



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:01 am GMT

PDB ID : 4V9S  
Title : Crystal structure of antibiotic GE82832 bound to 70S ribosome  
Authors : Bulkley, D.P.; Brandi, L.; Polikanov, Y.S.; Fabbretti, A.; O'Connor, M.;  
Gualerzi, C.O.; Steitz, T.A.  
Deposited on : 2013-12-05  
Resolution : 3.10 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28972

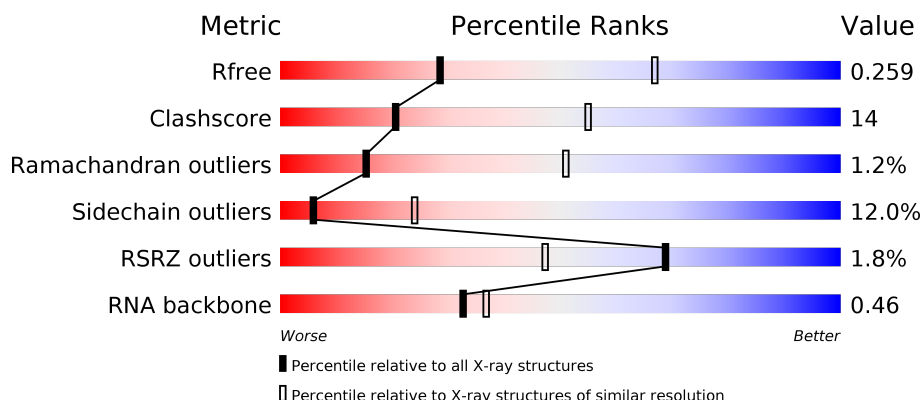
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

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	1522	<div> <div>2%</div> <div>36% 43% 17% . .</div> </div>
1	CA	1522	<div> <div>2%</div> <div>34% 43% 18% . .</div> </div>
2	AB	256	<div> <div>3%</div> <div>38% 39% 11% . 10%</div> </div>
2	CB	256	<div> <div>5%</div> <div>36% 44% 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	






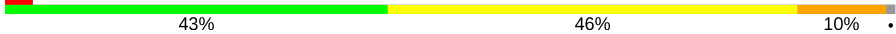



















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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AX	77	
23	CX	77	
24	AW	10	
24	CW	10	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BD	276	
27	DD	276	

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Mol	Chain	Length	Quality of chain
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	
39	DT	146	
40	BU	118	

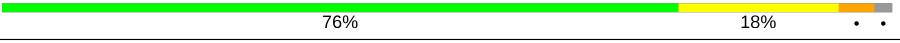


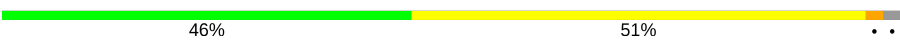


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Mol	Chain	Length	Quality of chain
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	

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Mol	Chain	Length	Quality of chain
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
24	2QY	CW	10	-	-	X	-
24	MVA	CW	9	-	-	X	-
56	MG	AA	3008	-	-	-	X
56	MG	AA	3010	-	-	-	X
56	MG	AA	3011	-	-	-	X
56	MG	AA	3019	-	-	-	X
56	MG	AA	3024	-	-	-	X
56	MG	AA	3031	-	-	-	X
56	MG	AA	3033	-	-	-	X
56	MG	AA	3035	-	-	-	X
56	MG	AA	3036	-	-	-	X
56	MG	AA	3038	-	-	-	X
56	MG	AA	3039	-	-	-	X
56	MG	AA	3050	-	-	-	X
56	MG	AA	3060	-	-	-	X
56	MG	AA	3064	-	-	-	X
56	MG	AA	3071	-	-	-	X
56	MG	AA	3072	-	-	-	X
56	MG	AA	3082	-	-	-	X
56	MG	AA	3084	-	-	-	X
56	MG	AA	3088	-	-	-	X
56	MG	AA	3095	-	-	-	X
56	MG	AA	3107	-	-	-	X
56	MG	AA	3108	-	-	-	X
56	MG	AA	3109	-	-	-	X
56	MG	AA	3120	-	-	-	X
56	MG	AA	3145	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	3146	-	-	-	X
56	MG	AA	3159	-	-	-	X
56	MG	AA	3160	-	-	-	X
56	MG	AA	3168	-	-	-	X
56	MG	AA	3171	-	-	-	X
56	MG	AA	3179	-	-	-	X
56	MG	AA	3180	-	-	-	X
56	MG	AA	3190	-	-	-	X
56	MG	AA	3208	-	-	-	X
56	MG	AA	3209	-	-	-	X
56	MG	B3	103	-	-	-	X
56	MG	B7	102	-	-	-	X
56	MG	B7	103	-	-	-	X
56	MG	B8	101	-	-	-	X
56	MG	BA	3014	-	-	-	X
56	MG	BA	3024	-	-	-	X
56	MG	BA	3025	-	-	-	X
56	MG	BA	3026	-	-	-	X
56	MG	BA	3033	-	-	-	X
56	MG	BA	3034	-	-	-	X
56	MG	BA	3036	-	-	-	X
56	MG	BA	3037	-	-	-	X
56	MG	BA	3038	-	-	-	X
56	MG	BA	3041	-	-	-	X
56	MG	BA	3042	-	-	-	X
56	MG	BA	3045	-	-	-	X
56	MG	BA	3047	-	-	-	X
56	MG	BA	3048	-	-	-	X
56	MG	BA	3057	-	-	-	X
56	MG	BA	3060	-	-	-	X
56	MG	BA	3079	-	-	-	X
56	MG	BA	3086	-	-	-	X
56	MG	BA	3093	-	-	-	X
56	MG	BA	3117	-	-	-	X
56	MG	BA	3121	-	-	-	X
56	MG	BA	3124	-	-	-	X
56	MG	BA	3128	-	-	-	X
56	MG	BA	3133	-	-	-	X
56	MG	BA	3139	-	-	-	X
56	MG	BA	3145	-	-	-	X
56	MG	BA	3147	-	-	-	X
56	MG	BA	3150	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3153	-	-	-	X
56	MG	BA	3155	-	-	-	X
56	MG	BA	3160	-	-	-	X
56	MG	BA	3178	-	-	-	X
56	MG	BA	3184	-	-	-	X
56	MG	BA	3187	-	-	-	X
56	MG	BA	3192	-	-	-	X
56	MG	BA	3193	-	-	-	X
56	MG	BA	3196	-	-	-	X
56	MG	BA	3197	-	-	-	X
56	MG	BA	3199	-	-	-	X
56	MG	BA	3200	-	-	-	X
56	MG	BA	3203	-	-	-	X
56	MG	BA	3211	-	-	-	X
56	MG	BA	3222	-	-	-	X
56	MG	BA	3223	-	-	-	X
56	MG	BA	3227	-	-	-	X
56	MG	BA	3228	-	-	-	X
56	MG	BA	3230	-	-	-	X
56	MG	BA	3264	-	-	-	X
56	MG	BA	3277	-	-	-	X
56	MG	BA	3297	-	-	-	X
56	MG	BA	3299	-	-	-	X
56	MG	BA	3304	-	-	-	X
56	MG	BA	3311	-	-	-	X
56	MG	BA	3324	-	-	-	X
56	MG	BA	3328	-	-	-	X
56	MG	BA	3332	-	-	-	X
56	MG	BA	3343	-	-	-	X
56	MG	BA	3346	-	-	-	X
56	MG	BA	3349	-	-	-	X
56	MG	BA	3353	-	-	-	X
56	MG	BA	3356	-	-	-	X
56	MG	BA	3368	-	-	-	X
56	MG	BA	3370	-	-	-	X
56	MG	BA	3379	-	-	-	X
56	MG	BA	3402	-	-	-	X
56	MG	BA	3414	-	-	-	X
56	MG	BA	3416	-	-	-	X
56	MG	BA	3431	-	-	-	X
56	MG	BA	3435	-	-	-	X
56	MG	BA	3441	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3451	-	-	-	X
56	MG	BA	3459	-	-	-	X
56	MG	BA	3480	-	-	-	X
56	MG	BA	3493	-	-	-	X
56	MG	BA	3503	-	-	-	X
56	MG	BA	3504	-	-	-	X
56	MG	BA	3512	-	-	-	X
56	MG	BA	3524	-	-	-	X
56	MG	BA	3525	-	-	-	X
56	MG	BA	3530	-	-	-	X
56	MG	BA	3544	-	-	-	X
56	MG	BA	3545	-	-	-	X
56	MG	BA	3546	-	-	-	X
56	MG	BA	3548	-	-	-	X
56	MG	BA	3550	-	-	-	X
56	MG	BA	3552	-	-	-	X
56	MG	BA	3557	-	-	-	X
56	MG	BA	3560	-	-	-	X
56	MG	BA	3576	-	-	-	X
56	MG	BA	3601	-	-	-	X
56	MG	BA	3607	-	-	-	X
56	MG	BA	3614	-	-	-	X
56	MG	BA	3622	-	-	-	X
56	MG	BA	3624	-	-	-	X
56	MG	BA	3630	-	-	-	X
56	MG	BA	3634	-	-	-	X
56	MG	BA	3637	-	-	-	X
56	MG	BA	3640	-	-	-	X
56	MG	BA	3642	-	-	-	X
56	MG	BA	3664	-	-	-	X
56	MG	BA	3671	-	-	-	X
56	MG	BA	3682	-	-	-	X
56	MG	BA	3689	-	-	-	X
56	MG	BA	3703	-	-	-	X
56	MG	BA	3719	-	-	-	X
56	MG	BA	3720	-	-	-	X
56	MG	BA	3726	-	-	-	X
56	MG	BA	3727	-	-	-	X
56	MG	BA	3729	-	-	-	X
56	MG	BA	3732	-	-	-	X
56	MG	BA	3737	-	-	-	X
56	MG	BA	3739	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BB	3003	-	-	-	X
56	MG	BB	3008	-	-	-	X
56	MG	BD	302	-	-	-	X
56	MG	BD	305	-	-	-	X
56	MG	BD	306	-	-	-	X
56	MG	BD	308	-	-	-	X
56	MG	BD	310	-	-	-	X
56	MG	BE	301	-	-	-	X
56	MG	BE	305	-	-	-	X
56	MG	BF	301	-	-	-	X
56	MG	BF	302	-	-	-	X
56	MG	BF	303	-	-	-	X
56	MG	BF	305	-	-	-	X
56	MG	BN	3001	-	-	-	X
56	MG	BN	3002	-	-	-	X
56	MG	BN	3003	-	-	-	X
56	MG	BN	3004	-	-	-	X
56	MG	BN	3005	-	-	-	X
56	MG	BP	201	-	-	-	X
56	MG	BP	203	-	-	-	X
56	MG	BQ	201	-	-	-	X
56	MG	BQ	202	-	-	-	X
56	MG	BQ	205	-	-	-	X
56	MG	BR	201	-	-	-	X
56	MG	BR	204	-	-	-	X
56	MG	BU	202	-	-	-	X
56	MG	BU	203	-	-	-	X
56	MG	BU	205	-	-	-	X
56	MG	BU	206	-	-	-	X
56	MG	BU	208	-	-	-	X
56	MG	BV	201	-	-	-	X
56	MG	BV	202	-	-	-	X
56	MG	BV	203	-	-	-	X
56	MG	BW	204	-	-	-	X
56	MG	BX	3001	-	-	-	X
56	MG	CA	3001	-	-	-	X
56	MG	CA	3007	-	-	-	X
56	MG	CA	3027	-	-	-	X
56	MG	CA	3032	-	-	-	X
56	MG	CA	3042	-	-	-	X
56	MG	CA	3043	-	-	-	X
56	MG	CA	3048	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	3053	-	-	-	X
56	MG	CA	3061	-	-	-	X
56	MG	CA	3072	-	-	-	X
56	MG	CA	3098	-	-	-	X
56	MG	CA	3099	-	-	-	X
56	MG	CA	3101	-	-	-	X
56	MG	CA	3114	-	-	-	X
56	MG	CA	3119	-	-	-	X
56	MG	CA	3135	-	-	-	X
56	MG	CA	3152	-	-	-	X
56	MG	CA	3162	-	-	-	X
56	MG	CA	3170	-	-	-	X
56	MG	CE	3001	-	-	-	X
56	MG	CT	3001	-	-	-	X
56	MG	D3	101	-	-	-	X
56	MG	D5	102	-	-	-	X
56	MG	DA	3002	-	-	-	X
56	MG	DA	3006	-	-	-	X
56	MG	DA	3011	-	-	-	X
56	MG	DA	3016	-	-	-	X
56	MG	DA	3018	-	-	-	X
56	MG	DA	3025	-	-	-	X
56	MG	DA	3026	-	-	-	X
56	MG	DA	3033	-	-	-	X
56	MG	DA	3035	-	-	-	X
56	MG	DA	3039	-	-	-	X
56	MG	DA	3056	-	-	-	X
56	MG	DA	3065	-	-	-	X
56	MG	DA	3070	-	-	-	X
56	MG	DA	3078	-	-	-	X
56	MG	DA	3079	-	-	-	X
56	MG	DA	3092	-	-	-	X
56	MG	DA	3094	-	-	-	X
56	MG	DA	3097	-	-	-	X
56	MG	DA	3099	-	-	-	X
56	MG	DA	3100	-	-	-	X
56	MG	DA	3112	-	-	-	X
56	MG	DA	3114	-	-	-	X
56	MG	DA	3116	-	-	-	X
56	MG	DA	3121	-	-	-	X
56	MG	DA	3142	-	-	-	X
56	MG	DA	3143	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3148	-	-	-	X
56	MG	DA	3164	-	-	-	X
56	MG	DA	3170	-	-	-	X
56	MG	DA	3171	-	-	-	X
56	MG	DA	3173	-	-	-	X
56	MG	DA	3176	-	-	-	X
56	MG	DA	3178	-	-	-	X
56	MG	DA	3191	-	-	-	X
56	MG	DA	3197	-	-	-	X
56	MG	DA	3215	-	-	-	X
56	MG	DA	3236	-	-	-	X
56	MG	DA	3261	-	-	-	X
56	MG	DA	3262	-	-	-	X
56	MG	DA	3264	-	-	-	X
56	MG	DA	3265	-	-	-	X
56	MG	DA	3266	-	-	-	X
56	MG	DA	3272	-	-	-	X
56	MG	DA	3279	-	-	-	X
56	MG	DA	3295	-	-	-	X
56	MG	DA	3298	-	-	-	X
56	MG	DA	3302	-	-	-	X
56	MG	DA	3306	-	-	-	X
56	MG	DA	3312	-	-	-	X
56	MG	DA	3324	-	-	-	X
56	MG	DA	3326	-	-	-	X
56	MG	DA	3335	-	-	-	X
56	MG	DA	3346	-	-	-	X
56	MG	DA	3347	-	-	-	X
56	MG	DA	3364	-	-	-	X
56	MG	DA	3379	-	-	-	X
56	MG	DA	3395	-	-	-	X
56	MG	DA	3397	-	-	-	X
56	MG	DA	3401	-	-	-	X
56	MG	DA	3407	-	-	-	X
56	MG	DA	3408	-	-	-	X
56	MG	DA	3414	-	-	-	X
56	MG	DA	3418	-	-	-	X
56	MG	DA	3424	-	-	-	X
56	MG	DA	3432	-	-	-	X
56	MG	DA	3440	-	-	-	X
56	MG	DA	3450	-	-	-	X
56	MG	DA	3461	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3469	-	-	-	X
56	MG	DA	3473	-	-	-	X
56	MG	DA	3476	-	-	-	X
56	MG	DA	3479	-	-	-	X
56	MG	DA	3518	-	-	-	X
56	MG	DA	3535	-	-	-	X
56	MG	DA	3553	-	-	-	X
56	MG	DA	3554	-	-	-	X
56	MG	DA	3577	-	-	-	X
56	MG	DA	3581	-	-	-	X
56	MG	DA	3608	-	-	-	X
56	MG	DA	3609	-	-	-	X
56	MG	DA	3615	-	-	-	X
56	MG	DA	3620	-	-	-	X
56	MG	DA	3623	-	-	-	X
56	MG	DA	3624	-	-	-	X
56	MG	DA	3627	-	-	-	X
56	MG	DA	3628	-	-	-	X
56	MG	DA	3631	-	-	-	X
56	MG	DA	3633	-	-	-	X
56	MG	DA	3637	-	-	-	X
56	MG	DA	3638	-	-	-	X
56	MG	DA	3639	-	-	-	X
56	MG	DA	3641	-	-	-	X
56	MG	DA	3643	-	-	-	X
56	MG	DA	3649	-	-	-	X
56	MG	DA	3651	-	-	-	X
56	MG	DA	3652	-	-	-	X
56	MG	DA	3653	-	-	-	X
56	MG	DB	3007	-	-	-	X
56	MG	DD	301	-	-	-	X
56	MG	DD	305	-	-	-	X
56	MG	DD	306	-	-	-	X
56	MG	DD	307	-	-	-	X
56	MG	DE	301	-	-	-	X
56	MG	DF	301	-	-	-	X
56	MG	DF	304	-	-	-	X
56	MG	DF	305	-	-	-	X
56	MG	DQ	205	-	-	-	X
56	MG	DV	201	-	-	-	X
56	MG	DV	202	-	-	-	X
56	MG	DV	203	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	FME	AX	101	-	-	-	X
59	FME	CX	101	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 286321 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	1498	Total	C	N	O	P	0	0	0
			32196	14328	5966	10404	1498			
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	7	Total	C	N	O	P	0	0	1
			114	49	22	37	6			
22	CV	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			
23	CX	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			

- Molecule 24 is a protein called GE82832.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AW	10	Total	C	N	O	0	0	0
			93	67	10	16			
24	CW	10	Total	C	N	O	0	0	0
			93	67	10	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2731	Total	C	N	O	P	0	0	0
			58834	26185	11020	18899	2730			
25	DA	2714	Total	C	N	O	P	0	0	0
			58458	26018	10942	18786	2712			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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	S	0	0	0
			877	553	175	149				
38	DS	110	Total	C	N	O	S	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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
			551	348	99	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			531	338	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
			511	328	99	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	738	Total	Mg	0	0
			738	738		
56	AK	1	Total	Mg	0	0
			1	1		
56	DQ	5	Total	Mg	0	0
			5	5		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	6	Total	Mg	0	0
			6	6		
56	B8	3	Total	Mg	0	0
			3	3		
56	BE	10	Total	Mg	0	0
			10	10		
56	B1	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AN	2	Total 2	Mg 2	0	0
56	BP	4	Total 4	Mg 4	0	0
56	AX	9	Total 9	Mg 9	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CA	172	Total 172	Mg 172	0	0
56	B5	1	Total 1	Mg 1	0	0
56	BB	18	Total 18	Mg 18	0	0
56	D8	1	Total 1	Mg 1	0	0
56	DG	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	8	Total 8	Mg 8	0	0
56	AV	1	Total 1	Mg 1	0	0
56	BX	1	Total 1	Mg 1	0	0
56	B2	1	Total 1	Mg 1	0	0
56	AA	221	Total 221	Mg 221	0	0
56	BQ	5	Total 5	Mg 5	0	0
56	CQ	1	Total 1	Mg 1	0	0
56	CX	3	Total 3	Mg 3	0	0
56	DV	4	Total 4	Mg 4	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	8	Total 8	Mg 8	0	0

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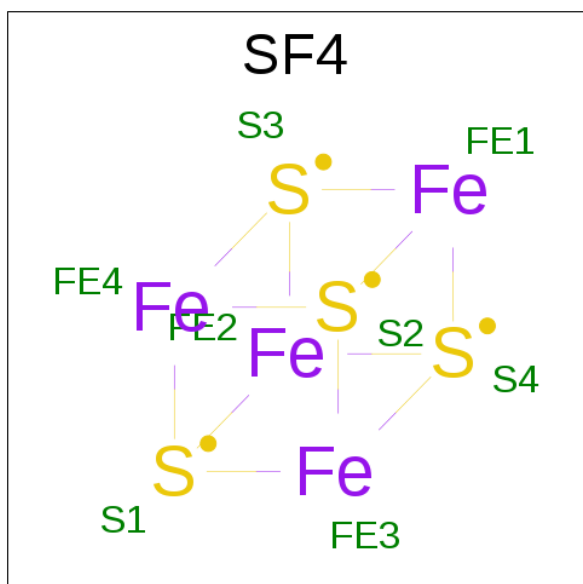
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DR	2	Total 2	Mg 2	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	6	Total 6	Mg 6	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	BG	4	Total 4	Mg 4	0	0
56	BY	1	Total 1	Mg 1	0	0
56	DE	6	Total 6	Mg 6	0	0
56	B3	3	Total 3	Mg 3	0	0
56	BR	4	Total 4	Mg 4	0	0
56	DA	653	Total 653	Mg 653	0	0
56	DW	2	Total 2	Mg 2	0	0
56	B7	4	Total 4	Mg 4	0	0
56	CF	1	Total 1	Mg 1	0	0
56	BV	4	Total 4	Mg 4	0	0
56	DO	1	Total 1	Mg 1	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	D5	2	Total 2	Mg 2	0	0
56	BD	12	Total 12	Mg 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B0	4	Total	Mg	0	0
			4	4		
56	CE	2	Total	Mg	0	0
			2	2		
56	BW	5	Total	Mg	0	0
			5	5		
56	DD	8	Total	Mg	0	0
			8	8		
56	AF	1	Total	Mg	0	0
			1	1		
56	DB	12	Total	Mg	0	0
			12	12		

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

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

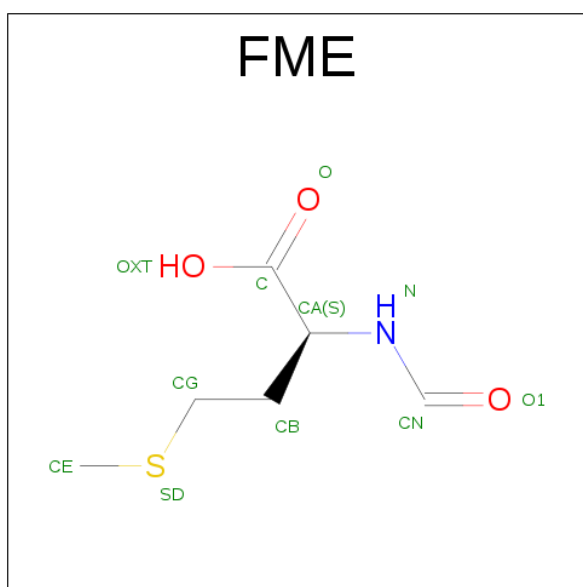
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B5	1	Total	Zn	0	0
			1	1		

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

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	AX	1	Total	C	N	O	S	0	0
			10	6	1	2	1		
59	CX	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	1	Total	K	0	0
			1	1		
60	DA	1	Total	K	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	148	Total	O	0	0
			148	148		
61	AD	1	Total	O	0	0
			1	1		
61	AE	3	Total	O	0	0
			3	3		
61	AJ	1	Total	O	0	0
			1	1		
61	AL	1	Total	O	0	0
			1	1		
61	AP	1	Total	O	0	0
			1	1		
61	AU	1	Total	O	0	0
			1	1		
61	AV	1	Total	O	0	0
			1	1		
61	AX	1	Total	O	0	0
			1	1		
61	BA	1092	Total	O	0	0
			1092	1092		
61	BB	26	Total	O	0	0
			26	26		
61	BD	8	Total	O	0	0
			8	8		
61	BE	9	Total	O	0	0
			9	9		
61	BF	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BG	1	Total 1	O 1	0	0
61	BN	3	Total 3	O 3	0	0
61	BO	2	Total 2	O 2	0	0
61	BP	15	Total 15	O 15	0	0
61	BQ	3	Total 3	O 3	0	0
61	BR	1	Total 1	O 1	0	0
61	BT	1	Total 1	O 1	0	0
61	BU	4	Total 4	O 4	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	2	Total 2	O 2	0	0
61	BX	4	Total 4	O 4	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	2	Total 2	O 2	0	0
61	B5	3	Total 3	O 3	0	0
61	B7	1	Total 1	O 1	0	0
61	B8	8	Total 8	O 8	0	0
61	CA	187	Total 187	O 187	0	0
61	CE	2	Total 2	O 2	0	0
61	CN	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CX	2	Total 2	O 2	0	0

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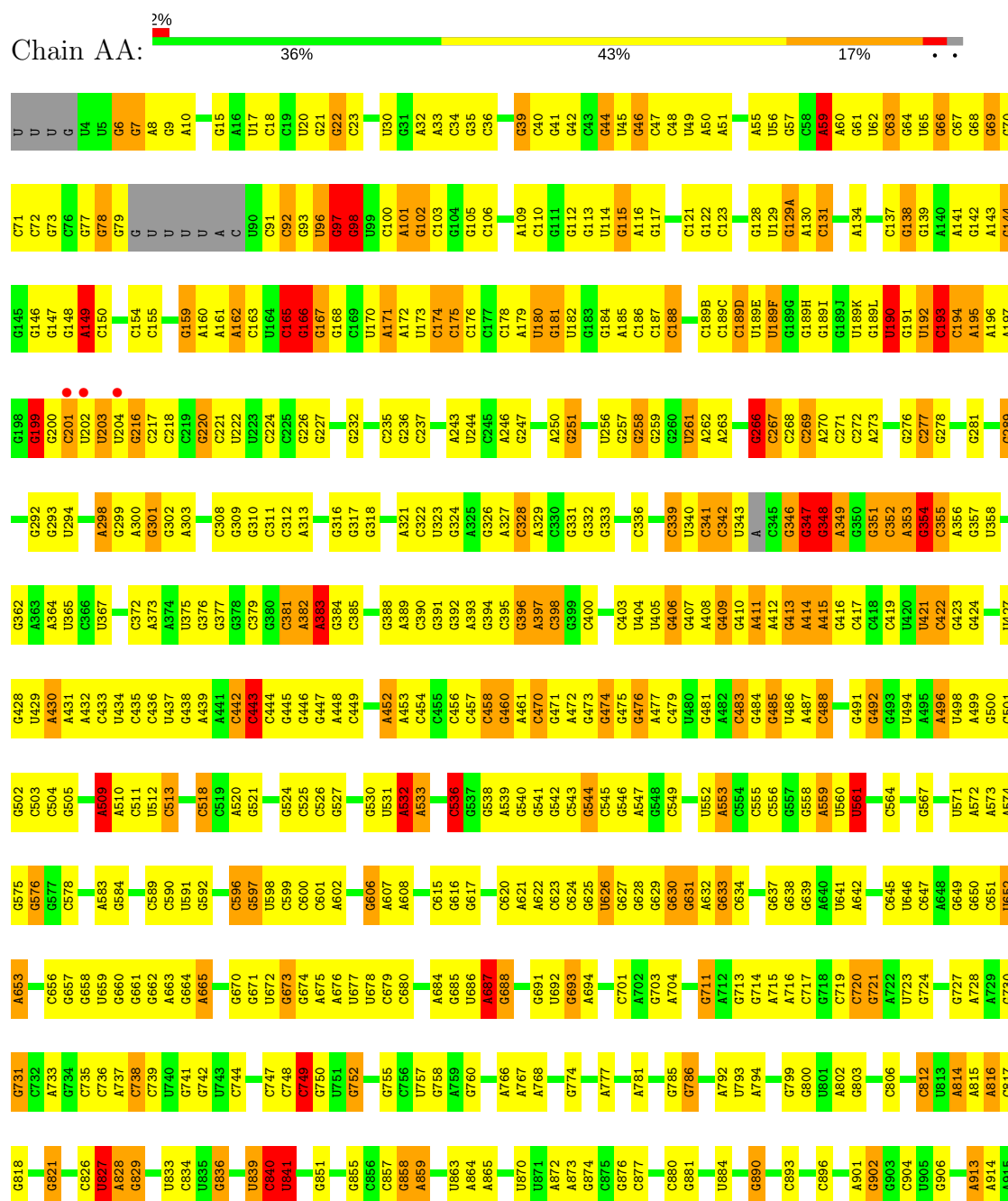
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DA	902	Total 902	O 902	0	0
61	DB	7	Total 7	O 7	0	0
61	DD	8	Total 8	O 8	0	0
61	DE	13	Total 13	O 13	0	0
61	DF	5	Total 5	O 5	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	14	Total 14	O 14	0	0
61	DQ	3	Total 3	O 3	0	0
61	DU	4	Total 4	O 4	0	0
61	DV	1	Total 1	O 1	0	0
61	DX	2	Total 2	O 2	0	0
61	DY	2	Total 2	O 2	0	0
61	D0	5	Total 5	O 5	0	0
61	D1	1	Total 1	O 1	0	0
61	D7	2	Total 2	O 2	0	0
61	D8	4	Total 4	O 4	0	0

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

#### • Molecule 1: 16S Ribosomal RNA



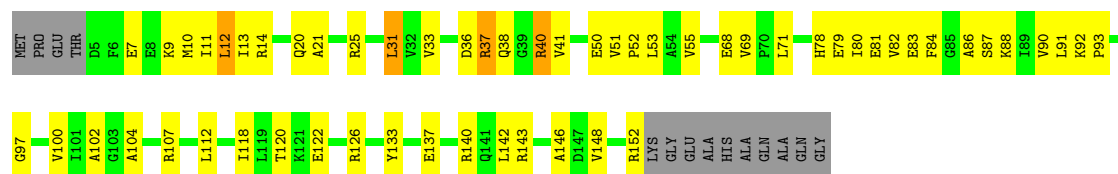


C1445	C1362	C1297	C1228	A1168	A1105	A1041	C985	A919	C934	G752	C680	A608	G538	C454	G388
U1446	C1363	C1298	C1233	A1169	G1106	G1042	A986	U920	U935	A753	G683	A609	A539	C455	A389
C1447	C1366	A1299	C1234	A1170	C1107	C1043	C989	U921	G936	G754	A684	G610	G540	C456	C390
G1452	C1367	G1300	G1235	G1171	G1108	A1044	C990	G922	G937	G755	G685	G611	G541	C457	G391
G1456	G1368	C1303	A1236	G1173	C1110	G1047	U991	G923	G938	G756	G686	G616	G542	C458	G392
G1458	C1369	G1304	C1237	G1174	A1111	G1048	U992	G924	U839	G757	U687	G617	C543	C460	A393
C1459	G1370	G1305	A1238	G1176	C1112	C1051	G993	G925	C940	G758	G688	U619	G544	A461	G396
A1460	A1376	A1239	A1239	A1176	C1113	C1052	A994	G926	U941	A759	G689	C620	C545	G471	A397
G1461	U1307	U1240	U1241	G1177	G1053	U1052	A996	G927	U850	G760	G690	A621	G546	A472	C398
G1373	G1378	G1241	G1378	G1178	G1053	G1053	U997	G928	U851	A767	G691	G622	A547	A473	G399
A1374	A1374	C1243	C1243	A1179	A1054	A1054	U997	G931	G851	A768	U692	C623	U551	G474	C400
A1375	G1310	C1242	C1242	A1180	A1055	A1055	G998	G932	G855	G769	U693	C624	U552	G475	C401
U1376	G1311	C1244	C1244	G1181	U1056	U1056	C999	G933	G855	G774	A694	C625	A553	G476	C402
A1377	G1312	A1245	A1245	G1182	G1057	G1057	U1000	C934	G858	G775	C701	G626	C554	G494	C403
C1378	G1313	C1246	C1246	A1183	U1120	G1058	A1001	C935	A859	G776	G705	U627	C555	G485	U404
U1379	G1314	C1249	C1249	G1184	U1122	C1059	G1001A	A936	G859	G777	A704	G628	C556	U486	U405
U1380	G1315	G1315	G1315	G1185	A1123	G1060	G1003	G937	A860	G778	U706	G629	G557	A487	G406
G1385	G1316	C1316	C1316	G1186	G1124	G1061	A1004	A938	G861	G779	U706	G630	G558	C488	G407
G1386	G1317	A1251	A1251	G1187	U1125	U1062	A1005	G939	A865	G783	A706	G631	A559	C489	A408
G1387	A1318	A1252	A1252	G1188	U1125	C1063	A1006	C940	C968	G784	C707	A652	U560	G490	G409
G1388	C1319	C1259	C1259	G1189	G1127	U1065	C1007	G941	G785	G785	G708	G633	U561	G491	G410
C1389	C1320	A1256	A1256	G1190	C1128	G1066	C1007	G942	C968	G786	G709	G634	C562	G492	A411
G1391	C1321	U1257	U1257	A1191	C1129	A1067	G1008	G947	G869	G790	G710	G635	G564	U494	A412
U1390	C1322	G1258	G1258	C1192	A1130	A1067	G1009	C948	A872	G791	A712	G638	C564	U495	G413
U1391	G1323	C1259	C1259	G1193	G1131	G1068	G1010	C948	A873	G792	A713	G639	U565	A496	A414
G1392	A1324	A1260	A1260	U1194	C1132	C1069	G1011	G951	A874	A793	G714	A640	U566	U498	A415
U1393	C1325	G1261	G1261	C1195	G1133	U1070	G1012	U952	G874	G794	G715	A641	G568	A499	C418
A1396	C1326	C1262	C1262	U1196	G1071	G1071	G1013	G953	G875	A794	A716	A642	U571	G500	C419
C1397	G1327	C1263	C1263	G1197	U1135	G1072	A1014	G954	G876	G797	G719	U646	A573	C501	G422
C1398	C1328	C1264	C1264	U1198	U1136	G1073	A1015	U955	G877	G798	G720	C647	C503	G502	G423
A1399	A1329	G1265	G1265	U1199	C1137	G1074	A1016	U956	G878	G799	G721	A648	G576	C503	G424
C1400	U1330	G1266	G1266	C1200	G1138	C1075	G1017	U957	C980	G800	A722	G649	G577	G505	G425
G1401	G1331	A1267	A1267	A1201	G1139	G1076	C1018	A958	G881	U801	G723	G650	G578	G505	G426
C1402	C1332	C1268	C1268	G1202	C1140	G1077	A1019	A959	C982	A802	U723	G651	G579	A509	U427
C1403	A1333	A1269	A1269	C1203	G1141	U1078	U1020	U960	G885	G803	G724	U652	U580	A510	G428
G1403	G1334	C1270	C1270	A1204	G1142	G1079	G1021	U961	G885	U804	G725	U653	U582	C511	U429
G1411	C1335	G1271	G1271	U1205	G1143	A1080	G1022	A964	G890	C806	G726	A654	U583	C513	A430
G1412	G1336	G1272	G1272	G1206	G1144	G1081	G1023	A965	U891	C811	G730	A655	A584	C518	A431
G1413	C1337	G1273	G1273	G1207	C1145	U1085	G1024	A966	U892	C812	G731	A656	G585	C519	A432
U1414	G1338	C1274	C1274	C1208	A1146	U1086	U1025	A967	A892	C813	G732	G660	G586	C520	A433
G1415	A1339	G1277	G1277	C1210	U1147	G1087	C1028	A968	C993	U814	A733	G661	G587	A520	A434
G1419	A1340	U1278	U1278	U1211	C1149	G1088	C1029	A969	G994	U813	G734	G662	G588	G521	C436
C1420	C1342	A1279	A1279	U1212	U1150	G1088	C1030	A970	C999	A814	G735	A663	C589	C522	U437
A1513	G1343	A1280	A1280	A1213	A1151	U1090	G1030A	G971	A900	A816	G736	G664	C590	G525	G438
C1514	C1344	U1281	U1281	C1214	A1152	U1091	C1030B	C972	A901	C817	G737	A665	U591	C526	A439
G1422	U1345	C1282	C1282	G1215	C1153	U1091	G1030C	G973	G902	G818	A737	G666	G592	G527	A441
G1423	A1346	G1283	G1283	G1216	G1154	A1092	U1030D	A974	G906	G821	C738	G667	C596	C528	C442
G1516	G1347	C1284	C1284	C1217	G1155	A1093	G1031	A975	G906	C826	U739	G671	C597	C529	C443
G1517	U1348	A1285	A1285	C1218	G1156	G1094	G1032	G976	A907	U827	G740	U672	G597	U531	C444
A1518	U1348	A1286	A1286	U1219	A1157	U1095	G1033	A977	A908	C826	G741	G673	C599	A532	G445
A1519	C1352	A1287	A1287	G1220	C1158	C1096	G1034	A978	A909	A828	G742	G674	C600	A533	G446
G1435	G1353	A1288	A1288	G1221	U1159	A1095	A1035	C979	A913	G829	G743	G675	C601	U534	G447
U1436	C1354	A1289	A1289	G1222	C1160	G1100	C1037	G981	A915	G830	C745	U677	C602	A535	A448
G1442	C1355	G1290	G1290	G1223	C1161	A1101	C1038	U982	A916	G831	C749	U678	G606	C536	A452
G1523	G1223	C1162	C1162	G1224	C1162	A1102	C1039	A983	G917	U831	G750	C679	G607	G537	A453
G1529	A1225	C1163	C1163	A1226	G1163	C1103	U1040	C984	A918	U832	U751		A507		
G1530	G1226	G1166	G1166	A1227	G1166	G1104									




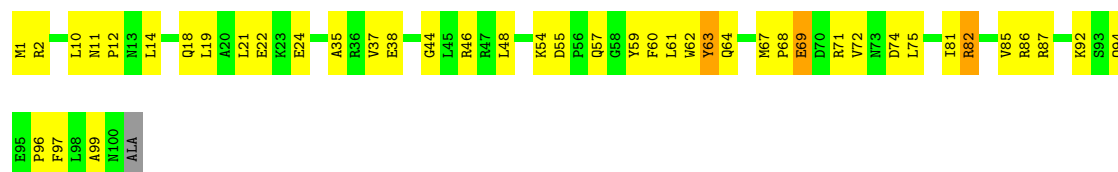


Chain CE: 



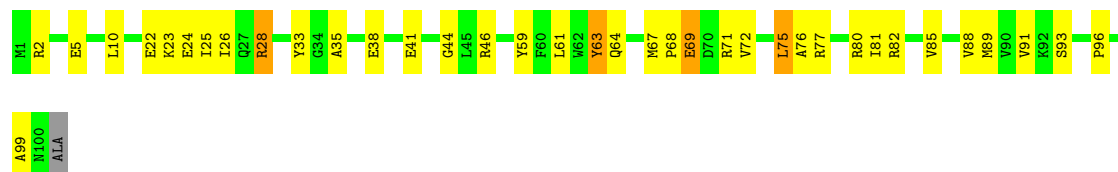
• Molecule 6: 30S Ribosomal Protein S6

Chain AF: 



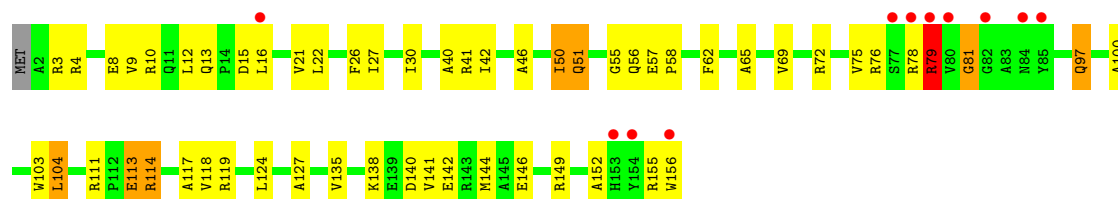
• Molecule 6: 30S Ribosomal Protein S6

Chain CF: 



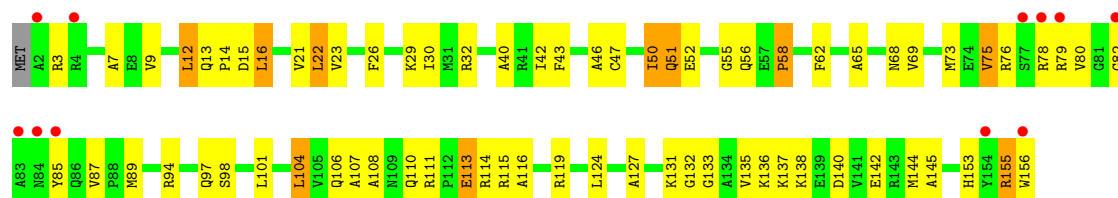
• Molecule 7: 30S Ribosomal Protein S7

Chain AG: 



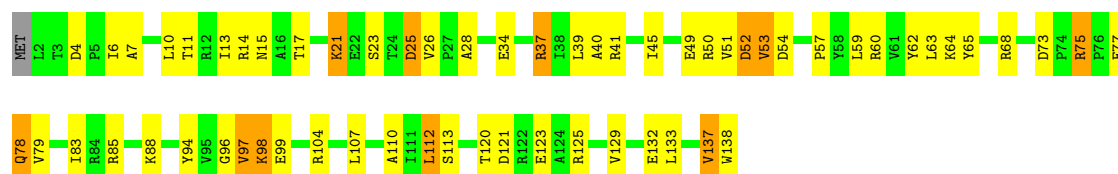
• Molecule 7: 30S Ribosomal Protein S7

Chain CG: 



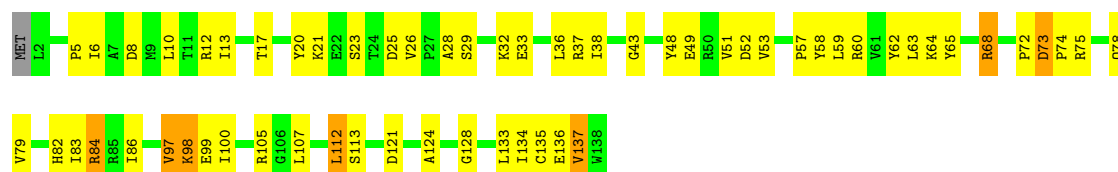
• Molecule 8: 30S Ribosomal Protein S8

Chain AH: 



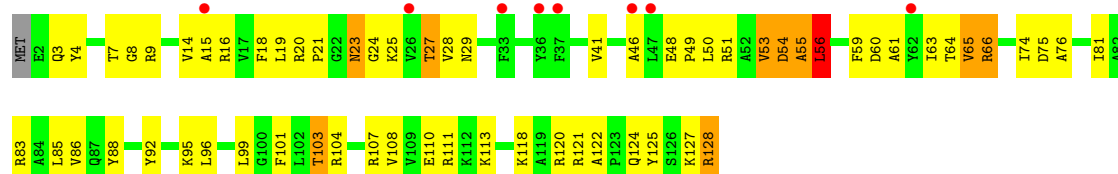
• Molecule 8: 30S Ribosomal Protein S8

Chain CH: 56% 38% 5% .



