



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2016 – 12:50 AM EDT

PDB ID : 5DFE  
Title : 70S termination complex containing E. coli RF2  
Authors : Hoffer, E.D.; Dunham, C.M.  
Deposited on : 2015-08-26  
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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

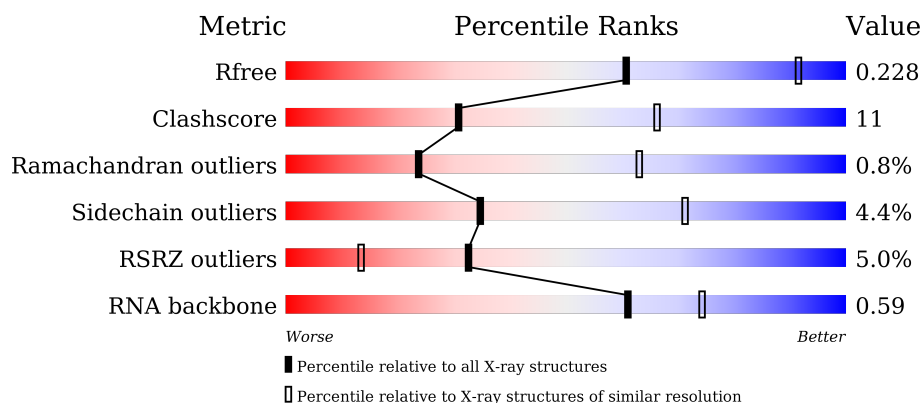
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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	QV	77	<div> <div>4%</div> <div>58% 32% 6% .</div> </div>
1	XV	77	<div> <div>3%</div> <div>64% 27% 8% .</div> </div>
2	QX	25	<div> <div>12%</div> <div>24% 12% . 60%</div> </div>
2	XX	25	<div> <div>12%</div> <div>20% 12% 8% 60%</div> </div>

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Mol	Chain	Length	Quality of chain
3	QY	380	
3	XY	380	
4	RA	2915	
4	YA	2915	
5	RB	122	
5	YB	122	
6	RD	276	
6	YD	276	
7	RE	206	
7	YE	206	
8	RF	210	
8	YF	210	
9	RG	182	
9	YG	182	
10	RH	180	
10	YH	180	
11	RI	148	
11	YI	148	
12	RN	140	
12	YN	140	
13	RO	122	
13	YO	122	
14	RP	150	
14	YP	150	
15	RQ	141	

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Mol	Chain	Length	Quality of chain
15	YQ	141	
16	RR	118	
16	YR	118	
17	RS	112	
17	YS	112	
18	RT	146	
18	YT	146	
19	RU	118	
19	YU	118	
20	RV	101	
20	YV	101	
21	RW	113	
21	YW	113	
22	RX	96	
22	YX	96	
23	RY	110	
23	YY	110	
24	RZ	206	
24	YZ	206	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	
27	Y2	72	

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Mol	Chain	Length	Quality of chain
28	R3	60	<div> <div>5%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
28	Y3	60	<div> <div>2%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
29	R4	71	<div> <div>11%</div> <div>55%</div> <div>34%</div> <div>7%</div> <div>..</div> </div>
29	Y4	71	<div> <div>11%</div> <div>48%</div> <div>39%</div> <div>6%</div> <div>..</div> </div>
30	R5	60	<div> <div>2%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
30	Y5	60	<div> <div>78%</div> <div>15%</div> <div>5%</div> <div>.</div> </div>
31	R6	54	<div> <div>50%</div> <div>69%</div> <div>26%</div> <div>...</div> </div>
31	Y6	54	<div> <div>28%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
32	R7	49	<div> <div>2%</div> <div>61%</div> <div>33%</div> <div>..</div> </div>
32	Y7	49	<div> <div>73%</div> <div>18%</div> <div>..</div> <div>..</div> </div>
33	R8	65	<div> <div>66%</div> <div>29%</div> <div>...</div> </div>
33	Y8	65	<div> <div>60%</div> <div>37%</div> <div>..</div> </div>
34	R9	37	<div> <div>8%</div> <div>70%</div> <div>24%</div> <div>..</div> </div>
34	Y9	37	<div> <div>3%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
35	QA	1521	<div> <div>2%</div> <div>52%</div> <div>39%</div> <div>7%</div> <div>.</div> </div>
35	XA	1521	<div> <div>3%</div> <div>54%</div> <div>38%</div> <div>6%</div> <div>..</div> </div>
36	QB	256	<div> <div>5%</div> <div>51%</div> <div>33%</div> <div>.</div> <div>.</div> <div>10%</div> </div>
36	XB	256	<div> <div>4%</div> <div>48%</div> <div>34%</div> <div>5%</div> <div>.</div> <div>10%</div> </div>
37	QC	239	<div> <div>4%</div> <div>63%</div> <div>21%</div> <div>.</div> <div>14%</div> </div>
37	XC	239	<div> <div>3%</div> <div>60%</div> <div>23%</div> <div>.</div> <div>14%</div> </div>
38	QD	209	<div> <div>59%</div> <div>36%</div> <div>..</div> </div>
38	XD	209	<div> <div>65%</div> <div>31%</div> <div>..</div> </div>
39	QE	162	<div> <div>63%</div> <div>25%</div> <div>..</div> <div>9%</div> </div>
39	XE	162	<div> <div>%</div> <div>56%</div> <div>32%</div> <div>..</div> <div>9%</div> </div>
40	QF	101	<div> <div>%</div> <div>63%</div> <div>26%</div> <div>10%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
40	XF	101	
41	QG	156	
41	XG	156	
42	QH	138	
42	XH	138	
43	QI	128	
43	XI	128	
44	QJ	105	
44	XJ	105	
45	QK	129	
45	XK	129	
46	QL	132	
46	XL	132	
47	QM	126	
47	XM	126	
48	QN	61	
48	XN	61	
49	QO	89	
49	XO	89	
50	QP	88	
50	XP	88	
51	QQ	105	
51	XQ	105	
52	QR	88	
52	XR	88	

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Mol	Chain	Length	Quality of chain
53	QS	93	
53	XS	93	
54	QT	106	
54	XT	106	
55	QU	27	
55	XU	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1606	-	-	-	X
56	MG	QA	1610	-	-	-	X
56	MG	QA	1621	-	-	-	X
56	MG	QA	1622	-	-	-	X
56	MG	QA	1623	-	-	-	X
56	MG	QA	1625	-	-	-	X
56	MG	QA	1645	-	-	-	X
56	MG	QA	1647	-	-	-	X
56	MG	QA	1654	-	-	-	X
56	MG	QA	1655	-	-	-	X
56	MG	QA	1661	-	-	-	X
56	MG	QA	1665	-	-	-	X
56	MG	QA	1672	-	-	-	X
56	MG	QA	1680	-	-	-	X
56	MG	QA	1682	-	-	-	X
56	MG	QA	1703	-	-	-	X
56	MG	QA	1707	-	-	-	X
56	MG	QA	1710	-	-	-	X
56	MG	QA	1714	-	-	-	X
56	MG	QA	1719	-	-	-	X
56	MG	QA	1721	-	-	-	X
56	MG	QA	1722	-	-	-	X
56	MG	QA	1729	-	-	-	X
56	MG	QA	1734	-	-	-	X
56	MG	QA	1757	-	-	-	X
56	MG	QA	1768	-	-	-	X
56	MG	QA	1778	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1800	-	-	-	X
56	MG	QA	1812	-	-	-	X
56	MG	QA	1821	-	-	-	X
56	MG	QA	1830	-	-	-	X
56	MG	QA	1833	-	-	-	X
56	MG	QA	1841	-	-	-	X
56	MG	QA	1843	-	-	-	X
56	MG	QA	1847	-	-	-	X
56	MG	QA	1852	-	-	-	X
56	MG	QA	1855	-	-	-	X
56	MG	QA	1858	-	-	-	X
56	MG	QA	1870	-	-	-	X
56	MG	QA	1876	-	-	-	X
56	MG	QL	201	-	-	-	X
56	MG	QN	103	-	-	-	X
56	MG	QT	201	-	-	-	X
56	MG	QY	402	-	-	-	X
56	MG	R0	103	-	-	-	X
56	MG	R1	102	-	-	-	X
56	MG	R3	102	-	-	-	X
56	MG	R5	101	-	-	-	X
56	MG	R8	101	-	-	-	X
56	MG	RA	3001	-	-	-	X
56	MG	RA	3014	-	-	-	X
56	MG	RA	3021	-	-	-	X
56	MG	RA	3022	-	-	-	X
56	MG	RA	3023	-	-	-	X
56	MG	RA	3027	-	-	-	X
56	MG	RA	3029	-	-	-	X
56	MG	RA	3030	-	-	-	X
56	MG	RA	3040	-	-	-	X
56	MG	RA	3045	-	-	-	X
56	MG	RA	3050	-	-	-	X
56	MG	RA	3064	-	-	-	X
56	MG	RA	3070	-	-	-	X
56	MG	RA	3073	-	-	-	X
56	MG	RA	3075	-	-	-	X
56	MG	RA	3077	-	-	-	X
56	MG	RA	3082	-	-	-	X
56	MG	RA	3088	-	-	-	X
56	MG	RA	3092	-	-	-	X
56	MG	RA	3101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3109	-	-	-	X
56	MG	RA	3116	-	-	-	X
56	MG	RA	3117	-	-	-	X
56	MG	RA	3118	-	-	-	X
56	MG	RA	3119	-	-	-	X
56	MG	RA	3122	-	-	-	X
56	MG	RA	3128	-	-	-	X
56	MG	RA	3132	-	-	-	X
56	MG	RA	3135	-	-	-	X
56	MG	RA	3141	-	-	-	X
56	MG	RA	3142	-	-	-	X
56	MG	RA	3146	-	-	-	X
56	MG	RA	3148	-	-	-	X
56	MG	RA	3163	-	-	-	X
56	MG	RA	3165	-	-	-	X
56	MG	RA	3168	-	-	-	X
56	MG	RA	3170	-	-	-	X
56	MG	RA	3177	-	-	-	X
56	MG	RA	3178	-	-	-	X
56	MG	RA	3184	-	-	-	X
56	MG	RA	3185	-	-	-	X
56	MG	RA	3196	-	-	-	X
56	MG	RA	3204	-	-	-	X
56	MG	RA	3207	-	-	-	X
56	MG	RA	3210	-	-	-	X
56	MG	RA	3216	-	-	-	X
56	MG	RA	3220	-	-	-	X
56	MG	RA	3225	-	-	-	X
56	MG	RA	3229	-	-	-	X
56	MG	RA	3230	-	-	-	X
56	MG	RA	3231	-	-	-	X
56	MG	RA	3233	-	-	-	X
56	MG	RA	3234	-	-	-	X
56	MG	RA	3240	-	-	-	X
56	MG	RA	3250	-	-	-	X
56	MG	RA	3264	-	-	-	X
56	MG	RA	3270	-	-	-	X
56	MG	RA	3274	-	-	-	X
56	MG	RA	3289	-	-	-	X
56	MG	RA	3298	-	-	-	X
56	MG	RA	3299	-	-	-	X
56	MG	RA	3301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3306	-	-	-	X
56	MG	RA	3312	-	-	-	X
56	MG	RA	3315	-	-	-	X
56	MG	RA	3321	-	-	-	X
56	MG	RA	3323	-	-	-	X
56	MG	RA	3328	-	-	-	X
56	MG	RA	3330	-	-	-	X
56	MG	RA	3332	-	-	-	X
56	MG	RA	3333	-	-	-	X
56	MG	RA	3335	-	-	-	X
56	MG	RA	3342	-	-	-	X
56	MG	RA	3348	-	-	-	X
56	MG	RA	3349	-	-	-	X
56	MG	RA	3351	-	-	-	X
56	MG	RA	3353	-	-	-	X
56	MG	RA	3355	-	-	-	X
56	MG	RA	3358	-	-	-	X
56	MG	RA	3360	-	-	-	X
56	MG	RA	3363	-	-	-	X
56	MG	RA	3365	-	-	-	X
56	MG	RA	3374	-	-	-	X
56	MG	RA	3378	-	-	-	X
56	MG	RA	3380	-	-	-	X
56	MG	RA	3381	-	-	-	X
56	MG	RA	3383	-	-	-	X
56	MG	RA	3384	-	-	-	X
56	MG	RA	3385	-	-	-	X
56	MG	RA	3386	-	-	-	X
56	MG	RA	3389	-	-	-	X
56	MG	RA	3390	-	-	-	X
56	MG	RA	3391	-	-	-	X
56	MG	RA	3393	-	-	-	X
56	MG	RA	3398	-	-	-	X
56	MG	RA	3400	-	-	-	X
56	MG	RA	3407	-	-	-	X
56	MG	RA	3408	-	-	-	X
56	MG	RA	3411	-	-	-	X
56	MG	RA	3418	-	-	-	X
56	MG	RA	3419	-	-	-	X
56	MG	RA	3423	-	-	-	X
56	MG	RA	3430	-	-	-	X
56	MG	RA	3435	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3443	-	-	-	X
56	MG	RA	3451	-	-	-	X
56	MG	RA	3454	-	-	-	X
56	MG	RA	3457	-	-	-	X
56	MG	RA	3461	-	-	-	X
56	MG	RA	3464	-	-	-	X
56	MG	RA	3465	-	-	-	X
56	MG	RA	3467	-	-	-	X
56	MG	RA	3469	-	-	-	X
56	MG	RA	3470	-	-	-	X
56	MG	RA	3471	-	-	-	X
56	MG	RA	3472	-	-	-	X
56	MG	RA	3475	-	-	-	X
56	MG	RA	3476	-	-	-	X
56	MG	RA	3478	-	-	-	X
56	MG	RA	3482	-	-	-	X
56	MG	RA	3483	-	-	-	X
56	MG	RA	3485	-	-	-	X
56	MG	RA	3490	-	-	-	X
56	MG	RA	3495	-	-	-	X
56	MG	RA	3496	-	-	-	X
56	MG	RA	3500	-	-	-	X
56	MG	RA	3501	-	-	-	X
56	MG	RA	3504	-	-	-	X
56	MG	RA	3506	-	-	-	X
56	MG	RA	3511	-	-	-	X
56	MG	RA	3517	-	-	-	X
56	MG	RA	3520	-	-	-	X
56	MG	RA	3523	-	-	-	X
56	MG	RA	3525	-	-	-	X
56	MG	RA	3529	-	-	-	X
56	MG	RA	3531	-	-	-	X
56	MG	RA	3534	-	-	-	X
56	MG	RA	3535	-	-	-	X
56	MG	RA	3536	-	-	-	X
56	MG	RA	3538	-	-	-	X
56	MG	RA	3550	-	-	-	X
56	MG	RA	3553	-	-	-	X
56	MG	RA	3565	-	-	-	X
56	MG	RA	3567	-	-	-	X
56	MG	RA	3571	-	-	-	X
56	MG	RA	3573	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3587	-	-	-	X
56	MG	RA	3597	-	-	-	X
56	MG	RA	3600	-	-	-	X
56	MG	RA	3602	-	-	-	X
56	MG	RA	3606	-	-	-	X
56	MG	RA	3608	-	-	-	X
56	MG	RA	3610	-	-	-	X
56	MG	RA	3613	-	-	-	X
56	MG	RA	3615	-	-	-	X
56	MG	RA	3621	-	-	-	X
56	MG	RA	3622	-	-	-	X
56	MG	RA	3623	-	-	-	X
56	MG	RA	3629	-	-	-	X
56	MG	RA	3630	-	-	-	X
56	MG	RA	3633	-	-	-	X
56	MG	RA	3634	-	-	-	X
56	MG	RA	3637	-	-	-	X
56	MG	RA	3643	-	-	-	X
56	MG	RA	3649	-	-	-	X
56	MG	RA	3658	-	-	-	X
56	MG	RA	3676	-	-	-	X
56	MG	RA	3678	-	-	-	X
56	MG	RA	3683	-	-	-	X
56	MG	RA	3695	-	-	-	X
56	MG	RA	3696	-	-	-	X
56	MG	RA	3701	-	-	-	X
56	MG	RA	3706	-	-	-	X
56	MG	RA	3707	-	-	-	X
56	MG	RA	3708	-	-	-	X
56	MG	RA	3711	-	-	-	X
56	MG	RA	3712	-	-	-	X
56	MG	RA	3714	-	-	-	X
56	MG	RA	3721	-	-	-	X
56	MG	RA	3723	-	-	-	X
56	MG	RA	3737	-	-	-	X
56	MG	RA	3743	-	-	-	X
56	MG	RA	3745	-	-	-	X
56	MG	RA	3750	-	-	-	X
56	MG	RA	3753	-	-	-	X
56	MG	RA	3766	-	-	-	X
56	MG	RA	3769	-	-	-	X
56	MG	RA	3770	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3772	-	-	-	X
56	MG	RA	3773	-	-	-	X
56	MG	RA	3783	-	-	-	X
56	MG	RA	3785	-	-	-	X
56	MG	RA	3794	-	-	-	X
56	MG	RA	3802	-	-	-	X
56	MG	RA	3804	-	-	-	X
56	MG	RA	3806	-	-	-	X
56	MG	RA	3808	-	-	-	X
56	MG	RA	3809	-	-	-	X
56	MG	RA	3811	-	-	-	X
56	MG	RA	3813	-	-	-	X
56	MG	RA	3814	-	-	-	X
56	MG	RA	3820	-	-	-	X
56	MG	RA	3822	-	-	-	X
56	MG	RA	3828	-	-	-	X
56	MG	RA	3838	-	-	-	X
56	MG	RA	3849	-	-	-	X
56	MG	RA	3853	-	-	-	X
56	MG	RA	3855	-	-	-	X
56	MG	RA	3857	-	-	-	X
56	MG	RA	3861	-	-	-	X
56	MG	RA	3873	-	-	-	X
56	MG	RA	3874	-	-	-	X
56	MG	RA	3881	-	-	-	X
56	MG	RA	3888	-	-	-	X
56	MG	RA	3891	-	-	-	X
56	MG	RA	3892	-	-	-	X
56	MG	RA	3899	-	-	-	X
56	MG	RA	3900	-	-	-	X
56	MG	RA	3901	-	-	-	X
56	MG	RA	3902	-	-	-	X
56	MG	RA	3905	-	-	-	X
56	MG	RA	3910	-	-	-	X
56	MG	RA	3923	-	-	-	X
56	MG	RA	3927	-	-	-	X
56	MG	RA	3938	-	-	-	X
56	MG	RA	3940	-	-	-	X
56	MG	RA	3951	-	-	-	X
56	MG	RA	3952	-	-	-	X
56	MG	RA	3966	-	-	-	X
56	MG	RA	3968	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3978	-	-	-	X
56	MG	RA	3988	-	-	-	X
56	MG	RA	3999	-	-	-	X
56	MG	RA	4000	-	-	-	X
56	MG	RA	4001	-	-	-	X
56	MG	RA	4003	-	-	-	X
56	MG	RA	4006	-	-	-	X
56	MG	RA	4009	-	-	-	X
56	MG	RA	4015	-	-	-	X
56	MG	RA	4016	-	-	-	X
56	MG	RA	4017	-	-	-	X
56	MG	RA	4018	-	-	-	X
56	MG	RA	4020	-	-	-	X
56	MG	RA	4022	-	-	-	X
56	MG	RA	4024	-	-	-	X
56	MG	RA	4028	-	-	-	X
56	MG	RA	4029	-	-	-	X
56	MG	RA	4030	-	-	-	X
56	MG	RA	4031	-	-	-	X
56	MG	RA	4032	-	-	-	X
56	MG	RA	4033	-	-	-	X
56	MG	RA	4034	-	-	-	X
56	MG	RA	4036	-	-	-	X
56	MG	RA	4037	-	-	-	X
56	MG	RA	4038	-	-	-	X
56	MG	RA	4039	-	-	-	X
56	MG	RA	4040	-	-	-	X
56	MG	RA	4041	-	-	-	X
56	MG	RA	4042	-	-	-	X
56	MG	RA	4043	-	-	-	X
56	MG	RA	4044	-	-	-	X
56	MG	RA	4045	-	-	-	X
56	MG	RA	4046	-	-	-	X
56	MG	RA	4047	-	-	-	X
56	MG	RA	4048	-	-	-	X
56	MG	RA	4049	-	-	-	X
56	MG	RA	4050	-	-	-	X
56	MG	RA	4052	-	-	-	X
56	MG	RA	4055	-	-	-	X
56	MG	RA	4057	-	-	-	X
56	MG	RA	4058	-	-	-	X
56	MG	RA	4059	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	4060	-	-	-	X
56	MG	RA	4061	-	-	-	X
56	MG	RA	4062	-	-	-	X
56	MG	RA	4063	-	-	-	X
56	MG	RA	4064	-	-	-	X
56	MG	RA	4065	-	-	-	X
56	MG	RA	4066	-	-	-	X
56	MG	RB	209	-	-	-	X
56	MG	RB	215	-	-	-	X
56	MG	RB	225	-	-	-	X
56	MG	RD	301	-	-	-	X
56	MG	RD	302	-	-	-	X
56	MG	RD	304	-	-	-	X
56	MG	RD	305	-	-	-	X
56	MG	RD	307	-	-	-	X
56	MG	RD	308	-	-	-	X
56	MG	RD	311	-	-	-	X
56	MG	RD	312	-	-	-	X
56	MG	RE	301	-	-	-	X
56	MG	RE	302	-	-	-	X
56	MG	RE	305	-	-	-	X
56	MG	RE	306	-	-	-	X
56	MG	RF	301	-	-	-	X
56	MG	RF	303	-	-	-	X
56	MG	RF	305	-	-	-	X
56	MG	RF	306	-	-	-	X
56	MG	RF	308	-	-	-	X
56	MG	RF	310	-	-	-	X
56	MG	RG	201	-	-	-	X
56	MG	RN	201	-	-	-	X
56	MG	RO	201	-	-	-	X
56	MG	RP	201	-	-	-	X
56	MG	RQ	204	-	-	-	X
56	MG	RR	3201	-	-	-	X
56	MG	RR	3202	-	-	-	X
56	MG	RR	3203	-	-	-	X
56	MG	RU	203	-	-	-	X
56	MG	RV	202	-	-	-	X
56	MG	RV	203	-	-	-	X
56	MG	RX	101	-	-	-	X
56	MG	XA	1605	-	-	-	X
56	MG	XA	1608	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	XA	1611	-	-	-	X
56	MG	XA	1617	-	-	-	X
56	MG	XA	1620	-	-	-	X
56	MG	XA	1622	-	-	-	X
56	MG	XA	1626	-	-	-	X
56	MG	XA	1627	-	-	-	X
56	MG	XA	1628	-	-	-	X
56	MG	XA	1630	-	-	-	X
56	MG	XA	1631	-	-	-	X
56	MG	XA	1632	-	-	-	X
56	MG	XA	1658	-	-	-	X
56	MG	XA	1672	-	-	-	X
56	MG	XA	1682	-	-	-	X
56	MG	XA	1687	-	-	-	X
56	MG	XA	1695	-	-	-	X
56	MG	XA	1699	-	-	-	X
56	MG	XA	1706	-	-	-	X
56	MG	XA	1719	-	-	-	X
56	MG	XA	1726	-	-	-	X
56	MG	XA	1730	-	-	-	X
56	MG	XA	1736	-	-	-	X
56	MG	XA	1737	-	-	-	X
56	MG	XA	1740	-	-	-	X
56	MG	XA	1743	-	-	-	X
56	MG	XA	1746	-	-	-	X
56	MG	XA	1756	-	-	-	X
56	MG	XA	1757	-	-	-	X
56	MG	XA	1758	-	-	-	X
56	MG	XA	1761	-	-	-	X
56	MG	XA	1762	-	-	-	X
56	MG	XA	1767	-	-	-	X
56	MG	XA	1768	-	-	-	X
56	MG	XA	1770	-	-	-	X
56	MG	XA	1772	-	-	-	X
56	MG	XA	1774	-	-	-	X
56	MG	XA	1775	-	-	-	X
56	MG	XA	1778	-	-	-	X
56	MG	XA	1779	-	-	-	X
56	MG	XA	1784	-	-	-	X
56	MG	XA	1788	-	-	-	X
56	MG	XF	203	-	-	-	X
56	MG	XF	204	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	XR	101	-	-	-	X
56	MG	XX	101	-	-	-	X
56	MG	Y8	101	-	-	-	X
56	MG	YA	3010	-	-	-	X
56	MG	YA	3012	-	-	-	X
56	MG	YA	3014	-	-	-	X
56	MG	YA	3015	-	-	-	X
56	MG	YA	3021	-	-	-	X
56	MG	YA	3022	-	-	-	X
56	MG	YA	3029	-	-	-	X
56	MG	YA	3030	-	-	-	X
56	MG	YA	3032	-	-	-	X
56	MG	YA	3035	-	-	-	X
56	MG	YA	3038	-	-	-	X
56	MG	YA	3051	-	-	-	X
56	MG	YA	3055	-	-	-	X
56	MG	YA	3056	-	-	-	X
56	MG	YA	3060	-	-	-	X
56	MG	YA	3062	-	-	-	X
56	MG	YA	3073	-	-	-	X
56	MG	YA	3079	-	-	-	X
56	MG	YA	3087	-	-	-	X
56	MG	YA	3089	-	-	-	X
56	MG	YA	3090	-	-	-	X
56	MG	YA	3093	-	-	-	X
56	MG	YA	3094	-	-	-	X
56	MG	YA	3096	-	-	-	X
56	MG	YA	3097	-	-	-	X
56	MG	YA	3109	-	-	-	X
56	MG	YA	3112	-	-	-	X
56	MG	YA	3114	-	-	-	X
56	MG	YA	3116	-	-	-	X
56	MG	YA	3124	-	-	-	X
56	MG	YA	3131	-	-	-	X
56	MG	YA	3133	-	-	-	X
56	MG	YA	3135	-	-	-	X
56	MG	YA	3136	-	-	-	X
56	MG	YA	3141	-	-	-	X
56	MG	YA	3142	-	-	-	X
56	MG	YA	3149	-	-	-	X
56	MG	YA	3154	-	-	-	X
56	MG	YA	3155	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3156	-	-	-	X
56	MG	YA	3159	-	-	-	X
56	MG	YA	3169	-	-	-	X
56	MG	YA	3173	-	-	-	X
56	MG	YA	3179	-	-	-	X
56	MG	YA	3186	-	-	-	X
56	MG	YA	3195	-	-	-	X
56	MG	YA	3202	-	-	-	X
56	MG	YA	3212	-	-	-	X
56	MG	YA	3213	-	-	-	X
56	MG	YA	3219	-	-	-	X
56	MG	YA	3240	-	-	-	X
56	MG	YA	3243	-	-	-	X
56	MG	YA	3250	-	-	-	X
56	MG	YA	3252	-	-	-	X
56	MG	YA	3255	-	-	-	X
56	MG	YA	3256	-	-	-	X
56	MG	YA	3271	-	-	-	X
56	MG	YA	3272	-	-	-	X
56	MG	YA	3273	-	-	-	X
56	MG	YA	3275	-	-	-	X
56	MG	YA	3287	-	-	-	X
56	MG	YA	3288	-	-	-	X
56	MG	YA	3294	-	-	-	X
56	MG	YA	3295	-	-	-	X
56	MG	YA	3298	-	-	-	X
56	MG	YA	3300	-	-	-	X
56	MG	YA	3302	-	-	-	X
56	MG	YA	3303	-	-	-	X
56	MG	YA	3314	-	-	-	X
56	MG	YA	3319	-	-	-	X
56	MG	YA	3321	-	-	-	X
56	MG	YA	3323	-	-	-	X
56	MG	YA	3324	-	-	-	X
56	MG	YA	3326	-	-	-	X
56	MG	YA	3327	-	-	-	X
56	MG	YA	3328	-	-	-	X
56	MG	YA	3329	-	-	-	X
56	MG	YA	3331	-	-	-	X
56	MG	YA	3338	-	-	-	X
56	MG	YA	3339	-	-	-	X
56	MG	YA	3342	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3346	-	-	-	X
56	MG	YA	3348	-	-	-	X
56	MG	YA	3353	-	-	-	X
56	MG	YA	3354	-	-	-	X
56	MG	YA	3358	-	-	-	X
56	MG	YA	3363	-	-	-	X
56	MG	YA	3371	-	-	-	X
56	MG	YA	3377	-	-	-	X
56	MG	YA	3380	-	-	-	X
56	MG	YA	3381	-	-	-	X
56	MG	YA	3385	-	-	-	X
56	MG	YA	3387	-	-	-	X
56	MG	YA	3389	-	-	-	X
56	MG	YA	3390	-	-	-	X
56	MG	YA	3394	-	-	-	X
56	MG	YA	3400	-	-	-	X
56	MG	YA	3401	-	-	-	X
56	MG	YA	3404	-	-	-	X
56	MG	YA	3407	-	-	-	X
56	MG	YA	3410	-	-	-	X
56	MG	YA	3412	-	-	-	X
56	MG	YA	3416	-	-	-	X
56	MG	YA	3425	-	-	-	X
56	MG	YA	3433	-	-	-	X
56	MG	YA	3434	-	-	-	X
56	MG	YA	3443	-	-	-	X
56	MG	YA	3444	-	-	-	X
56	MG	YA	3452	-	-	-	X
56	MG	YA	3453	-	-	-	X
56	MG	YA	3460	-	-	-	X
56	MG	YA	3472	-	-	-	X
56	MG	YA	3478	-	-	-	X
56	MG	YA	3479	-	-	-	X
56	MG	YA	3480	-	-	-	X
56	MG	YA	3489	-	-	-	X
56	MG	YA	3491	-	-	-	X
56	MG	YA	3499	-	-	-	X
56	MG	YA	3503	-	-	-	X
56	MG	YA	3507	-	-	-	X
56	MG	YA	3515	-	-	-	X
56	MG	YA	3518	-	-	-	X
56	MG	YA	3520	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3521	-	-	-	X
56	MG	YA	3522	-	-	-	X
56	MG	YA	3536	-	-	-	X
56	MG	YA	3538	-	-	-	X
56	MG	YA	3542	-	-	-	X
56	MG	YA	3544	-	-	-	X
56	MG	YA	3548	-	-	-	X
56	MG	YA	3551	-	-	-	X
56	MG	YA	3554	-	-	-	X
56	MG	YA	3556	-	-	-	X
56	MG	YA	3569	-	-	-	X
56	MG	YA	3574	-	-	-	X
56	MG	YA	3575	-	-	-	X
56	MG	YA	3581	-	-	-	X
56	MG	YA	3582	-	-	-	X
56	MG	YA	3584	-	-	-	X
56	MG	YA	3586	-	-	-	X
56	MG	YA	3591	-	-	-	X
56	MG	YA	3592	-	-	-	X
56	MG	YA	3604	-	-	-	X
56	MG	YA	3605	-	-	-	X
56	MG	YA	3610	-	-	-	X
56	MG	YA	3611	-	-	-	X
56	MG	YA	3614	-	-	-	X
56	MG	YA	3615	-	-	-	X
56	MG	YA	3616	-	-	-	X
56	MG	YA	3618	-	-	-	X
56	MG	YA	3620	-	-	-	X
56	MG	YA	3625	-	-	-	X
56	MG	YA	3627	-	-	-	X
56	MG	YA	3634	-	-	-	X
56	MG	YA	3636	-	-	-	X
56	MG	YA	3646	-	-	-	X
56	MG	YA	3651	-	-	-	X
56	MG	YA	3652	-	-	-	X
56	MG	YA	3654	-	-	-	X
56	MG	YA	3660	-	-	-	X
56	MG	YA	3662	-	-	-	X
56	MG	YA	3664	-	-	-	X
56	MG	YA	3668	-	-	-	X
56	MG	YA	3669	-	-	-	X
56	MG	YA	3672	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3678	-	-	-	X
56	MG	YA	3683	-	-	-	X
56	MG	YA	3685	-	-	-	X
56	MG	YA	3688	-	-	-	X
56	MG	YA	3692	-	-	-	X
56	MG	YA	3694	-	-	-	X
56	MG	YA	3704	-	-	-	X
56	MG	YA	3705	-	-	-	X
56	MG	YA	3707	-	-	-	X
56	MG	YA	3708	-	-	-	X
56	MG	YA	3712	-	-	-	X
56	MG	YA	3713	-	-	-	X
56	MG	YA	3718	-	-	-	X
56	MG	YA	3727	-	-	-	X
56	MG	YA	3728	-	-	-	X
56	MG	YA	3730	-	-	-	X
56	MG	YA	3734	-	-	-	X
56	MG	YA	3744	-	-	-	X
56	MG	YA	3747	-	-	-	X
56	MG	YA	3748	-	-	-	X
56	MG	YA	3749	-	-	-	X
56	MG	YA	3750	-	-	-	X
56	MG	YA	3751	-	-	-	X
56	MG	YA	3753	-	-	-	X
56	MG	YA	3754	-	-	-	X
56	MG	YA	3755	-	-	-	X
56	MG	YA	3756	-	-	-	X
56	MG	YA	3757	-	-	-	X
56	MG	YA	3758	-	-	-	X
56	MG	YA	3759	-	-	-	X
56	MG	YA	3760	-	-	-	X
56	MG	YB	217	-	-	-	X
56	MG	YD	303	-	-	-	X
56	MG	YD	304	-	-	-	X
56	MG	YD	305	-	-	-	X
56	MG	YD	306	-	-	-	X
56	MG	YD	308	-	-	-	X
56	MG	YD	309	-	-	-	X
56	MG	YE	302	-	-	-	X
56	MG	YE	303	-	-	-	X
56	MG	YE	304	-	-	-	X
56	MG	YE	305	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YF	303	-	-	-	X
56	MG	YQ	201	-	-	-	X
56	MG	YR	201	-	-	-	X
56	MG	YT	202	-	-	-	X
56	MG	YW	201	-	-	-	X
56	MG	YX	101	-	-	-	X
57	ZN	R4	101	-	-	-	X
57	ZN	Y4	101	-	-	-	X

