632	G1756	C1838	G1533	C1446	G1355	U1251	G1160	U1033	U963	A899	U826	G744
C1942	A1637	U1757	G1839	U	A1449	U1357	G1256	G1164	C1038	C964	A900	U827	G745
U1945	A1637	U1758	U1842	C1536	G1450	A1359	U1257	U1170	G1040	G973	A901	U828	A746
U1946	U1639	C1761	C1843	G1538	A1452	A1360	A1262	G1171	G1041	C975	C902	C831	G747
C1947	C1640	A1762	A1848	G1539	U1453	A1364	U1263	A	C1043	G974	C903	U833	U747
G1948	G1645	G1763	U1851	U1540	A1460	A1365	G1264	U	G	A973	U905	U834	G748
G1950	C1646	G1764	C1854	A1542	A1461	G1368	A1265	G	C1043	A974	C904	C834	C749
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A1952	C1648	U1778	G1855	C1545	U1467	G1374	A1268	U	A	G977	A911	C840	C753
A1953	G1651	U1779	G1856	C1546	G1465	C1375	A1269	C1178	A	A980	C912	C845	C755
U1954	A1652	C1781	G1857	U	C1466	C1375	G1271	C1179	G	A881	C914	C846	G760
U1955	G1653	A1781	G1858	C1550	C1467	G1378	C1270	C1180	A	C982	C916	U847	A761
C1958	A1654	C1782	A1859	A1554	C1468	A1378	A1272	A1182	C	A984	A917	C850	U762
U1963	A1665	A1783	A1864	A1554	C1469	A1379	U1273	G1183	A	G887	A918	U851	A763
A1966	G1666	A1784	G1865	A1558	C1470	G1380	A1274	G1184	G	A888	G919	G852	G771
C1967	G1667	U1785	A1786	G1559	A1471	G1384	A1278	U1188	A	G989	G921	G853	A774
A1970	A1668	C1790	C1881	A1566	A1472	C1385	G1279	A1189	G	A990	U922	G854	G775
A1971	A1669	A1791	C1882	A1566	G1478	C1387	G1287	G1191	U	C991	C923	C856	G776
A1972	C1670	U1794	A1885	A1569	G1482	U1384	U1300	U1198	G	C994	C925	U858	A782
C1983	C1674	C1795	C1886	U1576	G1484	A1395	A1301	U1199	C	C995	A926	G859	A783
U1991	C1686	C1797	A1889	C1577	G1485	U1396	A1302	C1200	U	A996	G927	U860	A784
U1992	G1687	U1798	A1890	U1578	A1486	U1397	G1303	C1201	U	G997	G928	A861	A785
U1993	U1688	C1799	C1895	A1580	G1487	U1400	G1310	A1204	A	C998	A933	G863	A788
C1996	A1689	G1800	C1896	G1581	A1490	G1401	U1313	U1205	G	A1000	C936	A866	G792
C1997	U1693	A1801	G1897	U1582	G1491	U1394	U1313	G1206	A	A1001	U937	C867	C795
G1997	C1696	A1802	A1898	C1583	G1492	U1405	G1314	U1209	G	G1002	G938	C867	C796
G1998	G1697	A1803	A1899	C1584	C1493	U1406	C1315	G1209	C	G1003	C939	G873	G797
C1999	A1698	G1804	A1900	A1586	A1494	U1407	U1316	A1210	A	C1005	G940	G874	G798
G2000	G1698	U1805	A1901	A1587	A1495	C1408	A1317	G1211	G	C1006	A941	G875	G798
A2001	A1698	C1812	G1906	C1588	A1496	G1409	C1318	G1212	C	C1007	G942	G878	G801
G2002	G1699	G1813	A1913	U1589	U1497	C1411	C1319	A1213	C	U1012	G943	A879	G805
	A1701	G1814		U1590	U1503		A1321	A1220	U	C1013	A945	G880	

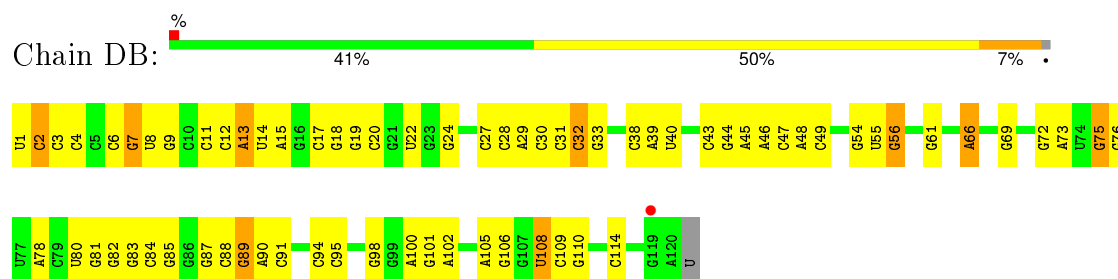


● Molecule 26: 5S Ribosomal RNA

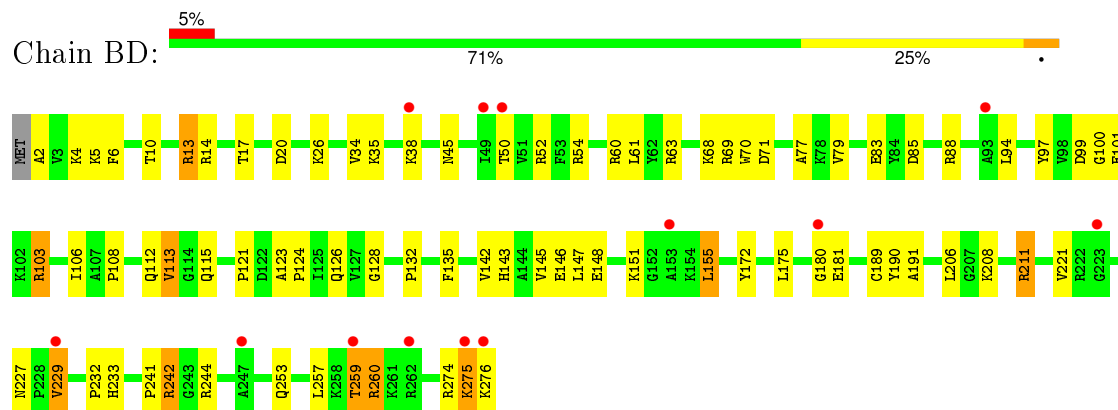
Chain BB: 68% 28%



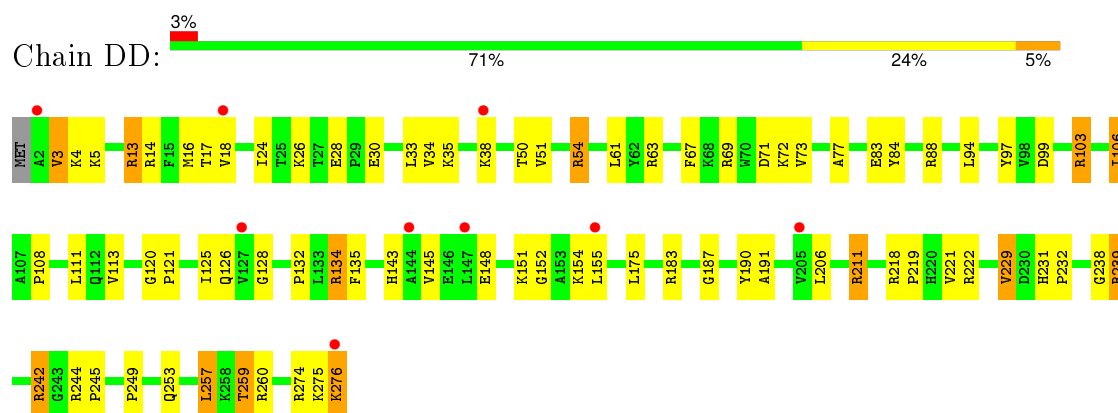
- Molecule 26: 5S Ribosomal RNA



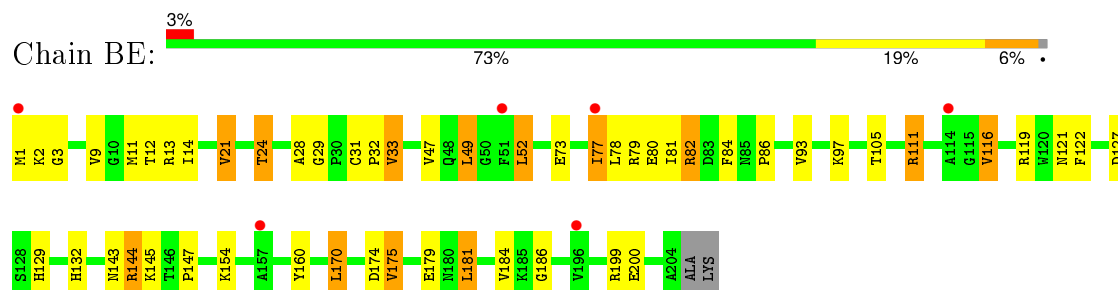
- Molecule 27: 50S Ribosomal Protein L2



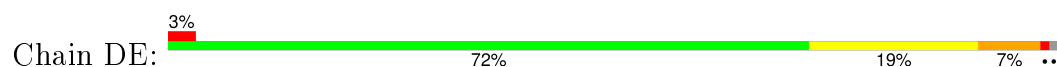
- Molecule 27: 50S Ribosomal Protein L2

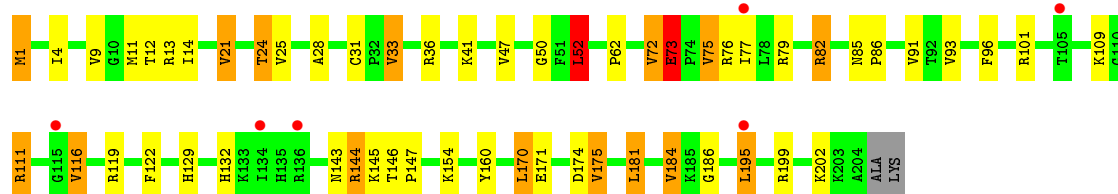


- Molecule 28: 50S Ribosomal Protein L3

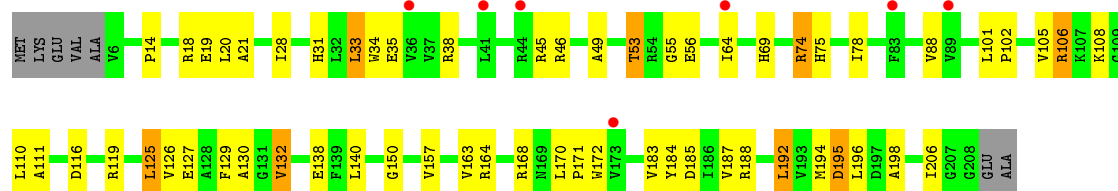


- Molecule 28: 50S Ribosomal Protein L3

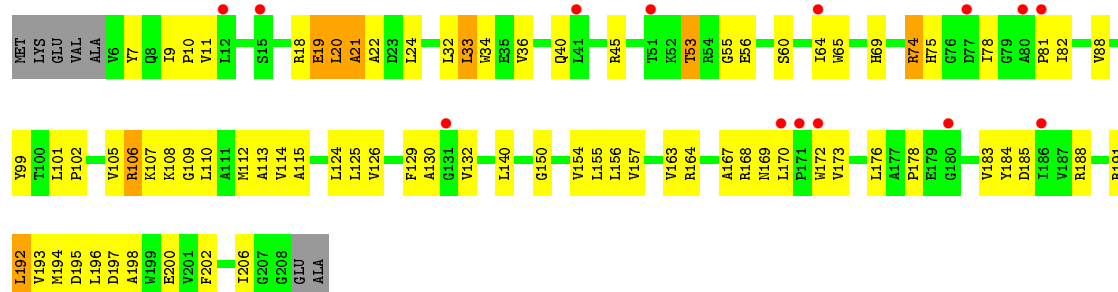




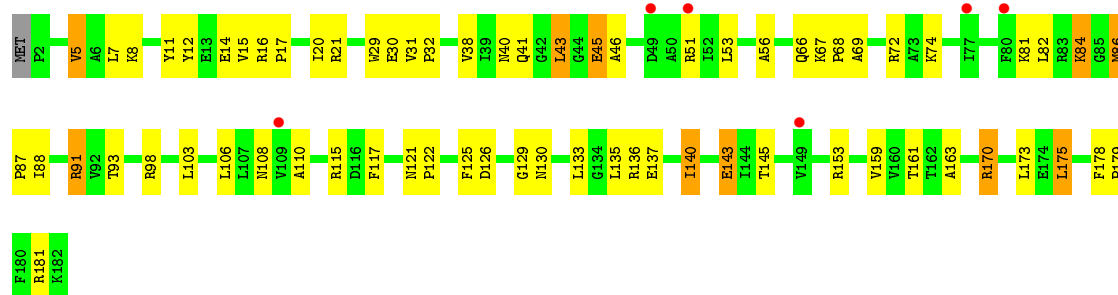
• Molecule 29: 50S Ribosomal Protein L4



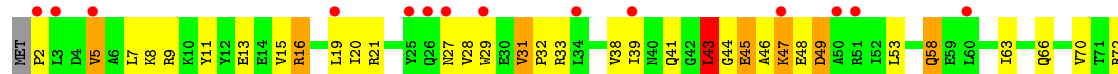
• Molecule 29: 50S Ribosomal Protein L4

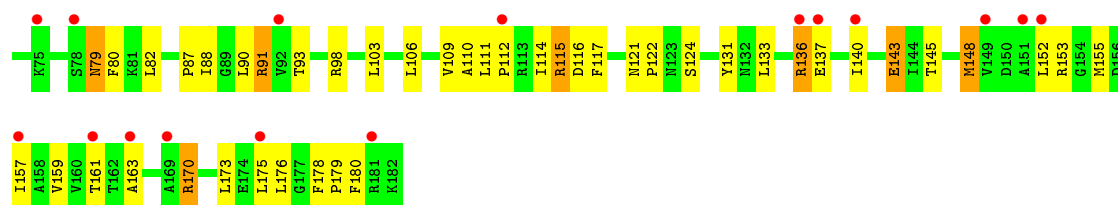


• Molecule 30: 50S Ribosomal Protein L5



• Molecule 30: 50S Ribosomal Protein L5

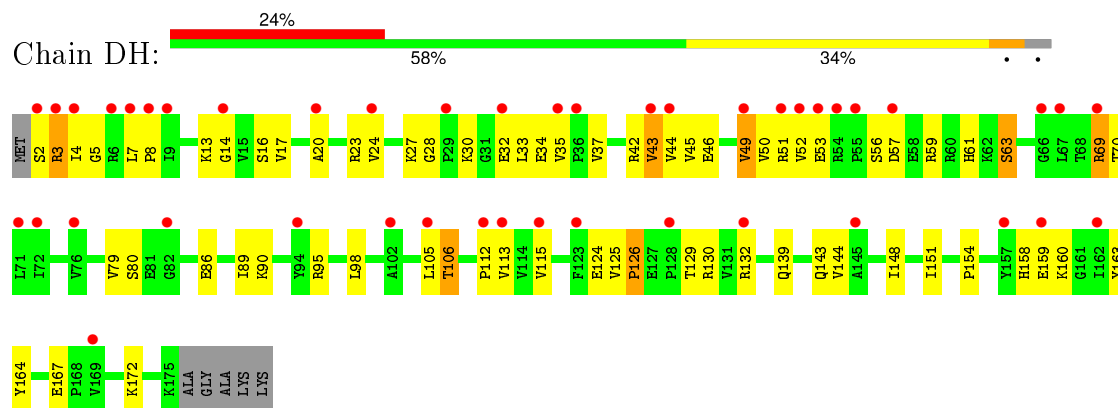




• Molecule 31: 50S Ribosomal Protein L6



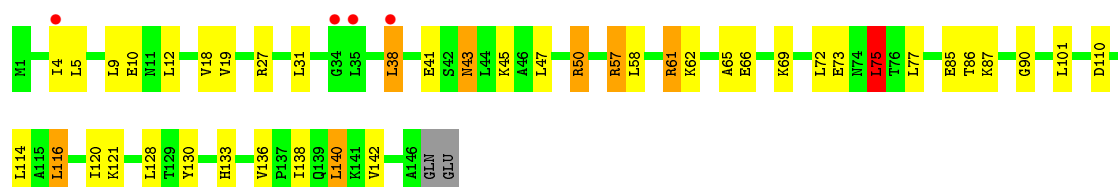
• Molecule 31: 50S Ribosomal Protein L6



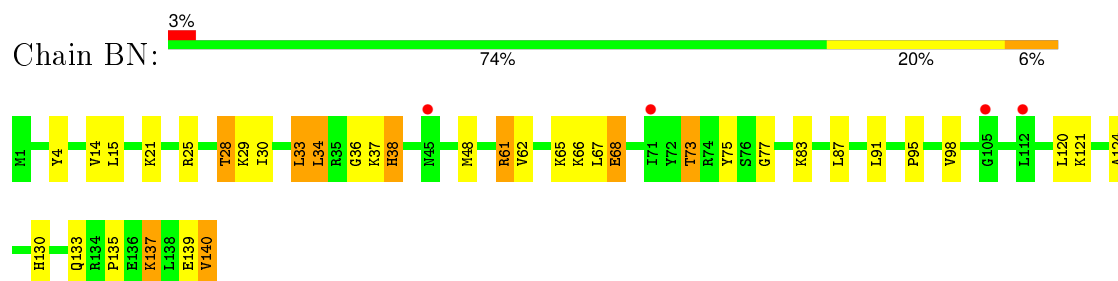
• Molecule 32: 50S Ribosomal Protein L9



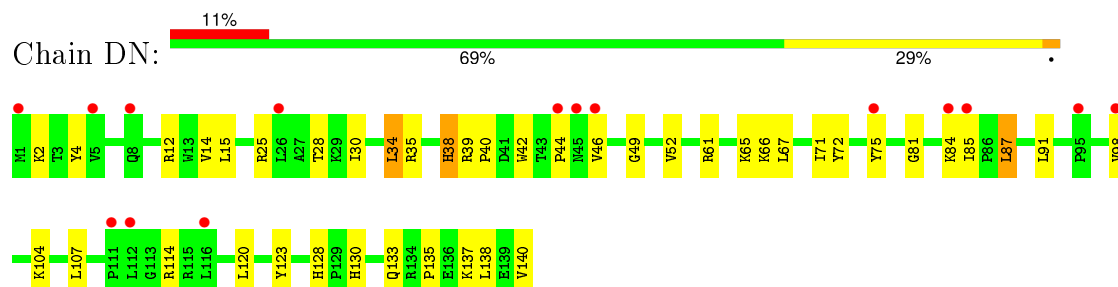
• Molecule 32: 50S Ribosomal Protein L9



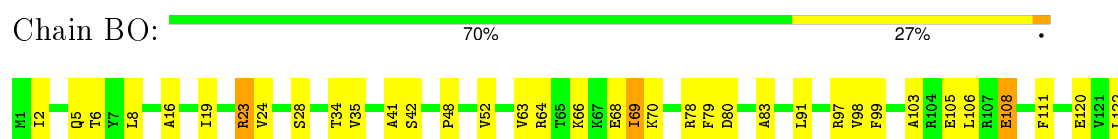
- Molecule 33: 50S Ribosomal Protein L13



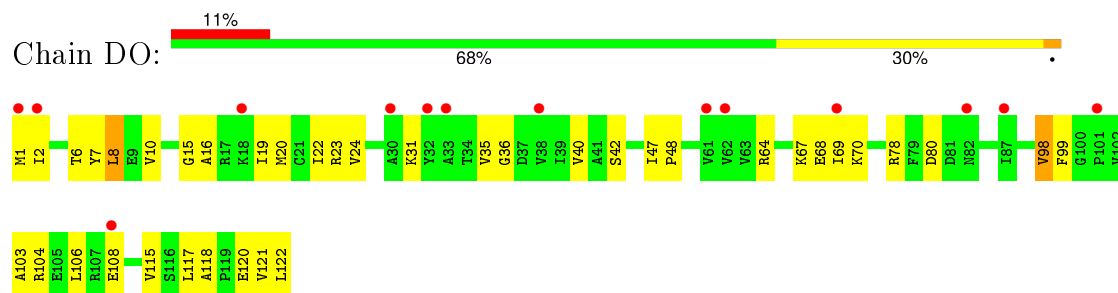
- Molecule 33: 50S Ribosomal Protein L13



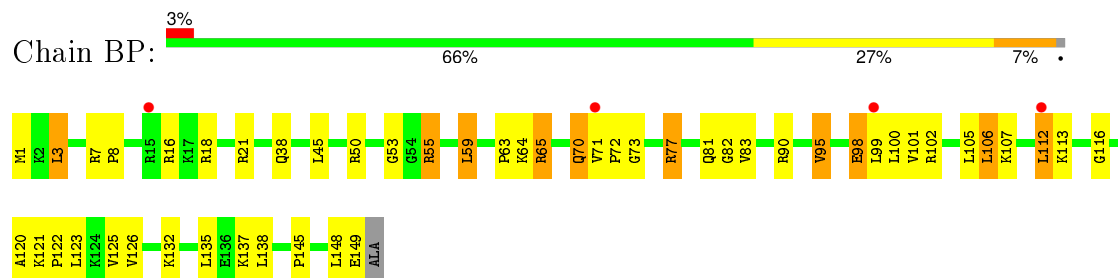
- Molecule 34: 50S Ribosomal Protein L14



- Molecule 34: 50S Ribosomal Protein L14



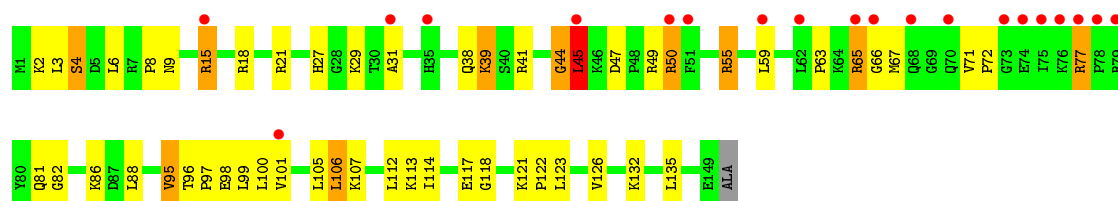
- Molecule 35: 50S Ribosomal Protein L15



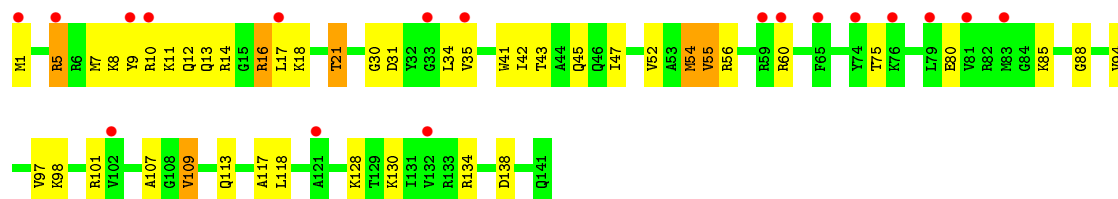
- Molecule 35: 50S Ribosomal Protein L15



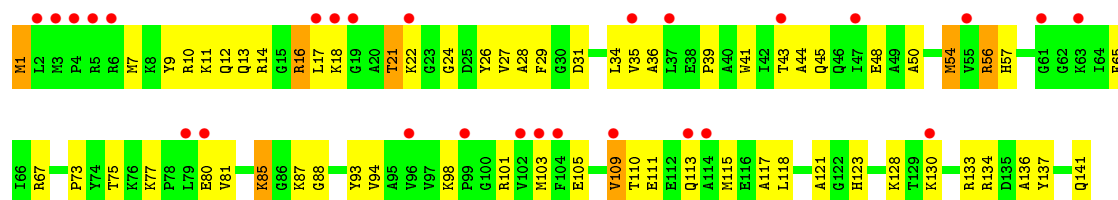




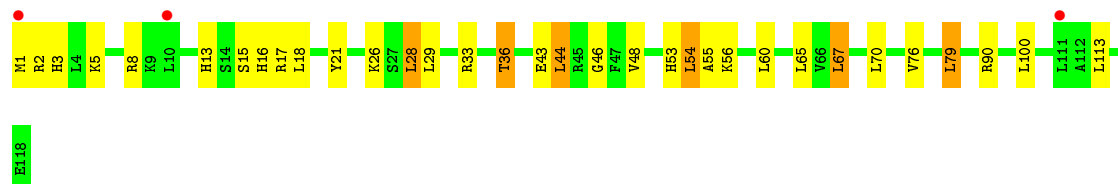
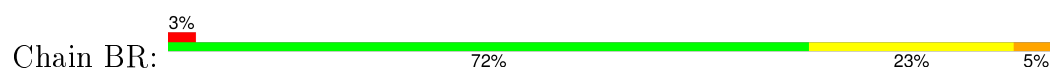
• Molecule 36: 50S Ribosomal Protein L16



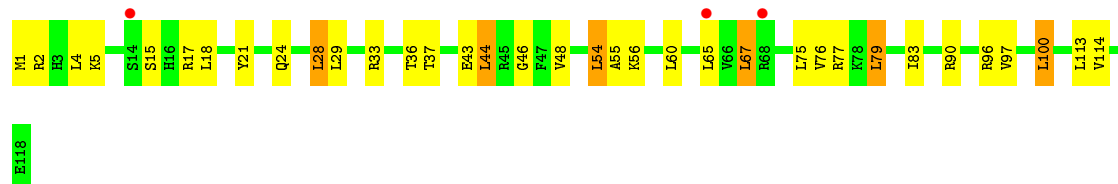
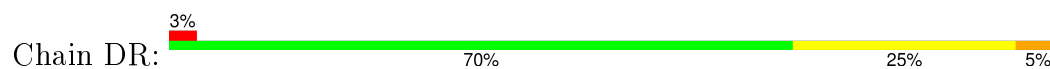
• Molecule 36: 50S Ribosomal Protein L16



• Molecule 37: 50S Ribosomal Protein L17

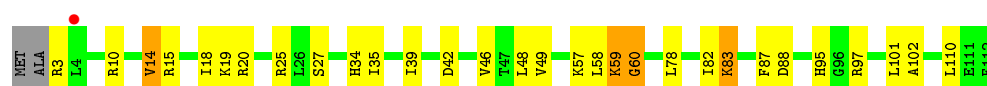


• Molecule 37: 50S Ribosomal Protein L17

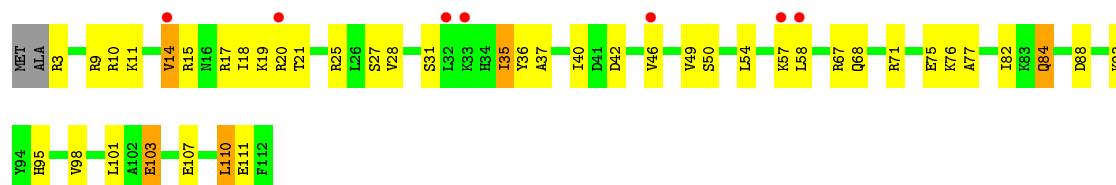


• Molecule 38: 50S Ribosomal Protein L18

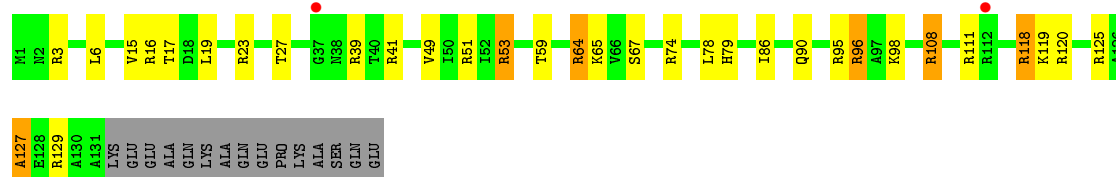




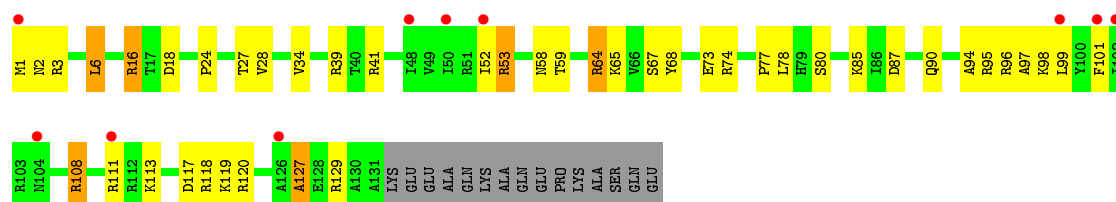
• Molecule 38: 50S Ribosomal Protein L18



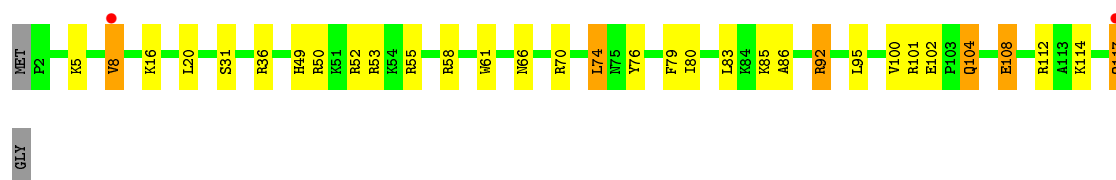
• Molecule 39: 50S Ribosomal Protein L19



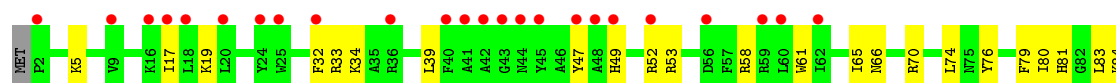
• Molecule 39: 50S Ribosomal Protein L19

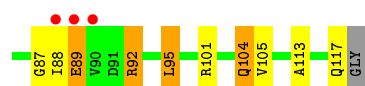


• Molecule 40: 50S Ribosomal Protein L20



• Molecule 40: 50S Ribosomal Protein L20





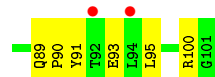
• Molecule 41: 50S Ribosomal Protein L21

Chain BV: 73% 23% .



• Molecule 41: 50S Ribosomal Protein L21

Chain DV: 21% 66% 29% . .



• Molecule 42: 50S Ribosomal Protein L22

Chain BW: 3% 68% 28% . .



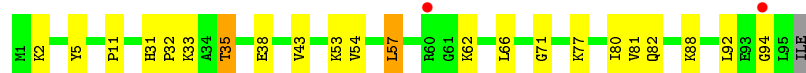
• Molecule 42: 50S Ribosomal Protein L22

Chain DW: 5% 74% 19% 5% .



• Molecule 43: 50S Ribosomal Protein L23

Chain BX: 2% 76% 21% . .



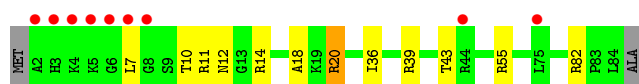
• Molecule 43: 50S Ribosomal Protein L23

Chain DX: 17% 74% 23% . .