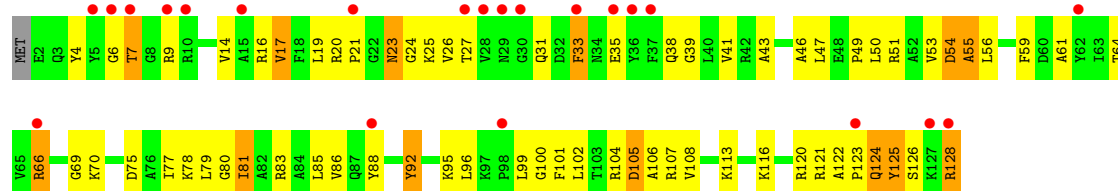
• Molecule 9: 30S Ribosomal Protein S9

Chain AI: 6% 50% 41% 7% ..



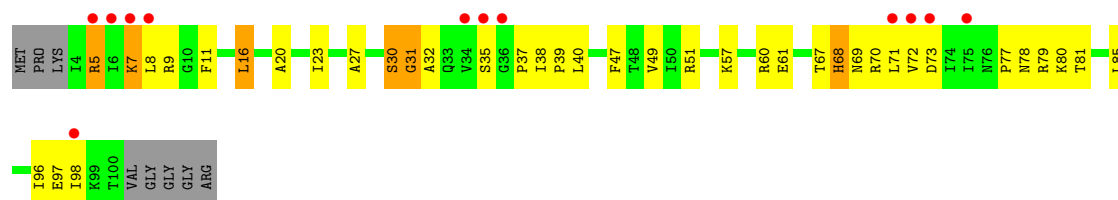
• Molecule 9: 30S Ribosomal Protein S9

Chain CI: 17% 45% 44% 10% .



• Molecule 10: 30S Ribosomal Protein S10

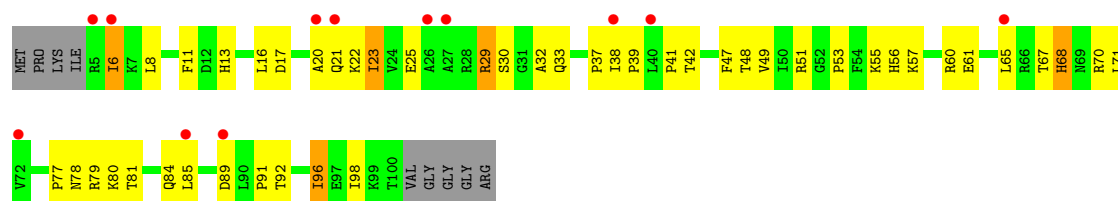
Chain AJ: 11% 55% 31% 6% 8%



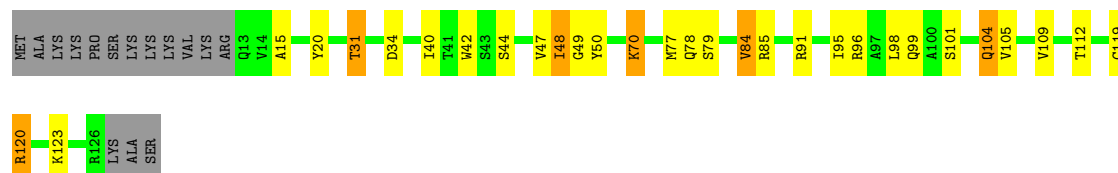
• Molecule 10: 30S Ribosomal Protein S10

Chain CJ: 11% 47% 40% 5% 9%

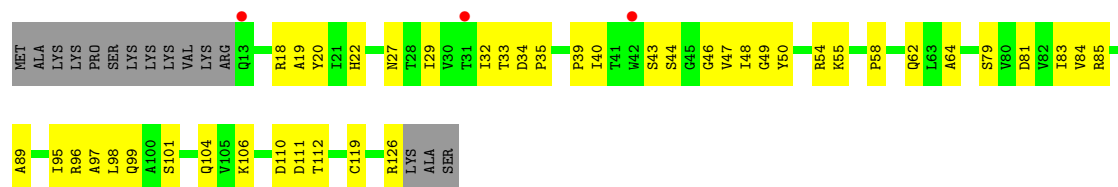




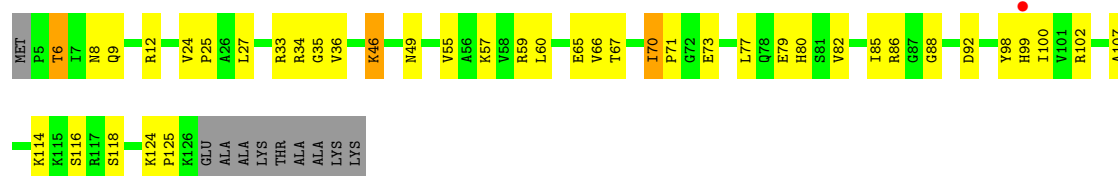
• Molecule 11: 30S Ribosomal Protein S11



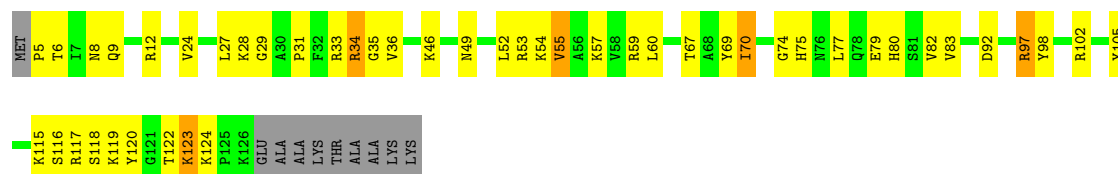
• Molecule 11: 30S Ribosomal Protein S11



• Molecule 12: 30S Ribosomal Protein S12

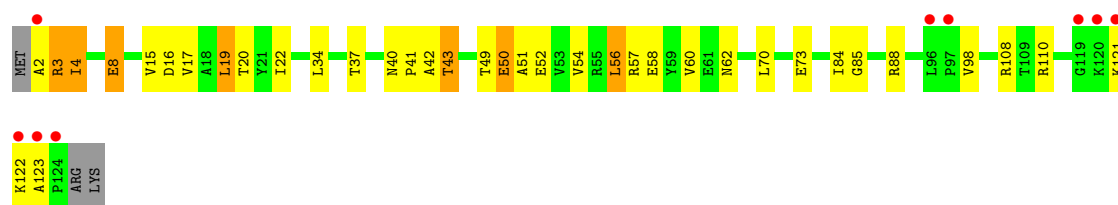


• Molecule 12: 30S Ribosomal Protein S12

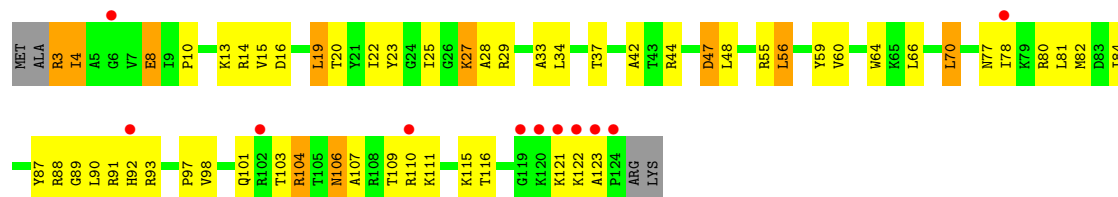


• Molecule 13: 30S Ribosomal Protein S13





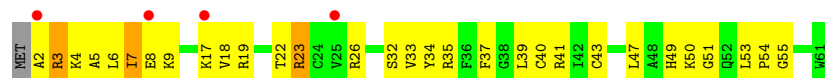
• Molecule 13: 30S Ribosomal Protein S13



• Molecule 14: 30S Ribosomal Protein S14



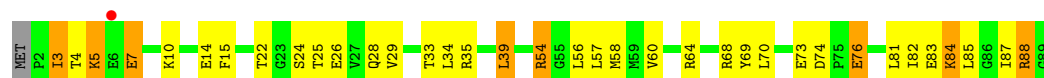
• Molecule 14: 30S Ribosomal Protein S14



• Molecule 15: 30S Ribosomal Protein S15

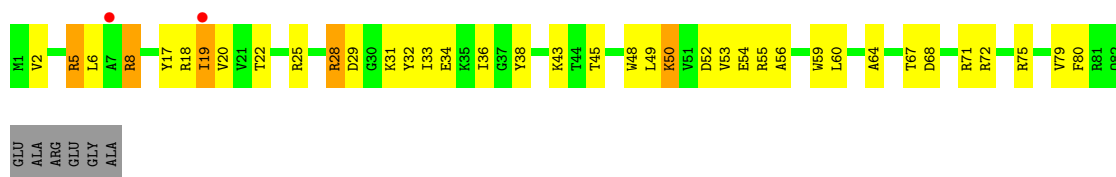


• Molecule 15: 30S Ribosomal Protein S15



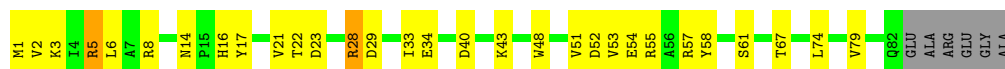
• Molecule 16: 30S Ribosomal Protein S16





• Molecule 16: 30S Ribosomal Protein S16

Chain CP: 59% 32% 7%



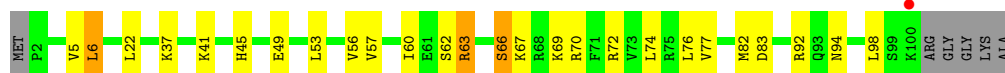
• Molecule 17: 30S Ribosomal Protein S17

Chain AQ: 68% 24% 6%



• Molecule 17: 30S Ribosomal Protein S17

Chain CQ: 70% 22% 6%



• Molecule 18: 30S Ribosomal Protein S18

Chain AR: 55% 20% 23%



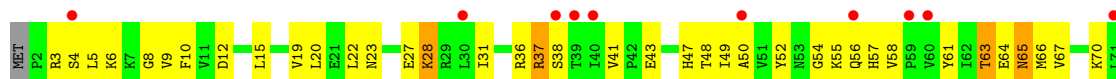
• Molecule 18: 30S Ribosomal Protein S18

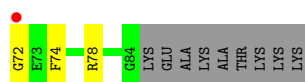
Chain CR: 41% 31% 5% 23%



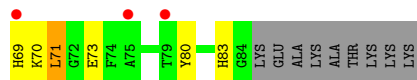
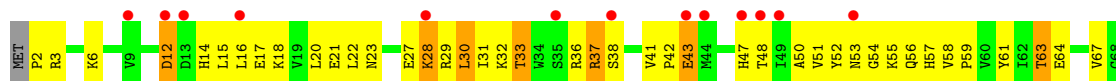
• Molecule 19: 30S Ribosomal Protein S19

Chain AS: 12% 45% 40% 11%

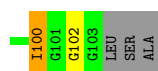




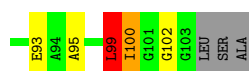
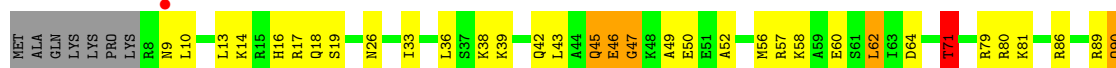
• Molecule 19: 30S Ribosomal Protein S19



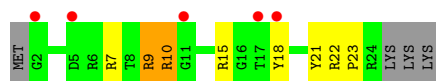
• Molecule 20: 30S Ribosomal Protein S20



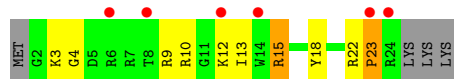
• Molecule 20: 30S Ribosomal Protein S20



• Molecule 21: 30S Ribosomal Protein THX

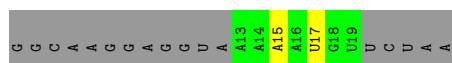


• Molecule 21: 30S Ribosomal Protein THX



• Molecule 22: mRNA





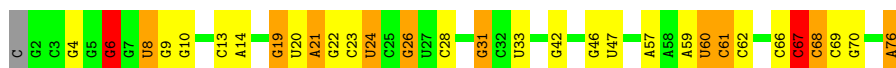
• Molecule 22: mRNA

Chain CV: 21% 75%



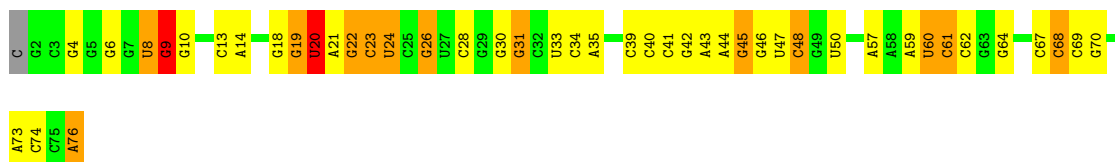
• Molecule 23: P-site tRNA

Chain AX: 58% 25% 13%



• Molecule 23: P-site tRNA

Chain CX: 40% 39% 17%



• Molecule 24: GE82832

Chain AW: 10% 80% 10%



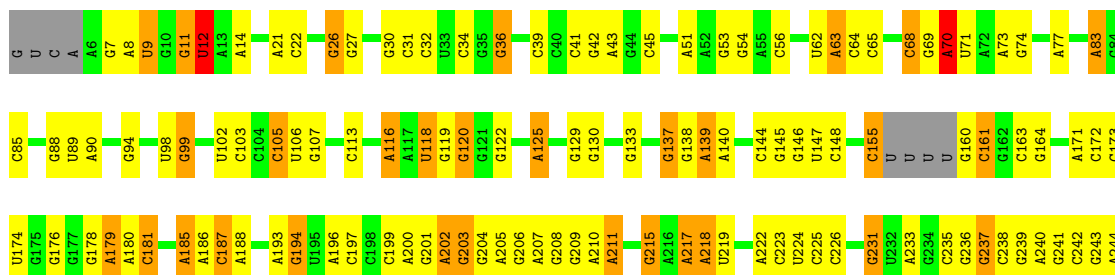
• Molecule 24: GE82832

Chain CW: 10% 70% 20%



• Molecule 25: 23S Ribosomal RNA

Chain BA: 47% 34% 10% 6%

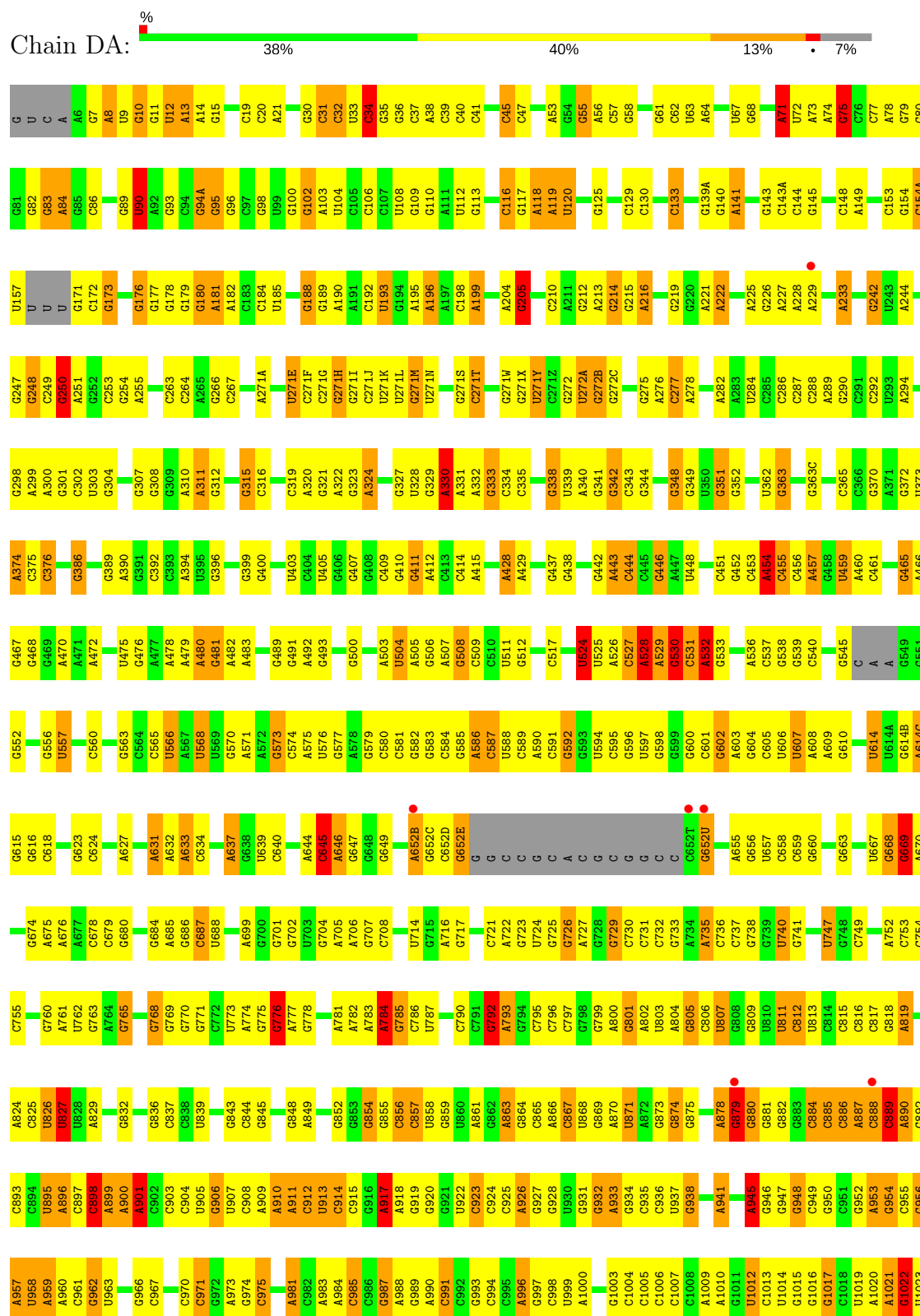




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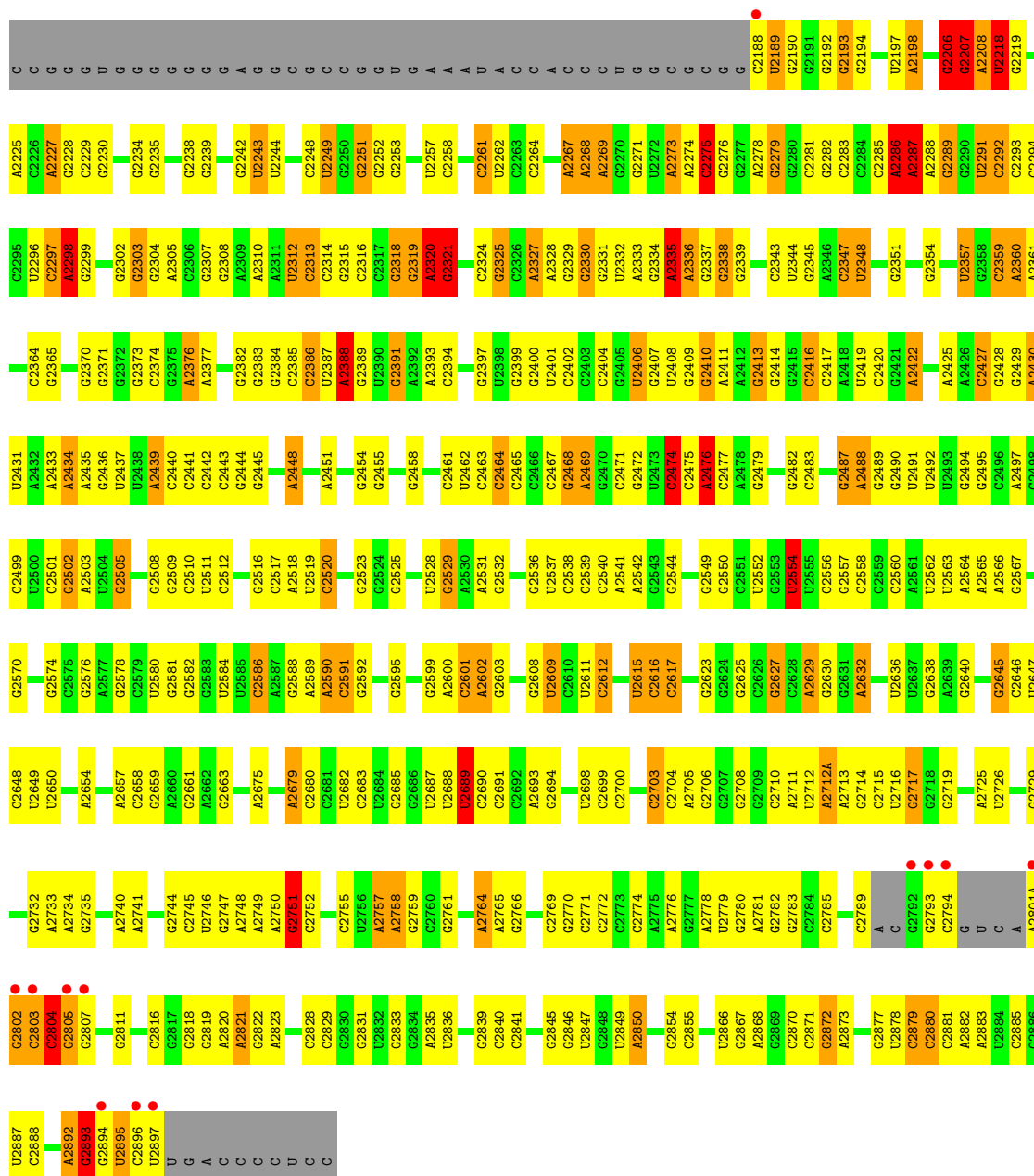
U  
C  
G

• Molecule 25: 23S Ribosomal RNA



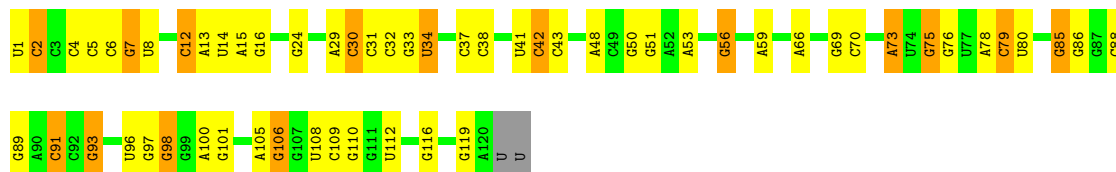


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C	U2075	U2011	A1928	C1767	A1668	C1669	C1588	U1513	U1438	G1364	U1291	C	
C	G2076	G2012	G1929	G1769	U1768	C1670	C1589	U1514	A1439	U1292	U1141	A	
C	A2077	A2013	C1930	U1841	C1769	U1671	U1590	G1515	G1440	C1293	U1142	U	
G	U2078	A2014	U1931	G1842	U1769	U1671	U1591	U1514	G1441	U1294	A1142A	C	
C	C2079	A2015	A1932	C1843	A1773	C1672	G1591	C1516		G1296	A1143	C	
C	G2080	U2016	C1933	C1844	C1774	U1673	C1592	G1517	A1445	G1369	G1297	U	
	C2081	U2017	C1934	U1775	U1775	C1674	C1593	U1518	C1445A	U1220	C1298	U	
										C1299	C1298	A	



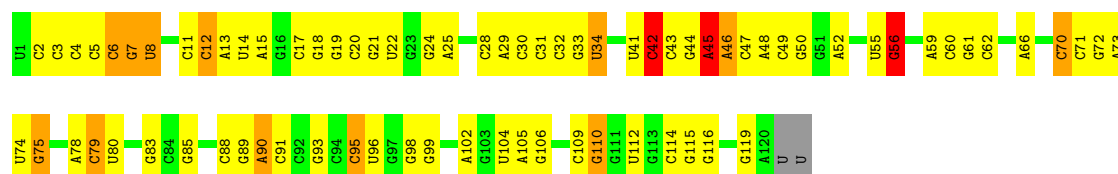
● Molecule 26: 5S Ribosomal RNA

Chain BB: 51% 35% 12%

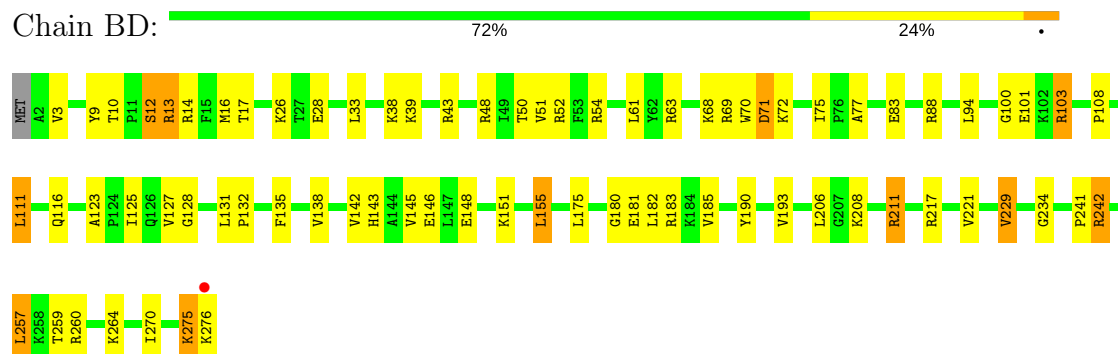


● Molecule 26: 5S Ribosomal RNA

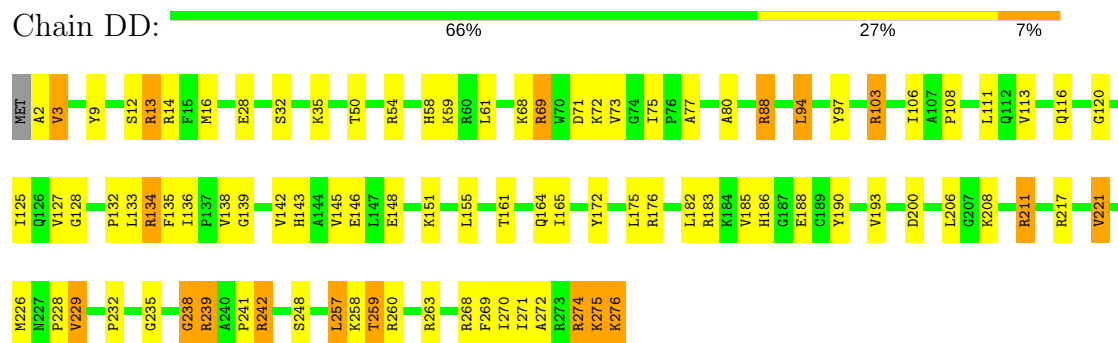
Chain DB: 36% 50% 10%



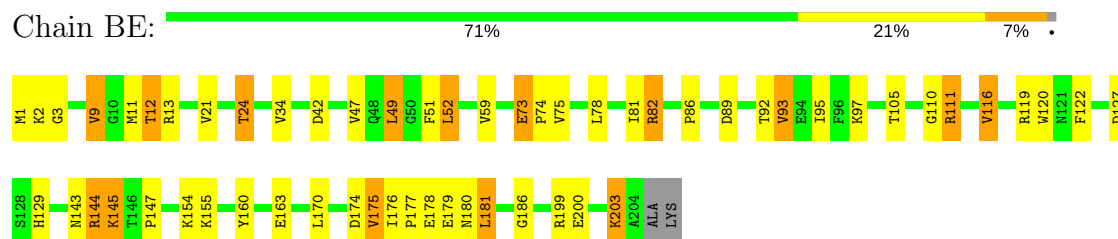
### • Molecule 27: 50S Ribosomal Protein L2



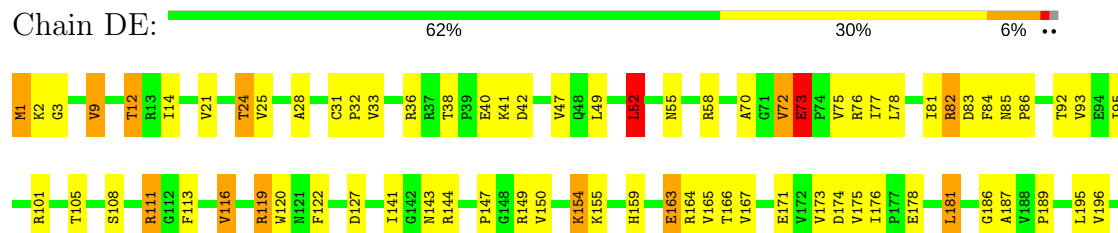
### • Molecule 27: 50S Ribosomal Protein L2

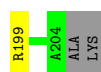


### • Molecule 28: 50S Ribosomal Protein L3



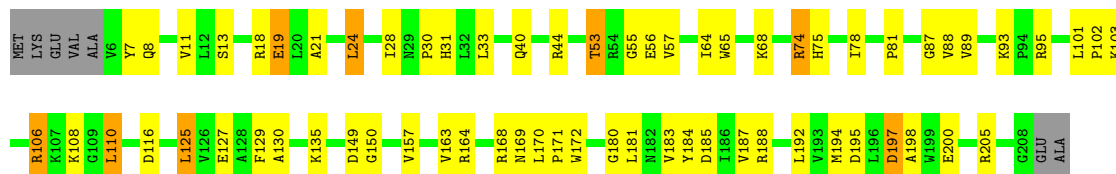
### • Molecule 28: 50S Ribosomal Protein L3





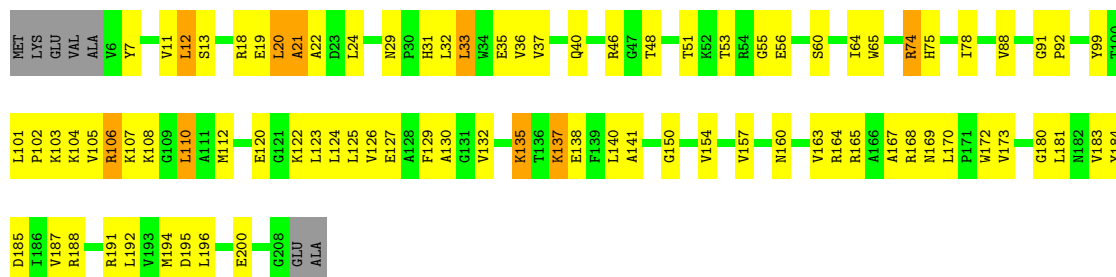
• Molecule 29: 50S Ribosomal Protein L4

Chain BF: 65% 28%



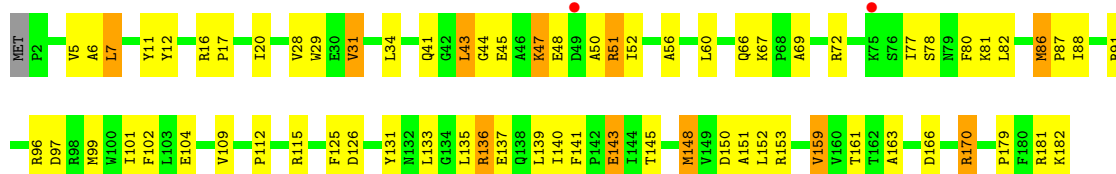
• Molecule 29: 50S Ribosomal Protein L4

Chain DF: 56% 36%



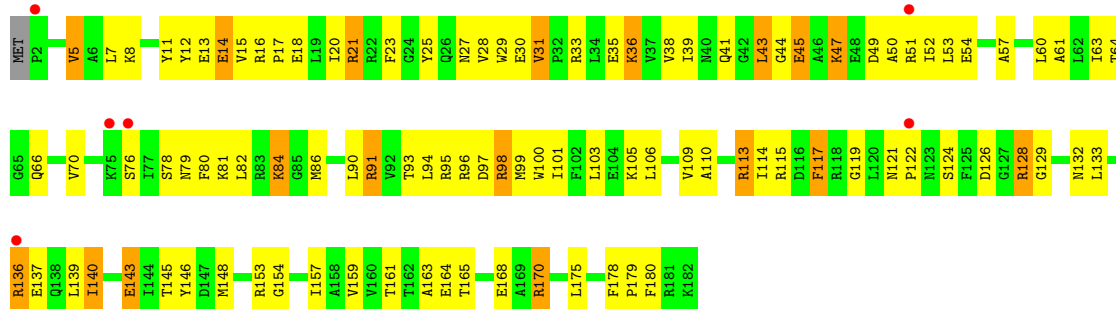
• Molecule 30: 50S Ribosomal Protein L5

Chain BG: 61% 32% 6%

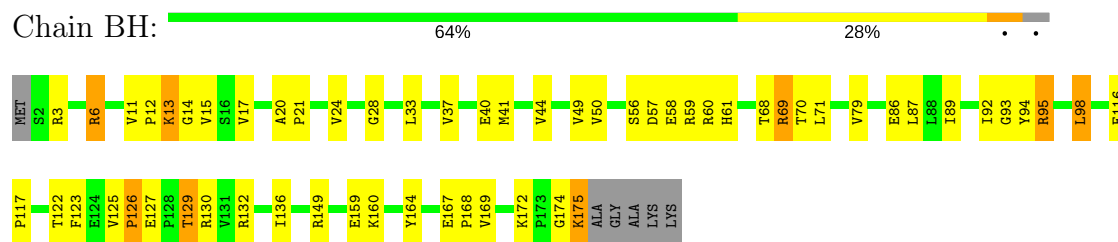


• Molecule 30: 50S Ribosomal Protein L5

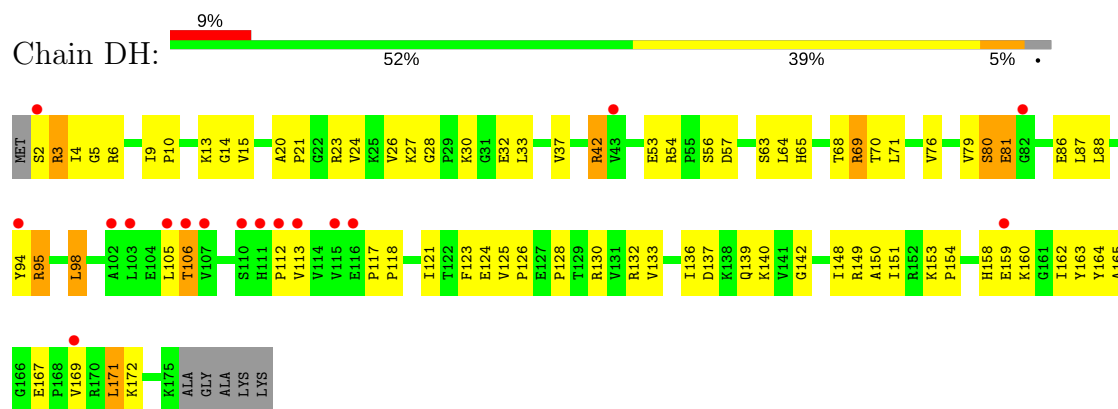
Chain DG: 43% 46% 10%



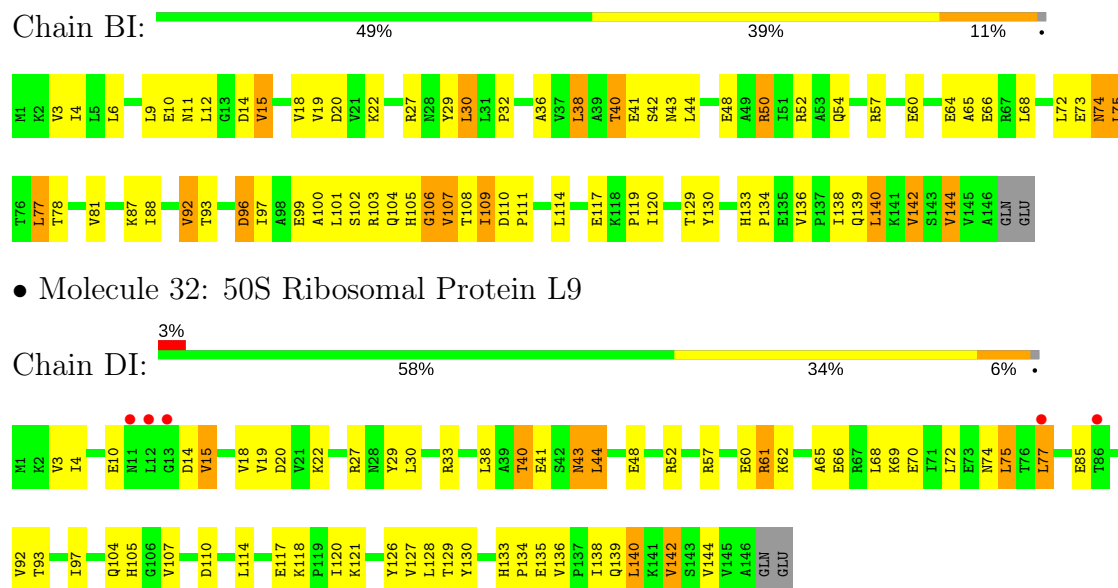
• Molecule 31: 50S Ribosomal Protein L6



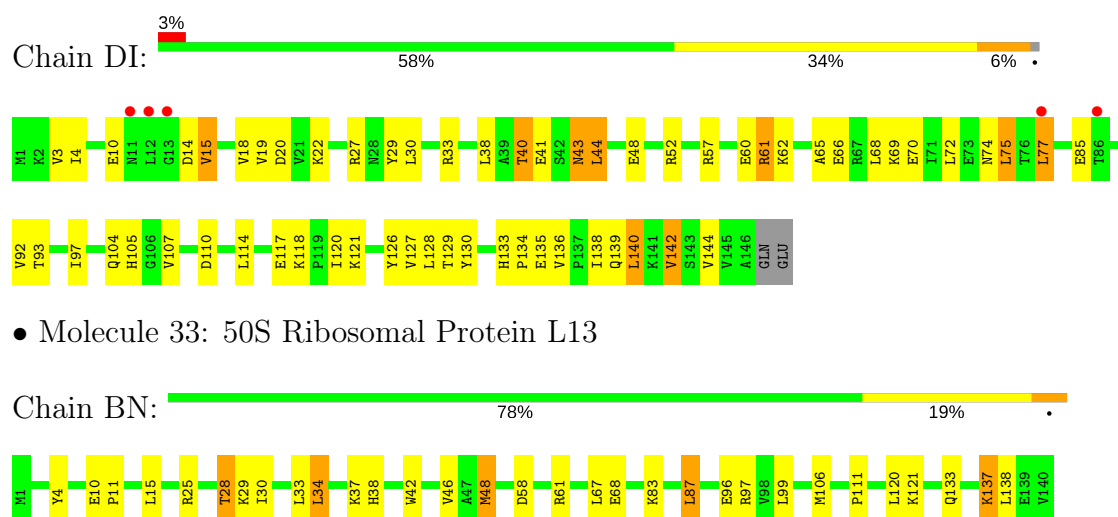
• Molecule 31: 50S Ribosomal Protein L6



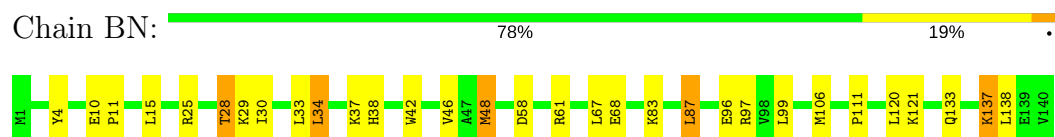
• Molecule 32: 50S Ribosomal Protein L9



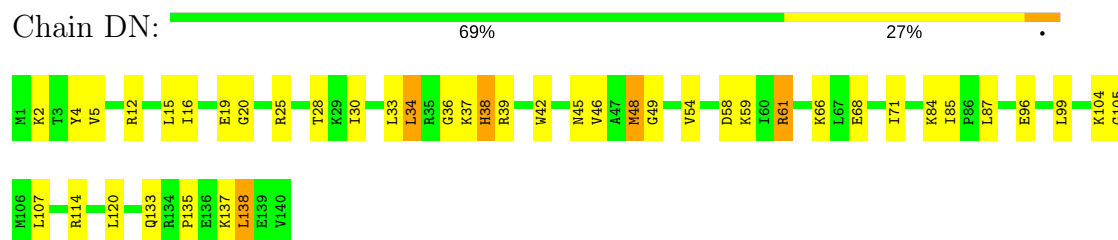
• Molecule 32: 50S Ribosomal Protein L9



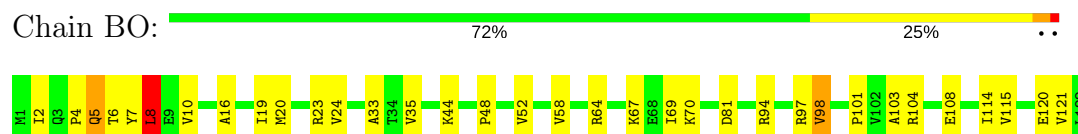
• Molecule 33: 50S Ribosomal Protein L13