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 296662 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 Escherichia coli strain Ecol\_745, complete genome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
1	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 2 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QX	10	Total	C	N	O	P	0	0	0
			215	97	42	66	10			
2	XX	10	Total	C	N	O	P	0	0	0
			215	97	42	66	10			

- Molecule 3 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QY	357	Total	C	N	O	S	0	0	0
			2833	1742	498	583	10			
3	XY	357	Total	C	N	O	S	0	0	0
			2833	1742	498	583	10			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QY	-14	MET	-	initiating methionine	UNP P07012
QY	-13	GLY	-	expression tag	UNP P07012
QY	-12	SER	-	expression tag	UNP P07012
QY	-11	SER	-	expression tag	UNP P07012
QY	-10	HIS	-	expression tag	UNP P07012
QY	-9	HIS	-	expression tag	UNP P07012
QY	-8	HIS	-	expression tag	UNP P07012
QY	-7	HIS	-	expression tag	UNP P07012

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Chain	Residue	Modelled	Actual	Comment	Reference
QY	-6	HIS	-	expression tag	UNP P07012
QY	-5	HIS	-	expression tag	UNP P07012
QY	-4	SER	-	expression tag	UNP P07012
QY	-3	GLU	-	expression tag	UNP P07012
QY	-2	ASP	-	expression tag	UNP P07012
QY	-1	PRO	-	expression tag	UNP P07012
QY	0	ALA	-	expression tag	UNP P07012
XY	-14	MET	-	initiating methionine	UNP P07012
XY	-13	GLY	-	expression tag	UNP P07012
XY	-12	SER	-	expression tag	UNP P07012
XY	-11	SER	-	expression tag	UNP P07012
XY	-10	HIS	-	expression tag	UNP P07012
XY	-9	HIS	-	expression tag	UNP P07012
XY	-8	HIS	-	expression tag	UNP P07012
XY	-7	HIS	-	expression tag	UNP P07012
XY	-6	HIS	-	expression tag	UNP P07012
XY	-5	HIS	-	expression tag	UNP P07012
XY	-4	SER	-	expression tag	UNP P07012
XY	-3	GLU	-	expression tag	UNP P07012
XY	-2	ASP	-	expression tag	UNP P07012
XY	-1	PRO	-	expression tag	UNP P07012
XY	0	ALA	-	expression tag	UNP P07012

- Molecule 4 is a RNA chain called *Thermus thermophilus* HB8 genomic DNA, complete genome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	YA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			
4	RA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- Molecule 5 is a RNA chain called *Thermus thermophilus* HB8 genomic DNA, complete genome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
5	RB	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	YD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
6	RD	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
7	RE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	YG	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			
9	RG	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	YH	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			
10	RH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	YI	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	RI	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	YN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
12	RN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
13	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
14	RP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
15	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
16	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	YS	110	Total	C	N	O	0	0	0
			870	549	173	148			
17	RS	110	Total	C	N	O	0	0	0
			877	553	175	149			

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	YT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			
18	RT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	YU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
19	RU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	YV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
20	RV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	YW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
21	RW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	YX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
22	RX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	YY	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			
23	RY	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	YZ	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			
24	RZ	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
25	R0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y1	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			
26	R1	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y3	59	Total	C	N	O		0	0	0
			464	296	90	78				
28	R3	59	Total	C	N	O		0	0	0
			469	298	90	81				

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			
29	R4	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
30	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Y6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			
31	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
32	R7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
33	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
34	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called Thermus thermophilus HB8 genomic DNA, complete genome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	XA	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			
35	QA	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	XB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			
36	QB	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	XC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			
37	QC	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	XD	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			
38	QD	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	XE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
39	QE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	XF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			
40	QF	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	XG	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			
41	QG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
42	QH	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	XI	126	Total	C	N	O		0	0	0
			966	613	186	167				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	QI	127	Total	C	N	O	0	0	0
			986	625	193	168			

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	XJ	96	Total	C	N	O	0	0	0
			710	442	137	131			
44	QJ	97	Total	C	N	O	0	0	0
			719	446	142	131			

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	XK	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			
45	QK	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	XL	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
46	QL	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	XM	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			
47	QM	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
48	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	XO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
49	QO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	XP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			
50	QP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	XQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
51	QQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	XR	68	Total	C	N	O	0	0	0
			555	355	108	92			
52	QR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	XS	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			
53	QS	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	XT	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			
54	QT	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			

- Molecule 55 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	XU	23	Total	C	N	O	0	0	0
			199	122	48	29			
55	QU	23	Total	C	N	O	0	0	0
			199	122	48	29			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	279	Total	Mg	0	0
			279	279		
56	YV	1	Total	Mg	0	0
			1	1		
56	RP	2	Total	Mg	0	0
			2	2		
56	R7	2	Total	Mg	0	0
			2	2		
56	YA	760	Total	Mg	0	0
			760	760		
56	Y5	1	Total	Mg	0	0
			1	1		
56	YR	1	Total	Mg	0	0
			1	1		
56	RT	3	Total	Mg	0	0
			3	3		
56	QD	3	Total	Mg	0	0
			3	3		
56	RN	3	Total	Mg	0	0
			3	3		
56	XE	2	Total	Mg	0	0
			2	2		
56	RG	4	Total	Mg	0	0
			4	4		
56	Y1	1	Total	Mg	0	0
			1	1		
56	YD	10	Total	Mg	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	XX	1	Total Mg 1 1	0	0
56	QV	2	Total Mg 2 2	0	0
56	RX	1	Total Mg 1 1	0	0
56	Y8	2	Total Mg 2 2	0	0
56	YO	1	Total Mg 1 1	0	0
56	XA	190	Total Mg 190 190	0	0
56	QI	1	Total Mg 1 1	0	0
56	RQ	4	Total Mg 4 4	0	0
56	R0	4	Total Mg 4 4	0	0
56	XT	1	Total Mg 1 1	0	0
56	QR	1	Total Mg 1 1	0	0
56	QL	3	Total Mg 3 3	0	0
56	RU	3	Total Mg 3 3	0	0
56	QG	3	Total Mg 3 3	0	0
56	RO	1	Total Mg 1 1	0	0
56	XJ	1	Total Mg 1 1	0	0
56	QO	1	Total Mg 1 1	0	0
56	Y0	1	Total Mg 1 1	0	0
56	YG	3	Total Mg 3 3	0	0
56	YQ	2	Total Mg 2 2	0	0
56	YN	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XF	4	Total 4	Mg 4	0	0
56	YX	1	Total 1	Mg 1	0	0
56	RR	5	Total 5	Mg 5	0	0
56	RD	13	Total 13	Mg 13	0	0
56	R1	3	Total 3	Mg 3	0	0
56	QU	1	Total 1	Mg 1	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	YT	3	Total 3	Mg 3	0	0
56	RV	4	Total 4	Mg 4	0	0
56	QF	1	Total 1	Mg 1	0	0
56	RH	2	Total 2	Mg 2	0	0
56	XK	1	Total 1	Mg 1	0	0
56	QH	2	Total 2	Mg 2	0	0
56	QQ	2	Total 2	Mg 2	0	0
56	RA	1066	Total 1066	Mg 1066	0	0
56	R4	1	Total 1	Mg 1	0	0
56	YF	3	Total 3	Mg 3	0	0
56	YP	1	Total 1	Mg 1	0	0
56	RZ	1	Total 1	Mg 1	0	0
56	QB	1	Total 1	Mg 1	0	0
56	QM	1	Total 1	Mg 1	0	0

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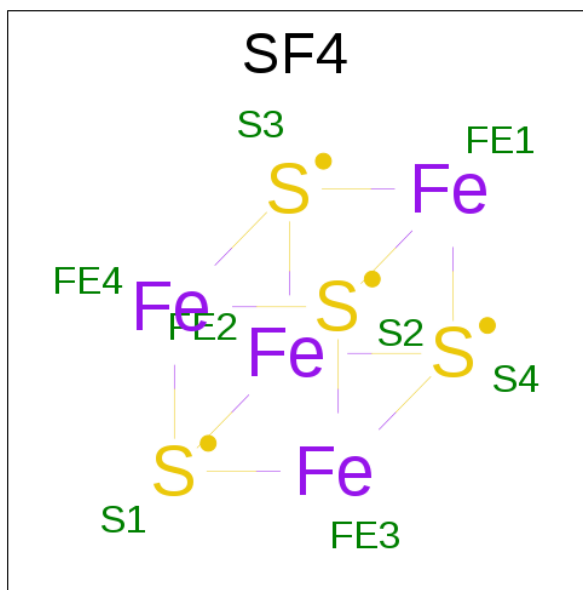
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	R9	2	Total 2	Mg 2	0	0
56	RE	6	Total 6	Mg 6	0	0
56	XL	1	Total 1	Mg 1	0	0
56	YB	19	Total 19	Mg 19	0	0
56	QT	1	Total 1	Mg 1	0	0
56	QN	2	Total 2	Mg 2	0	0
56	YW	2	Total 2	Mg 2	0	0
56	RW	2	Total 2	Mg 2	0	0
56	QY	3	Total 3	Mg 3	0	0
56	R8	1	Total 1	Mg 1	0	0
56	XH	1	Total 1	Mg 1	0	0
56	RB	29	Total 29	Mg 29	0	0
56	YI	1	Total 1	Mg 1	0	0
56	QE	2	Total 2	Mg 2	0	0
56	R5	3	Total 3	Mg 3	0	0
56	XR	1	Total 1	Mg 1	0	0
56	RF	12	Total 12	Mg 12	0	0
56	R3	2	Total 2	Mg 2	0	0
56	YE	7	Total 7	Mg 7	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	Y9	1	Total Zn 1 1	0	0
57	QN	1	Total Zn 1 1	0	0
57	Y6	1	Total Zn 1 1	0	0
57	XN	1	Total Zn 1 1	0	0
57	R9	1	Total Zn 1 1	0	0
57	Y4	1	Total Zn 1 1	0	0
57	R6	1	Total Zn 1 1	0	0
57	Y5	1	Total Zn 1 1	0	0
57	R5	1	Total Zn 1 1	0	0
57	YY	1	Total Zn 1 1	0	0
57	R4	1	Total Zn 1 1	0	0
57	RY	1	Total Zn 1 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

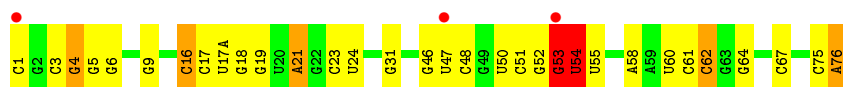


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	XD	1	Total 8	Fe 4	S 4	0	0
58	QD	1	Total 8	Fe 4	S 4	0	0

### 3 Residue-property plots [i](#)

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

- Molecule 1: Escherichia coli strain Ecol\_745, complete genome



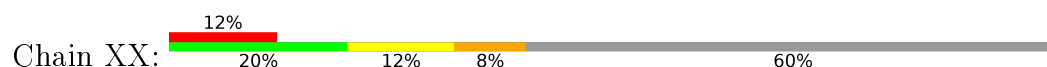
- Molecule 1: Escherichia coli strain Ecol\_745, complete genome



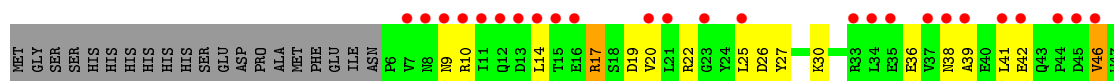
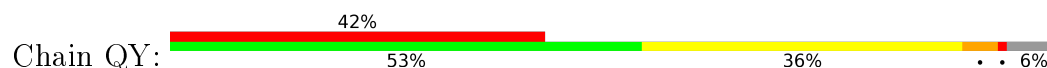
- Molecule 2: messenger RNA

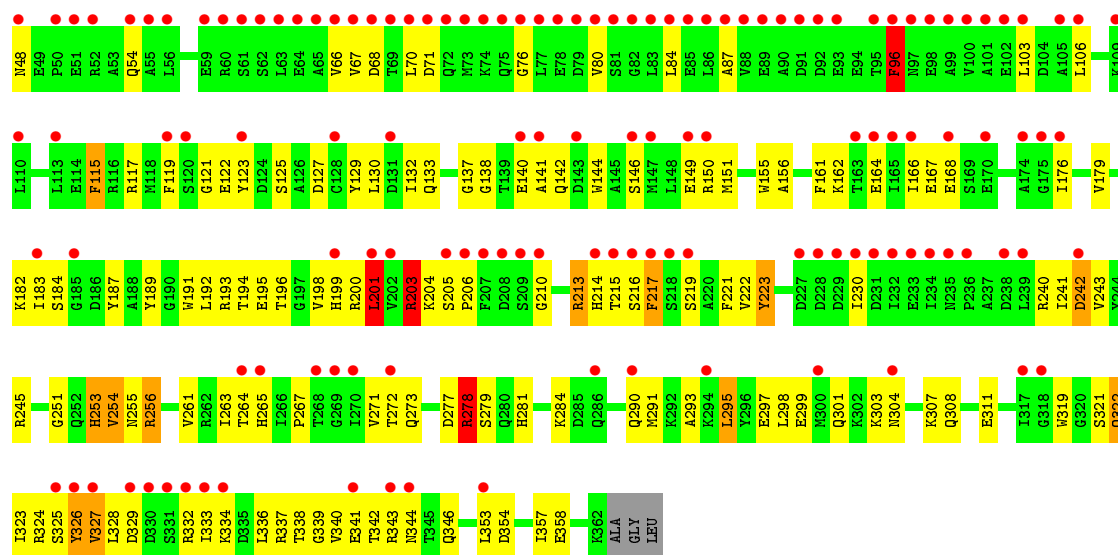


- Molecule 2: messenger RNA

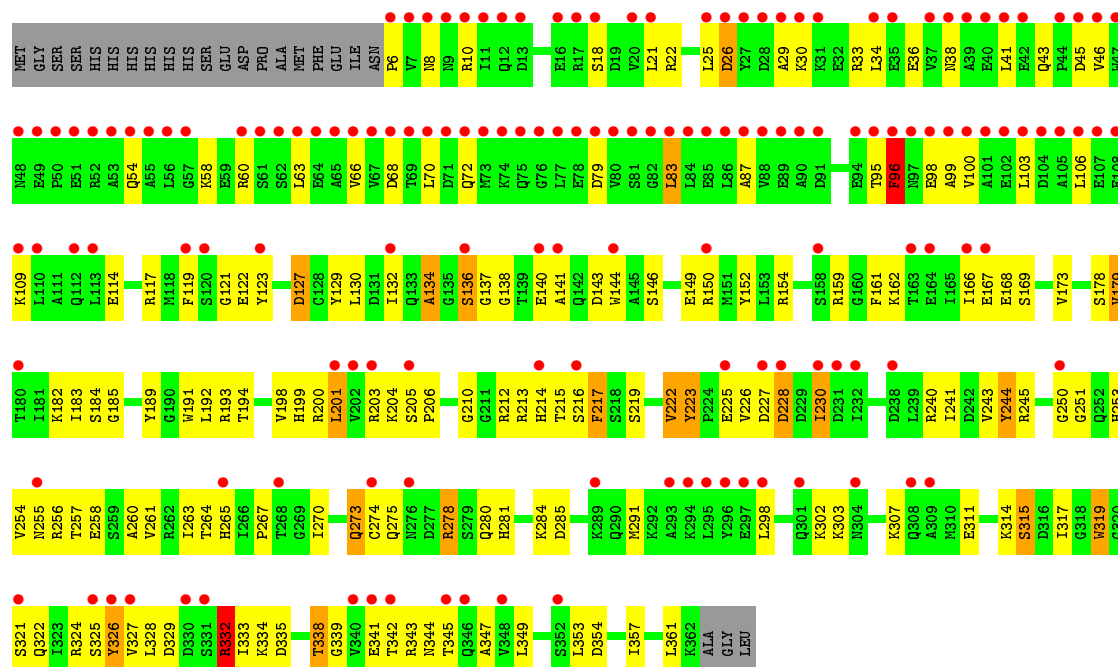
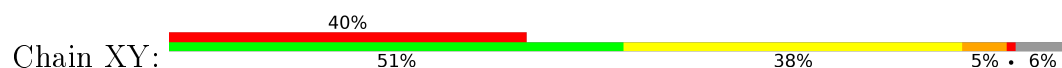


- Molecule 3: Peptide chain release factor 2

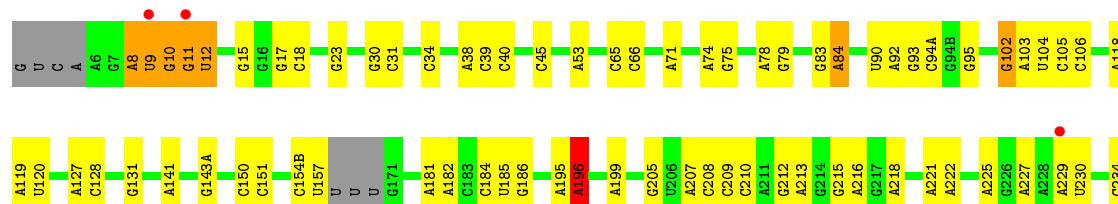




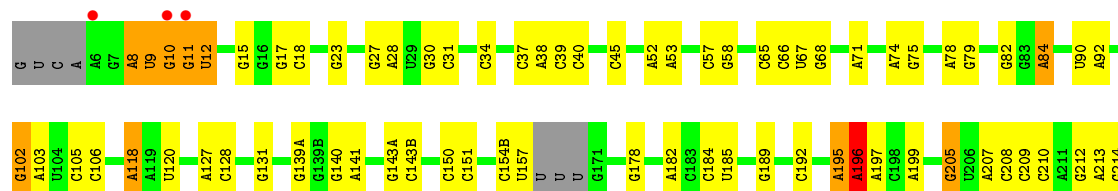
• Molecule 3: Peptide chain release factor 2



• Molecule 4: Thermus thermophilus HB8 genomic DNA, complete genome

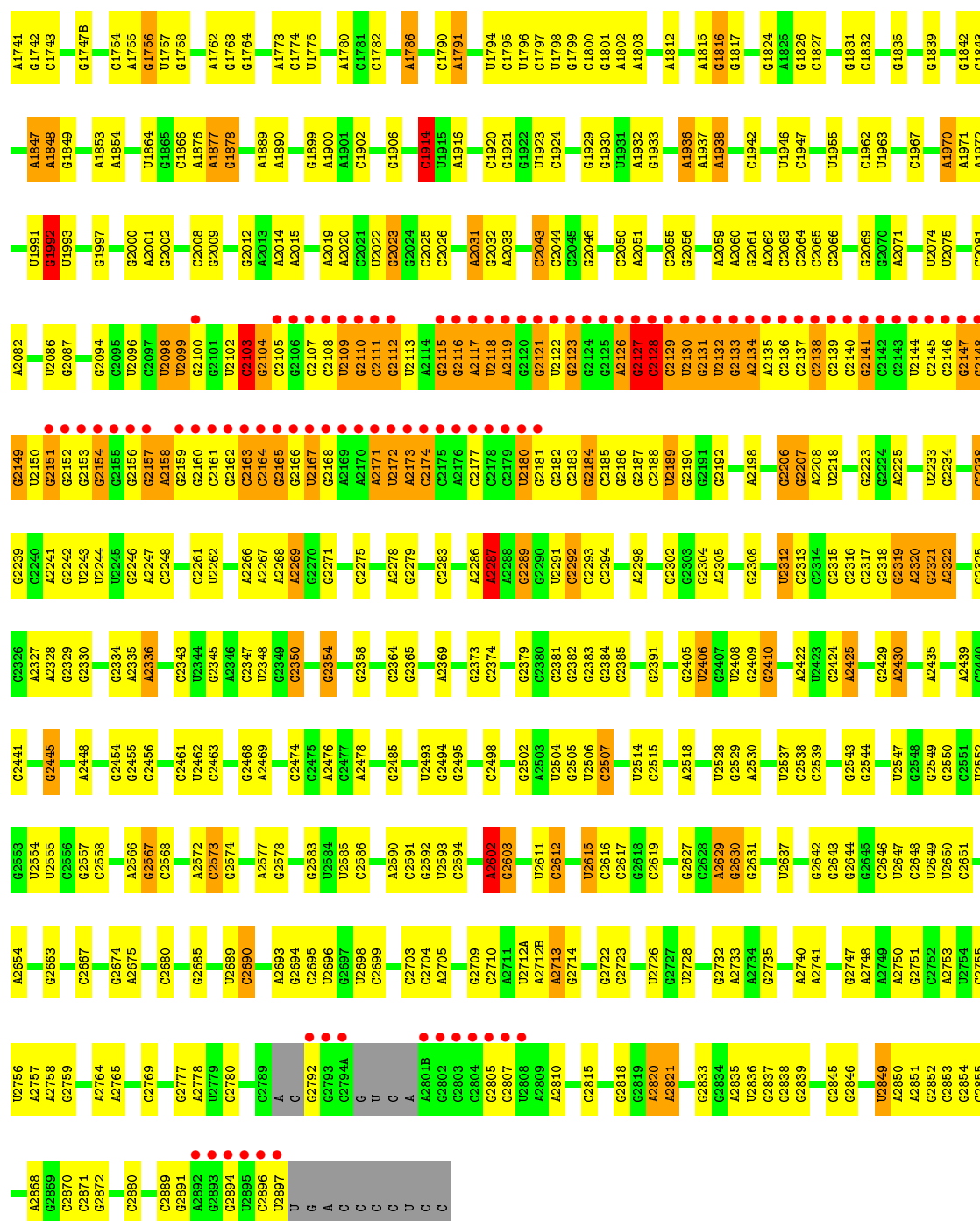






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A1609	A1509B	U1406	A1287	G1154	G1072	C998	A909	A827	G686	A627	G530	U405	A276	A216
A1610	A1509C	C1407	U1288	A1155	A1073	U999	A910	U827	G690	G630	C531	G411	G277	G217
G1628	C1511	G1416	C1289	G1157	G1075	A1001	C912	U833	G691	G631	A532	A412	A278	A218
G1629	U1514	G1417	C1290	U1164	A1077	C1007	C915	C834	A706	A632	G533	A411	U284	A221
G1630	G1515	G1418	C1291	U1165	U1078	U1012	G916	U839	G707	A633	G534	A412	A222	A222
G1631A	U1518	G1419	U1292	C1166	U1079	C1013	A917	C840	C719	A635	U534	A413	C285	
C1636	G1519	G1420	C1293	U1167	U1080	U1014	A918	A841	C721	G636	C535	C414	C286	
A1637	U1525	G1422	C1297	U1171	U1081	G1015	G919	U847	A722	A637	G538	U421	C297	A228
C1638	G1526	G1423	U1300	A1171	U1082	G1016	G920	G848		G638	C540	U427	A299	A229
U1639	U1529	C1428	A1301	G	U1083	G1017	G921	A849		U639	G545	A428	U230	U230
G1647	C1530	G1429	G1310	A	A1084	A1021	U922		C730	C640	C	A428	A300	
C1648	C1531	C1430	G1311	U	A1085	G1022	C923	G852	U740	C641	A	A443	G301	C234
G1651	C1532	U1431	U1312	C1178	G1087	A1023	C924	G853	U741	A642	G549	C444	U235	C236
A1654	G1533	G1444	U1313	C1179	U1088	G1024	C925	G854	G742	A643	G549	C445	U303	C237
A1655	U	A1446A	C1314	C1180	U1090	G1025	G931	G855	G743	A644	G549	C446	U305	
A1656	A	C1446B	C1315	C1181	C1092	U1026	G932	C856	G744	C645	G563		U306	G242
C1657	C1536	U1449	A1317	U1188	U1094	A1028	C936	C857	U747	C646	U568	A454	G307	
C1658	U1540	G1450A	A1321	C1196	A1095	U1033	G935	U858	A752	A652C	G573	A455	A310	G247
U1659	G1541	C1450B	A1322	G1197	A1096	G1034	C936	U859	C753	G652E	C574	C456	A311	G248
A1665	C1543	C1451	U1323	U1198	U1097	U1035	A941	G862		G652F	A575	A457	C249	C249
A1666	A1544	G1455	A1342	C1201	A1098	G1036	G945	A863	G760	g	G579	C456	G250	G250
A1667	C1547	G1459	C1351	C1202	U1101	C1038	G947	G864	A764	C	G580	A466	A251	A251
A1669	C1557	C1467	U1352	A1210	A1102	G1041	G948	U871	A774	A	C587	G469	A257	
G1674	A1558	A1468	A1353	U1211	U1103	G1044	C949	G873	G775	C	U588	A470	A271	A271
G1682	C1559	G1470	A1354	G1212	U1105	A1045	G950	G874	G776	C	C589	G476	A272A	A272A
U1688	U1566	A1471	U1357	A1220	G1110	A1046	G952	C876	A782	G	A590	A479	C272B	C272B
U1692	A1567	G1475	A1358	C1229	A1111	G1047	G953	A878	A783	G	C591	A480	C272C	C272C
U1693	U1578	C1476	A1360	G1239	U1112	A1048	G956	U879	A784	C	U594	A481	G272D	G272D
G1696	A1579	G1482	G1368	U1240	G1113	A1050	A959	G880	G785	C	C595	A482	U272E	U272E
A1700	U1580	G1491	A1378	G1260	G1115	C1053	G961	G882	A788	G652U	A603	C485	C272F	C272F
A1701	C1582	G1492	A1379	U1253	G1116	A1054	G966	C886	G792	A653	G604	C486	U272K	U272K
U1709	C1583	C1493	G1380	A1253	G1117	G1055	G966	A887	A793	A654	U607	A492	U272L	U272L
C1710	C1584	A1495	G1256	C1257	U1118	G1056	U969	C888	C796	A655	A608	A493	U272M	U272M
C1711	A1586	U1497	A1384	G1257	G1125	G1058	C970	C889	C797	A656	A609	G494	C272O	C272O
C1712	U1587	C1498	G1385	C1257	U1125	G1059	C971	A890	G892	U657	G610	A502	C372	
G1713	C1588	C1499	C1386	G1264	U1129	U1060	G972	C893	A802	C659	C611	A503	G375	G272X
G1714	U1589	G1500	C1387	A1265	U	G1062	A973	C894	U603	G660	U614A	A503	C376	C272Y
U1720	G1593	C1501	U1394	C1265	G1135	G1063	G974	U895	A804	G661	U614B	A505	C377	U272Z
G1721	U1594	G1502	A1395	A1269	C1136	C1064	C975A	A896	G805	G668	G614C	A508	G386	G273A
U1722	A1595	C1503	U1396	G1271	U1141	U1065	A933	C897	C812	A670	A614D	G508	G273B	U273B
U1739	A1596	C1504	A1272	A1273	U1144	A1067	G983	A900	C814	C671	G615	C509	G273D	G273D
G1740	A1597	A1507	G1401	C1145	G1444	G1068	C994	A901	C815	C672	G620	C510	G273E	G273E
	C1599	A1508			A1070	A1069	A996	C902	C816	G673	G623	C512	G273F	C273F
								C904	C817	G674			G273G	G273G