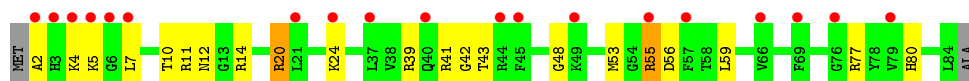
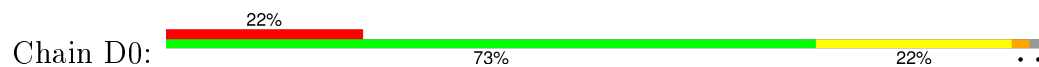


• Molecule 44: 50S Ribosomal Protein L24

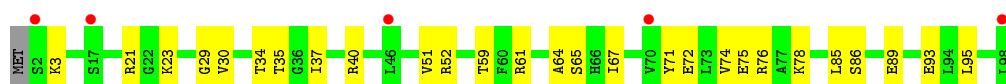
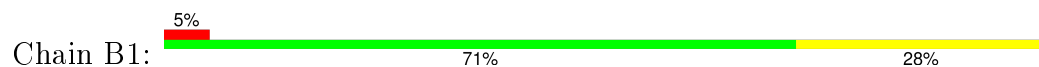




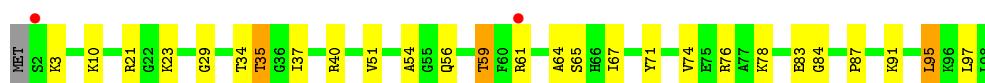
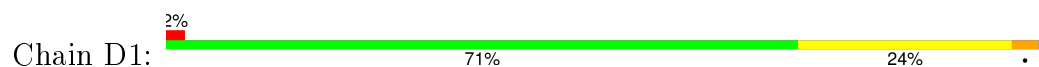
• Molecule 46: 50S Ribosomal Protein L27



• Molecule 47: 50S Ribosomal Protein L28



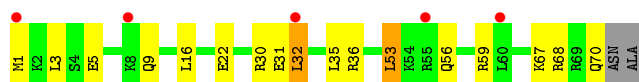
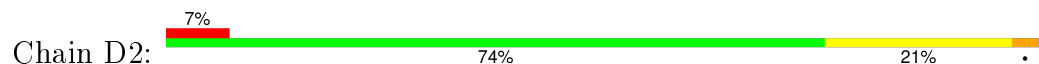
• Molecule 47: 50S Ribosomal Protein L28



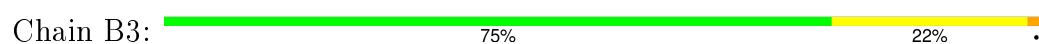
• Molecule 48: 50S Ribosomal Protein L29



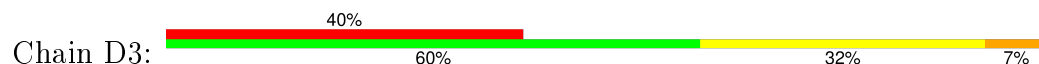
• Molecule 48: 50S Ribosomal Protein L29

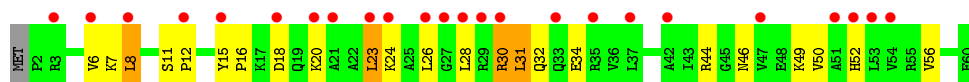


• Molecule 49: 50S Ribosomal Protein L30

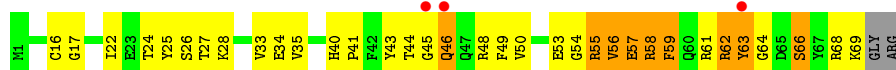


• Molecule 49: 50S Ribosomal Protein L30

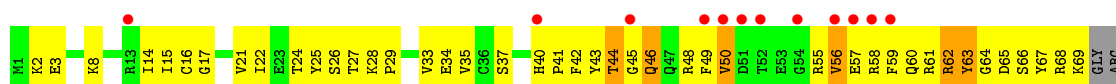




• Molecule 50: 50S Ribosomal Protein L31



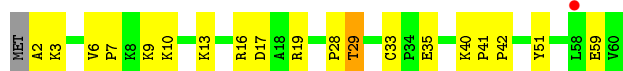
• Molecule 50: 50S Ribosomal Protein L31



• Molecule 51: 50S Ribosomal Protein L32



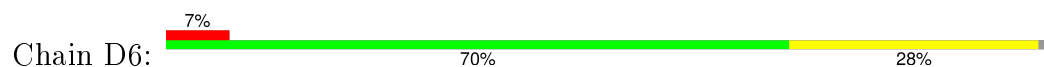
• Molecule 51: 50S Ribosomal Protein L32



• Molecule 52: 50S Ribosomal Protein L33

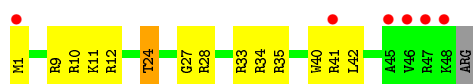


• Molecule 52: 50S Ribosomal Protein L33

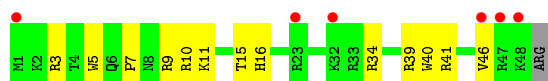
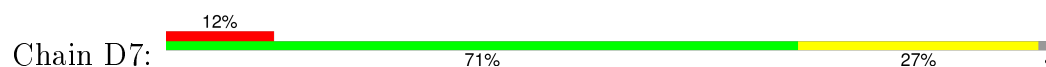


• Molecule 53: 50S Ribosomal Protein L34





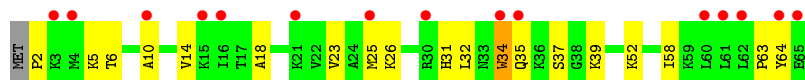
- Molecule 53: 50S Ribosomal Protein L34



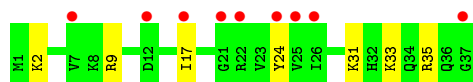
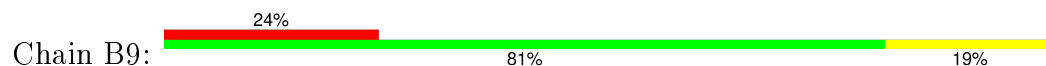
- Molecule 54: 50S Ribosomal Protein L35



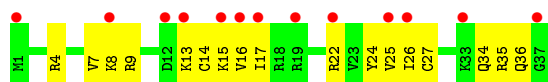
- Molecule 54: 50S Ribosomal Protein L35



- Molecule 55: 50S Ribosomal Protein L36



- Molecule 55: 50S Ribosomal Protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.25Å 443.61Å 619.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.25 – 2.70 360.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (124.25-2.70) 97.2 (360.63-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.210 , 0.257 0.218 , 0.263	Depositor DCC
$R_{free}$ test set	75600 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1504988 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	297376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MIA, NEG, SF4, MG, 5MC, 4SU, 7MG, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.44	0/36002	0.92	46/56188 (0.1%)
1	CA	0.42	0/36170	0.94	42/56452 (0.1%)
2	AB	0.32	0/1881	0.59	0/2542
2	CB	0.32	0/1860	0.62	1/2518 (0.0%)
3	AC	0.30	0/1576	0.50	0/2130
3	CC	0.30	0/1566	0.53	0/2119
4	AD	0.31	0/1689	0.53	0/2267
4	CD	0.31	0/1704	0.55	1/2284 (0.0%)
5	AE	0.33	0/1145	0.53	0/1543
5	CE	0.33	0/1149	0.57	0/1548
6	AF	0.32	0/819	0.54	0/1111
6	CF	0.31	0/829	0.51	1/1123 (0.1%)
7	AG	0.30	0/1250	0.49	0/1679
7	CG	0.29	0/1254	0.52	0/1683
8	AH	0.29	0/1108	0.51	0/1494
8	CH	0.30	0/1108	0.52	0/1494
9	AI	0.30	0/1002	0.55	0/1346
9	CI	0.32	0/997	0.56	0/1343
10	AJ	0.29	0/722	0.56	0/982
10	CJ	0.31	0/727	0.58	0/988
11	AK	0.30	0/844	0.51	0/1145
11	CK	0.31	0/848	0.51	0/1149
12	AL	0.34	0/946	0.55	1/1274 (0.1%)
12	CL	0.33	0/946	0.58	0/1274
13	AM	0.32	0/969	0.59	0/1302
13	CM	0.29	0/961	0.54	0/1291
14	AN	0.30	0/501	0.50	0/664
14	CN	0.34	0/501	0.54	0/664
15	AO	0.34	0/739	0.53	0/985
15	CO	0.31	0/739	0.49	0/985
16	AP	0.32	0/697	0.57	0/939
16	CP	0.31	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.31	0/836	0.52	0/1117
17	CQ	0.31	0/836	0.50	0/1117
18	AR	0.33	0/560	0.49	0/746
18	CR	0.28	0/560	0.51	0/746
19	AS	0.29	0/667	0.50	0/900
19	CS	0.32	0/661	0.63	0/893
20	AT	0.29	0/730	0.56	0/965
20	CT	0.29	0/729	0.52	0/965
21	AU	0.29	0/203	0.53	0/266
21	CU	0.34	0/203	0.52	0/266
22	AV	0.51	0/310	0.97	1/480 (0.2%)
22	CV	0.44	0/282	1.00	2/437 (0.5%)
23	AW	0.54	0/1602	1.16	6/2493 (0.2%)
23	AY	0.50	0/1602	1.09	2/2493 (0.1%)
23	CW	0.50	0/1556	1.10	2/2418 (0.1%)
23	CY	0.53	0/1579	1.15	2/2455 (0.1%)
24	AX	0.58	1/1725 (0.1%)	1.16	14/2689 (0.5%)
24	CX	0.52	0/1725	1.12	11/2689 (0.4%)
25	BA	0.65	6/68083 (0.0%)	1.00	128/106274 (0.1%)
25	DA	0.49	1/67542 (0.0%)	0.97	74/105428 (0.1%)
26	BB	0.51	0/2878	0.92	0/4490
26	DB	0.48	0/2878	0.91	2/4490 (0.0%)
27	BD	0.43	0/2186	0.62	0/2944
27	DD	0.39	0/2186	0.59	0/2944
28	BE	0.45	0/1592	0.58	0/2149
28	DE	0.37	0/1592	0.61	1/2149 (0.0%)
29	BF	0.39	0/1619	0.57	0/2193
29	DF	0.35	0/1615	0.58	0/2188
30	BG	0.32	0/1450	0.52	0/1959
30	DG	0.32	0/1449	0.55	0/1958
31	BH	0.36	0/1356	0.54	0/1834
31	DH	0.33	0/1356	0.53	0/1834
32	BI	0.32	0/1100	0.58	0/1501
32	DI	0.30	0/1076	0.56	1/1471 (0.1%)
33	BN	0.39	0/1144	0.53	0/1543
33	DN	0.33	0/1144	0.55	0/1543
34	BO	0.41	0/943	0.59	0/1269
34	DO	0.35	0/943	0.55	1/1269 (0.1%)
35	BP	0.39	0/1152	0.59	0/1533
35	DP	0.34	0/1152	0.64	1/1533 (0.1%)
36	BQ	0.41	0/1143	0.53	0/1527
36	DQ	0.35	0/1143	0.56	0/1527
37	BR	0.42	0/982	0.62	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DR	0.33	0/982	0.57	0/1312
38	BS	0.36	0/887	0.55	0/1180
38	DS	0.30	0/880	0.55	0/1172
39	BT	0.38	0/1105	0.58	0/1477
39	DT	0.32	0/1097	0.54	0/1468
40	BU	0.44	0/977	0.59	0/1301
40	DU	0.30	0/977	0.48	0/1301
41	BV	0.42	0/782	0.60	0/1049
41	DV	0.32	0/782	0.54	1/1049 (0.1%)
42	BW	0.44	0/897	0.57	0/1205
42	DW	0.34	0/897	0.52	0/1205
43	BX	0.43	0/764	0.61	1/1025 (0.1%)
43	DX	0.35	0/764	0.55	1/1025 (0.1%)
44	BY	0.40	0/819	0.59	0/1095
44	DY	0.33	0/819	0.53	0/1095
45	BZ	0.34	0/1379	0.59	0/1873
45	DZ	0.32	0/1390	0.56	0/1890
46	B0	0.42	0/662	0.63	0/881
46	D0	0.33	0/662	0.53	0/881
47	B1	0.41	0/762	0.56	0/1014
47	D1	0.35	0/762	0.54	0/1014
48	B2	0.38	0/590	0.58	0/781
48	D2	0.28	0/590	0.48	0/781
49	B3	0.37	0/474	0.58	0/635
49	D3	0.30	0/469	0.52	0/630
50	B4	0.37	0/571	0.71	0/768
50	D4	0.35	0/545	0.57	0/737
51	B5	0.43	0/469	0.64	0/635
51	D5	0.34	0/469	0.54	0/635
52	B6	0.41	0/460	0.57	0/613
52	D6	0.35	0/456	0.45	0/608
53	B7	0.44	0/426	0.60	0/561
53	D7	0.36	0/426	0.55	0/561
54	B8	0.43	0/525	0.61	0/691
54	D8	0.36	0/525	0.54	0/691
55	B9	0.42	0/310	0.50	0/407
55	D9	0.36	0/310	0.56	0/407
All	All	0.48	8/316673 (0.0%)	0.89	343/474091 (0.1%)

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
7	AG	0	1
7	CG	0	1
38	BS	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	553	A	N9-C4	-8.54	1.32	1.37
25	BA	354	A	N9-C4	-8.21	1.32	1.37
25	BA	1188	A	N9-C4	-7.54	1.33	1.37
25	BA	990	A	N9-C4	-6.34	1.34	1.37
25	BA	2299	A	N9-C4	-6.34	1.34	1.37

The worst 5 of 343 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	553	A	C2-N3-C4	-12.04	104.58	110.60
25	BA	354	A	C2-N3-C4	-11.68	104.76	110.60
1	AA	345	C	N1-C2-O2	11.09	125.55	118.90
25	BA	1686	U	O5'-P-OP2	-10.46	96.29	105.70
1	CA	1154	G	C5-C6-O6	10.31	134.78	128.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
7	AG	79	ARG	Peptide
38	BS	58	LEU	Peptide
7	CG	78	ARG	Peptide

## 5.2 Too-close contacts ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32163	0	16234	552	0
1	CA	32312	0	16308	628	0
2	AB	1846	0	1867	78	0
2	CB	1825	0	1828	97	0
3	AC	1552	0	1546	55	0
3	CC	1542	0	1517	57	0
4	AD	1659	0	1676	64	0
4	CD	1674	0	1714	46	0
5	AE	1129	0	1185	36	0
5	CE	1133	0	1191	38	0
6	AF	806	0	793	20	0
6	CF	816	0	808	29	0
7	AG	1231	0	1238	27	0
7	CG	1235	0	1249	37	0
8	AH	1088	0	1126	35	0
8	CH	1088	0	1126	39	0
9	AI	983	0	986	41	0
9	CI	978	0	966	45	0
10	AJ	709	0	650	32	0
10	CJ	714	0	672	46	0
11	AK	829	0	825	14	0
11	CK	833	0	836	20	0
12	AL	930	0	980	28	0
12	CL	930	0	980	31	0
13	AM	958	0	1002	41	0
13	CM	950	0	988	43	0
14	AN	492	0	529	22	0
14	CN	492	0	529	24	0
15	AO	728	0	760	20	0
15	CO	728	0	760	23	0
16	AP	681	0	697	21	0
16	CP	677	0	686	22	0
17	AQ	823	0	891	17	0
17	CQ	823	0	891	20	0
18	AR	555	0	618	16	0
18	CR	555	0	618	17	0
19	AS	652	0	662	38	0
19	CS	646	0	644	35	0
20	AT	728	0	798	21	0
20	CT	727	0	796	18	0
21	AU	199	0	208	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	199	0	208	4	0
22	AV	277	0	140	7	0
22	CV	252	0	130	6	0
23	AW	1588	0	820	66	0
23	AY	1581	0	805	62	0
23	CW	1541	0	784	47	0
23	CY	1561	0	796	65	0
24	AX	1625	0	828	13	0
24	CX	1625	0	828	31	0
25	BA	60792	0	30654	800	0
25	DA	60311	0	30412	1121	0
26	BB	2573	0	1306	23	0
26	DB	2573	0	1306	63	0
27	BD	2136	0	2218	67	0
27	DD	2136	0	2218	69	0
28	BE	1559	0	1618	35	0
28	DE	1559	0	1618	52	0
29	BF	1584	0	1625	41	0
29	DF	1580	0	1619	61	0
30	BG	1425	0	1443	41	0
30	DG	1424	0	1434	57	0
31	BH	1330	0	1407	30	0
31	DH	1330	0	1407	42	0
32	BI	1085	0	1114	38	0
32	DI	1061	0	1080	20	0
33	BN	1117	0	1184	24	0
33	DN	1117	0	1184	29	0
34	BO	933	0	996	22	0
34	DO	933	0	996	27	0
35	BP	1135	0	1212	44	0
35	DP	1135	0	1212	48	0
36	BQ	1122	0	1179	37	0
36	DQ	1122	0	1179	62	0
37	BR	968	0	1033	20	0
37	DR	968	0	1033	27	0
38	BS	877	0	938	20	0
38	DS	870	0	923	28	0
39	BT	1091	0	1151	22	0
39	DT	1083	0	1136	32	0
40	BU	959	0	1019	27	0
40	DU	959	0	1019	29	0
41	BV	771	0	830	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	DV	771	0	830	20	0
42	BW	886	0	940	21	0
42	DW	886	0	939	17	0
43	BX	750	0	814	18	0
43	DX	750	0	814	17	0
44	BY	806	0	881	26	0
44	DY	806	0	881	29	0
45	BZ	1349	0	1355	51	0
45	DZ	1360	0	1363	64	0
46	B0	653	0	674	13	0
46	D0	653	0	674	22	0
47	B1	755	0	826	17	0
47	D1	755	0	826	18	0
48	B2	588	0	643	11	0
48	D2	588	0	643	10	0
49	B3	469	0	518	6	0
49	D3	464	0	514	17	0
50	B4	558	0	544	27	0
50	D4	532	0	503	30	0
51	B5	455	0	465	15	0
51	D5	455	0	465	13	0
52	B6	453	0	473	10	0
52	D6	449	0	469	10	0
53	B7	418	0	467	18	0
53	D7	418	0	467	13	0
54	B8	517	0	582	25	0
54	D8	517	0	582	15	0
55	B9	307	0	335	4	0
55	D9	307	0	335	13	0
56	AA	218	0	0	0	0
56	AD	1	0	0	0	0
56	AE	2	0	0	0	0
56	AF	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	3	0	0	0	0
56	AO	1	0	0	0	0
56	AV	3	0	0	0	0
56	AW	4	0	0	0	0
56	AX	11	0	0	0	0
56	AY	3	0	0	0	0
56	B0	3	0	0	0	0
56	B1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B2	1	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	5	0	0	0	0
56	B6	1	0	0	0	0
56	B7	4	0	0	0	0
56	B8	1	0	0	0	0
56	B9	1	0	0	0	0
56	BA	785	0	0	0	0
56	BB	18	0	0	0	0
56	BD	11	0	0	0	0
56	BE	8	0	0	0	0
56	BF	11	0	0	0	0
56	BG	2	0	0	0	0
56	BN	6	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	5	0	0	0	0
56	BR	3	0	0	0	0
56	BT	1	0	0	0	0
56	BU	9	0	0	0	0
56	BV	7	0	0	0	0
56	BW	4	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	172	0	0	0	0
56	CD	1	0	0	0	0
56	CE	1	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CK	1	0	0	0	0
56	CN	1	0	0	0	0
56	CT	1	0	0	0	0
56	CV	1	0	0	0	0
56	CW	2	0	0	0	0
56	CX	2	0	0	0	0
56	CY	1	0	0	0	0
56	D0	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	1	0	0	0	0
56	D7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	D8	1	0	0	0	0
56	DA	623	0	0	0	0
56	DB	12	0	0	0	0
56	DD	9	0	0	0	0
56	DE	4	0	0	0	0
56	DF	6	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	2	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	2	0	0	0	0
56	DU	3	0	0	0	0
56	DV	3	0	0	0	0
56	DW	4	0	0	0	0
56	DY	1	0	0	0	0
57	AA	119	0	133	18	0
57	AW	17	0	19	2	0
57	AX	17	0	19	3	0
57	CA	136	0	152	13	0
57	CW	17	0	19	1	0
57	CX	17	0	19	5	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	247	0	0	9	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AL	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	AM	2	0	0	0	0
61	AO	1	0	0	0	0
61	AV	3	0	0	0	0
61	AW	13	0	0	2	0
61	AX	11	0	0	2	0
61	AY	1	0	0	0	0
61	B0	8	0	0	0	0
61	B3	1	0	0	0	0
61	B5	6	0	0	1	0
61	B6	1	0	0	0	0
61	B7	2	0	0	1	0
61	B8	7	0	0	1	0
61	BA	1396	0	0	65	0
61	BB	34	0	0	1	0
61	BD	12	0	0	2	0
61	BE	11	0	0	3	0
61	BF	5	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BN	1	0	0	0	0
61	BO	2	0	0	0	0
61	BP	23	0	0	1	0
61	BQ	3	0	0	0	0
61	BR	1	0	0	0	0
61	BT	2	0	0	0	0
61	BU	3	0	0	0	0
61	BV	2	0	0	0	0
61	BW	1	0	0	1	0
61	BX	2	0	0	0	0
61	BZ	1	0	0	1	0
61	CA	184	0	0	14	0
61	CJ	2	0	0	2	0
61	CP	1	0	0	0	0
61	CV	2	0	0	0	0
61	CW	3	0	0	1	0
61	CX	6	0	0	0	0
61	D0	8	0	0	1	0
61	D1	4	0	0	0	0
61	D7	2	0	0	0	0
61	D8	1	0	0	0	0
61	DA	960	0	0	63	0
61	DB	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DD	16	0	0	2	0
61	DE	9	0	0	0	0
61	DF	5	0	0	0	0
61	DN	3	0	0	0	0
61	DO	2	0	0	0	0
61	DP	15	0	0	0	0
61	DQ	1	0	0	1	0
61	DR	1	0	0	0	0
61	DU	1	0	0	0	0
61	DW	1	0	0	0	0
61	DX	1	0	0	0	0
61	DY	2	0	0	1	0
All	All	297376	0	196603	5587	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 5587 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:CW:27:G:H1	23:CW:43:C:N4	1.53	1.07
23:CY:7:A:N6	23:CY:66:U:H3	1.50	1.07
23:AY:49:C:N4	23:AY:65:G:H1	1.56	1.03
23:CY:15:G:N2	23:CY:48:C:H42	1.55	1.03
53:B7:24:THR:HG22	53:B7:27:GLY:H	1.24	1.02

There are no symmetry-related clashes.

## 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	229/256 (90%)	196 (86%)	24 (10%)	9 (4%)	4	8
2	CB	229/256 (90%)	195 (85%)	24 (10%)	10 (4%)	3	6
3	AC	204/239 (85%)	182 (89%)	18 (9%)	4 (2%)	9	24
3	CC	204/239 (85%)	182 (89%)	19 (9%)	3 (2%)	13	32
4	AD	206/209 (99%)	193 (94%)	12 (6%)	1 (0%)	34	63
4	CD	206/209 (99%)	196 (95%)	8 (4%)	2 (1%)	19	45
5	AE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	26	55
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	26	55
6	AF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
6	CF	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	19	45
7	AG	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	9	24
7	CG	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	9	24
8	AH	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	26	55
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	26	55
9	AI	125/128 (98%)	113 (90%)	10 (8%)	2 (2%)	12	30
9	CI	125/128 (98%)	112 (90%)	10 (8%)	3 (2%)	7	19
10	AJ	95/105 (90%)	82 (86%)	7 (7%)	6 (6%)	2	2
10	CJ	94/105 (90%)	81 (86%)	7 (7%)	6 (6%)	2	2
11	AK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	11	27
11	CK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	11	27
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
13	AM	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	24	51
13	CM	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	11	29
14	AN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	CN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	CO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	16	39
16	AP	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	15	37
16	CP	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	15	37
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	19	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	66/88 (75%)	65 (98%)	0	1 (2%)	13	32
18	CR	66/88 (75%)	65 (98%)	0	1 (2%)	13	32
19	AS	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	7	18
19	CS	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	7	18
20	AT	94/106 (89%)	86 (92%)	2 (2%)	6 (6%)	2	2
20	CT	94/106 (89%)	87 (93%)	1 (1%)	6 (6%)	2	2
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
27	BD	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	39	69
27	DD	273/276 (99%)	255 (93%)	16 (6%)	2 (1%)	26	55
28	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	34	63
28	DE	202/206 (98%)	195 (96%)	5 (2%)	2 (1%)	19	45
29	BF	201/210 (96%)	199 (99%)	1 (0%)	1 (0%)	34	63
29	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	19	45
30	BG	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	17	42
30	DG	179/182 (98%)	166 (93%)	10 (6%)	3 (2%)	11	29
31	BH	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	30	59
31	DH	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	30	59
32	BI	144/148 (97%)	128 (89%)	12 (8%)	4 (3%)	6	15
32	DI	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	14	35
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
33	DN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	26	55
34	BO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	24	51
34	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	26	55
35	DP	147/150 (98%)	137 (93%)	7 (5%)	3 (2%)	9	24
36	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
36	DQ	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	26	55
37	BR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
37	DR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
38	BS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	21	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	21	49
39	BT	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	24	51
39	DT	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	24	51
40	BU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
41	BV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	19	45
41	DV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	19	45
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
42	DW	110/113 (97%)	110 (100%)	0	0	100	100
43	BX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
43	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	BY	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	19	45
44	DY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
45	BZ	169/206 (82%)	145 (86%)	21 (12%)	3 (2%)	11	27
45	DZ	172/206 (84%)	153 (89%)	18 (10%)	1 (1%)	30	59
46	B0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
46	D0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	16	39
47	B1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
47	D1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
48	B2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	D3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	B4	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1	1
50	D4	67/71 (94%)	51 (76%)	8 (12%)	8 (12%)	0	0
51	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	D5	57/60 (95%)	57 (100%)	0	0	100	100
52	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	8	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	62 (100%)	0	0	100	100
55	B9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
55	D9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11409/12128 (94%)	10706 (94%)	562 (5%)	141 (1%)	16	39

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	HIS
2	AB	17	PHE
2	AB	231	GLU
7	AG	80	VAL
9	AI	44	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	162 (84%)	30 (16%)	3	8
2	CB	187/220 (85%)	163 (87%)	24 (13%)	5	12
3	AC	143/188 (76%)	132 (92%)	11 (8%)	16	36
3	CC	140/188 (74%)	130 (93%)	10 (7%)	18	41
4	AD	170/181 (94%)	161 (95%)	9 (5%)	28	57
4	CD	173/181 (96%)	159 (92%)	14 (8%)	15	33
5	AE	113/123 (92%)	106 (94%)	7 (6%)	23	49
5	CE	114/123 (93%)	103 (90%)	11 (10%)	10	24
6	AF	83/90 (92%)	79 (95%)	4 (5%)	31	62
6	CF	85/90 (94%)	77 (91%)	8 (9%)	11	25
7	AG	119/127 (94%)	112 (94%)	7 (6%)	24	51
7	CG	120/127 (94%)	114 (95%)	6 (5%)	30	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	114/119 (96%)	108 (95%)	6 (5%)	28	57
8	CH	114/119 (96%)	109 (96%)	5 (4%)	35	65
9	AI	90/99 (91%)	80 (89%)	10 (11%)	8	17
9	CI	89/99 (90%)	77 (86%)	12 (14%)	5	11
10	AJ	66/92 (72%)	62 (94%)	4 (6%)	23	49
10	CJ	69/92 (75%)	67 (97%)	2 (3%)	50	80
11	AK	82/99 (83%)	74 (90%)	8 (10%)	10	23
11	CK	83/99 (84%)	73 (88%)	10 (12%)	6	14
12	AL	97/109 (89%)	94 (97%)	3 (3%)	47	78
12	CL	97/109 (89%)	94 (97%)	3 (3%)	47	78
13	AM	93/101 (92%)	83 (89%)	10 (11%)	8	18
13	CM	92/101 (91%)	84 (91%)	8 (9%)	13	29
14	AN	49/50 (98%)	42 (86%)	7 (14%)	4	10
14	CN	49/50 (98%)	43 (88%)	6 (12%)	6	14
15	AO	78/80 (98%)	69 (88%)	9 (12%)	7	16
15	CO	78/80 (98%)	74 (95%)	4 (5%)	29	59
16	AP	69/74 (93%)	63 (91%)	6 (9%)	13	29
16	CP	68/74 (92%)	63 (93%)	5 (7%)	17	39
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	46	77
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	61	87
18	AR	59/77 (77%)	54 (92%)	5 (8%)	13	30
18	CR	59/77 (77%)	56 (95%)	3 (5%)	29	59
19	AS	69/80 (86%)	65 (94%)	4 (6%)	25	52
19	CS	67/80 (84%)	60 (90%)	7 (10%)	9	20
20	AT	70/82 (85%)	63 (90%)	7 (10%)	9	22
20	CT	70/82 (85%)	63 (90%)	7 (10%)	9	22
21	AU	18/22 (82%)	16 (89%)	2 (11%)	8	17
21	CU	18/22 (82%)	17 (94%)	1 (6%)	26	54
27	BD	215/218 (99%)	200 (93%)	15 (7%)	19	42
27	DD	215/218 (99%)	197 (92%)	18 (8%)	14	30
28	BE	164/166 (99%)	147 (90%)	17 (10%)	9	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	DE	164/166 (99%)	146 (89%)	18 (11%)	8	18
29	BF	160/166 (96%)	147 (92%)	13 (8%)	15	33
29	DF	159/166 (96%)	148 (93%)	11 (7%)	19	43
30	BG	143/156 (92%)	125 (87%)	18 (13%)	5	13
30	DG	142/156 (91%)	123 (87%)	19 (13%)	5	11
31	BH	144/148 (97%)	135 (94%)	9 (6%)	22	48
31	DH	144/148 (97%)	130 (90%)	14 (10%)	10	23
32	BI	110/124 (89%)	92 (84%)	18 (16%)	3	7
32	DI	104/124 (84%)	88 (85%)	16 (15%)	3	8
33	BN	118/119 (99%)	101 (86%)	17 (14%)	4	10
33	DN	118/119 (99%)	109 (92%)	9 (8%)	16	37
34	BO	100/100 (100%)	94 (94%)	6 (6%)	24	50
34	DO	100/100 (100%)	96 (96%)	4 (4%)	38	69
35	BP	115/116 (99%)	102 (89%)	13 (11%)	7	16
35	DP	115/116 (99%)	102 (89%)	13 (11%)	7	16
36	BQ	111/111 (100%)	101 (91%)	10 (9%)	12	27
36	DQ	111/111 (100%)	100 (90%)	11 (10%)	10	22
37	BR	101/101 (100%)	88 (87%)	13 (13%)	5	12
37	DR	101/101 (100%)	87 (86%)	14 (14%)	4	10
38	BS	87/88 (99%)	80 (92%)	7 (8%)	15	33
38	DS	85/88 (97%)	75 (88%)	10 (12%)	6	15
39	BT	115/127 (91%)	106 (92%)	9 (8%)	16	35
39	DT	113/127 (89%)	102 (90%)	11 (10%)	10	23
40	BU	93/94 (99%)	84 (90%)	9 (10%)	10	23
40	DU	93/94 (99%)	88 (95%)	5 (5%)	27	56
41	BV	80/82 (98%)	72 (90%)	8 (10%)	9	22
41	DV	80/82 (98%)	71 (89%)	9 (11%)	7	16
42	BW	90/92 (98%)	82 (91%)	8 (9%)	12	27
42	DW	90/92 (98%)	82 (91%)	8 (9%)	12	27
43	BX	77/78 (99%)	73 (95%)	4 (5%)	29	58
43	DX	77/78 (99%)	75 (97%)	2 (3%)	54	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BY	85/91 (93%)	78 (92%)	7 (8%)	14	32
44	DY	85/91 (93%)	82 (96%)	3 (4%)	43	74
45	BZ	145/179 (81%)	132 (91%)	13 (9%)	12	27
45	DZ	145/179 (81%)	130 (90%)	15 (10%)	9	20
46	B0	65/67 (97%)	61 (94%)	4 (6%)	23	49
46	D0	65/67 (97%)	62 (95%)	3 (5%)	33	64
47	B1	80/83 (96%)	73 (91%)	7 (9%)	12	28
47	D1	80/83 (96%)	74 (92%)	6 (8%)	17	38
48	B2	65/67 (97%)	61 (94%)	4 (6%)	23	49
48	D2	65/67 (97%)	61 (94%)	4 (6%)	23	49
49	B3	51/52 (98%)	46 (90%)	5 (10%)	10	23
49	D3	50/52 (96%)	43 (86%)	7 (14%)	4	10
50	B4	60/63 (95%)	50 (83%)	10 (17%)	3	7
50	D4	53/63 (84%)	44 (83%)	9 (17%)	2	6
51	B5	50/52 (96%)	43 (86%)	7 (14%)	4	10
51	D5	50/52 (96%)	45 (90%)	5 (10%)	9	22
52	B6	51/52 (98%)	47 (92%)	4 (8%)	16	35
52	D6	50/52 (96%)	49 (98%)	1 (2%)	63	87
53	B7	41/42 (98%)	39 (95%)	2 (5%)	31	61
53	D7	41/42 (98%)	41 (100%)	0	100	100
54	B8	54/55 (98%)	50 (93%)	4 (7%)	17	39
54	D8	54/55 (98%)	48 (89%)	6 (11%)	8	17
55	B9	34/34 (100%)	33 (97%)	1 (3%)	50	80
55	D9	34/34 (100%)	32 (94%)	2 (6%)	24	51
All	All	9321/10066 (93%)	8506 (91%)	815 (9%)	13	29

5 of 815 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	B0	55	ARG
4	CD	135	LEU
43	DX	88	LYS
48	B2	53	LEU
55	B9	33	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
40	BU	117	GLN
3	CC	104	GLN
39	DT	123	GLN
43	BX	82	GLN
48	B2	70	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1521 (98%)	280 (18%)	27 (1%)
1	CA	1501/1521 (98%)	280 (18%)	24 (1%)
22	AV	12/24 (50%)	2 (16%)	0
22	CV	11/24 (45%)	2 (18%)	0
23	AW	71/76 (93%)	31 (43%)	1 (1%)
23	AY	72/76 (94%)	33 (45%)	4 (5%)
23	CW	68/76 (89%)	30 (44%)	2 (2%)
23	CY	70/76 (92%)	31 (44%)	1 (1%)
24	AX	75/77 (97%)	21 (28%)	2 (2%)
24	CX	75/77 (97%)	21 (28%)	1 (1%)
25	BA	2814/2915 (96%)	455 (16%)	28 (0%)
25	DA	2791/2915 (95%)	518 (18%)	29 (1%)
26	BB	119/121 (98%)	13 (10%)	2 (1%)
26	DB	119/121 (98%)	14 (11%)	0
All	All	9291/9620 (96%)	1731 (18%)	121 (1%)

5 of 1731 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	32	A
1	AA	39	G

5 of 121 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2170	G
1	CA	266	G
25	DA	1992	G