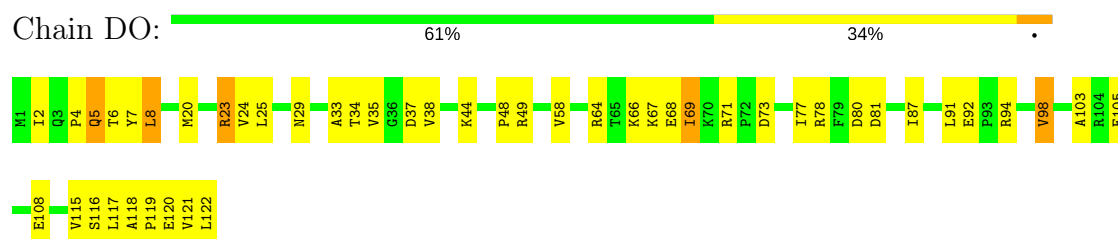
• Molecule 33: 50S Ribosomal Protein L13



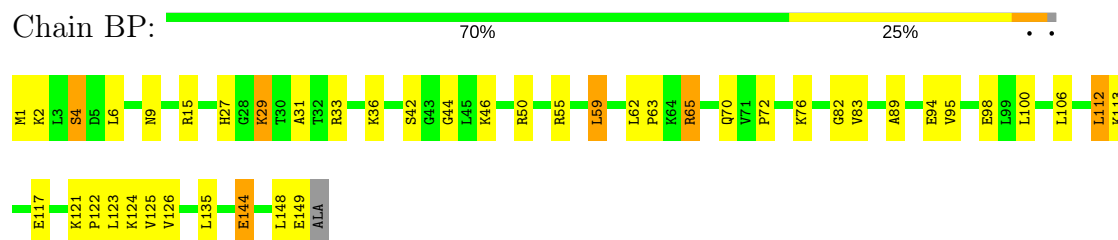
• Molecule 34: 50S Ribosomal Protein L14



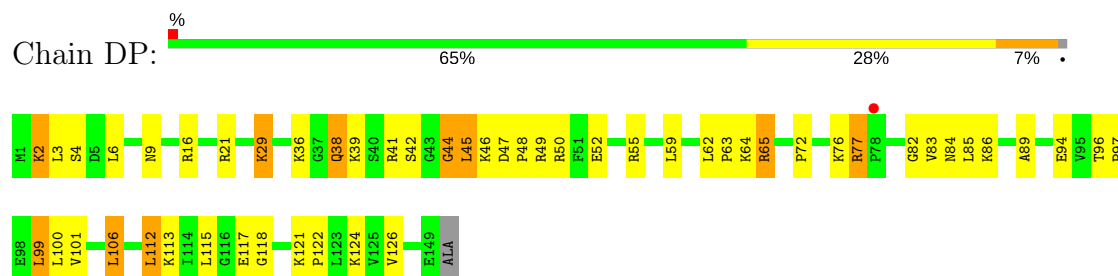
• Molecule 34: 50S Ribosomal Protein L14



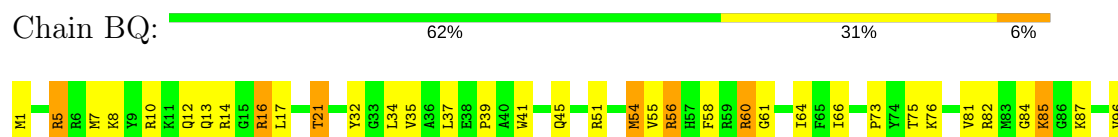
• Molecule 35: 50S Ribosomal Protein L15



• Molecule 35: 50S Ribosomal Protein L15

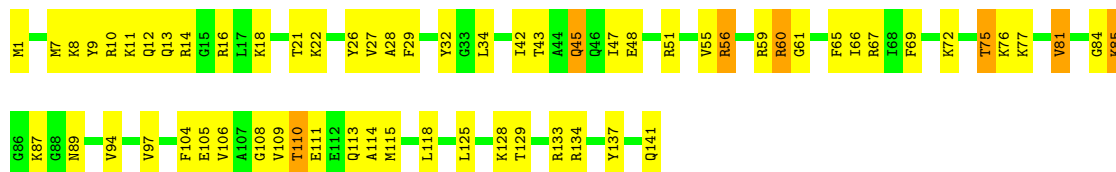


• Molecule 36: 50S Ribosomal Protein L16

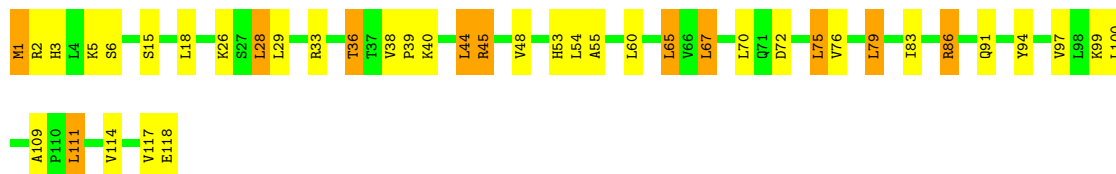




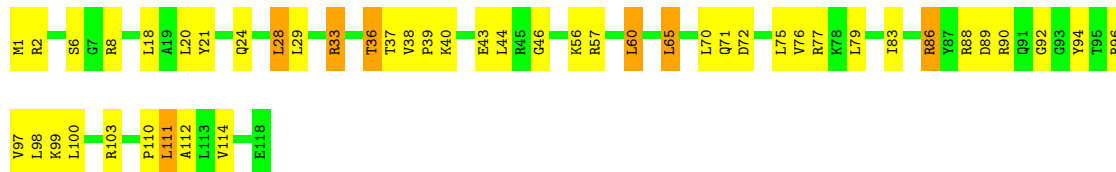
• Molecule 36: 50S Ribosomal Protein L16



• Molecule 37: 50S Ribosomal Protein L17



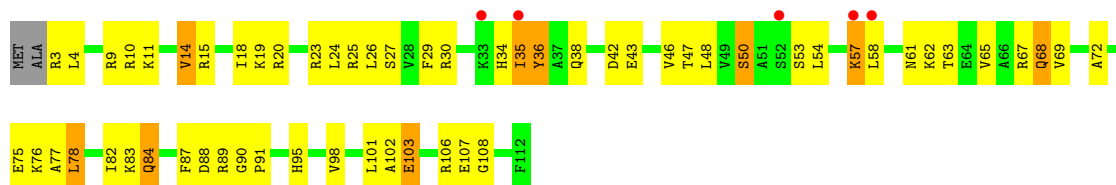
• Molecule 37: 50S Ribosomal Protein L17



• Molecule 38: 50S Ribosomal Protein L18

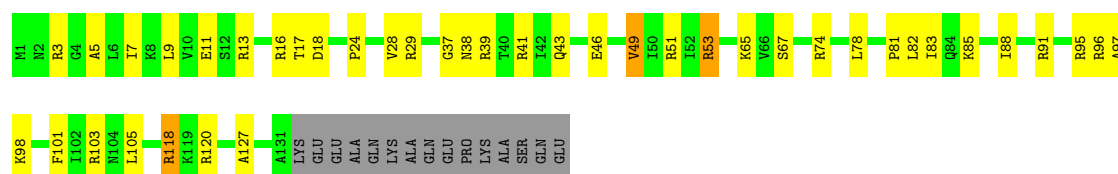


• Molecule 38: 50S Ribosomal Protein L18



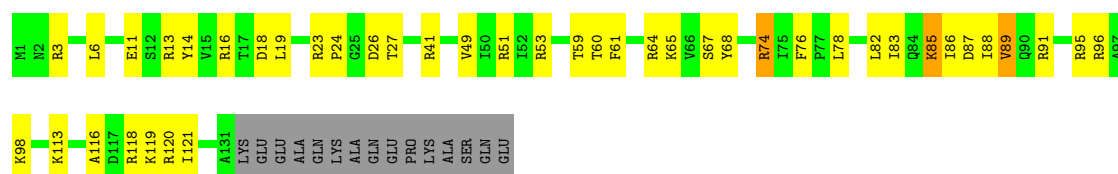
• Molecule 39: 50S Ribosomal Protein L19

Chain BT: 



• Molecule 39: 50S Ribosomal Protein L19

Chain DT: 



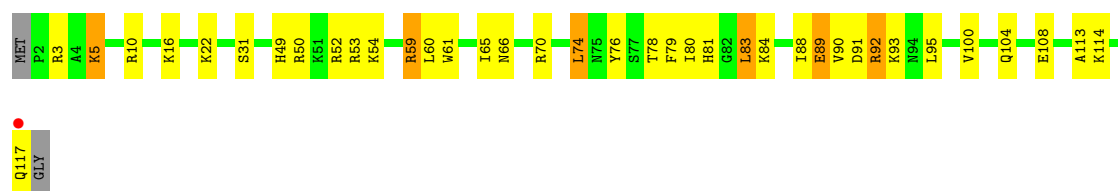
• Molecule 40: 50S Ribosomal Protein L20

Chain BU: 




• Molecule 40: 50S Ribosomal Protein L20

Chain DU: 



• Molecule 41: 50S Ribosomal Protein L21

Chain BV: 




• Molecule 41: 50S Ribosomal Protein L21

Chain DV: 





- Molecule 42: 50S Ribosomal Protein L22

Chain BW:  79% 17%



- Molecule 42: 50S Ribosomal Protein L22

Chain DW:  73% 23%



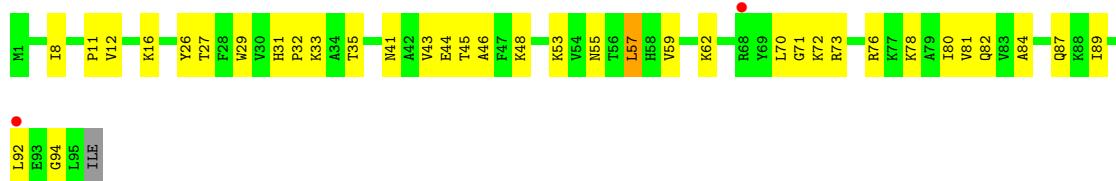
- Molecule 43: 50S Ribosomal Protein L23

Chain BX:  73% 24%



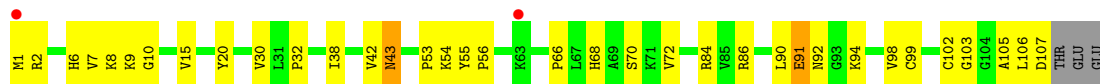
- Molecule 43: 50S Ribosomal Protein L23

Chain DX:  2% 61% 36%



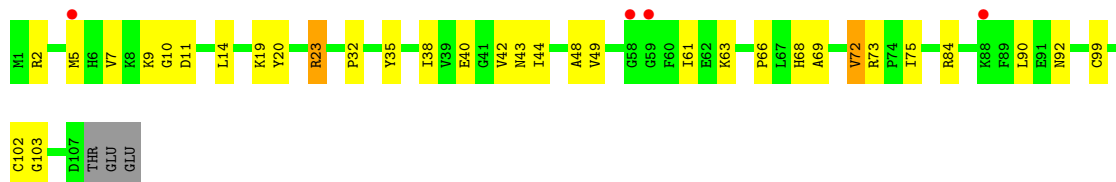
- Molecule 44: 50S Ribosomal Protein L24

Chain BY:  2% 65% 30%



- Molecule 44: 50S Ribosomal Protein L24

Chain DY:  4% 67% 28%



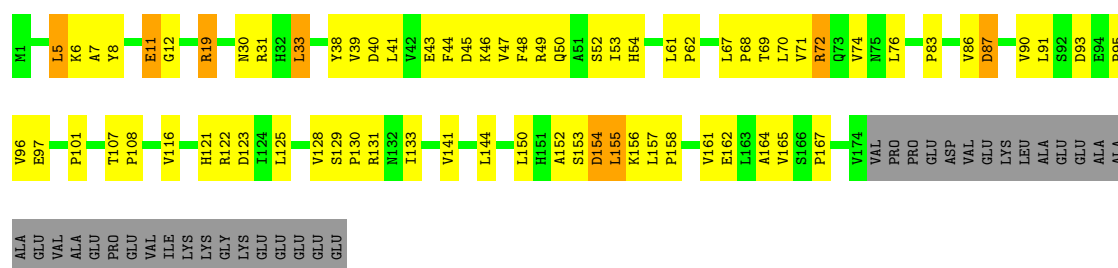
- Molecule 45: 50S Ribosomal Protein L25

Chain BZ:  48% 30% 5% 17%



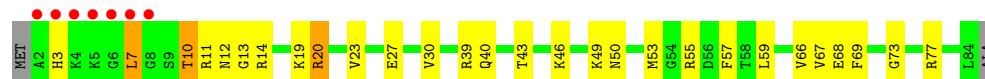
• Molecule 45: 50S Ribosomal Protein L25

Chain DZ: 50% 31% 16%



• Molecule 46: 50S Ribosomal Protein L27

Chain B0: 8% 65% 29%



• Molecule 46: 50S Ribosomal Protein L27

Chain D0: 12% 68% 24% 6%



• Molecule 47: 50S Ribosomal Protein L28

Chain B1: % 71% 21% 6%



• Molecule 47: 50S Ribosomal Protein L28

Chain D1: % 63% 30% 6%



• Molecule 48: 50S Ribosomal Protein L29

Chain B2: 



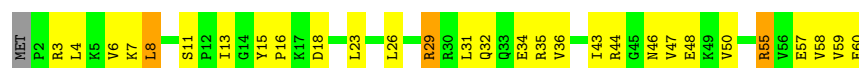
- Molecule 48: 50S Ribosomal Protein L29

Chain D2: 



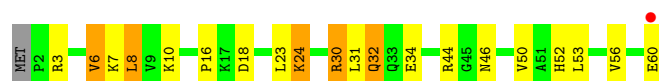
- Molecule 49: 50S Ribosomal Protein L30

Chain B3: 



- Molecule 49: 50S Ribosomal Protein L30

Chain D3: 



- Molecule 50: 50S Ribosomal Protein L31

Chain B4: 



- Molecule 50: 50S Ribosomal Protein L31

Chain D4: 



- Molecule 51: 50S Ribosomal Protein L32

Chain B5: 



- Molecule 51: 50S Ribosomal Protein L32

Chain D5: 



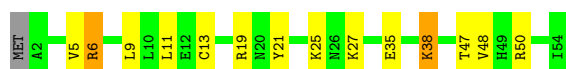
• Molecule 52: 50S Ribosomal Protein L33

Chain B6: 67% 22% 9%



• Molecule 52: 50S Ribosomal Protein L33

Chain D6: 72% 22%



• Molecule 53: 50S Ribosomal Protein L34

Chain B7: 76% 18%



• Molecule 53: 50S Ribosomal Protein L34

Chain D7: 2% 63% 35%



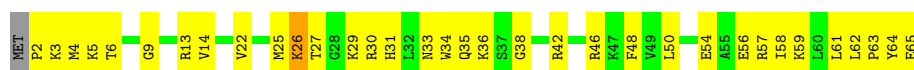
• Molecule 54: 50S Ribosomal Protein L35

Chain B8: 57% 42%



• Molecule 54: 50S Ribosomal Protein L35

Chain D8: 46% 51%

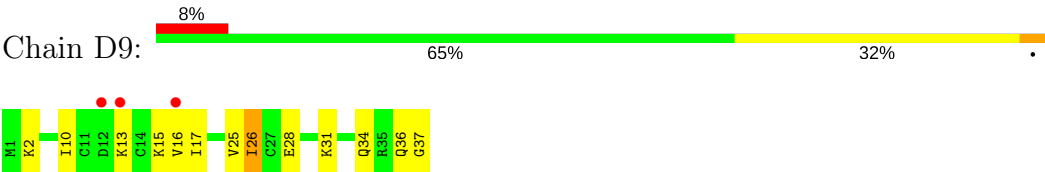


• Molecule 55: 50S Ribosomal Protein L36

Chain B9: 81% 19%



• 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, $\alpha$ , $\beta$ , $\gamma$	209.68Å 450.64Å 622.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.10 49.68 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.68-3.10) 98.2 (49.68-3.10)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.25	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.203 , 0.260 0.206 , 0.259	Depositor DCC
$R_{free}$ test set	51894 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	286321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, K, 2QZ, ZN, 2QY, MVA, 004, FME, 2R3, SF4, 2R1

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	0.75	2/36038 (0.0%)	1.31	240/56244 (0.4%)
1	CA	0.75	10/36170 (0.0%)	1.36	314/56452 (0.6%)
2	AB	0.49	0/1881	0.77	1/2542 (0.0%)
2	CB	0.54	0/1860	0.79	1/2518 (0.0%)
3	AC	0.47	0/1576	0.65	0/2130
3	CC	0.51	0/1566	0.71	2/2119 (0.1%)
4	AD	0.49	0/1689	0.73	0/2267
4	CD	0.49	0/1704	0.70	1/2284 (0.0%)
5	AE	0.47	0/1145	0.70	0/1543
5	CE	0.50	0/1149	0.71	0/1548
6	AF	0.47	0/819	0.69	0/1111
6	CF	0.52	0/829	0.74	1/1123 (0.1%)
7	AG	0.48	0/1250	0.67	1/1679 (0.1%)
7	CG	0.50	0/1254	0.71	1/1683 (0.1%)
8	AH	0.45	0/1108	0.66	0/1494
8	CH	0.48	0/1108	0.69	0/1494
9	AI	0.46	0/1002	0.72	0/1346
9	CI	0.56	0/997	0.75	1/1343 (0.1%)
10	AJ	0.47	0/722	0.68	0/982
10	CJ	0.51	0/727	0.68	0/988
11	AK	0.44	0/844	0.62	0/1145
11	CK	0.46	0/848	0.66	0/1149
12	AL	0.52	0/946	0.69	0/1274
12	CL	0.51	0/946	0.73	0/1274
13	AM	0.46	0/969	0.69	0/1302
13	CM	0.49	0/961	0.66	0/1291
14	AN	0.51	0/501	0.67	0/664
14	CN	0.54	0/501	0.68	0/664
15	AO	0.47	0/739	0.72	0/985
15	CO	0.46	0/739	0.73	0/985
16	AP	0.45	0/697	0.71	0/939
16	CP	0.47	0/693	0.65	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.48	0/836	0.66	0/1117
17	CQ	0.49	0/836	0.68	0/1117
18	AR	0.49	0/560	0.72	0/746
18	CR	0.51	0/560	0.75	1/746 (0.1%)
19	AS	0.47	0/667	0.68	0/900
19	CS	0.54	0/661	0.82	2/893 (0.2%)
20	AT	0.51	0/730	0.76	0/965
20	CT	0.44	0/729	0.68	0/965
21	AU	0.45	0/203	0.65	0/266
21	CU	0.51	0/203	0.68	0/266
22	AV	0.94	0/127	1.36	2/198 (1.0%)
22	CV	0.86	0/126	1.29	0/195
23	AX	0.85	5/1813 (0.3%)	1.59	36/2825 (1.3%)
23	CX	0.88	4/1813 (0.2%)	1.81	40/2825 (1.4%)
24	AW	0.50	0/20	0.80	0/23
24	CW	0.43	0/20	0.70	0/23
25	BA	1.06	33/65892 (0.1%)	1.42	649/102850 (0.6%)
25	DA	0.79	9/65466 (0.0%)	1.39	590/102184 (0.6%)
26	BB	0.82	0/2878	1.26	11/4490 (0.2%)
26	DB	0.89	0/2878	1.39	18/4490 (0.4%)
27	BD	0.67	1/2186 (0.0%)	0.78	1/2944 (0.0%)
27	DD	0.61	2/2186 (0.1%)	0.77	1/2944 (0.0%)
28	BE	0.69	0/1592	0.75	0/2149
28	DE	0.55	0/1592	0.77	1/2149 (0.0%)
29	BF	0.69	0/1619	0.76	0/2193
29	DF	0.53	0/1615	0.77	1/2188 (0.0%)
30	BG	0.46	0/1450	0.70	0/1959
30	DG	0.55	0/1449	0.74	0/1958
31	BH	0.60	0/1356	0.70	0/1834
31	DH	0.56	0/1356	0.70	0/1834
32	BI	0.49	0/1100	0.74	1/1501 (0.1%)
32	DI	0.48	0/1076	0.77	0/1471
33	BN	0.65	0/1144	0.73	0/1543
33	DN	0.50	0/1144	0.72	0/1543
34	BO	0.65	0/943	0.73	1/1269 (0.1%)
34	DO	0.54	0/943	0.73	1/1269 (0.1%)
35	BP	0.62	0/1152	0.77	0/1533
35	DP	0.53	0/1152	0.80	1/1533 (0.1%)
36	BQ	0.64	0/1143	0.76	0/1527
36	DQ	0.60	0/1143	0.79	0/1527
37	BR	0.59	0/982	0.78	0/1312
37	DR	0.49	0/982	0.71	0/1312
38	BS	0.54	0/887	0.77	0/1180



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DS	0.47	0/880	0.72	0/1172
39	BT	0.59	0/1105	0.79	1/1477 (0.1%)
39	DT	0.50	0/1097	0.72	0/1468
40	BU	0.71	1/977 (0.1%)	0.73	0/1301
40	DU	0.54	0/977	0.71	1/1301 (0.1%)
41	BV	0.68	0/782	0.74	1/1049 (0.1%)
41	DV	0.55	0/782	0.71	0/1049
42	BW	0.74	0/897	0.74	0/1205
42	DW	0.56	0/897	0.72	0/1205
43	BX	0.66	0/764	0.96	3/1025 (0.3%)
43	DX	0.55	0/764	0.75	1/1025 (0.1%)
44	BY	0.64	0/819	0.78	0/1095
44	DY	0.54	0/819	0.74	0/1095
45	BZ	0.56	0/1379	0.75	0/1873
45	DZ	0.53	0/1390	0.71	0/1890
46	B0	0.63	0/662	0.81	2/881 (0.2%)
46	D0	0.54	0/662	0.73	0/881
47	B1	0.61	0/762	0.74	0/1014
47	D1	0.51	0/762	0.75	1/1014 (0.1%)
48	B2	0.61	0/590	0.79	0/781
48	D2	0.48	0/590	0.66	0/781
49	B3	0.70	0/474	0.76	0/635
49	D3	0.45	0/469	0.67	0/630
50	B4	0.58	0/564	0.79	0/759
50	D4	0.59	0/544	0.86	1/735 (0.1%)
51	B5	0.66	0/469	0.78	0/635
51	D5	0.53	0/469	0.74	1/635 (0.2%)
52	B6	0.67	0/460	0.64	0/613
52	D6	0.53	0/456	0.70	0/608
53	B7	0.79	0/426	0.78	0/561
53	D7	0.62	0/426	0.76	1/561 (0.2%)
54	B8	0.70	0/519	0.71	0/684
54	D8	0.55	0/525	0.75	0/691
55	B9	0.69	0/310	0.76	0/407
55	D9	0.60	0/310	0.79	0/407
All	All	0.79	67/305966 (0.0%)	1.24	1933/457396 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	3
4	CD	0	1
7	AG	0	1
23	CX	1	0
24	AW	0	1
24	CW	0	1
27	DD	0	1
38	BS	0	1
45	BZ	0	1
50	B4	0	1
All	All	1	11

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AX	76	A	N7-C5	-11.16	1.32	1.39
1	CA	1154	G	C6-N1	-11.02	1.31	1.39
1	CA	1154	G	N1-C2	-10.69	1.29	1.37
25	BA	1188	A	N9-C4	-10.29	1.31	1.37
1	CA	1119	C	N3-C4	-10.20	1.26	1.33

The worst 5 of 1933 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CX	76	A	O4'-C1'-N9	38.71	139.17	108.20
1	CA	1119	C	N1-C2-O2	32.56	138.44	118.90
1	CA	1154	G	C5-C6-O6	28.63	145.78	128.60
1	CA	1154	G	N3-C2-N2	25.05	137.43	119.90
1	CA	1154	G	N1-C2-N2	-22.71	95.76	116.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	CX	76	A	C1'

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
24	AW	4	PRO	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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32196	0	16251	809	0
1	CA	32312	0	16307	915	0
2	AB	1846	0	1867	109	0
2	CB	1825	0	1828	119	0
3	AC	1552	0	1546	59	0
3	CC	1542	0	1517	66	0
4	AD	1659	0	1676	99	0
4	CD	1674	0	1714	78	0
5	AE	1129	0	1185	50	0
5	CE	1133	0	1191	45	0
6	AF	806	0	793	33	0
6	CF	816	0	808	27	0
7	AG	1231	0	1238	35	0
7	CG	1235	0	1249	56	0
8	AH	1088	0	1126	48	0
8	CH	1088	0	1126	46	0
9	AI	983	0	986	54	0
9	CI	978	0	966	57	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	47	0
11	AK	829	0	825	19	0
11	CK	833	0	836	29	0
12	AL	930	0	980	28	0
12	CL	930	0	980	34	0
13	AM	958	0	1002	25	0
13	CM	950	0	988	56	0
14	AN	492	0	529	26	0
14	CN	492	0	529	29	0
15	AO	728	0	760	16	0
15	CO	728	0	760	27	0
16	AP	681	0	697	29	0
16	CP	677	0	686	28	0
17	AQ	823	0	891	21	0
17	CQ	823	0	891	19	0
18	AR	555	0	618	17	0
18	CR	555	0	618	27	0
19	AS	652	0	662	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	646	0	644	56	0
20	AT	728	0	798	30	0
20	CT	727	0	796	28	0
21	AU	199	0	208	5	0
21	CU	199	0	208	7	0
22	AV	114	0	54	0	0
22	CV	113	0	54	0	0
23	AX	1623	0	823	18	0
23	CX	1623	0	824	24	0
24	AW	93	0	84	9	0
24	CW	93	0	84	14	0
25	BA	58834	0	29667	785	0
25	DA	58458	0	29482	1100	0
26	BB	2573	0	1306	38	0
26	DB	2573	0	1306	54	0
27	BD	2136	0	2218	64	0
27	DD	2136	0	2218	74	0
28	BE	1559	0	1618	38	0
28	DE	1559	0	1618	60	0
29	BF	1584	0	1625	46	0
29	DF	1580	0	1619	69	0
30	BG	1425	0	1443	45	0
30	DG	1424	0	1434	82	0
31	BH	1330	0	1407	33	0
31	DH	1330	0	1407	52	0
32	BI	1085	0	1114	42	0
32	DI	1061	0	1080	31	0
33	BN	1117	0	1183	17	0
33	DN	1117	0	1184	26	0
34	BO	933	0	996	24	0
34	DO	933	0	996	36	0
35	BP	1135	0	1212	37	0
35	DP	1135	0	1211	46	0
36	BQ	1122	0	1179	38	0
36	DQ	1122	0	1179	47	0
37	BR	968	0	1033	24	0
37	DR	968	0	1032	30	0
38	BS	877	0	938	25	0
38	DS	870	0	923	47	0
39	BT	1091	0	1151	28	0
39	DT	1083	0	1136	36	0
40	BU	959	0	1019	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DU	959	0	1019	37	0
41	BV	771	0	830	11	0
41	DV	771	0	830	23	0
42	BW	886	0	940	9	0
42	DW	886	0	940	17	0
43	BX	750	0	814	20	0
43	DX	750	0	814	25	0
44	BY	806	0	881	25	0
44	DY	806	0	881	21	0
45	BZ	1349	0	1355	47	0
45	DZ	1360	0	1363	48	0
46	B0	653	0	674	25	0
46	D0	653	0	674	23	0
47	B1	755	0	826	19	0
47	D1	755	0	826	26	0
48	B2	588	0	643	18	0
48	D2	588	0	643	20	0
49	B3	469	0	518	17	0
49	D3	464	0	514	12	0
50	B4	551	0	532	38	0
50	D4	531	0	502	32	0
51	B5	455	0	465	13	0
51	D5	455	0	465	11	0
52	B6	453	0	473	10	0
52	D6	449	0	469	10	0
53	B7	418	0	466	9	0
53	D7	418	0	467	9	0
54	B8	511	0	571	27	0
54	D8	517	0	582	27	0
55	B9	307	0	335	5	0
55	D9	307	0	335	10	0
56	AA	221	0	0	0	0
56	AD	1	0	0	0	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	2	0	0	0	0
56	AV	1	0	0	0	0
56	AX	9	0	0	0	0
56	B0	4	0	0	0	0
56	B1	1	0	0	0	0
56	B2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B3	3	0	0	0	0
56	B4	1	0	0	0	0
56	B5	1	0	0	0	0
56	B7	4	0	0	0	0
56	B8	3	0	0	0	0
56	B9	1	0	0	0	0
56	BA	738	0	0	0	0
56	BB	18	0	0	0	0
56	BD	12	0	0	0	0
56	BE	10	0	0	0	0
56	BF	8	0	0	0	0
56	BG	4	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	4	0	0	0	0
56	BU	8	0	0	0	0
56	BV	4	0	0	0	0
56	BW	5	0	0	0	0
56	BX	1	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	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CQ	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	3	0	0	0	0
56	D0	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	2	0	0	0	0
56	D8	1	0	0	0	0
56	DA	653	0	0	0	0
56	DB	12	0	0	0	0
56	DD	8	0	0	0	0
56	DE	6	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	1	0	0	0	0
56	DQ	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DR	2	0	0	0	0
56	DV	4	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	1	0
57	CD	8	0	0	1	0
58	AN	1	0	0	0	0
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
58	B6	1	0	0	0	0
58	B9	1	0	0	0	0
58	BY	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D5	1	0	0	0	0
58	D6	1	0	0	0	0
58	D9	1	0	0	0	0
58	DY	1	0	0	0	0
59	AX	10	0	10	0	0
59	CX	10	0	10	2	0
60	BA	1	0	0	0	0
60	DA	1	0	0	0	0
61	AA	148	0	0	27	0
61	AD	1	0	0	0	0
61	AE	3	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	1	0	0	0	0
61	AP	1	0	0	0	0
61	AU	1	0	0	0	0
61	AV	1	0	0	0	0
61	AX	1	0	0	0	0
61	B0	4	0	0	0	0
61	B1	2	0	0	0	0
61	B5	3	0	0	1	0
61	B7	1	0	0	1	0
61	B8	8	0	0	1	0
61	BA	1092	0	0	113	0
61	BB	26	0	0	0	0
61	BD	8	0	0	1	0
61	BE	9	0	0	4	0
61	BF	4	0	0	0	0
61	BG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BN	3	0	0	0	0
61	BO	2	0	0	0	0
61	BP	15	0	0	3	0
61	BQ	3	0	0	1	0
61	BR	1	0	0	0	0
61	BT	1	0	0	0	0
61	BU	4	0	0	0	0
61	BV	2	0	0	0	0
61	BW	2	0	0	0	0
61	BX	4	0	0	1	0
61	CA	187	0	0	24	0
61	CE	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CX	2	0	0	0	0
61	D0	5	0	0	1	0
61	D1	1	0	0	0	0
61	D7	2	0	0	0	0
61	D8	4	0	0	0	0
61	DA	902	0	0	120	0
61	DB	7	0	0	0	0
61	DD	8	0	0	0	0
61	DE	13	0	0	1	0
61	DF	5	0	0	0	0
61	DO	1	0	0	0	0
61	DP	14	0	0	0	0
61	DQ	3	0	0	1	0
61	DU	4	0	0	0	0
61	DV	1	0	0	0	0
61	DX	2	0	0	0	0
61	DY	2	0	0	0	0
All	All	286321	0	191126	6372	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 14.