• Molecule 5: Thermus thermophilus HB8 genomic DNA, complete genome

Chain YB: 70% 23% 5%

Chain RB: 75% 22%



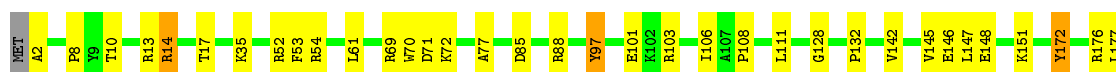
• Molecule 6: 50S ribosomal protein L2

Chain YD: 76% 20%



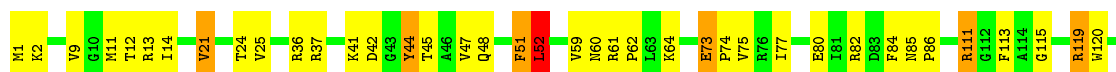
• Molecule 6: 50S ribosomal protein L2

Chain RD: 79% 18%



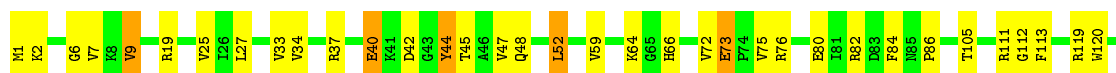
• Molecule 7: 50S ribosomal protein L3

Chain YE: 73% 23%



• Molecule 7: 50S ribosomal protein L3

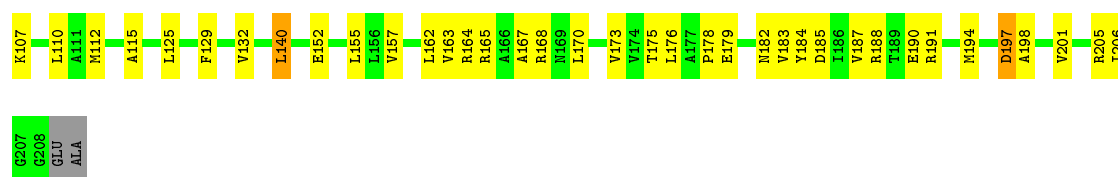
Chain RE: 75% 22%



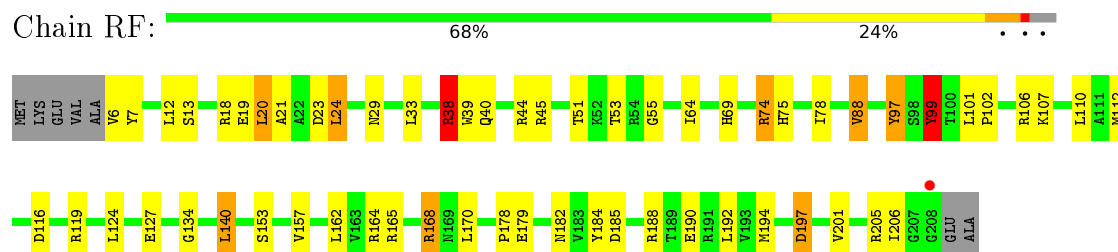
• Molecule 8: 50S ribosomal protein L4

Chain YF: 64% 30%

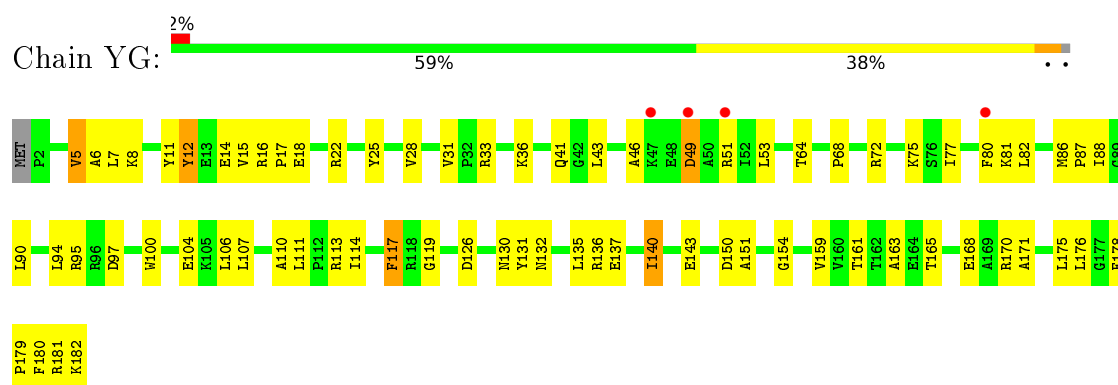




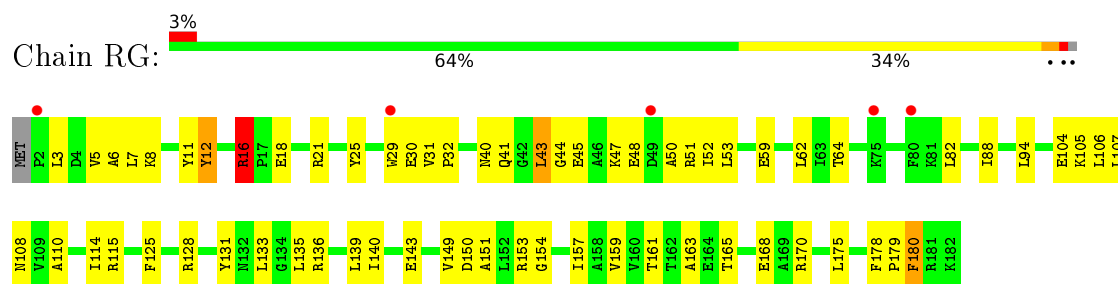
- Molecule 8: 50S ribosomal protein L4



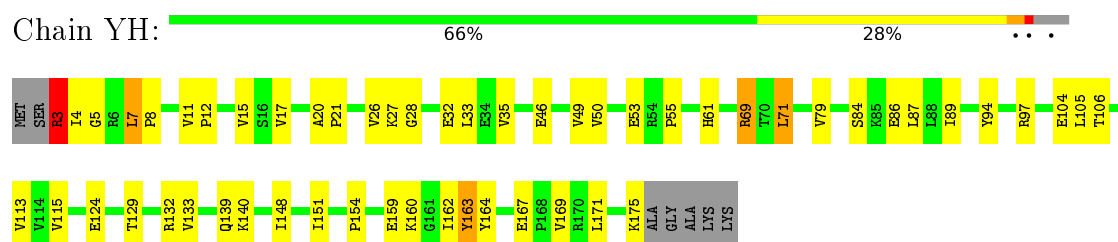
- Molecule 9: 50S ribosomal protein L5



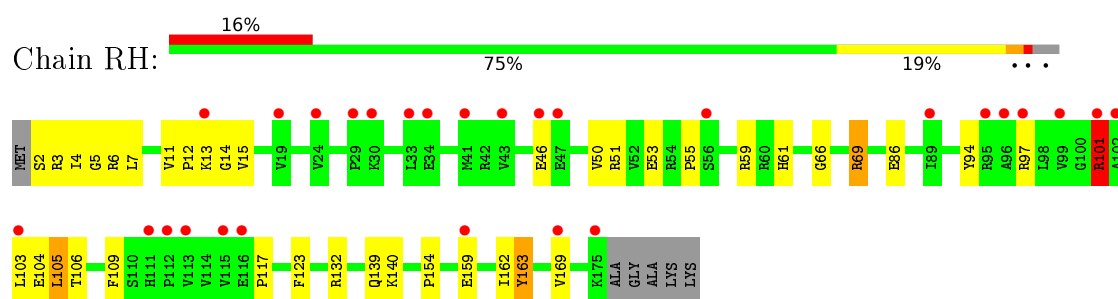
- Molecule 9: 50S ribosomal protein L5



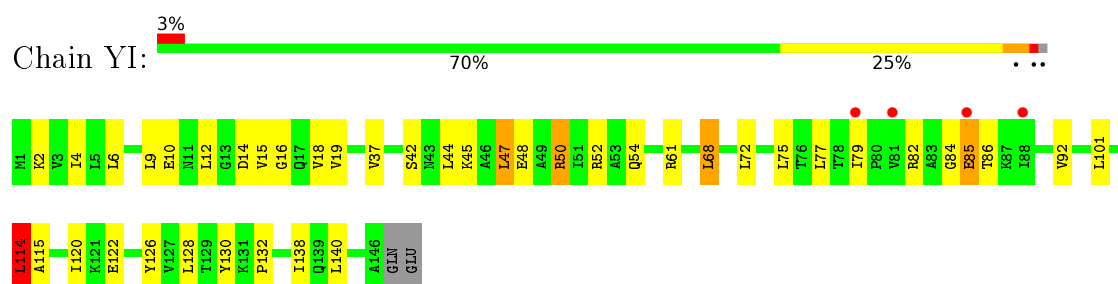
- Molecule 10: 50S ribosomal protein L6



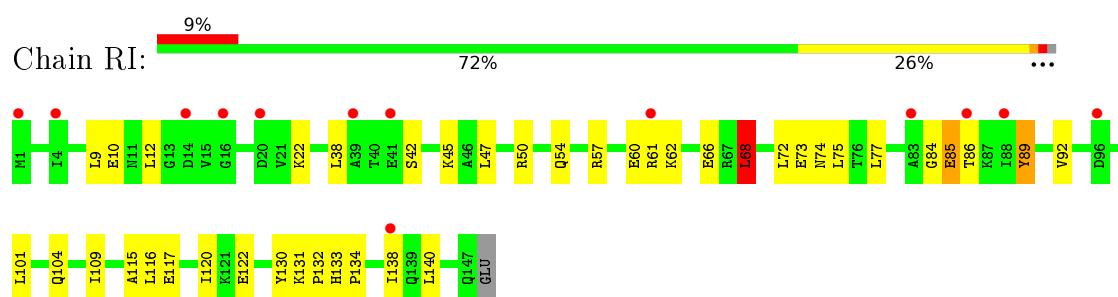
- Molecule 10: 50S ribosomal protein L6



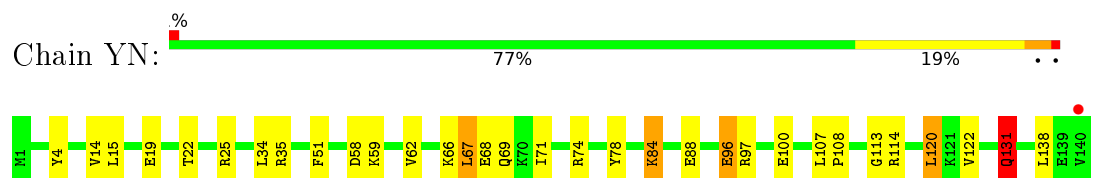
- Molecule 11: 50S ribosomal protein L9



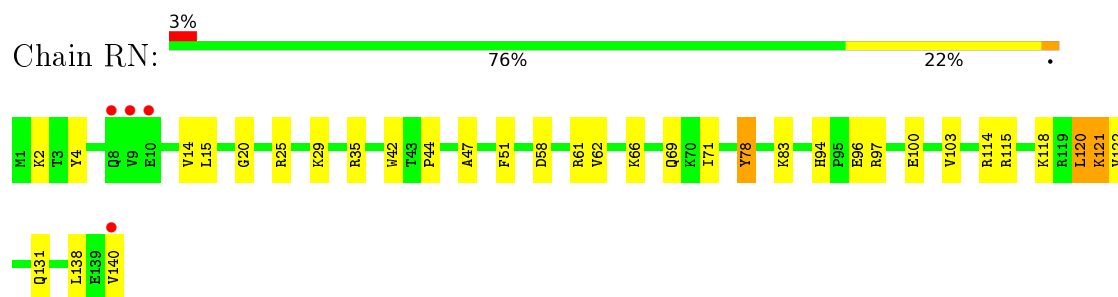
- Molecule 11: 50S ribosomal protein L9



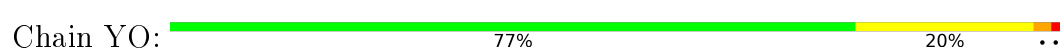
- Molecule 12: 50S ribosomal protein L13



- Molecule 12: 50S ribosomal protein L13



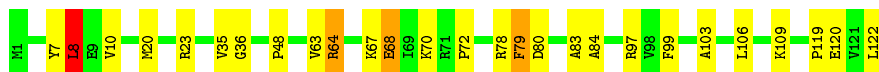
- Molecule 13: 50S ribosomal protein L14





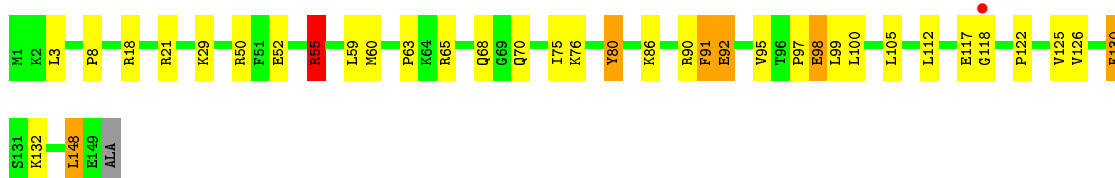
- Molecule 13: 50S ribosomal protein L14

Chain RO: 78% 19% ..



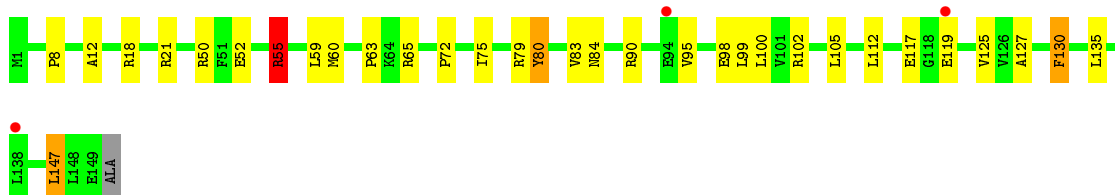
- Molecule 14: 50S ribosomal protein L15

Chain YP: 75% 19% ..



- Molecule 14: 50S ribosomal protein L15

Chain RP: 78% 19% ..



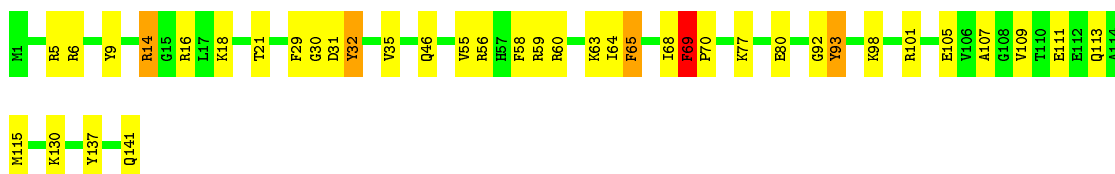
- Molecule 15: 50S ribosomal protein L16

Chain YQ: 77% 19% .



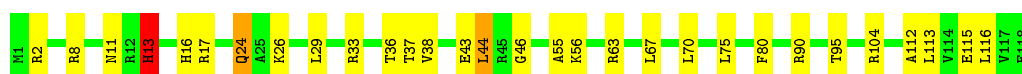
- Molecule 15: 50S ribosomal protein L16

Chain RQ: 72% 24% ..



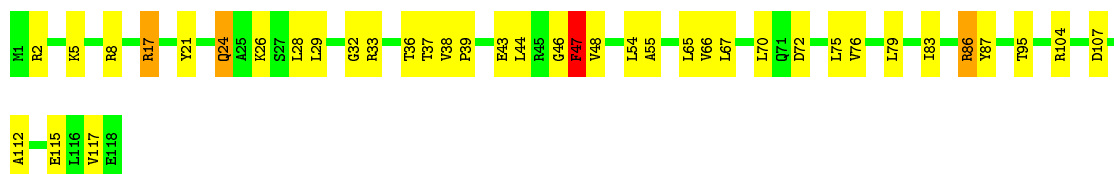
- Molecule 16: 50S ribosomal protein L17

Chain YR: 75% 23% ..



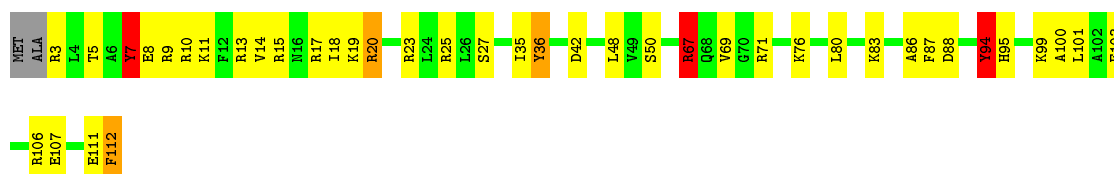
- Molecule 16: 50S ribosomal protein L17

Chain RR: 67% 30%



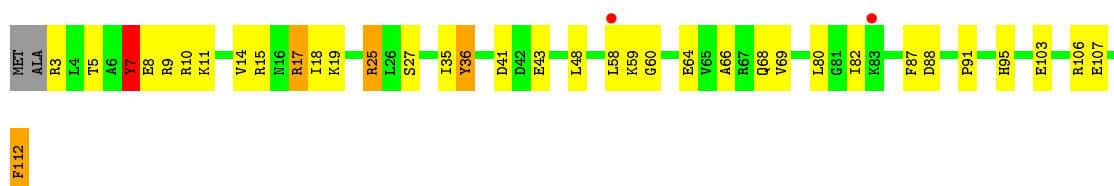
- Molecule 17: 50S ribosomal protein L18

Chain YS: 62% 31%



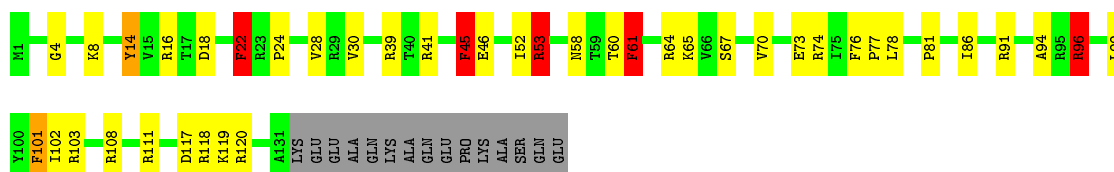
- Molecule 17: 50S ribosomal protein L18

Chain RS: 2% 66% 28%



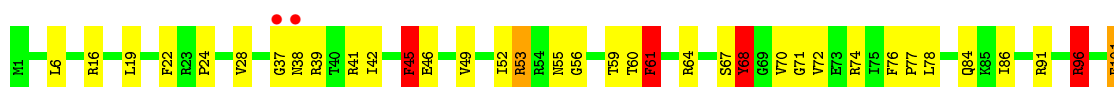
- Molecule 18: 50S ribosomal protein L19

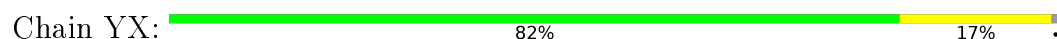
Chain YT: 61% 24% 10%

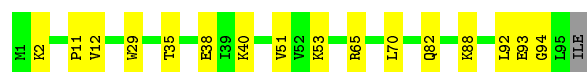


- Molecule 18: 50S ribosomal protein L19

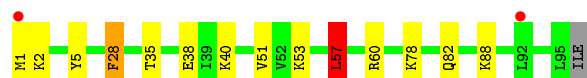
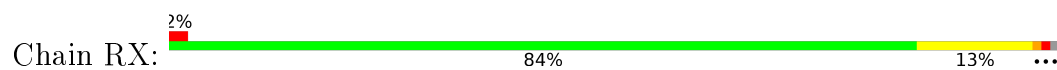
Chain RT: 60% 25% 10%



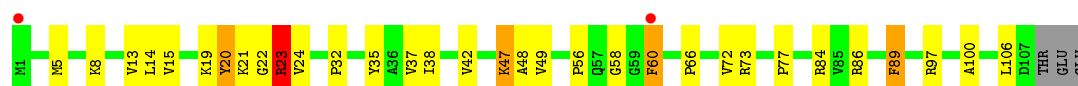




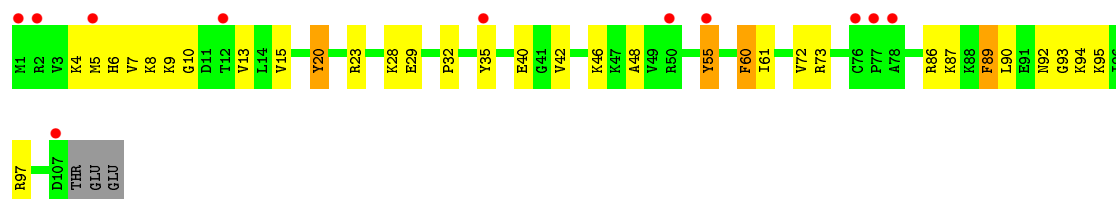
- Molecule 22: 50S ribosomal protein L23



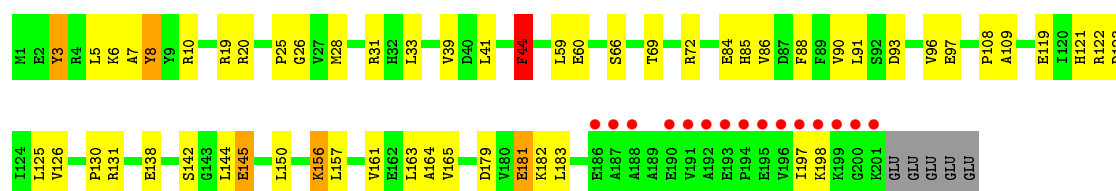
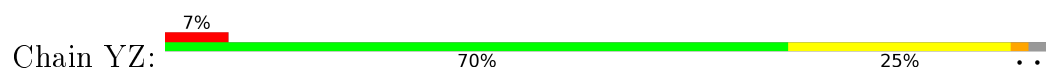
- Molecule 23: 50S ribosomal protein L24



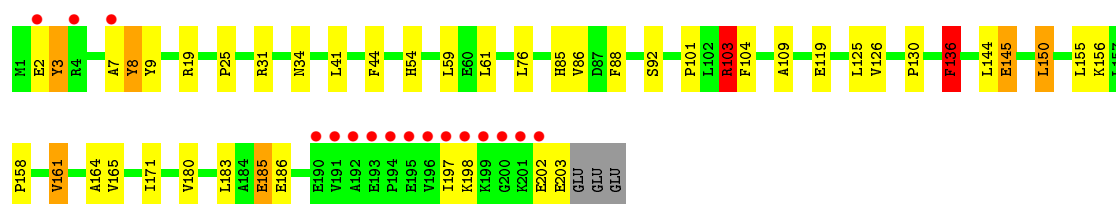
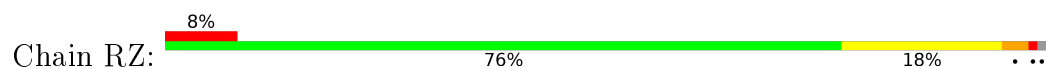
- Molecule 23: 50S ribosomal protein L24



- Molecule 24: 50S ribosomal protein L25

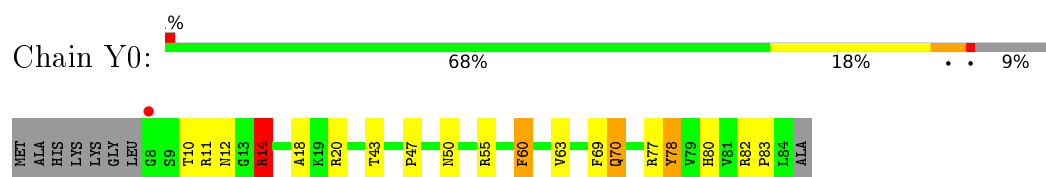


- Molecule 24: 50S ribosomal protein L25

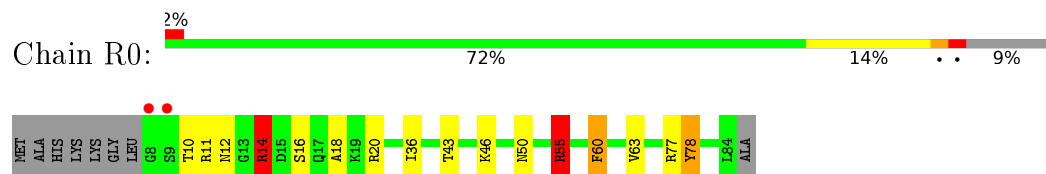


- Molecule 25: 50S ribosomal protein L27

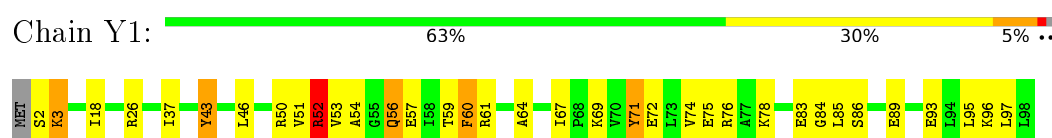




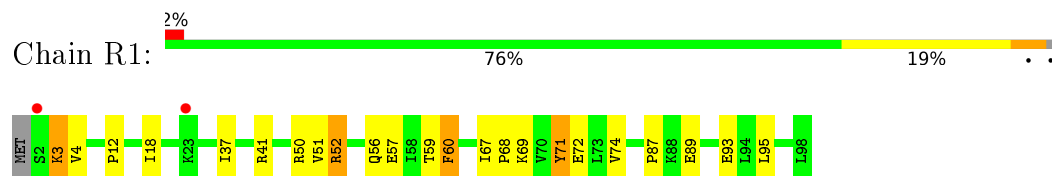
- Molecule 25: 50S ribosomal protein L27



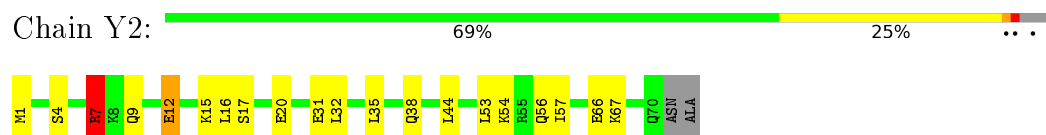
- Molecule 26: 50S ribosomal protein L28



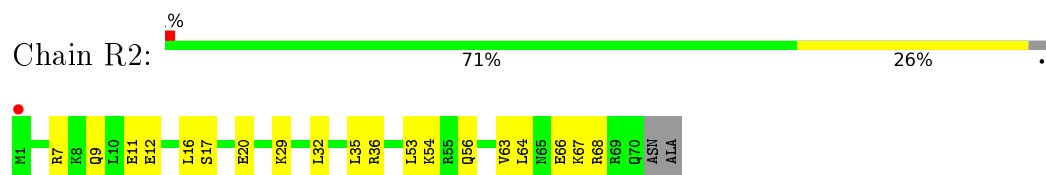
- Molecule 26: 50S ribosomal protein L28



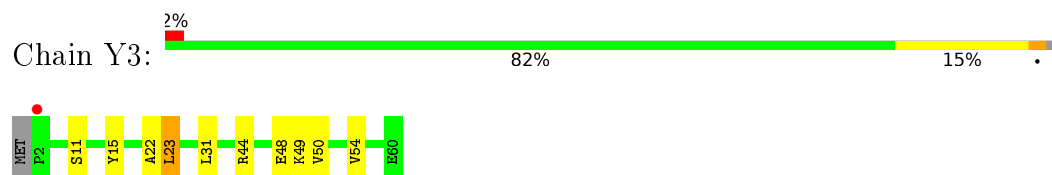
- Molecule 27: 50S ribosomal protein L29