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Mol	Chain	Res	Type
25	BA	2347	A
25	BA	2902	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
23	PSU	AW	32	23	13,21,22	1.21	1 (7%)	18,30,33	3.54	6 (33%)
23	MIA	AW	37	23	21,31,32	1.79	3 (14%)	26,44,47	1.57	7 (26%)
23	PSU	AW	39	23	13,21,22	1.39	1 (7%)	18,30,33	3.82	6 (33%)
23	7MG	AW	46	23	19,26,27	1.05	1 (5%)	24,39,42	2.85	6 (25%)
23	5MU	AW	54	23	12,22,23	0.31	0	14,32,35	2.53	2 (14%)
23	PSU	AW	55	23	13,21,22	1.14	1 (7%)	18,30,33	3.88	6 (33%)
23	4SU	AW	8	23	11,21,22	1.12	1 (9%)	13,30,33	1.37	1 (7%)
24	5MC	AX	32	24	13,22,23	1.30	1 (7%)	15,32,35	1.05	1 (6%)
24	5MU	AX	54	24	12,22,23	0.34	0	14,32,35	2.42	2 (14%)
24	PSU	AX	55	24	13,21,22	1.48	1 (7%)	18,30,33	3.34	6 (33%)
24	4SU	AX	8	24	11,21,22	1.17	1 (9%)	13,30,33	1.86	1 (7%)
23	PSU	AY	32	23	13,21,22	1.35	1 (7%)	18,30,33	3.23	6 (33%)
23	MIA	AY	37	23	15,24,32	1.24	2 (13%)	16,35,47	2.22	2 (12%)
23	PSU	AY	39	23	13,21,22	1.12	2 (15%)	18,30,33	3.30	5 (27%)
23	7MG	AY	46	23	19,26,27	1.12	1 (5%)	24,39,42	3.09	7 (29%)
23	5MU	AY	54	23	12,22,23	0.30	0	14,32,35	2.93	2 (14%)
23	PSU	AY	55	23	13,21,22	1.18	1 (7%)	18,30,33	3.18	5 (27%)
23	4SU	AY	8	23	11,21,22	1.12	1 (9%)	13,30,33	1.47	1 (7%)
23	PSU	CW	32	23	13,21,22	1.22	1 (7%)	18,30,33	3.37	6 (33%)
23	MIA	CW	37	23	15,24,32	1.19	2 (13%)	16,35,47	2.34	2 (12%)
23	PSU	CW	39	23	13,21,22	1.29	1 (7%)	18,30,33	3.28	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	7MG	CW	46	23	19,26,27	1.05	1 (5%)	24,39,42	3.03	7 (29%)
23	5MU	CW	54	23	12,22,23	0.43	0	14,32,35	2.88	2 (14%)
23	PSU	CW	55	23	13,21,22	1.03	1 (7%)	18,30,33	3.61	6 (33%)
23	4SU	CW	8	23	11,21,22	1.20	1 (9%)	13,30,33	1.23	1 (7%)
24	5MC	CX	32	24	13,22,23	1.38	1 (7%)	15,32,35	0.96	1 (6%)
24	5MU	CX	54	24	12,22,23	0.42	0	14,32,35	2.07	2 (14%)
24	PSU	CX	55	24	13,21,22	1.18	1 (7%)	18,30,33	3.42	6 (33%)
24	4SU	CX	8	24	11,21,22	1.15	1 (9%)	13,30,33	1.76	1 (7%)
23	PSU	CY	32	23	13,21,22	0.97	1 (7%)	18,30,33	3.45	5 (27%)
23	MIA	CY	37	23	15,24,32	1.26	2 (13%)	16,35,47	2.18	2 (12%)
23	PSU	CY	39	23	13,21,22	1.39	2 (15%)	18,30,33	2.93	6 (33%)
23	7MG	CY	46	23	19,26,27	1.12	1 (5%)	24,39,42	2.89	6 (25%)
23	5MU	CY	54	23	12,22,23	0.37	0	14,32,35	2.21	2 (14%)
23	PSU	CY	55	23	13,21,22	0.88	1 (7%)	18,30,33	3.64	6 (33%)
23	4SU	CY	8	23	11,21,22	1.20	1 (9%)	13,30,33	1.36	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	AW	32	23	-	0/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	0/11/33/34	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	0/7/37/38	0/3/3/3
23	5MU	AW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/3/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/3/25/26	0/2/2/2
23	PSU	AY	32	23	-	0/7/25/26	0/2/2/2
23	MIA	AY	37	23	-	0/3/25/34	0/3/3/3
23	PSU	AY	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AY	46	23	-	0/7/37/38	0/3/3/3
23	5MU	AY	54	23	-	0/3/25/26	0/2/2/2
23	PSU	AY	55	23	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	4SU	AY	8	23	-	0/3/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	0/7/37/38	0/3/3/3
23	5MU	CW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	CW	8	23	-	0/3/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/3/25/26	0/2/2/2
23	PSU	CY	32	23	-	0/7/25/26	0/2/2/2
23	MIA	CY	37	23	-	0/3/25/34	0/3/3/3
23	PSU	CY	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CY	46	23	-	0/7/37/38	0/3/3/3
23	5MU	CY	54	23	-	0/3/25/26	0/2/2/2
23	PSU	CY	55	23	-	0/7/25/26	0/2/2/2
23	4SU	CY	8	23	-	0/3/25/26	0/2/2/2

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C2-S10	-6.81	1.70	1.75
24	AX	55	PSU	C5-C1'	-4.77	1.48	1.52
23	AW	39	PSU	C5-C1'	-4.58	1.48	1.52
23	AY	32	PSU	C5-C1'	-4.40	1.48	1.52
23	CW	39	PSU	C5-C1'	-4.19	1.48	1.52

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	55	PSU	N1-C2-N3	-12.34	120.46	128.33
23	AW	39	PSU	N1-C2-N3	-11.99	120.68	128.33
23	CY	32	PSU	N1-C2-N3	-11.22	121.17	128.33
23	AW	32	PSU	N1-C2-N3	-11.12	121.24	128.33
24	CX	55	PSU	N1-C2-N3	-10.85	121.41	128.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	32	PSU	1	0
23	AW	39	PSU	1	0
23	AW	46	7MG	1	0
23	AW	54	5MU	2	0
23	AW	55	PSU	3	0
23	AW	8	4SU	1	0
24	AX	8	4SU	1	0
23	AY	37	MIA	2	0
23	AY	39	PSU	1	0
23	AY	54	5MU	3	0
23	AY	55	PSU	3	0
23	AY	8	4SU	4	0
23	CW	32	PSU	1	0
23	CW	39	PSU	3	0
23	CW	46	7MG	3	0
23	CW	8	4SU	2	0
24	CX	54	5MU	2	0
24	CX	55	PSU	1	0
24	CX	8	4SU	1	0
23	CY	37	MIA	1	0
23	CY	39	PSU	1	0
23	CY	46	7MG	5	0
23	CY	54	5MU	1	0
23	CY	55	PSU	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2048 ligands modelled in this entry, 2027 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	NEG	AA	3216	56	11,16,16	8.67	1 (9%)	12,20,20	3.24	4 (33%)
57	NEG	AA	3217	-	11,16,16	7.85	1 (9%)	12,20,20	2.91	4 (33%)
57	NEG	AA	3218	56	11,16,16	8.40	1 (9%)	12,20,20	1.84	3 (25%)
57	NEG	AA	3219	-	11,16,16	8.06	1 (9%)	12,20,20	2.34	4 (33%)
57	NEG	AA	3220	-	11,16,16	7.84	1 (9%)	12,20,20	2.14	3 (25%)
57	NEG	AA	3221	-	11,16,16	8.87	1 (9%)	12,20,20	2.05	3 (25%)
57	NEG	AA	3222	-	11,16,16	8.22	1 (9%)	12,20,20	1.76	2 (16%)
58	SF4	AD	501	4	0,12,12	0.00	-	0,24,24	0.00	-
57	NEG	AW	3004	-	11,16,16	7.94	1 (9%)	12,20,20	2.74	4 (33%)
57	NEG	AX	3013	-	11,16,16	8.77	1 (9%)	12,20,20	2.98	5 (41%)
57	NEG	CA	3170	56	11,16,16	8.43	1 (9%)	12,20,20	1.41	2 (16%)
57	NEG	CA	3171	-	11,16,16	7.92	1 (9%)	12,20,20	3.33	5 (41%)
57	NEG	CA	3172	-	11,16,16	8.61	1 (9%)	12,20,20	2.29	3 (25%)
57	NEG	CA	3173	-	11,16,16	8.19	1 (9%)	12,20,20	1.82	3 (25%)
57	NEG	CA	3174	-	11,16,16	7.74	1 (9%)	12,20,20	3.98	3 (25%)
57	NEG	CA	3175	-	11,16,16	8.50	2 (18%)	12,20,20	3.10	7 (58%)
57	NEG	CA	3176	-	11,16,16	8.37	1 (9%)	12,20,20	1.64	2 (16%)
57	NEG	CA	3177	-	11,16,16	7.43	2 (18%)	12,20,20	3.75	6 (50%)
58	SF4	CD	302	4	0,12,12	0.00	-	0,24,24	0.00	-
57	NEG	CW	3002	-	11,16,16	7.97	1 (9%)	12,20,20	2.47	4 (33%)
57	NEG	CX	3004	-	11,16,16	8.31	1 (9%)	12,20,20	1.83	3 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	NEG	AA	3216	56	-	0/15/18/18	0/0/0/0
57	NEG	AA	3217	-	-	0/15/18/18	0/0/0/0
57	NEG	AA	3218	56	-	0/15/18/18	0/0/0/0
57	NEG	AA	3219	-	-	0/15/18/18	0/0/0/0
57	NEG	AA	3220	-	-	0/15/18/18	0/0/0/0
57	NEG	AA	3221	-	-	0/15/18/18	0/0/0/0
57	NEG	AA	3222	-	-	0/15/18/18	0/0/0/0
58	SF4	AD	501	4	-	0/0/48/48	0/6/5/5
57	NEG	AW	3004	-	-	0/15/18/18	0/0/0/0
57	NEG	AX	3013	-	-	0/15/18/18	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	NEG	CA	3170	56	-	0/15/18/18	0/0/0/0
57	NEG	CA	3171	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3172	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3173	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3174	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3175	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3176	-	-	0/15/18/18	0/0/0/0
57	NEG	CA	3177	-	-	0/15/18/18	0/0/0/0
58	SF4	CD	302	4	-	0/0/48/48	0/6/5/5
57	NEG	CW	3002	-	-	0/15/18/18	0/0/0/0
57	NEG	CX	3004	-	-	0/15/18/18	0/0/0/0

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	3221	NEG	N2-N3	-29.34	1.11	1.41
57	AX	3013	NEG	N2-N3	-28.98	1.11	1.41
57	AA	3216	NEG	N2-N3	-28.69	1.11	1.41
57	CA	3172	NEG	N2-N3	-28.49	1.12	1.41
57	CA	3175	NEG	N2-N3	-28.07	1.12	1.41

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	3216	NEG	C4-C5-C6	-8.07	103.90	112.61
57	CA	3171	NEG	C4-C5-C6	-7.81	104.18	112.61
57	AW	3004	NEG	C4-C5-C6	-7.11	104.94	112.61
57	AA	3217	NEG	C4-C5-C6	-6.55	105.54	112.61
57	CA	3172	NEG	C6-N2-N3	-5.89	114.40	120.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	3216	NEG	7	0
57	AA	3217	NEG	1	0
57	AA	3218	NEG	1	0
57	AA	3219	NEG	1	0
57	AA	3220	NEG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	3221	NEG	4	0
57	AW	3004	NEG	2	0
57	AX	3013	NEG	3	0
57	CA	3171	NEG	1	0
57	CA	3173	NEG	2	0
57	CA	3174	NEG	5	0
57	CA	3175	NEG	3	0
57	CA	3177	NEG	2	0
57	CW	3002	NEG	1	0
57	CX	3004	NEG	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1496/1521 (98%)	0.58	34 (2%) 64 64	36, 68, 97, 112	0
1	CA	1503/1521 (98%)	0.43	33 (2%) 65 66	38, 71, 97, 111	0
2	AB	231/256 (90%)	0.59	15 (6%) 22 20	67, 83, 93, 99	0
2	CB	231/256 (90%)	1.07	45 (19%) 1 1	69, 85, 94, 100	0
3	AC	206/239 (86%)	0.87	32 (15%) 3 2	65, 78, 88, 96	0
3	CC	206/239 (86%)	1.14	41 (19%) 1 1	68, 80, 90, 96	0
4	AD	208/209 (99%)	0.92	30 (14%) 3 3	53, 68, 80, 87	0
4	CD	208/209 (99%)	0.90	17 (8%) 14 11	54, 67, 80, 90	0
5	AE	148/162 (91%)	0.82	10 (6%) 20 19	54, 70, 81, 86	0
5	CE	148/162 (91%)	0.95	17 (11%) 6 5	57, 72, 82, 88	0
6	AF	100/101 (99%)	0.55	2 (2%) 68 69	53, 67, 78, 87	0
6	CF	100/101 (99%)	0.20	0 100 100	54, 68, 80, 87	0
7	AG	155/156 (99%)	0.69	15 (9%) 10 7	62, 75, 86, 95	0
7	CG	155/156 (99%)	0.93	20 (12%) 5 4	63, 77, 86, 99	0
8	AH	137/138 (99%)	1.16	28 (20%) 1 1	57, 70, 78, 85	0
8	CH	137/138 (99%)	1.05	26 (18%) 2 1	60, 72, 81, 85	0
9	AI	127/128 (99%)	1.04	24 (18%) 2 1	57, 82, 90, 94	0
9	CI	127/128 (99%)	2.02	63 (49%) 0 0	65, 84, 91, 95	0
10	AJ	97/105 (92%)	1.31	33 (34%) 0 0	63, 85, 94, 98	0
10	CJ	96/105 (91%)	1.38	29 (30%) 1 0	65, 86, 94, 99	0
11	AK	114/129 (88%)	0.89	5 (4%) 38 37	47, 66, 78, 84	0
11	CK	114/129 (88%)	0.75	11 (9%) 10 8	49, 68, 79, 85	0
12	AL	122/132 (92%)	0.89	10 (8%) 14 11	48, 57, 69, 79	0
12	CL	122/132 (92%)	0.99	20 (16%) 2 2	50, 60, 71, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	123/126 (97%)	0.59	5 (4%) 41 41	52, 70, 84, 96	0
13	CM	122/126 (96%)	1.19	24 (19%) 1 1	70, 83, 93, 99	0
14	AN	60/61 (98%)	1.52	18 (30%) 1 0	64, 77, 83, 89	0
14	CN	60/61 (98%)	2.74	35 (58%) 0 0	67, 80, 87, 90	0
15	AO	88/89 (98%)	0.60	4 (4%) 37 36	49, 66, 77, 84	0
15	CO	88/89 (98%)	0.79	11 (12%) 5 4	51, 67, 79, 85	0
16	AP	82/88 (93%)	1.10	10 (12%) 5 4	53, 67, 78, 82	0
16	CP	82/88 (93%)	0.85	2 (2%) 62 62	54, 66, 77, 82	0
17	AQ	99/105 (94%)	0.85	8 (8%) 15 12	53, 69, 81, 83	0
17	CQ	99/105 (94%)	1.69	33 (33%) 0 0	55, 70, 81, 85	0
18	AR	68/88 (77%)	0.62	3 (4%) 38 37	54, 67, 80, 82	0
18	CR	68/88 (77%)	0.40	2 (2%) 55 55	54, 69, 81, 85	0
19	AS	83/93 (89%)	0.66	3 (3%) 46 46	68, 80, 88, 97	0
19	CS	83/93 (89%)	1.25	21 (25%) 1 1	71, 82, 91, 97	0
20	AT	96/106 (90%)	0.72	7 (7%) 18 16	57, 69, 85, 90	0
20	CT	96/106 (90%)	0.98	15 (15%) 3 2	56, 69, 85, 90	0
21	AU	23/27 (85%)	1.38	7 (30%) 1 0	62, 71, 78, 81	0
21	CU	23/27 (85%)	2.04	11 (47%) 0 0	65, 74, 80, 83	0
22	AV	13/24 (54%)	1.90	6 (46%) 0 0	51, 61, 91, 97	0
22	CV	12/24 (50%)	1.69	4 (33%) 0 0	55, 65, 91, 92	0
23	AW	67/76 (88%)	1.44	21 (31%) 1 0	50, 93, 102, 108	0
23	AY	67/76 (88%)	1.34	19 (28%) 1 0	37, 101, 106, 107	0
23	CW	65/76 (85%)	1.27	17 (26%) 1 1	69, 100, 108, 110	0
23	CY	66/76 (86%)	1.30	14 (21%) 1 1	40, 101, 106, 107	0
24	AX	72/77 (93%)	0.78	4 (5%) 28 26	45, 69, 85, 96	0
24	CX	72/77 (93%)	0.63	5 (6%) 20 18	46, 72, 87, 98	0
25	BA	2822/2915 (96%)	0.99	82 (2%) 55 55	22, 42, 94, 110	0
25	DA	2800/2915 (96%)	0.48	78 (2%) 56 57	25, 47, 96, 113	0
26	BB	120/121 (99%)	0.64	0 100 100	41, 61, 72, 92	0
26	DB	120/121 (99%)	0.08	1 (0%) 87 88	48, 67, 78, 93	0
27	BD	275/276 (99%)	1.00	13 (4%) 35 34	21, 38, 55, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
27	DD	275/276 (99%)	0.77	9 (3%)	50	50	23, 41, 57, 85	0
28	BE	204/206 (99%)	0.86	6 (2%)	55	55	19, 45, 67, 84	0
28	DE	204/206 (99%)	0.58	6 (2%)	55	55	22, 49, 69, 84	0
29	BF	203/210 (96%)	0.78	7 (3%)	49	49	23, 50, 74, 95	0
29	DF	203/210 (96%)	0.67	14 (6%)	20	18	25, 55, 77, 95	0
30	BG	181/182 (99%)	0.59	6 (3%)	50	50	52, 68, 82, 94	0
30	DG	181/182 (99%)	1.02	30 (16%)	2	2	57, 72, 84, 92	0
31	BH	174/180 (96%)	0.82	5 (2%)	55	55	51, 69, 80, 87	0
31	DH	174/180 (96%)	1.36	44 (25%)	1	1	57, 74, 84, 88	0
32	BI	146/148 (98%)	0.33	3 (2%)	67	68	45, 71, 84, 88	0
32	DI	146/148 (98%)	0.29	4 (2%)	58	58	46, 72, 84, 89	0
33	BN	140/140 (100%)	0.90	4 (2%)	55	55	32, 48, 69, 78	0
33	DN	140/140 (100%)	0.87	15 (10%)	8	6	37, 53, 72, 79	0
34	BO	122/122 (100%)	0.60	0	100	100	23, 39, 59, 65	0
34	DO	122/122 (100%)	1.06	14 (11%)	6	5	43, 58, 72, 84	0
35	BP	149/150 (99%)	0.82	4 (2%)	58	58	23, 53, 76, 82	0
35	DP	149/150 (99%)	0.95	20 (13%)	4	3	28, 57, 78, 83	0
36	BQ	141/141 (100%)	1.18	18 (12%)	5	4	32, 53, 69, 81	0
36	DQ	141/141 (100%)	1.14	27 (19%)	2	1	36, 58, 73, 82	0
37	BR	118/118 (100%)	0.79	3 (2%)	61	61	19, 33, 48, 59	0
37	DR	118/118 (100%)	0.74	3 (2%)	61	61	32, 51, 65, 78	0
38	BS	110/112 (98%)	0.73	1 (0%)	85	86	36, 50, 67, 72	0
38	DS	110/112 (98%)	0.54	7 (6%)	23	21	64, 77, 88, 94	0
39	BT	131/146 (89%)	0.50	2 (1%)	76	76	28, 41, 69, 88	0
39	DT	131/146 (89%)	0.83	10 (7%)	17	15	45, 60, 78, 88	0
40	BU	116/118 (98%)	0.84	2 (1%)	73	74	17, 29, 43, 67	0
40	DU	116/118 (98%)	1.23	27 (23%)	1	1	36, 64, 80, 89	0
41	BV	101/101 (100%)	0.46	0	100	100	18, 36, 55, 73	0
41	DV	101/101 (100%)	1.26	21 (20%)	1	1	42, 77, 87, 93	0
42	BW	112/113 (99%)	0.83	3 (2%)	58	58	17, 29, 52, 89	0
42	DW	112/113 (99%)	0.88	6 (5%)	29	28	35, 49, 71, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BX	95/96 (98%)	0.57	2 (2%) 67 68	15, 33, 65, 84	0
43	DX	95/96 (98%)	1.17	16 (16%) 2 2	38, 57, 76, 84	0
44	BY	107/110 (97%)	0.47	1 (0%) 85 86	33, 48, 75, 84	0
44	DY	107/110 (97%)	1.56	31 (28%) 1 0	54, 70, 86, 93	0
45	BZ	171/206 (83%)	1.32	30 (17%) 2 1	38, 69, 102, 108	0
45	DZ	174/206 (84%)	1.56	51 (29%) 1 0	71, 88, 101, 108	0
46	B0	83/85 (97%)	1.10	9 (10%) 8 6	25, 37, 67, 83	0
46	D0	83/85 (97%)	1.68	19 (22%) 1 1	46, 69, 81, 91	0
47	B1	97/98 (98%)	0.95	5 (5%) 31 30	19, 40, 69, 76	0
47	D1	97/98 (98%)	0.71	2 (2%) 67 68	33, 53, 77, 79	0
48	B2	70/72 (97%)	0.65	1 (1%) 78 77	32, 42, 62, 80	0
48	D2	70/72 (97%)	0.84	5 (7%) 19 17	54, 70, 81, 84	0
49	B3	59/60 (98%)	0.59	0 100 100	22, 36, 55, 80	0
49	D3	59/60 (98%)	1.97	24 (40%) 0 0	52, 67, 82, 85	0
50	B4	69/71 (97%)	0.37	3 (4%) 39 38	53, 73, 93, 94	0
50	D4	69/71 (97%)	0.87	12 (17%) 2 1	76, 87, 99, 107	0
51	B5	59/60 (98%)	0.84	2 (3%) 49 49	18, 31, 46, 68	0
51	D5	59/60 (98%)	0.66	1 (1%) 73 74	28, 50, 68, 77	0
52	B6	53/54 (98%)	0.63	0 100 100	29, 40, 59, 67	0
52	D6	53/54 (98%)	0.89	4 (7%) 17 15	47, 61, 75, 79	0
53	B7	48/49 (97%)	1.10	6 (12%) 5 4	16, 25, 55, 66	0
53	D7	48/49 (97%)	1.30	6 (12%) 5 4	28, 37, 62, 71	0
54	B8	64/65 (98%)	0.77	2 (3%) 52 52	23, 32, 43, 58	0
54	D8	64/65 (98%)	1.45	15 (23%) 1 1	43, 57, 65, 71	0
55	B9	37/37 (100%)	1.45	9 (24%) 1 1	31, 50, 69, 75	0
55	D9	37/37 (100%)	1.54	13 (35%) 0 0	49, 60, 73, 77	0
All	All	20900/21748 (96%)	0.81	1633 (7%) 16 14	15, 62, 92, 113	0

The worst 5 of 1633 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CG	82	GLY	17.6
13	CM	124	PRO	15.5

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Mol	Chain	Res	Type	RSRZ
13	AM	123	ALA	13.8
45	BZ	111	VAL	12.9
45	BZ	115	GLY	12.5