The worst 5 of 6372 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1002:G:H1	1:CA:1038:C:N4	1.42	1.16
1:AA:348:G:H2'	1:AA:349:A:H5'	1.36	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1125:U:N3	1:AA:1127:G:N7	2.06	1.03
39:BT:16:ARG:NH2	39:BT:83:ILE:O	1.92	1.02
2:CB:185:ILE:HG22	2:CB:199:TYR:HB2	1.40	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%)	200 (87%)	23 (10%)	6 (3%)	6	31
2	CB	229/256 (90%)	201 (88%)	18 (8%)	10 (4%)	3	18
3	AC	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	12	45
3	CC	204/239 (85%)	178 (87%)	24 (12%)	2 (1%)	18	57
4	AD	206/209 (99%)	182 (88%)	22 (11%)	2 (1%)	18	57
4	CD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	12	45
5	AE	146/162 (90%)	127 (87%)	15 (10%)	4 (3%)	6	30
5	CE	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	8	36
6	AF	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
6	CF	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
7	AG	153/156 (98%)	137 (90%)	14 (9%)	2 (1%)	14	48
7	CG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	25	64
8	AH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	25	64
9	AI	125/128 (98%)	111 (89%)	10 (8%)	4 (3%)	5	25
9	CI	125/128 (98%)	112 (90%)	11 (9%)	2 (2%)	11	43
10	AJ	95/105 (90%)	85 (90%)	7 (7%)	3 (3%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CJ	94/105 (90%)	86 (92%)	7 (7%)	1 (1%)	17	54
11	AK	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	20	60
11	CK	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	20	60
12	AL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
12	CL	120/132 (91%)	112 (93%)	8 (7%)	0	100	100
13	AM	121/126 (96%)	106 (88%)	15 (12%)	0	100	100
13	CM	120/126 (95%)	104 (87%)	14 (12%)	2 (2%)	11	42
14	AN	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	CO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	15	51
16	AP	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
16	CP	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
17	AQ	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	12	45
18	CR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	12	45
19	AS	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
19	CS	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
20	AT	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2	14
20	CT	94/106 (89%)	85 (90%)	3 (3%)	6 (6%)	1	9
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	1 (5%)	2 (10%)	1	4
24	AW	3/10 (30%)	1 (33%)	0	2 (67%)	0	0
24	CW	3/10 (30%)	1 (33%)	1 (33%)	1 (33%)	0	0
27	BD	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	38	75
27	DD	273/276 (99%)	257 (94%)	13 (5%)	3 (1%)	17	54
28	BE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	32	71
28	DE	202/206 (98%)	194 (96%)	6 (3%)	2 (1%)	18	57
29	BF	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	32	71
29	DF	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	18	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BG	179/182 (98%)	163 (91%)	13 (7%)	3 (2%)	11	42
30	DG	179/182 (98%)	160 (89%)	13 (7%)	6 (3%)	4	24
31	BH	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	28	67
31	DH	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	15	51
32	BI	144/148 (97%)	122 (85%)	17 (12%)	5 (4%)	4	23
32	DI	144/148 (97%)	123 (85%)	17 (12%)	4 (3%)	6	29
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
33	DN	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	25	64
34	BO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	22	62
34	DO	120/122 (98%)	117 (98%)	2 (2%)	1 (1%)	22	62
35	BP	147/150 (98%)	132 (90%)	14 (10%)	1 (1%)	25	64
35	DP	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	13	47
36	BQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	25	64
36	DQ	139/141 (99%)	129 (93%)	8 (6%)	2 (1%)	13	47
37	BR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	20	60
37	DR	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
38	BS	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	20	60
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	20	60
39	BT	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	22	62
39	DT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
41	BV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	18	57
41	DV	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	18	57
42	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
42	DW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
43	BX	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	17	54
43	DX	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
44	BY	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
44	DY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
45	BZ	169/206 (82%)	150 (89%)	17 (10%)	2 (1%)	15	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DZ	172/206 (84%)	157 (91%)	15 (9%)	0	100	100
46	B0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	15	51
46	D0	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
47	B1	95/98 (97%)	93 (98%)	0	2 (2%)	8	36
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	17	54
48	B2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
48	D2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
49	B3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
49	D3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	B4	67/71 (94%)	50 (75%)	9 (13%)	8 (12%)	0	2
50	D4	67/71 (94%)	50 (75%)	8 (12%)	9 (13%)	0	1
51	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
52	D6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
53	B7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	8	35
54	B8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	D8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11415/12148 (94%)	10525 (92%)	749 (7%)	141 (1%)	15	51

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	17	PHE
2	AB	125	PRO
3	AC	65	ALA
3	AC	107	GLN
4	AD	166	LYS

### 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%)	147 (77%)	45 (23%)	1	3
2	CB	187/220 (85%)	152 (81%)	35 (19%)	2	8
3	AC	143/188 (76%)	125 (87%)	18 (13%)	5	22
3	CC	140/188 (74%)	122 (87%)	18 (13%)	5	21
4	AD	170/181 (94%)	145 (85%)	25 (15%)	3	16
4	CD	173/181 (96%)	152 (88%)	21 (12%)	6	24
5	AE	113/123 (92%)	104 (92%)	9 (8%)	14	47
5	CE	114/123 (93%)	107 (94%)	7 (6%)	22	58
6	AF	83/90 (92%)	76 (92%)	7 (8%)	13	44
6	CF	85/90 (94%)	79 (93%)	6 (7%)	17	52
7	AG	119/127 (94%)	100 (84%)	19 (16%)	3	12
7	CG	120/127 (94%)	102 (85%)	18 (15%)	3	15
8	AH	114/119 (96%)	98 (86%)	16 (14%)	4	18
8	CH	114/119 (96%)	102 (90%)	12 (10%)	8	31
9	AI	90/99 (91%)	76 (84%)	14 (16%)	3	13
9	CI	89/99 (90%)	75 (84%)	14 (16%)	3	13
10	AJ	66/92 (72%)	60 (91%)	6 (9%)	11	39
10	CJ	69/92 (75%)	64 (93%)	5 (7%)	17	51
11	AK	82/99 (83%)	73 (89%)	9 (11%)	7	30
11	CK	83/99 (84%)	77 (93%)	6 (7%)	17	51
12	AL	97/109 (89%)	90 (93%)	7 (7%)	17	51
12	CL	97/109 (89%)	87 (90%)	10 (10%)	8	32
13	AM	93/101 (92%)	82 (88%)	11 (12%)	6	25
13	CM	92/101 (91%)	80 (87%)	12 (13%)	5	21
14	AN	49/50 (98%)	41 (84%)	8 (16%)	3	12
14	CN	49/50 (98%)	42 (86%)	7 (14%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	78/80 (98%)	69 (88%)	9 (12%)	6	27
15	CO	78/80 (98%)	66 (85%)	12 (15%)	3	14
16	AP	69/74 (93%)	60 (87%)	9 (13%)	5	21
16	CP	68/74 (92%)	63 (93%)	5 (7%)	16	49
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	26	63
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	16	49
18	AR	59/77 (77%)	55 (93%)	4 (7%)	18	53
18	CR	59/77 (77%)	52 (88%)	7 (12%)	6	25
19	AS	69/80 (86%)	63 (91%)	6 (9%)	12	43
19	CS	67/80 (84%)	57 (85%)	10 (15%)	3	15
20	AT	70/82 (85%)	61 (87%)	9 (13%)	5	21
20	CT	70/82 (85%)	60 (86%)	10 (14%)	4	17
21	AU	18/22 (82%)	14 (78%)	4 (22%)	1	4
21	CU	18/22 (82%)	16 (89%)	2 (11%)	7	29
24	AW	3/3 (100%)	2 (67%)	1 (33%)	0	0
24	CW	3/3 (100%)	2 (67%)	1 (33%)	0	0
27	BD	215/218 (99%)	198 (92%)	17 (8%)	14	47
27	DD	215/218 (99%)	190 (88%)	25 (12%)	6	26
28	BE	164/166 (99%)	142 (87%)	22 (13%)	4	19
28	DE	164/166 (99%)	144 (88%)	20 (12%)	6	23
29	BF	160/166 (96%)	143 (89%)	17 (11%)	8	30
29	DF	159/166 (96%)	145 (91%)	14 (9%)	12	42
30	BG	143/156 (92%)	123 (86%)	20 (14%)	4	18
30	DG	142/156 (91%)	116 (82%)	26 (18%)	2	9
31	BH	144/148 (97%)	129 (90%)	15 (10%)	8	31
31	DH	144/148 (97%)	131 (91%)	13 (9%)	11	40
32	BI	110/124 (89%)	82 (74%)	28 (26%)	0	2
32	DI	104/124 (84%)	86 (83%)	18 (17%)	2	10
33	BN	118/119 (99%)	103 (87%)	15 (13%)	5	21
33	DN	118/119 (99%)	102 (86%)	16 (14%)	4	19
34	BO	100/100 (100%)	94 (94%)	6 (6%)	22	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DO	100/100 (100%)	91 (91%)	9 (9%)	11	40
35	BP	115/116 (99%)	102 (89%)	13 (11%)	7	28
35	DP	115/116 (99%)	104 (90%)	11 (10%)	10	36
36	BQ	111/111 (100%)	94 (85%)	17 (15%)	3	14
36	DQ	111/111 (100%)	96 (86%)	15 (14%)	4	19
37	BR	101/101 (100%)	83 (82%)	18 (18%)	2	9
37	DR	101/101 (100%)	85 (84%)	16 (16%)	3	13
38	BS	87/88 (99%)	77 (88%)	10 (12%)	6	27
38	DS	85/88 (97%)	70 (82%)	15 (18%)	2	10
39	BT	115/127 (91%)	104 (90%)	11 (10%)	10	36
39	DT	113/127 (89%)	105 (93%)	8 (7%)	17	52
40	BU	93/94 (99%)	83 (89%)	10 (11%)	7	30
40	DU	93/94 (99%)	82 (88%)	11 (12%)	6	25
41	BV	80/82 (98%)	69 (86%)	11 (14%)	4	19
41	DV	80/82 (98%)	71 (89%)	9 (11%)	7	28
42	BW	90/92 (98%)	79 (88%)	11 (12%)	6	23
42	DW	90/92 (98%)	80 (89%)	10 (11%)	7	29
43	BX	77/78 (99%)	73 (95%)	4 (5%)	27	63
43	DX	77/78 (99%)	74 (96%)	3 (4%)	37	73
44	BY	85/91 (93%)	79 (93%)	6 (7%)	17	52
44	DY	85/91 (93%)	79 (93%)	6 (7%)	17	52
45	BZ	145/179 (81%)	121 (83%)	24 (17%)	2	11
45	DZ	145/179 (81%)	126 (87%)	19 (13%)	5	20
46	B0	65/67 (97%)	61 (94%)	4 (6%)	21	57
46	D0	65/67 (97%)	59 (91%)	6 (9%)	11	39
47	B1	80/83 (96%)	72 (90%)	8 (10%)	9	33
47	D1	80/83 (96%)	73 (91%)	7 (9%)	12	42
48	B2	65/67 (97%)	56 (86%)	9 (14%)	4	19
48	D2	65/67 (97%)	57 (88%)	8 (12%)	5	23
49	B3	51/52 (98%)	44 (86%)	7 (14%)	4	19
49	D3	50/52 (96%)	43 (86%)	7 (14%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B4	59/63 (94%)	48 (81%)	11 (19%)	2	8
50	D4	53/63 (84%)	45 (85%)	8 (15%)	3	15
51	B5	50/52 (96%)	45 (90%)	5 (10%)	9	33
51	D5	50/52 (96%)	45 (90%)	5 (10%)	9	33
52	B6	51/52 (98%)	45 (88%)	6 (12%)	6	25
52	D6	50/52 (96%)	46 (92%)	4 (8%)	14	47
53	B7	41/42 (98%)	37 (90%)	4 (10%)	9	35
53	D7	41/42 (98%)	39 (95%)	2 (5%)	29	66
54	B8	53/55 (96%)	49 (92%)	4 (8%)	16	49
54	D8	54/55 (98%)	50 (93%)	4 (7%)	16	49
55	B9	34/34 (100%)	33 (97%)	1 (3%)	48	80
55	D9	34/34 (100%)	33 (97%)	1 (3%)	48	80
All	All	9325/10072 (93%)	8209 (88%)	1116 (12%)	6	24

5 of 1116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BZ	87	ASP
3	CC	154	SER
42	DW	51	LEU
46	B0	55	ARG
53	B7	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
44	BY	43	ASN
3	CC	28	GLN
37	DR	71	GLN
45	BZ	32	HIS
49	B3	32	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1522 (98%)	393 (26%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CA	1501/1522 (98%)	388 (25%)	0
22	AV	4/24 (16%)	1 (25%)	0
22	CV	4/24 (16%)	1 (25%)	0
23	AX	75/77 (97%)	16 (21%)	0
23	CX	75/77 (97%)	16 (21%)	0
25	BA	2721/2915 (93%)	508 (18%)	0
25	DA	2704/2915 (92%)	535 (19%)	0
26	BB	119/122 (97%)	18 (15%)	0
26	DB	119/122 (97%)	24 (20%)	0
All	All	8817/9320 (94%)	1900 (21%)	0

5 of 1900 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	22	G
1	AA	32	A

There are no RNA pucker outliers to report.

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

14 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	$\# Z  > 2$
24	2QZ	AW	1	24	7,8,9	1.61	1 (14%)	4,10,12	5.47	1 (25%)
24	2QY	AW	10	24	13,13,14	2.66	2 (15%)	12,16,18	2.16	3 (25%)
24	004	AW	3	24	8,10,11	0.67	0	11,12,14	1.35	1 (9%)
24	MVA	AW	5	24	7,7,8	1.34	1 (14%)	7,8,10	1.63	1 (14%)
24	2R1	AW	6	24	10,10,11	1.76	3 (30%)	7,13,15	5.12	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	2R3	AW	8	24	14,14,15	0.81	0	16,18,20	1.56	5 (31%)
24	MVA	AW	9	24	7,7,8	1.21	1 (14%)	7,8,10	1.46	2 (28%)
24	2QZ	CW	1	24	7,8,9	1.17	1 (14%)	4,10,12	4.75	1 (25%)
24	2QY	CW	10	24	13,13,14	2.79	3 (23%)	12,16,18	1.54	1 (8%)
24	004	CW	3	24	8,10,11	1.07	1 (12%)	11,12,14	1.32	2 (18%)
24	MVA	CW	5	24	7,7,8	1.15	1 (14%)	7,8,10	1.44	1 (14%)
24	2R1	CW	6	24	10,10,11	1.83	2 (20%)	7,13,15	4.02	2 (28%)
24	2R3	CW	8	24	14,14,15	0.75	0	16,18,20	1.57	4 (25%)
24	MVA	CW	9	24	7,7,8	1.44	2 (28%)	7,8,10	1.80	3 (42%)

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
24	2QZ	AW	1	24	-	0/6/10/12	0/0/0/0
24	2QY	AW	10	24	-	0/3/8/10	0/1/1/1
24	004	AW	3	24	-	0/4/6/8	0/1/1/1
24	MVA	AW	5	24	-	1/5/8/10	0/0/0/0
24	2R1	AW	6	24	-	0/1/14/16	0/0/1/1
24	2R3	AW	8	24	-	0/10/12/14	0/1/1/1
24	MVA	AW	9	24	-	0/5/8/10	0/0/0/0
24	2QZ	CW	1	24	-	0/6/10/12	0/0/0/0
24	2QY	CW	10	24	-	0/3/8/10	0/1/1/1
24	004	CW	3	24	-	0/4/6/8	0/1/1/1
24	MVA	CW	5	24	-	0/5/8/10	0/0/0/0
24	2R1	CW	6	24	-	0/1/14/16	0/0/1/1
24	2R3	CW	8	24	-	0/10/12/14	0/1/1/1
24	MVA	CW	9	24	-	0/5/8/10	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CW	3	004	CB-CA	-2.87	1.49	1.52
24	AW	6	2R1	C-CA	2.14	1.48	1.45
24	CW	9	MVA	CB-CA	2.21	1.58	1.54
24	AW	6	2R1	OD1-CG1	2.31	1.55	1.43
24	CW	5	MVA	CA-C	2.55	1.53	1.50

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AW	6	2R1	OD2-CG2-CB	-12.42	88.98	112.09
24	CW	6	2R1	OD2-CG2-CB	-10.01	93.46	112.09
24	AW	10	2QY	O-C-CA	-5.68	118.21	125.47
24	CW	10	2QY	O-C-CA	-4.90	119.21	125.47
24	AW	6	2R1	CG2-CB-CA	-3.71	118.45	123.52

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AW	5	MVA	CB-CA-N-CN

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AW	1	2QZ	2	0
24	AW	10	2QY	5	0
24	AW	3	004	1	0
24	AW	6	2R1	1	0
24	AW	8	2R3	1	0
24	AW	9	MVA	3	0
24	CW	1	2QZ	2	0
24	CW	10	2QY	9	0
24	CW	3	004	1	0
24	CW	5	MVA	2	0
24	CW	6	2R1	1	0
24	CW	8	2R3	2	0
24	CW	9	MVA	6	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1991 ligands modelled in this entry, 1987 are monoatomic - leaving 4 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	SF4	AD	501	4	0,12,12	0.00	-	0,24,24	0.00	-
59	FME	AX	101	23	9,9,10	1.50	1 (11%)	7,9,11	1.36	1 (14%)
57	SF4	CD	501	4	0,12,12	0.00	-	0,24,24	0.00	-
59	FME	CX	101	23	9,9,10	1.42	2 (22%)	7,9,11	1.27	1 (14%)

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	SF4	AD	501	4	-	0/0/48/48	0/6/5/5
59	FME	AX	101	23	-	1/6/9/11	0/0/0/0
57	SF4	CD	501	4	-	0/0/48/48	0/6/5/5
59	FME	CX	101	23	-	1/6/9/11	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CX	101	FME	CA-N	2.06	1.49	1.46
59	CX	101	FME	CA-C	3.15	1.54	1.50
59	AX	101	FME	CA-C	3.72	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AX	101	FME	CA-N-CN	-2.85	118.44	122.82
59	CX	101	FME	CA-N-CN	-2.17	119.49	122.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	CX	101	FME	O1-CN-N-CA
59	AX	101	FME	O1-CN-N-CA

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AD	501	SF4	1	0
57	CD	501	SF4	1	0
59	CX	101	FME	2	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	1498/1522 (98%)	-0.17	32 (2%) 64 43	36, 80, 103, 123	0
1	CA	1503/1522 (98%)	-0.18	34 (2%) 61 39	38, 80, 103, 122	0
2	AB	231/256 (90%)	-0.08	7 (3%) 51 27	71, 88, 98, 107	0
2	CB	231/256 (90%)	0.21	12 (5%) 28 12	71, 89, 99, 108	0
3	AC	206/239 (86%)	0.18	6 (2%) 52 28	74, 87, 96, 108	0
3	CC	206/239 (86%)	0.33	13 (6%) 21 8	75, 89, 98, 106	0
4	AD	208/209 (99%)	0.06	4 (1%) 67 46	62, 80, 92, 99	0
4	CD	208/209 (99%)	-0.15	0 100 100	61, 79, 92, 99	0
5	AE	148/162 (91%)	-0.26	0 100 100	53, 73, 83, 96	0
5	CE	148/162 (91%)	-0.22	0 100 100	54, 74, 85, 98	0
6	AF	100/101 (99%)	-0.23	0 100 100	60, 78, 89, 92	0
6	CF	100/101 (99%)	-0.32	0 100 100	62, 79, 89, 94	0
7	AG	155/156 (99%)	0.28	11 (7%) 17 6	74, 85, 97, 104	0
7	CG	155/156 (99%)	0.35	11 (7%) 17 6	76, 86, 99, 105	0
8	AH	137/138 (99%)	-0.07	0 100 100	60, 75, 83, 90	0
8	CH	137/138 (99%)	-0.15	0 100 100	61, 76, 83, 90	0
9	AI	127/128 (99%)	0.44	8 (6%) 21 8	70, 92, 99, 103	0
9	CI	127/128 (99%)	0.98	22 (17%) 2 1	69, 93, 100, 105	0
10	AJ	97/105 (92%)	0.65	12 (12%) 4 2	71, 93, 101, 106	0
10	CJ	96/105 (91%)	0.68	12 (12%) 4 2	75, 95, 102, 107	0
11	AK	114/129 (88%)	-0.23	0 100 100	53, 74, 88, 93	0
11	CK	114/129 (88%)	-0.03	3 (2%) 56 33	54, 76, 88, 93	0
12	AL	122/132 (92%)	-0.18	1 (0%) 86 71	56, 68, 80, 86	0
12	CL	122/132 (92%)	-0.18	0 100 100	55, 68, 79, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	123/126 (97%)	0.29	9 (7%) 16 6	67, 83, 95, 104	0
13	CM	122/126 (96%)	0.58	11 (9%) 10 4	77, 91, 101, 105	0
14	AN	60/61 (98%)	0.17	2 (3%) 47 24	74, 85, 95, 97	0
14	CN	60/61 (98%)	0.54	4 (6%) 19 7	77, 88, 95, 100	0
15	AO	88/89 (98%)	-0.23	0 100 100	59, 73, 87, 94	0
15	CO	88/89 (98%)	0.04	1 (1%) 80 65	58, 73, 87, 95	0
16	AP	82/88 (93%)	0.40	2 (2%) 59 37	66, 77, 88, 95	0
16	CP	82/88 (93%)	-0.02	0 100 100	66, 76, 89, 93	0
17	AQ	99/105 (94%)	0.03	0 100 100	59, 73, 84, 87	0
17	CQ	99/105 (94%)	-0.08	1 (1%) 82 67	60, 73, 84, 85	0
18	AR	68/88 (77%)	0.15	1 (1%) 74 54	66, 76, 86, 90	0
18	CR	68/88 (77%)	0.39	0 100 100	67, 77, 87, 89	0
19	AS	83/93 (89%)	0.79	11 (13%) 4 1	79, 91, 100, 105	0
19	CS	83/93 (89%)	1.23	16 (19%) 1 0	82, 92, 102, 106	0
20	AT	96/106 (90%)	0.07	0 100 100	62, 75, 88, 91	0
20	CT	96/106 (90%)	0.09	1 (1%) 82 67	62, 75, 86, 94	0
21	AU	23/27 (85%)	1.21	5 (21%) 1 0	76, 87, 90, 91	0
21	CU	23/27 (85%)	1.17	6 (26%) 1 0	77, 87, 91, 92	0
22	AV	7/24 (29%)	0.03	0 100 100	61, 73, 97, 100	0
22	CV	6/24 (25%)	0.36	0 100 100	64, 75, 94, 103	0
23	AX	76/77 (98%)	0.02	0 100 100	48, 79, 96, 101	0
23	CX	76/77 (98%)	0.02	0 100 100	47, 81, 98, 101	0
24	AW	3/10 (30%)	0.01	0 100 100	78, 78, 93, 96	0
24	CW	3/10 (30%)	0.56	1 (33%) 0 0	67, 67, 87, 96	0
25	BA	2731/2915 (93%)	-0.28	11 (0%) 92 84	24, 44, 86, 114	0
25	DA	2714/2915 (93%)	-0.49	19 (0%) 87 75	27, 48, 87, 118	0
26	BB	120/122 (98%)	-0.40	0 100 100	41, 68, 81, 96	0
26	DB	120/122 (98%)	-0.33	0 100 100	47, 73, 86, 98	0
27	BD	275/276 (99%)	-0.47	1 (0%) 92 84	24, 41, 62, 85	0
27	DD	275/276 (99%)	-0.47	0 100 100	25, 44, 63, 86	0
28	BE	204/206 (99%)	-0.35	0 100 100	22, 45, 68, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DE	204/206 (99%)	-0.45	0 100 100	24, 47, 70, 90	0
29	BF	203/210 (96%)	-0.33	0 100 100	24, 53, 77, 97	0
29	DF	203/210 (96%)	-0.46	0 100 100	25, 56, 79, 96	0
30	BG	181/182 (99%)	-0.30	2 (1%) 80 65	61, 76, 89, 100	0
30	DG	181/182 (99%)	0.09	6 (3%) 47 24	65, 79, 91, 100	0
31	BH	174/180 (96%)	-0.32	0 100 100	49, 67, 81, 85	0
31	DH	174/180 (96%)	0.52	17 (9%) 8 3	54, 72, 85, 89	0
32	BI	146/148 (98%)	-0.16	0 100 100	49, 77, 88, 94	0
32	DI	146/148 (98%)	0.13	5 (3%) 46 23	49, 78, 88, 94	0
33	BN	140/140 (100%)	-0.37	0 100 100	33, 48, 71, 78	0
33	DN	140/140 (100%)	-0.43	0 100 100	35, 52, 73, 81	0
34	BO	122/122 (100%)	-0.50	0 100 100	23, 40, 61, 76	0
34	DO	122/122 (100%)	-0.47	0 100 100	37, 53, 71, 80	0
35	BP	149/150 (99%)	-0.32	0 100 100	25, 54, 77, 83	0
35	DP	149/150 (99%)	-0.07	1 (0%) 87 75	27, 57, 81, 87	0
36	BQ	141/141 (100%)	-0.34	0 100 100	36, 52, 68, 79	0
36	DQ	141/141 (100%)	-0.45	0 100 100	38, 55, 71, 81	0
37	BR	118/118 (100%)	-0.50	0 100 100	20, 35, 52, 64	0
37	DR	118/118 (100%)	-0.40	0 100 100	36, 52, 68, 84	0
38	BS	110/112 (98%)	-0.43	0 100 100	35, 54, 71, 85	0
38	DS	110/112 (98%)	0.27	5 (4%) 34 16	65, 81, 92, 95	0
39	BT	131/146 (89%)	-0.48	0 100 100	31, 45, 75, 92	0
39	DT	131/146 (89%)	-0.45	0 100 100	45, 59, 80, 90	0
40	BU	116/118 (98%)	-0.64	0 100 100	21, 31, 52, 63	0
40	DU	116/118 (98%)	-0.34	1 (0%) 84 69	36, 61, 78, 92	0
41	BV	101/101 (100%)	-0.42	0 100 100	27, 53, 73, 80	0
41	DV	101/101 (100%)	-0.19	0 100 100	29, 58, 78, 80	0
42	BW	112/113 (99%)	-0.43	0 100 100	27, 38, 62, 92	0
42	DW	112/113 (99%)	-0.26	0 100 100	30, 42, 64, 94	0
43	BX	95/96 (98%)	-0.37	0 100 100	29, 47, 72, 81	0
43	DX	95/96 (98%)	-0.29	2 (2%) 64 43	33, 51, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BY	107/110 (97%)	-0.19	2 (1%) 67 46	39, 61, 80, 89	0
44	DY	107/110 (97%)	0.27	4 (3%) 42 21	43, 65, 82, 92	0
45	BZ	171/206 (83%)	-0.38	0 100 100	53, 71, 85, 96	0
45	DZ	174/206 (84%)	-0.07	0 100 100	58, 74, 87, 95	0
46	B0	83/85 (97%)	-0.08	7 (8%) 12 4	25, 39, 80, 108	0
46	D0	83/85 (97%)	0.41	10 (12%) 5 2	42, 66, 86, 104	0
47	B1	97/98 (98%)	-0.27	1 (1%) 82 67	27, 44, 74, 83	0
47	D1	97/98 (98%)	-0.23	1 (1%) 82 67	35, 58, 79, 86	0
48	B2	70/72 (97%)	-0.54	0 100 100	35, 48, 64, 90	0
48	D2	70/72 (97%)	-0.27	0 100 100	59, 74, 83, 92	0
49	B3	59/60 (98%)	-0.36	0 100 100	24, 38, 63, 85	0
49	D3	59/60 (98%)	0.19	1 (1%) 70 49	45, 62, 80, 90	0
50	B4	69/71 (97%)	-0.17	1 (1%) 75 57	60, 85, 103, 105	0
50	D4	69/71 (97%)	0.37	5 (7%) 16 6	82, 96, 106, 112	0
51	B5	59/60 (98%)	-0.60	0 100 100	14, 36, 59, 74	0
51	D5	59/60 (98%)	-0.54	0 100 100	31, 50, 72, 82	0
52	B6	53/54 (98%)	-0.27	0 100 100	43, 53, 68, 75	0
52	D6	53/54 (98%)	-0.26	0 100 100	45, 56, 69, 73	0
53	B7	48/49 (97%)	-0.30	0 100 100	24, 32, 62, 84	0
53	D7	48/49 (97%)	-0.15	1 (2%) 64 43	26, 35, 63, 86	0
54	B8	64/65 (98%)	-0.30	0 100 100	31, 42, 51, 64	0
54	D8	64/65 (98%)	-0.30	0 100 100	34, 46, 56, 66	0
55	B9	37/37 (100%)	0.06	0 100 100	43, 53, 71, 77	0
55	D9	37/37 (100%)	0.63	3 (8%) 13 5	46, 58, 73, 78	0
All	All	20462/21468 (95%)	-0.18	365 (1%) 69 47	14, 65, 95, 123	0