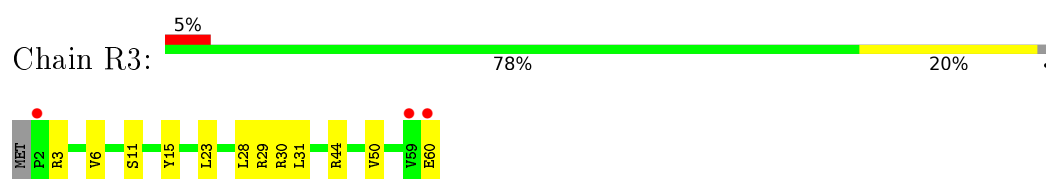
- Molecule 27: 50S ribosomal protein L29



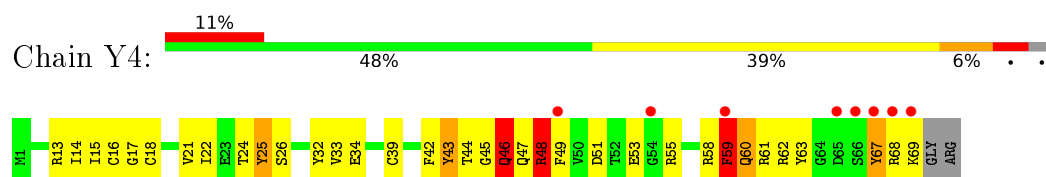
- Molecule 28: 50S ribosomal protein L30



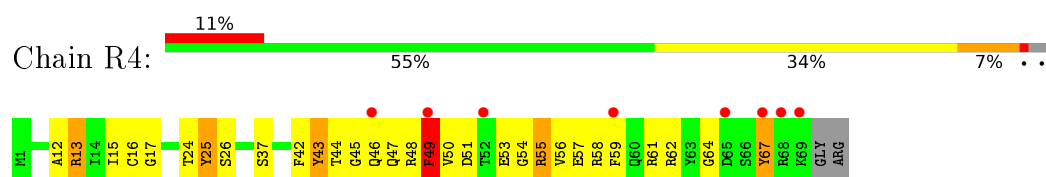
- Molecule 28: 50S ribosomal protein L30



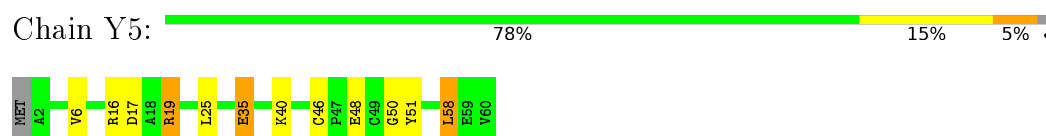
- Molecule 29: 50S ribosomal protein L31



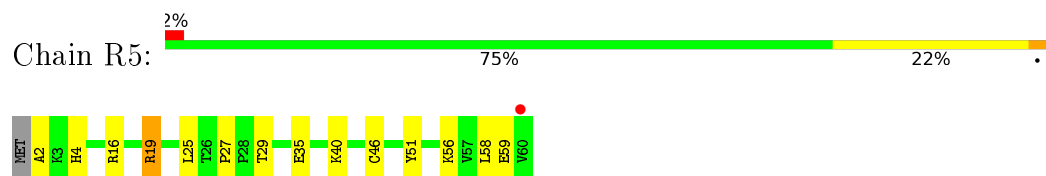
- Molecule 29: 50S ribosomal protein L31



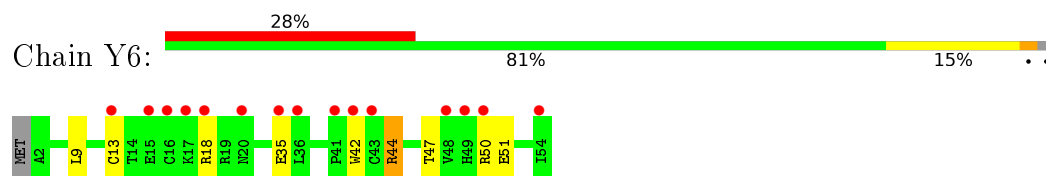
- Molecule 30: 50S ribosomal protein L32



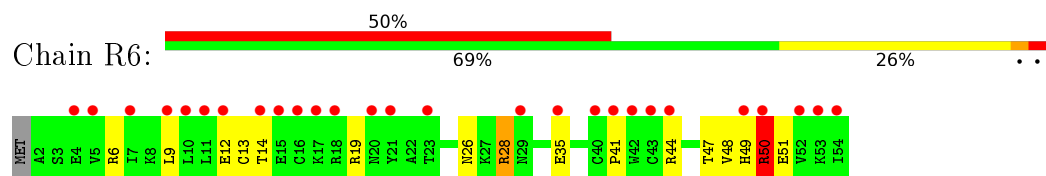
- Molecule 30: 50S ribosomal protein L32




- Molecule 31: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L33



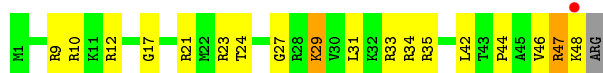
- Molecule 32: 50S ribosomal protein L34

Chain Y7:  73% 18% . . .



- Molecule 32: 50S ribosomal protein L34

Chain R7:  2% 61% 33% . . .



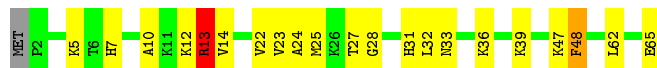
- Molecule 33: 50S ribosomal protein L35

Chain Y8:  60% 37% . . .




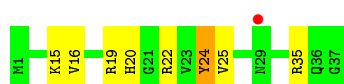
- Molecule 33: 50S ribosomal protein L35

Chain R8:  66% 29% . . .




- Molecule 34: 50S ribosomal protein L36

Chain Y9:  3% 78% 19% .



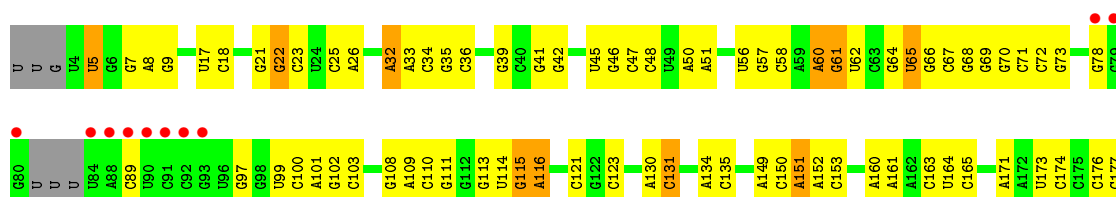
- Molecule 34: 50S ribosomal protein L36

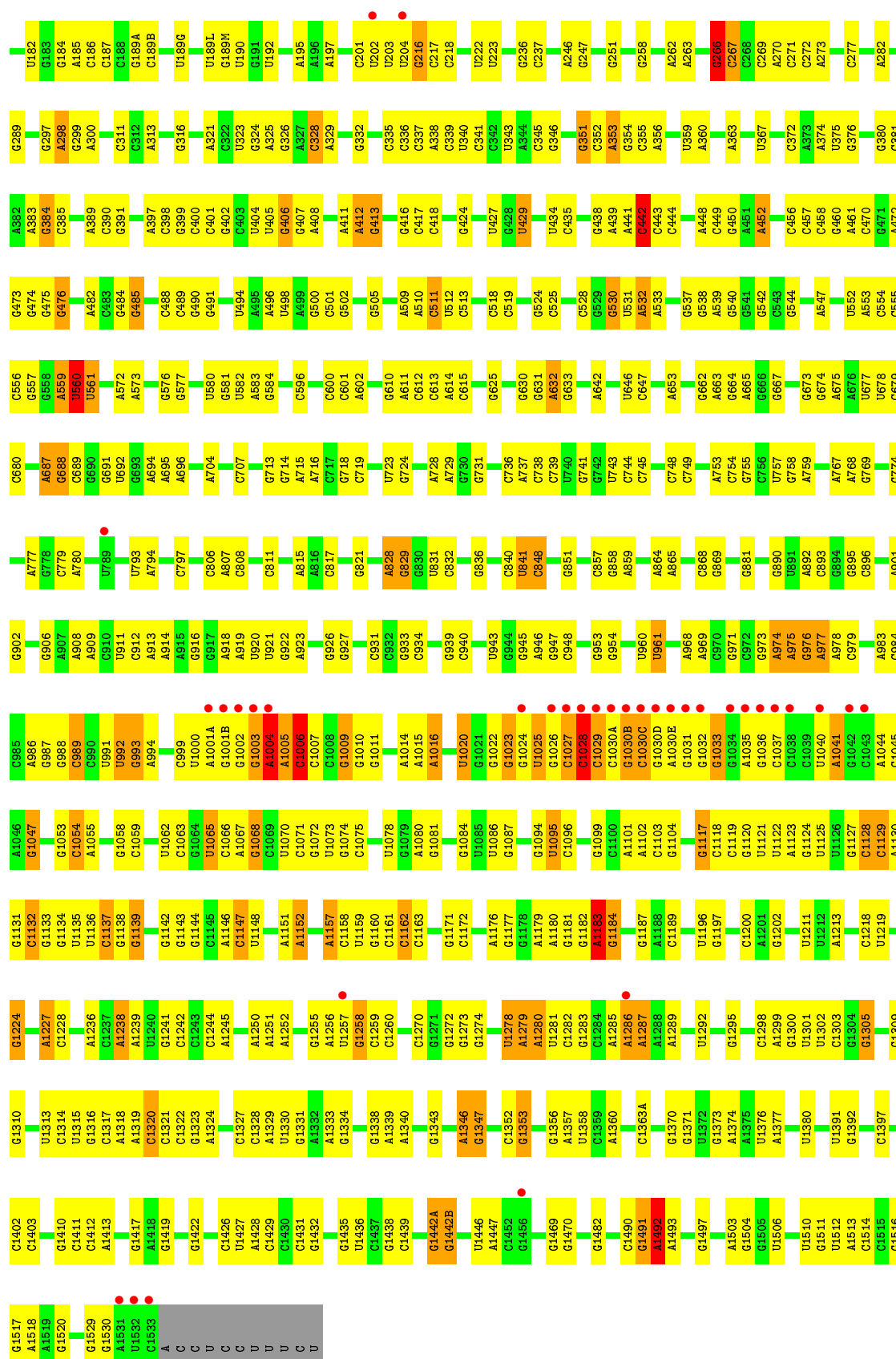
Chain R9:  8% 70% 24% . . .



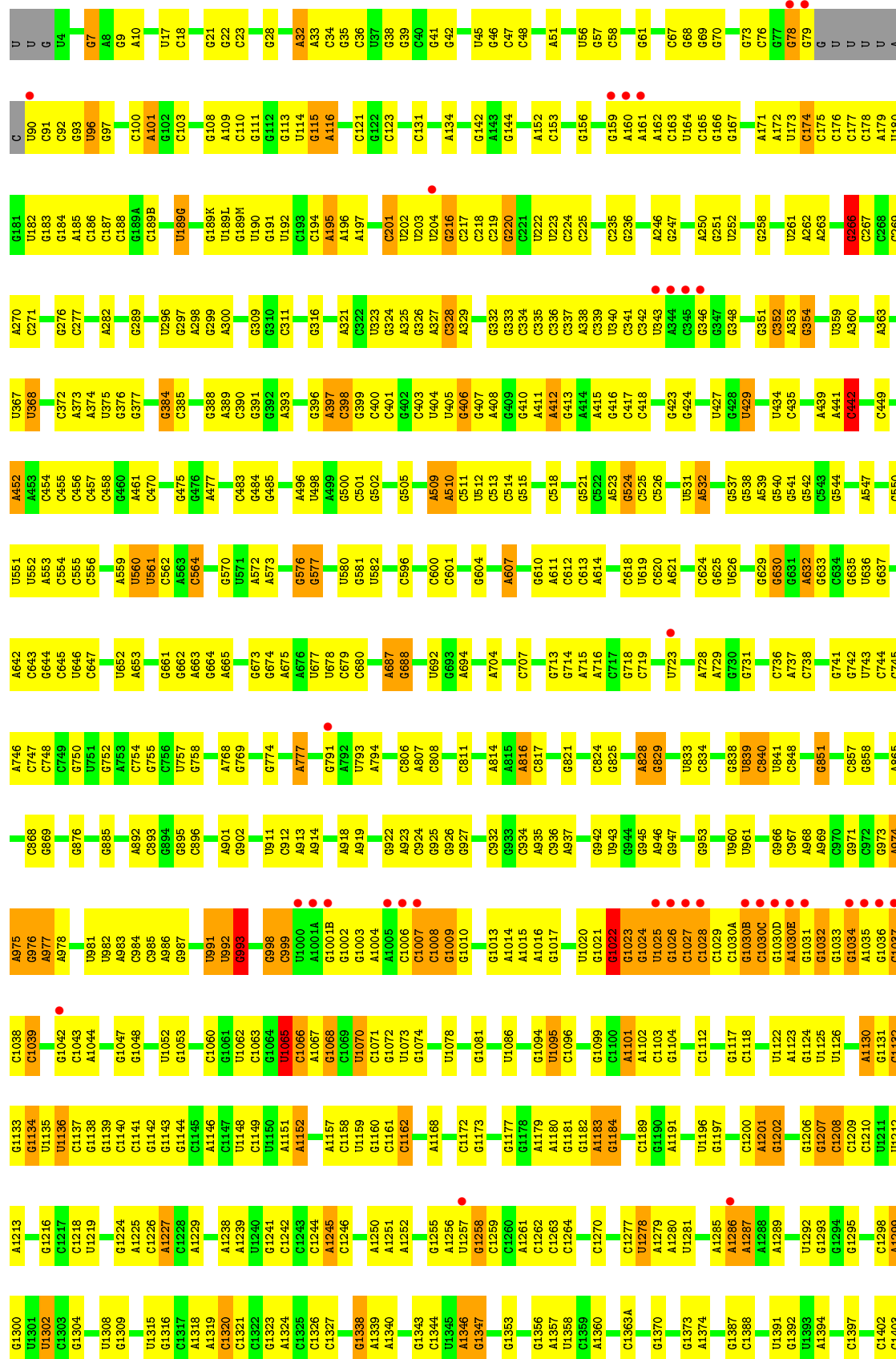
- Molecule 35: Thermus thermophilus HB8 genomic DNA, complete genome

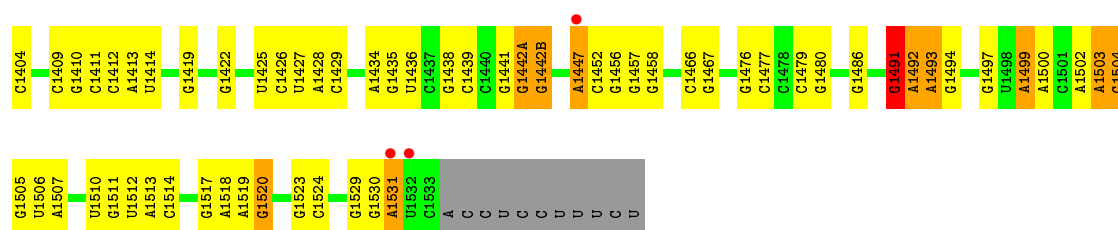
Chain XA:  3% 54% 38% 6% . . .



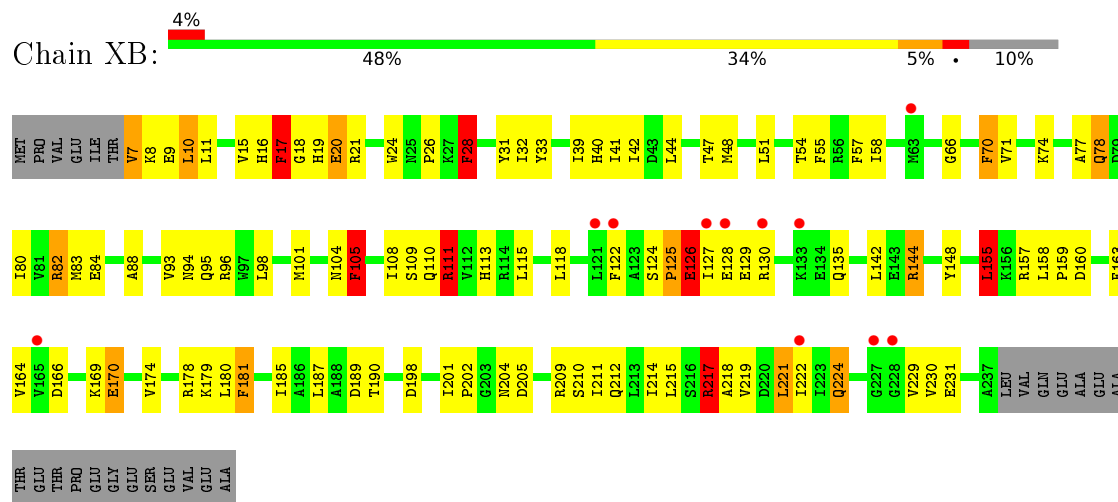


- Molecule 35: Thermus thermophilus HB8 genomic DNA, complete genome

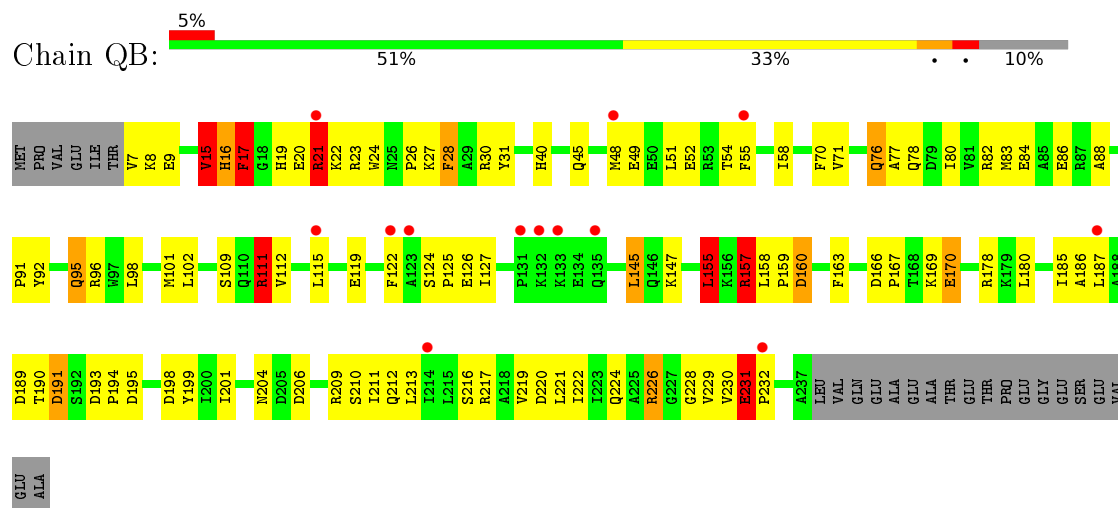




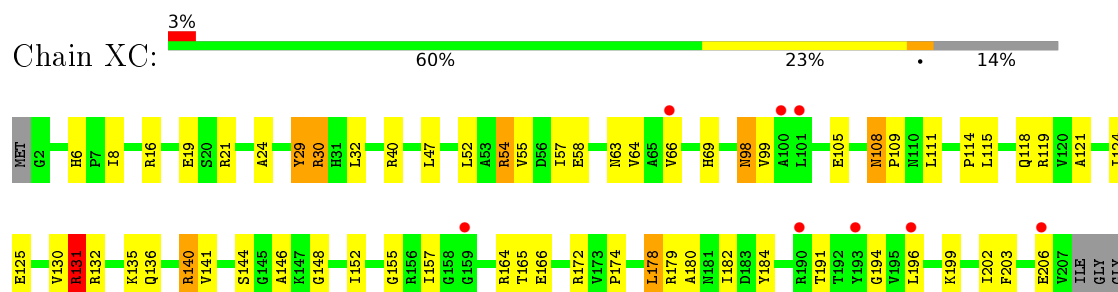
• Molecule 36: 30S ribosomal protein S2



• Molecule 36: 30S ribosomal protein S2



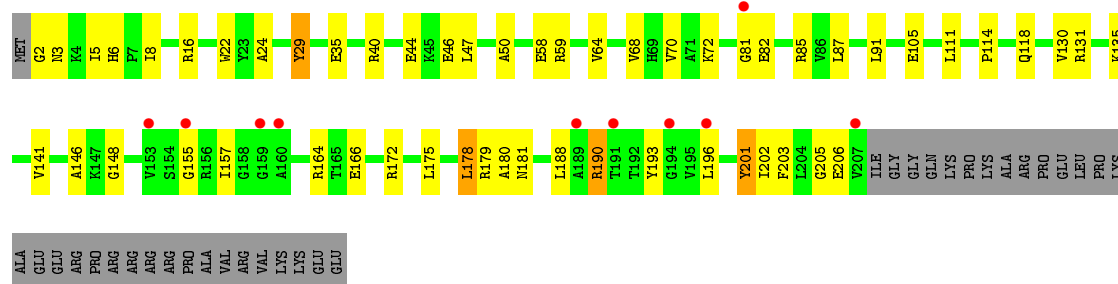
• Molecule 37: 30S ribosomal protein S3



GLN  
LYS  
PRO  
LYS  
LYS  
ALA  
ARG  
PRO  
GLU  
LEU  
PRO  
LYS  
LYS  
ALA  
GLU  
GLU  
ARG  
PRO  
ARG  
ARG  
ARG  
ARG  
PRO  
VAL  
VAL  
VAL  
LYS  
LYS  
GLU  
GLU

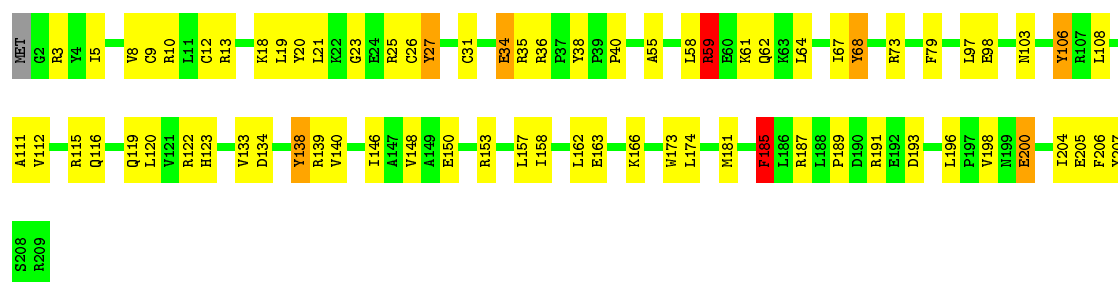
• Molecule 37: 30S ribosomal protein S3

Chain QC: 4% 63% 21% 14%



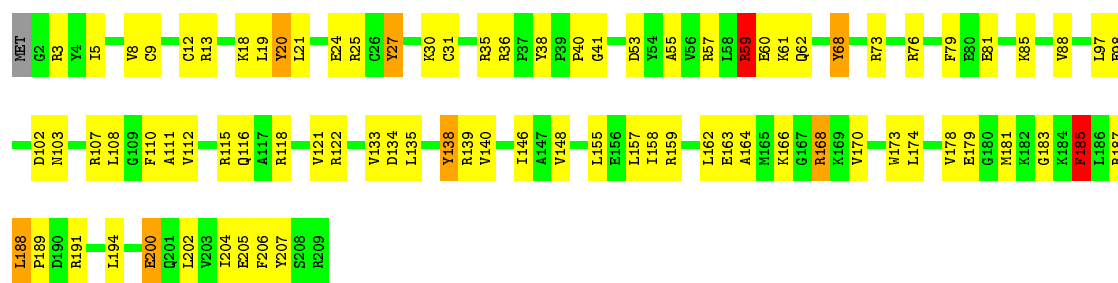
• Molecule 38: 30S ribosomal protein S4

Chain XD: 65% 31% 4%



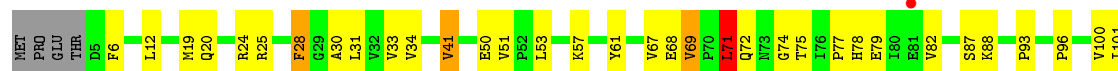
• Molecule 38: 30S ribosomal protein S4

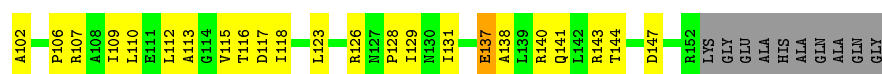
Chain QD: 59% 36% 5%



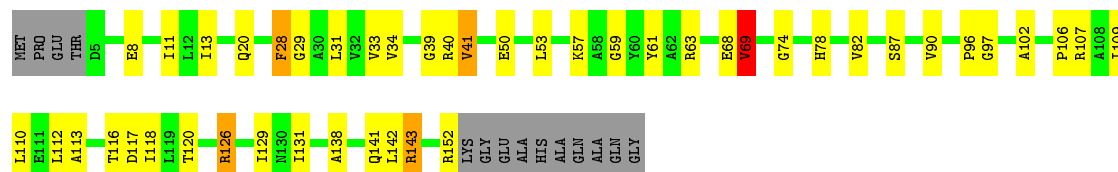
• Molecule 39: 30S ribosomal protein S5

Chain XE: 56% 32% 9% 3%





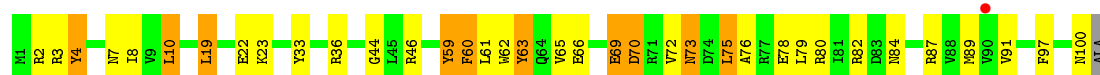
- Molecule 39: 30S ribosomal protein S5



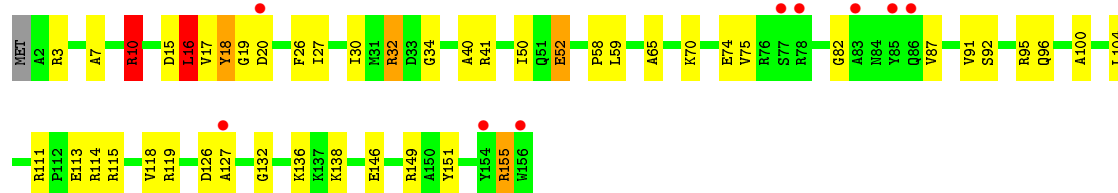
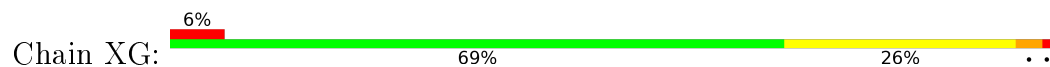
- Molecule 40: 30S ribosomal protein S6



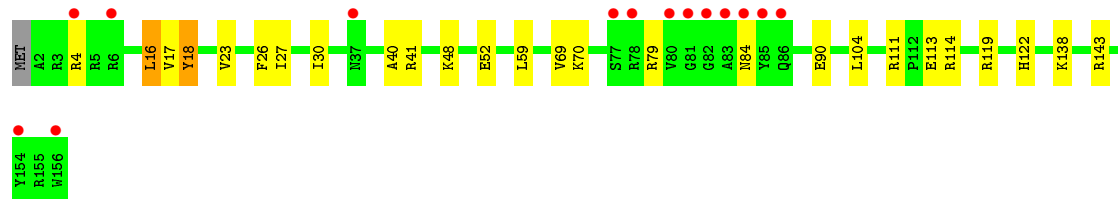
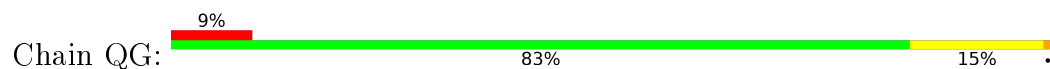
- Molecule 40: 30S ribosomal protein S6