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
23	PSU	AY	32	20/21	0.92	0.17	-	83,93,99,105	0
24	4SU	AX	8	20/21	0.95	0.20	-	47,62,81,87	0
24	5MC	CX	32	21/22	0.95	0.22	-	63,72,77,80	0
23	PSU	AW	32	20/21	0.96	0.21	-	39,59,64,65	0
23	5MU	CY	54	21/22	0.80	0.30	-	88,99,111,135	0
24	PSU	CX	55	20/21	0.91	0.15	-	62,70,83,92	0
23	5MU	CW	54	21/22	0.92	0.14	-	72,81,90,93	0
23	4SU	CW	8	20/21	0.72	0.22	-	85,105,116,130	0
23	4SU	AW	8	20/21	0.89	0.16	-	81,89,100,121	0
24	5MU	CX	54	21/22	0.94	0.24	-	69,80,89,95	0
23	PSU	CW	39	20/21	0.95	0.26	-	62,79,88,94	0
23	MIA	CW	37	22/30	0.94	0.20	-	53,72,83,85	0
24	PSU	AX	55	20/21	0.94	0.18	-	60,68,83,92	0
23	5MU	AW	54	21/22	0.93	0.23	-	57,76,85,89	0
23	7MG	CY	46	24/25	0.72	0.24	-	91,105,113,139	0
23	4SU	AY	8	20/21	0.77	0.20	-	99,105,115,127	0
23	PSU	CY	39	20/21	0.84	0.22	-	79,92,100,112	0
23	7MG	CW	46	24/25	0.82	0.24	-	93,104,114,127	0
23	4SU	CY	8	20/21	0.69	0.25	-	95,103,122,140	0
23	PSU	AW	39	20/21	0.96	0.21	-	37,57,68,72	0
23	MIA	AY	37	22/30	0.83	0.22	-	82,91,103,118	0
23	MIA	CY	37	22/30	0.86	0.27	-	75,93,102,117	0
23	PSU	CY	55	20/21	0.73	0.36	-	91,104,118,129	0
23	7MG	AY	46	24/25	0.81	0.28	-	92,100,111,135	0
23	7MG	AW	46	24/25	0.82	0.15	-	74,94,116,138	0
24	5MU	AX	54	21/22	0.95	0.17	-	60,70,77,80	0
24	4SU	CX	8	20/21	0.92	0.20	-	73,82,90,90	0
23	PSU	CW	32	20/21	0.95	0.23	-	62,82,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	PSU	CY	32	20/21	0.85	0.20	-	83,95,100,107	0
23	PSU	AY	55	20/21	0.70	0.25	-	88,103,115,132	0
23	PSU	CW	55	20/21	0.79	0.20	-	76,95,105,108	0
23	PSU	AW	55	20/21	0.81	0.26	-	57,85,93,93	0
23	5MU	AY	54	21/22	0.76	0.29	-	85,97,115,141	0
24	5MC	AX	32	21/22	0.97	0.24	-	38,56,66,77	0
23	PSU	AY	39	20/21	0.92	0.22	-	76,89,100,102	0
23	MIA	AW	37	29/30	0.96	0.27	-	36,49,67,72	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3182	1/1	0.90	0.92	83.37	50,50,50,50	0
56	MG	BA	3127	1/1	0.86	0.58	79.97	38,38,38,38	0
56	MG	DA	3086	1/1	0.83	0.90	66.41	42,42,42,42	0
56	MG	BA	3615	1/1	0.94	0.72	66.20	41,41,41,41	0
56	MG	BA	3160	1/1	0.92	0.64	58.15	58,58,58,58	0
56	MG	BA	3776	1/1	0.96	1.10	56.08	52,52,52,52	0
56	MG	BU	206	1/1	0.95	0.88	55.07	54,54,54,54	0
56	MG	BA	3164	1/1	0.96	0.54	35.67	33,33,33,33	0
56	MG	BA	3094	1/1	0.97	0.79	35.59	49,49,49,49	0
56	MG	DA	3023	1/1	0.90	1.12	29.37	44,44,44,44	0
56	MG	DA	3415	1/1	0.95	0.58	29.28	45,45,45,45	0
56	MG	BU	209	1/1	0.96	0.65	29.07	41,41,41,41	0
56	MG	BA	3238	1/1	0.98	0.63	28.01	35,35,35,35	0
56	MG	B5	103	1/1	0.77	0.68	26.65	51,51,51,51	0
56	MG	DF	306	1/1	0.94	1.20	24.96	55,55,55,55	0
56	MG	BA	3110	1/1	0.94	0.72	22.77	49,49,49,49	0
56	MG	BA	3089	1/1	0.95	0.59	22.36	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BV	205	1/1	0.94	0.71	21.81	37,37,37,37	0
56	MG	BQ	3001	1/1	0.94	0.98	20.30	52,52,52,52	0
56	MG	DA	3160	1/1	0.93	0.52	20.06	51,51,51,51	0
56	MG	BA	3188	1/1	0.98	0.53	19.76	41,41,41,41	0
56	MG	BF	308	1/1	0.96	0.72	19.13	40,40,40,40	0
56	MG	BA	3132	1/1	0.89	0.53	18.43	42,42,42,42	0
56	MG	BA	3026	1/1	0.98	0.39	16.16	41,41,41,41	0
56	MG	DR	3001	1/1	0.93	0.66	16.09	55,55,55,55	0
56	MG	BA	3131	1/1	0.91	0.46	15.84	35,35,35,35	0
56	MG	DA	3065	1/1	0.86	0.51	15.54	56,56,56,56	0
56	MG	BA	3116	1/1	0.91	0.42	15.53	68,68,68,68	0
56	MG	BA	3028	1/1	0.95	0.55	15.35	48,48,48,48	0
56	MG	AE	3002	1/1	0.89	0.50	15.02	67,67,67,67	0
56	MG	BA	3091	1/1	0.97	0.63	14.96	43,43,43,43	0
56	MG	BN	3004	1/1	0.93	0.78	14.93	60,60,60,60	0
56	MG	BA	3190	1/1	0.97	0.67	14.91	35,35,35,35	0
56	MG	BA	3027	1/1	0.97	0.44	14.73	41,41,41,41	0
56	MG	BN	3006	1/1	0.94	0.62	14.56	54,54,54,54	0
56	MG	BA	3777	1/1	0.94	0.55	14.33	40,40,40,40	0
56	MG	BE	304	1/1	0.95	0.50	14.19	42,42,42,42	0
56	MG	DU	3001	1/1	0.88	0.98	13.85	61,61,61,61	0
56	MG	BA	3774	1/1	0.97	0.64	13.67	32,32,32,32	0
56	MG	BU	205	1/1	0.94	0.63	13.59	39,39,39,39	0
56	MG	BA	3022	1/1	0.95	0.50	13.54	41,41,41,41	0
56	MG	CA	3092	1/1	0.90	0.23	13.51	55,55,55,55	0
56	MG	BA	3562	1/1	0.92	0.42	13.18	37,37,37,37	0
56	MG	AA	3127	1/1	0.90	0.29	12.90	52,52,52,52	0
56	MG	BA	3136	1/1	0.84	0.60	12.74	49,49,49,49	0
56	MG	BV	202	1/1	0.94	0.40	12.68	34,34,34,34	0
56	MG	BN	3001	1/1	0.86	0.62	12.57	51,51,51,51	0
56	MG	BF	305	1/1	0.95	0.46	12.37	40,40,40,40	0
56	MG	B5	101	1/1	0.94	0.62	12.26	42,42,42,42	0
56	MG	DE	301	1/1	0.98	0.89	12.04	50,50,50,50	0
56	MG	BU	202	1/1	0.95	0.45	11.93	32,32,32,32	0
56	MG	B7	102	1/1	0.94	0.47	11.50	40,40,40,40	0
56	MG	BF	309	1/1	0.95	0.49	11.30	40,40,40,40	0
56	MG	B5	102	1/1	0.92	0.57	11.13	42,42,42,42	0
56	MG	AA	3172	1/1	0.96	0.32	10.68	44,44,44,44	0
56	MG	AX	3010	1/1	0.87	0.49	10.56	54,54,54,54	0
56	MG	BD	311	1/1	0.90	0.71	10.48	46,46,46,46	0
56	MG	DA	3024	1/1	0.97	0.53	10.32	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3078	1/1	0.85	0.31	10.14	64,64,64,64	0
56	MG	BF	302	1/1	0.97	0.45	10.05	29,29,29,29	0
56	MG	BD	309	1/1	0.98	0.64	9.98	39,39,39,39	0
56	MG	BA	3672	1/1	0.97	0.34	9.49	37,37,37,37	0
56	MG	DD	308	1/1	0.97	0.55	9.27	45,45,45,45	0
56	MG	DA	3251	1/1	0.93	0.33	9.21	47,47,47,47	0
56	MG	BF	306	1/1	0.92	0.48	9.21	41,41,41,41	0
56	MG	BA	3327	1/1	0.61	0.37	9.13	74,74,74,74	0
56	MG	BA	3029	1/1	0.96	0.33	8.97	44,44,44,44	0
56	MG	DA	3361	1/1	0.94	0.35	8.82	45,45,45,45	0
56	MG	D7	101	1/1	0.94	0.48	8.81	33,33,33,33	0
56	MG	BA	3785	1/1	0.97	0.52	8.79	42,42,42,42	0
56	MG	BR	202	1/1	0.77	0.49	8.77	51,51,51,51	0
56	MG	BA	3460	1/1	0.93	0.43	8.57	45,45,45,45	0
56	MG	DA	3621	1/1	0.83	0.41	8.54	73,73,73,73	0
56	MG	B0	101	1/1	0.93	0.40	8.43	49,49,49,49	0
56	MG	CA	3035	1/1	0.94	0.29	8.08	52,52,52,52	0
56	MG	DD	306	1/1	0.97	0.55	8.05	35,35,35,35	0
56	MG	BA	3773	1/1	0.85	0.39	8.02	43,43,43,43	0
56	MG	BA	3143	1/1	0.88	0.37	7.79	35,35,35,35	0
56	MG	BA	3018	1/1	0.99	0.47	7.73	36,36,36,36	0
56	MG	DA	3449	1/1	0.94	0.35	7.68	49,49,49,49	0
56	MG	BR	201	1/1	0.92	0.55	7.59	40,40,40,40	0
56	MG	BF	301	1/1	0.94	0.41	7.41	39,39,39,39	0
56	MG	BA	3495	1/1	0.95	0.32	7.16	44,44,44,44	0
56	MG	DA	3037	1/1	0.89	0.40	7.12	46,46,46,46	0
56	MG	DD	304	1/1	0.96	0.44	7.10	56,56,56,56	0
56	MG	BA	3472	1/1	0.97	0.40	6.80	43,43,43,43	0
56	MG	DQ	3003	1/1	0.95	0.58	6.79	64,64,64,64	0
56	MG	BA	3141	1/1	0.93	0.42	6.69	55,55,55,55	0
56	MG	BD	307	1/1	0.95	0.38	6.64	38,38,38,38	0
56	MG	DA	3006	1/1	0.87	0.36	6.62	42,42,42,42	0
56	MG	DA	3025	1/1	0.91	0.71	6.22	49,49,49,49	0
56	MG	DA	3316	1/1	0.95	0.38	6.20	48,48,48,48	0
56	MG	BP	201	1/1	0.96	0.42	6.14	36,36,36,36	0
56	MG	DV	3002	1/1	0.98	0.70	6.02	51,51,51,51	0
56	MG	BA	3244	1/1	0.89	0.34	5.99	53,53,53,53	0
56	MG	BF	304	1/1	0.96	0.47	5.96	37,37,37,37	0
56	MG	AA	3094	1/1	0.90	0.30	5.83	53,53,53,53	0
57	NEG	AA	3221	17/17	0.90	0.34	5.80	44,57,69,70	0
56	MG	DA	3071	1/1	0.97	0.32	5.67	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3782	1/1	0.97	0.37	5.58	48,48,48,48	0
57	NEG	CA	3170	17/17	0.87	0.36	5.44	58,72,83,86	0
57	NEG	CA	3175	17/17	0.88	0.39	5.44	48,61,79,89	0
56	MG	DA	3186	1/1	0.94	0.47	5.39	41,41,41,41	0
56	MG	AA	3034	1/1	0.89	0.24	5.38	56,56,56,56	0
56	MG	BA	3642	1/1	0.97	0.28	5.24	38,38,38,38	0
56	MG	BD	304	1/1	0.97	0.41	5.01	50,50,50,50	0
56	MG	DA	3015	1/1	0.97	0.45	4.98	49,49,49,49	0
56	MG	CA	3048	1/1	0.93	0.25	4.93	54,54,54,54	0
56	MG	BA	3649	1/1	0.89	0.27	4.92	49,49,49,49	0
56	MG	BU	207	1/1	0.98	0.40	4.84	22,22,22,22	0
57	NEG	CA	3174	17/17	0.83	0.29	4.84	38,53,68,69	0
56	MG	BU	208	1/1	0.98	0.36	4.83	35,35,35,35	0
57	NEG	AA	3219	17/17	0.91	0.30	4.82	61,71,78,79	0
56	MG	BA	3769	1/1	0.97	0.34	4.75	52,52,52,52	0
57	NEG	CX	3004	17/17	0.86	0.26	4.74	32,64,79,84	0
56	MG	DF	305	1/1	0.93	0.46	4.74	45,45,45,45	0
56	MG	DA	3244	1/1	0.98	0.27	4.52	58,58,58,58	0
56	MG	BD	305	1/1	0.89	0.32	4.38	41,41,41,41	0
57	NEG	CA	3173	17/17	0.84	0.31	4.37	54,76,85,86	0
56	MG	BA	3237	1/1	0.98	0.38	4.36	43,43,43,43	0
56	MG	BV	207	1/1	0.93	0.30	4.30	42,42,42,42	0
56	MG	BA	3541	1/1	0.95	0.35	4.24	31,31,31,31	0
56	MG	BA	3106	1/1	0.98	0.43	4.21	42,42,42,42	0
56	MG	BQ	3005	1/1	0.95	0.49	4.10	49,49,49,49	0
56	MG	BX	102	1/1	0.92	0.29	4.03	40,40,40,40	0
56	MG	BA	3271	1/1	0.94	0.26	4.02	39,39,39,39	0
56	MG	BA	3440	1/1	0.93	0.33	4.01	41,41,41,41	0
57	NEG	CA	3177	17/17	0.90	0.24	3.89	36,63,74,81	0
56	MG	BA	3203	1/1	0.93	0.31	3.80	51,51,51,51	0
56	MG	BA	3354	1/1	0.95	0.27	3.68	39,39,39,39	0
56	MG	DD	307	1/1	0.97	0.33	3.66	56,56,56,56	0
56	MG	D3	3001	1/1	0.95	0.61	3.63	70,70,70,70	0
56	MG	DA	3125	1/1	0.88	0.51	3.63	56,56,56,56	0
56	MG	BA	3209	1/1	0.88	0.36	3.41	57,57,57,57	0
56	MG	BA	3025	1/1	0.94	0.33	3.39	37,37,37,37	0
57	NEG	AA	3216	17/17	0.94	0.31	3.37	34,56,70,74	0
56	MG	DA	3558	1/1	0.94	0.35	3.33	48,48,48,48	0
56	MG	BA	3757	1/1	0.87	0.28	3.30	47,47,47,47	0
56	MG	DA	3233	1/1	0.97	0.23	3.30	40,40,40,40	0
56	MG	BU	201	1/1	0.89	0.33	3.27	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3052	1/1	0.88	0.30	3.27	52,52,52,52	0
56	MG	DA	3617	1/1	0.95	0.38	3.23	55,55,55,55	0
56	MG	BA	3668	1/1	0.95	0.29	3.14	42,42,42,42	0
56	MG	BA	3061	1/1	0.92	0.31	3.11	48,48,48,48	0
57	NEG	AW	3004	17/17	0.89	0.37	3.02	37,50,72,73	0
56	MG	DA	3284	1/1	0.93	0.26	2.81	40,40,40,40	0
56	MG	DA	3156	1/1	0.96	0.23	2.81	45,45,45,45	0
56	MG	BA	3105	1/1	0.94	0.30	2.78	43,43,43,43	0
56	MG	BD	308	1/1	0.90	0.26	2.70	42,42,42,42	0
56	MG	DA	3553	1/1	0.91	0.23	2.67	45,45,45,45	0
57	NEG	AA	3222	17/17	0.90	0.29	2.66	30,45,63,66	0
56	MG	BP	202	1/1	0.96	0.32	2.64	36,36,36,36	0
56	MG	BA	3399	1/1	0.92	0.25	2.64	62,62,62,62	0
56	MG	CA	3140	1/1	0.95	0.27	2.60	49,49,49,49	0
56	MG	DA	3168	1/1	0.97	0.27	2.59	41,41,41,41	0
56	MG	BA	3220	1/1	0.96	0.26	2.56	45,45,45,45	0
56	MG	CA	3032	1/1	0.95	0.24	2.46	52,52,52,52	0
56	MG	AX	3002	1/1	0.79	0.24	2.35	71,71,71,71	0
56	MG	DV	3001	1/1	0.98	0.34	2.26	75,75,75,75	0
56	MG	AA	3130	1/1	0.87	0.21	2.26	74,74,74,74	0
56	MG	CA	3055	1/1	0.80	0.19	2.25	63,63,63,63	0
56	MG	DA	3471	1/1	0.90	0.20	2.24	58,58,58,58	0
56	MG	BA	3194	1/1	0.95	0.27	2.23	40,40,40,40	0
56	MG	BA	3783	1/1	0.89	0.29	2.16	36,36,36,36	0
56	MG	DW	3002	1/1	0.98	0.40	2.13	32,32,32,32	0
56	MG	BA	3479	1/1	0.94	0.27	2.06	36,36,36,36	0
56	MG	BA	3007	1/1	0.88	0.34	2.05	39,39,39,39	0
59	ZN	B5	105	1/1	0.99	0.26	2.02	52,52,52,52	0
56	MG	DA	3216	1/1	0.87	0.28	1.99	52,52,52,52	0
56	MG	CA	3168	1/1	0.92	0.26	1.99	62,62,62,62	0
56	MG	DO	201	1/1	0.73	0.38	1.90	59,59,59,59	0
56	MG	DA	3142	1/1	0.84	0.27	1.86	55,55,55,55	0
56	MG	BD	303	1/1	0.89	0.34	1.83	45,45,45,45	0
59	ZN	D5	501	1/1	0.99	0.21	1.81	57,57,57,57	0
56	MG	AA	3059	1/1	0.88	0.22	1.73	53,53,53,53	0
59	ZN	B4	501	1/1	0.98	0.18	1.69	86,86,86,86	0
56	MG	DA	3360	1/1	0.95	0.20	1.63	47,47,47,47	0
56	MG	BA	3505	1/1	0.87	0.29	1.62	54,54,54,54	0
57	NEG	CA	3176	17/17	0.91	0.30	1.59	46,65,76,84	0
56	MG	BD	302	1/1	0.97	0.30	1.58	33,33,33,33	0
56	MG	BN	3002	1/1	0.67	0.31	1.57	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B3	3001	1/1	0.95	0.33	1.55	41,41,41,41	0
56	MG	DA	3556	1/1	0.96	0.41	1.54	48,48,48,48	0
56	MG	AA	3146	1/1	0.82	0.21	1.52	65,65,65,65	0
56	MG	DA	3465	1/1	0.92	0.23	1.51	52,52,52,52	0
56	MG	CA	3089	1/1	0.97	0.25	1.50	46,46,46,46	0
57	NEG	AA	3217	17/17	0.90	0.27	1.48	45,55,78,95	0
56	MG	BA	3079	1/1	0.96	0.25	1.33	40,40,40,40	0
56	MG	DA	3424	1/1	0.96	0.31	1.33	35,35,35,35	0
57	NEG	CW	3002	17/17	0.88	0.31	1.31	41,56,78,84	0
56	MG	DU	3003	1/1	0.91	0.32	1.29	50,50,50,50	0
56	MG	BU	203	1/1	0.97	0.28	1.28	34,34,34,34	0
56	MG	DQ	3004	1/1	0.84	0.28	1.25	65,65,65,65	0
59	ZN	BY	501	1/1	0.98	0.20	1.25	60,60,60,60	0
56	MG	CA	3094	1/1	0.96	0.22	1.22	48,48,48,48	0
57	NEG	AX	3013	17/17	0.90	0.26	1.22	29,49,69,70	0
56	MG	BV	203	1/1	0.99	0.28	1.18	31,31,31,31	0
56	MG	BD	310	1/1	0.95	0.29	1.18	45,45,45,45	0
56	MG	BA	3260	1/1	0.91	0.28	1.17	52,52,52,52	0
56	MG	BA	3201	1/1	0.87	0.24	1.13	49,49,49,49	0
57	NEG	AA	3220	17/17	0.93	0.26	1.06	29,49,59,65	0
56	MG	BA	3198	1/1	0.93	0.28	1.05	35,35,35,35	0
56	MG	AA	3073	1/1	0.94	0.23	0.97	60,60,60,60	0
56	MG	BA	3637	1/1	0.67	0.27	0.97	34,34,34,34	0
56	MG	AA	3087	1/1	0.78	0.17	0.96	59,59,59,59	0
56	MG	AA	3215	1/1	0.87	0.24	0.91	56,56,56,56	0
56	MG	BA	3156	1/1	0.95	0.16	0.90	64,64,64,64	0
56	MG	BU	204	1/1	0.86	0.27	0.86	43,43,43,43	0
59	ZN	B6	102	1/1	0.99	0.23	0.84	43,43,43,43	0
56	MG	CA	3129	1/1	0.93	0.20	0.79	49,49,49,49	0
56	MG	BA	3423	1/1	0.98	0.23	0.76	43,43,43,43	0
56	MG	BA	3322	1/1	0.69	0.23	0.72	58,58,58,58	0
56	MG	AA	3211	1/1	0.94	0.23	0.71	41,41,41,41	0
56	MG	DA	3615	1/1	0.83	0.26	0.68	59,59,59,59	0
56	MG	AA	3012	1/1	0.98	0.22	0.67	43,43,43,43	0
56	MG	DF	302	1/1	0.91	0.22	0.66	60,60,60,60	0
56	MG	CA	3056	1/1	0.90	0.17	0.66	74,74,74,74	0
57	NEG	AA	3218	17/17	0.91	0.21	0.64	57,72,76,91	0
56	MG	DA	3292	1/1	0.90	0.23	0.62	36,36,36,36	0
56	MG	BA	3359	1/1	0.88	0.25	0.61	43,43,43,43	0
56	MG	AA	3145	1/1	0.92	0.23	0.55	36,36,36,36	0
56	MG	BR	203	1/1	0.97	0.25	0.41	36,36,36,36	0
57	NEG	CA	3171	17/17	0.90	0.24	0.40	53,72,80,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3166	1/1	0.85	0.15	0.38	57,57,57,57	0
56	MG	CA	3019	1/1	0.95	0.25	0.37	45,45,45,45	0
56	MG	BW	203	1/1	0.98	0.22	0.35	42,42,42,42	0
56	MG	BA	3298	1/1	0.97	0.26	0.33	24,24,24,24	0
56	MG	DA	3271	1/1	0.99	0.23	0.32	51,51,51,51	0
56	MG	AA	3091	1/1	0.96	0.21	0.31	62,62,62,62	0
56	MG	CN	101	1/1	0.98	0.20	0.26	69,69,69,69	0
56	MG	DA	3600	1/1	0.94	0.24	0.18	55,55,55,55	0
56	MG	BA	3536	1/1	0.99	0.25	0.16	30,30,30,30	0
56	MG	DA	3012	1/1	0.91	0.21	0.16	43,43,43,43	0
56	MG	CA	3086	1/1	0.94	0.20	0.15	53,53,53,53	0
56	MG	BA	3003	1/1	0.92	0.27	0.15	43,43,43,43	0
56	MG	BA	3639	1/1	0.65	0.25	0.13	55,55,55,55	0
56	MG	CA	3028	1/1	0.88	0.20	0.12	53,53,53,53	0
56	MG	DA	3619	1/1	0.89	0.21	0.08	57,57,57,57	0
56	MG	BA	3226	1/1	0.95	0.25	0.06	32,32,32,32	0
56	MG	DA	3381	1/1	0.91	0.21	0.04	55,55,55,55	0
56	MG	DA	3270	1/1	0.96	0.23	0.03	47,47,47,47	0
56	MG	BB	3001	1/1	0.73	0.21	-0.03	56,56,56,56	0
59	ZN	D6	501	1/1	0.93	0.20	-0.05	70,70,70,70	0
56	MG	AA	3131	1/1	0.98	0.22	-0.13	63,63,63,63	0
56	MG	DA	3096	1/1	0.98	0.21	-0.15	29,29,29,29	0
56	MG	DA	3191	1/1	0.97	0.20	-0.15	35,35,35,35	0
56	MG	DA	3428	1/1	0.98	0.20	-0.23	50,50,50,50	0
56	MG	DA	3128	1/1	0.94	0.22	-0.28	45,45,45,45	0
56	MG	DA	3386	1/1	0.91	0.14	-0.29	59,59,59,59	0
56	MG	CA	3103	1/1	0.94	0.20	-0.29	78,78,78,78	0
56	MG	DB	3006	1/1	0.91	0.19	-0.33	63,63,63,63	0
56	MG	BA	3055	1/1	0.94	0.22	-0.36	30,30,30,30	0
56	MG	DA	3140	1/1	0.92	0.21	-0.41	36,36,36,36	0
59	ZN	AN	501	1/1	0.98	0.20	-0.44	65,65,65,65	0
56	MG	DA	3406	1/1	0.93	0.20	-0.44	48,48,48,48	0
56	MG	BV	201	1/1	0.97	0.24	-0.46	26,26,26,26	0
56	MG	BA	3517	1/1	0.98	0.23	-0.47	26,26,26,26	0
56	MG	AA	3139	1/1	0.94	0.20	-0.47	50,50,50,50	0
56	MG	DA	3543	1/1	0.87	0.21	-0.47	63,63,63,63	0
56	MG	DA	3365	1/1	0.81	0.21	-0.48	54,54,54,54	0
56	MG	DA	3371	1/1	0.97	0.21	-0.49	68,68,68,68	0
56	MG	CA	3061	1/1	0.81	0.19	-0.50	61,61,61,61	0
56	MG	CA	3141	1/1	0.93	0.20	-0.50	61,61,61,61	0
56	MG	AA	3192	1/1	0.71	0.20	-0.53	71,71,71,71	0
56	MG	AA	3204	1/1	0.95	0.21	-0.55	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3146	1/1	0.88	0.14	-0.57	80,80,80,80	0
56	MG	DB	3007	1/1	0.89	0.15	-0.58	67,67,67,67	0
56	MG	BA	3527	1/1	0.95	0.23	-0.59	58,58,58,58	0
58	SF4	AD	501	8/8	0.99	0.18	-0.62	52,60,68,71	0
56	MG	DA	3620	1/1	0.88	0.17	-0.63	71,71,71,71	0
59	ZN	B9	501	1/1	0.99	0.21	-0.63	47,47,47,47	0
56	MG	CA	3004	1/1	0.60	0.18	-0.64	69,69,69,69	0
56	MG	CE	3001	1/1	0.97	0.14	-0.66	73,73,73,73	0
56	MG	CK	3001	1/1	0.97	0.17	-0.67	47,47,47,47	0
56	MG	DA	3393	1/1	0.93	0.19	-0.68	53,53,53,53	0
56	MG	BA	3032	1/1	0.92	0.22	-0.69	32,32,32,32	0
56	MG	DA	3076	1/1	0.94	0.20	-0.70	34,34,34,34	0
59	ZN	D4	501	1/1	0.69	0.12	-0.71	137,137,137,137	0
56	MG	CA	3030	1/1	0.97	0.20	-0.72	51,51,51,51	0
56	MG	AA	3125	1/1	0.96	0.20	-0.76	53,53,53,53	0
56	MG	CA	3159	1/1	0.92	0.17	-0.76	60,60,60,60	0
56	MG	DA	3537	1/1	0.97	0.21	-0.77	53,53,53,53	0
59	ZN	DY	501	1/1	0.97	0.13	-0.78	88,88,88,88	0
56	MG	AA	3150	1/1	0.92	0.20	-0.79	58,58,58,58	0
56	MG	BG	3001	1/1	0.93	0.19	-0.80	42,42,42,42	0
56	MG	CA	3027	1/1	0.93	0.15	-0.82	64,64,64,64	0
56	MG	CA	3132	1/1	0.95	0.20	-0.83	54,54,54,54	0
56	MG	BA	3383	1/1	0.94	0.21	-0.83	49,49,49,49	0
56	MG	DA	3477	1/1	0.95	0.18	-0.87	41,41,41,41	0
58	SF4	CD	302	8/8	0.99	0.17	-0.87	51,66,73,73	0
56	MG	AA	3114	1/1	0.96	0.19	-0.88	66,66,66,66	0
56	MG	BA	3308	1/1	0.96	0.21	-0.89	38,38,38,38	0
56	MG	CA	3049	1/1	0.89	0.19	-0.91	54,54,54,54	0
56	MG	BA	3122	1/1	0.98	0.25	-0.91	42,42,42,42	0
56	MG	DA	3378	1/1	0.87	0.20	-0.92	51,51,51,51	0
56	MG	BA	3178	1/1	0.89	0.23	-0.92	43,43,43,43	0
56	MG	BA	3459	1/1	0.93	0.21	-0.92	56,56,56,56	0
56	MG	BA	3342	1/1	0.95	0.16	-0.97	43,43,43,43	0
59	ZN	D9	501	1/1	0.94	0.09	-0.99	82,82,82,82	0
56	MG	AA	3072	1/1	0.96	0.20	-0.99	48,48,48,48	0
56	MG	DA	3515	1/1	0.80	0.12	-1.00	56,56,56,56	0
56	MG	BA	3052	1/1	0.94	0.20	-1.04	34,34,34,34	0
56	MG	BA	3638	1/1	0.80	0.22	-1.06	47,47,47,47	0
56	MG	DA	3472	1/1	0.74	0.16	-1.08	40,40,40,40	0
56	MG	CA	3110	1/1	0.93	0.19	-1.08	62,62,62,62	0
56	MG	DA	3043	1/1	0.94	0.16	-1.09	49,49,49,49	0
56	MG	DA	3274	1/1	0.96	0.20	-1.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3257	1/1	0.86	0.20	-1.10	58,58,58,58	0
56	MG	B9	502	1/1	0.84	0.20	-1.11	61,61,61,61	0
56	MG	BA	3568	1/1	0.92	0.20	-1.13	39,39,39,39	0
56	MG	DA	3114	1/1	0.70	0.21	-1.14	53,53,53,53	0
56	MG	AA	3166	1/1	0.99	0.19	-1.15	43,43,43,43	0
56	MG	AA	3046	1/1	0.91	0.21	-1.16	50,50,50,50	0
56	MG	DA	3494	1/1	0.96	0.20	-1.17	55,55,55,55	0
56	MG	BA	3781	1/1	0.92	0.23	-1.19	42,42,42,42	0
56	MG	B7	101	1/1	0.98	0.21	-1.20	35,35,35,35	0
56	MG	DA	3429	1/1	0.93	0.14	-1.21	57,57,57,57	0
56	MG	DA	3243	1/1	0.96	0.22	-1.22	42,42,42,42	0
56	MG	AN	504	1/1	0.92	0.20	-1.26	56,56,56,56	0
56	MG	BA	3592	1/1	0.99	0.18	-1.26	61,61,61,61	0
56	MG	DA	3536	1/1	0.94	0.14	-1.28	39,39,39,39	0
56	MG	DA	3215	1/1	0.95	0.22	-1.29	53,53,53,53	0
56	MG	DA	3306	1/1	0.69	0.14	-1.29	57,57,57,57	0
56	MG	DA	3144	1/1	0.84	0.11	-1.30	60,60,60,60	0
56	MG	CA	3091	1/1	0.98	0.17	-1.32	45,45,45,45	0
56	MG	DA	3499	1/1	0.99	0.17	-1.32	60,60,60,60	0
56	MG	BA	3695	1/1	0.86	0.23	-1.33	39,39,39,39	0
56	MG	DA	3542	1/1	0.91	0.12	-1.33	65,65,65,65	0
56	MG	AA	3092	1/1	0.82	0.18	-1.33	59,59,59,59	0
56	MG	DE	303	1/1	0.86	0.18	-1.35	40,40,40,40	0
56	MG	BA	3050	1/1	0.96	0.18	-1.36	34,34,34,34	0
56	MG	AA	3054	1/1	0.94	0.17	-1.37	46,46,46,46	0
56	MG	BQ	3002	1/1	0.97	0.23	-1.38	41,41,41,41	0
56	MG	BA	3275	1/1	0.89	0.19	-1.40	45,45,45,45	0
56	MG	DA	3368	1/1	0.94	0.17	-1.40	48,48,48,48	0
56	MG	DE	302	1/1	0.93	0.20	-1.44	30,30,30,30	0
56	MG	CA	3169	1/1	0.99	0.19	-1.44	49,49,49,49	0
56	MG	DD	305	1/1	0.90	0.18	-1.45	32,32,32,32	0
56	MG	DA	3395	1/1	0.92	0.21	-1.45	40,40,40,40	0
56	MG	AA	3018	1/1	0.87	0.21	-1.46	58,58,58,58	0
56	MG	DA	3405	1/1	0.90	0.15	-1.47	76,76,76,76	0
56	MG	DA	3011	1/1	0.92	0.14	-1.47	46,46,46,46	0
56	MG	DA	3033	1/1	0.93	0.19	-1.47	43,43,43,43	0
59	ZN	CN	102	1/1	0.95	0.09	-1.49	82,82,82,82	0
56	MG	BA	3049	1/1	0.90	0.23	-1.50	54,54,54,54	0
56	MG	CA	3002	1/1	0.74	0.12	-1.54	65,65,65,65	0
56	MG	BA	3473	1/1	0.92	0.21	-1.56	31,31,31,31	0
56	MG	DA	3126	1/1	0.88	0.13	-1.57	51,51,51,51	0
56	MG	CA	3036	1/1	0.68	0.15	-1.61	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BN	3003	1/1	0.84	0.16	-1.61	62,62,62,62	0
56	MG	CA	3025	1/1	0.84	0.16	-1.65	64,64,64,64	0
56	MG	DA	3366	1/1	0.91	0.15	-1.66	36,36,36,36	0
56	MG	DA	3265	1/1	0.97	0.17	-1.67	47,47,47,47	0
56	MG	AA	3006	1/1	0.92	0.23	-1.68	57,57,57,57	0
56	MG	AA	3214	1/1	0.83	0.13	-1.69	69,69,69,69	0
56	MG	BA	3014	1/1	0.94	0.17	-1.69	46,46,46,46	0
56	MG	BP	203	1/1	0.93	0.18	-1.70	37,37,37,37	0
56	MG	CA	3107	1/1	0.96	0.14	-1.72	63,63,63,63	0
56	MG	BA	3348	1/1	0.95	0.24	-1.74	35,35,35,35	0
56	MG	DA	3147	1/1	0.78	0.12	-1.75	49,49,49,49	0
56	MG	BD	306	1/1	0.90	0.19	-1.76	22,22,22,22	0