The worst 5 of 365 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	15.2
13	CM	123	ALA	12.7
13	AM	124	PRO	9.8
13	AM	123	ALA	9.6
46	B0	3	HIS	8.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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
24	2R3	CW	8	14/15	0.96	0.11	-	47,70,74,79	0
24	MVA	CW	5	8/9	0.94	0.20	-	51,78,86,88	0
24	MVA	AW	9	8/9	0.93	0.24	-	65,78,87,91	0
24	2QZ	AW	1	9/10	0.95	0.22	-	58,64,81,82	0
24	MVA	CW	9	8/9	0.92	0.21	-	61,72,80,84	0
24	2QY	AW	10	13/14	0.97	0.14	-	55,67,75,79	0
24	2R1	AW	6	10/11	0.90	0.12	-	68,82,98,104	0
24	2R3	AW	8	14/15	0.95	0.15	-	54,79,87,90	0
24	MVA	AW	5	8/9	0.93	0.19	-	66,87,90,90	0
24	2QZ	CW	1	9/10	0.95	0.24	-	57,72,81,93	0
24	004	CW	3	10/11	0.94	0.15	-	60,76,84,86	0
24	2R1	CW	6	10/11	0.94	0.11	-	79,86,90,94	0
24	2QY	CW	10	13/14	0.91	0.14	-	55,69,84,94	0
24	004	AW	3	10/11	0.82	0.13	-	71,89,99,106	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(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3581	1/1	0.71	0.86	126.13	73,73,73,73	0
56	MG	BA	3014	1/1	0.95	0.76	83.86	34,34,34,34	0
56	MG	AA	3011	1/1	0.91	1.19	73.14	55,55,55,55	0
56	MG	BA	3634	1/1	0.98	0.70	72.21	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	DA	3092	1/1	0.88	0.61	62.70	39,39,39,39	0
56	MG	BA	3223	1/1	0.96	0.68	61.58	47,47,47,47	0
56	MG	BA	3038	1/1	0.91	0.60	56.20	51,51,51,51	0
56	MG	BA	3042	1/1	0.95	0.76	55.48	47,47,47,47	0
56	MG	BA	3196	1/1	0.92	0.76	49.64	56,56,56,56	0
56	MG	BA	3297	1/1	0.73	1.46	48.81	53,53,53,53	0
56	MG	DF	301	1/1	0.91	0.51	43.16	32,32,32,32	0
56	MG	DD	306	1/1	0.95	1.14	42.96	44,44,44,44	0
56	MG	BA	3607	1/1	0.96	0.43	40.74	53,53,53,53	0
56	MG	CA	3007	1/1	0.82	0.56	39.00	68,68,68,68	0
56	MG	BA	3160	1/1	0.78	0.64	38.61	53,53,53,53	0
56	MG	BA	3187	1/1	0.91	0.64	36.94	50,50,50,50	0
56	MG	DA	3112	1/1	0.86	0.43	32.14	54,54,54,54	0
56	MG	BP	201	1/1	0.95	0.66	32.11	40,40,40,40	0
56	MG	CA	3053	1/1	0.61	1.18	30.79	73,73,73,73	0
56	MG	B8	101	1/1	0.93	0.46	30.44	49,49,49,49	0
56	MG	DA	3018	1/1	0.89	0.47	28.91	48,48,48,48	0
56	MG	BA	3150	1/1	0.98	0.45	28.65	34,34,34,34	0
56	MG	AA	3060	1/1	0.93	0.53	26.72	60,60,60,60	0
56	MG	D5	102	1/1	0.95	0.58	26.27	55,55,55,55	0
56	MG	DA	3639	1/1	0.96	0.30	26.18	15,15,15,15	0
56	MG	BA	3024	1/1	0.90	0.40	25.71	35,35,35,35	0
56	MG	CA	3042	1/1	0.57	0.55	24.99	85,85,85,85	0
56	MG	BU	208	1/1	0.95	0.88	22.96	56,56,56,56	0
56	MG	DA	3011	1/1	0.75	0.38	22.52	45,45,45,45	0
56	MG	BV	203	1/1	0.95	1.03	22.44	46,46,46,46	0
56	MG	DA	3643	1/1	0.92	0.72	22.16	53,53,53,53	0
56	MG	DA	3016	1/1	0.94	0.27	21.38	37,37,37,37	0
56	MG	BA	3034	1/1	0.96	0.41	21.31	52,52,52,52	0
56	MG	DA	3178	1/1	0.96	0.37	20.98	43,43,43,43	0
56	MG	DA	3197	1/1	0.95	0.45	20.76	36,36,36,36	0
56	MG	DA	3615	1/1	0.78	0.40	20.59	60,60,60,60	0
56	MG	BA	3664	1/1	0.89	0.26	20.17	68,68,68,68	0
56	MG	B7	103	1/1	0.90	0.85	19.81	48,48,48,48	0
56	MG	BP	203	1/1	0.97	0.70	19.23	29,29,29,29	0
56	MG	BF	301	1/1	0.97	0.52	19.13	45,45,45,45	0
56	MG	DV	203	1/1	0.86	0.74	19.12	54,54,54,54	0
56	MG	AA	3008	1/1	0.93	0.42	18.92	54,54,54,54	0
56	MG	BA	3727	1/1	0.87	0.66	18.44	68,68,68,68	0
56	MG	DA	3079	1/1	0.87	0.27	17.87	37,37,37,37	0
56	MG	BA	3199	1/1	0.96	0.46	17.87	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	DA	3173	1/1	0.97	0.41	17.87	39,39,39,39	0
56	MG	DF	305	1/1	0.94	0.73	17.84	39,39,39,39	0
56	MG	AA	3180	1/1	0.90	0.38	17.72	66,66,66,66	0
56	MG	DD	305	1/1	0.94	0.64	17.69	49,49,49,49	0
56	MG	AA	3159	1/1	0.99	0.32	17.67	57,57,57,57	0
56	MG	BA	3230	1/1	0.89	0.47	17.62	46,46,46,46	0
56	MG	AA	3107	1/1	0.96	0.31	17.57	44,44,44,44	0
56	MG	DA	3279	1/1	0.82	0.31	17.57	63,63,63,63	0
56	MG	BA	3047	1/1	0.90	0.41	17.35	47,47,47,47	0
56	MG	AA	3038	1/1	0.82	0.35	17.33	66,66,66,66	0
56	MG	DD	307	1/1	0.85	0.61	17.21	38,38,38,38	0
56	MG	BE	301	1/1	0.96	0.56	17.10	43,43,43,43	0
56	MG	BV	202	1/1	0.95	0.44	16.55	56,56,56,56	0
56	MG	BA	3041	1/1	0.96	0.37	16.12	32,32,32,32	0
56	MG	BA	3026	1/1	0.97	0.47	15.86	36,36,36,36	0
56	MG	BA	3622	1/1	0.65	0.52	15.82	77,77,77,77	0
56	MG	BD	306	1/1	0.93	0.45	15.77	46,46,46,46	0
56	MG	CA	3135	1/1	0.70	0.56	15.36	76,76,76,76	0
56	MG	DA	3624	1/1	0.90	0.40	15.34	51,51,51,51	0
56	MG	AA	3082	1/1	0.92	0.24	15.29	39,39,39,39	0
56	MG	DA	3056	1/1	0.76	0.38	15.24	43,43,43,43	0
56	MG	BA	3155	1/1	0.81	0.38	15.14	57,57,57,57	0
56	MG	BE	305	1/1	0.90	0.70	14.86	42,42,42,42	0
56	MG	AA	3209	1/1	0.94	0.40	14.82	70,70,70,70	0
56	MG	CA	3152	1/1	0.92	0.38	14.77	55,55,55,55	0
56	MG	BA	3739	1/1	0.82	0.77	14.57	50,50,50,50	0
56	MG	BA	3493	1/1	0.98	0.37	14.53	15,15,15,15	0
56	MG	AA	3208	1/1	0.97	0.34	14.18	46,46,46,46	0
56	MG	AA	3010	1/1	0.95	0.37	14.08	70,70,70,70	0
59	FME	CX	101	10/11	0.70	0.57	14.05	71,82,97,105	0
56	MG	AA	3108	1/1	0.96	0.46	13.89	67,67,67,67	0
56	MG	BA	3726	1/1	0.96	0.55	13.75	47,47,47,47	0
56	MG	BA	3227	1/1	0.98	0.31	13.48	32,32,32,32	0
56	MG	AA	3050	1/1	0.88	0.50	13.34	63,63,63,63	0
56	MG	BA	3184	1/1	0.97	0.38	13.23	49,49,49,49	0
56	MG	BR	201	1/1	0.98	0.60	12.92	51,51,51,51	0
56	MG	BA	3153	1/1	0.93	0.32	12.85	35,35,35,35	0
56	MG	BA	3145	1/1	0.95	0.40	12.78	38,38,38,38	0
56	MG	DA	3473	1/1	0.98	0.31	12.78	32,32,32,32	0
56	MG	BA	3211	1/1	0.94	0.29	12.63	38,38,38,38	0
56	MG	BA	3637	1/1	0.96	0.35	12.58	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3176	1/1	0.97	0.27	12.50	39,39,39,39	0
56	MG	BA	3614	1/1	0.99	0.42	12.48	30,30,30,30	0
56	MG	DA	3553	1/1	0.86	0.36	12.37	70,70,70,70	0
56	MG	BN	3005	1/1	0.95	0.84	12.28	52,52,52,52	0
56	MG	AA	3019	1/1	0.89	0.39	12.21	74,74,74,74	0
56	MG	BA	3060	1/1	0.93	0.40	12.17	40,40,40,40	0
56	MG	DA	3100	1/1	0.94	0.50	12.08	56,56,56,56	0
56	MG	DA	3033	1/1	0.91	0.25	12.07	39,39,39,39	0
56	MG	DV	202	1/1	0.85	0.84	11.94	63,63,63,63	0
56	MG	BD	302	1/1	0.96	0.36	11.84	58,58,58,58	0
56	MG	DA	3461	1/1	0.90	0.21	11.83	41,41,41,41	0
56	MG	BA	3133	1/1	0.93	0.27	11.78	32,32,32,32	0
56	MG	DA	3401	1/1	0.91	0.29	11.52	58,58,58,58	0
56	MG	AA	3120	1/1	0.77	0.63	11.52	71,71,71,71	0
56	MG	DA	3116	1/1	0.92	0.31	11.51	39,39,39,39	0
56	MG	BN	3001	1/1	0.91	0.76	11.50	54,54,54,54	0
56	MG	AA	3071	1/1	0.79	0.29	11.43	60,60,60,60	0
56	MG	DA	3039	1/1	0.96	0.40	11.17	59,59,59,59	0
56	MG	AA	3190	1/1	0.92	0.33	10.92	67,67,67,67	0
56	MG	BA	3729	1/1	0.97	0.40	10.80	46,46,46,46	0
56	MG	B3	103	1/1	0.93	0.63	10.79	41,41,41,41	0
56	MG	DA	3432	1/1	0.96	0.27	10.77	66,66,66,66	0
56	MG	BA	3524	1/1	0.96	0.25	10.69	55,55,55,55	0
56	MG	BU	206	1/1	0.76	0.38	10.59	60,60,60,60	0
56	MG	AA	3160	1/1	0.97	0.30	10.59	52,52,52,52	0
56	MG	DA	3265	1/1	0.96	0.27	10.41	51,51,51,51	0
56	MG	BF	303	1/1	0.99	0.27	10.29	36,36,36,36	0
56	MG	BA	3503	1/1	0.96	0.28	10.23	31,31,31,31	0
56	MG	AA	3109	1/1	0.94	0.33	10.15	65,65,65,65	0
56	MG	AA	3084	1/1	0.70	0.36	10.11	78,78,78,78	0
56	MG	BA	3033	1/1	0.97	0.37	10.09	35,35,35,35	0
59	FME	AX	101	10/11	0.86	0.44	10.03	48,75,97,113	0
56	MG	DA	3097	1/1	0.92	0.22	9.94	61,61,61,61	0
56	MG	DE	301	1/1	0.96	0.62	9.92	51,51,51,51	0
56	MG	DA	3651	1/1	0.92	0.60	9.90	52,52,52,52	0
56	MG	AA	3035	1/1	0.76	0.42	9.79	71,71,71,71	0
56	MG	DA	3191	1/1	0.89	0.44	9.59	47,47,47,47	0
56	MG	DA	3171	1/1	0.87	0.25	9.54	39,39,39,39	0
56	MG	AA	3033	1/1	0.88	0.38	9.43	64,64,64,64	0
56	MG	BA	3139	1/1	0.90	0.25	9.23	51,51,51,51	0
56	MG	AA	3168	1/1	0.95	0.31	9.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3045	1/1	0.88	0.29	9.12	34,34,34,34	0
56	MG	DA	3298	1/1	0.95	0.32	9.11	37,37,37,37	0
56	MG	BA	3530	1/1	0.97	0.28	8.98	31,31,31,31	0
56	MG	CA	3170	1/1	0.89	0.48	8.94	50,50,50,50	0
56	MG	CA	3043	1/1	0.97	0.34	8.89	49,49,49,49	0
56	MG	BR	204	1/1	0.92	0.62	8.83	43,43,43,43	0
56	MG	BA	3435	1/1	0.97	0.23	8.68	24,24,24,24	0
56	MG	BA	3197	1/1	0.89	0.30	8.54	39,39,39,39	0
56	MG	BA	3086	1/1	0.94	0.33	8.51	49,49,49,49	0
56	MG	BA	3025	1/1	0.96	0.25	8.50	28,28,28,28	0
56	MG	DA	3577	1/1	0.96	0.25	8.31	44,44,44,44	0
56	MG	DA	3479	1/1	0.94	0.19	8.27	57,57,57,57	0
56	MG	BA	3057	1/1	0.94	0.27	8.22	35,35,35,35	0
56	MG	BA	3192	1/1	0.88	0.48	8.13	58,58,58,58	0
56	MG	DA	3215	1/1	0.98	0.30	8.10	29,29,29,29	0
56	MG	BA	3222	1/1	0.98	0.29	7.99	25,25,25,25	0
56	MG	BA	3732	1/1	0.99	0.52	7.98	61,61,61,61	0
56	MG	AA	3088	1/1	0.77	0.33	7.88	63,63,63,63	0
56	MG	BA	3671	1/1	0.90	0.33	7.87	57,57,57,57	0
56	MG	DA	3469	1/1	0.94	0.22	7.85	47,47,47,47	0
56	MG	DA	3440	1/1	0.90	0.32	7.75	33,33,33,33	0
56	MG	BA	3576	1/1	0.95	0.26	7.61	23,23,23,23	0
56	MG	CA	3032	1/1	0.83	0.20	7.60	42,42,42,42	0
56	MG	CA	3114	1/1	0.82	0.26	7.41	82,82,82,82	0
56	MG	DA	3609	1/1	0.84	0.35	7.23	64,64,64,64	0
56	MG	BA	3546	1/1	0.94	0.31	7.19	48,48,48,48	0
56	MG	DA	3099	1/1	0.86	0.27	7.18	44,44,44,44	0
56	MG	BF	305	1/1	0.97	0.32	7.15	35,35,35,35	0
56	MG	BA	3550	1/1	0.97	0.24	7.13	45,45,45,45	0
56	MG	BD	308	1/1	0.97	0.32	7.11	23,23,23,23	0
56	MG	DA	3170	1/1	0.92	0.81	6.92	57,57,57,57	0
56	MG	AA	3031	1/1	0.89	0.21	6.81	41,41,41,41	0
56	MG	BW	204	1/1	0.96	0.35	6.78	35,35,35,35	0
56	MG	DB	3007	1/1	0.80	0.27	6.70	45,45,45,45	0
56	MG	BB	3003	1/1	0.82	0.24	6.66	43,43,43,43	0
56	MG	BN	3004	1/1	0.98	0.40	6.59	66,66,66,66	0
56	MG	BD	310	1/1	0.98	0.32	6.59	48,48,48,48	0
56	MG	BA	3441	1/1	0.95	0.25	6.58	25,25,25,25	0
56	MG	BA	3048	1/1	0.90	0.23	6.43	31,31,31,31	0
56	MG	DA	3295	1/1	0.92	0.24	6.29	39,39,39,39	0
56	MG	AA	3064	1/1	0.95	0.30	6.22	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3451	1/1	0.97	0.30	6.22	28,28,28,28	0
56	MG	DA	3407	1/1	0.95	0.24	6.20	21,21,21,21	0
56	MG	DD	301	1/1	0.95	0.32	6.19	46,46,46,46	0
56	MG	BA	3416	1/1	0.99	0.25	6.17	42,42,42,42	0
56	MG	DA	3264	1/1	0.90	0.32	6.12	49,49,49,49	0
56	MG	BA	3642	1/1	0.96	0.24	6.10	51,51,51,51	0
56	MG	DA	3094	1/1	0.96	0.18	6.05	26,26,26,26	0
56	MG	DA	3608	1/1	0.98	0.28	6.04	57,57,57,57	0
56	MG	DA	3346	1/1	0.99	0.23	6.02	29,29,29,29	0
56	MG	DA	3326	1/1	0.93	0.20	5.96	33,33,33,33	0
56	MG	BU	203	1/1	0.98	0.35	5.96	33,33,33,33	0
56	MG	AA	3039	1/1	0.89	0.24	5.94	60,60,60,60	0
56	MG	DA	3272	1/1	0.99	0.28	5.92	27,27,27,27	0
56	MG	DA	3266	1/1	0.96	0.23	5.90	43,43,43,43	0
56	MG	DA	3324	1/1	0.99	0.23	5.89	40,40,40,40	0
56	MG	BA	3277	1/1	0.86	0.37	5.79	45,45,45,45	0
56	MG	DA	3627	1/1	0.93	0.21	5.66	43,43,43,43	0
56	MG	AA	3095	1/1	0.93	0.24	5.65	58,58,58,58	0
56	MG	BQ	205	1/1	0.94	0.42	5.63	49,49,49,49	0
56	MG	CA	3099	1/1	0.93	0.33	5.62	65,65,65,65	0
56	MG	BA	3200	1/1	0.99	0.27	5.61	25,25,25,25	0
56	MG	BA	3630	1/1	0.96	0.25	5.61	52,52,52,52	0
56	MG	DA	3364	1/1	0.94	0.19	5.55	32,32,32,32	0
56	MG	DA	3070	1/1	0.86	0.27	5.53	44,44,44,44	0
56	MG	BU	202	1/1	0.95	0.36	5.51	32,32,32,32	0
56	MG	BA	3328	1/1	0.92	0.21	5.36	42,42,42,42	0
56	MG	DA	3142	1/1	0.96	0.24	5.34	33,33,33,33	0
56	MG	BA	3548	1/1	0.95	0.22	5.34	50,50,50,50	0
56	MG	DA	3335	1/1	0.97	0.26	5.26	38,38,38,38	0
56	MG	BV	201	1/1	0.96	0.39	5.21	53,53,53,53	0
56	MG	CA	3098	1/1	0.98	0.23	5.21	46,46,46,46	0
56	MG	BA	3459	1/1	0.98	0.22	5.14	31,31,31,31	0
56	MG	BA	3203	1/1	0.97	0.26	5.12	32,32,32,32	0
56	MG	DA	3236	1/1	0.98	0.17	5.08	46,46,46,46	0
56	MG	DA	3641	1/1	0.96	0.43	5.02	61,61,61,61	0
56	MG	BA	3178	1/1	0.94	0.28	4.98	48,48,48,48	0
56	MG	DA	3035	1/1	0.98	0.23	4.98	56,56,56,56	0
56	MG	BA	3353	1/1	0.95	0.24	4.91	57,57,57,57	0
56	MG	BA	3402	1/1	0.82	0.25	4.87	71,71,71,71	0
56	MG	DA	3312	1/1	0.99	0.27	4.83	43,43,43,43	0
56	MG	AA	3179	1/1	0.98	0.26	4.83	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BQ	202	1/1	0.94	0.30	4.79	28,28,28,28	0
56	MG	DA	3554	1/1	0.92	0.19	4.72	70,70,70,70	0
56	MG	BN	3003	1/1	0.89	0.39	4.71	59,59,59,59	0
56	MG	BX	3001	1/1	0.93	0.29	4.69	55,55,55,55	0
56	MG	AA	3145	1/1	0.94	0.25	4.68	63,63,63,63	0
56	MG	DA	3025	1/1	0.98	0.38	4.63	44,44,44,44	0
56	MG	BA	3552	1/1	0.97	0.23	4.59	29,29,29,29	0
56	MG	BA	3356	1/1	0.89	0.27	4.48	56,56,56,56	0
56	MG	BA	3193	1/1	0.93	0.57	4.46	52,52,52,52	0
56	MG	BA	3228	1/1	0.98	0.27	4.45	63,63,63,63	0
56	MG	BA	3370	1/1	0.81	0.19	4.44	54,54,54,54	0
56	MG	BA	3504	1/1	0.96	0.29	4.43	41,41,41,41	0
56	MG	BA	3512	1/1	0.96	0.23	4.38	40,40,40,40	0
56	MG	CA	3162	1/1	0.91	0.21	4.37	46,46,46,46	0
56	MG	BU	205	1/1	0.84	0.33	4.34	42,42,42,42	0
56	MG	DA	3535	1/1	0.95	0.19	4.31	33,33,33,33	0
56	MG	BA	3703	1/1	0.72	0.22	4.27	31,31,31,31	0
56	MG	DA	3631	1/1	0.83	0.17	4.26	56,56,56,56	0
56	MG	BA	3624	1/1	0.85	0.25	4.15	52,52,52,52	0
56	MG	BA	3117	1/1	0.96	0.24	4.11	25,25,25,25	0
56	MG	BQ	201	1/1	0.98	0.43	4.09	61,61,61,61	0
56	MG	BD	305	1/1	0.94	0.23	4.07	48,48,48,48	0
56	MG	BA	3346	1/1	0.88	0.23	4.06	37,37,37,37	0
56	MG	DA	3164	1/1	0.94	0.26	4.03	48,48,48,48	0
56	MG	DA	3026	1/1	0.98	0.21	4.01	37,37,37,37	0
56	MG	DA	3306	1/1	0.95	0.21	4.00	33,33,33,33	0
56	MG	BA	3560	1/1	0.90	0.20	3.99	61,61,61,61	0
56	MG	BA	3304	1/1	0.94	0.19	3.98	49,49,49,49	0
56	MG	BA	3124	1/1	0.94	0.23	3.93	39,39,39,39	0
56	MG	BB	3008	1/1	0.87	0.21	3.93	35,35,35,35	0
56	MG	BA	3079	1/1	0.94	0.28	3.91	42,42,42,42	0
56	MG	DA	3637	1/1	0.96	0.28	3.90	48,48,48,48	0
56	MG	DF	304	1/1	0.90	0.28	3.88	44,44,44,44	0
56	MG	BA	3480	1/1	0.98	0.20	3.84	17,17,17,17	0
56	MG	DA	3408	1/1	0.98	0.22	3.82	37,37,37,37	0
56	MG	DA	3476	1/1	0.98	0.21	3.80	45,45,45,45	0
56	MG	DA	3620	1/1	0.90	0.19	3.76	71,71,71,71	0
56	MG	BA	3557	1/1	0.98	0.23	3.75	31,31,31,31	0
56	MG	DA	3633	1/1	0.96	0.20	3.72	54,54,54,54	0
56	MG	DA	3078	1/1	0.88	0.17	3.70	44,44,44,44	0
56	MG	BA	3682	1/1	0.97	0.22	3.68	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	BA	3601	1/1	0.93	0.28	3.67	64,64,64,64	0
56	MG	BA	3379	1/1	0.97	0.22	3.65	22,22,22,22	0
56	MG	BA	3093	1/1	0.96	0.22	3.59	25,25,25,25	0
56	MG	BA	3640	1/1	0.93	0.25	3.58	60,60,60,60	0
56	MG	DA	3006	1/1	0.92	0.16	3.53	42,42,42,42	0
56	MG	DA	3347	1/1	0.94	0.19	3.50	62,62,62,62	0
56	MG	BA	3128	1/1	0.99	0.27	3.47	40,40,40,40	0
56	MG	BA	3036	1/1	0.98	0.18	3.47	38,38,38,38	0
56	MG	CA	3072	1/1	0.96	0.22	3.47	38,38,38,38	0
56	MG	DA	3114	1/1	0.94	0.19	3.42	37,37,37,37	0
56	MG	BN	3002	1/1	0.88	0.30	3.40	56,56,56,56	0
56	MG	DA	3628	1/1	0.96	0.22	3.36	63,63,63,63	0
56	MG	CE	3001	1/1	0.81	0.33	3.35	68,68,68,68	0
56	MG	BA	3737	1/1	0.96	0.25	3.32	60,60,60,60	0
56	MG	BA	3689	1/1	0.91	0.23	3.25	39,39,39,39	0
56	MG	DA	3302	1/1	0.97	0.18	3.22	22,22,22,22	0
56	MG	DA	3450	1/1	0.93	0.16	3.20	43,43,43,43	0
56	MG	BA	3343	1/1	0.96	0.19	3.20	40,40,40,40	0
56	MG	DQ	205	1/1	0.82	0.40	3.18	55,55,55,55	0
56	MG	BA	3368	1/1	0.96	0.19	3.18	35,35,35,35	0
56	MG	BA	3544	1/1	0.98	0.23	3.17	27,27,27,27	0
56	MG	BA	3147	1/1	0.89	0.24	3.17	46,46,46,46	0
56	MG	CT	3001	1/1	0.90	0.43	3.15	57,57,57,57	0
56	MG	BA	3311	1/1	0.97	0.23	3.15	42,42,42,42	0
56	MG	AA	3024	1/1	0.92	0.18	3.11	53,53,53,53	0
56	MG	CA	3001	1/1	0.99	0.21	3.10	55,55,55,55	0
56	MG	DA	3424	1/1	0.93	0.20	3.07	30,30,30,30	0
56	MG	BA	3264	1/1	0.98	0.17	3.06	30,30,30,30	0
56	MG	BA	3431	1/1	0.94	0.23	3.06	17,17,17,17	0
56	MG	DA	3379	1/1	0.99	0.22	3.04	28,28,28,28	0
56	MG	DA	3649	1/1	0.98	0.24	3.02	24,24,24,24	0
56	MG	BA	3414	1/1	0.99	0.21	3.00	19,19,19,19	0
56	MG	AA	3072	1/1	0.92	0.26	2.93	79,79,79,79	0
56	MG	DA	3065	1/1	0.85	0.18	2.89	38,38,38,38	0
56	MG	DA	3638	1/1	0.89	0.30	2.86	62,62,62,62	0
56	MG	BA	3545	1/1	0.95	0.24	2.85	47,47,47,47	0
56	MG	DA	3653	1/1	0.91	0.35	2.82	60,60,60,60	0
56	MG	BF	302	1/1	0.91	0.31	2.79	46,46,46,46	0
56	MG	DV	201	1/1	0.96	0.38	2.76	55,55,55,55	0
56	MG	DA	3397	1/1	0.96	0.18	2.72	41,41,41,41	0
56	MG	BA	3299	1/1	0.93	0.23	2.72	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3525	1/1	0.98	0.23	2.72	43,43,43,43	0
56	MG	DA	3262	1/1	0.97	0.22	2.71	44,44,44,44	0
56	MG	CA	3061	1/1	0.94	0.30	2.67	46,46,46,46	0
56	MG	DA	3002	1/1	0.93	0.19	2.63	55,55,55,55	0
56	MG	DA	3395	1/1	0.98	0.21	2.63	34,34,34,34	0
56	MG	DA	3261	1/1	0.95	0.22	2.61	35,35,35,35	0
56	MG	BA	3349	1/1	0.97	0.26	2.59	43,43,43,43	0
56	MG	BA	3037	1/1	0.95	0.20	2.55	31,31,31,31	0
56	MG	DA	3143	1/1	0.91	0.22	2.52	46,46,46,46	0
56	MG	BA	3324	1/1	0.96	0.18	2.49	36,36,36,36	0
56	MG	DA	3518	1/1	0.96	0.20	2.48	40,40,40,40	0
56	MG	DA	3148	1/1	0.91	0.23	2.43	47,47,47,47	0
56	MG	AA	3171	1/1	0.97	0.25	2.41	72,72,72,72	0
56	MG	D3	101	1/1	0.96	0.45	2.41	63,63,63,63	0
56	MG	B7	102	1/1	0.99	0.25	2.38	40,40,40,40	0
56	MG	AA	3146	1/1	0.93	0.20	2.37	48,48,48,48	0
56	MG	DA	3623	1/1	0.89	0.17	2.37	53,53,53,53	0
56	MG	CA	3119	1/1	0.91	0.23	2.30	64,64,64,64	0
56	MG	AA	3036	1/1	0.91	0.24	2.25	71,71,71,71	0
56	MG	BA	3332	1/1	0.95	0.19	2.24	39,39,39,39	0
56	MG	DA	3121	1/1	0.95	0.19	2.16	48,48,48,48	0
56	MG	BA	3720	1/1	0.97	0.20	2.15	33,33,33,33	0
56	MG	BA	3719	1/1	0.82	0.25	2.08	25,25,25,25	0
56	MG	CA	3048	1/1	0.83	0.20	2.07	62,62,62,62	0
56	MG	CA	3101	1/1	0.97	0.18	2.03	70,70,70,70	0
56	MG	CA	3027	1/1	0.88	0.17	2.03	57,57,57,57	0
56	MG	DA	3418	1/1	0.98	0.17	2.03	29,29,29,29	0
56	MG	BA	3121	1/1	0.96	0.27	2.02	57,57,57,57	0
56	MG	DA	3652	1/1	0.98	0.60	2.02	60,60,60,60	0
56	MG	DA	3414	1/1	0.93	0.17	2.00	49,49,49,49	0
56	MG	DA	3498	1/1	0.96	0.18	1.97	56,56,56,56	0
56	MG	DA	3133	1/1	0.96	0.15	1.95	33,33,33,33	0
56	MG	DA	3221	1/1	0.92	0.18	1.90	49,49,49,49	0
56	MG	BA	3125	1/1	0.90	0.20	1.89	39,39,39,39	0
56	MG	DA	3429	1/1	0.96	0.18	1.88	44,44,44,44	0
56	MG	BA	3098	1/1	0.93	0.15	1.88	35,35,35,35	0
56	MG	BB	3001	1/1	0.97	0.17	1.86	54,54,54,54	0
56	MG	DA	3595	1/1	0.95	0.18	1.81	72,72,72,72	0
56	MG	DA	3588	1/1	0.98	0.18	1.81	40,40,40,40	0
56	MG	CA	3171	1/1	0.97	0.32	1.78	67,67,67,67	0
56	MG	DA	3284	1/1	0.90	0.14	1.77	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3397	1/1	0.95	0.19	1.75	28,28,28,28	0
56	MG	BA	3393	1/1	0.98	0.18	1.72	38,38,38,38	0
56	MG	DA	3341	1/1	0.96	0.19	1.70	23,23,23,23	0
56	MG	DA	3613	1/1	0.85	0.16	1.67	54,54,54,54	0
56	MG	BA	3724	1/1	0.93	0.19	1.67	58,58,58,58	0
56	MG	BA	3185	1/1	0.94	0.20	1.64	47,47,47,47	0
56	MG	DD	304	1/1	0.97	0.22	1.59	35,35,35,35	0
56	MG	DA	3012	1/1	0.93	0.18	1.57	57,57,57,57	0
56	MG	B7	101	1/1	0.91	0.20	1.51	43,43,43,43	0
56	MG	BE	307	1/1	0.95	0.24	1.50	39,39,39,39	0
56	MG	BA	3403	1/1	0.93	0.21	1.50	41,41,41,41	0
56	MG	BA	3215	1/1	0.89	0.14	1.50	69,69,69,69	0
56	MG	AN	103	1/1	0.88	0.38	1.48	60,60,60,60	0
56	MG	DA	3579	1/1	0.93	0.17	1.46	23,23,23,23	0
56	MG	DA	3073	1/1	0.91	0.18	1.45	44,44,44,44	0
56	MG	AK	3001	1/1	0.90	0.18	1.43	45,45,45,45	0
56	MG	DA	3472	1/1	0.93	0.17	1.43	36,36,36,36	0
56	MG	AA	3054	1/1	0.94	0.20	1.42	45,45,45,45	0
56	MG	BA	3077	1/1	0.97	0.19	1.40	39,39,39,39	0
56	MG	BA	3331	1/1	0.91	0.19	1.38	47,47,47,47	0
56	MG	DA	3499	1/1	0.80	0.13	1.38	46,46,46,46	0
56	MG	BA	3162	1/1	0.97	0.19	1.37	23,23,23,23	0
56	MG	AA	3214	1/1	0.99	0.27	1.30	75,75,75,75	0
56	MG	BA	3575	1/1	0.96	0.19	1.27	51,51,51,51	0
56	MG	BA	3407	1/1	0.99	0.19	1.25	15,15,15,15	0
56	MG	DA	3017	1/1	0.95	0.16	1.20	46,46,46,46	0
56	MG	BA	3350	1/1	0.90	0.24	1.16	47,47,47,47	0
56	MG	BA	3281	1/1	0.98	0.18	1.15	52,52,52,52	0
56	MG	DA	3575	1/1	0.96	0.19	1.15	43,43,43,43	0
56	MG	BA	3359	1/1	0.96	0.20	1.15	23,23,23,23	0
56	MG	BA	3412	1/1	0.94	0.18	1.13	26,26,26,26	0
56	MG	BD	303	1/1	0.96	0.19	1.08	42,42,42,42	0
56	MG	DA	3569	1/1	0.98	0.19	0.98	37,37,37,37	0
56	MG	BA	3582	1/1	0.97	0.22	0.94	25,25,25,25	0
56	MG	BA	3009	1/1	0.85	0.17	0.93	25,25,25,25	0
56	MG	BA	3287	1/1	0.74	0.17	0.93	53,53,53,53	0
56	MG	BD	307	1/1	0.94	0.20	0.93	43,43,43,43	0
56	MG	DA	3328	1/1	0.96	0.15	0.86	28,28,28,28	0
56	MG	AA	3021	1/1	0.96	0.19	0.86	76,76,76,76	0
56	MG	BA	3039	1/1	0.92	0.14	0.82	42,42,42,42	0
56	MG	DA	3309	1/1	0.97	0.17	0.80	33,33,33,33	0
56	MG	CA	3089	1/1	0.93	0.15	0.77	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	CA	3004	1/1	0.96	0.21	0.77	96,96,96,96	0
56	MG	BA	3527	1/1	0.97	0.18	0.75	64,64,64,64	0
56	MG	BA	3249	1/1	0.86	0.24	0.72	40,40,40,40	0
56	MG	DA	3263	1/1	0.95	0.19	0.68	31,31,31,31	0
56	MG	CF	3001	1/1	0.94	0.22	0.68	55,55,55,55	0
56	MG	DA	3139	1/1	0.92	0.18	0.67	40,40,40,40	0
56	MG	DA	3219	1/1	0.90	0.17	0.66	60,60,60,60	0
56	MG	DA	3349	1/1	0.97	0.17	0.62	54,54,54,54	0
56	MG	DA	3301	1/1	0.99	0.14	0.62	45,45,45,45	0
56	MG	AA	3014	1/1	0.83	0.19	0.60	28,28,28,28	0
56	MG	AA	3103	1/1	0.98	0.19	0.59	38,38,38,38	0
56	MG	BA	3194	1/1	0.90	0.18	0.48	55,55,55,55	0
56	MG	AA	3023	1/1	0.68	0.17	0.43	65,65,65,65	0
56	MG	BA	3615	1/1	0.96	0.17	0.40	36,36,36,36	0
56	MG	CA	3124	1/1	0.94	0.17	0.40	61,61,61,61	0
56	MG	CQ	201	1/1	0.86	0.19	0.40	56,56,56,56	0
56	MG	DA	3119	1/1	0.88	0.15	0.38	44,44,44,44	0
56	MG	CA	3120	1/1	0.97	0.19	0.38	58,58,58,58	0
56	MG	AA	3219	1/1	0.91	0.20	0.38	57,57,57,57	0
56	MG	BA	3396	1/1	0.97	0.18	0.37	22,22,22,22	0
56	MG	DA	3182	1/1	0.96	0.17	0.37	32,32,32,32	0
56	MG	BE	308	1/1	0.98	0.18	0.32	52,52,52,52	0
56	MG	DA	3320	1/1	0.98	0.17	0.29	30,30,30,30	0
56	MG	BA	3108	1/1	0.92	0.14	0.27	55,55,55,55	0
56	MG	AA	3170	1/1	0.95	0.16	0.26	101,101,101,101	0
56	MG	DA	3500	1/1	0.87	0.17	0.25	50,50,50,50	0
56	MG	DA	3129	1/1	0.90	0.14	0.25	43,43,43,43	0
56	MG	DA	3110	1/1	0.88	0.14	0.23	49,49,49,49	0
56	MG	AA	3003	1/1	0.90	0.24	0.22	63,63,63,63	0
56	MG	CA	3020	1/1	0.95	0.18	0.21	47,47,47,47	0
56	MG	AX	110	1/1	0.97	0.20	0.20	42,42,42,42	0
56	MG	DA	3251	1/1	0.97	0.14	0.19	54,54,54,54	0
56	MG	DA	3398	1/1	0.88	0.15	0.17	35,35,35,35	0
56	MG	DA	3468	1/1	0.96	0.14	0.17	48,48,48,48	0
56	MG	BA	3438	1/1	0.97	0.18	0.15	30,30,30,30	0
56	MG	DA	3160	1/1	0.97	0.15	0.15	44,44,44,44	0
56	MG	BA	3734	1/1	0.97	0.26	0.13	45,45,45,45	0
56	MG	DA	3452	1/1	0.94	0.17	0.12	56,56,56,56	0
56	MG	BA	3583	1/1	0.98	0.20	0.10	27,27,27,27	0
56	MG	DA	3300	1/1	0.97	0.15	0.03	37,37,37,37	0
56	MG	DA	3555	1/1	0.95	0.12	0.02	41,41,41,41	0
56	MG	BA	3569	1/1	0.98	0.18	0.02	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3064	1/1	0.98	0.12	0.02	58,58,58,58	0
56	MG	DA	3330	1/1	0.98	0.14	0.00	37,37,37,37	0
56	MG	BA	3260	1/1	0.95	0.17	-0.01	22,22,22,22	0
56	MG	BF	306	1/1	0.97	0.18	-0.03	37,37,37,37	0
56	MG	BA	3468	1/1	0.92	0.17	-0.03	30,30,30,30	0
56	MG	DA	3297	1/1	0.96	0.14	-0.04	57,57,57,57	0
56	MG	AN	101	1/1	0.91	0.19	-0.05	63,63,63,63	0
56	MG	BA	3010	1/1	0.98	0.17	-0.05	32,32,32,32	0
56	MG	DA	3385	1/1	0.98	0.15	-0.07	35,35,35,35	0
56	MG	DA	3482	1/1	0.86	0.13	-0.07	55,55,55,55	0
56	MG	CA	3087	1/1	0.93	0.19	-0.08	41,41,41,41	0
56	MG	AA	3004	1/1	0.86	0.15	-0.10	55,55,55,55	0
56	MG	BA	3526	1/1	0.98	0.19	-0.10	19,19,19,19	0
56	MG	BA	3314	1/1	0.97	0.17	-0.10	24,24,24,24	0
56	MG	BA	3735	1/1	0.92	0.20	-0.12	45,45,45,45	0
56	MG	CA	3150	1/1	0.90	0.12	-0.15	59,59,59,59	0
56	MG	DA	3380	1/1	0.98	0.16	-0.16	26,26,26,26	0
56	MG	BA	3695	1/1	0.97	0.17	-0.16	15,15,15,15	0
56	MG	AA	3143	1/1	0.98	0.15	-0.19	45,45,45,45	0
56	MG	DA	3489	1/1	0.92	0.16	-0.20	36,36,36,36	0
56	MG	BE	303	1/1	0.86	0.17	-0.21	29,29,29,29	0
56	MG	DA	3419	1/1	0.91	0.17	-0.21	31,31,31,31	0
56	MG	DA	3654	1/1	0.94	0.17	-0.24	52,52,52,52	0
56	MG	BA	3432	1/1	0.92	0.16	-0.25	60,60,60,60	0
56	MG	DA	3391	1/1	0.90	0.14	-0.25	41,41,41,41	0
56	MG	DA	3576	1/1	0.95	0.15	-0.27	38,38,38,38	0
56	MG	DA	3040	1/1	0.92	0.10	-0.29	42,42,42,42	0
56	MG	BA	3511	1/1	0.94	0.16	-0.30	39,39,39,39	0
56	MG	BA	3003	1/1	0.97	0.16	-0.33	43,43,43,43	0
56	MG	CA	3097	1/1	0.93	0.15	-0.33	48,48,48,48	0
56	MG	DA	3394	1/1	0.98	0.14	-0.33	47,47,47,47	0
56	MG	BD	309	1/1	0.96	0.14	-0.44	42,42,42,42	0
56	MG	BA	3592	1/1	0.93	0.17	-0.47	28,28,28,28	0
56	MG	BA	3229	1/1	0.95	0.15	-0.51	22,22,22,22	0
56	MG	DA	3338	1/1	0.99	0.14	-0.51	29,29,29,29	0
56	MG	AA	3075	1/1	0.87	0.11	-0.54	52,52,52,52	0
56	MG	DA	3162	1/1	0.66	0.13	-0.54	71,71,71,71	0
56	MG	AA	3025	1/1	0.92	0.14	-0.55	69,69,69,69	0
56	MG	BA	3070	1/1	0.98	0.14	-0.57	35,35,35,35	0
56	MG	AA	3156	1/1	0.97	0.18	-0.57	62,62,62,62	0
56	MG	BA	3188	1/1	0.92	0.15	-0.59	37,37,37,37	0
56	MG	CA	3006	1/1	0.91	0.17	-0.60	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DE	306	1/1	0.95	0.14	-0.62	32,32,32,32	0
56	MG	D0	101	1/1	0.97	0.13	-0.65	63,63,63,63	0