- Molecule 41: 30S ribosomal protein S7

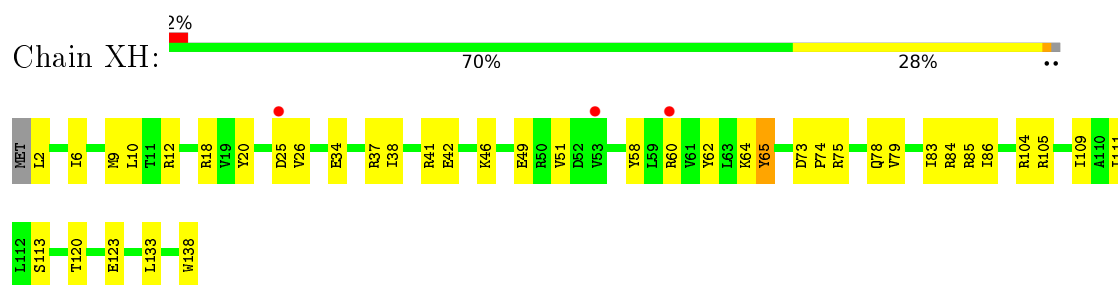


- Molecule 41: 30S ribosomal protein S7

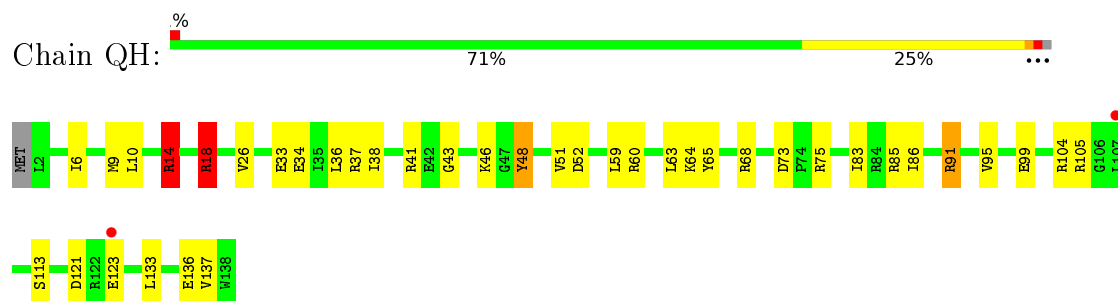


- Molecule 42: 30S ribosomal protein S8

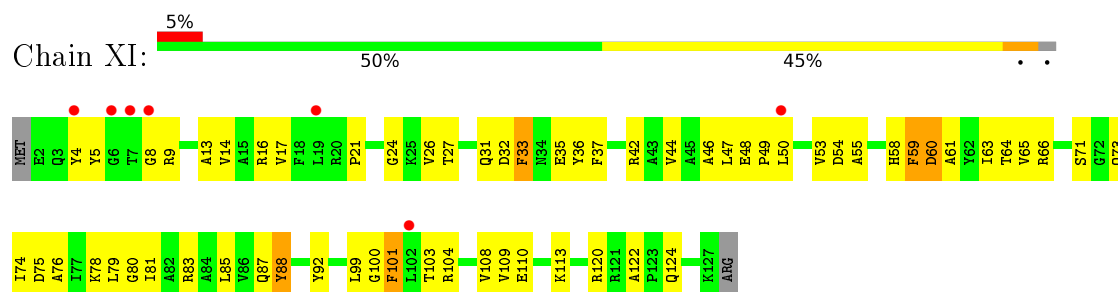




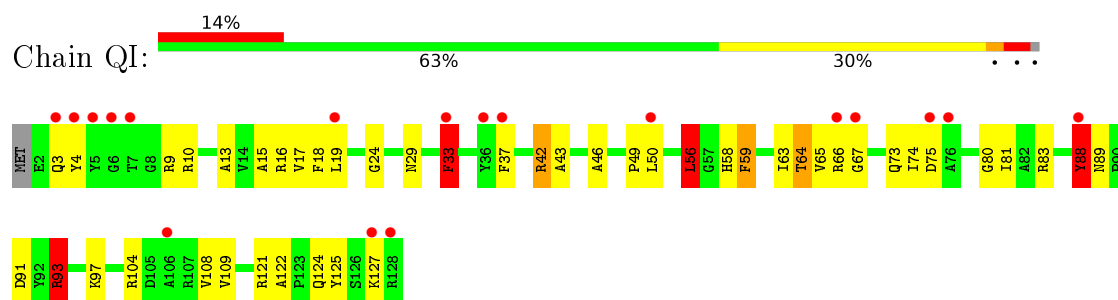
- Molecule 42: 30S ribosomal protein S8



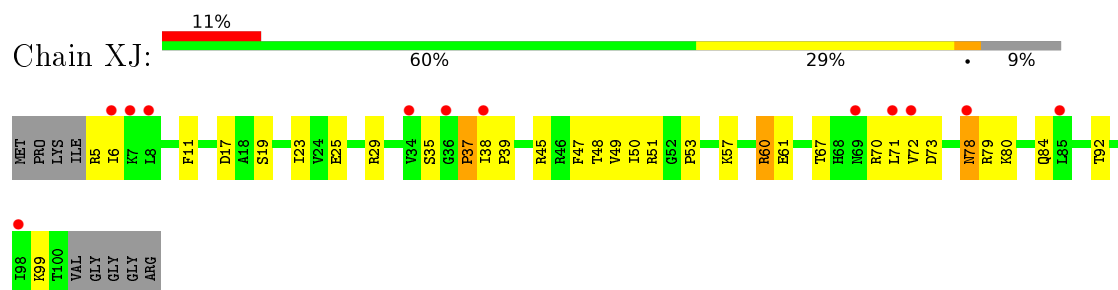
- Molecule 43: 30S ribosomal protein S9



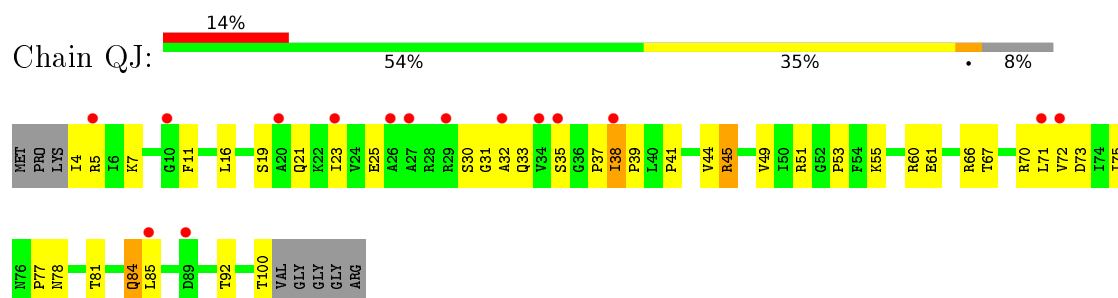
- Molecule 43: 30S ribosomal protein S9



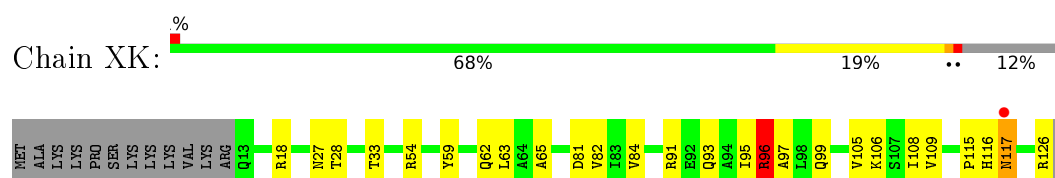
- Molecule 44: 30S ribosomal protein S10



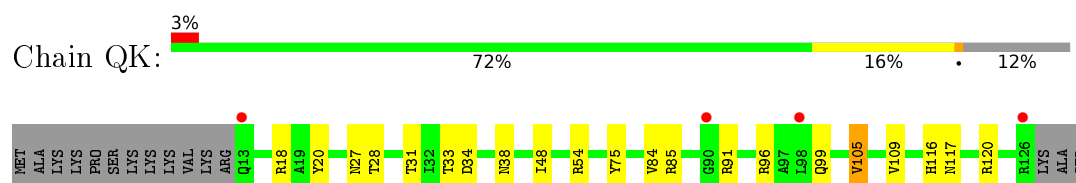
- Molecule 44: 30S ribosomal protein S10



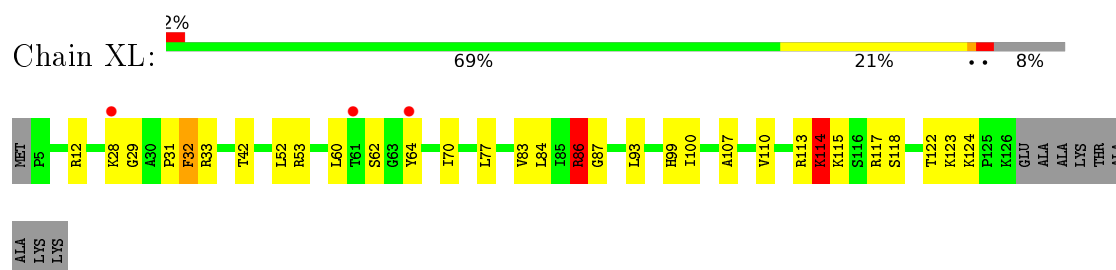
- Molecule 45: 30S ribosomal protein S11



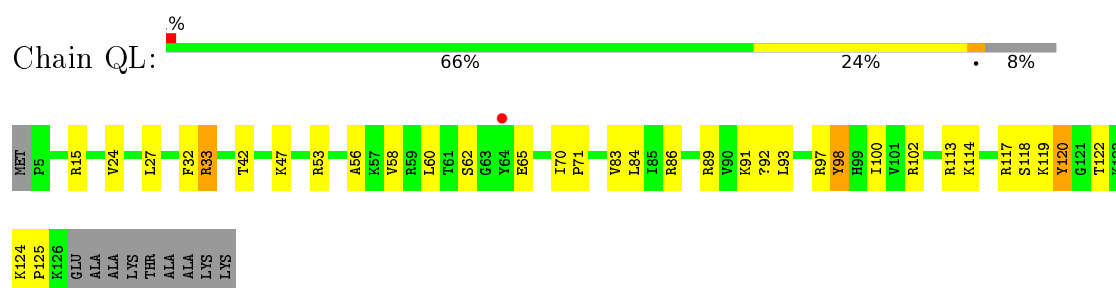
- Molecule 45: 30S ribosomal protein S11



- Molecule 46: 30S ribosomal protein S12

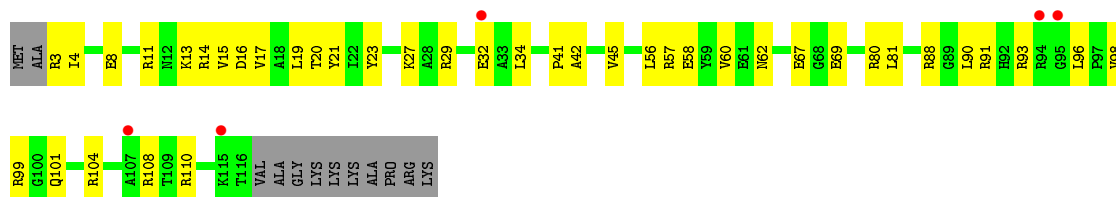


- Molecule 46: 30S ribosomal protein S12

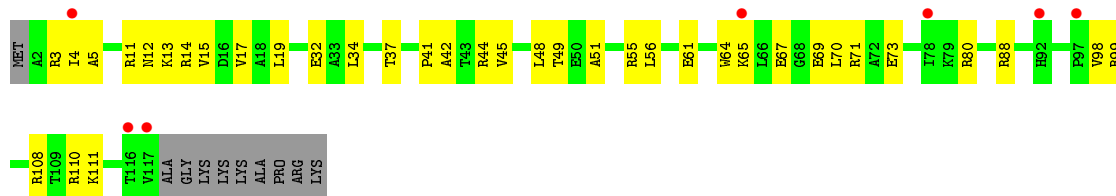


- Molecule 47: 30S ribosomal protein S13

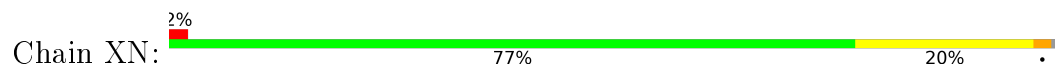




- Molecule 47: 30S ribosomal protein S13



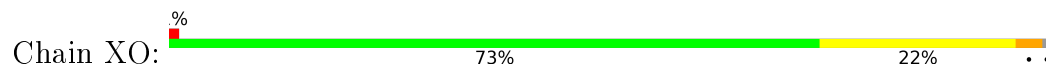
- Molecule 48: 30S ribosomal protein S14 type Z



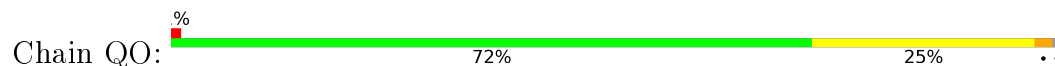
- Molecule 48: 30S ribosomal protein S14 type Z



- Molecule 49: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S15



- Molecule 50: 30S ribosomal protein S16

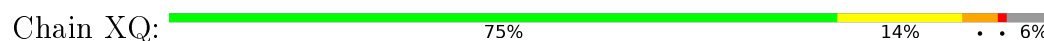




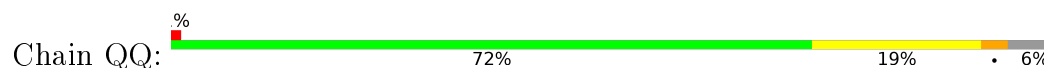
- Molecule 50: 30S ribosomal protein S16



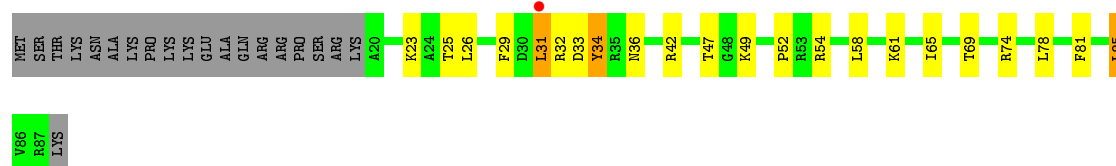
- Molecule 51: 30S ribosomal protein S17



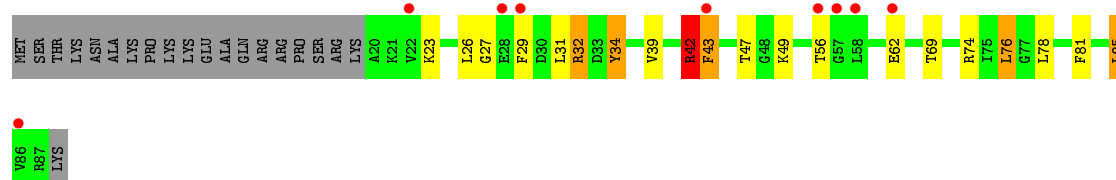
- Molecule 51: 30S ribosomal protein S17



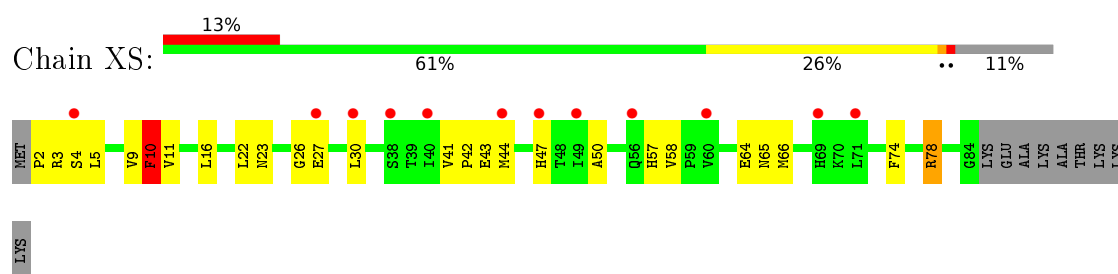
- Molecule 52: 30S ribosomal protein S18



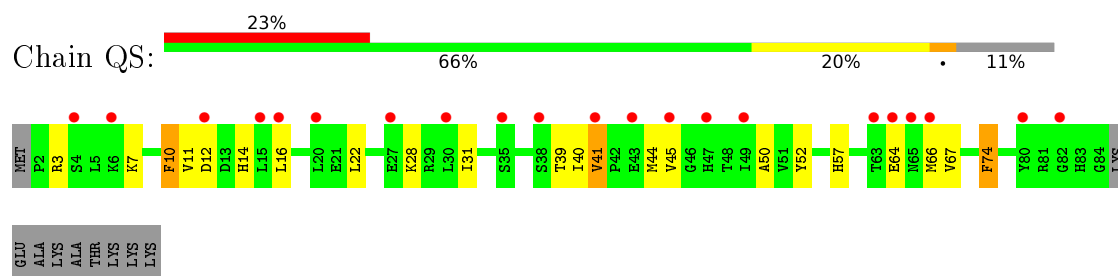
- Molecule 52: 30S ribosomal protein S18



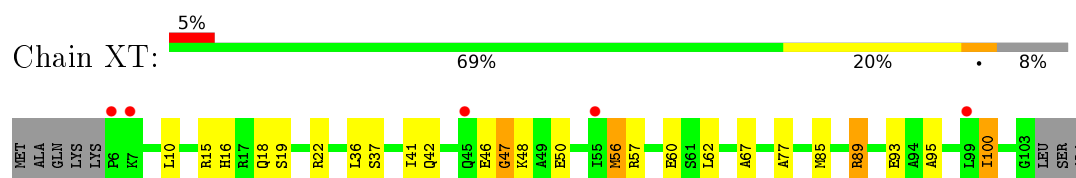
- Molecule 53: 30S ribosomal protein S19



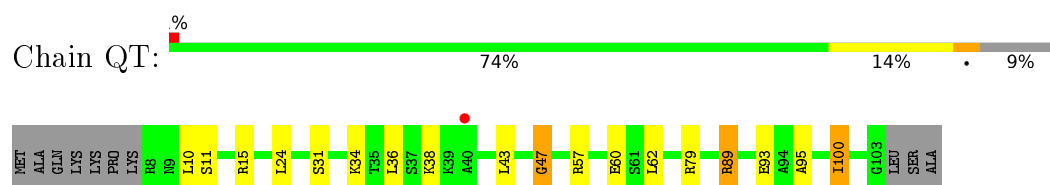
- Molecule 53: 30S ribosomal protein S19



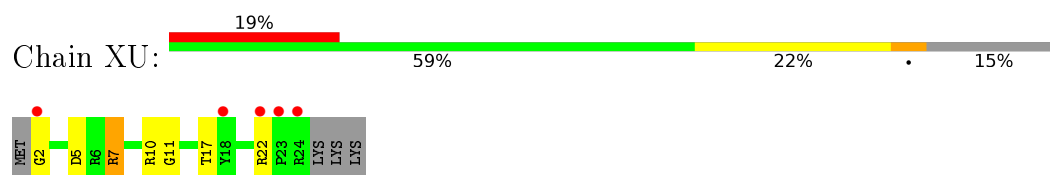
- Molecule 54: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein S20



- Molecule 55: 30S ribosomal protein Thx



- Molecule 55: 30S ribosomal protein Thx



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.48 Å   450.41 Å   622.55 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.88 – 3.10 49.88 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.88-3.10) 100.0 (49.88-3.10)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 3.12 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.10.1_2155)	Depositor
R, $R_{free}$	0.196 , 0.227 0.199 , 0.228	Depositor DCC
$R_{free}$ test set	49511 reflections (4.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 74.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	296662	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: 5MU, ZN, OMG, MA6, SF4, 0TD, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	QV	0.39	1/1836 (0.1%)	0.88	5/2859 (0.2%)
1	XV	0.35	1/1836 (0.1%)	0.81	2/2859 (0.1%)
2	QX	0.31	0/241	0.88	0/373
2	XX	0.29	0/241	0.85	0/373
3	QY	0.39	1/2873 (0.0%)	0.88	12/3870 (0.3%)
3	XY	0.38	1/2873 (0.0%)	0.77	9/3870 (0.2%)
4	RA	0.28	0/68901	0.90	93/107544 (0.1%)
4	YA	0.30	0/68901	0.88	81/107544 (0.1%)
5	RB	0.24	0/2876	0.85	0/4486
5	YB	0.27	0/2878	0.88	0/4490
6	RD	0.39	1/2181 (0.0%)	0.71	2/2940 (0.1%)
6	YD	0.47	2/2186 (0.1%)	0.88	9/2944 (0.3%)
7	RE	0.35	0/1592	0.68	0/2149
7	YE	0.48	3/1592 (0.2%)	0.74	4/2149 (0.2%)
8	RF	0.34	0/1619	0.75	4/2193 (0.2%)
8	YF	0.33	0/1615	0.71	2/2188 (0.1%)
9	RG	0.49	1/1451 (0.1%)	0.75	3/1961 (0.2%)
9	YG	0.36	0/1449	0.75	0/1957
10	RH	0.35	1/1356 (0.1%)	0.68	1/1834 (0.1%)
10	YH	0.40	1/1350 (0.1%)	0.79	5/1826 (0.3%)
11	RI	0.39	1/1109 (0.1%)	0.75	2/1512 (0.1%)
11	YI	0.41	1/1091 (0.1%)	0.82	6/1490 (0.4%)
12	RN	0.62	3/1148 (0.3%)	0.77	2/1547 (0.1%)
12	YN	0.44	1/1144 (0.1%)	0.71	3/1543 (0.2%)
13	RO	0.32	0/943	0.67	3/1269 (0.2%)
13	YO	0.38	1/943 (0.1%)	0.69	2/1269 (0.2%)
14	RP	0.35	0/1152	0.81	3/1533 (0.2%)
14	YP	0.36	0/1152	0.82	3/1533 (0.2%)
15	RQ	0.37	0/1143	0.78	5/1527 (0.3%)
15	YQ	0.39	0/1143	0.70	1/1527 (0.1%)
16	RR	0.42	1/982 (0.1%)	0.87	6/1312 (0.5%)
16	YR	0.41	1/982 (0.1%)	0.75	2/1312 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	RS	0.39	0/887	0.78	3/1180 (0.3%)
17	YS	0.40	0/880	0.96	4/1172 (0.3%)
18	RT	0.37	0/1105	0.87	6/1477 (0.4%)
18	YT	0.36	0/1097	0.90	7/1468 (0.5%)
19	RU	0.61	3/977 (0.3%)	1.20	9/1301 (0.7%)
19	YU	0.66	3/977 (0.3%)	1.09	8/1301 (0.6%)
20	RV	0.51	1/786 (0.1%)	1.31	5/1053 (0.5%)
20	YV	0.39	0/782	0.80	2/1049 (0.2%)
21	RW	0.31	0/897	0.71	3/1205 (0.2%)
21	YW	0.32	0/897	0.72	3/1205 (0.2%)
22	RX	0.31	0/764	0.66	1/1025 (0.1%)
22	YX	0.30	0/764	0.62	0/1025
23	RY	0.32	0/823	0.67	0/1099
23	YY	0.51	1/823 (0.1%)	0.92	4/1100 (0.4%)
24	RZ	0.36	0/1620	0.77	5/2200 (0.2%)
24	YZ	0.40	1/1590 (0.1%)	0.78	6/2162 (0.3%)
25	R0	0.46	0/616	1.07	5/821 (0.6%)
25	Y0	0.48	1/616 (0.2%)	0.87	2/821 (0.2%)
26	R1	0.33	0/761	0.75	2/1013 (0.2%)
26	Y1	0.73	5/766 (0.7%)	0.85	5/1018 (0.5%)
27	R2	0.35	0/590	0.70	0/781
27	Y2	0.56	2/594 (0.3%)	0.82	3/785 (0.4%)
28	R3	0.41	1/474 (0.2%)	0.63	0/635
28	Y3	0.28	0/469	0.61	0/630
29	R4	0.68	3/559 (0.5%)	1.06	4/754 (0.5%)
29	Y4	0.64	2/549 (0.4%)	1.05	6/741 (0.8%)
30	R5	0.54	1/473 (0.2%)	0.87	2/639 (0.3%)
30	Y5	0.52	0/469	0.73	0/635
31	R6	0.69	2/460 (0.4%)	1.23	5/613 (0.8%)
31	Y6	0.34	0/456	0.62	0/608
32	R7	0.59	2/426 (0.5%)	0.97	2/561 (0.4%)
32	Y7	0.37	0/426	0.92	4/561 (0.7%)
33	R8	0.33	0/525	0.87	2/691 (0.3%)
33	Y8	0.31	0/525	0.66	0/691
34	R9	0.48	1/310 (0.3%)	1.08	4/407 (1.0%)
34	Y9	0.29	0/310	0.69	0/407
35	QA	0.25	0/35795	0.86	32/55864 (0.1%)
35	XA	0.26	0/35890	0.88	34/56012 (0.1%)
36	QB	0.43	1/1876 (0.1%)	0.93	12/2533 (0.5%)
36	XB	0.47	1/1860 (0.1%)	1.14	14/2518 (0.6%)
37	QC	0.36	0/1582	0.69	1/2137 (0.0%)
37	XC	0.43	1/1566 (0.1%)	0.87	6/2119 (0.3%)
38	QD	0.36	0/1695	0.82	6/2274 (0.3%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	XD	0.41	0/1698	0.79	2/2277 (0.1%)
39	QE	0.40	1/1149 (0.1%)	0.79	6/1548 (0.4%)
39	XE	0.41	1/1149 (0.1%)	0.65	1/1548 (0.1%)
40	QF	0.46	0/827	0.87	3/1120 (0.3%)
40	XF	0.39	0/829	0.83	1/1123 (0.1%)
41	QG	0.33	0/1254	0.66	1/1683 (0.1%)
41	XG	0.50	0/1248	0.84	7/1676 (0.4%)
42	QH	0.45	3/1118 (0.3%)	1.03	6/1506 (0.4%)
42	XH	0.41	0/1108	0.79	4/1494 (0.3%)
43	QI	0.71	1/1005 (0.1%)	0.92	5/1351 (0.4%)
43	XI	0.36	0/985	0.76	0/1329
44	QJ	0.36	0/732	0.80	3/993 (0.3%)
44	XJ	0.28	0/723	0.59	0/984
45	QK	0.34	0/849	0.71	2/1150 (0.2%)
45	XK	0.33	0/848	0.70	2/1149 (0.2%)
46	QL	0.34	0/937	0.71	1/1260 (0.1%)
46	XL	0.47	1/937 (0.1%)	0.74	2/1260 (0.2%)
47	QM	0.34	0/924	0.68	0/1242
47	XM	0.29	0/905	0.65	0/1217
48	QN	0.44	0/501	0.97	5/664 (0.8%)
48	XN	0.38	0/501	0.83	4/664 (0.6%)
49	QO	0.49	0/739	1.17	9/985 (0.9%)
49	XO	0.37	0/739	0.76	2/985 (0.2%)
50	QP	0.37	0/697	0.73	0/939
50	XP	0.60	1/693 (0.1%)	1.37	6/935 (0.6%)
51	QQ	0.34	0/836	0.69	0/1117
51	XQ	0.44	1/836 (0.1%)	0.68	1/1117 (0.1%)
52	QR	0.34	0/560	0.92	3/746 (0.4%)
52	XR	0.30	0/560	0.71	0/746
53	QS	0.61	2/663 (0.3%)	0.74	1/895 (0.1%)
53	XS	0.30	0/660	0.69	3/893 (0.3%)
54	QT	0.37	1/734 (0.1%)	0.65	1/969 (0.1%)
54	XT	0.41	1/736 (0.1%)	0.68	3/976 (0.3%)
55	QU	0.35	0/203	0.75	0/266
55	XU	0.32	0/203	0.68	0/266
All	All	0.33	67/318172 (0.0%)	0.86	571/475147 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	QY	0	3
8	RF	0	1
11	YI	0	1
17	RS	0	1
19	RU	0	1
25	R0	0	1
26	Y1	0	1
29	R4	0	1
29	Y4	0	1
31	R6	0	1
34	R9	0	1
36	QB	0	2
36	XB	0	2
37	QC	0	1
44	QJ	0	1
44	XJ	0	1
45	XK	0	1
46	XL	0	2
48	XN	0	1
51	XQ	0	1
All	All	0	25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	QI	93	ARG	CB-CG	-17.94	1.04	1.52
53	QS	28	LYS	CD-CE	-11.05	1.23	1.51
26	Y1	52	ARG	CZ-NH2	10.67	1.47	1.33
1	QV	1	C	OP3-P	-10.63	1.48	1.61
1	XV	1	C	OP3-P	-10.63	1.48	1.61

The worst 5 of 571 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	RA	2603	G	O5'-P-OP1	-35.76	67.78	110.70
36	XB	217	ARG	NE-CZ-NH2	-28.77	105.92	120.30
20	RV	21	ARG	NE-CZ-NH2	-27.66	106.47	120.30
50	XP	71	ARG	NE-CZ-NH2	-21.01	109.79	120.30
42	QH	14	ARG	NE-CZ-NH1	19.41	130.01	120.30