56	MG	DA	3295	1/1	0.94	0.18	-1.78	34,34,34,34	0
56	MG	BA	3448	1/1	0.96	0.20	-1.78	60,60,60,60	0
56	MG	BA	3362	1/1	0.90	0.20	-1.80	25,25,25,25	0
56	MG	DA	3035	1/1	0.95	0.17	-1.82	39,39,39,39	0
56	MG	BA	3552	1/1	0.94	0.18	-1.82	32,32,32,32	0
56	MG	DA	3063	1/1	0.85	0.14	-1.83	52,52,52,52	0
56	MG	AA	3041	1/1	0.75	0.14	-1.85	64,64,64,64	0
56	MG	DA	3034	1/1	0.97	0.20	-1.87	35,35,35,35	0
56	MG	DA	3290	1/1	0.94	0.20	-1.87	36,36,36,36	0
56	MG	BA	3652	1/1	0.91	0.21	-1.88	25,25,25,25	0
56	MG	DA	3403	1/1	0.85	0.17	-1.89	54,54,54,54	0
56	MG	CA	3051	1/1	0.77	0.15	-1.92	78,78,78,78	0
56	MG	BA	3037	1/1	0.97	0.22	-1.93	33,33,33,33	0
56	MG	BF	303	1/1	0.95	0.19	-1.93	36,36,36,36	0
56	MG	CA	3104	1/1	0.95	0.17	-1.94	51,51,51,51	0
56	MG	BA	3729	1/1	0.79	0.18	-1.96	55,55,55,55	0
56	MG	AA	3002	1/1	0.85	0.15	-1.97	59,59,59,59	0
56	MG	D0	101	1/1	0.96	0.17	-1.98	73,73,73,73	0
56	MG	BA	3607	1/1	0.95	0.21	-1.98	45,45,45,45	0
56	MG	AA	3212	1/1	0.94	0.15	-2.01	33,33,33,33	0
56	MG	BA	3441	1/1	0.94	0.12	-2.01	37,37,37,37	0
56	MG	DQ	3001	1/1	0.98	0.11	-2.03	57,57,57,57	0
56	MG	AA	3001	1/1	0.98	0.15	-2.06	37,37,37,37	0
56	MG	BA	3390	1/1	0.95	0.23	-2.06	26,26,26,26	0
56	MG	DA	3438	1/1	0.84	0.14	-2.07	55,55,55,55	0
56	MG	AX	3005	1/1	0.92	0.12	-2.07	66,66,66,66	0
56	MG	BA	3332	1/1	0.93	0.20	-2.08	48,48,48,48	0
56	MG	DA	3203	1/1	0.91	0.18	-2.09	46,46,46,46	0
56	MG	DA	3004	1/1	0.97	0.18	-2.11	18,18,18,18	0
56	MG	BV	204	1/1	0.89	0.19	-2.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3295	1/1	0.88	0.13	-2.13	66,66,66,66	0
56	MG	DF	304	1/1	0.87	0.12	-2.14	48,48,48,48	0
56	MG	BV	206	1/1	0.96	0.17	-2.15	38,38,38,38	0
56	MG	CA	3063	1/1	0.94	0.18	-2.15	59,59,59,59	0
56	MG	CA	3152	1/1	0.97	0.18	-2.16	58,58,58,58	0
56	MG	BA	3174	1/1	0.89	0.18	-2.17	52,52,52,52	0
56	MG	BA	3338	1/1	0.84	0.20	-2.19	39,39,39,39	0
56	MG	DA	3111	1/1	0.94	0.11	-2.19	49,49,49,49	0
56	MG	CT	3001	1/1	0.84	0.13	-2.21	50,50,50,50	0
56	MG	BA	3312	1/1	0.91	0.22	-2.22	41,41,41,41	0
56	MG	BA	3378	1/1	0.94	0.21	-2.23	24,24,24,24	0
56	MG	AA	3213	1/1	0.87	0.12	-2.27	44,44,44,44	0
56	MG	CA	3167	1/1	0.89	0.10	-2.30	55,55,55,55	0
56	MG	DA	3018	1/1	0.94	0.15	-2.33	29,29,29,29	0
56	MG	DG	3001	1/1	0.86	0.12	-2.33	55,55,55,55	0
56	MG	BA	3516	1/1	0.98	0.20	-2.34	36,36,36,36	0
56	MG	DA	3409	1/1	0.83	0.15	-2.36	41,41,41,41	0
56	MG	AE	3001	1/1	0.91	0.09	-2.38	77,77,77,77	0
56	MG	BA	3035	1/1	0.92	0.22	-2.38	25,25,25,25	0
56	MG	DA	3188	1/1	0.96	0.12	-2.38	61,61,61,61	0
56	MG	DA	3119	1/1	0.84	0.17	-2.41	50,50,50,50	0
56	MG	DA	3124	1/1	0.93	0.12	-2.43	43,43,43,43	0
56	MG	BA	3770	1/1	0.96	0.19	-2.44	20,20,20,20	0
56	MG	DA	3313	1/1	0.98	0.19	-2.46	46,46,46,46	0
56	MG	CA	3082	1/1	0.90	0.18	-2.47	41,41,41,41	0
56	MG	DA	3091	1/1	0.80	0.15	-2.48	57,57,57,57	0
56	MG	DA	3275	1/1	0.93	0.13	-2.49	51,51,51,51	0
56	MG	AA	3137	1/1	0.91	0.16	-2.49	49,49,49,49	0
56	MG	CA	3050	1/1	0.86	0.10	-2.49	55,55,55,55	0
56	MG	CA	3166	1/1	0.96	0.11	-2.50	42,42,42,42	0
56	MG	DA	3088	1/1	0.93	0.17	-2.50	39,39,39,39	0
56	MG	BA	3303	1/1	0.82	0.20	-2.50	27,27,27,27	0
56	MG	BA	3534	1/1	0.91	0.20	-2.53	54,54,54,54	0
56	MG	BA	3016	1/1	0.98	0.21	-2.54	22,22,22,22	0
56	MG	BA	3024	1/1	0.99	0.19	-2.57	19,19,19,19	0
56	MG	CA	3106	1/1	0.90	0.15	-2.61	55,55,55,55	0
56	MG	AA	3029	1/1	0.93	0.15	-2.63	60,60,60,60	0
56	MG	BA	3487	1/1	0.96	0.20	-2.64	37,37,37,37	0
56	MG	BA	3693	1/1	0.83	0.19	-2.65	38,38,38,38	0
56	MG	AN	503	1/1	0.94	0.14	-2.66	59,59,59,59	0
56	MG	DA	3087	1/1	0.68	0.10	-2.68	49,49,49,49	0
56	MG	BA	3343	1/1	0.91	0.18	-2.70	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3616	1/1	0.87	0.13	-2.72	47,47,47,47	0
56	MG	BA	3344	1/1	0.93	0.19	-2.73	36,36,36,36	0
56	MG	BA	3076	1/1	0.90	0.13	-2.76	58,58,58,58	0
56	MG	AA	3099	1/1	0.78	0.11	-2.78	59,59,59,59	0
56	MG	BA	3231	1/1	0.91	0.17	-2.80	42,42,42,42	0
56	MG	DA	3234	1/1	0.98	0.13	-2.84	42,42,42,42	0
56	MG	AA	3187	1/1	0.98	0.15	-2.89	56,56,56,56	0
56	MG	BA	3537	1/1	0.85	0.17	-2.89	55,55,55,55	0
56	MG	DA	3504	1/1	0.89	0.12	-2.90	55,55,55,55	0
56	MG	BA	3523	1/1	0.90	0.18	-2.90	39,39,39,39	0
56	MG	DA	3583	1/1	0.73	0.13	-2.91	44,44,44,44	0
56	MG	CA	3007	1/1	0.60	0.16	-2.91	69,69,69,69	0
56	MG	DA	3250	1/1	0.93	0.15	-2.93	37,37,37,37	0
56	MG	DB	3003	1/1	0.96	0.12	-2.99	62,62,62,62	0
56	MG	BA	3250	1/1	0.97	0.19	-3.00	40,40,40,40	0
56	MG	DA	3473	1/1	0.95	0.10	-3.02	60,60,60,60	0
56	MG	BA	3763	1/1	0.99	0.19	-3.02	10,10,10,10	0
56	MG	BA	3083	1/1	0.95	0.20	-3.02	30,30,30,30	0
56	MG	AA	3076	1/1	0.95	0.17	-3.04	45,45,45,45	0
56	MG	AM	201	1/1	0.82	0.10	-3.07	61,61,61,61	0
56	MG	BA	3628	1/1	0.83	0.18	-3.09	55,55,55,55	0
56	MG	DA	3487	1/1	0.96	0.14	-3.09	37,37,37,37	0
56	MG	BA	3778	1/1	0.96	0.14	-3.10	36,36,36,36	0
56	MG	DA	3372	1/1	0.91	0.11	-3.11	67,67,67,67	0
56	MG	CA	3071	1/1	0.90	0.08	-3.11	58,58,58,58	0
56	MG	BA	3291	1/1	0.96	0.20	-3.11	26,26,26,26	0
56	MG	DA	3414	1/1	0.85	0.17	-3.13	46,46,46,46	0
56	MG	BA	3480	1/1	0.69	0.20	-3.14	29,29,29,29	0
56	MG	BA	3571	1/1	0.91	0.14	-3.15	40,40,40,40	0
56	MG	BE	301	1/1	0.91	0.19	-3.16	36,36,36,36	0
56	MG	AA	3036	1/1	0.98	0.16	-3.17	24,24,24,24	0
56	MG	BA	3236	1/1	0.98	0.16	-3.17	34,34,34,34	0
56	MG	DA	3380	1/1	0.88	0.14	-3.17	43,43,43,43	0
56	MG	DA	3137	1/1	0.95	0.13	-3.19	57,57,57,57	0
56	MG	BA	3585	1/1	0.84	0.18	-3.21	61,61,61,61	0
56	MG	DA	3502	1/1	0.95	0.12	-3.26	47,47,47,47	0
56	MG	DA	3541	1/1	0.95	0.17	-3.30	46,46,46,46	0
56	MG	BA	3361	1/1	0.92	0.17	-3.31	29,29,29,29	0
56	MG	BA	3043	1/1	0.97	0.17	-3.36	34,34,34,34	0
56	MG	DA	3296	1/1	0.95	0.14	-3.37	38,38,38,38	0
56	MG	BA	3513	1/1	0.95	0.17	-3.39	42,42,42,42	0
56	MG	BA	3273	1/1	0.97	0.18	-3.39	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3184	1/1	0.93	0.18	-3.42	33,33,33,33	0
56	MG	DA	3337	1/1	0.94	0.13	-3.42	42,42,42,42	0
56	MG	BA	3382	1/1	0.91	0.19	-3.42	30,30,30,30	0
56	MG	DA	3606	1/1	0.86	0.12	-3.44	54,54,54,54	0
56	MG	AA	3154	1/1	0.92	0.13	-3.45	67,67,67,67	0
56	MG	DA	3442	1/1	0.86	0.15	-3.45	46,46,46,46	0
56	MG	AA	3060	1/1	0.94	0.14	-3.46	42,42,42,42	0
56	MG	BA	3005	1/1	0.98	0.13	-3.47	41,41,41,41	0
56	MG	DA	3182	1/1	0.91	0.11	-3.49	52,52,52,52	0
56	MG	DA	3505	1/1	0.95	0.18	-3.49	41,41,41,41	0
56	MG	DA	3085	1/1	0.79	0.12	-3.51	65,65,65,65	0
56	MG	BA	3744	1/1	0.95	0.15	-3.54	27,27,27,27	0
56	MG	DA	3280	1/1	0.97	0.15	-3.56	26,26,26,26	0
56	MG	BB	3003	1/1	0.90	0.17	-3.57	37,37,37,37	0
56	MG	BA	3054	1/1	0.87	0.18	-3.59	51,51,51,51	0
56	MG	BA	3369	1/1	0.97	0.19	-3.59	23,23,23,23	0
56	MG	BA	3663	1/1	0.93	0.16	-3.59	26,26,26,26	0
56	MG	BA	3063	1/1	0.93	0.15	-3.62	39,39,39,39	0
56	MG	DA	3278	1/1	0.87	0.12	-3.63	44,44,44,44	0
56	MG	DA	3315	1/1	0.93	0.09	-3.65	28,28,28,28	0
56	MG	BF	307	1/1	0.93	0.20	-3.68	46,46,46,46	0
56	MG	BA	3766	1/1	0.96	0.20	-3.69	43,43,43,43	0
56	MG	BA	3316	1/1	0.94	0.20	-3.73	58,58,58,58	0
56	MG	BA	3372	1/1	0.93	0.20	-3.73	33,33,33,33	0
56	MG	DA	3369	1/1	0.92	0.19	-3.75	47,47,47,47	0
56	MG	BA	3755	1/1	0.91	0.16	-3.77	42,42,42,42	0
56	MG	BA	3526	1/1	0.86	0.18	-3.79	38,38,38,38	0
56	MG	DA	3005	1/1	0.98	0.15	-3.81	39,39,39,39	0
56	MG	DA	3136	1/1	0.94	0.15	-3.84	35,35,35,35	0
56	MG	BA	3352	1/1	0.94	0.15	-3.85	22,22,22,22	0
56	MG	DA	3089	1/1	0.90	0.10	-3.85	57,57,57,57	0
56	MG	AA	3119	1/1	0.96	0.17	-3.87	36,36,36,36	0
56	MG	CA	3023	1/1	0.97	0.11	-3.87	54,54,54,54	0
56	MG	BA	3510	1/1	0.89	0.17	-3.88	43,43,43,43	0
56	MG	DA	3319	1/1	0.97	0.13	-3.89	21,21,21,21	0
56	MG	BA	3439	1/1	0.93	0.20	-3.93	15,15,15,15	0
56	MG	BA	3347	1/1	0.96	0.19	-3.96	26,26,26,26	0
56	MG	BA	3768	1/1	0.90	0.18	-3.97	48,48,48,48	0
56	MG	BA	3294	1/1	0.92	0.16	-3.99	45,45,45,45	0
56	MG	BA	3366	1/1	0.92	0.16	-3.99	23,23,23,23	0
56	MG	DA	3614	1/1	0.76	0.14	-3.99	34,34,34,34	0
56	MG	BA	3357	1/1	0.97	0.18	-4.03	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3267	1/1	0.95	0.14	-4.04	42,42,42,42	0
56	MG	BA	3259	1/1	0.95	0.16	-4.04	32,32,32,32	0
56	MG	BA	3261	1/1	0.91	0.21	-4.05	49,49,49,49	0
56	MG	CA	3165	1/1	0.89	0.15	-4.06	57,57,57,57	0
56	MG	DA	3008	1/1	0.95	0.14	-4.07	38,38,38,38	0
56	MG	DA	3497	1/1	0.94	0.14	-4.07	27,27,27,27	0
56	MG	DA	3392	1/1	0.97	0.16	-4.09	34,34,34,34	0
56	MG	BA	3167	1/1	0.96	0.19	-4.09	28,28,28,28	0
56	MG	BA	3494	1/1	0.86	0.16	-4.10	41,41,41,41	0
56	MG	AA	3023	1/1	0.92	0.13	-4.11	51,51,51,51	0
56	MG	DA	3579	1/1	0.86	0.10	-4.12	69,69,69,69	0
56	MG	BA	3764	1/1	0.92	0.17	-4.12	26,26,26,26	0
56	MG	DA	3399	1/1	0.98	0.16	-4.14	35,35,35,35	0
56	MG	AA	3111	1/1	0.77	0.16	-4.17	65,65,65,65	0
56	MG	DA	3440	1/1	0.97	0.13	-4.19	49,49,49,49	0
56	MG	DA	3554	1/1	0.84	0.13	-4.21	45,45,45,45	0
56	MG	AA	3123	1/1	0.96	0.15	-4.25	25,25,25,25	0
56	MG	BA	3640	1/1	0.94	0.11	-4.26	61,61,61,61	0
56	MG	DA	3416	1/1	0.97	0.13	-4.28	39,39,39,39	0
56	MG	BA	3572	1/1	0.91	0.13	-4.32	55,55,55,55	0
56	MG	DA	3236	1/1	0.95	0.14	-4.36	59,59,59,59	0
56	MG	AA	3143	1/1	0.89	0.12	-4.38	57,57,57,57	0
56	MG	AA	3031	1/1	0.86	0.15	-4.38	63,63,63,63	0
56	MG	AA	3013	1/1	0.94	0.12	-4.39	66,66,66,66	0
56	MG	DA	3566	1/1	0.88	0.12	-4.40	51,51,51,51	0
56	MG	DA	3408	1/1	0.96	0.10	-4.43	25,25,25,25	0
56	MG	BA	3619	1/1	0.94	0.11	-4.49	49,49,49,49	0
56	MG	BA	3570	1/1	0.92	0.18	-4.50	57,57,57,57	0
56	MG	BA	3462	1/1	0.84	0.16	-4.52	59,59,59,59	0
56	MG	BA	3317	1/1	0.98	0.13	-4.56	47,47,47,47	0
56	MG	DA	3056	1/1	0.94	0.08	-4.60	51,51,51,51	0
56	MG	BA	3629	1/1	0.97	0.17	-4.68	62,62,62,62	0
56	MG	BA	3654	1/1	0.98	0.17	-4.68	24,24,24,24	0
56	MG	B0	102	1/1	0.95	0.09	-4.68	54,54,54,54	0
56	MG	DA	3102	1/1	0.94	0.10	-4.69	50,50,50,50	0
56	MG	BA	3468	1/1	0.91	0.14	-4.72	31,31,31,31	0
56	MG	DA	3030	1/1	0.79	0.13	-4.75	54,54,54,54	0
56	MG	BA	3096	1/1	0.96	0.16	-4.77	29,29,29,29	0
56	MG	AA	3014	1/1	0.72	0.10	-4.78	64,64,64,64	0
56	MG	BA	3279	1/1	0.91	0.14	-4.78	52,52,52,52	0
56	MG	DA	3252	1/1	0.98	0.09	-4.80	43,43,43,43	0
56	MG	DA	3204	1/1	0.96	0.13	-4.86	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BB	3006	1/1	0.94	0.13	-4.86	46,46,46,46	0
56	MG	CA	3038	1/1	0.93	0.13	-4.90	31,31,31,31	0
56	MG	AA	3048	1/1	0.93	0.14	-4.90	55,55,55,55	0
56	MG	BA	3493	1/1	0.97	0.14	-4.91	29,29,29,29	0
56	MG	BA	3427	1/1	0.97	0.17	-4.93	22,22,22,22	0
56	MG	DA	3404	1/1	0.95	0.12	-4.94	36,36,36,36	0
56	MG	AV	102	1/1	0.83	0.18	-4.95	52,52,52,52	0
56	MG	DA	3354	1/1	0.94	0.10	-4.95	56,56,56,56	0
56	MG	AA	3064	1/1	0.96	0.13	-4.95	47,47,47,47	0
56	MG	BA	3596	1/1	0.94	0.14	-4.96	52,52,52,52	0
56	MG	DE	304	1/1	0.93	0.14	-4.97	45,45,45,45	0
56	MG	AA	3183	1/1	0.68	0.16	-4.97	63,63,63,63	0
56	MG	BA	3353	1/1	0.93	0.16	-4.98	27,27,27,27	0
56	MG	DA	3391	1/1	0.96	0.14	-4.99	40,40,40,40	0
56	MG	BA	3511	1/1	0.97	0.19	-5.07	31,31,31,31	0
56	MG	BA	3145	1/1	0.81	0.14	-5.09	41,41,41,41	0
56	MG	CA	3015	1/1	0.95	0.10	-5.13	45,45,45,45	0
56	MG	BA	3270	1/1	0.95	0.14	-5.13	47,47,47,47	0
56	MG	DA	3538	1/1	0.95	0.07	-5.14	50,50,50,50	0
56	MG	BA	3213	1/1	0.84	0.14	-5.15	48,48,48,48	0
56	MG	BA	3469	1/1	0.94	0.18	-5.17	49,49,49,49	0
56	MG	DA	3346	1/1	0.86	0.14	-5.18	29,29,29,29	0
56	MG	BE	302	1/1	0.95	0.20	-5.19	28,28,28,28	0
56	MG	BA	3144	1/1	0.85	0.16	-5.20	37,37,37,37	0
56	MG	BA	3355	1/1	0.92	0.17	-5.20	26,26,26,26	0
56	MG	BA	3334	1/1	0.99	0.18	-5.20	23,23,23,23	0
56	MG	DA	3282	1/1	0.96	0.14	-5.22	43,43,43,43	0
56	MG	DA	3327	1/1	0.97	0.12	-5.22	32,32,32,32	0
56	MG	DA	3559	1/1	0.94	0.09	-5.24	49,49,49,49	0
56	MG	BA	3319	1/1	0.95	0.17	-5.28	38,38,38,38	0
56	MG	BA	3381	1/1	0.92	0.17	-5.30	33,33,33,33	0
56	MG	DA	3317	1/1	0.96	0.05	-5.34	47,47,47,47	0
56	MG	BA	3414	1/1	0.99	0.16	-5.35	26,26,26,26	0
56	MG	DA	3110	1/1	0.96	0.09	-5.35	30,30,30,30	0
56	MG	DA	3237	1/1	0.97	0.09	-5.38	42,42,42,42	0
56	MG	BA	3720	1/1	0.98	0.10	-5.39	28,28,28,28	0
56	MG	BB	3014	1/1	0.93	0.16	-5.43	39,39,39,39	0
56	MG	BA	3465	1/1	0.93	0.21	-5.45	20,20,20,20	0
56	MG	BA	3349	1/1	0.91	0.19	-5.45	25,25,25,25	0
56	MG	BA	3478	1/1	0.96	0.19	-5.49	36,36,36,36	0
56	MG	AA	3040	1/1	0.88	0.10	-5.49	41,41,41,41	0
56	MG	AA	3180	1/1	0.94	0.12	-5.50	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3535	1/1	0.94	0.16	-5.53	46,46,46,46	0
56	MG	BA	3034	1/1	0.95	0.15	-5.53	34,34,34,34	0
56	MG	BA	3708	1/1	0.97	0.13	-5.58	7,7,7,7	0
56	MG	BA	3709	1/1	0.98	0.20	-5.59	42,42,42,42	0
56	MG	CA	3012	1/1	0.95	0.13	-5.64	56,56,56,56	0
56	MG	BA	3496	1/1	0.89	0.20	-5.66	53,53,53,53	0
56	MG	BA	3426	1/1	0.97	0.15	-5.67	29,29,29,29	0
56	MG	BA	3564	1/1	0.95	0.15	-5.67	49,49,49,49	0
56	MG	DA	3362	1/1	0.88	0.16	-5.71	22,22,22,22	0
56	MG	AA	3163	1/1	0.92	0.20	-5.71	53,53,53,53	0
56	MG	BA	3461	1/1	0.88	0.18	-5.74	21,21,21,21	0
56	MG	BA	3310	1/1	0.93	0.11	-5.82	41,41,41,41	0
56	MG	DA	3045	1/1	0.87	0.12	-5.82	44,44,44,44	0
56	MG	DA	3238	1/1	0.94	0.11	-5.84	40,40,40,40	0
56	MG	BA	3604	1/1	0.90	0.14	-5.89	46,46,46,46	0
56	MG	DA	3286	1/1	0.91	0.14	-5.90	39,39,39,39	0
56	MG	BA	3758	1/1	0.95	0.14	-5.90	38,38,38,38	0
56	MG	BA	3109	1/1	0.86	0.16	-5.90	49,49,49,49	0
56	MG	DA	3115	1/1	0.96	0.08	-5.92	51,51,51,51	0
56	MG	DA	3277	1/1	0.95	0.14	-5.99	52,52,52,52	0
56	MG	BA	3038	1/1	0.99	0.17	-5.99	31,31,31,31	0
56	MG	DA	3329	1/1	0.92	0.09	-6.09	62,62,62,62	0
56	MG	DA	3235	1/1	0.97	0.09	-6.09	29,29,29,29	0
56	MG	DA	3299	1/1	0.95	0.12	-6.12	40,40,40,40	0
56	MG	BA	3664	1/1	0.93	0.17	-6.12	25,25,25,25	0
56	MG	CA	3022	1/1	0.94	0.11	-6.16	53,53,53,53	0
56	MG	BE	308	1/1	0.92	0.12	-6.16	34,34,34,34	0
56	MG	DA	3092	1/1	0.97	0.12	-6.22	43,43,43,43	0
56	MG	BA	3682	1/1	0.87	0.11	-6.24	73,73,73,73	0
56	MG	BA	3078	1/1	0.75	0.13	-6.27	48,48,48,48	0
56	MG	DA	3232	1/1	0.94	0.09	-6.27	57,57,57,57	0
56	MG	BA	3456	1/1	0.88	0.12	-6.29	63,63,63,63	0
56	MG	AA	3070	1/1	0.93	0.12	-6.30	31,31,31,31	0
56	MG	DA	3325	1/1	0.92	0.13	-6.31	32,32,32,32	0
56	MG	DO	202	1/1	0.97	0.10	-6.33	57,57,57,57	0
56	MG	DA	3249	1/1	0.87	0.10	-6.41	43,43,43,43	0
56	MG	DA	3258	1/1	0.94	0.10	-6.42	24,24,24,24	0
56	MG	AA	3010	1/1	0.93	0.14	-6.42	22,22,22,22	0
56	MG	DA	3026	1/1	0.96	0.11	-6.45	24,24,24,24	0
56	MG	BA	3765	1/1	0.92	0.15	-6.49	59,59,59,59	0
56	MG	BA	3274	1/1	0.91	0.15	-6.52	29,29,29,29	0
56	MG	AA	3077	1/1	0.94	0.06	-6.53	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3014	1/1	0.91	0.09	-6.53	46,46,46,46	0
56	MG	BB	3015	1/1	0.84	0.12	-6.55	54,54,54,54	0
56	MG	BA	3500	1/1	0.96	0.11	-6.68	37,37,37,37	0
56	MG	BA	3006	1/1	0.99	0.15	-6.69	26,26,26,26	0
56	MG	BA	3397	1/1	0.95	0.15	-6.71	29,29,29,29	0
56	MG	DA	3019	1/1	0.93	0.11	-6.74	40,40,40,40	0
56	MG	BA	3180	1/1	0.86	0.14	-6.74	46,46,46,46	0
56	MG	DA	3510	1/1	0.89	0.13	-6.76	32,32,32,32	0
56	MG	BA	3340	1/1	0.88	0.18	-6.81	34,34,34,34	0
56	MG	BA	3711	1/1	0.95	0.13	-6.86	51,51,51,51	0
56	MG	DA	3531	1/1	0.96	0.11	-7.07	40,40,40,40	0
56	MG	BA	3492	1/1	0.91	0.14	-7.15	33,33,33,33	0
56	MG	BA	3004	1/1	0.95	0.09	-7.17	25,25,25,25	0
56	MG	BA	3723	1/1	0.87	0.12	-7.18	41,41,41,41	0
56	MG	BA	3165	1/1	0.82	0.13	-7.20	53,53,53,53	0
56	MG	DA	3506	1/1	0.98	0.14	-7.21	37,37,37,37	0
56	MG	BA	3417	1/1	0.87	0.14	-7.22	56,56,56,56	0
56	MG	BA	3442	1/1	0.93	0.14	-7.22	31,31,31,31	0
56	MG	DA	3032	1/1	0.90	0.15	-7.22	40,40,40,40	0
56	MG	BA	3759	1/1	0.98	0.17	-7.27	29,29,29,29	0
56	MG	BA	3566	1/1	0.94	0.15	-7.27	28,28,28,28	0
56	MG	BA	3346	1/1	0.97	0.17	-7.30	28,28,28,28	0
56	MG	CA	3158	1/1	0.93	0.13	-7.33	72,72,72,72	0
56	MG	AA	3129	1/1	0.95	0.06	-7.37	77,77,77,77	0
56	MG	DA	3304	1/1	0.93	0.12	-7.52	32,32,32,32	0
56	MG	BA	3613	1/1	0.85	0.13	-7.52	53,53,53,53	0
56	MG	BA	3304	1/1	0.93	0.19	-7.52	21,21,21,21	0
56	MG	DA	3518	1/1	0.97	0.06	-7.55	57,57,57,57	0
56	MG	BA	3292	1/1	0.97	0.15	-7.63	26,26,26,26	0
56	MG	BA	3337	1/1	0.93	0.16	-7.67	25,25,25,25	0
56	MG	BA	3680	1/1	0.82	0.15	-7.68	32,32,32,32	0
56	MG	AA	3085	1/1	0.94	0.12	-7.69	63,63,63,63	0
56	MG	BA	3447	1/1	0.92	0.13	-7.73	38,38,38,38	0
56	MG	DA	3281	1/1	0.97	0.12	-7.75	39,39,39,39	0
56	MG	DA	3187	1/1	0.93	0.16	-7.77	41,41,41,41	0
56	MG	DA	3014	1/1	0.95	0.11	-7.82	37,37,37,37	0
56	MG	BA	3452	1/1	0.98	0.10	-7.86	41,41,41,41	0
56	MG	BA	3722	1/1	0.92	0.12	-7.90	46,46,46,46	0
56	MG	AA	3202	1/1	0.89	0.08	-7.92	63,63,63,63	0
56	MG	BA	3688	1/1	0.94	0.12	-7.98	24,24,24,24	0
56	MG	BA	3706	1/1	0.82	0.18	-8.00	52,52,52,52	0
56	MG	BA	3409	1/1	0.92	0.15	-8.04	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3084	1/1	0.92	0.12	-8.14	46,46,46,46	0
56	MG	BA	3703	1/1	0.82	0.15	-8.14	56,56,56,56	0
56	MG	BA	3196	1/1	0.90	0.15	-8.21	46,46,46,46	0
56	MG	DA	3338	1/1	0.92	0.10	-8.35	60,60,60,60	0
56	MG	BA	3671	1/1	0.92	0.17	-8.36	33,33,33,33	0
56	MG	DA	3377	1/1	0.86	0.11	-8.40	48,48,48,48	0
56	MG	DA	3246	1/1	0.97	0.09	-8.53	53,53,53,53	0
56	MG	DA	3294	1/1	0.92	0.08	-8.60	53,53,53,53	0
56	MG	DA	3452	1/1	0.92	0.15	-8.61	44,44,44,44	0
56	MG	BA	3115	1/1	0.97	0.17	-8.67	13,13,13,13	0
56	MG	DA	3020	1/1	0.97	0.13	-8.71	33,33,33,33	0
56	MG	BA	3046	1/1	0.83	0.15	-8.72	50,50,50,50	0
56	MG	DA	3132	1/1	0.96	0.09	-8.81	39,39,39,39	0
56	MG	DA	3227	1/1	0.93	0.10	-8.82	47,47,47,47	0
56	MG	DA	3309	1/1	0.97	0.10	-8.91	42,42,42,42	0
56	MG	BA	3471	1/1	0.85	0.12	-8.93	33,33,33,33	0
56	MG	DA	3307	1/1	0.96	0.10	-9.04	28,28,28,28	0
56	MG	BA	3017	1/1	0.98	0.13	-9.28	32,32,32,32	0
56	MG	BA	3320	1/1	0.98	0.15	-9.38	28,28,28,28	0
56	MG	AA	3022	1/1	0.94	0.09	-9.38	58,58,58,58	0
56	MG	BA	3147	1/1	0.90	0.09	-9.46	60,60,60,60	0
56	MG	AA	3065	1/1	0.94	0.11	-9.46	40,40,40,40	0
56	MG	BA	3262	1/1	0.86	0.13	-9.88	51,51,51,51	0
56	MG	DA	3314	1/1	0.81	0.09	-10.14	46,46,46,46	0
56	MG	BA	3269	1/1	0.96	0.15	-10.45	40,40,40,40	0
56	MG	BA	3333	1/1	0.92	0.11	-10.64	39,39,39,39	0
56	MG	DA	3441	1/1	0.93	0.10	-10.66	39,39,39,39	0
56	MG	DA	3618	1/1	0.94	0.10	-10.70	57,57,57,57	0
56	MG	DA	3121	1/1	0.95	0.11	-10.83	33,33,33,33	0
56	MG	BA	3010	1/1	0.90	0.13	-11.11	58,58,58,58	0
56	MG	DA	3490	1/1	0.80	0.08	-11.12	49,49,49,49	0
56	MG	BA	3289	1/1	0.98	0.14	-11.21	24,24,24,24	0
56	MG	DA	3302	1/1	0.86	0.13	-11.54	38,38,38,38	0
56	MG	AA	3071	1/1	0.96	0.13	-11.73	52,52,52,52	0
56	MG	BA	3699	1/1	0.95	0.12	-11.77	39,39,39,39	0
56	MG	BA	3376	1/1	0.96	0.17	-11.84	23,23,23,23	0
56	MG	BA	3626	1/1	0.97	0.12	-12.59	40,40,40,40	0
56	MG	BA	3276	1/1	0.87	0.14	-12.68	40,40,40,40	0
56	MG	CA	3078	1/1	0.95	0.12	-12.99	41,41,41,41	0
56	MG	BA	3257	1/1	0.88	0.16	-13.30	48,48,48,48	0
56	MG	BA	3392	1/1	0.97	0.14	-13.75	17,17,17,17	0
56	MG	BA	3567	1/1	0.91	0.09	-14.59	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3569	1/1	0.93	0.12	-14.61	44,44,44,44	0
56	MG	BA	3263	1/1	0.96	0.10	-14.66	47,47,47,47	0
56	MG	BA	3282	1/1	0.97	0.08	-14.82	59,59,59,59	0
56	MG	DA	3478	1/1	0.95	0.08	-15.31	54,54,54,54	0
56	MG	DA	3101	1/1	0.98	0.09	-15.71	28,28,28,28	0
56	MG	BA	3393	1/1	0.96	0.17	-17.14	48,48,48,48	0
56	MG	BA	3296	1/1	0.95	0.10	-18.15	47,47,47,47	0
56	MG	DA	3219	1/1	0.91	0.10	-19.23	35,35,35,35	0
56	MG	BA	3245	1/1	0.90	0.12	-19.41	47,47,47,47	0
56	MG	BA	3488	1/1	0.97	0.12	-22.38	28,28,28,28	0
56	MG	DA	3344	1/1	0.97	0.07	-	54,54,54,54	0
56	MG	BA	3750	1/1	0.95	0.19	-	52,52,52,52	0
56	MG	AA	3053	1/1	0.95	0.15	-	41,41,41,41	0
56	MG	DA	3573	1/1	0.73	0.11	-	69,69,69,69	0
56	MG	BA	3082	1/1	0.98	0.17	-	27,27,27,27	0
56	MG	BA	3692	1/1	0.86	0.24	-	73,73,73,73	0
56	MG	BA	3632	1/1	0.95	0.15	-	53,53,53,53	0
56	MG	BA	3307	1/1	0.72	0.13	-	57,57,57,57	0
56	MG	BA	3721	1/1	0.88	0.18	-	74,74,74,74	0
56	MG	CA	3090	1/1	0.72	0.14	-	70,70,70,70	0
56	MG	DA	3532	1/1	0.96	0.16	-	53,53,53,53	0
56	MG	DA	3199	1/1	0.79	0.30	-	57,57,57,57	0
56	MG	AA	3015	1/1	0.59	0.16	-	56,56,56,56	0
56	MG	DA	3591	1/1	0.98	0.14	-	46,46,46,46	0
56	MG	DA	3217	1/1	0.94	0.12	-	43,43,43,43	0
56	MG	DA	3483	1/1	0.92	0.07	-	64,64,64,64	0
56	MG	BA	3272	1/1	0.98	0.20	-	41,41,41,41	0
56	MG	DA	3396	1/1	0.97	0.10	-	27,27,27,27	0
56	MG	DA	3151	1/1	0.85	0.12	-	52,52,52,52	0
56	MG	DA	3098	1/1	0.89	0.21	-	61,61,61,61	0
56	MG	DA	3268	1/1	0.97	0.19	-	53,53,53,53	0