56	MG	DA	3636	1/1	0.93	0.14	-0.65	61,61,61,61	0
56	MG	BA	3404	1/1	0.97	0.15	-0.65	35,35,35,35	0
56	MG	BA	3559	1/1	0.97	0.14	-0.67	48,48,48,48	0
56	MG	DA	3507	1/1	0.95	0.15	-0.68	54,54,54,54	0
56	MG	BB	3016	1/1	0.98	0.12	-0.72	21,21,21,21	0
56	MG	DA	3423	1/1	0.84	0.14	-0.74	29,29,29,29	0
56	MG	DA	3282	1/1	0.97	0.14	-0.75	36,36,36,36	0
56	MG	DQ	204	1/1	0.97	0.13	-0.78	43,43,43,43	0
56	MG	AA	3216	1/1	0.95	0.14	-0.81	58,58,58,58	0
58	ZN	D6	501	1/1	0.97	0.12	-0.82	61,61,61,61	0
56	MG	DA	3010	1/1	0.95	0.14	-0.89	39,39,39,39	0
56	MG	DA	3250	1/1	0.98	0.14	-0.89	31,31,31,31	0
56	MG	AA	3161	1/1	0.96	0.12	-0.90	72,72,72,72	0
57	SF4	CD	501	8/8	0.99	0.14	-0.91	64,75,91,95	0
56	MG	BA	3424	1/1	0.98	0.17	-0.93	15,15,15,15	0
58	ZN	CN	501	1/1	0.93	0.12	-0.95	108,108,108,108	0
58	ZN	B6	501	1/1	1.00	0.13	-0.95	49,49,49,49	0
56	MG	AA	3091	1/1	0.98	0.15	-0.96	75,75,75,75	0
58	ZN	B5	501	1/1	0.99	0.11	-0.99	54,54,54,54	0
58	ZN	B9	501	1/1	1.00	0.12	-1.01	48,48,48,48	0
57	SF4	AD	501	8/8	0.99	0.14	-1.01	59,72,92,96	0
56	MG	CA	3023	1/1	0.83	0.14	-1.03	37,37,37,37	0
56	MG	BA	3589	1/1	0.93	0.15	-1.03	51,51,51,51	0
56	MG	DA	3227	1/1	0.98	0.14	-1.04	53,53,53,53	0
58	ZN	BY	202	1/1	0.98	0.09	-1.05	71,71,71,71	0
56	MG	BA	3394	1/1	0.93	0.12	-1.05	49,49,49,49	0
56	MG	DA	3568	1/1	0.96	0.10	-1.17	42,42,42,42	0
56	MG	CA	3080	1/1	0.99	0.14	-1.20	55,55,55,55	0
56	MG	BA	3533	1/1	0.98	0.18	-1.21	32,32,32,32	0
56	MG	AA	3175	1/1	0.96	0.14	-1.34	76,76,76,76	0
56	MG	CA	3050	1/1	0.97	0.13	-1.35	43,43,43,43	0
56	MG	B3	101	1/1	0.98	0.15	-1.35	28,28,28,28	0
58	ZN	D5	103	1/1	0.99	0.07	-1.36	70,70,70,70	0
56	MG	DA	3446	1/1	0.97	0.11	-1.42	52,52,52,52	0
56	MG	CE	3002	1/1	0.98	0.07	-1.45	55,55,55,55	0
56	MG	BA	3389	1/1	0.98	0.12	-1.47	48,48,48,48	0
56	MG	DA	3190	1/1	0.99	0.13	-1.47	37,37,37,37	0
56	MG	BA	3538	1/1	0.96	0.16	-1.51	36,36,36,36	0
56	MG	DA	3601	1/1	0.95	0.12	-1.53	77,77,77,77	0
56	MG	BA	3316	1/1	0.98	0.16	-1.54	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3012	1/1	0.96	0.12	-1.54	49,49,49,49	0
56	MG	DG	3001	1/1	0.79	0.14	-1.57	63,63,63,63	0
56	MG	BA	3716	1/1	0.93	0.11	-1.61	27,27,27,27	0
56	MG	BA	3050	1/1	0.93	0.15	-1.64	21,21,21,21	0
56	MG	DA	3514	1/1	0.97	0.12	-1.64	39,39,39,39	0
56	MG	BA	3712	1/1	0.86	0.09	-1.68	58,58,58,58	0
58	ZN	AN	102	1/1	0.93	0.12	-1.71	90,90,90,90	0
56	MG	BA	3051	1/1	0.99	0.15	-1.72	20,20,20,20	0
58	ZN	D4	501	1/1	0.85	0.09	-1.73	153,153,153,153	0
56	MG	DE	303	1/1	0.98	0.11	-1.73	41,41,41,41	0
56	MG	DA	3356	1/1	0.97	0.11	-1.75	27,27,27,27	0
58	ZN	B4	3002	1/1	0.72	0.07	-1.78	165,165,165,165	0
56	MG	CX	104	1/1	0.97	0.14	-1.79	40,40,40,40	0
56	MG	BA	3447	1/1	0.97	0.13	-1.79	37,37,37,37	0
56	MG	AA	3201	1/1	0.93	0.12	-1.80	67,67,67,67	0
56	MG	DA	3009	1/1	0.87	0.12	-1.81	31,31,31,31	0
56	MG	BA	3600	1/1	0.97	0.15	-1.81	47,47,47,47	0
56	MG	BA	3366	1/1	0.96	0.09	-1.81	63,63,63,63	0
56	MG	DA	3552	1/1	0.94	0.12	-1.84	34,34,34,34	0
56	MG	DB	3004	1/1	0.96	0.14	-1.85	68,68,68,68	0
56	MG	CA	3056	1/1	0.91	0.11	-1.85	64,64,64,64	0
58	ZN	D9	501	1/1	0.96	0.05	-1.87	66,66,66,66	0
56	MG	BA	3418	1/1	0.98	0.15	-1.87	27,27,27,27	0
56	MG	DA	3390	1/1	0.98	0.09	-1.89	42,42,42,42	0
58	ZN	DY	501	1/1	0.97	0.05	-1.93	83,83,83,83	0
56	MG	BA	3539	1/1	0.97	0.16	-1.93	35,35,35,35	0
56	MG	CA	3068	1/1	0.86	0.11	-1.94	41,41,41,41	0
56	MG	DA	3544	1/1	0.96	0.11	-1.98	51,51,51,51	0
56	MG	DA	3019	1/1	0.98	0.13	-2.01	30,30,30,30	0
56	MG	DA	3646	1/1	0.94	0.07	-2.02	38,38,38,38	0
56	MG	BG	3002	1/1	0.88	0.11	-2.03	42,42,42,42	0
56	MG	DA	3318	1/1	0.84	0.11	-2.03	45,45,45,45	0
56	MG	BA	3283	1/1	0.98	0.15	-2.12	17,17,17,17	0
56	MG	DA	3382	1/1	0.95	0.14	-2.12	25,25,25,25	0
56	MG	BA	3413	1/1	0.96	0.14	-2.12	20,20,20,20	0
56	MG	AM	3001	1/1	0.94	0.06	-2.13	65,65,65,65	0
56	MG	DA	3562	1/1	0.92	0.10	-2.13	61,61,61,61	0
56	MG	CA	3066	1/1	0.95	0.10	-2.14	55,55,55,55	0
56	MG	BA	3011	1/1	0.90	0.09	-2.15	37,37,37,37	0
56	MG	BA	3388	1/1	0.98	0.14	-2.16	34,34,34,34	0
56	MG	DA	3317	1/1	0.98	0.11	-2.21	32,32,32,32	0
56	MG	DA	3547	1/1	0.97	0.10	-2.23	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	3553	1/1	0.99	0.13	-2.26	31,31,31,31	0
56	MG	BA	3329	1/1	0.97	0.13	-2.28	29,29,29,29	0
56	MG	BP	202	1/1	0.97	0.11	-2.31	40,40,40,40	0
56	MG	BA	3446	1/1	0.93	0.13	-2.34	49,49,49,49	0
56	MG	DA	3054	1/1	0.93	0.11	-2.35	51,51,51,51	0
56	MG	BA	3506	1/1	0.95	0.14	-2.36	30,30,30,30	0
56	MG	DA	3448	1/1	0.98	0.08	-2.46	57,57,57,57	0
56	MG	BA	3536	1/1	0.96	0.14	-2.48	27,27,27,27	0
56	MG	DA	3047	1/1	0.95	0.08	-2.52	34,34,34,34	0
56	MG	DA	3459	1/1	0.92	0.11	-2.53	33,33,33,33	0
56	MG	BA	3365	1/1	0.89	0.14	-2.54	20,20,20,20	0
56	MG	DA	3294	1/1	0.96	0.10	-2.60	47,47,47,47	0
56	MG	CA	3058	1/1	0.94	0.09	-2.70	40,40,40,40	0
56	MG	DA	3304	1/1	1.00	0.11	-2.72	35,35,35,35	0
56	MG	DA	3183	1/1	0.91	0.11	-2.73	54,54,54,54	0
56	MG	BA	3378	1/1	0.99	0.12	-2.80	20,20,20,20	0
56	MG	AA	3020	1/1	0.73	0.10	-2.93	77,77,77,77	0
56	MG	CA	3125	1/1	0.87	0.13	-2.93	72,72,72,72	0
56	MG	DA	3205	1/1	0.98	0.09	-2.93	38,38,38,38	0
56	MG	DA	3059	1/1	0.98	0.08	-2.97	46,46,46,46	0
56	MG	BA	3723	1/1	0.98	0.14	-2.97	49,49,49,49	0
56	MG	CA	3167	1/1	0.94	0.09	-2.99	78,78,78,78	0
56	MG	BA	3406	1/1	0.92	0.14	-2.99	28,28,28,28	0
56	MG	AA	3182	1/1	0.97	0.12	-3.06	49,49,49,49	0
56	MG	BA	3429	1/1	0.98	0.14	-3.10	20,20,20,20	0
56	MG	BA	3593	1/1	0.97	0.14	-3.23	74,74,74,74	0
56	MG	BA	3688	1/1	0.94	0.11	-3.28	54,54,54,54	0
56	MG	BA	3074	1/1	0.94	0.08	-3.29	42,42,42,42	0
56	MG	CA	3118	1/1	0.97	0.08	-3.29	37,37,37,37	0
56	MG	DA	3028	1/1	0.99	0.06	-3.31	35,35,35,35	0
56	MG	DA	3402	1/1	0.80	0.08	-3.34	61,61,61,61	0
56	MG	BA	3477	1/1	0.96	0.11	-3.35	25,25,25,25	0
56	MG	DA	3431	1/1	0.97	0.12	-3.37	41,41,41,41	0
56	MG	BA	3341	1/1	0.98	0.10	-3.37	33,33,33,33	0
56	MG	CA	3026	1/1	0.96	0.07	-3.42	52,52,52,52	0
56	MG	BA	3521	1/1	0.97	0.12	-3.43	49,49,49,49	0
56	MG	DA	3565	1/1	0.95	0.07	-3.45	57,57,57,57	0
56	MG	BB	3007	1/1	0.96	0.09	-3.47	47,47,47,47	0
56	MG	BA	3326	1/1	0.95	0.09	-3.49	41,41,41,41	0
56	MG	BA	3715	1/1	0.97	0.13	-3.56	47,47,47,47	0
56	MG	CA	3071	1/1	0.88	0.08	-3.56	63,63,63,63	0
56	MG	BA	3458	1/1	0.96	0.12	-3.60	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	BA	3318	1/1	0.99	0.13	-3.63	33,33,33,33	0
56	MG	AA	3102	1/1	0.97	0.06	-3.63	64,64,64,64	0
56	MG	BA	3421	1/1	0.95	0.12	-3.65	36,36,36,36	0
56	MG	BA	3408	1/1	0.93	0.15	-3.71	24,24,24,24	0
56	MG	DA	3490	1/1	0.95	0.10	-3.87	39,39,39,39	0
56	MG	DA	3504	1/1	0.97	0.08	-3.89	44,44,44,44	0
56	MG	AA	3124	1/1	0.90	0.10	-3.89	57,57,57,57	0
56	MG	BA	3013	1/1	0.96	0.14	-3.93	40,40,40,40	0
56	MG	DA	3311	1/1	0.96	0.09	-3.95	32,32,32,32	0
56	MG	DA	3345	1/1	0.96	0.09	-3.95	31,31,31,31	0
56	MG	DA	3247	1/1	0.96	0.08	-4.19	31,31,31,31	0
56	MG	CA	3019	1/1	0.93	0.07	-4.20	49,49,49,49	0
56	MG	BA	3423	1/1	0.99	0.07	-4.37	26,26,26,26	0
56	MG	DA	3315	1/1	0.91	0.09	-4.50	31,31,31,31	0
56	MG	BA	3357	1/1	0.93	0.13	-4.55	49,49,49,49	0
56	MG	DA	3149	1/1	0.92	0.06	-4.56	47,47,47,47	0
56	MG	DA	3625	1/1	0.99	0.10	-4.60	35,35,35,35	0
56	MG	DA	3524	1/1	0.89	0.12	-4.65	28,28,28,28	0
56	MG	BA	3602	1/1	0.98	0.09	-4.72	35,35,35,35	0
56	MG	AA	3198	1/1	0.92	0.11	-5.27	87,87,87,87	0
56	MG	BA	3113	1/1	0.98	0.08	-5.48	32,32,32,32	0
56	MG	BA	3580	1/1	0.95	0.12	-5.49	58,58,58,58	0
56	MG	AA	3057	1/1	0.97	0.09	-5.60	37,37,37,37	0
56	MG	BA	3721	1/1	0.97	0.08	-5.62	25,25,25,25	0
56	MG	AA	3062	1/1	0.98	0.08	-5.63	32,32,32,32	0
56	MG	AA	3152	1/1	0.93	0.09	-5.77	19,19,19,19	0
56	MG	DA	3644	1/1	0.98	0.07	-5.77	42,42,42,42	0
56	MG	AA	3027	1/1	0.98	0.06	-5.84	55,55,55,55	0
56	MG	BA	3112	1/1	0.96	0.09	-6.02	38,38,38,38	0
56	MG	DA	3436	1/1	0.97	0.07	-6.08	62,62,62,62	0
56	MG	BA	3217	1/1	0.96	0.09	-6.46	28,28,28,28	0
56	MG	BA	3564	1/1	0.97	0.07	-6.58	52,52,52,52	0
56	MG	CA	3083	1/1	0.97	0.07	-6.68	39,39,39,39	0
56	MG	BA	3636	1/1	0.97	0.11	-7.29	36,36,36,36	0
56	MG	BA	3516	1/1	0.99	0.09	-7.40	47,47,47,47	0
56	MG	DA	3177	1/1	0.98	0.08	-7.77	33,33,33,33	0
56	MG	BA	3220	1/1	0.97	0.10	-8.95	57,57,57,57	0
56	MG	BA	3351	1/1	0.97	0.07	-9.61	30,30,30,30	0
56	MG	BA	3434	1/1	0.96	0.12	-9.64	32,32,32,32	0
56	MG	BA	3635	1/1	0.94	0.10	-9.81	78,78,78,78	0
56	MG	BA	3454	1/1	0.98	0.09	-14.15	22,22,22,22	0
56	MG	DA	3517	1/1	0.90	0.19	-	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	CA	3028	1/1	0.96	0.44	-	43,43,43,43	0
56	MG	DA	3455	1/1	0.97	0.17	-	60,60,60,60	0
56	MG	BA	3486	1/1	0.97	0.06	-	38,38,38,38	0
56	MG	CA	3014	1/1	0.94	0.18	-	50,50,50,50	0
56	MG	AA	3069	1/1	0.92	0.14	-	84,84,84,84	0
56	MG	BA	3373	1/1	0.88	0.28	-	36,36,36,36	0
56	MG	DB	3012	1/1	0.93	0.27	-	59,59,59,59	0
56	MG	BA	3507	1/1	0.91	0.10	-	68,68,68,68	0
56	MG	AA	3155	1/1	0.95	0.17	-	70,70,70,70	0
56	MG	CA	3055	1/1	0.73	0.29	-	62,62,62,62	0
56	MG	AA	3206	1/1	0.93	0.07	-	70,70,70,70	0
56	MG	DA	3519	1/1	0.93	0.14	-	44,44,44,44	0
56	MG	BA	3710	1/1	0.97	0.21	-	48,48,48,48	0
56	MG	BA	3065	1/1	0.73	0.44	-	50,50,50,50	0
56	MG	DA	3352	1/1	0.79	0.38	-	47,47,47,47	0
56	MG	CA	3107	1/1	0.93	0.12	-	60,60,60,60	0
56	MG	BA	3623	1/1	0.97	0.21	-	47,47,47,47	0
56	MG	CA	3057	1/1	0.81	0.25	-	49,49,49,49	0
56	MG	DA	3399	1/1	0.96	0.19	-	41,41,41,41	0
56	MG	DA	3283	1/1	0.95	0.21	-	33,33,33,33	0
56	MG	CA	3005	1/1	0.85	0.31	-	54,54,54,54	0
56	MG	DA	3027	1/1	0.94	0.43	-	39,39,39,39	0
56	MG	BA	3020	1/1	0.91	0.11	-	45,45,45,45	0
56	MG	BB	3002	1/1	0.96	0.19	-	59,59,59,59	0
56	MG	AA	3172	1/1	0.98	0.05	-	53,53,53,53	0
56	MG	DA	3267	1/1	0.95	0.17	-	61,61,61,61	0
56	MG	DA	3229	1/1	0.94	0.11	-	40,40,40,40	0
56	MG	BA	3152	1/1	0.83	0.33	-	46,46,46,46	0
56	MG	DA	3200	1/1	0.89	0.20	-	42,42,42,42	0
56	MG	DA	3616	1/1	0.97	0.23	-	62,62,62,62	0
56	MG	BA	3006	1/1	0.87	0.27	-	42,42,42,42	0
56	MG	DB	3009	1/1	0.94	0.37	-	40,40,40,40	0
56	MG	BA	3428	1/1	0.97	0.11	-	45,45,45,45	0
56	MG	DA	3072	1/1	0.93	0.14	-	41,41,41,41	0
56	MG	DA	3233	1/1	0.93	0.19	-	42,42,42,42	0
56	MG	DA	3086	1/1	0.88	0.30	-	43,43,43,43	0
56	MG	DA	3291	1/1	0.97	0.24	-	35,35,35,35	0
56	MG	BA	3303	1/1	0.91	0.16	-	35,35,35,35	0
56	MG	DQ	201	1/1	0.88	0.42	-	48,48,48,48	0
56	MG	BA	3442	1/1	0.98	0.15	-	12,12,12,12	0
56	MG	B1	3001	1/1	0.74	0.86	-	54,54,54,54	0
56	MG	CA	3154	1/1	0.99	0.14	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3063	1/1	0.78	0.30	-	61,61,61,61	0
56	MG	DA	3090	1/1	0.94	0.34	-	47,47,47,47	0
56	MG	BA	3092	1/1	0.88	0.27	-	51,51,51,51	0
56	MG	AA	3087	1/1	0.64	0.36	-	72,72,72,72	0
56	MG	CA	3127	1/1	0.76	0.25	-	79,79,79,79	0
56	MG	DA	3387	1/1	0.89	0.14	-	56,56,56,56	0
56	MG	DA	3118	1/1	0.95	0.10	-	39,39,39,39	0
56	MG	CA	3141	1/1	0.93	0.25	-	70,70,70,70	0
56	MG	BA	3061	1/1	0.89	0.49	-	51,51,51,51	0
56	MG	DA	3246	1/1	0.92	0.17	-	24,24,24,24	0
56	MG	BA	3143	1/1	0.91	0.31	-	40,40,40,40	0
56	MG	DA	3370	1/1	0.98	0.15	-	38,38,38,38	0
56	MG	BU	207	1/1	0.98	0.22	-	40,40,40,40	0
56	MG	DA	3488	1/1	0.96	0.04	-	46,46,46,46	0
56	MG	BA	3080	1/1	0.97	0.52	-	45,45,45,45	0
56	MG	DA	3460	1/1	0.89	0.36	-	50,50,50,50	0
56	MG	DA	3600	1/1	0.98	0.07	-	45,45,45,45	0
56	MG	BA	3122	1/1	0.92	0.27	-	52,52,52,52	0
56	MG	DA	3102	1/1	0.88	0.25	-	41,41,41,41	0
56	MG	AA	3030	1/1	0.81	0.32	-	69,69,69,69	0
56	MG	AA	3078	1/1	0.95	0.27	-	42,42,42,42	0
56	MG	BA	3494	1/1	0.99	0.34	-	18,18,18,18	0
56	MG	AA	3074	1/1	0.87	0.44	-	47,47,47,47	0
56	MG	BA	3668	1/1	0.97	0.13	-	38,38,38,38	0
56	MG	BA	3030	1/1	0.93	0.44	-	51,51,51,51	0
56	MG	BA	3625	1/1	0.96	0.13	-	51,51,51,51	0
56	MG	DA	3611	1/1	0.91	0.09	-	42,42,42,42	0
56	MG	CA	3132	1/1	0.96	0.11	-	70,70,70,70	0
56	MG	BA	3577	1/1	0.90	0.10	-	52,52,52,52	0
56	MG	CA	3041	1/1	0.50	0.69	-	75,75,75,75	0
56	MG	BA	3455	1/1	0.97	0.14	-	47,47,47,47	0
56	MG	BA	3075	1/1	0.76	0.26	-	45,45,45,45	0
56	MG	BA	3173	1/1	0.97	0.59	-	37,37,37,37	0
56	MG	BA	3452	1/1	0.82	0.26	-	47,47,47,47	0
56	MG	BA	3251	1/1	0.89	0.21	-	61,61,61,61	0
56	MG	DA	3258	1/1	0.97	0.18	-	32,32,32,32	0
56	MG	DA	3310	1/1	0.88	0.21	-	53,53,53,53	0
56	MG	DA	3015	1/1	0.93	0.26	-	49,49,49,49	0
56	MG	DA	3409	1/1	0.96	0.15	-	32,32,32,32	0
56	MG	AX	107	1/1	0.91	0.25	-	66,66,66,66	0
56	MG	DA	3058	1/1	0.87	0.34	-	47,47,47,47	0
56	MG	DA	3463	1/1	0.96	0.37	-	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	3051	1/1	0.91	0.12	-	46,46,46,46	0
56	MG	CA	3100	1/1	0.98	0.11	-	60,60,60,60	0
56	MG	BA	3261	1/1	0.94	0.26	-	34,34,34,34	0
56	MG	BA	3296	1/1	0.97	0.24	-	46,46,46,46	0
56	MG	DA	3362	1/1	0.94	0.13	-	41,41,41,41	0
56	MG	BA	3520	1/1	0.99	0.14	-	34,34,34,34	0
56	MG	DA	3120	1/1	0.95	0.76	-	51,51,51,51	0
56	MG	DA	3111	1/1	0.92	0.23	-	53,53,53,53	0
56	MG	AA	3192	1/1	0.98	0.08	-	57,57,57,57	0
56	MG	BA	3244	1/1	0.82	0.47	-	65,65,65,65	0
56	MG	DA	3495	1/1	0.97	0.22	-	39,39,39,39	0
56	MG	BE	302	1/1	0.98	0.22	-	33,33,33,33	0
56	MG	BA	3490	1/1	0.97	0.26	-	38,38,38,38	0
56	MG	CA	3110	1/1	0.86	0.21	-	97,97,97,97	0
56	MG	BA	3551	1/1	0.96	0.22	-	25,25,25,25	0
56	MG	BB	3014	1/1	0.92	0.13	-	69,69,69,69	0
56	MG	BA	3372	1/1	0.91	0.17	-	38,38,38,38	0
56	MG	DA	3578	1/1	0.94	0.38	-	49,49,49,49	0
56	MG	DA	3467	1/1	0.98	0.09	-	35,35,35,35	0
56	MG	CX	102	1/1	0.97	0.06	-	61,61,61,61	0
56	MG	BA	3054	1/1	0.96	0.29	-	46,46,46,46	0
56	MG	DA	3635	1/1	0.91	0.32	-	58,58,58,58	0
56	MG	BA	3195	1/1	0.98	0.33	-	47,47,47,47	0
56	MG	BA	3056	1/1	0.91	0.42	-	44,44,44,44	0
56	MG	DA	3196	1/1	0.94	0.34	-	44,44,44,44	0
56	MG	BA	3571	1/1	0.96	0.08	-	65,65,65,65	0
56	MG	AA	3015	1/1	0.85	0.16	-	73,73,73,73	0
56	MG	AA	3093	1/1	0.38	0.58	-	88,88,88,88	0
56	MG	DA	3525	1/1	0.81	0.70	-	70,70,70,70	0
56	MG	BA	3436	1/1	0.98	0.09	-	37,37,37,37	0
56	MG	DA	3001	1/1	0.95	0.30	-	78,78,78,78	0
56	MG	DE	305	1/1	0.94	0.63	-	65,65,65,65	0
56	MG	DA	3573	1/1	0.97	0.20	-	40,40,40,40	0
56	MG	DB	3010	1/1	0.95	0.18	-	73,73,73,73	0
56	MG	DA	3439	1/1	0.96	0.19	-	28,28,28,28	0
56	MG	DA	3091	1/1	0.96	0.38	-	44,44,44,44	0
56	MG	CA	3149	1/1	0.94	0.17	-	74,74,74,74	0
56	MG	DA	3357	1/1	0.85	0.20	-	56,56,56,56	0
56	MG	BA	3599	1/1	0.93	0.31	-	46,46,46,46	0
56	MG	BA	3298	1/1	0.88	0.33	-	49,49,49,49	0
56	MG	DA	3610	1/1	0.90	0.28	-	54,54,54,54	0
56	MG	DA	3238	1/1	0.85	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	BA	3648	1/1	0.96	0.30	-	49,49,49,49	0
56	MG	AA	3001	1/1	0.86	0.18	-	68,68,68,68	0
56	MG	BA	3409	1/1	0.99	0.23	-	27,27,27,27	0
56	MG	AA	3073	1/1	0.99	0.07	-	46,46,46,46	0
56	MG	DA	3632	1/1	0.86	0.18	-	71,71,71,71	0
56	MG	DA	3457	1/1	0.96	0.12	-	37,37,37,37	0
56	MG	AA	3013	1/1	0.86	0.23	-	78,78,78,78	0
56	MG	BA	3271	1/1	0.95	0.12	-	36,36,36,36	0
56	MG	CA	3105	1/1	0.92	0.09	-	79,79,79,79	0
56	MG	DA	3184	1/1	0.97	0.32	-	45,45,45,45	0
56	MG	BA	3238	1/1	0.93	0.16	-	51,51,51,51	0
56	MG	BA	3180	1/1	0.81	0.98	-	43,43,43,43	0
56	MG	CA	3081	1/1	0.84	0.10	-	72,72,72,72	0
56	MG	AA	3026	1/1	0.93	0.17	-	41,41,41,41	0
56	MG	AA	3048	1/1	0.71	0.24	-	57,57,57,57	0
56	MG	BA	3629	1/1	0.97	0.13	-	47,47,47,47	0
56	MG	DA	3062	1/1	0.86	0.34	-	55,55,55,55	0
56	MG	BA	3049	1/1	0.92	0.38	-	35,35,35,35	0
56	MG	DA	3277	1/1	0.98	0.25	-	49,49,49,49	0
56	MG	BA	3290	1/1	0.82	0.24	-	49,49,49,49	0
56	MG	DA	3316	1/1	0.98	0.17	-	58,58,58,58	0
56	MG	DA	3165	1/1	0.98	0.23	-	44,44,44,44	0
56	MG	BA	3069	1/1	0.80	0.44	-	41,41,41,41	0
56	MG	BA	3183	1/1	0.90	0.24	-	48,48,48,48	0
56	MG	BA	3342	1/1	0.99	0.19	-	31,31,31,31	0
56	MG	BA	3400	1/1	0.97	0.19	-	24,24,24,24	0
56	MG	DA	3212	1/1	0.93	0.10	-	48,48,48,48	0
56	MG	BA	3067	1/1	0.93	0.33	-	53,53,53,53	0
56	MG	AA	3173	1/1	0.93	0.24	-	32,32,32,32	0
56	MG	DA	3260	1/1	0.87	0.10	-	40,40,40,40	0
56	MG	BA	3465	1/1	0.94	0.12	-	40,40,40,40	0
56	MG	BA	3278	1/1	0.93	0.17	-	34,34,34,34	0
56	MG	BA	3262	1/1	0.91	0.20	-	56,56,56,56	0
56	MG	CA	3161	1/1	0.82	0.12	-	54,54,54,54	0
56	MG	DA	3538	1/1	0.90	0.18	-	44,44,44,44	0
56	MG	BA	3684	1/1	0.93	0.17	-	58,58,58,58	0
56	MG	CA	3049	1/1	0.97	0.24	-	53,53,53,53	0
56	MG	DA	3415	1/1	0.93	0.25	-	56,56,56,56	0
56	MG	DA	3465	1/1	0.90	0.17	-	49,49,49,49	0
56	MG	DA	3135	1/1	0.65	0.23	-	50,50,50,50	0
56	MG	DA	3211	1/1	0.69	0.10	-	51,51,51,51	0
56	MG	CA	3160	1/1	0.89	0.13	-	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	3047	1/1	0.89	0.32	-	61,61,61,61	0
56	MG	DA	3031	1/1	0.95	0.29	-	55,55,55,55	0
56	MG	BA	3385	1/1	0.96	0.24	-	26,26,26,26	0
56	MG	BA	3198	1/1	0.86	0.14	-	52,52,52,52	0
56	MG	BA	3405	1/1	0.97	0.14	-	34,34,34,34	0
56	MG	DA	3587	1/1	0.77	0.14	-	64,64,64,64	0
56	MG	B8	103	1/1	0.97	0.19	-	24,24,24,24	0
56	MG	BA	3363	1/1	0.97	0.15	-	39,39,39,39	0
56	MG	DF	303	1/1	0.90	0.33	-	43,43,43,43	0
56	MG	BA	3179	1/1	0.98	0.20	-	43,43,43,43	0
56	MG	DA	3526	1/1	0.91	0.19	-	54,54,54,54	0
56	MG	DA	3064	1/1	0.76	0.41	-	50,50,50,50	0
56	MG	DA	3617	1/1	0.94	0.19	-	58,58,58,58	0
56	MG	AA	3077	1/1	0.84	0.41	-	65,65,65,65	0
56	MG	DA	3104	1/1	0.84	0.28	-	62,62,62,62	0
56	MG	B4	3001	1/1	0.61	0.27	-	100,100,100,100	0
56	MG	DA	3208	1/1	0.88	0.93	-	43,43,43,43	0
56	MG	BA	3327	1/1	0.97	0.15	-	38,38,38,38	0
56	MG	AA	3163	1/1	0.98	0.17	-	28,28,28,28	0
56	MG	AA	3210	1/1	0.94	0.06	-	40,40,40,40	0
56	MG	BA	3567	1/1	0.98	0.22	-	37,37,37,37	0
56	MG	DA	3140	1/1	0.83	0.34	-	54,54,54,54	0
56	MG	BA	3698	1/1	0.93	0.20	-	41,41,41,41	0
56	MG	BA	3651	1/1	0.96	0.13	-	45,45,45,45	0
56	MG	DA	3101	1/1	0.94	0.33	-	48,48,48,48	0
56	MG	BA	3685	1/1	0.96	0.10	-	67,67,67,67	0
56	MG	AA	3144	1/1	0.99	0.08	-	48,48,48,48	0
56	MG	CA	3163	1/1	0.85	0.24	-	65,65,65,65	0
56	MG	BA	3254	1/1	0.92	0.19	-	59,59,59,59	0
56	MG	AA	3139	1/1	0.89	0.34	-	56,56,56,56	0
56	MG	BA	3472	1/1	0.96	0.08	-	30,30,30,30	0
56	MG	BA	3172	1/1	0.91	0.98	-	48,48,48,48	0
56	MG	BA	3555	1/1	0.93	0.18	-	53,53,53,53	0
56	MG	BA	3411	1/1	0.98	0.15	-	38,38,38,38	0
56	MG	CA	3051	1/1	0.98	0.10	-	63,63,63,63	0
56	MG	BA	3390	1/1	0.97	0.25	-	30,30,30,30	0
56	MG	D5	101	1/1	0.86	0.48	-	53,53,53,53	0
56	MG	CA	3153	1/1	0.91	0.10	-	83,83,83,83	0
56	MG	BA	3528	1/1	0.99	0.22	-	33,33,33,33	0
56	MG	DA	3350	1/1	0.95	0.04	-	32,32,32,32	0
56	MG	DA	3404	1/1	0.98	0.16	-	47,47,47,47	0
56	MG	DA	3185	1/1	0.88	0.59	-	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	3347	1/1	0.98	0.27	-	25,25,25,25	0
56	MG	DA	3203	1/1	0.96	0.13	-	41,41,41,41	0
56	MG	DA	3014	1/1	0.92	0.21	-	34,34,34,34	0
56	MG	BA	3463	1/1	0.90	0.20	-	55,55,55,55	0
56	MG	BA	3012	1/1	0.93	0.16	-	40,40,40,40	0
56	MG	DQ	202	1/1	0.95	0.22	-	34,34,34,34	0
56	MG	DA	3137	1/1	0.93	0.28	-	56,56,56,56	0
56	MG	BA	3491	1/1	0.99	0.19	-	23,23,23,23	0
56	MG	DA	3354	1/1	0.98	0.15	-	27,27,27,27	0
56	MG	DA	3296	1/1	0.92	0.08	-	31,31,31,31	0
56	MG	CA	3091	1/1	0.87	0.17	-	72,72,72,72	0
56	MG	AA	3123	1/1	0.91	0.43	-	39,39,39,39	0
56	MG	BA	3621	1/1	0.97	0.36	-	74,74,74,74	0
56	MG	AA	3068	1/1	0.93	0.08	-	66,66,66,66	0
56	MG	BB	3013	1/1	0.98	0.10	-	39,39,39,39	0
56	MG	BA	3662	1/1	0.99	0.12	-	39,39,39,39	0
56	MG	BA	3613	1/1	0.64	0.29	-	76,76,76,76	0
56	MG	BA	3291	1/1	0.96	0.17	-	41,41,41,41	0
56	MG	CA	3075	1/1	0.95	0.17	-	76,76,76,76	0
56	MG	DA	3605	1/1	0.96	0.15	-	44,44,44,44	0
56	MG	BQ	203	1/1	0.90	0.23	-	58,58,58,58	0
56	MG	BA	3232	1/1	0.97	0.15	-	29,29,29,29	0
56	MG	BA	3460	1/1	0.99	0.13	-	33,33,33,33	0
56	MG	AD	502	1/1	0.96	0.46	-	43,43,43,43	0
56	MG	BA	3647	1/1	0.93	0.10	-	34,34,34,34	0
56	MG	AA	3041	1/1	0.92	0.15	-	49,49,49,49	0
56	MG	BA	3522	1/1	0.98	0.14	-	49,49,49,49	0
56	MG	DA	3477	1/1	0.98	0.09	-	49,49,49,49	0
56	MG	AA	3199	1/1	0.93	0.17	-	88,88,88,88	0
56	MG	AA	3067	1/1	0.87	0.37	-	87,87,87,87	0
56	MG	AA	3101	1/1	0.91	0.15	-	56,56,56,56	0
56	MG	AA	3115	1/1	0.90	0.10	-	48,48,48,48	0
56	MG	DA	3095	1/1	0.86	0.23	-	61,61,61,61	0
56	MG	BA	3134	1/1	0.82	0.32	-	47,47,47,47	0
56	MG	BA	3481	1/1	0.91	0.23	-	38,38,38,38	0
56	MG	DA	3210	1/1	0.88	0.15	-	40,40,40,40	0
56	MG	AA	3122	1/1	0.95	0.55	-	44,44,44,44	0
56	MG	BA	3654	1/1	0.95	0.16	-	25,25,25,25	0
56	MG	BA	3594	1/1	0.95	0.31	-	42,42,42,42	0
56	MG	BA	3305	1/1	0.98	0.13	-	44,44,44,44	0
56	MG	CA	3013	1/1	0.95	0.12	-	51,51,51,51	0
56	MG	BA	3015	1/1	0.96	0.34	-	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	0.87	0.33	-	44,44,44,44	0
56	MG	DA	3537	1/1	0.93	0.22	-	65,65,65,65	0
56	MG	BA	3371	1/1	0.99	0.18	-	15,15,15,15	0
56	MG	BA	3489	1/1	0.97	0.15	-	43,43,43,43	0
56	MG	DA	3063	1/1	0.94	0.12	-	52,52,52,52	0
56	MG	DA	3186	1/1	0.68	0.51	-	53,53,53,53	0
56	MG	CA	3003	1/1	0.83	0.11	-	66,66,66,66	0
56	MG	CA	3109	1/1	0.85	0.11	-	83,83,83,83	0
56	MG	DA	3022	1/1	0.86	0.26	-	45,45,45,45	0
56	MG	BA	3040	1/1	0.85	0.35	-	51,51,51,51	0
56	MG	DO	5001	1/1	0.97	0.12	-	35,35,35,35	0
56	MG	BA	3216	1/1	0.88	0.22	-	41,41,41,41	0
56	MG	BA	3002	1/1	0.97	0.20	-	54,54,54,54	0
56	MG	BA	3694	1/1	0.97	0.37	-	56,56,56,56	0
56	MG	DA	3057	1/1	0.94	0.16	-	52,52,52,52	0
56	MG	AA	3135	1/1	0.93	0.24	-	41,41,41,41	0
56	MG	BA	3295	1/1	0.39	0.57	-	75,75,75,75	0
56	MG	BA	3241	1/1	0.79	0.38	-	63,63,63,63	0
56	MG	BA	3667	1/1	0.96	0.10	-	63,63,63,63	0
56	MG	BA	3660	1/1	0.94	0.27	-	71,71,71,71	0
56	MG	DA	3249	1/1	0.96	0.21	-	28,28,28,28	0
56	MG	CA	3166	1/1	0.97	0.23	-	59,59,59,59	0
56	MG	CA	3133	1/1	0.98	0.05	-	49,49,49,49	0
56	MG	BA	3335	1/1	0.91	0.17	-	35,35,35,35	0
56	MG	DA	3206	1/1	0.96	0.26	-	42,42,42,42	0
56	MG	BA	3508	1/1	0.99	0.14	-	34,34,34,34	0
56	MG	BA	3306	1/1	0.94	0.14	-	48,48,48,48	0
56	MG	BB	3009	1/1	0.91	0.16	-	48,48,48,48	0
56	MG	DA	3359	1/1	0.89	0.23	-	46,46,46,46	0
56	MG	BA	3027	1/1	0.86	0.23	-	45,45,45,45	0
56	MG	AA	3118	1/1	0.80	0.31	-	52,52,52,52	0
56	MG	DA	3383	1/1	0.94	0.09	-	56,56,56,56	0
56	MG	DA	3438	1/1	0.74	0.51	-	70,70,70,70	0
56	MG	BA	3355	1/1	0.89	0.23	-	64,64,64,64	0
56	MG	DA	3008	1/1	0.93	0.23	-	51,51,51,51	0
56	MG	BA	3427	1/1	0.96	0.12	-	48,48,48,48	0
56	MG	DA	3366	1/1	0.93	0.35	-	36,36,36,36	0
56	MG	DA	3327	1/1	0.98	0.18	-	29,29,29,29	0
56	MG	DA	3523	1/1	0.98	0.06	-	55,55,55,55	0
56	MG	AA	3106	1/1	0.96	0.25	-	56,56,56,56	0
56	MG	DA	3505	1/1	0.92	0.06	-	65,65,65,65	0
56	MG	BA	3156	1/1	0.87	0.39	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3627	1/1	0.95	0.20	-	50,50,50,50	0
56	MG	BV	204	1/1	0.96	0.20	-	20,20,20,20	0
56	MG	CA	3078	1/1	0.96	0.29	-	46,46,46,46	0
56	MG	DA	3245	1/1	0.95	0.15	-	37,37,37,37	0
56	MG	DA	3406	1/1	0.95	0.12	-	40,40,40,40	0
56	MG	CA	3134	1/1	0.93	0.16	-	82,82,82,82	0
56	MG	BA	3064	1/1	0.97	0.19	-	39,39,39,39	0
56	MG	BA	3484	1/1	0.95	0.17	-	54,54,54,54	0
56	MG	BA	3563	1/1	0.95	0.21	-	37,37,37,37	0
56	MG	DA	3136	1/1	0.97	0.11	-	49,49,49,49	0
56	MG	CA	3088	1/1	0.97	0.26	-	43,43,43,43	0
56	MG	DA	3270	1/1	0.96	0.20	-	36,36,36,36	0
56	MG	DA	3532	1/1	0.92	0.10	-	57,57,57,57	0
56	MG	AA	3194	1/1	0.92	0.19	-	54,54,54,54	0
56	MG	CA	3142	1/1	0.87	0.18	-	59,59,59,59	0
56	MG	DA	3369	1/1	0.90	0.13	-	47,47,47,47	0
56	MG	DA	3466	1/1	0.90	0.14	-	56,56,56,56	0
56	MG	DA	3400	1/1	0.93	0.19	-	42,42,42,42	0
56	MG	DA	3648	1/1	0.95	0.17	-	52,52,52,52	0
56	MG	BA	3462	1/1	0.86	0.12	-	52,52,52,52	0
56	MG	BA	3448	1/1	0.98	0.09	-	29,29,29,29	0
56	MG	BA	3110	1/1	0.86	0.34	-	55,55,55,55	0
56	MG	AA	3165	1/1	0.98	0.15	-	23,23,23,23	0
56	MG	AA	3220	1/1	0.98	0.12	-	40,40,40,40	0
56	MG	BA	3597	1/1	0.93	0.35	-	60,60,60,60	0
56	MG	DA	3240	1/1	0.88	0.26	-	51,51,51,51	0
56	MG	DA	3207	1/1	0.94	0.13	-	58,58,58,58	0
56	MG	DF	302	1/1	0.85	0.27	-	43,43,43,43	0
56	MG	BA	3091	1/1	0.94	0.60	-	45,45,45,45	0
56	MG	BA	3628	1/1	0.95	0.21	-	41,41,41,41	0
56	MG	BA	3537	1/1	0.96	0.38	-	31,31,31,31	0
56	MG	BA	3420	1/1	0.98	0.30	-	33,33,33,33	0
56	MG	BA	3482	1/1	0.94	0.17	-	72,72,72,72	0
56	MG	DA	3141	1/1	0.95	0.13	-	62,62,62,62	0
56	MG	DA	3451	1/1	0.95	0.07	-	49,49,49,49	0
56	MG	DA	3511	1/1	0.95	0.08	-	65,65,65,65	0
56	MG	DA	3454	1/1	0.80	0.31	-	55,55,55,55	0
56	MG	DB	3011	1/1	0.88	0.34	-	55,55,55,55	0
56	MG	BA	3325	1/1	0.92	0.19	-	58,58,58,58	0
56	MG	BB	3010	1/1	0.99	0.26	-	40,40,40,40	0
56	MG	DA	3098	1/1	0.78	1.25	-	43,43,43,43	0