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	QY	115	PHE	Peptide
3	QY	201	LEU	Peptide
3	QY	48	ASN	Sidechain
26	Y1	52	ARG	Sidechain
11	YI	84	GLY	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	QV	1644	0	836	29	0
1	XV	1644	0	836	19	0
2	QX	215	0	109	3	0
2	XX	215	0	108	6	0
3	QY	2833	0	2729	139	0
3	XY	2833	0	2729	155	0
4	RA	61758	0	31149	799	0
4	YA	61758	0	31152	795	0
5	RB	2572	0	1305	19	0
5	YB	2573	0	1306	17	0
6	RD	2131	0	2207	63	0
6	YD	2136	0	2217	65	0
7	RE	1559	0	1618	41	0
7	YE	1559	0	1618	43	0
8	RF	1584	0	1625	58	0
8	YF	1580	0	1619	68	0
9	RG	1426	0	1445	51	0
9	YG	1424	0	1441	60	0
10	RH	1330	0	1407	30	0
10	YH	1324	0	1402	43	0
11	RI	1094	0	1127	34	0
11	YI	1076	0	1094	24	0
12	RN	1121	0	1195	27	0
12	YN	1117	0	1184	22	0
13	RO	933	0	996	28	0
13	YO	933	0	996	26	0
14	RP	1135	0	1212	33	0
14	YP	1135	0	1212	44	0
15	RQ	1122	0	1179	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	YQ	1122	0	1179	38	0
16	RR	968	0	1033	32	0
16	YR	968	0	1033	21	0
17	RS	877	0	938	38	0
17	YS	870	0	923	41	0
18	RT	1091	0	1151	44	0
18	YT	1083	0	1136	54	0
19	RU	959	0	1019	31	0
19	YU	959	0	1019	27	0
20	RV	775	0	841	23	0
20	YV	771	0	830	21	0
21	RW	886	0	940	18	0
21	YW	886	0	940	21	0
22	RX	750	0	814	13	0
22	YX	750	0	814	8	0
23	RY	810	0	892	35	0
23	YY	810	0	887	34	0
24	RZ	1587	0	1598	48	0
24	YZ	1557	0	1564	53	0
25	R0	608	0	622	19	0
25	Y0	608	0	622	21	0
26	R1	754	0	823	17	0
26	Y1	759	0	837	27	0
27	R2	588	0	643	13	0
27	Y2	592	0	654	17	0
28	R3	469	0	518	8	0
28	Y3	464	0	514	5	0
29	R4	546	0	522	37	0
29	Y4	536	0	514	45	0
30	R5	459	0	476	13	0
30	Y5	455	0	465	9	0
31	R6	453	0	473	9	0
31	Y6	449	0	469	6	0
32	R7	418	0	467	16	0
32	Y7	418	0	467	11	0
33	R8	517	0	582	21	0
33	Y8	517	0	582	26	0
34	R9	307	0	335	9	0
34	Y9	307	0	335	6	0
35	QA	32246	0	16294	525	0
35	XA	32331	0	16339	485	0
36	QB	1842	0	1862	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	XB	1825	0	1828	104	0
37	QC	1558	0	1557	50	0
37	XC	1542	0	1517	49	0
38	QD	1665	0	1688	86	0
38	XD	1668	0	1704	75	0
39	QE	1133	0	1191	33	0
39	XE	1133	0	1191	41	0
40	QF	814	0	808	44	0
40	XF	816	0	808	32	0
41	QG	1235	0	1249	23	0
41	XG	1229	0	1238	34	0
42	QH	1098	0	1143	33	0
42	XH	1088	0	1126	28	0
43	QI	986	0	990	50	0
43	XI	966	0	953	65	0
44	QJ	719	0	672	35	0
44	XJ	710	0	661	27	0
45	QK	834	0	838	13	0
45	XK	833	0	836	21	0
46	QL	932	0	981	36	0
46	XL	932	0	981	31	0
47	QM	914	0	954	36	0
47	XM	895	0	920	34	0
48	QN	492	0	529	29	0
48	XN	492	0	529	16	0
49	QO	728	0	760	16	0
49	XO	728	0	760	17	0
50	QP	681	0	697	30	0
50	XP	677	0	686	33	0
51	QQ	823	0	891	22	0
51	XQ	823	0	891	18	0
52	QR	555	0	618	22	0
52	XR	555	0	618	20	0
53	QS	648	0	658	22	0
53	XS	645	0	635	27	0
54	QT	732	0	809	13	0
54	XT	733	0	795	16	0
55	QU	199	0	208	10	0
55	XU	199	0	208	5	0
56	QA	279	0	0	0	0
56	QB	1	0	0	0	0
56	QD	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QE	2	0	0	0	0
56	QF	1	0	0	0	0
56	QG	3	0	0	0	0
56	QH	2	0	0	0	0
56	QI	1	0	0	0	0
56	QL	3	0	0	0	0
56	QM	1	0	0	0	0
56	QN	2	0	0	0	0
56	QO	1	0	0	0	0
56	QQ	2	0	0	0	0
56	QR	1	0	0	0	0
56	QT	1	0	0	0	0
56	QU	1	0	0	0	0
56	QV	2	0	0	0	0
56	QY	3	0	0	0	0
56	R0	4	0	0	0	0
56	R1	3	0	0	0	0
56	R3	2	0	0	0	0
56	R4	1	0	0	0	0
56	R5	3	0	0	0	0
56	R7	2	0	0	0	0
56	R8	1	0	0	0	0
56	R9	2	0	0	0	0
56	RA	1066	0	0	0	0
56	RB	29	0	0	0	0
56	RD	13	0	0	0	0
56	RE	6	0	0	0	0
56	RF	12	0	0	0	0
56	RG	4	0	0	0	0
56	RH	2	0	0	0	0
56	RN	3	0	0	0	0
56	RO	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	4	0	0	0	0
56	RR	5	0	0	0	0
56	RT	3	0	0	0	0
56	RU	3	0	0	0	0
56	RV	4	0	0	0	0
56	RW	2	0	0	0	0
56	RX	1	0	0	0	0
56	RZ	1	0	0	0	0
56	XA	190	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	XE	2	0	0	0	0
56	XF	4	0	0	0	0
56	XH	1	0	0	0	0
56	XJ	1	0	0	0	0
56	XK	1	0	0	0	0
56	XL	1	0	0	0	0
56	XR	1	0	0	0	0
56	XT	1	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	2	0	0	0	0
56	YA	760	0	0	0	0
56	YB	19	0	0	0	0
56	YD	10	0	0	0	0
56	YE	7	0	0	0	0
56	YF	3	0	0	0	0
56	YG	3	0	0	0	0
56	YI	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	1	0	0	0	0
56	YQ	2	0	0	0	0
56	YR	1	0	0	0	0
56	YT	3	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
56	YX	1	0	0	0	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
All	All	296662	0	200145	5370	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 11.

The worst 5 of 5370 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)
12:RN:121:LYS:CE	12:RN:121:LYS:CD	1.75	1.59
4:YA:2012:G:OP1	21:YW:11:ARG:NH2	1.88	1.07
36:QB:15:VAL:HG23	36:QB:209:ARG:HB3	1.36	1.06
35:XA:1003:G:H2'	35:XA:1004:A:H4'	1.33	1.05
3:XY:281:HIS:HE1	4:YA:2493:U:H1'	1.22	1.04

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	
3	QY	355/380 (93%)	304 (86%)	43 (12%)	8 (2%)	8	35
3	XY	355/380 (93%)	310 (87%)	33 (9%)	12 (3%)	5	25
6	RD	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
6	YD	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	39	75
7	RE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	34	72
7	YE	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	19	58
8	RF	201/210 (96%)	197 (98%)	4 (2%)	0	100	100
8	YF	201/210 (96%)	197 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	RG	179/182 (98%)	166 (93%)	10 (6%)	3 (2%)	11	43
9	YG	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	30	68
10	RH	172/180 (96%)	163 (95%)	9 (5%)	0	100	100
10	YH	171/180 (95%)	159 (93%)	12 (7%)	0	100	100
11	RI	145/148 (98%)	130 (90%)	13 (9%)	2 (1%)	14	48
11	YI	144/148 (97%)	136 (94%)	6 (4%)	2 (1%)	14	48
12	RN	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
12	YN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	26	65
13	RO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
13	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
14	RP	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
14	YP	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	14	48
15	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
15	YQ	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	26	65
16	RR	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
16	YR	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
17	RS	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
17	YS	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
18	RT	129/146 (88%)	120 (93%)	7 (5%)	2 (2%)	12	44
18	YT	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
19	RU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
19	YU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
20	RV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	19	58
20	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	19	58
21	RW	110/113 (97%)	110 (100%)	0	0	100	100
21	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
22	RX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
22	YX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	17	55
23	RY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
23	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
24	RZ	201/206 (98%)	192 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	YZ	199/206 (97%)	188 (94%)	11 (6%)	0	100	100
25	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
25	Y0	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
26	R1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	55
26	Y1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	17	55
27	R2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
27	Y2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
28	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
29	R4	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	7
29	Y4	67/71 (94%)	57 (85%)	7 (10%)	3 (4%)	3	17
30	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
31	R6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
31	Y6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
32	R7	46/49 (94%)	46 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
33	Y8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
36	QB	229/256 (90%)	197 (86%)	20 (9%)	12 (5%)	2	15
36	XB	229/256 (90%)	198 (86%)	24 (10%)	7 (3%)	5	27
37	QC	204/239 (85%)	195 (96%)	9 (4%)	0	100	100
37	XC	204/239 (85%)	193 (95%)	9 (4%)	2 (1%)	19	58
38	QD	206/209 (99%)	190 (92%)	15 (7%)	1 (0%)	34	72
38	XD	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	34	72
39	QE	146/162 (90%)	143 (98%)	3 (2%)	0	100	100
39	XE	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
40	QF	98/101 (97%)	90 (92%)	6 (6%)	2 (2%)	9	38
40	XF	98/101 (97%)	93 (95%)	3 (3%)	2 (2%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
41	XG	153/156 (98%)	147 (96%)	4 (3%)	2 (1%)	15	50
42	QH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	26	65
42	XH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
43	QI	125/128 (98%)	117 (94%)	7 (6%)	1 (1%)	24	63
43	XI	124/128 (97%)	113 (91%)	9 (7%)	2 (2%)	12	44
44	QJ	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	5	26
44	XJ	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	5	26
45	QK	112/129 (87%)	108 (96%)	3 (3%)	1 (1%)	21	61
45	XK	112/129 (87%)	110 (98%)	2 (2%)	0	100	100
46	QL	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
46	XL	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
47	QM	114/126 (90%)	106 (93%)	7 (6%)	1 (1%)	21	61
47	XM	112/126 (89%)	104 (93%)	7 (6%)	1 (1%)	21	61
48	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
48	XN	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
49	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
49	XO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
50	QP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
50	XP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
51	QQ	97/105 (92%)	91 (94%)	4 (4%)	2 (2%)	9	37
51	XQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
52	QR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
52	XR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
53	QS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
53	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
54	QT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	5	26
54	XT	96/106 (91%)	91 (95%)	2 (2%)	3 (3%)	5	27
55	QU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	3	17
55	XU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	3	17
All	All	12150/12888 (94%)	11432 (94%)	615 (5%)	103 (1%)	24	63

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	QY	254	VAL
3	XY	122	GLU
3	XY	230	ILE
3	XY	315	SER
9	YG	81	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	
3	QY	304/324 (94%)	290 (95%)	14 (5%)	33	70
3	XY	304/324 (94%)	292 (96%)	12 (4%)	39	75
6	RD	214/218 (98%)	206 (96%)	8 (4%)	41	76
6	YD	215/218 (99%)	208 (97%)	7 (3%)	45	79
7	RE	164/166 (99%)	158 (96%)	6 (4%)	41	76
7	YE	164/166 (99%)	156 (95%)	8 (5%)	31	68
8	RF	160/166 (96%)	149 (93%)	11 (7%)	19	55
8	YF	159/166 (96%)	152 (96%)	7 (4%)	35	71
9	RG	144/156 (92%)	139 (96%)	5 (4%)	43	78
9	YG	142/156 (91%)	137 (96%)	5 (4%)	43	78
10	RH	144/148 (97%)	140 (97%)	4 (3%)	51	82
10	YH	143/148 (97%)	136 (95%)	7 (5%)	31	68
11	RI	111/124 (90%)	105 (95%)	6 (5%)	27	64
11	YI	108/124 (87%)	105 (97%)	3 (3%)	51	82
12	RN	119/119 (100%)	114 (96%)	5 (4%)	36	73
12	YN	118/119 (99%)	111 (94%)	7 (6%)	24	60
13	RO	100/100 (100%)	96 (96%)	4 (4%)	38	75
13	YO	100/100 (100%)	96 (96%)	4 (4%)	38	75
14	RP	115/116 (99%)	111 (96%)	4 (4%)	43	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	YP	115/116 (99%)	109 (95%)	6 (5%)	29	65
15	RQ	111/111 (100%)	107 (96%)	4 (4%)	42	77
15	YQ	111/111 (100%)	106 (96%)	5 (4%)	34	70
16	RR	101/101 (100%)	100 (99%)	1 (1%)	82	93
16	YR	101/101 (100%)	99 (98%)	2 (2%)	63	86
17	RS	87/88 (99%)	83 (95%)	4 (5%)	33	70
17	YS	85/88 (97%)	77 (91%)	8 (9%)	11	39
18	RT	115/127 (91%)	106 (92%)	9 (8%)	16	49
18	YT	113/127 (89%)	105 (93%)	8 (7%)	18	54
19	RU	93/94 (99%)	84 (90%)	9 (10%)	10	36
19	YU	93/94 (99%)	85 (91%)	8 (9%)	13	45
20	RV	81/82 (99%)	76 (94%)	5 (6%)	23	59
20	YV	80/82 (98%)	75 (94%)	5 (6%)	22	58
21	RW	90/92 (98%)	85 (94%)	5 (6%)	26	62
21	YW	90/92 (98%)	84 (93%)	6 (7%)	20	56
22	RX	77/78 (99%)	75 (97%)	2 (3%)	54	83
22	YX	77/78 (99%)	77 (100%)	0	100	100
23	RY	86/91 (94%)	80 (93%)	6 (7%)	19	54
23	YY	86/91 (94%)	82 (95%)	4 (5%)	32	70
24	RZ	169/179 (94%)	160 (95%)	9 (5%)	28	64
24	YZ	165/179 (92%)	159 (96%)	6 (4%)	42	77
25	R0	61/67 (91%)	57 (93%)	4 (7%)	21	56
25	Y0	61/67 (91%)	57 (93%)	4 (7%)	21	56
26	R1	79/83 (95%)	76 (96%)	3 (4%)	40	76
26	Y1	81/83 (98%)	77 (95%)	4 (5%)	31	68
27	R2	65/67 (97%)	65 (100%)	0	100	100
27	Y2	66/67 (98%)	63 (96%)	3 (4%)	34	70
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	50/52 (96%)	48 (96%)	2 (4%)	38	75
29	R4	58/63 (92%)	54 (93%)	4 (7%)	19	55
29	Y4	54/63 (86%)	47 (87%)	7 (13%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	50/52 (96%)	46 (92%)	4 (8%)	15	48
31	R6	51/52 (98%)	50 (98%)	1 (2%)	63	86
31	Y6	50/52 (96%)	49 (98%)	1 (2%)	63	86
32	R7	41/42 (98%)	40 (98%)	1 (2%)	57	84
32	Y7	41/42 (98%)	39 (95%)	2 (5%)	31	68
33	R8	54/55 (98%)	52 (96%)	2 (4%)	41	76
33	Y8	54/55 (98%)	53 (98%)	1 (2%)	65	87
34	R9	34/34 (100%)	32 (94%)	2 (6%)	24	60
34	Y9	34/34 (100%)	33 (97%)	1 (3%)	50	81
36	QB	191/220 (87%)	181 (95%)	10 (5%)	29	65
36	XB	187/220 (85%)	171 (91%)	16 (9%)	13	45
37	QC	144/188 (77%)	141 (98%)	3 (2%)	61	86
37	XC	140/188 (74%)	134 (96%)	6 (4%)	35	72
38	QD	171/181 (94%)	163 (95%)	8 (5%)	32	70
38	XD	172/181 (95%)	163 (95%)	9 (5%)	29	65
39	QE	114/123 (93%)	111 (97%)	3 (3%)	54	83
39	XE	114/123 (93%)	110 (96%)	4 (4%)	43	78
40	QF	85/90 (94%)	78 (92%)	7 (8%)	14	47
40	XF	85/90 (94%)	79 (93%)	6 (7%)	18	54
41	QG	120/127 (94%)	117 (98%)	3 (2%)	55	84
41	XG	119/127 (94%)	115 (97%)	4 (3%)	44	79
42	QH	116/119 (98%)	112 (97%)	4 (3%)	44	79
42	XH	114/119 (96%)	112 (98%)	2 (2%)	66	88
43	QI	91/99 (92%)	83 (91%)	8 (9%)	12	43
43	XI	88/99 (89%)	83 (94%)	5 (6%)	25	62
44	QJ	68/92 (74%)	66 (97%)	2 (3%)	50	81
44	XJ	68/92 (74%)	68 (100%)	0	100	100
45	QK	83/99 (84%)	81 (98%)	2 (2%)	57	84
45	XK	83/99 (84%)	82 (99%)	1 (1%)	78	92
46	QL	96/108 (89%)	93 (97%)	3 (3%)	47	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	XL	96/108 (89%)	89 (93%)	7 (7%)	17	52
47	QM	90/101 (89%)	89 (99%)	1 (1%)	80	93
47	XM	87/101 (86%)	86 (99%)	1 (1%)	80	93
48	QN	49/50 (98%)	43 (88%)	6 (12%)	6	24
48	XN	49/50 (98%)	49 (100%)	0	100	100
49	QO	78/80 (98%)	76 (97%)	2 (3%)	54	83
49	XO	78/80 (98%)	75 (96%)	3 (4%)	40	76
50	QP	69/74 (93%)	66 (96%)	3 (4%)	35	72
50	XP	68/74 (92%)	62 (91%)	6 (9%)	12	43
51	QQ	94/97 (97%)	93 (99%)	1 (1%)	80	93
51	XQ	94/97 (97%)	90 (96%)	4 (4%)	35	72
52	QR	59/77 (77%)	54 (92%)	5 (8%)	13	45
52	XR	59/77 (77%)	56 (95%)	3 (5%)	29	66
53	QS	68/80 (85%)	65 (96%)	3 (4%)	35	71
53	XS	67/80 (84%)	65 (97%)	2 (3%)	48	81
54	QT	71/82 (87%)	71 (100%)	0	100	100
54	XT	70/82 (85%)	70 (100%)	0	100	100
55	QU	18/22 (82%)	17 (94%)	1 (6%)	26	62
55	XU	18/22 (82%)	18 (100%)	0	100	100
All	All	9971/10712 (93%)	9532 (96%)	439 (4%)	35	71

5 of 439 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	XF	60	PHE
36	QB	145	LEU
22	RX	28	PHE
41	XG	18	TYR
49	XO	6	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
43	XI	124	GLN

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Mol	Chain	Res	Type
36	QB	78	GLN
21	RW	60	ASN
45	XK	116	HIS
36	QB	113	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QV	76/77 (98%)	17 (22%)	1 (1%)
1	XV	76/77 (98%)	16 (21%)	1 (1%)
2	QX	9/25 (36%)	3 (33%)	0
2	XX	9/25 (36%)	4 (44%)	0
35	QA	1494/1521 (98%)	229 (15%)	14 (0%)
35	XA	1498/1521 (98%)	226 (15%)	18 (1%)
4	RA	2855/2915 (97%)	452 (15%)	28 (0%)
4	YA	2855/2915 (97%)	457 (16%)	26 (0%)
5	RB	119/122 (97%)	9 (7%)	0
5	YB	119/122 (97%)	14 (11%)	0
All	All	9110/9320 (97%)	1427 (15%)	88 (0%)

5 of 1427 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QV	4	G
1	QV	5	G
1	QV	6	G
1	QV	9	G
1	QV	16	C

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	XA	992	U
35	QA	560	U
4	RA	2171	A
35	XA	1065	U
35	XA	1256	A



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

48 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$
35	2MG	QA	1207	56,35	18,26,27	1.23	2 (11%)	21,38,41	2.36	7 (33%)
35	5MC	QA	1400	35	14,22,23	1.36	1 (7%)	17,32,35	0.84	1 (5%)
35	4OC	QA	1402	35	15,23,24	0.59	0	21,32,35	1.87	3 (14%)
35	5MC	QA	1404	35	14,22,23	1.32	1 (7%)	17,32,35	0.89	1 (5%)
35	5MC	QA	1407	35	14,22,23	1.31	1 (7%)	17,32,35	0.98	1 (5%)
35	UR3	QA	1498	35	13,22,23	0.71	0	18,32,35	0.75	0
35	MA6	QA	1518	35	18,26,27	0.97	1 (5%)	15,38,41	2.29	4 (26%)
35	MA6	QA	1519	35	18,26,27	0.98	1 (5%)	15,38,41	2.18	2 (13%)
35	PSU	QA	516	56,35	15,21,22	1.25	2 (13%)	16,30,33	2.20	3 (18%)
35	7MG	QA	527	56,35	20,26,27	1.45	2 (10%)	23,39,42	3.27	5 (21%)
35	M2G	QA	966	35	18,27,28	1.39	3 (16%)	22,40,43	1.84	4 (18%)
35	5MC	QA	967	35	14,22,23	1.31	1 (7%)	17,32,35	0.89	1 (5%)
46	0TD	QL	92	46	4,9,10	0.64	0	4,11,13	1.59	1 (25%)
4	PSU	RA	1911	4	15,21,22	1.38	1 (6%)	16,30,33	2.20	4 (25%)
4	5MU	RA	1915	56,4	13,22,23	0.55	0	16,32,35	2.83	2 (12%)
4	PSU	RA	1917	4	15,21,22	1.27	1 (6%)	16,30,33	2.25	4 (25%)
4	4OC	RA	1920	4	15,22,24	0.58	0	20,31,35	1.42	1 (5%)
4	5MU	RA	1939	4	13,22,23	0.59	0	16,32,35	2.55	2 (12%)
4	5MC	RA	1942	56,4	14,22,23	1.30	1 (7%)	17,32,35	0.93	1 (5%)
4	5MC	RA	1962	56,4	14,22,23	1.32	1 (7%)	17,32,35	0.88	1 (5%)
4	OMG	RA	2251	1,56,4	18,26,27	1.13	2 (11%)	21,38,41	1.83	4 (19%)
4	2MA	RA	2503	56,4	17,25,26	1.58	3 (17%)	18,37,40	2.95	1 (5%)
4	2MU	RA	2552	56,4	14,22,24	0.78	0	19,31,36	1.61	1 (5%)
4	PSU	RA	2605	4	15,21,22	1.30	1 (6%)	16,30,33	2.36	4 (25%)
35	2MG	XA	1207	35	18,26,27	1.20	2 (11%)	21,38,41	2.22	6 (28%)
35	5MC	XA	1400	35	14,22,23	1.30	1 (7%)	17,32,35	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	4OC	XA	1402	35	15,23,24	0.60	0	21,32,35	1.90	3 (14%)
35	5MC	XA	1404	35	14,22,23	1.31	1 (7%)	17,32,35	0.93	1 (5%)
35	5MC	XA	1407	35	14,22,23	1.28	1 (7%)	17,32,35	1.01	1 (5%)
35	UR3	XA	1498	56,35	13,22,23	0.72	1 (7%)	18,32,35	0.73	0
35	MA6	XA	1518	35	18,26,27	0.96	1 (5%)	15,38,41	2.22	2 (13%)
35	MA6	XA	1519	35	18,26,27	0.96	1 (5%)	15,38,41	2.36	3 (20%)
35	PSU	XA	516	35	15,21,22	1.29	1 (6%)	16,30,33	2.14	3 (18%)
35	7MG	XA	527	35	20,26,27	1.46	2 (10%)	23,39,42	3.18	5 (21%)
35	M2G	XA	966	35	18,27,28	1.42	3 (16%)	22,40,43	1.91	5 (22%)
35	5MC	XA	967	35	14,22,23	1.31	1 (7%)	17,32,35	0.88	1 (5%)
46	0TD	XL	92	46	4,9,10	0.58	0	4,11,13	1.63	1 (25%)
4	PSU	YA	1911	4	15,21,22	1.36	1 (6%)	16,30,33	2.32	4 (25%)
4	5MU	YA	1915	4	13,22,23	0.57	0	16,32,35	2.70	2 (12%)
4	PSU	YA	1917	4	15,21,22	1.23	1 (6%)	16,30,33	2.22	4 (25%)
4	4OC	YA	1920	4	15,22,24	0.57	0	20,31,35	1.27	1 (5%)
4	5MU	YA	1939	56,4	13,22,23	0.64	0	16,32,35	2.43	2 (12%)
4	5MC	YA	1942	4	14,22,23	1.25	1 (7%)	17,32,35	0.96	1 (5%)
4	5MC	YA	1962	56,4	14,22,23	1.30	1 (7%)	17,32,35	0.95	1 (5%)
4	OMG	YA	2251	1,56,4	18,26,27	1.17	2 (11%)	21,38,41	1.82	4 (19%)
4	2MA	YA	2503	56,4	17,25,26	1.56	3 (17%)	18,37,40	2.90	1 (5%)
4	2MU	YA	2552	56,4	14,22,24	0.79	0	19,31,36	1.66	1 (5%)
4	PSU	YA	2605	4	15,21,22	1.43	1 (6%)	16,30,33	2.31	4 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	2MG	QA	1207	56,35	-	0/5/27/28	0/3/3/3
35	5MC	QA	1400	35	-	0/3/25/26	0/2/2/2
35	4OC	QA	1402	35	-	0/7/29/30	0/2/2/2
35	5MC	QA	1404	35	-	0/3/25/26	0/2/2/2
35	5MC	QA	1407	35	-	0/3/25/26	0/2/2/2
35	UR3	QA	1498	35	-	0/3/25/26	0/2/2/2
35	MA6	QA	1518	35	-	0/7/29/30	0/3/3/3
35	MA6	QA	1519	35	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	QA	516	56,35	-	0/7/25/26	0/2/2/2
35	7MG	QA	527	56,35	-	0/7/37/38	0/3/3/3
35	M2G	QA	966	35	-	0/7/29/30	0/3/3/3
35	5MC	QA	967	35	-	0/3/25/26	0/2/2/2
46	0TD	QL	92	46	-	0/2/12/14	0/0/0/0
4	PSU	RA	1911	4	-	0/7/25/26	0/2/2/2
4	5MU	RA	1915	56,4	-	0/3/25/26	0/2/2/2
4	PSU	RA	1917	4	-	0/7/25/26	0/2/2/2
4	4OC	RA	1920	4	-	0/5/27/30	0/2/2/2
4	5MU	RA	1939	4	-	0/3/25/26	0/2/2/2
4	5MC	RA	1942	56,4	-	0/3/25/26	0/2/2/2
4	5MC	RA	1962	56,4	-	0/3/25/26	0/2/2/2
4	OMG	RA	2251	1,56,4	-	0/5/27/28	0/3/3/3
4	2MA	RA	2503	56,4	-	0/3/25/26	0/3/3/3
4	2MU	RA	2552	56,4	-	0/5/27/28	0/2/2/2
4	PSU	RA	2605	4	-	0/7/25/26	0/2/2/2
35	2MG	XA	1207	35	-	0/5/27/28	0/3/3/3
35	5MC	XA	1400	35	-	0/3/25/26	0/2/2/2
35	4OC	XA	1402	35	-	2/7/29/30	0/2/2/2
35	5MC	XA	1404	35	-	0/3/25/26	0/2/2/2
35	5MC	XA	1407	35	-	0/3/25/26	0/2/2/2
35	UR3	XA	1498	56,35	-	0/3/25/26	0/2/2/2
35	MA6	XA	1518	35	-	0/7/29/30	0/3/3/3
35	MA6	XA	1519	35	-	0/7/29/30	0/3/3/3
35	PSU	XA	516	35	-	0/7/25/26	0/2/2/2
35	7MG	XA	527	35	-	0/7/37/38	0/3/3/3
35	M2G	XA	966	35	-	0/7/29/30	0/3/3/3
35	5MC	XA	967	35	-	0/3/25/26	0/2/2/2
46	0TD	XL	92	46	-	0/2/12/14	0/0/0/0
4	PSU	YA	1911	4	-	0/7/25/26	0/2/2/2
4	5MU	YA	1915	4	-	0/3/25/26	0/2/2/2
4	PSU	YA	1917	4	-	0/7/25/26	0/2/2/2
4	4OC	YA	1920	4	-	0/5/27/30	0/2/2/2
4	5MU	YA	1939	56,4	-	0/3/25/26	0/2/2/2
4	5MC	YA	1942	4	-	0/3/25/26	0/2/2/2
4	5MC	YA	1962	56,4	-	0/3/25/26	0/2/2/2
4	OMG	YA	2251	1,56,4	-	0/5/27/28	0/3/3/3
4	2MA	YA	2503	56,4	-	0/3/25/26	0/3/3/3
4	2MU	YA	2552	56,4	-	0/5/27/28	0/2/2/2
4	PSU	YA	2605	4	-	0/7/25/26	0/2/2/2

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	YA	2605	PSU	C5-C1'	-4.46	1.48	1.52
4	RA	1911	PSU	C5-C1'	-4.31	1.48	1.52
4	YA	1911	PSU	C5-C1'	-4.20	1.48	1.52
4	RA	2605	PSU	C5-C1'	-3.99	1.48	1.52
35	XA	516	PSU	C5-C1'	-3.84	1.48	1.52

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	QA	527	7MG	C5-C4-N3	-8.85	117.73	126.74
35	XA	527	7MG	C5-C4-N3	-8.56	118.02	126.74
4	RA	1915	5MU	C5-C4-N3	-8.09	118.56	125.35
4	RA	1939	5MU	C5-C4-N3	-7.60	118.97	125.35
4	YA	1915	5MU	C5-C4-N3	-7.50	119.05	125.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	XA	1402	4OC	N3-C4-N4-CM4
35	XA	1402	4OC	C5-C4-N4-CM4

There are no ring outliers.