56	MG	DA	3129	1/1	0.94	0.15	-	42,42,42,42	0
56	MG	AV	103	1/1	0.91	0.13	-	70,70,70,70	0
56	MG	DA	3401	1/1	0.97	0.12	-	50,50,50,50	0
56	MG	AA	3104	1/1	0.84	0.16	-	44,44,44,44	0
56	MG	DA	3522	1/1	0.87	0.12	-	57,57,57,57	0
56	MG	BA	3044	1/1	0.92	0.14	-	39,39,39,39	0
56	MG	AA	3081	1/1	0.96	0.19	-	52,52,52,52	0
56	MG	BA	3756	1/1	0.95	0.12	-	56,56,56,56	0
56	MG	DW	3001	1/1	0.92	0.52	-	45,45,45,45	0
56	MG	DA	3589	1/1	0.96	0.13	-	55,55,55,55	0
56	MG	BA	3559	1/1	0.85	0.11	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3206	1/1	0.69	0.24	-	62,62,62,62	0
56	MG	AA	3074	1/1	0.83	0.29	-	59,59,59,59	0
56	MG	DA	3220	1/1	0.94	0.08	-	45,45,45,45	0
56	MG	BA	3530	1/1	0.84	0.10	-	56,56,56,56	0
56	MG	AA	3004	1/1	0.81	0.10	-	67,67,67,67	0
56	MG	CA	3008	1/1	0.95	0.11	-	45,45,45,45	0
56	MG	BA	3126	1/1	0.89	0.43	-	48,48,48,48	0
56	MG	DA	3017	1/1	0.93	0.26	-	46,46,46,46	0
56	MG	DA	3563	1/1	0.97	0.06	-	45,45,45,45	0
56	MG	DA	3422	1/1	0.94	0.18	-	52,52,52,52	0
56	MG	BA	3424	1/1	0.94	0.22	-	51,51,51,51	0
56	MG	DA	3491	1/1	0.56	0.12	-	69,69,69,69	0
56	MG	DA	3310	1/1	0.96	0.07	-	39,39,39,39	0
56	MG	CA	3005	1/1	0.72	0.12	-	62,62,62,62	0
56	MG	AA	3117	1/1	0.91	0.14	-	66,66,66,66	0
56	MG	AA	3191	1/1	0.93	0.18	-	49,49,49,49	0
56	MG	DA	3482	1/1	0.90	0.15	-	42,42,42,42	0
56	MG	BA	3386	1/1	0.97	0.20	-	36,36,36,36	0
56	MG	DA	3458	1/1	0.90	0.12	-	56,56,56,56	0
56	MG	BA	3225	1/1	0.91	0.17	-	43,43,43,43	0
56	MG	AA	3090	1/1	0.91	0.28	-	50,50,50,50	0
56	MG	AA	3151	1/1	0.95	0.19	-	65,65,65,65	0
56	MG	DA	3324	1/1	0.93	0.19	-	46,46,46,46	0
56	MG	BA	3402	1/1	0.92	0.19	-	67,67,67,67	0
56	MG	BA	3092	1/1	0.94	0.12	-	27,27,27,27	0
56	MG	BA	3600	1/1	0.90	0.09	-	59,59,59,59	0
56	MG	BA	3540	1/1	0.93	0.11	-	28,28,28,28	0
56	MG	BA	3690	1/1	0.92	0.16	-	44,44,44,44	0
56	MG	DA	3150	1/1	0.92	0.17	-	49,49,49,49	0
56	MG	DA	3016	1/1	0.85	0.31	-	34,34,34,34	0
56	MG	BA	3379	1/1	0.95	0.18	-	22,22,22,22	0
56	MG	CA	3113	1/1	0.85	0.11	-	79,79,79,79	0
56	MG	BA	3578	1/1	0.95	0.15	-	49,49,49,49	0
56	MG	DA	3127	1/1	0.89	0.16	-	53,53,53,53	0
56	MG	B8	101	1/1	0.92	0.19	-	35,35,35,35	0
56	MG	CA	3043	1/1	0.95	0.14	-	56,56,56,56	0
56	MG	AA	3088	1/1	0.81	0.15	-	63,63,63,63	0
56	MG	DA	3108	1/1	0.83	0.17	-	48,48,48,48	0
56	MG	AA	3209	1/1	0.97	0.09	-	62,62,62,62	0
56	MG	CA	3040	1/1	0.90	0.15	-	70,70,70,70	0
56	MG	DA	3453	1/1	0.75	0.31	-	77,77,77,77	0
56	MG	BA	3177	1/1	0.82	0.19	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3539	1/1	0.91	0.15	-	58,58,58,58	0
56	MG	BA	3712	1/1	0.92	0.13	-	35,35,35,35	0
56	MG	DA	3247	1/1	0.86	0.08	-	51,51,51,51	0
56	MG	BA	3205	1/1	0.88	0.22	-	45,45,45,45	0
56	MG	DA	3516	1/1	0.95	0.14	-	35,35,35,35	0
56	MG	BA	3189	1/1	0.90	0.43	-	55,55,55,55	0
56	MG	BA	3446	1/1	0.96	0.22	-	40,40,40,40	0
56	MG	DR	3002	1/1	0.91	0.10	-	55,55,55,55	0
56	MG	DA	3107	1/1	0.83	0.17	-	47,47,47,47	0
56	MG	DA	3131	1/1	0.80	0.16	-	63,63,63,63	0
56	MG	BA	3554	1/1	0.88	0.07	-	56,56,56,56	0
56	MG	BP	204	1/1	0.81	0.13	-	54,54,54,54	0
56	MG	AA	3116	1/1	0.92	0.14	-	57,57,57,57	0
56	MG	BA	3148	1/1	0.88	0.19	-	50,50,50,50	0
56	MG	BA	3515	1/1	0.91	0.11	-	57,57,57,57	0
56	MG	BA	3665	1/1	0.81	0.18	-	45,45,45,45	0
56	MG	BA	3104	1/1	0.97	0.95	-	44,44,44,44	0
56	MG	AA	3142	1/1	0.98	0.13	-	38,38,38,38	0
56	MG	BA	3445	1/1	0.89	0.24	-	53,53,53,53	0
56	MG	BA	3589	1/1	0.95	0.18	-	41,41,41,41	0
56	MG	AA	3203	1/1	0.83	0.23	-	62,62,62,62	0
56	MG	B6	101	1/1	0.90	0.11	-	49,49,49,49	0
56	MG	BA	3197	1/1	0.90	0.15	-	46,46,46,46	0
56	MG	DA	3427	1/1	0.97	0.09	-	61,61,61,61	0
56	MG	DA	3256	1/1	0.94	0.17	-	48,48,48,48	0
56	MG	AA	3027	1/1	0.86	0.12	-	58,58,58,58	0
56	MG	BA	3501	1/1	0.90	0.28	-	74,74,74,74	0
56	MG	D8	5001	1/1	0.92	0.16	-	52,52,52,52	0
56	MG	CA	3134	1/1	0.57	0.14	-	78,78,78,78	0
56	MG	BA	3158	1/1	0.93	0.19	-	47,47,47,47	0
56	MG	AA	3126	1/1	0.83	0.33	-	65,65,65,65	0
56	MG	AA	3141	1/1	0.92	0.18	-	67,67,67,67	0
56	MG	AA	3101	1/1	0.87	0.21	-	52,52,52,52	0
56	MG	AA	3045	1/1	0.78	0.29	-	68,68,68,68	0
56	MG	DA	3577	1/1	0.79	0.46	-	72,72,72,72	0
56	MG	AA	3068	1/1	0.63	0.18	-	70,70,70,70	0
56	MG	CA	3080	1/1	0.97	0.13	-	62,62,62,62	0
56	MG	BD	301	1/1	0.91	0.54	-	45,45,45,45	0
56	MG	DA	3495	1/1	0.36	0.10	-	57,57,57,57	0
56	MG	AA	3208	1/1	0.87	0.28	-	67,67,67,67	0
56	MG	AA	3188	1/1	0.69	0.12	-	69,69,69,69	0
56	MG	BA	3051	1/1	0.83	0.17	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3195	1/1	0.91	0.19	-	58,58,58,58	0
56	MG	DA	3155	1/1	0.96	0.15	-	53,53,53,53	0
56	MG	BA	3406	1/1	0.86	0.13	-	50,50,50,50	0
56	MG	DA	3066	1/1	0.83	0.13	-	39,39,39,39	0
56	MG	BA	3586	1/1	0.88	0.25	-	58,58,58,58	0
56	MG	BA	3107	1/1	0.99	0.73	-	49,49,49,49	0
56	MG	DA	3099	1/1	0.98	0.20	-	39,39,39,39	0
56	MG	CA	3102	1/1	0.94	0.11	-	48,48,48,48	0
56	MG	CA	3099	1/1	0.84	0.13	-	82,82,82,82	0
56	MG	DA	3492	1/1	0.94	0.43	-	51,51,51,51	0
56	MG	DA	3529	1/1	0.94	0.11	-	55,55,55,55	0
56	MG	BA	3149	1/1	0.94	0.19	-	57,57,57,57	0
56	MG	BA	3728	1/1	0.90	0.10	-	65,65,65,65	0
56	MG	DA	3174	1/1	0.94	0.11	-	42,42,42,42	0
56	MG	BA	3072	1/1	0.98	0.16	-	42,42,42,42	0
56	MG	BA	3644	1/1	0.94	0.31	-	34,34,34,34	0
56	MG	BA	3293	1/1	0.96	0.18	-	40,40,40,40	0
56	MG	DA	3212	1/1	0.88	0.26	-	52,52,52,52	0
56	MG	BA	3560	1/1	0.92	0.25	-	47,47,47,47	0
56	MG	BA	3179	1/1	0.84	0.25	-	61,61,61,61	0
56	MG	DA	3576	1/1	0.98	0.14	-	46,46,46,46	0
56	MG	BA	3609	1/1	0.85	0.15	-	62,62,62,62	0
56	MG	BA	3647	1/1	0.97	0.15	-	48,48,48,48	0
56	MG	AA	3147	1/1	0.94	0.09	-	47,47,47,47	0
56	MG	DA	3133	1/1	0.86	0.15	-	50,50,50,50	0
56	MG	AA	3135	1/1	0.99	0.11	-	34,34,34,34	0
56	MG	BA	3657	1/1	0.91	0.16	-	54,54,54,54	0
56	MG	BA	3129	1/1	0.96	0.36	-	49,49,49,49	0
56	MG	BA	3233	1/1	0.89	0.13	-	49,49,49,49	0
56	MG	BA	3222	1/1	0.85	0.20	-	60,60,60,60	0
56	MG	BA	3090	1/1	0.92	0.23	-	40,40,40,40	0
56	MG	BA	3557	1/1	0.92	0.12	-	58,58,58,58	0
56	MG	BA	3313	1/1	0.93	0.13	-	32,32,32,32	0
56	MG	DA	3498	1/1	0.93	0.15	-	66,66,66,66	0
56	MG	DA	3503	1/1	0.96	0.06	-	58,58,58,58	0
56	MG	AX	3006	1/1	0.87	0.14	-	80,80,80,80	0
56	MG	DA	3348	1/1	0.96	0.15	-	46,46,46,46	0
56	MG	BQ	3003	1/1	0.81	0.26	-	67,67,67,67	0
56	MG	CA	3029	1/1	0.93	0.15	-	37,37,37,37	0
56	MG	BA	3241	1/1	0.93	0.22	-	59,59,59,59	0
56	MG	DB	3004	1/1	0.92	0.14	-	54,54,54,54	0
56	MG	BA	3111	1/1	0.91	0.32	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3095	1/1	0.89	0.12	-	63,63,63,63	0
56	MG	DA	3350	1/1	0.87	0.16	-	61,61,61,61	0
56	MG	CA	3041	1/1	0.95	0.16	-	63,63,63,63	0
56	MG	DA	3263	1/1	0.96	0.06	-	48,48,48,48	0
56	MG	BA	3704	1/1	0.86	0.14	-	75,75,75,75	0
56	MG	BA	3040	1/1	0.93	0.13	-	60,60,60,60	0
56	MG	BA	3324	1/1	0.98	0.16	-	44,44,44,44	0
56	MG	BA	3389	1/1	0.90	0.14	-	51,51,51,51	0
56	MG	BA	3166	1/1	0.96	0.15	-	47,47,47,47	0
56	MG	CA	3010	1/1	0.93	0.21	-	60,60,60,60	0
56	MG	CA	3067	1/1	0.93	0.20	-	57,57,57,57	0
56	MG	BA	3302	1/1	0.95	0.11	-	46,46,46,46	0
56	MG	DA	3116	1/1	0.92	0.08	-	58,58,58,58	0
56	MG	BA	3407	1/1	0.93	0.22	-	44,44,44,44	0
56	MG	BA	3713	1/1	0.93	0.21	-	68,68,68,68	0
56	MG	AW	3005	1/1	0.96	0.12	-	52,52,52,52	0
56	MG	BA	3678	1/1	0.97	0.14	-	41,41,41,41	0
56	MG	DA	3394	1/1	0.94	0.11	-	50,50,50,50	0
56	MG	BA	3734	1/1	0.88	0.16	-	24,24,24,24	0
60	K	CX	3001	1/1	0.89	0.46	-	84,84,84,84	0
56	MG	CA	3034	1/1	0.95	0.22	-	46,46,46,46	0
56	MG	CA	3079	1/1	0.92	0.12	-	61,61,61,61	0
56	MG	AA	3199	1/1	0.86	0.20	-	68,68,68,68	0
56	MG	DA	3117	1/1	0.91	0.10	-	46,46,46,46	0
56	MG	DA	3159	1/1	0.83	0.14	-	60,60,60,60	0
56	MG	BA	3351	1/1	0.97	0.16	-	61,61,61,61	0
56	MG	DA	3240	1/1	0.96	0.15	-	36,36,36,36	0
56	MG	BA	3561	1/1	0.83	0.22	-	64,64,64,64	0
56	MG	DA	3622	1/1	0.92	0.37	-	61,61,61,61	0
56	MG	BA	3252	1/1	0.92	0.27	-	61,61,61,61	0
56	MG	DA	3050	1/1	0.85	0.27	-	60,60,60,60	0
56	MG	DA	3417	1/1	0.53	0.18	-	71,71,71,71	0
56	MG	CA	3072	1/1	0.94	0.17	-	57,57,57,57	0
56	MG	AA	3043	1/1	0.92	0.11	-	62,62,62,62	0
56	MG	DA	3134	1/1	0.92	0.26	-	60,60,60,60	0
56	MG	AA	3190	1/1	0.91	0.08	-	61,61,61,61	0
56	MG	BA	3400	1/1	0.87	0.15	-	53,53,53,53	0
56	MG	BA	3735	1/1	0.92	0.13	-	41,41,41,41	0
56	MG	BA	3155	1/1	0.85	0.35	-	63,63,63,63	0
56	MG	BA	3264	1/1	0.93	0.19	-	19,19,19,19	0
56	MG	DA	3100	1/1	0.93	0.16	-	45,45,45,45	0
56	MG	BA	3202	1/1	0.92	0.25	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3130	1/1	0.97	0.30	-	44,44,44,44	0
56	MG	DA	3287	1/1	0.78	0.21	-	50,50,50,50	0
56	MG	AA	3179	1/1	0.74	0.12	-	85,85,85,85	0
56	MG	DA	3145	1/1	0.95	0.26	-	61,61,61,61	0
56	MG	BA	3590	1/1	0.94	0.18	-	38,38,38,38	0
56	MG	DA	3339	1/1	0.85	0.33	-	46,46,46,46	0
56	MG	AA	3120	1/1	0.99	0.12	-	72,72,72,72	0
56	MG	BA	3522	1/1	0.91	0.25	-	59,59,59,59	0
56	MG	BA	3387	1/1	0.93	0.29	-	43,43,43,43	0
56	MG	CA	3112	1/1	0.96	0.29	-	59,59,59,59	0
56	MG	BA	3506	1/1	0.91	0.05	-	43,43,43,43	0
56	MG	AA	3138	1/1	0.93	0.08	-	73,73,73,73	0
56	MG	DA	3407	1/1	0.94	0.24	-	41,41,41,41	0
56	MG	DA	3605	1/1	0.80	0.12	-	53,53,53,53	0
56	MG	BA	3717	1/1	0.90	0.15	-	34,34,34,34	0
56	MG	DA	3437	1/1	0.62	0.14	-	47,47,47,47	0
56	MG	DA	3221	1/1	0.89	0.12	-	56,56,56,56	0
56	MG	CA	3161	1/1	0.97	0.10	-	59,59,59,59	0
56	MG	DA	3358	1/1	0.95	0.12	-	51,51,51,51	0
56	MG	BA	3064	1/1	0.94	0.34	-	46,46,46,46	0
56	MG	DA	3430	1/1	0.93	0.10	-	51,51,51,51	0
56	MG	DA	3570	1/1	0.94	0.10	-	62,62,62,62	0
56	MG	BA	3345	1/1	0.96	0.19	-	20,20,20,20	0
56	MG	DA	3072	1/1	0.97	0.19	-	60,60,60,60	0
56	MG	BA	3073	1/1	0.94	0.17	-	25,25,25,25	0
56	MG	AA	3113	1/1	0.85	0.13	-	57,57,57,57	0
56	MG	DA	3613	1/1	0.92	0.10	-	57,57,57,57	0
56	MG	BA	3335	1/1	0.91	0.12	-	50,50,50,50	0
56	MG	DA	3002	1/1	0.92	0.12	-	51,51,51,51	0
56	MG	BA	3573	1/1	0.94	0.13	-	53,53,53,53	0
56	MG	DA	3311	1/1	0.80	0.13	-	54,54,54,54	0
56	MG	DA	3106	1/1	0.92	0.27	-	56,56,56,56	0
56	MG	CA	3151	1/1	0.96	0.14	-	59,59,59,59	0
56	MG	BA	3176	1/1	0.76	0.19	-	41,41,41,41	0
56	MG	DA	3172	1/1	0.92	0.18	-	56,56,56,56	0
56	MG	BA	3048	1/1	0.93	0.14	-	56,56,56,56	0
56	MG	DA	3183	1/1	0.79	0.18	-	57,57,57,57	0
56	MG	BA	3433	1/1	0.96	0.15	-	48,48,48,48	0
56	MG	DA	3211	1/1	0.91	0.18	-	49,49,49,49	0
56	MG	AD	502	1/1	0.96	0.26	-	58,58,58,58	0
56	MG	DA	3261	1/1	0.87	0.34	-	60,60,60,60	0
56	MG	BA	3548	1/1	0.81	0.15	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3326	1/1	0.89	0.22	-	31,31,31,31	0
56	MG	DA	3500	1/1	0.89	0.12	-	56,56,56,56	0
56	MG	AA	3186	1/1	0.88	0.17	-	65,65,65,65	0
56	MG	BA	3674	1/1	0.95	0.15	-	42,42,42,42	0
56	MG	DA	3374	1/1	0.97	0.13	-	52,52,52,52	0
56	MG	BA	3702	1/1	0.93	0.18	-	60,60,60,60	0
56	MG	BA	3685	1/1	0.93	0.22	-	43,43,43,43	0
56	MG	DA	3347	1/1	0.94	0.15	-	53,53,53,53	0
56	MG	CA	3156	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	DA	3513	1/1	0.71	0.09	-	58,58,58,58	0
56	MG	DA	3321	1/1	0.82	0.17	-	58,58,58,58	0
56	MG	BA	3616	1/1	0.78	0.11	-	43,43,43,43	0
56	MG	DA	3567	1/1	0.97	0.07	-	52,52,52,52	0
56	MG	BA	3737	1/1	0.79	0.12	-	68,68,68,68	0
56	MG	DA	3080	1/1	0.89	0.20	-	48,48,48,48	0
56	MG	BA	3491	1/1	0.93	0.16	-	52,52,52,52	0
56	MG	DA	3333	1/1	0.92	0.07	-	53,53,53,53	0
56	MG	DA	3242	1/1	0.77	0.13	-	56,56,56,56	0
56	MG	DA	3139	1/1	0.96	0.24	-	59,59,59,59	0
56	MG	DA	3521	1/1	0.98	0.16	-	29,29,29,29	0
56	MG	BA	3084	1/1	0.82	0.40	-	46,46,46,46	0
56	MG	BA	3039	1/1	0.86	0.22	-	34,34,34,34	0
56	MG	BA	3726	1/1	0.74	0.18	-	61,61,61,61	0
56	MG	AA	3189	1/1	0.83	0.10	-	56,56,56,56	0
56	MG	BA	3062	1/1	0.93	0.32	-	35,35,35,35	0
56	MG	DA	3460	1/1	0.93	0.08	-	64,64,64,64	0
56	MG	DA	3201	1/1	0.95	0.17	-	56,56,56,56	0
56	MG	DA	3001	1/1	0.84	0.27	-	49,49,49,49	0
56	MG	CA	3017	1/1	0.92	0.27	-	53,53,53,53	0
56	MG	BA	3724	1/1	0.91	0.14	-	84,84,84,84	0
56	MG	BA	3204	1/1	0.96	0.30	-	35,35,35,35	0
56	MG	DA	3209	1/1	0.89	0.19	-	52,52,52,52	0
56	MG	BA	3673	1/1	0.99	0.28	-	22,22,22,22	0
56	MG	DA	3331	1/1	0.96	0.14	-	46,46,46,46	0
56	MG	BA	3464	1/1	0.95	0.21	-	53,53,53,53	0
56	MG	DA	3420	1/1	0.96	0.08	-	40,40,40,40	0
56	MG	DA	3269	1/1	0.98	0.11	-	46,46,46,46	0
56	MG	BA	3211	1/1	0.88	0.20	-	57,57,57,57	0
56	MG	AA	3084	1/1	0.91	0.12	-	53,53,53,53	0
56	MG	DA	3146	1/1	0.94	0.13	-	50,50,50,50	0
56	MG	AA	3067	1/1	0.94	0.31	-	53,53,53,53	0
56	MG	BA	3443	1/1	0.94	0.15	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3623	1/1	0.94	0.66	-	48,48,48,48	0
56	MG	DA	3041	1/1	0.95	0.40	-	51,51,51,51	0
56	MG	DA	3042	1/1	0.81	0.14	-	71,71,71,71	0
56	MG	DA	3575	1/1	0.67	0.19	-	58,58,58,58	0
56	MG	DA	3485	1/1	0.91	0.38	-	60,60,60,60	0
56	MG	BA	3658	1/1	0.89	0.15	-	41,41,41,41	0
56	MG	CA	3042	1/1	0.85	0.15	-	61,61,61,61	0
56	MG	DA	3213	1/1	0.81	0.21	-	58,58,58,58	0
56	MG	DA	3432	1/1	0.93	0.11	-	43,43,43,43	0
56	MG	BA	3731	1/1	0.80	0.13	-	57,57,57,57	0
56	MG	BA	3747	1/1	0.97	0.23	-	50,50,50,50	0
56	MG	AA	3100	1/1	0.88	0.25	-	53,53,53,53	0
56	MG	DA	3083	1/1	0.95	0.50	-	46,46,46,46	0
56	MG	AA	3205	1/1	0.94	0.07	-	66,66,66,66	0
56	MG	AA	3083	1/1	0.94	0.17	-	57,57,57,57	0
56	MG	BA	3030	1/1	0.80	0.12	-	50,50,50,50	0
56	MG	BA	3574	1/1	0.97	0.26	-	60,60,60,60	0
56	MG	DA	3163	1/1	0.81	0.68	-	63,63,63,63	0
56	MG	BA	3101	1/1	0.98	0.28	-	36,36,36,36	0
56	MG	BA	3200	1/1	0.84	0.16	-	50,50,50,50	0
56	MG	DA	3184	1/1	0.91	0.23	-	56,56,56,56	0
56	MG	BA	3520	1/1	0.96	0.23	-	25,25,25,25	0
56	MG	BA	3434	1/1	0.89	0.15	-	65,65,65,65	0
56	MG	CA	3066	1/1	0.84	0.16	-	58,58,58,58	0
56	MG	AA	3112	1/1	0.90	0.15	-	53,53,53,53	0
56	MG	AA	3155	1/1	0.91	0.14	-	60,60,60,60	0
56	MG	CA	3003	1/1	0.78	0.20	-	65,65,65,65	0
56	MG	BA	3183	1/1	0.82	0.73	-	47,47,47,47	0
56	MG	BA	3474	1/1	0.95	0.17	-	37,37,37,37	0
56	MG	BA	3364	1/1	0.89	0.12	-	50,50,50,50	0
56	MG	DA	3384	1/1	0.94	0.21	-	55,55,55,55	0
56	MG	DA	3512	1/1	0.90	0.12	-	52,52,52,52	0
56	MG	DA	3509	1/1	0.98	0.13	-	38,38,38,38	0
56	MG	BA	3477	1/1	0.91	0.20	-	35,35,35,35	0
56	MG	DA	3488	1/1	0.88	0.11	-	66,66,66,66	0
56	MG	BA	3772	1/1	0.94	0.15	-	52,52,52,52	0
56	MG	AA	3132	1/1	0.97	0.19	-	75,75,75,75	0
56	MG	DA	3210	1/1	0.96	0.21	-	35,35,35,35	0
56	MG	DA	3550	1/1	0.87	0.11	-	61,61,61,61	0
56	MG	BA	3725	1/1	0.87	0.09	-	63,63,63,63	0
56	MG	BA	3662	1/1	0.95	0.11	-	56,56,56,56	0
56	MG	DA	3095	1/1	0.96	0.08	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3374	1/1	0.92	0.20	-	34,34,34,34	0
56	MG	AA	3224	1/1	0.93	0.19	-	61,61,61,61	0
56	MG	DA	3202	1/1	0.94	0.15	-	51,51,51,51	0
56	MG	DA	3149	1/1	0.91	0.18	-	48,48,48,48	0
56	MG	DA	3511	1/1	0.94	0.12	-	62,62,62,62	0
56	MG	BA	3542	1/1	0.89	0.15	-	66,66,66,66	0
56	MG	AX	3011	1/1	0.85	0.13	-	62,62,62,62	0
56	MG	DA	3514	1/1	0.80	0.13	-	67,67,67,67	0
56	MG	BA	3365	1/1	0.93	0.09	-	47,47,47,47	0
56	MG	DA	3434	1/1	0.94	0.31	-	46,46,46,46	0
56	MG	BB	3005	1/1	0.87	0.19	-	54,54,54,54	0
56	MG	BA	3251	1/1	0.98	0.13	-	51,51,51,51	0
56	MG	BA	3732	1/1	0.88	0.14	-	57,57,57,57	0
56	MG	BO	5001	1/1	0.96	0.22	-	70,70,70,70	0
56	MG	BA	3584	1/1	0.93	0.20	-	47,47,47,47	0
56	MG	DA	3198	1/1	0.98	0.22	-	32,32,32,32	0
56	MG	BA	3253	1/1	0.90	0.17	-	30,30,30,30	0
56	MG	CA	3018	1/1	0.89	0.15	-	69,69,69,69	0
56	MG	BA	3216	1/1	0.95	0.14	-	53,53,53,53	0
56	MG	DA	3097	1/1	0.91	0.14	-	52,52,52,52	0
56	MG	BA	3377	1/1	0.94	0.20	-	39,39,39,39	0
56	MG	DA	3535	1/1	0.96	0.10	-	38,38,38,38	0
56	MG	DA	3254	1/1	0.97	0.12	-	53,53,53,53	0
56	MG	B2	3001	1/1	0.77	0.28	-	54,54,54,54	0
56	MG	CA	3077	1/1	0.96	0.17	-	36,36,36,36	0
56	MG	AA	3158	1/1	0.97	0.14	-	62,62,62,62	0
56	MG	DA	3467	1/1	0.84	0.25	-	69,69,69,69	0
56	MG	DA	3120	1/1	0.94	0.18	-	42,42,42,42	0
56	MG	BA	3013	1/1	0.87	0.19	-	46,46,46,46	0
56	MG	BA	3171	1/1	0.94	0.10	-	58,58,58,58	0
56	MG	BA	3208	1/1	0.81	0.21	-	47,47,47,47	0
56	MG	CA	3033	1/1	0.97	0.19	-	44,44,44,44	0
56	MG	DA	3462	1/1	0.86	0.12	-	36,36,36,36	0
56	MG	AA	3011	1/1	0.84	0.19	-	66,66,66,66	0
56	MG	DA	3192	1/1	0.76	0.16	-	49,49,49,49	0
56	MG	BA	3133	1/1	0.95	0.30	-	43,43,43,43	0
56	MG	CA	3045	1/1	0.87	0.19	-	68,68,68,68	0
56	MG	BA	3463	1/1	0.98	0.16	-	34,34,34,34	0
56	MG	DA	3153	1/1	0.86	0.13	-	40,40,40,40	0
56	MG	BA	3278	1/1	0.97	0.12	-	48,48,48,48	0
56	MG	DA	3013	1/1	0.92	0.14	-	49,49,49,49	0
56	MG	DA	3519	1/1	0.97	0.06	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3517	1/1	0.91	0.29	-	60,60,60,60	0
56	MG	BA	3482	1/1	0.88	0.32	-	27,27,27,27	0
56	MG	DD	301	1/1	0.93	0.22	-	44,44,44,44	0
56	MG	BA	3733	1/1	0.62	0.07	-	78,78,78,78	0
56	MG	BA	3760	1/1	0.93	0.12	-	78,78,78,78	0
56	MG	BA	3305	1/1	0.95	0.26	-	61,61,61,61	0
56	MG	DA	3525	1/1	0.97	0.07	-	33,33,33,33	0
56	MG	BA	3314	1/1	0.94	0.14	-	41,41,41,41	0
56	MG	DB	3012	1/1	0.96	0.08	-	61,61,61,61	0
56	MG	DA	3093	1/1	0.83	0.11	-	59,59,59,59	0
56	MG	AA	3058	1/1	0.88	0.23	-	63,63,63,63	0
56	MG	DA	3446	1/1	0.94	0.18	-	52,52,52,52	0
56	MG	DA	3051	1/1	0.98	0.14	-	54,54,54,54	0
56	MG	AA	3032	1/1	0.74	0.18	-	62,62,62,62	0
56	MG	BA	3457	1/1	0.97	0.10	-	46,46,46,46	0
56	MG	CA	3096	1/1	0.96	0.16	-	51,51,51,51	0
56	MG	DA	3308	1/1	0.91	0.25	-	57,57,57,57	0
56	MG	AA	3181	1/1	0.95	0.10	-	65,65,65,65	0
56	MG	AA	3160	1/1	0.94	0.23	-	70,70,70,70	0
56	MG	AA	3198	1/1	0.92	0.13	-	82,82,82,82	0
56	MG	DA	3584	1/1	0.91	0.16	-	45,45,45,45	0
56	MG	BA	3551	1/1	0.94	0.15	-	56,56,56,56	0
56	MG	CA	3024	1/1	0.97	0.07	-	53,53,53,53	0
56	MG	BB	3009	1/1	0.93	0.14	-	49,49,49,49	0
56	MG	CA	3163	1/1	0.94	0.16	-	49,49,49,49	0
56	MG	BA	3161	1/1	0.90	0.46	-	40,40,40,40	0
56	MG	CA	3137	1/1	0.99	0.08	-	52,52,52,52	0
56	MG	BA	3247	1/1	0.75	0.20	-	49,49,49,49	0
56	MG	AA	3164	1/1	0.93	0.12	-	71,71,71,71	0
56	MG	BA	3301	1/1	0.85	0.11	-	55,55,55,55	0
56	MG	CX	3003	1/1	0.95	0.19	-	64,64,64,64	0
56	MG	BA	3780	1/1	0.94	0.52	-	45,45,45,45	0
56	MG	BA	3512	1/1	0.89	0.14	-	65,65,65,65	0
56	MG	DA	3260	1/1	0.96	0.19	-	36,36,36,36	0
56	MG	BA	3367	1/1	0.93	0.12	-	58,58,58,58	0
56	MG	BA	3114	1/1	0.94	0.61	-	49,49,49,49	0
56	MG	DA	3486	1/1	0.81	0.12	-	47,47,47,47	0
56	MG	BA	3287	1/1	0.94	0.14	-	21,21,21,21	0
56	MG	BA	3606	1/1	0.95	0.16	-	62,62,62,62	0
56	MG	CA	3070	1/1	0.96	0.33	-	52,52,52,52	0
56	MG	BA	3467	1/1	0.87	0.21	-	48,48,48,48	0
56	MG	DA	3177	1/1	0.93	0.23	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B5	106	1/1	0.97	0.15	-	55,55,55,55	0
56	MG	B3	3002	1/1	0.93	0.13	-	65,65,65,65	0
56	MG	AA	3193	1/1	0.87	0.25	-	69,69,69,69	0
56	MG	DA	3431	1/1	0.90	0.16	-	44,44,44,44	0
56	MG	BA	3329	1/1	0.75	0.30	-	57,57,57,57	0
56	MG	BA	3591	1/1	0.83	0.13	-	58,58,58,58	0
56	MG	DA	3064	1/1	0.95	0.22	-	52,52,52,52	0
56	MG	AA	3055	1/1	0.95	0.10	-	40,40,40,40	0
56	MG	DA	3581	1/1	0.85	0.16	-	67,67,67,67	0
56	MG	DA	3544	1/1	0.95	0.12	-	49,49,49,49	0
56	MG	AX	3008	1/1	0.98	0.18	-	52,52,52,52	0
56	MG	DA	3539	1/1	0.93	0.19	-	64,64,64,64	0
56	MG	DA	3320	1/1	0.91	0.15	-	53,53,53,53	0
56	MG	BA	3221	1/1	0.96	0.19	-	47,47,47,47	0
56	MG	DA	3528	1/1	0.90	0.15	-	70,70,70,70	0
56	MG	DA	3228	1/1	0.94	0.15	-	29,29,29,29	0
56	MG	BA	3385	1/1	0.96	0.20	-	50,50,50,50	0
56	MG	DA	3185	1/1	0.93	0.24	-	53,53,53,53	0
56	MG	DF	301	1/1	0.96	0.16	-	49,49,49,49	0
56	MG	B5	104	1/1	0.90	0.42	-	55,55,55,55	0
56	MG	CA	3122	1/1	0.89	0.19	-	70,70,70,70	0
56	MG	DA	3105	1/1	0.87	0.20	-	54,54,54,54	0
56	MG	DA	3508	1/1	0.89	0.06	-	68,68,68,68	0
56	MG	BA	3670	1/1	0.90	0.19	-	55,55,55,55	0
56	MG	BA	3075	1/1	0.83	0.32	-	48,48,48,48	0
56	MG	BA	3268	1/1	0.98	0.19	-	40,40,40,40	0
56	MG	CA	3125	1/1	0.87	0.08	-	76,76,76,76	0
56	MG	DA	3572	1/1	0.86	0.14	-	70,70,70,70	0
56	MG	BA	3743	1/1	0.97	0.15	-	18,18,18,18	0
56	MG	DA	3461	1/1	0.96	0.14	-	49,49,49,49	0
56	MG	BA	3603	1/1	0.93	0.24	-	28,28,28,28	0
56	MG	BA	3435	1/1	0.89	0.34	-	52,52,52,52	0
56	MG	CA	3160	1/1	0.98	0.22	-	53,53,53,53	0
56	MG	BA	3476	1/1	0.93	0.21	-	37,37,37,37	0
56	MG	BA	3384	1/1	0.98	0.14	-	43,43,43,43	0
56	MG	AA	3175	1/1	0.84	0.10	-	54,54,54,54	0
56	MG	DB	3005	1/1	0.81	0.35	-	77,77,77,77	0
56	MG	DA	3349	1/1	0.88	0.12	-	46,46,46,46	0
56	MG	DA	3169	1/1	0.90	0.12	-	61,61,61,61	0
56	MG	CA	3143	1/1	0.90	0.25	-	59,59,59,59	0
56	MG	DA	3300	1/1	0.91	0.13	-	27,27,27,27	0