56	MG	DA	3223	1/1	0.70	0.26	-	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	3076	1/1	0.79	0.29	-	66,66,66,66	0
56	MG	BA	3076	1/1	0.96	0.23	-	41,41,41,41	0
56	MG	BA	3191	1/1	0.96	0.19	-	52,52,52,52	0
56	MG	BD	312	1/1	0.91	0.85	-	80,80,80,80	0
56	MG	BA	3352	1/1	0.97	0.12	-	34,34,34,34	0
56	MG	DA	3109	1/1	0.92	0.56	-	66,66,66,66	0
56	MG	BA	3053	1/1	0.95	0.34	-	39,39,39,39	0
56	MG	DA	3041	1/1	0.90	0.45	-	57,57,57,57	0
56	MG	BA	3474	1/1	0.86	0.21	-	42,42,42,42	0
56	MG	DA	3456	1/1	0.85	0.13	-	47,47,47,47	0
56	MG	CA	3102	1/1	0.95	0.09	-	41,41,41,41	0
56	MG	DA	3285	1/1	0.94	0.26	-	55,55,55,55	0
56	MG	BA	3141	1/1	0.92	0.30	-	43,43,43,43	0
56	MG	BA	3738	1/1	0.89	0.35	-	59,59,59,59	0
56	MG	DA	3049	1/1	0.74	0.30	-	58,58,58,58	0
56	MG	BA	3631	1/1	0.94	0.14	-	78,78,78,78	0
56	MG	DA	3443	1/1	0.93	0.17	-	53,53,53,53	0
56	MG	BA	3100	1/1	0.88	0.24	-	48,48,48,48	0
56	MG	BA	3609	1/1	0.90	0.12	-	46,46,46,46	0
56	MG	BA	3728	1/1	0.93	0.52	-	32,32,32,32	0
56	MG	DA	3377	1/1	0.98	0.24	-	59,59,59,59	0
56	MG	DA	3201	1/1	0.96	0.12	-	48,48,48,48	0
56	MG	DA	3024	1/1	0.82	0.36	-	65,65,65,65	0
56	MG	DA	3393	1/1	0.94	0.19	-	41,41,41,41	0
56	MG	BA	3344	1/1	0.94	0.09	-	30,30,30,30	0
56	MG	BA	3419	1/1	0.94	0.14	-	24,24,24,24	0
56	MG	DA	3218	1/1	0.90	0.25	-	62,62,62,62	0
56	MG	AA	3002	1/1	0.89	0.20	-	57,57,57,57	0
56	MG	AA	3022	1/1	0.83	0.27	-	48,48,48,48	0
56	MG	AA	3133	1/1	0.88	0.35	-	63,63,63,63	0
56	MG	BB	3017	1/1	0.85	0.20	-	64,64,64,64	0
56	MG	DA	3340	1/1	0.92	0.14	-	47,47,47,47	0
56	MG	DA	3358	1/1	0.94	0.18	-	46,46,46,46	0
56	MG	BA	3235	1/1	0.71	0.28	-	47,47,47,47	0
56	MG	B7	104	1/1	0.85	0.13	-	51,51,51,51	0
56	MG	BA	3616	1/1	0.95	0.10	-	33,33,33,33	0
56	MG	DA	3640	1/1	0.90	0.68	-	56,56,56,56	0
56	MG	AX	106	1/1	0.86	0.17	-	73,73,73,73	0
56	MG	DA	3271	1/1	0.99	0.21	-	37,37,37,37	0
56	MG	CA	3025	1/1	0.70	0.18	-	94,94,94,94	0
56	MG	CA	3126	1/1	0.88	0.24	-	61,61,61,61	0
56	MG	BA	3367	1/1	0.96	0.16	-	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	CA	3039	1/1	0.85	0.36	-	72,72,72,72	0
56	MG	DA	3586	1/1	0.97	0.09	-	29,29,29,29	0
56	MG	D8	5001	1/1	0.91	0.41	-	47,47,47,47	0
56	MG	BA	3500	1/1	0.95	0.15	-	37,37,37,37	0
56	MG	DA	3626	1/1	0.95	0.07	-	68,68,68,68	0
56	MG	DA	3598	1/1	0.83	0.30	-	66,66,66,66	0
56	MG	BA	3270	1/1	0.71	0.31	-	50,50,50,50	0
56	MG	DA	3584	1/1	0.97	0.15	-	61,61,61,61	0
56	MG	BD	304	1/1	0.92	0.51	-	58,58,58,58	0
56	MG	BA	3322	1/1	0.97	0.24	-	22,22,22,22	0
56	MG	BA	3499	1/1	0.94	0.17	-	55,55,55,55	0
56	MG	BA	3686	1/1	0.94	0.14	-	25,25,25,25	0
56	MG	DE	302	1/1	0.81	0.38	-	44,44,44,44	0
56	MG	DA	3564	1/1	0.94	0.77	-	61,61,61,61	0
56	MG	BA	3568	1/1	0.91	0.23	-	47,47,47,47	0
56	MG	AA	3090	1/1	0.77	0.17	-	68,68,68,68	0
56	MG	DA	3378	1/1	0.94	0.15	-	45,45,45,45	0
56	MG	DA	3464	1/1	0.60	0.57	-	50,50,50,50	0
56	MG	BD	301	1/1	0.85	0.27	-	28,28,28,28	0
56	MG	DA	3458	1/1	0.84	0.15	-	71,71,71,71	0
56	MG	BA	3358	1/1	0.95	0.09	-	33,33,33,33	0
56	MG	AA	3176	1/1	0.97	0.09	-	63,63,63,63	0
56	MG	DA	3220	1/1	0.95	0.12	-	37,37,37,37	0
56	MG	BA	3202	1/1	0.95	0.25	-	41,41,41,41	0
56	MG	DA	3123	1/1	0.76	0.23	-	59,59,59,59	0
56	MG	DA	3152	1/1	0.96	0.23	-	50,50,50,50	0
56	MG	BB	3011	1/1	0.99	0.15	-	37,37,37,37	0
56	MG	CA	3136	1/1	0.92	0.18	-	45,45,45,45	0
56	MG	DA	3551	1/1	0.98	0.08	-	52,52,52,52	0
56	MG	DA	3549	1/1	0.99	0.24	-	52,52,52,52	0
56	MG	AA	3154	1/1	0.92	0.08	-	63,63,63,63	0
56	MG	BA	3610	1/1	0.94	0.21	-	40,40,40,40	0
56	MG	DA	3255	1/1	0.92	0.20	-	40,40,40,40	0
56	MG	BA	3700	1/1	0.95	0.12	-	67,67,67,67	0
56	MG	BA	3212	1/1	0.97	0.28	-	43,43,43,43	0
56	MG	DA	3093	1/1	0.86	0.20	-	53,53,53,53	0
56	MG	DA	3235	1/1	0.96	0.20	-	50,50,50,50	0
56	MG	BA	3470	1/1	0.95	0.24	-	54,54,54,54	0
56	MG	DA	3412	1/1	0.97	0.28	-	30,30,30,30	0
56	MG	BA	3717	1/1	0.94	0.22	-	57,57,57,57	0
56	MG	BA	3488	1/1	0.96	0.35	-	35,35,35,35	0
56	MG	BA	3483	1/1	0.96	0.26	-	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	BA	3337	1/1	0.98	0.17	-	23,23,23,23	0
56	MG	BA	3226	1/1	0.91	0.30	-	32,32,32,32	0
56	MG	DA	3322	1/1	0.95	0.13	-	55,55,55,55	0
56	MG	DA	3313	1/1	0.98	0.17	-	52,52,52,52	0
56	MG	DA	3287	1/1	0.96	0.27	-	53,53,53,53	0
56	MG	BA	3126	1/1	0.99	0.22	-	24,24,24,24	0
56	MG	AA	3196	1/1	0.95	0.31	-	65,65,65,65	0
56	MG	CA	3090	1/1	0.95	0.19	-	73,73,73,73	0
56	MG	BA	3096	1/1	0.97	0.35	-	62,62,62,62	0
56	MG	BA	3071	1/1	0.83	0.30	-	55,55,55,55	0
56	MG	BA	3643	1/1	0.87	0.28	-	43,43,43,43	0
56	MG	DA	3036	1/1	0.86	0.30	-	35,35,35,35	0
56	MG	DA	3131	1/1	0.67	0.23	-	54,54,54,54	0
56	MG	DA	3179	1/1	0.92	0.22	-	46,46,46,46	0
56	MG	BA	3510	1/1	0.95	0.23	-	40,40,40,40	0
56	MG	DA	3372	1/1	0.98	0.12	-	45,45,45,45	0
56	MG	DA	3343	1/1	0.88	0.21	-	41,41,41,41	0
56	MG	BA	3088	1/1	0.85	0.36	-	56,56,56,56	0
56	MG	BA	3658	1/1	0.80	0.27	-	79,79,79,79	0
56	MG	BA	3498	1/1	0.95	0.15	-	39,39,39,39	0
56	MG	AA	3092	1/1	0.90	0.51	-	50,50,50,50	0
56	MG	BA	3205	1/1	0.88	0.19	-	40,40,40,40	0
56	MG	AA	3211	1/1	0.92	0.20	-	36,36,36,36	0
56	MG	DA	3572	1/1	0.94	0.11	-	53,53,53,53	0
56	MG	BA	3072	1/1	0.92	0.28	-	45,45,45,45	0
56	MG	DA	3146	1/1	0.94	0.18	-	34,34,34,34	0
56	MG	DA	3060	1/1	0.87	0.26	-	55,55,55,55	0
56	MG	BA	3705	1/1	0.97	0.05	-	39,39,39,39	0
56	MG	BA	3505	1/1	0.91	0.19	-	59,59,59,59	0
56	MG	BA	3515	1/1	0.93	0.05	-	56,56,56,56	0
56	MG	BA	3492	1/1	0.99	0.25	-	23,23,23,23	0
56	MG	DA	3084	1/1	0.84	0.32	-	70,70,70,70	0
56	MG	BA	3225	1/1	0.92	0.33	-	62,62,62,62	0
56	MG	CA	3144	1/1	0.81	0.59	-	63,63,63,63	0
56	MG	BA	3681	1/1	0.98	0.14	-	40,40,40,40	0
56	MG	BA	3214	1/1	0.87	0.09	-	53,53,53,53	0
56	MG	BA	3354	1/1	0.88	0.15	-	74,74,74,74	0
56	MG	CA	3104	1/1	0.92	0.19	-	62,62,62,62	0
56	MG	AA	3104	1/1	0.96	0.16	-	37,37,37,37	0
56	MG	AA	3099	1/1	0.96	0.41	-	60,60,60,60	0
56	MG	DA	3122	1/1	0.88	0.15	-	62,62,62,62	0
56	MG	DA	3561	1/1	0.98	0.19	-	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	DA	3336	1/1	0.93	0.12	-	27,27,27,27	0
56	MG	B0	101	1/1	0.93	0.20	-	36,36,36,36	0
56	MG	BA	3619	1/1	0.91	0.27	-	40,40,40,40	0
56	MG	AA	3150	1/1	0.97	0.27	-	46,46,46,46	0
56	MG	BB	3012	1/1	0.98	0.15	-	56,56,56,56	0
56	MG	BA	3395	1/1	0.96	0.20	-	25,25,25,25	0
56	MG	AA	3134	1/1	0.89	0.43	-	70,70,70,70	0
56	MG	DA	3365	1/1	0.98	0.06	-	40,40,40,40	0
56	MG	BA	3541	1/1	0.95	0.23	-	30,30,30,30	0
56	MG	BN	3006	1/1	0.99	0.12	-	24,24,24,24	0
56	MG	BE	309	1/1	0.98	0.26	-	25,25,25,25	0
56	MG	DB	3003	1/1	0.69	0.12	-	63,63,63,63	0
56	MG	BA	3708	1/1	0.90	0.23	-	40,40,40,40	0
56	MG	DA	3125	1/1	0.69	0.55	-	48,48,48,48	0
56	MG	DA	3254	1/1	0.90	0.22	-	30,30,30,30	0
56	MG	DA	3368	1/1	0.97	0.12	-	39,39,39,39	0
56	MG	DA	3046	1/1	0.90	0.18	-	56,56,56,56	0
56	MG	DA	3486	1/1	0.96	0.12	-	38,38,38,38	0
56	MG	BA	3579	1/1	0.71	0.24	-	63,63,63,63	0
56	MG	BA	3240	1/1	0.84	0.17	-	28,28,28,28	0
56	MG	DA	3521	1/1	0.93	0.12	-	62,62,62,62	0
56	MG	AX	104	1/1	0.95	0.14	-	76,76,76,76	0
56	MG	CA	3021	1/1	0.79	0.21	-	53,53,53,53	0
56	MG	DA	3607	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	CA	3155	1/1	0.87	0.16	-	71,71,71,71	0
56	MG	AA	3121	1/1	0.91	0.53	-	51,51,51,51	0
56	MG	DA	3541	1/1	0.98	0.28	-	35,35,35,35	0
56	MG	BA	3382	1/1	0.98	0.13	-	51,51,51,51	0
56	MG	DA	3228	1/1	0.76	0.25	-	45,45,45,45	0
56	MG	BA	3676	1/1	0.91	0.22	-	51,51,51,51	0
56	MG	BA	3673	1/1	0.83	0.20	-	53,53,53,53	0
56	MG	DA	3497	1/1	0.82	0.23	-	60,60,60,60	0
56	MG	BA	3018	1/1	0.94	0.34	-	40,40,40,40	0
56	MG	BA	3653	1/1	0.91	0.15	-	69,69,69,69	0
56	MG	DA	3543	1/1	0.92	0.15	-	42,42,42,42	0
56	MG	BA	3562	1/1	0.82	0.10	-	73,73,73,73	0
56	MG	AA	3142	1/1	0.91	0.25	-	38,38,38,38	0
56	MG	DA	3071	1/1	0.83	0.52	-	46,46,46,46	0
56	MG	DA	3430	1/1	0.91	0.28	-	55,55,55,55	0
56	MG	DA	3417	1/1	0.96	0.15	-	34,34,34,34	0
56	MG	DA	3043	1/1	0.97	0.45	-	54,54,54,54	0
56	MG	CA	3085	1/1	0.98	0.30	-	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	3137	1/1	0.92	0.29	-	42,42,42,42	0
56	MG	BA	3286	1/1	0.95	0.26	-	32,32,32,32	0
56	MG	BA	3340	1/1	0.96	0.13	-	57,57,57,57	0
56	MG	BA	3476	1/1	0.94	0.13	-	40,40,40,40	0
56	MG	BA	3129	1/1	0.95	0.25	-	36,36,36,36	0
56	MG	BF	307	1/1	0.73	0.40	-	47,47,47,47	0
56	MG	BA	3218	1/1	0.89	0.20	-	62,62,62,62	0
56	MG	BA	3106	1/1	0.91	0.12	-	48,48,48,48	0
56	MG	BA	3323	1/1	0.97	0.14	-	23,23,23,23	0
56	MG	BR	203	1/1	0.97	0.18	-	15,15,15,15	0
56	MG	DA	3332	1/1	0.99	0.13	-	33,33,33,33	0
56	MG	AA	3040	1/1	0.95	0.12	-	55,55,55,55	0
56	MG	DA	3478	1/1	0.92	0.25	-	46,46,46,46	0
56	MG	BA	3585	1/1	0.89	0.17	-	51,51,51,51	0
56	MG	BA	3532	1/1	0.97	0.18	-	34,34,34,34	0
56	MG	DA	3303	1/1	0.94	0.17	-	47,47,47,47	0
56	MG	BA	3257	1/1	0.93	0.30	-	38,38,38,38	0
56	MG	BA	3495	1/1	0.87	0.33	-	84,84,84,84	0
56	MG	AA	3189	1/1	0.93	0.10	-	77,77,77,77	0
56	MG	CA	3069	1/1	0.99	0.11	-	69,69,69,69	0
56	MG	DA	3494	1/1	0.95	0.09	-	78,78,78,78	0
56	MG	DA	3167	1/1	0.89	0.23	-	48,48,48,48	0
56	MG	DA	3166	1/1	0.96	0.08	-	32,32,32,32	0
56	MG	BA	3587	1/1	0.97	0.18	-	23,23,23,23	0
56	MG	DA	3038	1/1	0.94	0.15	-	39,39,39,39	0
56	MG	DA	3280	1/1	0.93	0.20	-	57,57,57,57	0
56	MG	BA	3115	1/1	0.97	0.26	-	36,36,36,36	0
56	MG	DA	3566	1/1	0.94	0.14	-	71,71,71,71	0
56	MG	CA	3108	1/1	0.95	0.22	-	52,52,52,52	0
56	MG	BA	3683	1/1	0.90	0.22	-	60,60,60,60	0
56	MG	DA	3032	1/1	0.87	0.13	-	46,46,46,46	0
56	MG	CA	3146	1/1	0.87	0.20	-	69,69,69,69	0
56	MG	BG	3003	1/1	0.96	0.15	-	42,42,42,42	0
56	MG	CA	3070	1/1	0.84	0.34	-	55,55,55,55	0
56	MG	BA	3733	1/1	0.98	0.11	-	27,27,27,27	0
56	MG	DA	3619	1/1	0.95	0.22	-	48,48,48,48	0
56	MG	DA	3308	1/1	0.98	0.32	-	30,30,30,30	0
56	MG	BA	3255	1/1	0.89	0.18	-	41,41,41,41	0
56	MG	DA	3083	1/1	0.95	0.25	-	41,41,41,41	0
56	MG	BA	3219	1/1	0.96	0.21	-	65,65,65,65	0
56	MG	BA	3714	1/1	0.90	0.21	-	58,58,58,58	0
56	MG	BA	3267	1/1	0.97	0.16	-	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	3693	1/1	0.88	0.14	-	64,64,64,64	0
56	MG	BA	3207	1/1	0.98	0.22	-	35,35,35,35	0
56	MG	BA	3574	1/1	0.98	0.08	-	54,54,54,54	0
56	MG	AA	3051	1/1	0.76	0.51	-	73,73,73,73	0
56	MG	BA	3028	1/1	0.93	0.21	-	48,48,48,48	0
56	MG	CA	3037	1/1	0.90	0.30	-	67,67,67,67	0
56	MG	AV	101	1/1	0.93	0.17	-	36,36,36,36	0
56	MG	BA	3561	1/1	0.96	0.19	-	24,24,24,24	0
56	MG	AA	3009	1/1	0.88	0.23	-	79,79,79,79	0
56	MG	AA	3053	1/1	0.94	0.33	-	49,49,49,49	0
56	MG	BA	3068	1/1	0.83	0.45	-	54,54,54,54	0
56	MG	DA	3106	1/1	0.94	0.21	-	41,41,41,41	0
56	MG	BA	3282	1/1	0.87	0.37	-	49,49,49,49	0
56	MG	DA	3539	1/1	0.94	0.17	-	53,53,53,53	0
56	MG	DA	3226	1/1	0.91	0.21	-	50,50,50,50	0
56	MG	BA	3595	1/1	0.95	0.16	-	41,41,41,41	0
56	MG	BA	3245	1/1	0.92	0.30	-	47,47,47,47	0
56	MG	AA	3080	1/1	0.90	0.17	-	53,53,53,53	0
56	MG	DA	3621	1/1	0.91	0.14	-	54,54,54,54	0
56	MG	BZ	3001	1/1	0.83	0.28	-	61,61,61,61	0
56	MG	DA	3612	1/1	0.99	0.14	-	39,39,39,39	0
56	MG	BA	3334	1/1	0.83	0.30	-	73,73,73,73	0
56	MG	DA	3435	1/1	0.94	0.21	-	46,46,46,46	0
56	MG	CA	3024	1/1	0.72	0.44	-	65,65,65,65	0
56	MG	DA	3181	1/1	0.99	0.30	-	36,36,36,36	0
56	MG	BA	3265	1/1	0.96	0.11	-	20,20,20,20	0
56	MG	DA	3567	1/1	0.91	0.15	-	62,62,62,62	0
56	MG	DA	3630	1/1	0.97	0.20	-	40,40,40,40	0
56	MG	DA	3510	1/1	0.93	0.23	-	63,63,63,63	0
56	MG	BA	3603	1/1	0.95	0.08	-	39,39,39,39	0
56	MG	BA	3617	1/1	0.92	0.23	-	62,62,62,62	0
56	MG	DA	3428	1/1	0.97	0.27	-	51,51,51,51	0
56	MG	AA	3167	1/1	0.93	0.19	-	67,67,67,67	0
56	MG	BA	3330	1/1	0.95	0.16	-	39,39,39,39	0
56	MG	AA	3174	1/1	0.96	0.22	-	33,33,33,33	0
56	MG	BA	3101	1/1	0.95	0.17	-	35,35,35,35	0
56	MG	CA	3073	1/1	0.82	0.39	-	55,55,55,55	0
56	MG	BA	3626	1/1	0.85	0.11	-	43,43,43,43	0
56	MG	BA	3107	1/1	0.94	0.23	-	40,40,40,40	0
56	MG	BA	3170	1/1	0.97	0.66	-	48,48,48,48	0
56	MG	CA	3131	1/1	0.86	0.10	-	55,55,55,55	0
56	MG	BA	3464	1/1	0.91	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	3528	1/1	0.94	0.09	-	56,56,56,56	0
56	MG	DA	3044	1/1	0.90	0.13	-	46,46,46,46	0
56	MG	BA	3016	1/1	0.92	0.24	-	33,33,33,33	0
56	MG	AA	3128	1/1	0.71	0.20	-	68,68,68,68	0
56	MG	DA	3158	1/1	0.96	0.34	-	57,57,57,57	0
56	MG	DA	3373	1/1	0.93	0.23	-	29,29,29,29	0
56	MG	BA	3711	1/1	0.93	0.17	-	86,86,86,86	0
56	MG	DA	3550	1/1	0.95	0.17	-	53,53,53,53	0
56	MG	AA	3185	1/1	0.97	0.28	-	46,46,46,46	0
56	MG	CA	3156	1/1	0.95	0.15	-	70,70,70,70	0
56	MG	DB	3001	1/1	0.81	0.25	-	68,68,68,68	0
56	MG	DA	3508	1/1	0.97	0.19	-	38,38,38,38	0
56	MG	DA	3534	1/1	0.95	0.18	-	45,45,45,45	0
56	MG	BU	204	1/1	0.93	0.38	-	44,44,44,44	0
56	MG	DA	3371	1/1	0.97	0.07	-	44,44,44,44	0
56	MG	DA	3453	1/1	0.92	0.36	-	61,61,61,61	0
56	MG	BA	3208	1/1	0.98	0.29	-	41,41,41,41	0
56	MG	DA	3582	1/1	0.90	0.11	-	52,52,52,52	0
56	MG	DA	3222	1/1	0.85	0.13	-	71,71,71,71	0
56	MG	BA	3639	1/1	0.95	0.16	-	50,50,50,50	0
56	MG	BA	3572	1/1	0.97	0.20	-	36,36,36,36	0
56	MG	BA	3046	1/1	0.99	0.14	-	29,29,29,29	0
56	MG	CA	3129	1/1	0.98	0.14	-	45,45,45,45	0
56	MG	CA	3067	1/1	0.73	0.30	-	80,80,80,80	0
56	MG	BA	3253	1/1	0.86	0.16	-	51,51,51,51	0
56	MG	AA	3217	1/1	0.90	0.64	-	67,67,67,67	0
56	MG	BA	3201	1/1	0.95	0.29	-	36,36,36,36	0
56	MG	BA	3004	1/1	0.95	0.12	-	24,24,24,24	0
56	MG	BA	3132	1/1	0.91	0.25	-	35,35,35,35	0
56	MG	DA	3189	1/1	0.82	0.11	-	55,55,55,55	0
56	MG	BA	3123	1/1	0.82	0.33	-	69,69,69,69	0
56	MG	BA	3136	1/1	0.85	0.23	-	58,58,58,58	0
56	MG	DA	3503	1/1	0.90	0.17	-	71,71,71,71	0
56	MG	BA	3604	1/1	0.96	0.11	-	72,72,72,72	0
56	MG	BA	3479	1/1	0.97	0.10	-	56,56,56,56	0
56	MG	DA	3470	1/1	0.93	0.28	-	52,52,52,52	0
56	MG	BA	3336	1/1	0.89	0.21	-	54,54,54,54	0
56	MG	BA	3426	1/1	0.96	0.27	-	51,51,51,51	0
56	MG	CA	3165	1/1	0.98	0.08	-	40,40,40,40	0
56	MG	BA	3399	1/1	0.99	0.19	-	18,18,18,18	0
56	MG	BA	3645	1/1	0.95	0.09	-	56,56,56,56	0
56	MG	BA	3146	1/1	0.80	0.28	-	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	DA	3422	1/1	0.96	0.11	-	38,38,38,38	0
56	MG	DA	3007	1/1	0.96	0.23	-	30,30,30,30	0
56	MG	DA	3323	1/1	0.98	0.18	-	30,30,30,30	0
56	MG	DA	3355	1/1	0.99	0.27	-	18,18,18,18	0
56	MG	BA	3517	1/1	0.97	0.08	-	49,49,49,49	0
56	MG	DA	3256	1/1	0.84	0.18	-	63,63,63,63	0
56	MG	AA	3094	1/1	0.85	0.21	-	68,68,68,68	0
56	MG	DA	3075	1/1	0.90	0.34	-	44,44,44,44	0
56	MG	CA	3011	1/1	0.95	0.28	-	42,42,42,42	0
56	MG	AA	3097	1/1	0.98	0.25	-	43,43,43,43	0
56	MG	AA	3138	1/1	0.88	0.54	-	37,37,37,37	0
56	MG	AA	3184	1/1	0.90	0.10	-	72,72,72,72	0
56	MG	AA	3151	1/1	0.99	0.08	-	41,41,41,41	0
56	MG	AA	3178	1/1	0.96	0.18	-	65,65,65,65	0
56	MG	CA	3040	1/1	0.88	0.35	-	42,42,42,42	0
56	MG	BA	3672	1/1	0.95	0.31	-	48,48,48,48	0
56	MG	B2	101	1/1	0.82	0.36	-	40,40,40,40	0
56	MG	DA	3204	1/1	0.94	0.41	-	34,34,34,34	0
56	MG	BA	3233	1/1	0.95	0.18	-	47,47,47,47	0
56	MG	BA	3263	1/1	0.72	0.24	-	79,79,79,79	0
56	MG	BA	3111	1/1	0.85	0.40	-	53,53,53,53	0
56	MG	DA	3293	1/1	0.80	0.28	-	53,53,53,53	0
56	MG	BB	3004	1/1	0.82	0.26	-	54,54,54,54	0
56	MG	CA	3035	1/1	0.83	0.23	-	52,52,52,52	0
56	MG	BA	3031	1/1	0.97	0.79	-	41,41,41,41	0
56	MG	AA	3110	1/1	0.80	0.24	-	48,48,48,48	0
56	MG	AA	3187	1/1	0.95	0.04	-	62,62,62,62	0
56	MG	BA	3159	1/1	0.90	0.31	-	48,48,48,48	0
56	MG	AA	3018	1/1	0.94	0.27	-	38,38,38,38	0
56	MG	DA	3591	1/1	0.86	0.26	-	58,58,58,58	0
56	MG	BA	3439	1/1	0.94	0.16	-	34,34,34,34	0
56	MG	DA	3188	1/1	0.92	0.34	-	47,47,47,47	0
56	MG	DA	3493	1/1	0.97	0.15	-	29,29,29,29	0
56	MG	AA	3052	1/1	0.90	0.25	-	60,60,60,60	0
56	MG	BA	3605	1/1	0.95	0.30	-	59,59,59,59	0
56	MG	BA	3035	1/1	0.96	0.09	-	37,37,37,37	0
56	MG	DA	3286	1/1	0.89	0.17	-	62,62,62,62	0
56	MG	AA	3169	1/1	0.91	0.16	-	76,76,76,76	0
56	MG	DA	3003	1/1	0.81	0.35	-	56,56,56,56	0
56	MG	DA	3599	1/1	0.88	0.23	-	72,72,72,72	0
56	MG	BA	3062	1/1	0.88	0.34	-	42,42,42,42	0
56	MG	CA	3093	1/1	0.98	0.06	-	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	BA	3293	1/1	0.94	0.18	-	45,45,45,45	0
56	MG	DA	3126	1/1	0.90	0.34	-	43,43,43,43	0
56	MG	CA	3016	1/1	0.64	0.48	-	76,76,76,76	0
56	MG	CA	3145	1/1	0.96	0.08	-	43,43,43,43	0
56	MG	DA	3273	1/1	0.93	0.13	-	30,30,30,30	0
56	MG	DA	3384	1/1	0.95	0.11	-	23,23,23,23	0
56	MG	DA	3290	1/1	0.98	0.07	-	42,42,42,42	0
56	MG	BA	3166	1/1	0.84	0.53	-	59,59,59,59	0
56	MG	CA	3018	1/1	0.76	0.31	-	54,54,54,54	0
56	MG	AA	3136	1/1	0.91	0.08	-	62,62,62,62	0
56	MG	DA	3020	1/1	0.93	0.30	-	52,52,52,52	0
56	MG	DA	3475	1/1	0.98	0.11	-	36,36,36,36	0
56	MG	DA	3420	1/1	0.96	0.13	-	51,51,51,51	0
56	MG	BA	3234	1/1	0.96	0.30	-	55,55,55,55	0
56	MG	AA	3058	1/1	0.93	0.16	-	50,50,50,50	0
56	MG	BA	3017	1/1	0.88	0.54	-	44,44,44,44	0
56	MG	DD	308	1/1	0.93	0.15	-	55,55,55,55	0
56	MG	DA	3563	1/1	0.97	0.14	-	64,64,64,64	0
56	MG	DA	3403	1/1	0.96	0.14	-	28,28,28,28	0
56	MG	CA	3096	1/1	0.96	0.10	-	60,60,60,60	0
56	MG	AA	3181	1/1	0.89	0.28	-	57,57,57,57	0
56	MG	CA	3128	1/1	0.98	0.26	-	41,41,41,41	0
56	MG	DA	3292	1/1	0.87	0.22	-	37,37,37,37	0
56	MG	DA	3187	1/1	0.82	0.44	-	59,59,59,59	0
56	MG	DA	3444	1/1	0.95	0.13	-	43,43,43,43	0
56	MG	BA	3501	1/1	0.87	0.26	-	59,59,59,59	0
56	MG	CA	3123	1/1	0.82	0.14	-	77,77,77,77	0
56	MG	DA	3281	1/1	0.93	0.21	-	42,42,42,42	0
56	MG	BA	3437	1/1	0.97	0.15	-	42,42,42,42	0
56	MG	AA	3070	1/1	0.95	0.10	-	75,75,75,75	0
56	MG	BA	3650	1/1	0.94	0.15	-	45,45,45,45	0
56	MG	CA	3015	1/1	0.83	0.34	-	51,51,51,51	0
56	MG	DA	3442	1/1	0.94	0.19	-	40,40,40,40	0
56	MG	BA	3142	1/1	0.94	0.71	-	46,46,46,46	0
56	MG	DA	3474	1/1	0.93	0.08	-	61,61,61,61	0
56	MG	AA	3195	1/1	0.95	0.17	-	71,71,71,71	0
56	MG	BA	3339	1/1	0.95	0.22	-	43,43,43,43	0
56	MG	CA	3112	1/1	0.97	0.23	-	59,59,59,59	0
56	MG	DA	3156	1/1	0.94	0.56	-	29,29,29,29	0
56	MG	DA	3153	1/1	0.96	0.20	-	38,38,38,38	0
56	MG	CA	3076	1/1	0.94	0.33	-	40,40,40,40	0
56	MG	DA	3405	1/1	0.88	0.11	-	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	BW	203	1/1	0.87	0.32	-	45,45,45,45	0
56	MG	BA	3487	1/1	0.98	0.12	-	31,31,31,31	0
56	MG	BA	3272	1/1	0.97	0.34	-	7,7,7,7	0
56	MG	DA	3209	1/1	0.94	0.17	-	41,41,41,41	0
56	MG	DA	3248	1/1	0.96	0.29	-	51,51,51,51	0
56	MG	DW	201	1/1	0.93	0.31	-	46,46,46,46	0
56	MG	CA	3140	1/1	0.92	0.16	-	73,73,73,73	0
56	MG	DN	5001	1/1	0.96	0.12	-	75,75,75,75	0
56	MG	BA	3246	1/1	0.93	0.24	-	46,46,46,46	0
56	MG	AA	3212	1/1	0.85	0.15	-	79,79,79,79	0
56	MG	BA	3130	1/1	0.96	0.59	-	43,43,43,43	0
56	MG	BA	3247	1/1	0.51	0.96	-	68,68,68,68	0
56	MG	DA	3193	1/1	0.91	0.22	-	65,65,65,65	0
56	MG	DA	3172	1/1	0.91	0.44	-	51,51,51,51	0
56	MG	DA	3381	1/1	0.96	0.27	-	47,47,47,47	0
56	MG	AA	3117	1/1	0.75	0.26	-	71,71,71,71	0
56	MG	BA	3259	1/1	0.94	0.49	-	27,27,27,27	0
56	MG	DA	3441	1/1	0.89	0.30	-	53,53,53,53	0
56	MG	DA	3077	1/1	0.90	0.28	-	50,50,50,50	0
56	MG	BA	3055	1/1	0.91	0.23	-	44,44,44,44	0
56	MG	BA	3531	1/1	0.99	0.29	-	38,38,38,38	0
56	MG	BA	3558	1/1	0.89	0.22	-	35,35,35,35	0
56	MG	AA	3158	1/1	0.97	0.20	-	44,44,44,44	0
56	MG	BA	3032	1/1	0.97	0.19	-	49,49,49,49	0
56	MG	BA	3102	1/1	0.84	0.32	-	52,52,52,52	0
56	MG	CA	3074	1/1	0.93	0.18	-	54,54,54,54	0
56	MG	DA	3529	1/1	0.98	0.10	-	63,63,63,63	0
56	MG	DA	3557	1/1	0.96	0.12	-	45,45,45,45	0
56	MG	BA	3485	1/1	0.96	0.29	-	44,44,44,44	0
56	MG	BA	3513	1/1	0.96	0.11	-	45,45,45,45	0
56	MG	BA	3590	1/1	0.86	0.13	-	64,64,64,64	0
56	MG	BA	3058	1/1	0.88	0.45	-	38,38,38,38	0
56	MG	AA	3186	1/1	0.97	0.07	-	49,49,49,49	0
56	MG	BD	311	1/1	0.82	0.54	-	45,45,45,45	0
56	MG	BA	3084	1/1	0.94	0.14	-	33,33,33,33	0
56	MG	DA	3055	1/1	0.95	0.20	-	48,48,48,48	0
56	MG	DA	3288	1/1	0.94	0.17	-	47,47,47,47	0
56	MG	AA	3045	1/1	0.64	0.31	-	61,61,61,61	0
56	MG	CA	3002	1/1	0.88	0.07	-	62,62,62,62	0
56	MG	DA	3342	1/1	0.91	0.12	-	52,52,52,52	0
56	MG	CA	3151	1/1	0.91	0.25	-	80,80,80,80	0
56	MG	AA	3017	1/1	0.94	0.27	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3095	1/1	0.96	0.11	-	39,39,39,39	0
56	MG	DQ	203	1/1	0.97	0.32	-	57,57,57,57	0
56	MG	CX	103	1/1	0.76	0.25	-	60,60,60,60	0
56	MG	BA	3044	1/1	0.94	0.30	-	42,42,42,42	0
56	MG	BA	3095	1/1	0.98	0.47	-	55,55,55,55	0
56	MG	CA	3158	1/1	0.85	0.23	-	76,76,76,76	0
56	MG	AX	105	1/1	0.91	0.69	-	56,56,56,56	0
56	MG	BA	3210	1/1	0.97	0.11	-	34,34,34,34	0
56	MG	BA	3308	1/1	0.98	0.08	-	44,44,44,44	0
56	MG	BA	3097	1/1	0.95	0.19	-	33,33,33,33	0
56	MG	BA	3702	1/1	0.98	0.12	-	56,56,56,56	0
56	MG	DA	3314	1/1	0.80	0.19	-	64,64,64,64	0
56	MG	DW	202	1/1	0.73	0.42	-	58,58,58,58	0
56	MG	CA	3143	1/1	0.88	0.07	-	87,87,87,87	0
56	MG	DA	3634	1/1	0.94	0.14	-	51,51,51,51	0
56	MG	CA	3115	1/1	0.96	0.09	-	55,55,55,55	0
56	MG	BA	3675	1/1	0.98	0.12	-	49,49,49,49	0
56	MG	DA	3593	1/1	0.89	0.23	-	73,73,73,73	0
56	MG	DA	3023	1/1	0.97	0.28	-	52,52,52,52	0
56	MG	BA	3157	1/1	0.82	0.39	-	63,63,63,63	0
56	MG	BA	3570	1/1	0.94	0.12	-	61,61,61,61	0
56	MG	DA	3559	1/1	0.92	0.19	-	46,46,46,46	0
56	MG	BA	3549	1/1	0.93	0.22	-	27,27,27,27	0
56	MG	CA	3138	1/1	0.80	0.24	-	72,72,72,72	0
56	MG	DA	3144	1/1	0.93	0.39	-	36,36,36,36	0
56	MG	DA	3392	1/1	0.94	0.17	-	35,35,35,35	0
56	MG	DA	3081	1/1	0.88	0.20	-	48,48,48,48	0
56	MG	DA	3168	1/1	0.86	0.38	-	48,48,48,48	0
56	MG	AA	3034	1/1	0.93	0.18	-	48,48,48,48	0
56	MG	BA	3120	1/1	0.97	0.09	-	51,51,51,51	0
56	MG	DA	3145	1/1	0.89	0.46	-	65,65,65,65	0
56	MG	DA	3590	1/1	0.89	0.17	-	80,80,80,80	0
56	MG	BW	202	1/1	0.96	0.18	-	34,34,34,34	0
56	MG	BA	3313	1/1	0.98	0.27	-	36,36,36,36	0
56	MG	BA	3680	1/1	0.97	0.35	-	37,37,37,37	0
56	MG	DA	3533	1/1	0.98	0.08	-	68,68,68,68	0
56	MG	AA	3197	1/1	0.94	0.30	-	69,69,69,69	0
56	MG	DA	3127	1/1	0.93	0.09	-	48,48,48,48	0
56	MG	CA	3060	1/1	0.81	0.37	-	43,43,43,43	0
56	MG	BA	3158	1/1	0.80	0.53	-	64,64,64,64	0
56	MG	DA	3367	1/1	0.83	0.26	-	42,42,42,42	0
56	MG	BA	3275	1/1	0.78	0.21	-	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	3598	1/1	0.84	0.12	-	56,56,56,56	0
56	MG	AA	3153	1/1	0.96	0.13	-	45,45,45,45	0
56	MG	BA	3736	1/1	0.82	0.25	-	48,48,48,48	0
56	MG	BA	3066	1/1	0.94	0.26	-	44,44,44,44	0
56	MG	AA	3215	1/1	0.90	0.10	-	53,53,53,53	0
56	MG	BA	3250	1/1	0.93	0.21	-	45,45,45,45	0
56	MG	BA	3566	1/1	0.96	0.09	-	53,53,53,53	0
56	MG	BA	3655	1/1	0.98	0.21	-	52,52,52,52	0
56	MG	BA	3186	1/1	0.98	0.14	-	53,53,53,53	0
56	MG	DA	3105	1/1	0.90	0.38	-	48,48,48,48	0
56	MG	DA	3050	1/1	0.92	0.57	-	31,31,31,31	0
56	MG	AA	3191	1/1	0.93	0.13	-	71,71,71,71	0
56	MG	BA	3401	1/1	0.92	0.12	-	42,42,42,42	0
56	MG	DA	3234	1/1	0.98	0.23	-	33,33,33,33	0
56	MG	BA	3073	1/1	0.95	0.86	-	41,41,41,41	0
56	MG	CA	3017	1/1	0.98	0.25	-	42,42,42,42	0
56	MG	BA	3556	1/1	0.98	0.31	-	27,27,27,27	0
56	MG	CA	3009	1/1	0.95	0.14	-	47,47,47,47	0
56	MG	CA	3106	1/1	0.91	0.35	-	64,64,64,64	0
56	MG	BA	3175	1/1	0.85	0.25	-	48,48,48,48	0
56	MG	DA	3108	1/1	0.87	0.47	-	37,37,37,37	0
56	MG	DA	3325	1/1	0.95	0.17	-	36,36,36,36	0
56	MG	BA	3417	1/1	0.94	0.18	-	18,18,18,18	0
56	MG	DA	3214	1/1	0.88	0.27	-	64,64,64,64	0
56	MG	BA	3190	1/1	0.93	0.20	-	42,42,42,42	0
56	MG	DA	3213	1/1	0.90	0.21	-	44,44,44,44	0
56	MG	BA	3285	1/1	0.85	0.14	-	32,32,32,32	0
56	MG	DA	3481	1/1	0.87	0.27	-	47,47,47,47	0
56	MG	DA	3501	1/1	0.94	0.20	-	23,23,23,23	0
56	MG	AA	3028	1/1	0.65	0.47	-	60,60,60,60	0
56	MG	BA	3302	1/1	0.97	0.13	-	27,27,27,27	0
56	MG	BY	201	1/1	0.94	0.43	-	58,58,58,58	0
56	MG	BA	3375	1/1	0.98	0.24	-	31,31,31,31	0
56	MG	BA	3236	1/1	0.87	0.17	-	36,36,36,36	0
56	MG	BA	3103	1/1	0.89	0.12	-	53,53,53,53	0
56	MG	AA	3119	1/1	0.90	0.37	-	63,63,63,63	0
56	MG	CA	3010	1/1	0.91	0.11	-	32,32,32,32	0
56	MG	DA	3269	1/1	0.97	0.12	-	48,48,48,48	0
56	MG	DA	3276	1/1	0.96	0.22	-	36,36,36,36	0
56	MG	AA	3203	1/1	0.97	0.12	-	63,63,63,63	0
56	MG	BA	3652	1/1	0.92	0.20	-	64,64,64,64	0
56	MG	DA	3319	1/1	0.95	0.18	-	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	DA	3515	1/1	0.83	0.22	-	48,48,48,48	0
56	MG	DA	3169	1/1	0.89	0.38	-	57,57,57,57	0
56	MG	BA	3392	1/1	0.97	0.26	-	56,56,56,56	0
56	MG	DA	3259	1/1	0.96	0.15	-	47,47,47,47	0
56	MG	AA	3137	1/1	0.87	0.21	-	42,42,42,42	0
56	MG	BA	3730	1/1	0.90	0.64	-	45,45,45,45	0
56	MG	DA	3329	1/1	0.95	0.16	-	53,53,53,53	0
56	MG	BA	3475	1/1	0.96	0.21	-	36,36,36,36	0
56	MG	BA	3307	1/1	0.98	0.20	-	33,33,33,33	0
56	MG	CA	3084	1/1	0.94	0.11	-	64,64,64,64	0