19 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	QA	1207	2MG	2	0
35	QA	1402	4OC	1	0
35	QA	1404	5MC	1	0
35	QA	1518	MA6	2	0
35	QA	1519	MA6	2	0
35	QA	966	M2G	1	0
35	QA	967	5MC	1	0
46	QL	92	0TD	2	0
4	RA	1920	4OC	1	0
4	RA	1942	5MC	1	0
4	RA	1962	5MC	1	0
4	RA	2552	2MU	1	0
35	XA	1402	4OC	1	0
35	XA	1518	MA6	1	0
4	YA	1915	5MU	4	0
4	YA	1920	4OC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	YA	1962	5MC	1	0
4	YA	2251	OMG	1	0
4	YA	2503	2MA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2527 ligands modelled in this entry, 2525 are monoatomic - leaving 2 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	$\# Z  > 2$
58	SF4	QD	302	38	0,12,12	0.00	-	0,24,24	0.00	-
58	SF4	XD	301	38	0,12,12	0.00	-	0,24,24	0.00	-

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
58	SF4	QD	302	38	-	0/0/48/48	0/6/5/5
58	SF4	XD	301	38	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	QV	77/77 (100%)	0.23	3 (3%) 43 21	57, 94, 173, 210	0
1	XV	77/77 (100%)	0.30	2 (2%) 59 35	49, 84, 141, 212	0
2	QX	10/25 (40%)	1.09	3 (30%) 1 0	69, 105, 168, 212	0
2	XX	10/25 (40%)	1.03	3 (30%) 1 0	52, 112, 150, 183	0
3	QY	357/380 (93%)	2.04	158 (44%) 0 0	77, 135, 202, 220	0
3	XY	357/380 (93%)	2.11	151 (42%) 0 0	73, 132, 203, 228	0
4	RA	2856/2915 (97%)	0.01	131 (4%) 36 17	22, 55, 177, 347	0
4	YA	2856/2915 (97%)	-0.02	124 (4%) 39 18	14, 41, 183, 343	0
5	RB	120/122 (98%)	-0.21	0 100 100	56, 91, 116, 152	0
5	YB	120/122 (98%)	-0.32	0 100 100	39, 63, 85, 130	0
6	RD	275/276 (99%)	-0.31	1 (0%) 93 85	25, 47, 71, 109	0
6	YD	275/276 (99%)	-0.35	1 (0%) 93 85	16, 39, 69, 132	0
7	RE	204/206 (99%)	-0.19	0 100 100	26, 53, 85, 119	0
7	YE	204/206 (99%)	-0.19	0 100 100	19, 46, 86, 135	0
8	RF	203/210 (96%)	-0.16	1 (0%) 91 83	29, 67, 110, 133	0
8	YF	203/210 (96%)	-0.31	1 (0%) 91 83	15, 45, 89, 139	0
9	RG	181/182 (99%)	0.17	5 (2%) 56 32	76, 103, 134, 155	0
9	YG	181/182 (99%)	-0.11	4 (2%) 65 42	55, 78, 121, 184	0
10	RH	174/180 (96%)	0.79	28 (16%) 3 1	74, 111, 147, 158	0
10	YH	173/180 (96%)	-0.14	0 100 100	40, 64, 95, 139	0
11	RI	147/148 (99%)	0.59	13 (8%) 12 4	59, 103, 135, 164	0
11	YI	146/148 (98%)	0.32	4 (2%) 58 34	51, 92, 127, 150	0
12	RN	140/140 (100%)	0.03	4 (2%) 55 31	40, 62, 101, 140	0
12	YN	140/140 (100%)	-0.23	1 (0%) 89 78	27, 47, 87, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	RO	122/122 (100%)	-0.27	0 100 100	33, 52, 78, 113	0
13	YO	122/122 (100%)	-0.26	0 100 100	27, 45, 71, 83	0
14	RP	149/150 (99%)	0.10	3 (2%) 68 46	29, 72, 109, 138	0
14	YP	149/150 (99%)	-0.13	1 (0%) 89 78	18, 52, 84, 115	0
15	RQ	141/141 (100%)	-0.26	0 100 100	43, 67, 88, 112	0
15	YQ	141/141 (100%)	-0.30	0 100 100	30, 48, 74, 124	0
16	RR	118/118 (100%)	-0.25	0 100 100	31, 50, 77, 93	0
16	YR	118/118 (100%)	-0.31	0 100 100	28, 43, 67, 89	0
17	RS	110/112 (98%)	0.15	2 (1%) 71 50	66, 89, 113, 133	0
17	YS	110/112 (98%)	-0.08	0 100 100	47, 62, 89, 106	0
18	RT	131/146 (89%)	-0.23	2 (1%) 76 58	37, 59, 105, 155	0
18	YT	131/146 (89%)	-0.25	0 100 100	36, 53, 98, 122	0
19	RU	116/118 (98%)	-0.20	1 (0%) 85 72	33, 57, 91, 113	0
19	YU	116/118 (98%)	-0.41	0 100 100	23, 37, 67, 104	0
20	RV	101/101 (100%)	-0.21	0 100 100	37, 74, 100, 122	0
20	YV	101/101 (100%)	-0.13	1 (0%) 84 69	21, 50, 88, 109	0
21	RW	112/113 (99%)	-0.19	0 100 100	34, 48, 81, 122	0
21	YW	112/113 (99%)	-0.33	0 100 100	25, 37, 68, 143	0
22	RX	95/96 (98%)	0.02	2 (2%) 67 44	45, 60, 87, 120	0
22	YX	95/96 (98%)	-0.28	0 100 100	28, 42, 80, 115	0
23	RY	107/110 (97%)	0.85	11 (10%) 9 3	57, 83, 131, 176	0
23	YY	107/110 (97%)	0.14	2 (1%) 70 48	38, 64, 107, 150	0
24	RZ	203/206 (98%)	0.60	16 (7%) 15 5	71, 100, 156, 194	0
24	YZ	201/206 (97%)	0.17	15 (7%) 17 6	50, 77, 135, 178	0
25	R0	77/85 (90%)	0.22	2 (2%) 59 35	50, 62, 90, 109	0
25	Y0	77/85 (90%)	-0.06	1 (1%) 79 62	31, 45, 80, 110	0
26	R1	97/98 (98%)	0.01	2 (2%) 67 44	33, 58, 89, 111	0
26	Y1	97/98 (98%)	-0.06	0 100 100	27, 47, 95, 114	0
27	R2	70/72 (97%)	0.02	1 (1%) 78 60	53, 74, 106, 130	0
27	Y2	70/72 (97%)	-0.22	0 100 100	34, 55, 82, 142	0
28	R3	59/60 (98%)	0.46	3 (5%) 32 13	42, 63, 107, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	Y3	59/60 (98%)	-0.06	1 (1%) 73 52	28, 43, 106, 122	0
29	R4	69/71 (97%)	0.79	8 (11%) 6 2	99, 136, 177, 184	0
29	Y4	69/71 (97%)	0.48	8 (11%) 6 2	75, 124, 168, 178	0
30	R5	59/60 (98%)	-0.16	1 (1%) 73 52	29, 51, 94, 160	0
30	Y5	59/60 (98%)	-0.32	0 100 100	18, 42, 91, 141	0
31	R6	53/54 (98%)	2.07	27 (50%) 0 0	82, 102, 143, 150	0
31	Y6	53/54 (98%)	1.49	15 (28%) 1 0	75, 88, 116, 130	0
32	R7	48/49 (97%)	-0.08	1 (2%) 67 44	28, 42, 83, 120	0
32	Y7	48/49 (97%)	-0.16	0 100 100	17, 31, 69, 115	0
33	R8	64/65 (98%)	-0.15	0 100 100	39, 54, 73, 107	0
33	Y8	64/65 (98%)	-0.26	0 100 100	24, 38, 58, 71	0
34	R9	37/37 (100%)	0.82	3 (8%) 15 5	58, 77, 101, 112	0
34	Y9	37/37 (100%)	0.60	1 (2%) 58 34	49, 61, 81, 93	0
35	QA	1488/1521 (97%)	0.01	38 (2%) 59 35	42, 86, 173, 260	0
35	XA	1492/1521 (98%)	0.02	44 (2%) 55 31	32, 84, 168, 253	0
36	QB	231/256 (90%)	0.39	13 (5%) 28 11	85, 122, 153, 178	0
36	XB	231/256 (90%)	0.27	11 (4%) 34 15	80, 110, 143, 161	0
37	QC	206/239 (86%)	0.35	10 (4%) 33 14	88, 115, 144, 168	0
37	XC	206/239 (86%)	0.24	8 (3%) 43 21	80, 104, 134, 167	0
38	QD	208/209 (99%)	-0.04	0 100 100	62, 91, 125, 150	0
38	XD	208/209 (99%)	0.09	0 100 100	68, 97, 133, 152	0
39	QE	148/162 (91%)	-0.03	0 100 100	64, 86, 114, 143	0
39	XE	148/162 (91%)	0.08	1 (0%) 89 78	62, 78, 114, 139	0
40	QF	100/101 (99%)	-0.04	1 (1%) 84 69	71, 95, 118, 132	0
40	XF	100/101 (99%)	-0.24	0 100 100	62, 81, 109, 124	0
41	QG	155/156 (99%)	0.52	14 (9%) 12 4	82, 109, 137, 157	0
41	XG	155/156 (99%)	0.44	9 (5%) 26 11	78, 100, 130, 155	0
42	QH	137/138 (99%)	0.19	2 (1%) 76 58	55, 86, 114, 123	0
42	XH	137/138 (99%)	0.09	3 (2%) 65 42	60, 86, 113, 120	0
43	QI	127/128 (99%)	0.93	18 (14%) 4 2	78, 123, 151, 175	0
43	XI	126/128 (98%)	0.43	7 (5%) 28 11	68, 111, 139, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	QJ	97/105 (92%)	1.06	15 (15%) 3 1	90, 121, 149, 161	0
44	XJ	96/105 (91%)	0.82	12 (12%) 5 2	78, 116, 144, 146	0
45	QK	114/129 (88%)	0.35	4 (3%) 48 23	63, 86, 113, 138	0
45	XK	114/129 (88%)	0.13	1 (0%) 85 72	47, 75, 105, 132	0
46	QL	121/132 (91%)	-0.10	1 (0%) 87 75	47, 66, 90, 105	0
46	XL	121/132 (91%)	0.04	3 (2%) 61 37	48, 66, 94, 116	0
47	QM	116/126 (92%)	0.34	7 (6%) 25 10	85, 114, 138, 148	0
47	XM	114/126 (90%)	0.42	5 (4%) 38 17	84, 107, 128, 144	0
48	QN	60/61 (98%)	0.69	6 (10%) 9 3	88, 111, 129, 146	0
48	XN	60/61 (98%)	0.27	1 (1%) 73 52	73, 92, 115, 127	0
49	QO	88/89 (98%)	0.07	1 (1%) 82 66	60, 80, 109, 121	0
49	XO	88/89 (98%)	0.15	1 (1%) 82 66	48, 80, 112, 123	0
50	QP	82/88 (93%)	0.37	3 (3%) 45 22	58, 76, 104, 114	0
50	XP	82/88 (93%)	0.57	5 (6%) 25 10	71, 93, 118, 141	0
51	QQ	99/105 (94%)	0.27	1 (1%) 84 69	53, 78, 114, 138	0
51	XQ	99/105 (94%)	0.03	0 100 100	59, 78, 101, 126	0
52	QR	68/88 (77%)	0.76	9 (13%) 4 2	72, 90, 119, 139	0
52	XR	68/88 (77%)	0.32	1 (1%) 76 58	56, 83, 114, 124	0
53	QS	83/93 (89%)	1.21	21 (25%) 1 0	87, 120, 146, 161	0
53	XS	83/93 (89%)	1.01	12 (14%) 3 1	89, 118, 142, 183	0
54	QT	96/106 (90%)	0.15	1 (1%) 84 69	54, 80, 116, 120	0
54	XT	98/106 (92%)	0.46	5 (5%) 32 13	65, 88, 120, 128	0
55	QU	23/27 (85%)	2.09	14 (60%) 0 0	88, 103, 130, 145	0
55	XU	23/27 (85%)	1.31	5 (21%) 1 0	81, 102, 117, 119	0
All	All	21456/22208 (96%)	0.14	1081 (5%) 32 13	14, 73, 148, 347	0

The worst 5 of 1081 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	XA	88	A	13.9
4	YA	2141	G	11.3
3	XY	50	PRO	10.6
24	YZ	192	ALA	10.2
24	YZ	193	GLU	9.8