56	MG	BA	3538	1/1	0.98	0.10	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3421	1/1	0.93	0.14	-	55,55,55,55	0
56	MG	BA	3002	1/1	0.75	0.17	-	36,36,36,36	0
56	MG	BA	3715	1/1	0.86	0.14	-	48,48,48,48	0
56	MG	DA	3048	1/1	0.78	0.13	-	58,58,58,58	0
56	MG	CA	3044	1/1	0.90	0.16	-	62,62,62,62	0
56	MG	CA	3095	1/1	0.88	0.08	-	47,47,47,47	0
56	MG	AA	3168	1/1	0.71	0.18	-	76,76,76,76	0
56	MG	CA	3117	1/1	0.94	0.18	-	71,71,71,71	0
56	MG	BA	3656	1/1	0.71	0.19	-	34,34,34,34	0
56	MG	DA	3264	1/1	0.93	0.12	-	44,44,44,44	0
56	MG	BA	3283	1/1	0.89	0.17	-	39,39,39,39	0
56	MG	DA	3061	1/1	0.77	0.14	-	63,63,63,63	0
56	MG	CA	3097	1/1	0.82	0.13	-	66,66,66,66	0
56	MG	BA	3008	1/1	0.94	0.23	-	27,27,27,27	0
56	MG	CA	3098	1/1	0.94	0.14	-	59,59,59,59	0
56	MG	BA	3614	1/1	0.94	0.14	-	54,54,54,54	0
56	MG	AA	3106	1/1	0.77	0.14	-	62,62,62,62	0
56	MG	DA	3197	1/1	0.89	0.12	-	57,57,57,57	0
56	MG	DA	3480	1/1	0.94	0.19	-	48,48,48,48	0
56	MG	BA	3550	1/1	0.63	0.49	-	74,74,74,74	0
56	MG	BA	3074	1/1	0.74	0.17	-	58,58,58,58	0
56	MG	DF	303	1/1	0.85	0.36	-	46,46,46,46	0
56	MG	BA	3015	1/1	0.88	0.27	-	52,52,52,52	0
56	MG	DA	3022	1/1	0.87	0.24	-	50,50,50,50	0
56	MG	BA	3752	1/1	0.96	0.22	-	48,48,48,48	0
56	MG	DA	3245	1/1	0.94	0.13	-	28,28,28,28	0
56	MG	BA	3120	1/1	0.98	0.40	-	45,45,45,45	0
56	MG	BA	3428	1/1	0.94	0.22	-	42,42,42,42	0
56	MG	DA	3113	1/1	0.93	0.27	-	51,51,51,51	0
56	MG	BA	3719	1/1	0.90	0.19	-	49,49,49,49	0
56	MG	DA	3448	1/1	0.97	0.19	-	40,40,40,40	0
56	MG	AA	3144	1/1	0.83	0.08	-	62,62,62,62	0
56	MG	AA	3140	1/1	0.91	0.21	-	61,61,61,61	0
56	MG	CV	101	1/1	0.98	0.17	-	56,56,56,56	0
56	MG	BW	201	1/1	0.94	0.20	-	45,45,45,45	0
56	MG	BE	307	1/1	0.92	0.08	-	71,71,71,71	0
56	MG	DA	3459	1/1	0.94	0.11	-	63,63,63,63	0
56	MG	AA	3118	1/1	0.94	0.12	-	40,40,40,40	0
56	MG	DA	3293	1/1	0.94	0.13	-	59,59,59,59	0
56	MG	BA	3300	1/1	0.90	0.17	-	55,55,55,55	0
56	MG	BA	3444	1/1	0.89	0.16	-	37,37,37,37	0
56	MG	AF	3001	1/1	0.76	0.14	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3103	1/1	0.78	0.12	-	60,60,60,60	0
56	MG	BA	3021	1/1	0.98	0.31	-	32,32,32,32	0
56	MG	AA	3110	1/1	0.95	0.15	-	53,53,53,53	0
56	MG	DA	3044	1/1	0.92	0.25	-	60,60,60,60	0
56	MG	DA	3413	1/1	0.97	0.25	-	40,40,40,40	0
56	MG	DA	3376	1/1	0.89	0.15	-	46,46,46,46	0
56	MG	BA	3235	1/1	0.80	0.16	-	65,65,65,65	0
56	MG	DB	3008	1/1	0.97	0.10	-	62,62,62,62	0
56	MG	BA	3748	1/1	0.95	0.19	-	63,63,63,63	0
56	MG	BA	3341	1/1	0.95	0.17	-	59,59,59,59	0
56	MG	BA	3646	1/1	0.78	0.42	-	48,48,48,48	0
56	MG	BA	3746	1/1	0.92	0.10	-	71,71,71,71	0
56	MG	AA	3173	1/1	0.95	0.11	-	55,55,55,55	0
56	MG	DA	3334	1/1	0.95	0.24	-	51,51,51,51	0
56	MG	BA	3232	1/1	0.99	0.28	-	44,44,44,44	0
56	MG	BA	3173	1/1	0.95	0.44	-	46,46,46,46	0
56	MG	DA	3586	1/1	0.90	0.19	-	49,49,49,49	0
56	MG	DA	3356	1/1	0.96	0.09	-	47,47,47,47	0
56	MG	BA	3594	1/1	0.98	0.15	-	37,37,37,37	0
56	MG	DA	3602	1/1	0.96	0.19	-	62,62,62,62	0
56	MG	CA	3060	1/1	0.93	0.15	-	58,58,58,58	0
56	MG	DA	3598	1/1	0.97	0.24	-	63,63,63,63	0
56	MG	BA	3169	1/1	0.95	0.18	-	28,28,28,28	0
56	MG	DA	3054	1/1	0.62	0.32	-	59,59,59,59	0
56	MG	DA	3322	1/1	0.77	0.09	-	46,46,46,46	0
56	MG	CA	3006	1/1	0.94	0.27	-	50,50,50,50	0
56	MG	BA	3419	1/1	0.93	0.20	-	50,50,50,50	0
56	MG	BA	3081	1/1	0.85	0.15	-	61,61,61,61	0
56	MG	BA	3620	1/1	0.91	0.21	-	42,42,42,42	0
56	MG	BA	3418	1/1	0.90	0.14	-	57,57,57,57	0
56	MG	AA	3177	1/1	0.92	0.21	-	66,66,66,66	0
56	MG	AA	3037	1/1	0.98	0.14	-	55,55,55,55	0
56	MG	DA	3077	1/1	0.88	0.17	-	40,40,40,40	0
56	MG	BA	3290	1/1	0.91	0.19	-	61,61,61,61	0
56	MG	BA	3255	1/1	0.98	0.22	-	56,56,56,56	0
56	MG	BA	3618	1/1	0.75	0.19	-	64,64,64,64	0
56	MG	BA	3519	1/1	0.67	0.15	-	56,56,56,56	0
56	MG	BA	3455	1/1	0.98	0.13	-	28,28,28,28	0
56	MG	BA	3580	1/1	0.80	0.15	-	61,61,61,61	0
56	MG	DA	3122	1/1	0.41	0.30	-	71,71,71,71	0
56	MG	BA	3532	1/1	0.75	0.14	-	73,73,73,73	0
56	MG	DA	3332	1/1	0.92	0.13	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3019	1/1	0.91	0.31	-	38,38,38,38	0
56	MG	BA	3224	1/1	0.95	0.17	-	55,55,55,55	0
56	MG	BA	3151	1/1	0.94	0.36	-	51,51,51,51	0
56	MG	BA	3277	1/1	0.98	0.17	-	40,40,40,40	0
56	MG	CA	3108	1/1	0.97	0.10	-	56,56,56,56	0
56	MG	BA	3701	1/1	0.89	0.12	-	66,66,66,66	0
56	MG	DA	3564	1/1	0.88	0.14	-	64,64,64,64	0
56	MG	BA	3565	1/1	0.94	0.12	-	50,50,50,50	0
56	MG	DA	3027	1/1	0.85	0.15	-	43,43,43,43	0
56	MG	DA	3164	1/1	0.95	0.06	-	58,58,58,58	0
56	MG	DA	3253	1/1	0.96	0.20	-	57,57,57,57	0
56	MG	BA	3627	1/1	0.93	0.19	-	52,52,52,52	0
56	MG	CA	3120	1/1	0.91	0.12	-	70,70,70,70	0
56	MG	CA	3111	1/1	0.92	0.12	-	69,69,69,69	0
56	MG	DA	3560	1/1	0.95	0.49	-	59,59,59,59	0
56	MG	BA	3625	1/1	0.89	0.14	-	49,49,49,49	0
56	MG	DA	3171	1/1	0.93	0.16	-	41,41,41,41	0
56	MG	BA	3036	1/1	0.91	0.21	-	50,50,50,50	0
56	MG	AA	3003	1/1	0.81	0.23	-	79,79,79,79	0
56	MG	AO	3101	1/1	0.83	0.19	-	58,58,58,58	0
56	MG	AA	3079	1/1	0.85	0.25	-	66,66,66,66	0
56	MG	BA	3068	1/1	0.92	0.77	-	56,56,56,56	0
56	MG	BA	3098	1/1	0.87	0.11	-	51,51,51,51	0
56	MG	AA	3128	1/1	0.79	0.14	-	60,60,60,60	0
56	MG	BA	3700	1/1	0.86	0.13	-	73,73,73,73	0
56	MG	BA	3306	1/1	0.95	0.21	-	51,51,51,51	0
56	MG	DA	3549	1/1	0.90	0.23	-	53,53,53,53	0
56	MG	BA	3531	1/1	0.87	0.09	-	56,56,56,56	0
56	MG	DA	3218	1/1	0.80	0.11	-	53,53,53,53	0
56	MG	BA	3223	1/1	0.89	0.19	-	42,42,42,42	0
56	MG	BA	3370	1/1	0.84	0.23	-	51,51,51,51	0
56	MG	BA	3311	1/1	0.94	0.18	-	34,34,34,34	0
56	MG	AA	3194	1/1	0.91	0.07	-	66,66,66,66	0
56	MG	BA	3410	1/1	0.98	0.18	-	33,33,33,33	0
56	MG	DA	3370	1/1	0.96	0.14	-	49,49,49,49	0
56	MG	BB	3018	1/1	0.90	0.17	-	46,46,46,46	0
56	MG	CA	3100	1/1	0.88	0.10	-	52,52,52,52	0
56	MG	BA	3449	1/1	0.87	0.16	-	59,59,59,59	0
56	MG	BA	3309	1/1	0.92	0.15	-	41,41,41,41	0
56	MG	BT	201	1/1	0.98	0.19	-	49,49,49,49	0
56	MG	DB	3011	1/1	0.91	0.14	-	49,49,49,49	0
56	MG	CA	3149	1/1	0.96	0.10	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AX	3004	1/1	0.87	0.22	-	67,67,67,67	0
56	MG	BA	3775	1/1	0.86	0.24	-	47,47,47,47	0
56	MG	DA	3433	1/1	0.87	0.11	-	58,58,58,58	0
56	MG	BA	3634	1/1	0.86	0.12	-	50,50,50,50	0
56	MG	DA	3444	1/1	0.96	0.17	-	59,59,59,59	0
56	MG	DA	3526	1/1	0.65	0.21	-	64,64,64,64	0
56	MG	BA	3503	1/1	0.87	0.20	-	43,43,43,43	0
56	MG	BA	3041	1/1	0.93	0.26	-	51,51,51,51	0
56	MG	BA	3421	1/1	0.83	0.12	-	46,46,46,46	0
56	MG	BA	3045	1/1	0.83	0.21	-	41,41,41,41	0
56	MG	BA	3123	1/1	0.95	0.58	-	39,39,39,39	0
56	MG	AA	3062	1/1	0.91	0.30	-	58,58,58,58	0
56	MG	DA	3601	1/1	0.70	0.16	-	75,75,75,75	0
56	MG	BA	3121	1/1	0.91	0.35	-	64,64,64,64	0
56	MG	AW	3001	1/1	0.93	0.12	-	67,67,67,67	0
56	MG	BA	3258	1/1	0.89	0.18	-	57,57,57,57	0
56	MG	BA	3099	1/1	0.62	0.37	-	58,58,58,58	0
56	MG	BA	3163	1/1	0.95	0.19	-	57,57,57,57	0
56	MG	DA	3067	1/1	0.95	0.09	-	52,52,52,52	0
56	MG	BB	3012	1/1	0.93	0.10	-	42,42,42,42	0
56	MG	DA	3040	1/1	0.95	0.12	-	47,47,47,47	0
56	MG	BA	3714	1/1	0.82	0.17	-	73,73,73,73	0
56	MG	BA	3398	1/1	0.96	0.18	-	37,37,37,37	0
56	MG	DA	3208	1/1	0.89	0.15	-	61,61,61,61	0
56	MG	BB	3011	1/1	0.83	0.13	-	56,56,56,56	0
56	MG	AW	3002	1/1	0.94	0.20	-	54,54,54,54	0
56	MG	DA	3104	1/1	0.97	0.25	-	49,49,49,49	0
56	MG	BA	3080	1/1	0.90	0.30	-	49,49,49,49	0
56	MG	BA	3498	1/1	0.92	0.05	-	70,70,70,70	0
56	MG	BA	3001	1/1	0.93	0.17	-	23,23,23,23	0
56	MG	DA	3489	1/1	0.92	0.07	-	53,53,53,53	0
56	MG	DA	3055	1/1	0.93	0.12	-	44,44,44,44	0
56	MG	AA	3103	1/1	0.89	0.22	-	59,59,59,59	0
56	MG	AA	3149	1/1	0.92	0.08	-	71,71,71,71	0
56	MG	BA	3544	1/1	0.74	0.26	-	57,57,57,57	0
56	MG	DA	3196	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	BA	3395	1/1	0.87	0.13	-	65,65,65,65	0
56	MG	DA	3205	1/1	0.85	0.14	-	45,45,45,45	0
56	MG	B4	502	1/1	0.83	0.22	-	73,73,73,73	0
56	MG	DA	3009	1/1	0.92	0.11	-	46,46,46,46	0
56	MG	BA	3404	1/1	0.87	0.12	-	59,59,59,59	0
56	MG	BA	3484	1/1	0.87	0.13	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3321	1/1	0.97	0.18	-	43,43,43,43	0
56	MG	AA	3017	1/1	0.87	0.14	-	49,49,49,49	0
56	MG	AA	3056	1/1	0.96	0.10	-	56,56,56,56	0
56	MG	BA	3667	1/1	0.92	0.12	-	64,64,64,64	0
56	MG	DA	3457	1/1	0.97	0.23	-	46,46,46,46	0
56	MG	CA	3148	1/1	0.86	0.11	-	72,72,72,72	0
56	MG	BA	3415	1/1	0.87	0.12	-	62,62,62,62	0
56	MG	B1	101	1/1	0.97	0.71	-	45,45,45,45	0
56	MG	BA	3718	1/1	0.93	0.17	-	49,49,49,49	0
56	MG	BA	3413	1/1	0.95	0.19	-	53,53,53,53	0
56	MG	AA	3196	1/1	0.96	0.17	-	66,66,66,66	0
56	MG	BA	3643	1/1	0.93	0.47	-	38,38,38,38	0
56	MG	BA	3242	1/1	0.88	0.21	-	58,58,58,58	0
56	MG	DA	3328	1/1	0.92	0.17	-	49,49,49,49	0
56	MG	AA	3049	1/1	0.81	0.13	-	59,59,59,59	0
56	MG	DA	3557	1/1	0.87	0.10	-	67,67,67,67	0
56	MG	DA	3229	1/1	0.94	0.16	-	49,49,49,49	0
56	MG	AX	3003	1/1	0.80	0.13	-	74,74,74,74	0
56	MG	DA	3336	1/1	0.98	0.12	-	30,30,30,30	0
56	MG	AA	3033	1/1	0.93	0.32	-	45,45,45,45	0
56	MG	DA	3190	1/1	0.95	0.10	-	58,58,58,58	0
56	MG	BA	3545	1/1	0.84	0.18	-	58,58,58,58	0
56	MG	DA	3597	1/1	0.92	0.24	-	56,56,56,56	0
56	MG	AA	3008	1/1	0.90	0.18	-	53,53,53,53	0
56	MG	BA	3288	1/1	0.91	0.17	-	36,36,36,36	0
56	MG	DA	3595	1/1	0.87	0.12	-	34,34,34,34	0
56	MG	BA	3762	1/1	0.91	0.23	-	58,58,58,58	0
56	MG	BA	3749	1/1	0.90	0.12	-	38,38,38,38	0
56	MG	DD	302	1/1	0.92	0.44	-	40,40,40,40	0
56	MG	BA	3266	1/1	0.93	0.13	-	38,38,38,38	0
56	MG	DA	3158	1/1	0.85	0.30	-	55,55,55,55	0
56	MG	CA	3053	1/1	0.89	0.22	-	63,63,63,63	0
56	MG	AA	3066	1/1	0.91	0.11	-	53,53,53,53	0
56	MG	DA	3400	1/1	0.93	0.13	-	61,61,61,61	0
56	MG	DA	3578	1/1	0.83	0.10	-	71,71,71,71	0
56	MG	BA	3140	1/1	0.92	0.52	-	41,41,41,41	0
56	MG	BA	3033	1/1	0.91	0.12	-	45,45,45,45	0
56	MG	DA	3359	1/1	0.95	0.15	-	54,54,54,54	0
56	MG	DA	3443	1/1	0.93	0.15	-	49,49,49,49	0
56	MG	AA	3109	1/1	0.91	0.21	-	51,51,51,51	0
56	MG	DA	3450	1/1	0.97	0.08	-	50,50,50,50	0
56	MG	DA	3343	1/1	0.94	0.11	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3481	1/1	0.92	0.16	-	51,51,51,51	0
56	MG	DA	3175	1/1	0.82	0.18	-	43,43,43,43	0
56	MG	AA	3020	1/1	0.84	0.25	-	53,53,53,53	0
56	MG	BA	3218	1/1	0.94	0.10	-	52,52,52,52	0
56	MG	BA	3191	1/1	0.85	0.45	-	50,50,50,50	0
56	MG	DA	3082	1/1	0.92	0.08	-	48,48,48,48	0
56	MG	BA	3583	1/1	0.95	0.12	-	46,46,46,46	0
56	MG	BA	3113	1/1	0.92	0.94	-	44,44,44,44	0
56	MG	BA	3429	1/1	0.90	0.09	-	71,71,71,71	0
56	MG	AA	3035	1/1	0.69	0.16	-	69,69,69,69	0
56	MG	DA	3588	1/1	0.90	0.18	-	57,57,57,57	0
56	MG	CA	3179	1/1	0.98	0.16	-	53,53,53,53	0
56	MG	BA	3508	1/1	0.69	0.31	-	61,61,61,61	0
56	MG	DA	3484	1/1	0.96	0.06	-	59,59,59,59	0
56	MG	DA	3419	1/1	0.92	0.07	-	59,59,59,59	0
56	MG	BA	3767	1/1	0.98	0.14	-	31,31,31,31	0
56	MG	CA	3126	1/1	0.60	0.23	-	76,76,76,76	0
56	MG	AA	3165	1/1	0.93	0.14	-	51,51,51,51	0
56	MG	DA	3389	1/1	0.88	0.14	-	63,63,63,63	0
56	MG	BA	3128	1/1	0.96	0.39	-	46,46,46,46	0
56	MG	BA	3142	1/1	0.92	0.32	-	47,47,47,47	0
56	MG	BA	3648	1/1	0.82	0.14	-	39,39,39,39	0
56	MG	AA	3080	1/1	0.92	0.26	-	58,58,58,58	0
56	MG	DA	3226	1/1	0.73	0.26	-	70,70,70,70	0
56	MG	CA	3081	1/1	0.92	0.11	-	51,51,51,51	0
56	MG	DA	3596	1/1	0.91	0.11	-	64,64,64,64	0
56	MG	BA	3088	1/1	0.92	0.40	-	46,46,46,46	0
56	MG	BA	3100	1/1	0.93	0.35	-	46,46,46,46	0
56	MG	DA	3412	1/1	0.91	0.35	-	52,52,52,52	0
56	MG	BA	3576	1/1	0.97	0.10	-	56,56,56,56	0
56	MG	CA	3105	1/1	0.84	0.11	-	76,76,76,76	0
56	MG	CA	3130	1/1	0.91	0.11	-	70,70,70,70	0
56	MG	AA	3050	1/1	0.88	0.13	-	65,65,65,65	0
56	MG	BA	3754	1/1	0.94	0.21	-	36,36,36,36	0
56	MG	BF	310	1/1	0.82	0.20	-	44,44,44,44	0
56	MG	CA	3083	1/1	0.89	0.08	-	58,58,58,58	0
56	MG	DA	3231	1/1	0.97	0.10	-	54,54,54,54	0
56	MG	CA	3154	1/1	0.93	0.14	-	62,62,62,62	0
56	MG	CA	3139	1/1	0.83	0.11	-	63,63,63,63	0
56	MG	DA	3207	1/1	0.89	0.13	-	58,58,58,58	0
56	MG	CA	3074	1/1	0.93	0.09	-	62,62,62,62	0
56	MG	DA	3276	1/1	0.78	0.15	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3127	1/1	0.85	0.13	-	69,69,69,69	0
56	MG	BA	3284	1/1	0.97	0.20	-	35,35,35,35	0
56	MG	BA	3697	1/1	0.94	0.13	-	34,34,34,34	0
56	MG	BA	3684	1/1	0.98	0.08	-	39,39,39,39	0
56	MG	DA	3239	1/1	0.87	0.09	-	61,61,61,61	0
56	MG	DA	3574	1/1	0.92	0.13	-	68,68,68,68	0
56	MG	BA	3575	1/1	0.90	0.17	-	48,48,48,48	0
56	MG	BA	3707	1/1	0.86	0.21	-	62,62,62,62	0
56	MG	CA	3021	1/1	0.81	0.12	-	66,66,66,66	0
56	MG	CA	3016	1/1	0.84	0.09	-	56,56,56,56	0
56	MG	AA	3207	1/1	0.95	0.13	-	57,57,57,57	0
56	MG	BA	3193	1/1	0.94	0.14	-	24,24,24,24	0
56	MG	DA	3474	1/1	0.82	0.14	-	55,55,55,55	0
56	MG	BA	3602	1/1	0.94	0.11	-	61,61,61,61	0
56	MG	DA	3038	1/1	0.94	0.14	-	56,56,56,56	0
56	MG	BB	3002	1/1	0.96	0.28	-	51,51,51,51	0
56	MG	BA	3059	1/1	0.81	0.15	-	40,40,40,40	0
56	MG	BA	3219	1/1	0.85	0.16	-	39,39,39,39	0
56	MG	BA	3502	1/1	0.90	0.14	-	62,62,62,62	0
56	MG	AA	3201	1/1	0.84	0.10	-	60,60,60,60	0
56	MG	BA	3563	1/1	0.94	0.20	-	43,43,43,43	0
56	MG	CA	3020	1/1	0.84	0.15	-	48,48,48,48	0
56	MG	DA	3418	1/1	0.94	0.11	-	55,55,55,55	0
56	MG	BA	3009	1/1	0.86	0.30	-	41,41,41,41	0
56	MG	DA	3561	1/1	0.92	0.18	-	65,65,65,65	0
56	MG	DA	3036	1/1	0.79	0.34	-	48,48,48,48	0
56	MG	AA	3170	1/1	0.91	0.07	-	66,66,66,66	0
56	MG	BA	3599	1/1	0.75	0.10	-	59,59,59,59	0
56	MG	BA	3254	1/1	0.93	0.11	-	56,56,56,56	0
56	MG	DA	3555	1/1	0.94	0.22	-	48,48,48,48	0
56	MG	BA	3103	1/1	0.94	0.16	-	45,45,45,45	0
56	MG	CA	3085	1/1	0.89	0.13	-	60,60,60,60	0
56	MG	DA	3262	1/1	0.91	0.16	-	41,41,41,41	0
56	MG	DA	3568	1/1	0.95	0.11	-	61,61,61,61	0
56	MG	CY	3001	1/1	0.94	0.15	-	63,63,63,63	0
56	MG	BA	3315	1/1	0.98	0.11	-	40,40,40,40	0
56	MG	DA	3148	1/1	0.74	0.14	-	53,53,53,53	0
56	MG	DA	3342	1/1	0.86	0.10	-	55,55,55,55	0
56	MG	CA	3121	1/1	0.82	0.14	-	88,88,88,88	0
56	MG	AA	3069	1/1	0.91	0.13	-	59,59,59,59	0
56	MG	BA	3543	1/1	0.90	0.12	-	62,62,62,62	0
56	MG	DA	3367	1/1	0.96	0.20	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3753	1/1	0.95	0.12	-	76,76,76,76	0
56	MG	BA	3328	1/1	0.95	0.10	-	56,56,56,56	0
56	MG	DA	3266	1/1	0.97	0.24	-	61,61,61,61	0
56	MG	DA	3189	1/1	0.96	0.21	-	42,42,42,42	0
56	MG	AA	3171	1/1	0.92	0.15	-	56,56,56,56	0
56	MG	DA	3161	1/1	0.88	0.30	-	57,57,57,57	0
56	MG	CA	3039	1/1	0.84	0.14	-	70,70,70,70	0
56	MG	CA	3069	1/1	0.89	0.20	-	75,75,75,75	0
56	MG	BA	3153	1/1	0.88	0.22	-	56,56,56,56	0
56	MG	BA	3675	1/1	0.91	0.28	-	39,39,39,39	0
56	MG	BA	3420	1/1	0.90	0.17	-	61,61,61,61	0
56	MG	BA	3394	1/1	0.93	0.17	-	53,53,53,53	0
56	MG	DA	3540	1/1	0.74	0.11	-	65,65,65,65	0
56	MG	DA	3464	1/1	0.95	0.15	-	51,51,51,51	0
56	MG	BA	3533	1/1	0.86	0.12	-	27,27,27,27	0
56	MG	BA	3521	1/1	0.88	0.21	-	28,28,28,28	0
56	MG	AA	3009	1/1	0.92	0.23	-	64,64,64,64	0
56	MG	DA	3323	1/1	0.95	0.10	-	44,44,44,44	0
56	MG	CA	3047	1/1	0.93	0.28	-	56,56,56,56	0
56	MG	CA	3009	1/1	0.85	0.27	-	55,55,55,55	0
56	MG	DA	3388	1/1	0.99	0.15	-	49,49,49,49	0
56	MG	DU	3002	1/1	0.93	0.80	-	58,58,58,58	0
56	MG	DA	3173	1/1	0.87	0.25	-	49,49,49,49	0
56	MG	BA	3168	1/1	0.89	0.15	-	57,57,57,57	0
56	MG	DA	3425	1/1	0.89	0.14	-	69,69,69,69	0
56	MG	DA	3355	1/1	0.94	0.12	-	53,53,53,53	0
56	MG	BA	3581	1/1	0.93	0.14	-	47,47,47,47	0
56	MG	DA	3003	1/1	0.93	0.09	-	55,55,55,55	0
56	MG	DA	3353	1/1	0.87	0.06	-	65,65,65,65	0
60	K	AX	3001	1/1	0.93	0.28	-	73,73,73,73	0
56	MG	BA	3240	1/1	0.93	0.19	-	43,43,43,43	0
56	MG	BA	3186	1/1	0.81	0.24	-	59,59,59,59	0
56	MG	BA	3779	1/1	0.73	0.40	-	52,52,52,52	0
56	MG	DA	3318	1/1	0.91	0.08	-	60,60,60,60	0
56	MG	AA	3021	1/1	0.87	0.16	-	60,60,60,60	0
56	MG	AA	3005	1/1	0.94	0.36	-	55,55,55,55	0
56	MG	AA	3097	1/1	0.95	0.17	-	45,45,45,45	0
56	MG	DA	3301	1/1	0.95	0.09	-	60,60,60,60	0
56	MG	BA	3047	1/1	0.94	0.13	-	51,51,51,51	0
56	MG	DA	3112	1/1	0.90	0.12	-	49,49,49,49	0
56	MG	DA	3590	1/1	0.85	0.12	-	61,61,61,61	0
56	MG	BG	3002	1/1	0.91	0.12	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3162	1/1	0.98	0.16	-	37,37,37,37	0
56	MG	DA	3248	1/1	0.92	0.10	-	39,39,39,39	0
56	MG	DA	3527	1/1	0.94	0.17	-	67,67,67,67	0
56	MG	CX	3002	1/1	0.88	0.17	-	67,67,67,67	0
56	MG	BA	3181	1/1	0.84	0.17	-	48,48,48,48	0
56	MG	BA	3416	1/1	0.93	0.16	-	53,53,53,53	0
56	MG	DA	3345	1/1	0.92	0.10	-	57,57,57,57	0
56	MG	BA	3060	1/1	0.81	0.32	-	61,61,61,61	0
56	MG	DA	3241	1/1	0.91	0.14	-	51,51,51,51	0
56	MG	BA	3633	1/1	0.72	0.09	-	58,58,58,58	0
56	MG	BA	3553	1/1	0.98	0.11	-	49,49,49,49	0
56	MG	DB	3009	1/1	0.92	0.12	-	70,70,70,70	0
56	MG	BA	3159	1/1	0.93	0.14	-	45,45,45,45	0
56	MG	AA	3225	1/1	0.81	0.16	-	55,55,55,55	0
56	MG	BA	3453	1/1	0.83	0.16	-	59,59,59,59	0
56	MG	BA	3612	1/1	0.86	0.16	-	65,65,65,65	0
56	MG	CJ	5001	1/1	0.75	0.10	-	75,75,75,75	0
56	MG	DA	3195	1/1	0.75	0.15	-	56,56,56,56	0
56	MG	AA	3078	1/1	0.95	0.18	-	59,59,59,59	0
56	MG	CA	3157	1/1	0.95	0.13	-	57,57,57,57	0
56	MG	BA	3112	1/1	0.97	0.07	-	50,50,50,50	0
56	MG	BA	3071	1/1	0.90	0.12	-	48,48,48,48	0
56	MG	BA	3546	1/1	0.84	0.12	-	57,57,57,57	0
56	MG	BA	3396	1/1	0.96	0.17	-	24,24,24,24	0
56	MG	DA	3469	1/1	0.94	0.05	-	56,56,56,56	0
56	MG	AA	3162	1/1	0.95	0.08	-	70,70,70,70	0
56	MG	BA	3299	1/1	0.97	0.07	-	53,53,53,53	0
56	MG	BA	3281	1/1	0.86	0.09	-	55,55,55,55	0
56	MG	CF	3001	1/1	0.91	0.17	-	44,44,44,44	0
56	MG	DA	3436	1/1	0.90	0.14	-	63,63,63,63	0
56	MG	CA	3162	1/1	0.91	0.07	-	57,57,57,57	0
56	MG	DA	3021	1/1	0.95	0.35	-	44,44,44,44	0
56	MG	DN	5001	1/1	0.88	0.15	-	75,75,75,75	0
56	MG	AA	3075	1/1	0.71	0.24	-	81,81,81,81	0
56	MG	BA	3138	1/1	0.97	0.17	-	50,50,50,50	0
56	MG	DA	3060	1/1	0.90	0.30	-	50,50,50,50	0
56	MG	DA	3058	1/1	0.90	0.14	-	48,48,48,48	0
56	MG	DA	3547	1/1	0.95	0.51	-	41,41,41,41	0
56	MG	DA	3423	1/1	0.96	0.18	-	34,34,34,34	0
56	MG	DA	3385	1/1	0.91	0.27	-	55,55,55,55	0
56	MG	BA	3330	1/1	0.98	0.18	-	35,35,35,35	0
56	MG	BA	3660	1/1	0.95	0.17	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3042	1/1	0.89	0.14	-	52,52,52,52	0
56	MG	BA	3326	1/1	0.94	0.09	-	50,50,50,50	0
56	MG	BA	3108	1/1	0.87	0.38	-	52,52,52,52	0
56	MG	BA	3339	1/1	0.92	0.16	-	31,31,31,31	0
56	MG	BA	3117	1/1	0.93	0.45	-	41,41,41,41	0
56	MG	BA	3528	1/1	0.93	0.16	-	29,29,29,29	0
56	MG	BA	3736	1/1	0.73	0.09	-	73,73,73,73	0
56	MG	BA	3212	1/1	0.88	0.26	-	47,47,47,47	0
56	MG	BA	3597	1/1	0.84	0.09	-	51,51,51,51	0
56	MG	DA	3138	1/1	0.80	0.20	-	46,46,46,46	0
56	MG	DA	3507	1/1	0.95	0.19	-	54,54,54,54	0
56	MG	BA	3152	1/1	0.94	0.19	-	48,48,48,48	0
56	MG	BA	3653	1/1	0.84	0.14	-	23,23,23,23	0
56	MG	BA	3689	1/1	0.90	0.19	-	68,68,68,68	0
56	MG	DA	3193	1/1	0.87	0.09	-	57,57,57,57	0
56	MG	DA	3551	1/1	0.95	0.18	-	66,66,66,66	0
56	MG	AA	3161	1/1	0.94	0.07	-	59,59,59,59	0
56	MG	BA	3558	1/1	0.87	0.16	-	72,72,72,72	0
56	MG	CA	3116	1/1	0.90	0.17	-	64,64,64,64	0
56	MG	BA	3624	1/1	0.94	0.11	-	50,50,50,50	0
56	MG	BA	3086	1/1	0.84	0.20	-	67,67,67,67	0
56	MG	AA	3167	1/1	0.91	0.19	-	71,71,71,71	0
56	MG	DA	3070	1/1	0.90	0.12	-	34,34,34,34	0
56	MG	CA	3114	1/1	0.93	0.09	-	52,52,52,52	0
56	MG	DA	3496	1/1	0.96	0.27	-	51,51,51,51	0
56	MG	BA	3601	1/1	0.86	0.56	-	72,72,72,72	0
56	MG	AY	3003	1/1	0.57	0.26	-	78,78,78,78	0
56	MG	DA	3289	1/1	0.92	0.17	-	23,23,23,23	0
56	MG	DA	3611	1/1	0.94	0.09	-	53,53,53,53	0
56	MG	AA	3016	1/1	0.98	0.11	-	48,48,48,48	0
56	MG	DA	3341	1/1	0.88	0.09	-	54,54,54,54	0
56	MG	BA	3631	1/1	0.87	0.17	-	63,63,63,63	0
56	MG	DA	3206	1/1	0.96	0.17	-	45,45,45,45	0
56	MG	BQ	3004	1/1	0.90	0.27	-	48,48,48,48	0
56	MG	BA	3368	1/1	0.98	0.12	-	56,56,56,56	0
56	MG	BA	3093	1/1	0.94	0.23	-	39,39,39,39	0
56	MG	CA	3123	1/1	0.84	0.26	-	77,77,77,77	0
56	MG	BA	3053	1/1	0.94	0.15	-	56,56,56,56	0
56	MG	DD	309	1/1	0.86	0.36	-	65,65,65,65	0
56	MG	BN	3005	1/1	0.91	0.15	-	46,46,46,46	0
56	MG	DA	3470	1/1	0.71	0.13	-	65,65,65,65	0
56	MG	BE	305	1/1	0.97	0.28	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3170	1/1	0.90	0.25	-	39,39,39,39	0
56	MG	AA	3024	1/1	0.94	0.11	-	49,49,49,49	0
56	MG	BB	3016	1/1	0.79	0.14	-	63,63,63,63	0
56	MG	DA	3398	1/1	0.79	0.17	-	73,73,73,73	0
56	MG	CA	3101	1/1	0.97	0.19	-	64,64,64,64	0
56	MG	DA	3179	1/1	0.74	0.19	-	61,61,61,61	0
56	MG	CA	3135	1/1	0.94	0.43	-	75,75,75,75	0
56	MG	AA	3156	1/1	0.91	0.08	-	65,65,65,65	0
56	MG	BX	101	1/1	0.91	0.15	-	48,48,48,48	0