56	MG	DA	3066	1/1	0.90	0.37	-	53,53,53,53	0
56	MG	DA	3548	1/1	0.90	0.13	-	37,37,37,37	0
56	MG	BA	3440	1/1	0.96	0.40	-	38,38,38,38	0
56	MG	AA	3043	1/1	0.51	0.50	-	74,74,74,74	0
56	MG	DA	3348	1/1	0.95	0.32	-	37,37,37,37	0
56	MG	DA	3052	1/1	0.94	0.20	-	23,23,23,23	0
56	MG	BA	3677	1/1	0.82	0.27	-	67,67,67,67	0
56	MG	DA	3516	1/1	0.95	0.17	-	40,40,40,40	0
56	MG	DA	3061	1/1	0.85	0.45	-	52,52,52,52	0
56	MG	DA	3421	1/1	0.97	0.19	-	34,34,34,34	0
56	MG	DA	3202	1/1	0.92	0.33	-	42,42,42,42	0
56	MG	CA	3052	1/1	0.97	0.12	-	39,39,39,39	0
56	MG	AA	3066	1/1	0.93	0.30	-	38,38,38,38	0
56	MG	BA	3273	1/1	0.93	0.39	-	42,42,42,42	0
56	MG	AX	102	1/1	0.69	0.25	-	74,74,74,74	0
56	MG	BA	3461	1/1	0.95	0.24	-	36,36,36,36	0
56	MG	AA	3125	1/1	0.91	0.16	-	47,47,47,47	0
56	MG	B8	102	1/1	0.98	0.10	-	60,60,60,60	0
56	MG	BA	3690	1/1	0.93	0.17	-	53,53,53,53	0
56	MG	DY	502	1/1	0.94	0.10	-	60,60,60,60	0
56	MG	AA	3204	1/1	0.97	0.14	-	54,54,54,54	0
56	MG	DA	3252	1/1	0.88	0.12	-	45,45,45,45	0
56	MG	BA	3687	1/1	0.93	0.22	-	38,38,38,38	0
56	MG	DA	3096	1/1	0.90	0.17	-	60,60,60,60	0
56	MG	BA	3001	1/1	0.96	0.15	-	69,69,69,69	0
56	MG	BA	3644	1/1	0.97	0.16	-	43,43,43,43	0
56	MG	CA	3045	1/1	0.97	0.09	-	54,54,54,54	0
56	MG	CA	3077	1/1	0.99	0.22	-	53,53,53,53	0
56	MG	DA	3614	1/1	0.95	0.20	-	48,48,48,48	0
56	MG	AA	3089	1/1	0.80	0.43	-	78,78,78,78	0
56	MG	BA	3209	1/1	0.79	0.38	-	40,40,40,40	0
56	MG	BA	3019	1/1	0.90	0.18	-	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	3380	1/1	0.96	0.13	-	53,53,53,53	0
56	MG	AA	3044	1/1	0.71	0.22	-	66,66,66,66	0
56	MG	DA	3331	1/1	0.99	0.09	-	34,34,34,34	0
56	MG	AA	3056	1/1	0.95	0.19	-	39,39,39,39	0
56	MG	BA	3177	1/1	0.89	0.21	-	62,62,62,62	0
56	MG	CA	3082	1/1	0.95	0.08	-	47,47,47,47	0
56	MG	DA	3574	1/1	0.94	0.17	-	56,56,56,56	0
56	MG	BA	3456	1/1	0.97	0.10	-	52,52,52,52	0
56	MG	BA	3116	1/1	0.97	0.20	-	31,31,31,31	0
56	MG	B5	502	1/1	0.95	0.10	-	54,54,54,54	0
56	MG	CA	3086	1/1	0.88	0.20	-	80,80,80,80	0
56	MG	BA	3312	1/1	0.95	0.10	-	58,58,58,58	0
56	MG	BA	3008	1/1	0.98	0.13	-	50,50,50,50	0
56	MG	BA	3608	1/1	0.93	0.13	-	68,68,68,68	0
56	MG	BA	3310	1/1	0.98	0.17	-	13,13,13,13	0
56	MG	BA	3692	1/1	0.94	0.40	-	36,36,36,36	0
56	MG	BA	3450	1/1	0.97	0.27	-	46,46,46,46	0
56	MG	BA	3360	1/1	0.97	0.19	-	38,38,38,38	0
56	MG	BF	304	1/1	0.92	0.09	-	35,35,35,35	0
56	MG	BA	3167	1/1	0.97	0.39	-	39,39,39,39	0
56	MG	BA	3410	1/1	0.99	0.15	-	27,27,27,27	0
56	MG	DA	3150	1/1	0.88	0.21	-	64,64,64,64	0
56	MG	BA	3430	1/1	0.92	0.32	-	49,49,49,49	0
56	MG	BA	3547	1/1	0.95	0.18	-	31,31,31,31	0
56	MG	DA	3351	1/1	0.98	0.38	-	35,35,35,35	0
56	MG	BA	3082	1/1	0.94	0.29	-	41,41,41,41	0
56	MG	DA	3485	1/1	0.96	0.09	-	38,38,38,38	0
56	MG	BA	3266	1/1	0.96	0.33	-	46,46,46,46	0
56	MG	DA	3037	1/1	0.97	0.30	-	35,35,35,35	0
56	MG	AA	3188	1/1	0.99	0.24	-	53,53,53,53	0
56	MG	CA	3062	1/1	0.80	0.26	-	57,57,57,57	0
56	MG	BA	3151	1/1	0.96	0.06	-	52,52,52,52	0
56	MG	DA	3571	1/1	0.97	0.13	-	46,46,46,46	0
56	MG	BA	3280	1/1	0.88	0.70	-	69,69,69,69	0
56	MG	DA	3216	1/1	0.95	0.17	-	31,31,31,31	0
56	MG	BA	3386	1/1	0.94	0.14	-	58,58,58,58	0
56	MG	BA	3242	1/1	0.82	0.36	-	48,48,48,48	0
56	MG	BA	3171	1/1	0.97	0.41	-	40,40,40,40	0
56	MG	BA	3333	1/1	0.97	0.12	-	49,49,49,49	0
56	MG	AA	3061	1/1	0.80	0.19	-	82,82,82,82	0
56	MG	BO	201	1/1	0.97	0.14	-	70,70,70,70	0
56	MG	DA	3068	1/1	0.67	0.33	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3471	1/1	0.99	0.17	-	51,51,51,51	0
56	MG	AA	3105	1/1	0.92	0.22	-	46,46,46,46	0
56	MG	DA	3433	1/1	0.94	0.17	-	48,48,48,48	0
56	MG	DA	3082	1/1	0.96	0.10	-	19,19,19,19	0
56	MG	BA	3666	1/1	0.91	0.31	-	61,61,61,61	0
56	MG	BA	3104	1/1	0.89	0.28	-	45,45,45,45	0
56	MG	DA	3650	1/1	0.97	0.59	-	48,48,48,48	0
56	MG	BA	3731	1/1	0.80	0.36	-	55,55,55,55	0
56	MG	BA	3606	1/1	0.96	0.23	-	25,25,25,25	0
56	MG	BA	3586	1/1	0.98	0.19	-	29,29,29,29	0
56	MG	DA	3622	1/1	0.96	0.08	-	55,55,55,55	0
56	MG	BA	3204	1/1	0.97	0.40	-	25,25,25,25	0
56	MG	DA	3536	1/1	0.92	0.16	-	80,80,80,80	0
56	MG	CA	3029	1/1	0.89	0.15	-	59,59,59,59	0
56	MG	AA	3037	1/1	0.72	0.41	-	61,61,61,61	0
56	MG	BA	3540	1/1	0.95	0.27	-	34,34,34,34	0
56	MG	DF	306	1/1	0.96	0.23	-	50,50,50,50	0
56	MG	DA	3487	1/1	0.89	0.19	-	57,57,57,57	0
56	MG	AA	3029	1/1	0.84	0.69	-	52,52,52,52	0
56	MG	CA	3033	1/1	0.76	0.19	-	68,68,68,68	0
56	MG	BA	3391	1/1	0.91	0.14	-	48,48,48,48	0
56	MG	DA	3128	1/1	0.90	0.19	-	52,52,52,52	0
56	MG	AA	3205	1/1	0.98	0.19	-	61,61,61,61	0
56	MG	B0	102	1/1	0.84	0.61	-	40,40,40,40	0
56	MG	DA	3239	1/1	0.97	0.21	-	39,39,39,39	0
56	MG	DA	3556	1/1	0.93	0.08	-	56,56,56,56	0
56	MG	DA	3502	1/1	0.92	0.13	-	65,65,65,65	0
56	MG	BA	3518	1/1	0.97	0.10	-	41,41,41,41	0
56	MG	AX	103	1/1	0.81	0.08	-	66,66,66,66	0
56	MG	BA	3081	1/1	0.98	0.08	-	14,14,14,14	0
56	MG	BA	3284	1/1	0.95	0.10	-	54,54,54,54	0
56	MG	DA	3103	1/1	0.70	0.78	-	48,48,48,48	0
56	MG	BA	3699	1/1	0.74	0.51	-	56,56,56,56	0
56	MG	BA	3466	1/1	0.91	0.14	-	61,61,61,61	0
56	MG	BE	304	1/1	0.97	0.09	-	49,49,49,49	0
56	MG	DA	3386	1/1	0.96	0.18	-	56,56,56,56	0
56	MG	DA	3232	1/1	0.95	0.25	-	50,50,50,50	0
56	MG	DA	3496	1/1	0.91	0.15	-	53,53,53,53	0
56	MG	DA	3449	1/1	0.97	0.09	-	43,43,43,43	0
56	MG	BA	3638	1/1	0.91	0.21	-	37,37,37,37	0
56	MG	CA	3038	1/1	0.68	0.46	-	70,70,70,70	0
56	MG	BA	3301	1/1	0.94	0.13	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3086	1/1	0.74	0.30	-	51,51,51,51	0
56	MG	BA	3213	1/1	0.96	0.05	-	41,41,41,41	0
56	MG	DA	3363	1/1	0.90	0.09	-	57,57,57,57	0
56	MG	BA	3029	1/1	0.80	0.38	-	53,53,53,53	0
56	MG	DA	3257	1/1	0.96	0.10	-	48,48,48,48	0
56	MG	CA	3031	1/1	0.84	0.39	-	53,53,53,53	0
56	MG	DA	3080	1/1	0.87	0.14	-	44,44,44,44	0
56	MG	BA	3268	1/1	0.87	0.17	-	46,46,46,46	0
56	MG	AA	3079	1/1	0.60	1.07	-	74,74,74,74	0
56	MG	DA	3427	1/1	0.58	0.54	-	60,60,60,60	0
56	MG	BW	205	1/1	0.93	0.46	-	41,41,41,41	0
56	MG	CA	3172	1/1	0.81	0.15	-	51,51,51,51	0
56	MG	BA	3620	1/1	0.95	0.12	-	47,47,47,47	0
56	MG	DA	3396	1/1	0.95	0.19	-	35,35,35,35	0
56	MG	BA	3243	1/1	0.90	0.15	-	48,48,48,48	0
56	MG	AA	3126	1/1	0.95	0.16	-	54,54,54,54	0
56	MG	BE	306	1/1	0.93	0.44	-	46,46,46,46	0
56	MG	BA	3231	1/1	0.76	0.54	-	38,38,38,38	0
56	MG	BA	3252	1/1	0.87	0.17	-	55,55,55,55	0
56	MG	BA	3163	1/1	0.88	0.18	-	50,50,50,50	0
56	MG	BA	3384	1/1	0.96	0.40	-	60,60,60,60	0
56	MG	AA	3046	1/1	0.88	0.12	-	73,73,73,73	0
56	MG	BA	3237	1/1	0.89	0.55	-	51,51,51,51	0
56	MG	BA	3189	1/1	0.95	0.16	-	54,54,54,54	0
56	MG	BA	3149	1/1	0.89	0.55	-	40,40,40,40	0
56	MG	AA	3148	1/1	0.95	0.21	-	66,66,66,66	0
56	MG	BA	3127	1/1	0.89	0.38	-	50,50,50,50	0
56	MG	AA	3200	1/1	0.92	0.24	-	68,68,68,68	0
56	MG	DA	3522	1/1	0.95	0.17	-	61,61,61,61	0
56	MG	BA	3364	1/1	0.97	0.24	-	29,29,29,29	0
56	MG	BA	3449	1/1	0.94	0.12	-	21,21,21,21	0
56	MG	DA	3045	1/1	0.93	0.37	-	41,41,41,41	0
56	MG	BA	3174	1/1	0.90	0.09	-	48,48,48,48	0
56	MG	DA	3530	1/1	0.96	0.15	-	49,49,49,49	0
56	MG	DA	3580	1/1	0.93	0.14	-	46,46,46,46	0
56	MG	DB	3002	1/1	0.95	0.25	-	56,56,56,56	0
56	MG	BA	3083	1/1	0.82	0.23	-	63,63,63,63	0
56	MG	AA	3132	1/1	0.88	0.36	-	76,76,76,76	0
56	MG	DA	3604	1/1	0.87	0.20	-	54,54,54,54	0
56	MG	CA	3094	1/1	0.95	0.18	-	43,43,43,43	0
56	MG	AA	3005	1/1	0.90	0.20	-	66,66,66,66	0
56	MG	BA	3443	1/1	0.91	0.17	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3480	1/1	0.98	0.09	-	52,52,52,52	0
56	MG	DA	3299	1/1	0.95	0.22	-	40,40,40,40	0
56	MG	BA	3519	1/1	0.98	0.12	-	39,39,39,39	0
56	MG	DA	3531	1/1	0.85	0.09	-	57,57,57,57	0
56	MG	DA	3175	1/1	0.94	0.17	-	40,40,40,40	0
56	MG	BA	3422	1/1	0.95	0.23	-	42,42,42,42	0
56	MG	DA	3570	1/1	0.95	0.22	-	28,28,28,28	0
56	MG	DA	3606	1/1	0.96	0.10	-	58,58,58,58	0
56	MG	DA	3224	1/1	0.88	0.15	-	47,47,47,47	0
56	MG	CA	3044	1/1	0.94	0.20	-	63,63,63,63	0
56	MG	BA	3119	1/1	0.97	0.25	-	58,58,58,58	0
56	MG	BA	3663	1/1	0.96	0.23	-	56,56,56,56	0
56	MG	DA	3334	1/1	0.93	0.15	-	49,49,49,49	0
56	MG	BA	3618	1/1	0.95	0.27	-	46,46,46,46	0
56	MG	BA	3090	1/1	0.92	0.20	-	46,46,46,46	0
56	MG	AA	3147	1/1	0.63	0.48	-	61,61,61,61	0
56	MG	BE	310	1/1	0.97	0.24	-	50,50,50,50	0
56	MG	BA	3118	1/1	0.96	0.18	-	39,39,39,39	0
56	MG	BA	3669	1/1	0.85	0.24	-	75,75,75,75	0
56	MG	DA	3540	1/1	0.99	0.23	-	54,54,54,54	0
56	MG	CA	3103	1/1	0.85	0.19	-	83,83,83,83	0
56	MG	BA	3279	1/1	0.83	0.22	-	48,48,48,48	0
56	MG	BA	3022	1/1	0.80	0.34	-	52,52,52,52	0
56	MG	AA	3177	1/1	0.93	0.14	-	80,80,80,80	0
56	MG	BA	3292	1/1	0.89	0.21	-	63,63,63,63	0
56	MG	BA	3043	1/1	0.95	0.18	-	52,52,52,52	0
56	MG	DA	3124	1/1	0.84	0.13	-	67,67,67,67	0
56	MG	BA	3656	1/1	0.98	0.11	-	33,33,33,33	0
56	MG	DA	3426	1/1	0.96	0.15	-	74,74,74,74	0
56	MG	DA	3596	1/1	0.97	0.10	-	67,67,67,67	0
56	MG	AA	3221	1/1	0.97	0.10	-	64,64,64,64	0
56	MG	BA	3165	1/1	0.84	0.31	-	53,53,53,53	0
56	MG	DV	204	1/1	0.89	0.21	-	41,41,41,41	0
56	MG	BA	3425	1/1	0.96	0.36	-	36,36,36,36	0
56	MG	AA	3032	1/1	0.88	0.28	-	57,57,57,57	0
56	MG	BA	3535	1/1	0.94	0.19	-	37,37,37,37	0
56	MG	AX	109	1/1	0.99	0.09	-	43,43,43,43	0
56	MG	BR	202	1/1	0.94	0.29	-	27,27,27,27	0
56	MG	AA	3218	1/1	0.85	0.54	-	65,65,65,65	0
56	MG	DA	3115	1/1	0.87	0.09	-	63,63,63,63	0
56	MG	DA	3447	1/1	0.93	0.05	-	56,56,56,56	0
56	MG	DA	3376	1/1	0.91	0.08	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	K	DA	3231	1/1	0.93	0.22	-	96,96,96,96	0
56	MG	DA	3483	1/1	0.84	0.19	-	49,49,49,49	0
56	MG	CA	3159	1/1	0.88	0.61	-	91,91,91,91	0
56	MG	DA	3243	1/1	0.89	0.21	-	67,67,67,67	0
56	MG	DA	3161	1/1	0.87	0.30	-	60,60,60,60	0
56	MG	AA	3006	1/1	0.73	0.08	-	78,78,78,78	0
56	MG	CA	3022	1/1	0.98	0.04	-	70,70,70,70	0
56	MG	DA	3048	1/1	0.89	0.37	-	37,37,37,37	0
56	MG	AA	3149	1/1	0.96	0.09	-	50,50,50,50	0
56	MG	DA	3339	1/1	0.91	0.10	-	37,37,37,37	0
56	MG	DA	3337	1/1	0.98	0.09	-	27,27,27,27	0
56	MG	BA	3670	1/1	0.98	0.08	-	59,59,59,59	0
56	MG	CA	3148	1/1	0.98	0.19	-	68,68,68,68	0
56	MG	BA	3529	1/1	0.98	0.21	-	35,35,35,35	0
56	MG	BA	3138	1/1	0.95	0.17	-	46,46,46,46	0
56	MG	BA	3309	1/1	0.89	0.13	-	46,46,46,46	0
56	MG	DA	3194	1/1	0.89	0.13	-	48,48,48,48	0
56	MG	DA	3199	1/1	0.93	0.13	-	42,42,42,42	0
56	MG	AA	3164	1/1	0.85	0.38	-	69,69,69,69	0
56	MG	DA	3069	1/1	0.91	0.12	-	51,51,51,51	0
56	MG	BA	3140	1/1	0.85	0.19	-	64,64,64,64	0
56	MG	AA	3085	1/1	0.81	0.32	-	69,69,69,69	0
56	MG	BA	3321	1/1	0.99	0.16	-	29,29,29,29	0
56	MG	BA	3445	1/1	0.98	0.20	-	25,25,25,25	0
56	MG	AA	3012	1/1	0.81	0.14	-	56,56,56,56	0
56	MG	BA	3374	1/1	0.92	0.19	-	44,44,44,44	0
56	MG	DA	3274	1/1	0.97	0.09	-	52,52,52,52	0
56	MG	BA	3596	1/1	0.90	0.12	-	51,51,51,51	0
56	MG	DA	3013	1/1	0.92	0.09	-	47,47,47,47	0
56	MG	DA	3132	1/1	0.89	0.70	-	54,54,54,54	0
56	MG	DA	3159	1/1	0.89	0.24	-	51,51,51,51	0
56	MG	BA	3078	1/1	0.95	0.26	-	17,17,17,17	0
56	MG	BA	3496	1/1	0.83	0.40	-	57,57,57,57	0
56	MG	DA	3353	1/1	0.95	0.10	-	62,62,62,62	0
56	MG	BA	3679	1/1	0.98	0.40	-	27,27,27,27	0
56	MG	AA	3016	1/1	0.94	0.07	-	63,63,63,63	0
56	MG	BA	3289	1/1	0.73	0.34	-	60,60,60,60	0
56	MG	AA	3157	1/1	0.96	0.08	-	35,35,35,35	0
56	MG	BA	3181	1/1	0.90	0.34	-	38,38,38,38	0
56	MG	DA	3603	1/1	0.93	0.16	-	55,55,55,55	0
56	MG	DA	3004	1/1	0.95	0.19	-	29,29,29,29	0
56	MG	DA	3237	1/1	0.94	0.15	-	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	BA	3387	1/1	0.93	0.07	-	48,48,48,48	0
56	MG	CA	3059	1/1	0.97	0.26	-	51,51,51,51	0
56	MG	BG	3004	1/1	0.95	0.04	-	62,62,62,62	0
56	MG	AA	3130	1/1	0.95	0.23	-	46,46,46,46	0
56	MG	BA	3697	1/1	0.95	0.14	-	78,78,78,78	0
56	MG	DA	3113	1/1	0.80	0.57	-	43,43,43,43	0
56	MG	BA	3317	1/1	0.97	0.15	-	40,40,40,40	0
56	MG	DA	3416	1/1	0.96	0.07	-	44,44,44,44	0
56	MG	DA	3217	1/1	0.88	0.56	-	54,54,54,54	0
56	MG	BA	3348	1/1	0.95	0.20	-	64,64,64,64	0
56	MG	DA	3361	1/1	0.89	0.11	-	61,61,61,61	0
56	MG	BA	3701	1/1	0.97	0.13	-	32,32,32,32	0
56	MG	CA	3054	1/1	0.86	0.39	-	48,48,48,48	0
56	MG	DA	3445	1/1	0.97	0.23	-	39,39,39,39	0
56	MG	BA	3478	1/1	0.98	0.15	-	29,29,29,29	0
56	MG	BA	3444	1/1	0.82	0.15	-	74,74,74,74	0
56	MG	BA	3661	1/1	0.94	0.15	-	68,68,68,68	0
56	MG	DA	3647	1/1	0.81	0.37	-	66,66,66,66	0
56	MG	DA	3520	1/1	0.95	0.20	-	51,51,51,51	0
56	MG	AA	3096	1/1	0.78	0.28	-	44,44,44,44	0
56	MG	DA	3107	1/1	0.92	0.30	-	55,55,55,55	0
56	MG	CA	3169	1/1	0.97	0.16	-	57,57,57,57	0
56	MG	BA	3578	1/1	0.90	0.32	-	54,54,54,54	0
56	MG	BA	3514	1/1	0.89	0.14	-	37,37,37,37	0
56	MG	BB	3005	1/1	0.79	0.28	-	61,61,61,61	0
56	MG	DA	3147	1/1	0.88	0.11	-	53,53,53,53	0
56	MG	DA	3029	1/1	0.92	0.10	-	61,61,61,61	0
56	MG	AA	3055	1/1	0.96	0.20	-	50,50,50,50	0
56	MG	BA	3725	1/1	0.98	0.12	-	49,49,49,49	0
56	MG	BA	3612	1/1	0.98	0.15	-	37,37,37,37	0
56	MG	BA	3274	1/1	0.97	0.16	-	52,52,52,52	0
56	MG	BA	3573	1/1	0.94	0.16	-	56,56,56,56	0
56	MG	BA	3258	1/1	0.92	0.23	-	40,40,40,40	0
56	MG	BA	3534	1/1	0.97	0.12	-	41,41,41,41	0
56	MG	BA	3161	1/1	0.94	0.65	-	49,49,49,49	0
56	MG	AA	3007	1/1	0.95	0.18	-	82,82,82,82	0
56	MG	BB	3015	1/1	0.97	0.10	-	37,37,37,37	0
56	MG	BA	3320	1/1	0.88	0.29	-	57,57,57,57	0
56	MG	DA	3602	1/1	0.90	0.19	-	52,52,52,52	0
56	MG	AA	3127	1/1	0.78	0.18	-	62,62,62,62	0
56	MG	AA	3081	1/1	0.91	0.23	-	41,41,41,41	0
56	MG	DA	3275	1/1	0.97	0.07	-	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	BA	3361	1/1	0.96	0.26	-	34,34,34,34	0
56	MG	DA	3157	1/1	0.85	0.99	-	62,62,62,62	0
56	MG	AA	3113	1/1	0.79	0.28	-	68,68,68,68	0
56	MG	BA	3649	1/1	0.96	0.17	-	66,66,66,66	0
56	MG	BA	3581	1/1	0.98	0.10	-	51,51,51,51	0
56	MG	BA	3148	1/1	0.94	0.35	-	52,52,52,52	0
56	MG	DA	3546	1/1	0.97	0.12	-	44,44,44,44	0
56	MG	B9	502	1/1	0.86	0.27	-	49,49,49,49	0
56	MG	AA	3114	1/1	0.60	0.51	-	66,66,66,66	0
56	MG	BA	3154	1/1	0.99	0.17	-	61,61,61,61	0
56	MG	BA	3221	1/1	0.87	0.27	-	44,44,44,44	0
56	MG	BA	3588	1/1	0.95	0.21	-	48,48,48,48	0
56	MG	DA	3471	1/1	0.97	0.14	-	37,37,37,37	0
56	MG	BA	3094	1/1	0.40	0.86	-	61,61,61,61	0
56	MG	DD	302	1/1	0.87	0.23	-	46,46,46,46	0
56	MG	BA	3085	1/1	0.73	0.46	-	48,48,48,48	0
56	MG	BA	3176	1/1	0.96	0.19	-	38,38,38,38	0
56	MG	DA	3087	1/1	0.83	0.16	-	49,49,49,49	0
56	MG	CA	3130	1/1	0.97	0.08	-	65,65,65,65	0
56	MG	CA	3111	1/1	0.92	0.12	-	64,64,64,64	0
56	MG	BA	3377	1/1	0.94	0.14	-	32,32,32,32	0
56	MG	B3	102	1/1	0.98	0.13	-	59,59,59,59	0
56	MG	BA	3168	1/1	0.89	0.28	-	42,42,42,42	0
56	MG	DA	3085	1/1	0.96	0.12	-	36,36,36,36	0
56	MG	AA	3141	1/1	0.98	0.21	-	48,48,48,48	0
56	MG	DA	3138	1/1	0.95	0.23	-	42,42,42,42	0
56	MG	BA	3383	1/1	0.99	0.18	-	38,38,38,38	0
56	MG	DA	3629	1/1	0.96	0.17	-	19,19,19,19	0
56	MG	BA	3182	1/1	0.93	0.31	-	51,51,51,51	0
56	MG	BA	3665	1/1	0.96	0.21	-	39,39,39,39	0
56	MG	CA	3034	1/1	0.88	0.26	-	65,65,65,65	0
56	MG	AA	3193	1/1	0.98	0.09	-	60,60,60,60	0
56	MG	BA	3021	1/1	0.96	0.27	-	42,42,42,42	0
56	MG	BA	3502	1/1	0.91	0.20	-	43,43,43,43	0
56	MG	DA	3305	1/1	0.93	0.09	-	33,33,33,33	0
56	MG	BA	3542	1/1	0.96	0.23	-	19,19,19,19	0
56	MG	BB	3006	1/1	0.93	0.24	-	39,39,39,39	0
56	MG	DA	3134	1/1	0.88	0.23	-	46,46,46,46	0
56	MG	DA	3344	1/1	0.97	0.11	-	26,26,26,26	0
56	MG	CA	3164	1/1	0.88	0.39	-	49,49,49,49	0
56	MG	DA	3642	1/1	0.96	0.13	-	35,35,35,35	0
56	MG	BA	3691	1/1	0.66	0.39	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3083	1/1	0.95	0.09	-	65,65,65,65	0
56	MG	DA	3592	1/1	0.86	0.15	-	65,65,65,65	0
56	MG	AA	3049	1/1	0.93	0.50	-	51,51,51,51	0
56	MG	DA	3089	1/1	0.79	0.39	-	57,57,57,57	0
56	MG	CA	3116	1/1	0.94	0.17	-	76,76,76,76	0
56	MG	AA	3116	1/1	0.61	0.53	-	52,52,52,52	0
56	MG	BA	3381	1/1	0.98	0.10	-	37,37,37,37	0
56	MG	DA	3030	1/1	0.95	0.28	-	51,51,51,51	0
56	MG	BA	3248	1/1	0.91	0.24	-	43,43,43,43	0
56	MG	AA	3100	1/1	0.78	0.68	-	40,40,40,40	0
56	MG	BA	3523	1/1	0.89	0.12	-	48,48,48,48	0
56	MG	DA	3151	1/1	0.92	0.29	-	60,60,60,60	0
56	MG	BA	3114	1/1	0.90	0.36	-	51,51,51,51	0
56	MG	BA	3641	1/1	0.86	0.12	-	45,45,45,45	0
56	MG	BA	3591	1/1	0.98	0.32	-	48,48,48,48	0
56	MG	AA	3162	1/1	0.92	0.23	-	74,74,74,74	0
56	MG	CA	3008	1/1	0.84	0.79	-	53,53,53,53	0
56	MG	BA	3005	1/1	0.89	0.18	-	36,36,36,36	0
56	MG	DA	3117	1/1	0.71	0.17	-	53,53,53,53	0
56	MG	DA	3053	1/1	0.87	0.15	-	42,42,42,42	0
56	MG	DA	3542	1/1	0.99	0.18	-	32,32,32,32	0
56	MG	BA	3565	1/1	0.94	0.11	-	55,55,55,55	0
56	MG	DA	3268	1/1	0.98	0.17	-	40,40,40,40	0
56	MG	BA	3369	1/1	0.97	0.22	-	45,45,45,45	0
56	MG	BA	3007	1/1	0.90	0.23	-	35,35,35,35	0
56	MG	BA	3659	1/1	0.94	0.21	-	46,46,46,46	0
56	MG	AF	3001	1/1	0.94	0.17	-	61,61,61,61	0
56	MG	BP	204	1/1	0.96	0.17	-	55,55,55,55	0
56	MG	DA	3289	1/1	0.96	0.14	-	26,26,26,26	0
56	MG	DA	3583	1/1	0.97	0.28	-	48,48,48,48	0
56	MG	DA	3491	1/1	0.96	0.15	-	56,56,56,56	0
56	MG	DA	3597	1/1	0.92	0.22	-	47,47,47,47	0
56	MG	DA	3512	1/1	0.92	0.25	-	61,61,61,61	0
56	MG	BU	201	1/1	0.92	0.75	-	39,39,39,39	0
56	MG	BW	201	1/1	0.81	0.89	-	53,53,53,53	0
56	MG	CA	3046	1/1	0.90	0.38	-	53,53,53,53	0
56	MG	DA	3594	1/1	0.91	0.30	-	47,47,47,47	0
60	K	BA	3300	1/1	0.87	0.28	-	100,100,100,100	0
56	MG	DB	3006	1/1	0.95	0.13	-	42,42,42,42	0
56	MG	BA	3706	1/1	0.82	0.46	-	63,63,63,63	0
56	MG	DA	3195	1/1	0.89	0.10	-	50,50,50,50	0
56	MG	BA	3288	1/1	0.84	0.22	-	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	BA	3633	1/1	0.92	0.13	-	58,58,58,58	0
56	MG	DA	3225	1/1	0.92	0.16	-	45,45,45,45	0
56	MG	CA	3137	1/1	0.94	0.13	-	48,48,48,48	0
56	MG	DA	3241	1/1	0.97	0.21	-	15,15,15,15	0
56	MG	CA	3079	1/1	0.89	0.14	-	48,48,48,48	0
56	MG	BA	3398	1/1	0.98	0.11	-	41,41,41,41	0
56	MG	AA	3213	1/1	0.95	0.16	-	29,29,29,29	0
56	MG	DA	3088	1/1	0.97	0.16	-	46,46,46,46	0
56	MG	AX	108	1/1	0.77	0.21	-	61,61,61,61	0
56	MG	DA	3174	1/1	0.98	0.26	-	41,41,41,41	0
56	MG	BA	3457	1/1	0.90	0.12	-	57,57,57,57	0
56	MG	DA	3180	1/1	0.97	0.21	-	46,46,46,46	0
56	MG	BA	3345	1/1	0.96	0.21	-	33,33,33,33	0
56	MG	BA	3109	1/1	0.96	0.09	-	36,36,36,36	0
56	MG	B0	103	1/1	0.80	0.84	-	59,59,59,59	0
56	MG	DA	3410	1/1	0.76	0.22	-	69,69,69,69	0
56	MG	DA	3360	1/1	0.91	0.25	-	41,41,41,41	0
56	MG	BA	3099	1/1	0.92	0.17	-	44,44,44,44	0
56	MG	DA	3074	1/1	0.92	0.21	-	54,54,54,54	0
56	MG	DE	304	1/1	0.96	0.20	-	41,41,41,41	0
56	MG	BA	3611	1/1	0.82	0.28	-	52,52,52,52	0
56	MG	DA	3545	1/1	0.67	0.62	-	75,75,75,75	0
56	MG	BA	3509	1/1	0.89	0.16	-	27,27,27,27	0
56	MG	DA	3198	1/1	0.84	0.28	-	48,48,48,48	0
56	MG	DA	3527	1/1	0.93	0.10	-	46,46,46,46	0
56	MG	DA	3437	1/1	0.93	0.14	-	49,49,49,49	0
56	MG	CA	3147	1/1	0.80	0.27	-	66,66,66,66	0
56	MG	DR	202	1/1	0.94	0.18	-	37,37,37,37	0
56	MG	BA	3453	1/1	0.94	0.19	-	18,18,18,18	0
56	MG	DD	303	1/1	0.97	0.20	-	19,19,19,19	0
56	MG	AA	3111	1/1	0.95	0.17	-	95,95,95,95	0
56	MG	BA	3362	1/1	0.97	0.09	-	43,43,43,43	0
56	MG	BA	3722	1/1	0.93	0.17	-	32,32,32,32	0
56	MG	DA	3042	1/1	0.90	0.25	-	36,36,36,36	0
56	MG	DA	3506	1/1	0.95	0.07	-	59,59,59,59	0
56	MG	CA	3168	1/1	0.98	0.38	-	77,77,77,77	0
56	MG	DA	3154	1/1	0.95	0.61	-	45,45,45,45	0
56	MG	AA	3202	1/1	0.93	0.23	-	76,76,76,76	0
56	MG	BA	3554	1/1	0.97	0.20	-	31,31,31,31	0
56	MG	BA	3269	1/1	0.91	0.65	-	34,34,34,34	0
56	MG	BA	3169	1/1	0.95	0.70	-	46,46,46,46	0
56	MG	BA	3224	1/1	0.95	0.74	-	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	3415	1/1	0.99	0.24	-	27,27,27,27	0
56	MG	DA	3333	1/1	0.96	0.24	-	58,58,58,58	0
56	MG	DA	3253	1/1	0.89	0.14	-	42,42,42,42	0
56	MG	DA	3411	1/1	0.95	0.16	-	21,21,21,21	0
56	MG	BA	3433	1/1	0.98	0.24	-	39,39,39,39	0
56	MG	DA	3155	1/1	0.93	0.17	-	50,50,50,50	0
56	MG	BA	3256	1/1	0.92	0.18	-	58,58,58,58	0
56	MG	AA	3183	1/1	0.96	0.10	-	42,42,42,42	0
56	MG	DA	3618	1/1	0.99	0.12	-	39,39,39,39	0
56	MG	BA	3497	1/1	0.96	0.14	-	62,62,62,62	0
56	MG	DA	3560	1/1	0.89	0.11	-	34,34,34,34	0
56	MG	DA	3307	1/1	0.95	0.30	-	37,37,37,37	0
56	MG	BA	3467	1/1	0.98	0.06	-	40,40,40,40	0
56	MG	BA	3707	1/1	0.96	0.20	-	36,36,36,36	0
56	MG	DA	3192	1/1	0.97	0.12	-	47,47,47,47	0
56	MG	DA	3513	1/1	0.96	0.22	-	49,49,49,49	0
56	MG	DA	3163	1/1	0.83	0.18	-	39,39,39,39	0
56	MG	BA	3144	1/1	0.90	0.27	-	74,74,74,74	0
56	MG	BA	3319	1/1	0.96	0.17	-	25,25,25,25	0
56	MG	BA	3105	1/1	0.90	0.44	-	34,34,34,34	0
56	MG	B0	104	1/1	0.94	0.10	-	43,43,43,43	0
56	MG	BA	3315	1/1	0.97	0.11	-	37,37,37,37	0
56	MG	BB	3018	1/1	0.94	0.19	-	60,60,60,60	0
56	MG	DA	3389	1/1	0.96	0.28	-	27,27,27,27	0
56	MG	BA	3632	1/1	0.73	0.30	-	57,57,57,57	0
56	MG	BA	3704	1/1	0.93	0.19	-	85,85,85,85	0
56	MG	DA	3005	1/1	0.88	0.21	-	42,42,42,42	0
56	MG	BA	3709	1/1	0.96	0.12	-	86,86,86,86	0
56	MG	BG	3001	1/1	0.93	0.13	-	64,64,64,64	0
56	MG	DA	3558	1/1	0.95	0.18	-	37,37,37,37	0
56	MG	DA	3375	1/1	0.97	0.14	-	60,60,60,60	0
56	MG	BA	3543	1/1	0.96	0.29	-	52,52,52,52	0
56	MG	AA	3166	1/1	0.87	0.18	-	48,48,48,48	0
56	MG	CA	3122	1/1	0.99	0.07	-	47,47,47,47	0
56	MG	BA	3131	1/1	0.98	0.72	-	54,54,54,54	0
56	MG	DR	201	1/1	0.85	0.62	-	65,65,65,65	0
56	MG	BA	3087	1/1	0.78	0.45	-	61,61,61,61	0
56	MG	BA	3276	1/1	0.95	0.32	-	40,40,40,40	0
56	MG	AA	3207	1/1	0.97	0.27	-	45,45,45,45	0
56	MG	DA	3034	1/1	0.95	0.15	-	40,40,40,40	0
56	MG	DA	3374	1/1	0.97	0.05	-	37,37,37,37	0
56	MG	DB	3008	1/1	0.94	0.08	-	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	DA	3278	1/1	0.93	0.17	-	47,47,47,47	0
56	MG	DA	3462	1/1	0.90	0.11	-	55,55,55,55	0
56	MG	BA	3678	1/1	0.99	0.17	-	53,53,53,53	0
56	MG	DA	3589	1/1	0.95	0.18	-	59,59,59,59	0
56	MG	AA	3112	1/1	0.94	0.12	-	51,51,51,51	0
56	MG	AA	3065	1/1	0.73	0.27	-	60,60,60,60	0
56	MG	AA	3131	1/1	0.88	0.50	-	56,56,56,56	0
56	MG	CA	3063	1/1	0.86	0.10	-	61,61,61,61	0
56	MG	DA	3509	1/1	0.92	0.14	-	55,55,55,55	0
56	MG	CA	3113	1/1	0.96	0.23	-	77,77,77,77	0
56	MG	BA	3473	1/1	0.97	0.12	-	51,51,51,51	0
56	MG	AA	3129	1/1	0.65	0.30	-	77,77,77,77	0
56	MG	CA	3047	1/1	0.91	0.16	-	63,63,63,63	0
56	MG	DA	3230	1/1	0.99	0.16	-	62,62,62,62	0
56	MG	BA	3294	1/1	0.97	0.28	-	37,37,37,37	0
56	MG	BA	3646	1/1	0.97	0.23	-	52,52,52,52	0
56	MG	CA	3121	1/1	0.97	0.26	-	53,53,53,53	0
56	MG	CA	3030	1/1	0.71	0.45	-	73,73,73,73	0
56	MG	DA	3067	1/1	0.88	0.54	-	43,43,43,43	0
56	MG	DA	3585	1/1	0.95	0.15	-	62,62,62,62	0
56	MG	DA	3425	1/1	0.96	0.11	-	27,27,27,27	0
56	MG	DA	3492	1/1	0.81	0.37	-	68,68,68,68	0
56	MG	DA	3242	1/1	0.97	0.23	-	35,35,35,35	0
56	MG	CA	3139	1/1	0.83	0.27	-	75,75,75,75	0
56	MG	BA	3696	1/1	0.97	0.26	-	39,39,39,39	0
56	MG	DA	3130	1/1	0.96	0.12	-	32,32,32,32	0
56	MG	DB	3005	1/1	0.90	0.26	-	43,43,43,43	0
56	MG	DA	3434	1/1	0.95	0.26	-	49,49,49,49	0
56	MG	BQ	204	1/1	0.97	0.18	-	12,12,12,12	0
56	MG	BA	3164	1/1	0.83	0.72	-	56,56,56,56	0
56	MG	BA	3239	1/1	0.97	0.10	-	33,33,33,33	0
56	MG	DA	3321	1/1	0.96	0.23	-	41,41,41,41	0
56	MG	CA	3092	1/1	0.98	0.12	-	47,47,47,47	0
56	MG	CA	3117	1/1	0.92	0.15	-	68,68,68,68	0
56	MG	BA	3657	1/1	0.96	0.16	-	56,56,56,56	0
56	MG	BA	3063	1/1	0.97	0.28	-	43,43,43,43	0
56	MG	BA	3059	1/1	0.95	0.60	-	45,45,45,45	0
56	MG	BA	3718	1/1	0.78	0.37	-	57,57,57,57	0
56	MG	AA	3098	1/1	0.92	0.35	-	72,72,72,72	0
56	MG	DA	3244	1/1	0.98	0.31	-	29,29,29,29	0
56	MG	AA	3059	1/1	0.84	1.19	-	54,54,54,54	0
56	MG	BA	3713	1/1	0.97	0.10	-	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	3140	1/1	0.84	0.12	-	70,70,70,70	0
56	MG	BA	3584	1/1	0.96	0.18	-	22,22,22,22	0
56	MG	BA	3052	1/1	0.92	0.25	-	29,29,29,29	0
56	MG	BA	3469	1/1	0.97	0.09	-	38,38,38,38	0
56	MG	CA	3157	1/1	0.88	0.11	-	54,54,54,54	0
56	MG	BA	3089	1/1	0.74	0.58	-	61,61,61,61	0
56	MG	DA	3413	1/1	0.99	0.20	-	53,53,53,53	0
56	MG	DA	3484	1/1	0.85	0.25	-	51,51,51,51	0
56	MG	CA	3065	1/1	0.92	0.23	-	75,75,75,75	0
56	MG	BA	3135	1/1	0.85	0.17	-	42,42,42,42	0
56	MG	DA	3645	1/1	0.98	0.09	-	30,30,30,30	0
56	MG	BA	3023	1/1	0.88	0.13	-	66,66,66,66	0
56	MG	BA	3376	1/1	0.96	0.10	-	48,48,48,48	0
56	MG	BA	3338	1/1	0.97	0.21	-	50,50,50,50	0
56	MG	BA	3206	1/1	0.76	0.35	-	57,57,57,57	0
56	MG	CA	3036	1/1	0.89	0.52	-	68,68,68,68	0
56	MG	DA	3076	1/1	0.93	0.56	-	44,44,44,44	0
56	MG	BF	308	1/1	0.86	0.25	-	28,28,28,28	0
56	MG	BA	3674	1/1	0.95	0.18	-	55,55,55,55	0
56	MG	DA	3388	1/1	0.82	0.16	-	54,54,54,54	0
56	MG	DA	3021	1/1	0.95	0.15	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.