56	MG	BA	3408	1/1	0.89	0.10	-	71,71,71,71	0
56	MG	BA	3745	1/1	0.96	0.16	-	27,27,27,27	0
56	MG	DA	3520	1/1	0.87	0.11	-	61,61,61,61	0
56	MG	DA	3493	1/1	0.88	0.16	-	64,64,64,64	0
56	MG	DA	3352	1/1	0.86	0.18	-	45,45,45,45	0
56	MG	BA	3388	1/1	0.96	0.17	-	40,40,40,40	0
56	MG	BA	3065	1/1	0.95	0.23	-	33,33,33,33	0
56	MG	AA	3121	1/1	0.88	0.10	-	54,54,54,54	0
57	NEG	CA	3172	17/17	0.83	0.23	-	61,76,83,84	0
56	MG	DA	3402	1/1	0.95	0.10	-	57,57,57,57	0
56	MG	AA	3152	1/1	0.92	0.09	-	63,63,63,63	0
56	MG	AA	3051	1/1	0.90	0.12	-	64,64,64,64	0
56	MG	BA	3239	1/1	0.98	0.30	-	30,30,30,30	0
56	MG	DA	3230	1/1	0.98	0.12	-	23,23,23,23	0
56	MG	BA	3470	1/1	0.94	0.24	-	46,46,46,46	0
56	MG	BA	3358	1/1	0.94	0.14	-	30,30,30,30	0
56	MG	BA	3617	1/1	0.97	0.06	-	46,46,46,46	0
56	MG	BA	3023	1/1	0.97	0.32	-	38,38,38,38	0
56	MG	DA	3176	1/1	0.84	0.15	-	49,49,49,49	0
56	MG	DA	3109	1/1	0.91	0.34	-	47,47,47,47	0
56	MG	DA	3007	1/1	0.93	0.18	-	53,53,53,53	0
56	MG	D5	502	1/1	0.93	0.54	-	50,50,50,50	0
56	MG	BA	3514	1/1	0.90	0.12	-	50,50,50,50	0
56	MG	DA	3123	1/1	0.97	0.39	-	40,40,40,40	0
56	MG	DA	3297	1/1	0.93	0.50	-	70,70,70,70	0
56	MG	CA	3068	1/1	0.68	0.15	-	77,77,77,77	0
56	MG	AA	3026	1/1	0.96	0.11	-	68,68,68,68	0
56	MG	BA	3451	1/1	0.98	0.21	-	53,53,53,53	0
56	MG	DA	3612	1/1	0.92	0.57	-	38,38,38,38	0
56	MG	BA	3119	1/1	0.97	0.34	-	44,44,44,44	0
56	MG	BA	3622	1/1	0.88	0.21	-	48,48,48,48	0
56	MG	CA	3136	1/1	0.78	0.20	-	73,73,73,73	0
56	MG	CA	3119	1/1	0.91	0.15	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3439	1/1	0.96	0.10	-	58,58,58,58	0
56	MG	BA	3154	1/1	0.78	0.29	-	58,58,58,58	0
56	MG	BW	204	1/1	0.96	0.48	-	41,41,41,41	0
56	MG	DA	3379	1/1	0.97	0.18	-	38,38,38,38	0
56	MG	DB	3002	1/1	0.95	0.20	-	58,58,58,58	0
56	MG	DA	3610	1/1	0.84	0.10	-	65,65,65,65	0
56	MG	AA	3061	1/1	0.96	0.17	-	44,44,44,44	0
56	MG	DB	3001	1/1	0.88	0.25	-	56,56,56,56	0
56	MG	AA	3096	1/1	0.89	0.16	-	53,53,53,53	0
56	MG	BA	3556	1/1	0.97	0.20	-	50,50,50,50	0
56	MG	AA	3197	1/1	0.91	0.12	-	64,64,64,64	0
56	MG	BW	202	1/1	0.94	0.18	-	43,43,43,43	0
56	MG	AA	3028	1/1	0.97	0.23	-	46,46,46,46	0
56	MG	AA	3038	1/1	0.91	0.25	-	56,56,56,56	0
56	MG	BA	3234	1/1	0.90	0.14	-	52,52,52,52	0
56	MG	BA	3422	1/1	0.97	0.12	-	45,45,45,45	0
56	MG	AA	3124	1/1	0.90	0.16	-	63,63,63,63	0
56	MG	DA	3604	1/1	0.82	0.10	-	58,58,58,58	0
56	MG	BA	3621	1/1	0.91	0.26	-	48,48,48,48	0
56	MG	BA	3659	1/1	0.96	0.19	-	24,24,24,24	0
56	MG	DA	3157	1/1	0.84	0.22	-	58,58,58,58	0
56	MG	DA	3475	1/1	0.93	0.17	-	32,32,32,32	0
56	MG	BA	3412	1/1	0.92	0.15	-	50,50,50,50	0
56	MG	DA	3143	1/1	0.94	0.13	-	35,35,35,35	0
56	MG	BA	3582	1/1	0.80	0.13	-	63,63,63,63	0
56	MG	CA	3013	1/1	0.91	0.14	-	52,52,52,52	0
56	MG	DA	3594	1/1	0.93	0.14	-	52,52,52,52	0
56	MG	DA	3059	1/1	0.90	0.12	-	49,49,49,49	0
56	MG	AA	3148	1/1	0.99	0.18	-	50,50,50,50	0
56	MG	AA	3185	1/1	0.98	0.21	-	51,51,51,51	0
56	MG	BA	3608	1/1	0.90	0.12	-	68,68,68,68	0
56	MG	CW	3003	1/1	0.96	0.10	-	64,64,64,64	0
56	MG	DA	3463	1/1	0.63	0.20	-	53,53,53,53	0
56	MG	CA	3138	1/1	0.89	0.11	-	52,52,52,52	0
56	MG	BA	3199	1/1	0.66	0.28	-	55,55,55,55	0
56	MG	DA	3397	1/1	0.91	0.12	-	50,50,50,50	0
56	MG	DA	3225	1/1	0.92	0.15	-	56,56,56,56	0
56	MG	DA	3426	1/1	0.80	0.11	-	53,53,53,53	0
56	MG	DW	3004	1/1	0.88	0.21	-	50,50,50,50	0
56	MG	AA	3105	1/1	0.77	0.10	-	66,66,66,66	0
56	MG	BA	3215	1/1	0.92	0.15	-	47,47,47,47	0
56	MG	BA	3375	1/1	0.85	0.20	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3630	1/1	0.89	0.14	-	44,44,44,44	0
56	MG	CA	3058	1/1	0.79	0.20	-	64,64,64,64	0
56	MG	DA	3582	1/1	0.92	0.15	-	65,65,65,65	0
56	MG	BA	3771	1/1	0.93	0.10	-	73,73,73,73	0
56	MG	BA	3431	1/1	0.94	0.15	-	54,54,54,54	0
56	MG	DA	3053	1/1	0.84	0.21	-	61,61,61,61	0
56	MG	BA	3331	1/1	0.81	0.15	-	51,51,51,51	0
56	MG	BA	3489	1/1	0.97	0.09	-	43,43,43,43	0
56	MG	CA	3011	1/1	0.96	0.25	-	71,71,71,71	0
56	MG	DA	3523	1/1	0.92	0.33	-	62,62,62,62	0
56	MG	BA	3323	1/1	0.87	0.16	-	60,60,60,60	0
56	MG	BA	3373	1/1	0.84	0.12	-	35,35,35,35	0
56	MG	DA	3062	1/1	0.95	0.32	-	49,49,49,49	0
56	MG	BA	3466	1/1	0.95	0.30	-	52,52,52,52	0
56	MG	BA	3610	1/1	0.72	0.20	-	64,64,64,64	0
56	MG	CA	3128	1/1	0.95	0.08	-	72,72,72,72	0
56	MG	AA	3102	1/1	0.97	0.17	-	50,50,50,50	0
56	MG	CA	3065	1/1	0.85	0.31	-	73,73,73,73	0
56	MG	BA	3438	1/1	0.83	0.15	-	44,44,44,44	0
56	MG	AA	3082	1/1	0.75	0.16	-	70,70,70,70	0
56	MG	CA	3073	1/1	0.90	0.20	-	70,70,70,70	0
56	MG	BA	3579	1/1	0.89	0.25	-	57,57,57,57	0
56	MG	BA	3012	1/1	0.88	0.11	-	49,49,49,49	0
56	MG	BA	3325	1/1	0.95	0.14	-	42,42,42,42	0
56	MG	BA	3696	1/1	0.94	0.13	-	38,38,38,38	0
56	MG	DA	3562	1/1	0.86	0.10	-	67,67,67,67	0
56	MG	DA	3273	1/1	0.94	0.17	-	36,36,36,36	0
56	MG	BA	3371	1/1	0.95	0.19	-	50,50,50,50	0
56	MG	AA	3178	1/1	0.81	0.11	-	60,60,60,60	0
56	MG	CA	3131	1/1	0.88	0.09	-	62,62,62,62	0
56	MG	BA	3475	1/1	0.96	0.17	-	52,52,52,52	0
56	MG	DA	3455	1/1	0.95	0.29	-	50,50,50,50	0
56	MG	BE	303	1/1	0.80	0.26	-	61,61,61,61	0
56	MG	DA	3447	1/1	0.94	0.17	-	49,49,49,49	0
56	MG	BA	3739	1/1	0.90	0.29	-	75,75,75,75	0
56	MG	BA	3683	1/1	0.92	0.19	-	50,50,50,50	0
56	MG	BA	3524	1/1	0.96	0.17	-	44,44,44,44	0
56	MG	DA	3081	1/1	0.79	0.20	-	53,53,53,53	0
56	MG	DA	3608	1/1	0.96	0.09	-	47,47,47,47	0
56	MG	BA	3246	1/1	0.94	0.15	-	57,57,57,57	0
56	MG	AW	3003	1/1	0.97	0.21	-	44,44,44,44	0
56	MG	CA	3037	1/1	0.87	0.16	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3730	1/1	0.76	0.28	-	45,45,45,45	0
56	MG	BA	3588	1/1	0.89	0.17	-	62,62,62,62	0
56	MG	CD	301	1/1	0.94	0.12	-	67,67,67,67	0
56	MG	BA	3118	1/1	0.82	0.31	-	46,46,46,46	0
56	MG	BA	3437	1/1	0.92	0.10	-	55,55,55,55	0
56	MG	DA	3524	1/1	0.94	0.09	-	58,58,58,58	0
56	MG	BA	3710	1/1	0.93	0.15	-	51,51,51,51	0
56	MG	BA	3097	1/1	0.73	0.40	-	33,33,33,33	0
56	MG	BA	3095	1/1	0.93	0.32	-	39,39,39,39	0
56	MG	DA	3162	1/1	0.94	0.39	-	45,45,45,45	0
56	MG	AX	3007	1/1	0.91	0.24	-	66,66,66,66	0
56	MG	BA	3336	1/1	0.89	0.21	-	31,31,31,31	0
56	MG	DA	3351	1/1	0.89	0.11	-	40,40,40,40	0
56	MG	DA	3305	1/1	0.94	0.16	-	42,42,42,42	0
56	MG	BA	3669	1/1	0.88	0.30	-	45,45,45,45	0
56	MG	AA	3108	1/1	0.95	0.08	-	59,59,59,59	0
56	MG	DA	3364	1/1	0.96	0.20	-	54,54,54,54	0
56	MG	DP	201	1/1	0.72	0.26	-	50,50,50,50	0
56	MG	BA	3207	1/1	0.90	0.08	-	52,52,52,52	0
56	MG	BA	3077	1/1	0.76	0.17	-	59,59,59,59	0
56	MG	DA	3118	1/1	0.90	0.16	-	50,50,50,50	0
56	MG	DW	3003	1/1	0.94	0.58	-	71,71,71,71	0
56	MG	BA	3280	1/1	0.95	0.22	-	25,25,25,25	0
56	MG	CA	3142	1/1	0.90	0.17	-	69,69,69,69	0
56	MG	DA	3180	1/1	0.77	0.12	-	50,50,50,50	0
56	MG	DA	3135	1/1	0.97	0.27	-	44,44,44,44	0
56	MG	BA	3518	1/1	0.95	0.17	-	25,25,25,25	0
56	MG	DA	3194	1/1	0.97	0.13	-	52,52,52,52	0
56	MG	BA	3056	1/1	0.93	0.27	-	26,26,26,26	0
56	MG	BA	3485	1/1	0.93	0.15	-	25,25,25,25	0
56	MG	CA	3064	1/1	0.86	0.10	-	67,67,67,67	0
56	MG	DA	3049	1/1	0.88	0.16	-	48,48,48,48	0
56	MG	BA	3641	1/1	0.97	0.26	-	46,46,46,46	0
56	MG	DA	3373	1/1	0.95	0.22	-	51,51,51,51	0
56	MG	BA	3458	1/1	0.98	0.21	-	52,52,52,52	0
56	MG	BA	3486	1/1	0.95	0.21	-	30,30,30,30	0
56	MG	DA	3039	1/1	0.80	0.21	-	50,50,50,50	0
56	MG	BA	3411	1/1	0.97	0.24	-	49,49,49,49	0
56	MG	BA	3686	1/1	0.92	0.12	-	61,61,61,61	0
56	MG	DA	3454	1/1	0.93	0.12	-	47,47,47,47	0
56	MG	DA	3363	1/1	0.85	0.16	-	61,61,61,61	0
56	MG	CA	3153	1/1	0.94	0.24	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3609	1/1	0.92	0.14	-	47,47,47,47	0
56	MG	AA	3107	1/1	0.96	0.18	-	66,66,66,66	0
56	MG	BA	3636	1/1	0.93	0.22	-	61,61,61,61	0
56	MG	DD	303	1/1	0.95	0.27	-	60,60,60,60	0
56	MG	BA	3430	1/1	0.96	0.17	-	48,48,48,48	0
56	MG	BA	3217	1/1	0.72	0.28	-	66,66,66,66	0
56	MG	CA	3124	1/1	0.56	0.19	-	90,90,90,90	0
56	MG	AA	3210	1/1	0.92	0.10	-	65,65,65,65	0
56	MG	BA	3784	1/1	0.87	0.09	-	62,62,62,62	0
56	MG	AA	3134	1/1	0.92	0.17	-	73,73,73,73	0
56	MG	BA	3170	1/1	0.90	0.20	-	30,30,30,30	0
56	MG	BA	3256	1/1	0.83	0.25	-	25,25,25,25	0
56	MG	BA	3187	1/1	0.86	0.21	-	42,42,42,42	0
56	MG	DA	3335	1/1	0.97	0.07	-	41,41,41,41	0
56	MG	AA	3025	1/1	0.97	0.25	-	54,54,54,54	0
56	MG	DA	3200	1/1	0.93	0.09	-	52,52,52,52	0
56	MG	DA	3178	1/1	0.93	0.09	-	45,45,45,45	0
56	MG	BA	3716	1/1	0.86	0.15	-	48,48,48,48	0
56	MG	AV	101	1/1	0.96	0.10	-	47,47,47,47	0
56	MG	DA	3028	1/1	0.88	0.21	-	52,52,52,52	0
56	MG	BA	3403	1/1	0.91	0.19	-	53,53,53,53	0
56	MG	BE	306	1/1	0.98	0.21	-	15,15,15,15	0
56	MG	DA	3593	1/1	0.87	0.23	-	57,57,57,57	0
56	MG	AA	3223	1/1	0.96	0.12	-	52,52,52,52	0
56	MG	BA	3195	1/1	0.71	0.50	-	53,53,53,53	0
56	MG	AA	3174	1/1	0.88	0.09	-	59,59,59,59	0
56	MG	BA	3230	1/1	0.97	0.20	-	53,53,53,53	0
56	MG	CA	3076	1/1	0.93	0.15	-	54,54,54,54	0
56	MG	DA	3383	1/1	0.95	0.20	-	40,40,40,40	0
56	MG	BB	3007	1/1	0.85	0.23	-	84,84,84,84	0
56	MG	BA	3681	1/1	0.92	0.22	-	47,47,47,47	0
56	MG	DA	3084	1/1	0.83	0.20	-	53,53,53,53	0
56	MG	DA	3073	1/1	0.77	0.24	-	50,50,50,50	0
56	MG	DQ	3002	1/1	0.92	0.13	-	50,50,50,50	0
56	MG	BA	3087	1/1	0.93	0.13	-	63,63,63,63	0
56	MG	CA	3109	1/1	0.98	0.14	-	67,67,67,67	0
56	MG	BA	3635	1/1	0.96	0.19	-	56,56,56,56	0
56	MG	BA	3595	1/1	0.85	0.07	-	65,65,65,65	0
56	MG	BA	3206	1/1	0.95	0.31	-	49,49,49,49	0
56	MG	BA	3577	1/1	0.82	0.19	-	62,62,62,62	0
56	MG	DA	3167	1/1	0.92	0.77	-	51,51,51,51	0
56	MG	AY	3002	1/1	0.92	0.13	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3229	1/1	0.89	0.09	-	38,38,38,38	0
56	MG	BA	3042	1/1	0.88	0.20	-	54,54,54,54	0
56	MG	AA	3115	1/1	0.86	0.14	-	61,61,61,61	0
56	MG	DA	3312	1/1	0.95	0.14	-	40,40,40,40	0
56	MG	CA	3150	1/1	0.93	0.08	-	80,80,80,80	0
56	MG	DA	3214	1/1	0.90	0.11	-	58,58,58,58	0
56	MG	CA	3178	1/1	0.93	0.09	-	54,54,54,54	0
56	MG	BA	3436	1/1	0.88	0.13	-	67,67,67,67	0
56	MG	DA	3291	1/1	0.87	0.14	-	41,41,41,41	0
56	MG	CA	3118	1/1	0.92	0.21	-	61,61,61,61	0
56	MG	BA	3751	1/1	0.77	0.14	-	51,51,51,51	0
56	MG	BB	3013	1/1	0.93	0.24	-	46,46,46,46	0
56	MG	DA	3052	1/1	0.90	0.09	-	44,44,44,44	0
56	MG	DA	3533	1/1	0.86	0.13	-	50,50,50,50	0
56	MG	CA	3180	1/1	0.92	0.12	-	61,61,61,61	0
56	MG	DA	3283	1/1	0.86	0.10	-	53,53,53,53	0
56	MG	DA	3476	1/1	0.89	0.09	-	62,62,62,62	0
56	MG	BA	3499	1/1	0.94	0.12	-	57,57,57,57	0
56	MG	BA	3598	1/1	0.93	0.07	-	58,58,58,58	0
56	MG	DA	3222	1/1	0.96	0.10	-	46,46,46,46	0
56	MG	BA	3450	1/1	0.92	0.15	-	59,59,59,59	0
56	MG	BA	3137	1/1	0.89	0.21	-	41,41,41,41	0
56	MG	BA	3727	1/1	0.95	0.09	-	57,57,57,57	0
56	MG	BA	3391	1/1	0.93	0.13	-	36,36,36,36	0
56	MG	BA	3687	1/1	0.94	0.18	-	56,56,56,56	0
56	MG	BA	3067	1/1	0.91	0.44	-	35,35,35,35	0
56	MG	DA	3580	1/1	0.91	0.09	-	44,44,44,44	0
56	MG	BA	3125	1/1	0.97	0.37	-	34,34,34,34	0
56	MG	DA	3046	1/1	0.95	0.17	-	30,30,30,30	0
56	MG	CA	3145	1/1	0.70	0.14	-	62,62,62,62	0
56	MG	DA	3181	1/1	0.95	0.28	-	50,50,50,50	0
56	MG	DA	3224	1/1	0.77	0.22	-	27,27,27,27	0
56	MG	CA	3147	1/1	0.93	0.12	-	51,51,51,51	0
56	MG	B0	103	1/1	0.91	0.14	-	61,61,61,61	0
56	MG	CA	3087	1/1	0.93	0.17	-	65,65,65,65	0
56	MG	DA	3390	1/1	0.97	0.15	-	48,48,48,48	0
56	MG	AN	502	1/1	0.95	0.22	-	56,56,56,56	0
56	MG	BA	3360	1/1	0.87	0.21	-	41,41,41,41	0
56	MG	DA	3445	1/1	0.93	0.30	-	50,50,50,50	0
56	MG	DA	3069	1/1	0.91	0.13	-	49,49,49,49	0
56	MG	BA	3157	1/1	0.95	0.34	-	59,59,59,59	0
56	MG	BA	3228	1/1	0.95	0.32	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3330	1/1	0.84	0.12	-	54,54,54,54	0
56	MG	BA	3102	1/1	0.92	0.35	-	47,47,47,47	0
56	MG	BA	3741	1/1	0.72	0.15	-	68,68,68,68	0
56	MG	BA	3676	1/1	0.95	0.14	-	55,55,55,55	0
56	MG	DA	3382	1/1	0.97	0.14	-	53,53,53,53	0
56	MG	AA	3157	1/1	0.94	0.16	-	46,46,46,46	0
56	MG	DA	3165	1/1	0.93	0.18	-	69,69,69,69	0
56	MG	DA	3152	1/1	0.93	0.27	-	53,53,53,53	0
56	MG	BZ	3001	1/1	0.85	0.17	-	52,52,52,52	0
56	MG	CA	3115	1/1	0.89	0.06	-	58,58,58,58	0
56	MG	B7	103	1/1	0.94	0.14	-	69,69,69,69	0
56	MG	BA	3401	1/1	0.93	0.59	-	67,67,67,67	0
56	MG	DA	3501	1/1	0.83	0.18	-	67,67,67,67	0
56	MG	DA	3592	1/1	0.96	0.10	-	57,57,57,57	0
56	MG	CA	3088	1/1	0.96	0.15	-	48,48,48,48	0
56	MG	DA	3599	1/1	0.95	0.10	-	72,72,72,72	0
56	MG	DA	3552	1/1	0.95	0.13	-	43,43,43,43	0
56	MG	AA	3030	1/1	0.90	0.20	-	65,65,65,65	0
56	MG	DA	3466	1/1	0.93	0.20	-	46,46,46,46	0
56	MG	BA	3265	1/1	0.94	0.25	-	55,55,55,55	0
56	MG	CA	3031	1/1	0.69	0.22	-	71,71,71,71	0
56	MG	BB	3008	1/1	0.89	0.11	-	71,71,71,71	0
56	MG	BA	3645	1/1	0.82	0.33	-	47,47,47,47	0
56	MG	CA	3155	1/1	0.91	0.18	-	61,61,61,61	0
56	MG	CW	3001	1/1	0.94	0.65	-	69,69,69,69	0
56	MG	AA	3047	1/1	0.93	0.25	-	68,68,68,68	0
56	MG	DA	3411	1/1	0.94	0.41	-	43,43,43,43	0
56	MG	BA	3175	1/1	0.89	0.18	-	44,44,44,44	0
56	MG	BA	3172	1/1	0.94	0.30	-	58,58,58,58	0
56	MG	BF	311	1/1	0.95	0.08	-	60,60,60,60	0
56	MG	BA	3139	1/1	0.88	0.16	-	52,52,52,52	0
56	MG	BA	3593	1/1	0.98	0.20	-	53,53,53,53	0
56	MG	BA	3031	1/1	0.79	0.21	-	49,49,49,49	0
56	MG	BA	3214	1/1	0.71	0.26	-	64,64,64,64	0
56	MG	BA	3249	1/1	0.92	0.20	-	33,33,33,33	0
56	MG	DA	3255	1/1	0.95	0.12	-	50,50,50,50	0
56	MG	BA	3070	1/1	0.90	0.25	-	48,48,48,48	0
56	MG	BA	3363	1/1	0.92	0.16	-	53,53,53,53	0
56	MG	BA	3150	1/1	0.95	0.18	-	47,47,47,47	0
56	MG	DA	3057	1/1	0.86	0.20	-	54,54,54,54	0
56	MG	BA	3192	1/1	0.92	0.32	-	56,56,56,56	0
56	MG	BA	3509	1/1	0.94	0.17	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3279	1/1	0.89	0.09	-	51,51,51,51	0
56	MG	BA	3481	1/1	0.94	0.18	-	32,32,32,32	0
56	MG	BA	3651	1/1	0.91	0.13	-	38,38,38,38	0
56	MG	DA	3571	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	AA	3136	1/1	0.85	0.12	-	59,59,59,59	0
56	MG	DA	3357	1/1	0.97	0.12	-	44,44,44,44	0
56	MG	BA	3243	1/1	0.87	0.18	-	57,57,57,57	0
56	MG	AA	3044	1/1	0.76	0.17	-	67,67,67,67	0
56	MG	DA	3534	1/1	0.97	0.18	-	59,59,59,59	0
56	MG	AA	3176	1/1	0.88	0.18	-	69,69,69,69	0
56	MG	DA	3031	1/1	0.94	0.21	-	51,51,51,51	0
56	MG	BA	3267	1/1	0.99	0.20	-	14,14,14,14	0
56	MG	BB	3004	1/1	0.93	0.13	-	64,64,64,64	0
56	MG	BA	3066	1/1	0.93	0.41	-	40,40,40,40	0
56	MG	BA	3135	1/1	0.83	0.14	-	51,51,51,51	0
56	MG	DA	3607	1/1	0.94	0.05	-	60,60,60,60	0
56	MG	DA	3272	1/1	0.96	0.18	-	43,43,43,43	0
56	MG	AA	3098	1/1	0.95	0.17	-	59,59,59,59	0
56	MG	BA	3761	1/1	0.70	0.17	-	65,65,65,65	0
56	MG	BA	3611	1/1	0.95	0.20	-	23,23,23,23	0
56	MG	BA	3655	1/1	0.97	0.15	-	29,29,29,29	0
56	MG	DA	3079	1/1	0.75	0.16	-	60,60,60,60	0
56	MG	DA	3223	1/1	0.92	0.14	-	63,63,63,63	0
56	MG	DA	3565	1/1	0.91	0.16	-	48,48,48,48	0
56	MG	DA	3029	1/1	0.80	0.16	-	52,52,52,52	0
56	MG	DA	3435	1/1	0.92	0.25	-	59,59,59,59	0
56	MG	BA	3405	1/1	0.94	0.15	-	47,47,47,47	0
56	MG	DA	3387	1/1	0.95	0.14	-	47,47,47,47	0
56	MG	BA	3020	1/1	0.97	0.45	-	32,32,32,32	0
56	MG	CA	3046	1/1	0.92	0.22	-	68,68,68,68	0
56	MG	AA	3089	1/1	0.91	0.17	-	54,54,54,54	0
56	MG	CA	3164	1/1	0.98	0.19	-	65,65,65,65	0
56	MG	BA	3185	1/1	0.92	0.30	-	38,38,38,38	0
56	MG	CA	3054	1/1	0.84	0.16	-	65,65,65,65	0
56	MG	DA	3154	1/1	0.96	0.12	-	43,43,43,43	0
56	MG	BA	3605	1/1	0.90	0.21	-	69,69,69,69	0
56	MG	AA	3133	1/1	0.97	0.12	-	35,35,35,35	0
56	MG	AA	3159	1/1	0.78	0.11	-	70,70,70,70	0
56	MG	DA	3047	1/1	0.93	0.16	-	46,46,46,46	0
56	MG	DA	3545	1/1	0.93	0.13	-	68,68,68,68	0
56	MG	DA	3569	1/1	0.91	0.11	-	75,75,75,75	0
56	MG	BA	3623	1/1	0.91	0.15	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3007	1/1	0.92	0.23	-	49,49,49,49	0
56	MG	BA	3497	1/1	0.95	0.23	-	24,24,24,24	0
56	MG	AA	3057	1/1	0.95	0.19	-	58,58,58,58	0
56	MG	CA	3052	1/1	0.84	0.09	-	65,65,65,65	0
56	MG	BA	3248	1/1	0.89	0.13	-	27,27,27,27	0
56	MG	AA	3093	1/1	0.85	0.16	-	58,58,58,58	0
56	MG	BA	3454	1/1	0.88	0.15	-	43,43,43,43	0
56	MG	DA	3010	1/1	0.80	0.20	-	55,55,55,55	0
56	MG	DA	3456	1/1	0.95	0.11	-	50,50,50,50	0
56	MG	DA	3410	1/1	0.95	0.09	-	37,37,37,37	0
56	MG	BA	3318	1/1	0.95	0.08	-	36,36,36,36	0
56	MG	DA	3075	1/1	0.89	0.25	-	51,51,51,51	0
56	MG	AA	3122	1/1	0.89	0.13	-	74,74,74,74	0
56	MG	BA	3547	1/1	0.95	0.17	-	47,47,47,47	0
56	MG	DA	3259	1/1	0.97	0.12	-	50,50,50,50	0
56	MG	BA	3738	1/1	0.85	0.15	-	41,41,41,41	0
56	MG	BA	3356	1/1	0.88	0.21	-	24,24,24,24	0
56	MG	AA	3184	1/1	0.92	0.09	-	75,75,75,75	0
56	MG	DA	3546	1/1	0.89	0.14	-	64,64,64,64	0
56	MG	DY	502	1/1	0.89	0.20	-	86,86,86,86	0
56	MG	BA	3380	1/1	0.97	0.18	-	59,59,59,59	0
56	MG	BA	3432	1/1	0.96	0.13	-	48,48,48,48	0
56	MG	BA	3227	1/1	0.78	0.19	-	38,38,38,38	0
56	MG	BA	3650	1/1	0.97	0.10	-	38,38,38,38	0
56	MG	DA	3303	1/1	0.95	0.12	-	44,44,44,44	0
56	MG	BA	3549	1/1	0.89	0.22	-	53,53,53,53	0
56	MG	BA	3297	1/1	0.92	0.16	-	45,45,45,45	0
56	MG	BA	3661	1/1	0.87	0.13	-	61,61,61,61	0
56	MG	DA	3530	1/1	0.92	0.21	-	69,69,69,69	0
56	MG	BA	3705	1/1	0.92	0.16	-	52,52,52,52	0
56	MG	CA	3057	1/1	0.89	0.20	-	73,73,73,73	0
56	MG	BA	3694	1/1	0.85	0.22	-	57,57,57,57	0
56	MG	BA	3555	1/1	0.81	0.19	-	49,49,49,49	0
56	MG	AA	3086	1/1	0.88	0.18	-	53,53,53,53	0
56	MG	BA	3507	1/1	0.94	0.15	-	53,53,53,53	0
56	MG	DA	3141	1/1	0.95	0.32	-	56,56,56,56	0
56	MG	BA	3124	1/1	0.93	0.26	-	33,33,33,33	0
56	MG	BA	3679	1/1	0.94	0.16	-	47,47,47,47	0
56	MG	BA	3134	1/1	0.64	0.18	-	57,57,57,57	0
56	MG	DA	3375	1/1	0.98	0.17	-	42,42,42,42	0
56	MG	BA	3210	1/1	0.96	0.42	-	34,34,34,34	0
56	MG	CA	3133	1/1	0.93	0.22	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3548	1/1	0.93	0.13	-	67,67,67,67	0
56	MG	BA	3011	1/1	0.89	0.32	-	51,51,51,51	0
56	MG	DA	3090	1/1	0.97	0.21	-	67,67,67,67	0
56	MG	BA	3425	1/1	0.94	0.13	-	31,31,31,31	0
56	MG	BA	3740	1/1	0.89	0.12	-	49,49,49,49	0
56	MG	BA	3525	1/1	0.98	0.20	-	40,40,40,40	0
56	MG	DA	3094	1/1	0.84	0.11	-	55,55,55,55	0
56	MG	BA	3504	1/1	0.91	0.23	-	57,57,57,57	0
56	MG	DA	3479	1/1	0.93	0.12	-	52,52,52,52	0
56	MG	AA	3039	1/1	0.93	0.19	-	57,57,57,57	0
56	MG	CA	3093	1/1	0.92	0.09	-	57,57,57,57	0
56	MG	DB	3010	1/1	0.92	0.24	-	72,72,72,72	0
56	MG	AY	3001	1/1	0.39	0.25	-	92,92,92,92	0
56	MG	BA	3069	1/1	0.78	0.19	-	46,46,46,46	0
56	MG	BA	3057	1/1	0.95	0.57	-	48,48,48,48	0
56	MG	AA	3019	1/1	0.91	0.18	-	53,53,53,53	0
56	MG	CA	3144	1/1	0.97	0.12	-	54,54,54,54	0
56	MG	AA	3153	1/1	0.91	0.19	-	44,44,44,44	0
56	MG	BA	3742	1/1	0.90	0.35	-	44,44,44,44	0
56	MG	BA	3666	1/1	0.99	0.18	-	11,11,11,11	0
56	MG	BA	3285	1/1	0.94	0.20	-	55,55,55,55	0
56	MG	CA	3059	1/1	0.89	0.39	-	70,70,70,70	0
56	MG	BA	3085	1/1	0.96	0.19	-	50,50,50,50	0
56	MG	DA	3468	1/1	0.95	0.06	-	54,54,54,54	0
56	MG	AX	3009	1/1	0.79	0.19	-	72,72,72,72	0
56	MG	DV	3003	1/1	0.88	0.18	-	62,62,62,62	0
56	MG	DA	3451	1/1	0.94	0.23	-	56,56,56,56	0
56	MG	BA	3677	1/1	0.92	0.20	-	63,63,63,63	0
56	MG	BY	502	1/1	0.92	0.15	-	60,60,60,60	0
56	MG	BA	3483	1/1	0.92	0.19	-	50,50,50,50	0
56	MG	AA	3169	1/1	0.94	0.11	-	57,57,57,57	0
56	MG	DA	3130	1/1	0.92	0.23	-	52,52,52,52	0
56	MG	DA	3585	1/1	0.90	0.13	-	55,55,55,55	0
56	MG	B7	104	1/1	0.87	0.20	-	55,55,55,55	0
56	MG	BB	3010	1/1	0.98	0.19	-	51,51,51,51	0
56	MG	BA	3490	1/1	0.91	0.07	-	66,66,66,66	0
56	MG	DA	3068	1/1	0.92	0.34	-	52,52,52,52	0
56	MG	BA	3058	1/1	0.96	0.14	-	23,23,23,23	0
56	MG	DA	3298	1/1	0.89	0.10	-	57,57,57,57	0
56	MG	AA	3200	1/1	0.96	0.14	-	61,61,61,61	0
56	MG	DA	3603	1/1	0.89	0.21	-	45,45,45,45	0
56	MG	AX	3012	1/1	0.97	0.22	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3350	1/1	0.94	0.11	-	43,43,43,43	0
56	MG	DA	3074	1/1	0.85	0.36	-	49,49,49,49	0
56	MG	BA	3286	1/1	0.95	0.08	-	48,48,48,48	0
56	MG	BA	3587	1/1	0.93	0.36	-	58,58,58,58	0
56	MG	DA	3288	1/1	0.96	0.15	-	43,43,43,43	0
56	MG	BB	3017	1/1	0.94	0.14	-	48,48,48,48	0
56	MG	AA	3182	1/1	0.94	0.20	-	76,76,76,76	0
56	MG	CA	3001	1/1	0.74	0.14	-	59,59,59,59	0
56	MG	BA	3691	1/1	0.94	0.09	-	60,60,60,60	0
56	MG	CA	3062	1/1	0.91	0.22	-	65,65,65,65	0
56	MG	DA	3285	1/1	0.94	0.12	-	43,43,43,43	0
56	MG	BA	3529	1/1	0.98	0.17	-	57,57,57,57	0
56	MG	CA	3026	1/1	0.87	0.19	-	61,61,61,61	0
56	MG	AA	3063	1/1	0.90	0.23	-	56,56,56,56	0
56	MG	CA	3075	1/1	0.83	0.20	-	53,53,53,53	0
56	MG	BA	3698	1/1	0.94	0.10	-	59,59,59,59	0
56	MG	DA	3587	1/1	0.93	0.16	-	45,45,45,45	0
56	MG	BA	3146	1/1	0.92	0.17	-	36,36,36,36	0
56	MG	DA	3340	1/1	0.65	0.18	-	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.