## 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
35	5MC	XA	1404	21/22	0.97	0.18	-	34,45,58,63	0
4	4OC	YA	1920	21/23	0.97	0.16	-	40,47,55,60	0
35	4OC	XA	1402	22/23	0.94	0.23	-	45,57,67,81	0
4	PSU	YA	1917	20/21	0.93	0.17	-	51,62,88,91	0
35	MA6	XA	1519	24/25	0.98	0.18	-	28,45,53,54	0
35	MA6	XA	1518	24/25	0.98	0.20	-	31,41,46,52	0
4	2MU	YA	2552	21/23	0.98	0.18	-	19,28,42,46	0
35	5MC	XA	1407	21/22	0.97	0.20	-	46,49,58,59	0
4	2MA	YA	2503	23/24	0.98	0.18	-	8,22,36,38	0
35	2MG	QA	1207	24/25	0.94	0.13	-	101,124,131,134	0
4	5MC	YA	1942	21/22	0.98	0.16	-	25,38,47,50	0
35	UR3	QA	1498	21/22	0.97	0.18	-	44,57,69,72	0
35	UR3	XA	1498	21/22	0.98	0.15	-	34,43,57,66	0
4	OMG	RA	2251	24/25	0.98	0.18	-	31,38,50,55	0
4	PSU	RA	2605	20/21	0.97	0.17	-	19,36,47,48	0
35	5MC	QA	1400	21/22	0.96	0.21	-	66,75,85,88	0
4	5MC	YA	1962	21/22	0.98	0.15	-	25,33,47,55	0
4	PSU	RA	1917	20/21	0.93	0.17	-	53,73,89,103	0
4	5MC	RA	1962	21/22	0.98	0.15	-	39,46,52,62	0
35	5MC	QA	1407	21/22	0.98	0.15	-	44,51,62,68	0
4	OMG	YA	2251	24/25	0.98	0.19	-	13,25,35,41	0
4	PSU	YA	2605	20/21	0.97	0.21	-	10,25,42,59	0
35	7MG	QA	527	24/25	0.94	0.21	-	51,70,76,76	0
35	5MC	QA	967	21/22	0.94	0.22	-	71,84,95,99	0
4	5MU	YA	1915	21/22	0.91	0.18	-	52,76,85,87	0
4	5MU	RA	1915	21/22	0.91	0.13	-	92,100,114,117	0
35	M2G	XA	966	25/26	0.94	0.19	-	56,75,94,105	0
4	5MC	RA	1942	21/22	0.97	0.20	-	41,50,62,64	0
46	0TD	XL	92	10/11	0.92	0.20	-	58,67,84,87	0
35	5MC	QA	1404	21/22	0.96	0.20	-	55,62,67,73	0
35	MA6	QA	1518	24/25	0.96	0.19	-	48,58,67,72	0
35	PSU	QA	516	20/21	0.93	0.13	-	71,77,87,88	0
35	5MC	XA	1400	21/22	0.96	0.18	-	50,65,74,85	0
35	M2G	QA	966	25/26	0.93	0.21	-	71,80,92,93	0
4	2MU	RA	2552	21/23	0.98	0.17	-	19,33,40,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	MA6	QA	1519	24/25	0.96	0.25	-	41,56,68,79	0
4	4OC	RA	1920	21/23	0.95	0.20	-	55,62,85,94	0
4	5MU	RA	1939	21/22	0.97	0.19	-	23,37,44,52	0
35	7MG	XA	527	24/25	0.96	0.20	-	54,63,74,79	0
35	PSU	XA	516	20/21	0.93	0.18	-	75,86,95,95	0
46	0TD	QL	92	10/11	0.94	0.18	-	59,72,74,78	0
35	5MC	XA	967	21/22	0.95	0.20	-	62,75,84,92	0
4	PSU	YA	1911	20/21	0.97	0.17	-	45,57,62,63	0
4	PSU	RA	1911	20/21	0.96	0.15	-	55,66,73,74	0
35	4OC	QA	1402	22/23	0.92	0.23	-	55,67,72,74	0
4	5MU	YA	1939	21/22	0.98	0.17	-	15,27,36,48	0
4	2MA	RA	2503	23/24	0.98	0.16	-	16,24,31,37	0
35	2MG	XA	1207	24/25	0.94	0.17	-	85,98,106,107	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3264	1/1	0.75	1.24	138.91	63,63,63,63	0
56	MG	RA	4015	1/1	0.21	0.92	123.17	89,89,89,89	0
56	MG	RA	3696	1/1	0.86	1.18	109.91	74,74,74,74	0
56	MG	RA	3088	1/1	0.80	1.56	102.48	89,89,89,89	0
56	MG	RA	3457	1/1	0.50	1.10	100.26	81,81,81,81	0
56	MG	RA	3968	1/1	0.61	0.74	74.01	66,66,66,66	0
56	MG	RA	3511	1/1	0.38	1.14	72.77	62,62,62,62	0
56	MG	RA	3196	1/1	0.84	0.97	67.94	104,104,104,104	0
56	MG	RA	3360	1/1	0.70	0.93	67.86	66,66,66,66	0
56	MG	RA	3141	1/1	0.95	0.60	66.68	93,93,93,93	0
56	MG	YA	3491	1/1	0.73	0.66	66.06	53,53,53,53	0
56	MG	YA	3662	1/1	0.56	0.79	62.49	91,91,91,91	0
56	MG	YA	3654	1/1	0.92	0.78	61.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3828	1/1	-0.18	1.87	61.21	94,94,94,94	0
56	MG	YA	3302	1/1	0.34	0.79	60.28	72,72,72,72	0
56	MG	YA	3273	1/1	0.53	0.90	59.55	72,72,72,72	0
56	MG	RA	3881	1/1	0.92	1.20	59.41	68,68,68,68	0
56	MG	YA	3056	1/1	0.17	1.07	59.27	81,81,81,81	0
56	MG	YA	3090	1/1	0.85	0.91	58.63	54,54,54,54	0
56	MG	YA	3377	1/1	0.89	0.81	56.63	52,52,52,52	0
56	MG	XA	1719	1/1	0.24	0.94	54.90	95,95,95,95	0
56	MG	RA	3177	1/1	0.68	0.70	54.29	72,72,72,72	0
56	MG	RA	3374	1/1	0.88	0.69	52.51	92,92,92,92	0
56	MG	RA	4039	1/1	0.92	1.34	50.16	73,73,73,73	0
56	MG	R0	103	1/1	0.50	1.31	48.73	81,81,81,81	0
56	MG	RA	3630	1/1	0.64	0.64	48.42	90,90,90,90	0
56	MG	RA	3804	1/1	0.90	0.57	47.90	78,78,78,78	0
56	MG	QA	1812	1/1	0.53	0.97	47.81	68,68,68,68	0
56	MG	YA	3688	1/1	0.88	0.55	47.71	62,62,62,62	0
56	MG	RA	3637	1/1	0.63	0.66	46.70	66,66,66,66	0
56	MG	RA	3022	1/1	0.98	0.69	46.65	76,76,76,76	0
56	MG	YA	3574	1/1	0.92	0.45	46.10	30,30,30,30	0
56	MG	RA	3045	1/1	0.94	0.68	44.23	71,71,71,71	0
56	MG	RA	3855	1/1	0.91	0.82	44.22	62,62,62,62	0
56	MG	RA	3418	1/1	0.97	0.69	44.10	36,36,36,36	0
56	MG	YA	3712	1/1	0.97	0.54	43.82	51,51,51,51	0
56	MG	RA	3365	1/1	0.70	0.56	43.54	61,61,61,61	0
56	MG	RA	3750	1/1	0.93	0.93	43.15	66,66,66,66	0
56	MG	YA	3586	1/1	0.87	0.82	42.48	48,48,48,48	0
56	MG	RA	3853	1/1	0.86	1.12	41.47	64,64,64,64	0
56	MG	RA	3711	1/1	0.96	0.60	41.45	80,80,80,80	0
56	MG	YA	3155	1/1	0.73	0.81	40.95	65,65,65,65	0
56	MG	YA	3610	1/1	0.99	0.42	40.75	20,20,20,20	0
56	MG	QA	1870	1/1	0.87	0.62	40.10	47,47,47,47	0
56	MG	RA	3910	1/1	0.78	0.86	39.90	66,66,66,66	0
56	MG	RA	3363	1/1	0.87	0.50	39.78	50,50,50,50	0
56	MG	RA	3475	1/1	0.95	0.56	39.74	46,46,46,46	0
56	MG	RA	3386	1/1	0.95	0.40	38.90	26,26,26,26	0
56	MG	XA	1767	1/1	0.96	0.44	38.54	37,37,37,37	0
56	MG	RA	3978	1/1	0.95	0.52	38.54	55,55,55,55	0
56	MG	RA	3587	1/1	0.96	0.85	38.37	53,53,53,53	0
56	MG	RA	3523	1/1	0.56	0.93	38.29	64,64,64,64	0
56	MG	RA	3353	1/1	0.92	0.50	37.91	35,35,35,35	0
56	MG	RA	3118	1/1	0.93	0.48	37.52	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3483	1/1	0.96	0.45	37.40	21,21,21,21	0
56	MG	RA	3301	1/1	0.88	0.83	37.28	66,66,66,66	0
56	MG	RA	3163	1/1	0.83	0.95	37.14	93,93,93,93	0
56	MG	RA	3204	1/1	0.93	0.68	37.07	59,59,59,59	0
56	MG	RA	3772	1/1	0.73	0.41	36.97	57,57,57,57	0
56	MG	YA	3404	1/1	0.97	0.53	36.80	13,13,13,13	0
56	MG	RA	3116	1/1	0.86	0.76	36.72	104,104,104,104	0
56	MG	RA	3029	1/1	0.86	0.73	36.72	66,66,66,66	0
56	MG	RA	3435	1/1	0.98	0.59	36.67	23,23,23,23	0
56	MG	RA	3383	1/1	0.89	0.54	36.39	40,40,40,40	0
56	MG	RA	4020	1/1	0.96	0.88	36.38	88,88,88,88	0
56	MG	YA	3133	1/1	0.88	0.52	36.16	91,91,91,91	0
56	MG	RA	3207	1/1	0.74	0.82	36.00	69,69,69,69	0
56	MG	YA	3575	1/1	0.98	0.52	35.97	30,30,30,30	0
56	MG	RD	304	1/1	0.79	1.94	35.59	86,86,86,86	0
56	MG	YA	3416	1/1	0.84	0.84	35.40	39,39,39,39	0
56	MG	RU	203	1/1	0.94	0.79	35.34	64,64,64,64	0
56	MG	QA	1858	1/1	0.21	0.95	35.24	115,115,115,115	0
56	MG	RA	3082	1/1	0.90	0.96	34.44	62,62,62,62	0
56	MG	YE	305	1/1	0.82	0.42	34.01	57,57,57,57	0
56	MG	RA	3602	1/1	0.80	0.96	33.79	80,80,80,80	0
56	MG	QA	1623	1/1	0.84	0.48	33.52	74,74,74,74	0
56	MG	RA	3966	1/1	0.92	0.71	32.42	65,65,65,65	0
56	MG	XA	1784	1/1	0.79	0.78	32.41	72,72,72,72	0
56	MG	YA	3288	1/1	0.93	0.46	32.35	53,53,53,53	0
56	MG	YA	3327	1/1	0.98	0.48	32.35	7,7,7,7	0
56	MG	RA	3407	1/1	0.95	0.50	32.27	34,34,34,34	0
56	MG	RA	3888	1/1	0.97	0.47	32.05	24,24,24,24	0
56	MG	RA	3482	1/1	0.96	0.50	31.68	21,21,21,21	0
56	MG	YA	3298	1/1	0.94	0.56	31.41	19,19,19,19	0
56	MG	RA	3384	1/1	0.98	0.60	31.25	21,21,21,21	0
56	MG	QA	1778	1/1	0.79	0.83	31.25	61,61,61,61	0
56	MG	QA	1721	1/1	0.66	0.58	30.94	75,75,75,75	0
56	MG	RA	3814	1/1	0.87	0.79	30.72	63,63,63,63	0
56	MG	RA	3485	1/1	0.96	0.76	30.57	65,65,65,65	0
56	MG	YA	3634	1/1	0.93	0.77	30.43	48,48,48,48	0
56	MG	RA	3525	1/1	0.25	0.87	30.33	65,65,65,65	0
56	MG	RA	3469	1/1	0.97	0.66	30.33	40,40,40,40	0
56	MG	YA	3581	1/1	0.97	0.56	30.23	24,24,24,24	0
56	MG	RA	3391	1/1	0.98	0.48	30.20	17,17,17,17	0
56	MG	YA	3326	1/1	0.95	0.47	30.00	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3613	1/1	0.98	0.41	29.83	35,35,35,35	0
56	MG	YA	3727	1/1	0.63	0.49	29.67	59,59,59,59	0
56	MG	RA	3467	1/1	0.98	0.39	29.61	21,21,21,21	0
56	MG	RA	3849	1/1	0.44	0.62	29.49	52,52,52,52	0
56	MG	YA	3708	1/1	0.89	0.64	29.29	37,37,37,37	0
56	MG	YA	3678	1/1	0.93	0.56	28.84	50,50,50,50	0
56	MG	XA	1626	1/1	0.64	0.82	28.77	77,77,77,77	0
56	MG	YA	3618	1/1	0.98	0.34	28.57	24,24,24,24	0
56	MG	YA	3759	1/1	0.89	0.59	28.11	64,64,64,64	0
56	MG	RA	3553	1/1	0.64	0.83	28.02	87,87,87,87	0
56	MG	YA	3713	1/1	0.87	0.70	27.83	67,67,67,67	0
56	MG	RA	3342	1/1	0.93	0.45	27.68	60,60,60,60	0
56	MG	RA	3571	1/1	0.76	0.46	27.61	94,94,94,94	0
56	MG	RA	3822	1/1	0.71	0.41	27.56	37,37,37,37	0
56	MG	R3	102	1/1	0.78	1.19	27.43	80,80,80,80	0
56	MG	RA	3658	1/1	0.91	0.71	27.30	95,95,95,95	0
56	MG	QA	1847	1/1	0.59	1.06	27.11	64,64,64,64	0
56	MG	YA	3390	1/1	0.97	0.56	27.08	33,33,33,33	0
56	MG	RA	3988	1/1	0.80	0.65	26.85	75,75,75,75	0
56	MG	XA	1775	1/1	0.89	0.82	26.72	72,72,72,72	0
56	MG	YA	3518	1/1	0.98	0.35	26.68	16,16,16,16	0
56	MG	YA	3412	1/1	0.92	0.55	26.62	72,72,72,72	0
56	MG	YA	3760	1/1	0.95	0.49	26.43	85,85,85,85	0
56	MG	RA	3573	1/1	0.69	1.08	26.42	91,91,91,91	0
56	MG	RA	3633	1/1	0.91	0.40	26.40	74,74,74,74	0
56	MG	YA	3060	1/1	0.65	0.41	26.35	62,62,62,62	0
56	MG	RA	4063	1/1	0.84	1.41	26.33	68,68,68,68	0
56	MG	RF	306	1/1	0.90	0.66	26.28	79,79,79,79	0
56	MG	RA	3476	1/1	0.97	0.45	26.21	30,30,30,30	0
56	MG	RA	3606	1/1	0.93	0.80	26.19	53,53,53,53	0
56	MG	RA	3451	1/1	0.95	0.46	26.12	27,27,27,27	0
56	MG	XF	203	1/1	-0.28	1.43	25.95	109,109,109,109	0
56	MG	RA	3783	1/1	0.97	0.45	25.95	42,42,42,42	0
56	MG	QA	1661	1/1	0.62	0.61	25.86	81,81,81,81	0
56	MG	YA	3472	1/1	0.98	0.44	25.84	23,23,23,23	0
56	MG	RP	201	1/1	0.83	0.77	25.83	72,72,72,72	0
56	MG	YA	3363	1/1	0.99	0.58	25.74	11,11,11,11	0
56	MG	YA	3109	1/1	0.93	0.42	25.70	35,35,35,35	0
56	MG	RA	3109	1/1	0.86	0.54	25.66	66,66,66,66	0
56	MG	YA	3616	1/1	0.96	0.63	25.63	53,53,53,53	0
56	MG	XA	1682	1/1	0.37	0.73	25.56	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3672	1/1	0.94	0.70	25.39	26,26,26,26	0
56	MG	RA	3122	1/1	0.73	0.67	25.36	92,92,92,92	0
56	MG	YA	3358	1/1	0.99	0.60	25.36	18,18,18,18	0
56	MG	YA	3756	1/1	0.95	0.61	25.31	80,80,80,80	0
56	MG	RA	3184	1/1	0.92	0.56	25.27	60,60,60,60	0
56	MG	RA	3389	1/1	0.97	0.39	25.22	23,23,23,23	0
56	MG	YA	3346	1/1	0.98	0.53	25.17	16,16,16,16	0
56	MG	RF	310	1/1	0.48	0.69	25.02	88,88,88,88	0
56	MG	YA	3615	1/1	0.99	0.52	24.87	11,11,11,11	0
56	MG	YA	3371	1/1	0.99	0.44	24.71	14,14,14,14	0
56	MG	RA	3892	1/1	0.77	0.52	24.57	55,55,55,55	0
56	MG	YA	3548	1/1	0.91	0.56	24.34	32,32,32,32	0
56	MG	YA	3272	1/1	0.88	0.39	24.29	39,39,39,39	0
56	MG	YA	3683	1/1	0.91	0.56	24.19	39,39,39,39	0
56	MG	YA	3479	1/1	0.71	0.54	24.14	50,50,50,50	0
56	MG	YA	3627	1/1	0.87	0.45	24.11	38,38,38,38	0
56	MG	QA	1757	1/1	0.05	0.97	23.95	86,86,86,86	0
56	MG	RA	3378	1/1	0.98	0.41	23.84	25,25,25,25	0
56	MG	R5	101	1/1	0.81	1.13	23.83	105,105,105,105	0
56	MG	YA	3156	1/1	0.96	0.38	23.81	40,40,40,40	0
56	MG	YA	3694	1/1	0.75	0.47	23.73	80,80,80,80	0
56	MG	XA	1758	1/1	0.86	0.55	23.70	60,60,60,60	0
56	MG	YA	3089	1/1	0.81	0.37	23.69	80,80,80,80	0
56	MG	YA	3544	1/1	0.57	0.54	23.64	81,81,81,81	0
56	MG	YA	3271	1/1	0.94	0.36	23.54	70,70,70,70	0
56	MG	YA	3186	1/1	0.74	0.43	23.46	39,39,39,39	0
56	MG	YA	3124	1/1	0.94	0.56	23.00	54,54,54,54	0
56	MG	YA	3755	1/1	0.87	0.61	22.96	80,80,80,80	0
56	MG	RA	3940	1/1	0.47	0.65	22.80	83,83,83,83	0
56	MG	RA	3289	1/1	0.77	0.75	22.74	83,83,83,83	0
56	MG	YA	3240	1/1	0.90	0.71	22.65	70,70,70,70	0
56	MG	RN	201	1/1	0.65	0.82	22.51	85,85,85,85	0
56	MG	YA	3319	1/1	0.99	0.44	22.51	20,20,20,20	0
56	MG	YA	3029	1/1	0.82	0.55	22.40	57,57,57,57	0
56	MG	RA	3240	1/1	0.79	0.45	22.39	92,92,92,92	0
56	MG	YA	3169	1/1	0.80	0.59	22.24	91,91,91,91	0
56	MG	YA	3394	1/1	0.95	0.46	21.90	19,19,19,19	0
56	MG	YA	3718	1/1	0.62	0.35	21.87	60,60,60,60	0
56	MG	YA	3651	1/1	0.98	0.56	21.70	15,15,15,15	0
56	MG	RR	3201	1/1	0.89	0.59	21.59	62,62,62,62	0
56	MG	RA	3385	1/1	0.94	0.52	21.56	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	4045	1/1	0.94	0.73	21.48	71,71,71,71	0
56	MG	RA	3766	1/1	0.87	0.53	21.43	29,29,29,29	0
56	MG	RA	3951	1/1	0.50	0.51	21.43	87,87,87,87	0
56	MG	YA	3664	1/1	0.84	0.44	21.40	42,42,42,42	0
56	MG	R1	102	1/1	0.40	0.93	21.29	71,71,71,71	0
56	MG	RA	4041	1/1	0.80	1.06	21.25	77,77,77,77	0
56	MG	YA	3097	1/1	0.90	0.52	21.23	37,37,37,37	0
56	MG	RA	3838	1/1	0.97	0.53	21.11	17,17,17,17	0
56	MG	XA	1746	1/1	0.96	0.45	21.05	35,35,35,35	0
56	MG	XA	1774	1/1	0.96	0.38	21.03	59,59,59,59	0
56	MG	YA	3669	1/1	0.98	0.38	20.98	15,15,15,15	0
56	MG	RA	3615	1/1	0.98	0.58	20.80	34,34,34,34	0
56	MG	YA	3478	1/1	0.41	0.46	20.76	67,67,67,67	0
56	MG	YA	3584	1/1	0.65	0.51	20.44	56,56,56,56	0
56	MG	RA	3443	1/1	0.97	0.55	20.38	20,20,20,20	0
56	MG	RA	3411	1/1	0.93	0.34	20.31	31,31,31,31	0
56	MG	YA	3400	1/1	0.69	0.57	20.27	74,74,74,74	0
56	MG	RA	3165	1/1	0.97	0.49	20.18	99,99,99,99	0
56	MG	YA	3401	1/1	0.97	0.52	20.14	19,19,19,19	0
56	MG	RA	3501	1/1	0.98	0.65	20.14	22,22,22,22	0
56	MG	RA	3891	1/1	0.66	0.55	19.95	59,59,59,59	0
56	MG	RA	3101	1/1	0.88	0.38	19.91	68,68,68,68	0
56	MG	RA	3496	1/1	0.98	0.43	19.80	16,16,16,16	0
56	MG	RA	3274	1/1	0.86	0.36	19.78	101,101,101,101	0
56	MG	RF	305	1/1	0.87	0.88	19.71	69,69,69,69	0
56	MG	RA	3623	1/1	0.98	0.53	19.70	34,34,34,34	0
56	MG	YA	3136	1/1	0.94	0.48	19.66	59,59,59,59	0
56	MG	XA	1632	1/1	0.76	0.83	19.62	59,59,59,59	0
56	MG	YA	3652	1/1	0.98	0.47	19.59	24,24,24,24	0
56	MG	RA	3753	1/1	0.95	0.51	19.59	48,48,48,48	0
56	MG	YA	3275	1/1	0.90	0.50	19.58	53,53,53,53	0
56	MG	RA	4061	1/1	0.89	0.48	19.55	96,96,96,96	0
56	MG	RA	3495	1/1	0.98	0.49	19.52	43,43,43,43	0
56	MG	YA	3252	1/1	0.88	0.50	19.48	70,70,70,70	0
56	MG	YA	3515	1/1	0.99	0.41	19.37	12,12,12,12	0
56	MG	RA	3027	1/1	0.89	0.48	19.30	103,103,103,103	0
56	MG	RA	3225	1/1	0.76	0.42	19.25	109,109,109,109	0
56	MG	YA	3380	1/1	0.98	0.37	19.00	7,7,7,7	0
56	MG	YA	3381	1/1	0.96	0.36	18.87	11,11,11,11	0
56	MG	RA	4030	1/1	0.96	0.85	18.87	71,71,71,71	0
56	MG	RA	3148	1/1	0.94	0.37	18.78	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	RA	3536	1/1	0.89	0.37	18.65	64,64,64,64	0
56	MG	QN	103	1/1	0.45	0.95	18.53	80,80,80,80	0
56	MG	RA	3092	1/1	0.96	0.64	18.40	79,79,79,79	0
56	MG	RA	3465	1/1	0.98	0.37	18.35	27,27,27,27	0
56	MG	YA	3707	1/1	0.76	0.59	18.35	95,95,95,95	0
56	MG	YA	3321	1/1	0.96	0.43	18.31	29,29,29,29	0
56	MG	YA	3668	1/1	0.97	0.42	18.27	28,28,28,28	0
56	MG	YA	3250	1/1	0.84	0.30	18.26	45,45,45,45	0
56	MG	RD	308	1/1	0.78	0.57	18.23	80,80,80,80	0
56	MG	QA	1719	1/1	0.96	0.49	18.11	32,32,32,32	0
56	MG	RA	3419	1/1	0.96	0.45	18.09	17,17,17,17	0
56	MG	RA	3714	1/1	0.96	0.39	18.02	36,36,36,36	0
56	MG	RA	3478	1/1	0.98	0.38	18.02	34,34,34,34	0
56	MG	XA	1779	1/1	0.85	0.82	18.00	60,60,60,60	0
56	MG	YA	3480	1/1	0.98	0.40	17.99	17,17,17,17	0
56	MG	RA	3629	1/1	0.86	0.43	17.84	60,60,60,60	0
56	MG	RA	3785	1/1	0.91	0.43	17.78	56,56,56,56	0
56	MG	RA	3220	1/1	0.92	0.39	17.71	75,75,75,75	0
56	MG	RA	3231	1/1	0.82	0.59	17.65	97,97,97,97	0
56	MG	XA	1788	1/1	0.72	0.68	17.63	62,62,62,62	0
56	MG	QA	1722	1/1	0.96	0.71	17.55	61,61,61,61	0
56	MG	RA	3332	1/1	0.83	0.33	17.51	53,53,53,53	0
56	MG	QA	1703	1/1	0.92	0.27	17.50	60,60,60,60	0
56	MG	YA	3685	1/1	0.97	0.46	17.49	19,19,19,19	0
56	MG	RA	3927	1/1	0.85	0.38	17.47	81,81,81,81	0
56	MG	QA	1734	1/1	0.64	0.63	17.46	85,85,85,85	0
56	MG	YA	3522	1/1	0.80	0.48	17.36	65,65,65,65	0
56	MG	RA	3901	1/1	0.98	0.38	17.36	16,16,16,16	0
56	MG	YA	3407	1/1	0.97	0.47	17.34	18,18,18,18	0
56	MG	XA	1672	1/1	0.49	0.64	17.21	91,91,91,91	0
56	MG	XA	1778	1/1	0.89	0.70	17.19	60,60,60,60	0
56	MG	YA	3434	1/1	0.90	0.36	17.02	55,55,55,55	0
56	MG	RA	3490	1/1	0.23	0.49	16.89	86,86,86,86	0
56	MG	XA	1737	1/1	0.97	0.45	16.84	47,47,47,47	0
56	MG	RA	3517	1/1	0.57	0.44	16.80	107,107,107,107	0
56	MG	YA	3173	1/1	0.72	0.42	16.80	85,85,85,85	0
56	MG	QA	1645	1/1	0.49	0.36	16.73	75,75,75,75	0
56	MG	YA	3331	1/1	0.95	0.41	16.72	9,9,9,9	0
56	MG	YA	3551	1/1	0.76	0.51	16.67	60,60,60,60	0
56	MG	YA	3605	1/1	0.99	0.31	16.61	19,19,19,19	0
56	MG	RA	3707	1/1	0.84	0.43	16.53	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3354	1/1	0.94	0.47	16.52	47,47,47,47	0
56	MG	YA	3149	1/1	0.95	0.38	16.42	56,56,56,56	0
56	MG	RA	3408	1/1	0.95	0.33	16.41	24,24,24,24	0
56	MG	XA	1743	1/1	0.95	0.76	16.39	44,44,44,44	0
56	MG	RA	4064	1/1	0.88	1.01	16.19	64,64,64,64	0
56	MG	RD	312	1/1	0.67	0.47	16.16	76,76,76,76	0
56	MG	YA	3159	1/1	0.80	0.39	16.12	91,91,91,91	0
56	MG	RA	4059	1/1	0.67	0.61	16.05	101,101,101,101	0
56	MG	YA	3591	1/1	0.95	0.43	16.03	42,42,42,42	0
56	MG	YE	302	1/1	0.79	0.53	16.02	79,79,79,79	0
56	MG	YA	3489	1/1	0.98	0.37	15.94	15,15,15,15	0
56	MG	RA	3461	1/1	0.64	0.78	15.88	76,76,76,76	0
56	MG	RA	3423	1/1	0.99	0.41	15.80	21,21,21,21	0
56	MG	XA	1627	1/1	0.87	0.48	15.75	62,62,62,62	0
56	MG	YA	3212	1/1	0.91	0.49	15.72	62,62,62,62	0
56	MG	YA	3303	1/1	0.85	0.39	15.71	85,85,85,85	0
56	MG	YA	3339	1/1	0.95	0.50	15.64	15,15,15,15	0
56	MG	RA	3538	1/1	0.45	0.36	15.56	80,80,80,80	0
56	MG	RA	3634	1/1	0.49	0.61	15.55	81,81,81,81	0
56	MG	RA	3794	1/1	0.90	0.71	15.51	86,86,86,86	0
56	MG	YW	201	1/1	0.87	0.66	15.44	75,75,75,75	0
56	MG	RA	3400	1/1	0.98	0.46	15.33	21,21,21,21	0
56	MG	YA	3324	1/1	0.82	0.51	15.12	39,39,39,39	0
56	MG	RA	3808	1/1	0.91	0.36	14.98	56,56,56,56	0
56	MG	RA	3809	1/1	0.31	0.65	14.98	76,76,76,76	0
56	MG	RA	4058	1/1	0.65	0.53	14.91	120,120,120,120	0
56	MG	RA	3621	1/1	0.91	0.35	14.87	61,61,61,61	0
56	MG	RA	3348	1/1	0.97	0.39	14.70	34,34,34,34	0
56	MG	YA	3705	1/1	0.91	0.41	14.61	32,32,32,32	0
56	MG	YA	3748	1/1	0.86	0.49	14.57	95,95,95,95	0
56	MG	RA	4040	1/1	0.85	0.54	14.54	69,69,69,69	0
56	MG	YA	3256	1/1	0.89	0.37	14.54	43,43,43,43	0
56	MG	RA	3393	1/1	0.98	0.47	14.53	14,14,14,14	0
56	MG	YA	3734	1/1	0.96	0.49	14.46	41,41,41,41	0
56	MG	YD	303	1/1	0.90	0.75	14.46	44,44,44,44	0
56	MG	RA	4017	1/1	0.83	0.59	14.46	90,90,90,90	0
56	MG	RA	4018	1/1	0.69	0.68	14.42	70,70,70,70	0
56	MG	YA	3294	1/1	0.91	0.36	14.37	52,52,52,52	0
56	MG	QA	1654	1/1	0.88	0.37	14.34	64,64,64,64	0
56	MG	RA	3706	1/1	0.77	0.43	14.28	58,58,58,58	0
56	MG	YX	101	1/1	0.97	0.31	14.26	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	4038	1/1	0.83	0.61	14.17	66,66,66,66	0
56	MG	YA	3338	1/1	0.99	0.43	14.17	16,16,16,16	0
56	MG	RA	3146	1/1	0.86	0.21	13.99	37,37,37,37	0
56	MG	XA	1772	1/1	0.84	0.41	13.99	51,51,51,51	0
56	MG	RA	3649	1/1	0.63	0.40	13.86	85,85,85,85	0
56	MG	YA	3757	1/1	0.90	0.51	13.84	70,70,70,70	0
56	MG	RD	302	1/1	0.94	0.67	13.71	53,53,53,53	0
56	MG	RA	3500	1/1	0.92	0.50	13.68	25,25,25,25	0
56	MG	RA	4048	1/1	0.85	0.55	13.59	81,81,81,81	0
56	MG	YA	3131	1/1	0.50	0.32	13.58	88,88,88,88	0
56	MG	RA	3695	1/1	0.61	0.34	13.51	52,52,52,52	0
56	MG	YA	3660	1/1	0.96	0.25	13.45	34,34,34,34	0
56	MG	RA	4037	1/1	0.91	0.49	13.40	69,69,69,69	0
56	MG	YB	217	1/1	0.85	0.33	13.26	77,77,77,77	0
56	MG	RA	3178	1/1	0.82	0.57	13.24	79,79,79,79	0
56	MG	RA	3349	1/1	0.91	0.29	13.21	40,40,40,40	0
56	MG	RA	4036	1/1	0.97	0.75	13.20	85,85,85,85	0
56	MG	YA	3051	1/1	0.78	0.40	13.15	64,64,64,64	0
56	MG	RA	3873	1/1	0.98	0.45	13.11	31,31,31,31	0
56	MG	YA	3015	1/1	0.83	0.39	13.08	23,23,23,23	0
56	MG	YA	3444	1/1	0.97	0.43	13.04	27,27,27,27	0
56	MG	YA	3604	1/1	0.98	0.42	12.98	11,11,11,11	0
56	MG	YA	3614	1/1	0.99	0.44	12.94	26,26,26,26	0
56	MG	RA	3470	1/1	0.96	0.40	12.92	34,34,34,34	0
56	MG	RA	3229	1/1	0.75	0.46	12.89	82,82,82,82	0
56	MG	RA	4066	1/1	0.78	0.70	12.87	78,78,78,78	0
56	MG	RA	3355	1/1	0.99	0.57	12.86	24,24,24,24	0
56	MG	RA	3185	1/1	0.91	0.46	12.85	94,94,94,94	0
56	MG	YA	3443	1/1	0.58	0.79	12.82	81,81,81,81	0
56	MG	YA	3032	1/1	0.86	0.28	12.74	80,80,80,80	0
56	MG	RA	3643	1/1	0.83	0.75	12.71	71,71,71,71	0
56	MG	RA	3520	1/1	0.82	0.25	12.67	34,34,34,34	0
56	MG	YA	3329	1/1	0.97	0.34	12.63	19,19,19,19	0
56	MG	XA	1706	1/1	0.85	0.24	12.55	67,67,67,67	0
56	MG	RA	3900	1/1	0.91	0.26	12.54	30,30,30,30	0
56	MG	RA	3077	1/1	0.78	0.25	12.51	70,70,70,70	0
56	MG	RA	3380	1/1	0.95	0.46	12.48	43,43,43,43	0
56	MG	RA	3390	1/1	0.99	0.31	12.46	27,27,27,27	0
56	MG	RA	3075	1/1	0.78	0.32	12.36	56,56,56,56	0
56	MG	YA	3328	1/1	0.97	0.35	12.32	15,15,15,15	0
56	MG	RA	4006	1/1	0.85	0.80	12.31	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3550	1/1	0.88	0.34	12.26	70,70,70,70	0
56	MG	YD	306	1/1	0.99	0.41	12.25	53,53,53,53	0
56	MG	QA	1621	1/1	0.86	0.41	12.19	71,71,71,71	0
56	MG	YA	3073	1/1	0.96	0.58	12.18	67,67,67,67	0
56	MG	RA	4032	1/1	0.98	0.46	12.09	76,76,76,76	0
56	MG	XA	1630	1/1	0.83	0.35	12.02	62,62,62,62	0
56	MG	RA	3021	1/1	0.89	0.71	11.90	101,101,101,101	0
56	MG	RA	4047	1/1	0.47	0.62	11.85	117,117,117,117	0
56	MG	YD	305	1/1	0.78	0.41	11.73	82,82,82,82	0
56	MG	QA	1833	1/1	0.91	0.55	11.71	51,51,51,51	0
56	MG	YA	3219	1/1	0.85	0.42	11.66	60,60,60,60	0
56	MG	RA	3135	1/1	0.94	0.36	11.65	77,77,77,77	0
56	MG	YA	3750	1/1	0.99	0.43	11.60	22,22,22,22	0
56	MG	XA	1699	1/1	0.93	0.42	11.56	44,44,44,44	0
56	MG	YA	3094	1/1	0.41	0.40	11.53	68,68,68,68	0
56	MG	RA	3454	1/1	0.76	0.29	11.51	51,51,51,51	0
56	MG	XA	1740	1/1	0.75	0.30	11.47	65,65,65,65	0
56	MG	RA	4050	1/1	0.96	0.46	11.41	59,59,59,59	0
56	MG	RA	4060	1/1	0.87	0.58	11.39	82,82,82,82	0
56	MG	RA	3128	1/1	0.93	0.36	11.39	48,48,48,48	0
56	MG	RA	4043	1/1	0.93	0.60	11.14	86,86,86,86	0
56	MG	YA	3022	1/1	0.97	0.39	11.12	62,62,62,62	0
56	MG	RA	3472	1/1	0.72	0.27	11.11	51,51,51,51	0
56	MG	RA	3210	1/1	0.98	0.33	11.09	67,67,67,67	0
56	MG	YA	3348	1/1	0.94	0.33	11.07	17,17,17,17	0
56	MG	YA	3704	1/1	0.93	0.44	11.07	29,29,29,29	0
56	MG	RA	4057	1/1	0.91	0.67	11.06	77,77,77,77	0
56	MG	QA	1682	1/1	0.49	0.37	11.02	93,93,93,93	0
56	MG	RA	3770	1/1	0.97	0.35	11.02	22,22,22,22	0
56	MG	YA	3625	1/1	0.95	0.31	11.01	19,19,19,19	0
56	MG	RA	3142	1/1	0.47	0.41	10.99	76,76,76,76	0
56	MG	RF	303	1/1	0.95	0.46	10.97	80,80,80,80	0
56	MG	RD	301	1/1	0.81	0.57	10.93	76,76,76,76	0
56	MG	RA	3230	1/1	0.98	0.53	10.82	81,81,81,81	0
56	MG	RA	4031	1/1	0.71	0.40	10.78	102,102,102,102	0
56	MG	RR	3202	1/1	0.87	0.38	10.65	69,69,69,69	0
56	MG	RA	3806	1/1	0.82	0.30	10.63	78,78,78,78	0
56	MG	Y8	101	1/1	0.76	0.88	10.63	70,70,70,70	0
56	MG	RA	4029	1/1	0.88	0.72	10.59	91,91,91,91	0
56	MG	RA	4024	1/1	0.88	0.51	10.58	59,59,59,59	0
56	MG	XA	1695	1/1	0.81	0.64	10.56	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	YA	3035	1/1	0.89	0.29	10.50	73,73,73,73	0
56	MG	RA	3802	1/1	0.86	1.16	10.46	89,89,89,89	0
56	MG	YA	3499	1/1	0.91	0.44	10.41	38,38,38,38	0
56	MG	RA	4065	1/1	0.71	0.61	10.38	86,86,86,86	0
56	MG	RA	3813	1/1	0.96	0.36	10.34	23,23,23,23	0
56	MG	YT	202	1/1	0.35	0.83	10.24	84,84,84,84	0
56	MG	RA	3857	1/1	0.97	0.34	10.22	35,35,35,35	0
56	MG	RA	3600	1/1	0.72	0.46	10.15	87,87,87,87	0
56	MG	YA	3179	1/1	0.79	0.43	10.09	69,69,69,69	0
56	MG	YA	3287	1/1	0.97	0.42	10.07	35,35,35,35	0
56	MG	RA	3471	1/1	0.96	0.42	10.01	42,42,42,42	0
56	MG	RA	3170	1/1	0.90	0.24	9.96	66,66,66,66	0
56	MG	YA	3744	1/1	0.93	0.37	9.94	33,33,33,33	0
56	MG	RA	4003	1/1	0.70	0.34	9.94	51,51,51,51	0
56	MG	XA	1736	1/1	0.90	0.30	9.92	58,58,58,58	0
56	MG	YA	3195	1/1	0.96	0.26	9.82	33,33,33,33	0
56	MG	RA	3678	1/1	0.92	0.28	9.77	31,31,31,31	0
56	MG	YA	3342	1/1	0.96	0.29	9.75	20,20,20,20	0
56	MG	RB	225	1/1	0.60	0.45	9.75	76,76,76,76	0
56	MG	RA	3298	1/1	0.92	0.28	9.74	24,24,24,24	0
56	MG	RA	3683	1/1	0.60	0.50	9.73	96,96,96,96	0
56	MG	YA	3692	1/1	0.87	0.29	9.73	39,39,39,39	0
56	MG	RA	3040	1/1	0.73	0.48	9.72	76,76,76,76	0
56	MG	RA	3874	1/1	0.93	0.40	9.67	25,25,25,25	0
56	MG	RA	3070	1/1	0.97	0.59	9.67	78,78,78,78	0
56	MG	XA	1622	1/1	0.79	0.22	9.66	42,42,42,42	0
56	MG	YA	3135	1/1	0.91	1.19	9.61	89,89,89,89	0
56	MG	YA	3730	1/1	0.85	0.51	9.60	87,87,87,87	0
56	MG	YA	3758	1/1	0.90	0.55	9.58	76,76,76,76	0
56	MG	RA	4046	1/1	0.64	0.59	9.54	86,86,86,86	0
56	MG	YA	3569	1/1	0.96	0.41	9.50	32,32,32,32	0
56	MG	RA	4009	1/1	0.97	0.61	9.49	70,70,70,70	0
56	MG	XA	1611	1/1	0.97	0.42	9.42	73,73,73,73	0
56	MG	RA	3023	1/1	0.74	0.35	9.41	73,73,73,73	0
56	MG	RA	3721	1/1	0.82	0.58	9.36	73,73,73,73	0
56	MG	YA	3592	1/1	0.98	0.40	9.34	28,28,28,28	0
56	MG	YA	3520	1/1	0.89	0.65	9.32	68,68,68,68	0
56	MG	YA	3636	1/1	0.93	0.25	9.27	45,45,45,45	0
56	MG	YA	3433	1/1	0.90	0.29	9.23	19,19,19,19	0
56	MG	YA	3213	1/1	0.97	0.30	9.22	67,67,67,67	0
56	MG	QA	1647	1/1	-0.54	0.48	9.18	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3335	1/1	0.96	0.29	9.17	46,46,46,46	0
56	MG	XA	1687	1/1	0.87	0.68	9.14	101,101,101,101	0
56	MG	RF	301	1/1	0.64	0.55	9.13	101,101,101,101	0
56	MG	RA	3358	1/1	0.70	0.50	9.07	99,99,99,99	0
56	MG	RA	3769	1/1	0.93	0.40	9.03	46,46,46,46	0
56	MG	RA	3743	1/1	0.86	0.29	9.03	35,35,35,35	0
56	MG	RA	3504	1/1	0.97	0.36	8.96	38,38,38,38	0
56	MG	YA	3425	1/1	0.90	0.27	8.93	49,49,49,49	0
56	MG	YA	3154	1/1	0.80	0.59	8.78	86,86,86,86	0
56	MG	RA	4034	1/1	0.86	0.71	8.76	73,73,73,73	0
56	MG	RA	4022	1/1	0.88	0.40	8.73	73,73,73,73	0
56	MG	RA	3923	1/1	0.84	0.29	8.68	79,79,79,79	0
56	MG	RV	202	1/1	0.93	0.33	8.68	55,55,55,55	0
56	MG	QA	1622	1/1	0.91	0.31	8.51	62,62,62,62	0
56	MG	YA	3611	1/1	0.90	0.27	8.50	31,31,31,31	0
56	MG	RD	305	1/1	0.94	0.42	8.40	86,86,86,86	0
56	MG	RA	3321	1/1	0.98	0.28	8.32	19,19,19,19	0
56	MG	YA	3055	1/1	0.88	0.32	8.30	45,45,45,45	0
56	MG	RA	4062	1/1	0.90	0.38	8.22	78,78,78,78	0
56	MG	YA	3542	1/1	0.94	0.30	8.17	21,21,21,21	0
56	MG	QA	1729	1/1	0.93	0.38	8.16	50,50,50,50	0
56	MG	RF	308	1/1	0.86	0.51	8.14	74,74,74,74	0
56	MG	RB	209	1/1	0.73	0.42	8.14	92,92,92,92	0
56	MG	XF	204	1/1	0.77	0.67	8.02	101,101,101,101	0
56	MG	YD	304	1/1	0.92	0.34	8.00	49,49,49,49	0
56	MG	QA	1841	1/1	0.96	0.34	8.00	28,28,28,28	0
56	MG	RE	301	1/1	0.80	0.38	7.98	81,81,81,81	0
56	MG	RA	3737	1/1	0.83	0.28	7.98	77,77,77,77	0
56	MG	YA	3521	1/1	0.92	0.42	7.94	95,95,95,95	0
56	MG	RA	3398	1/1	0.98	0.44	7.90	20,20,20,20	0
56	MG	XA	1617	1/1	0.93	0.29	7.86	44,44,44,44	0
56	MG	YA	3353	1/1	0.96	0.29	7.81	14,14,14,14	0
56	MG	QA	1855	1/1	0.88	0.31	7.79	56,56,56,56	0
56	MG	XX	101	1/1	0.78	0.79	7.78	122,122,122,122	0
56	MG	YA	3620	1/1	0.93	0.27	7.77	34,34,34,34	0
56	MG	YA	3389	1/1	0.89	0.30	7.75	50,50,50,50	0
56	MG	RA	3312	1/1	0.46	1.07	7.71	124,124,124,124	0
56	MG	QA	1610	1/1	0.83	0.35	7.71	105,105,105,105	0
56	MG	YA	3749	1/1	0.90	0.32	7.71	54,54,54,54	0
56	MG	YA	3751	1/1	0.93	0.27	7.63	39,39,39,39	0
56	MG	RA	3565	1/1	0.91	0.30	7.63	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	RA	3250	1/1	0.73	0.43	7.62	69,69,69,69	0
56	MG	XA	1628	1/1	0.89	0.25	7.58	56,56,56,56	0
56	MG	YA	3554	1/1	0.96	0.23	7.58	44,44,44,44	0
56	MG	RA	3745	1/1	0.96	0.30	7.46	21,21,21,21	0
56	MG	YA	3323	1/1	0.89	0.33	7.41	37,37,37,37	0
56	MG	RA	3712	1/1	0.94	0.66	7.40	53,53,53,53	0
56	MG	RA	3306	1/1	0.97	1.00	7.39	66,66,66,66	0
56	MG	YA	3753	1/1	0.94	0.50	7.37	54,54,54,54	0
56	MG	RA	3132	1/1	0.72	0.25	7.36	63,63,63,63	0
56	MG	RA	3535	1/1	0.74	0.26	7.33	57,57,57,57	0
56	MG	RA	4016	1/1	0.91	0.35	7.33	68,68,68,68	0
56	MG	QA	1821	1/1	0.65	0.85	7.31	90,90,90,90	0
56	MG	RA	3333	1/1	0.98	0.37	7.25	24,24,24,24	0
56	MG	YA	3536	1/1	0.91	0.23	7.23	42,42,42,42	0
56	MG	YA	3021	1/1	0.92	0.38	7.16	69,69,69,69	0
56	MG	QA	1852	1/1	0.83	0.38	7.14	60,60,60,60	0
56	MG	QA	1768	1/1	0.34	0.29	7.09	91,91,91,91	0
56	MG	YA	3556	1/1	0.97	0.31	6.96	41,41,41,41	0
56	MG	RA	4028	1/1	0.97	0.30	6.91	78,78,78,78	0
56	MG	YA	3243	1/1	0.85	0.32	6.85	67,67,67,67	0
56	MG	RA	3315	1/1	0.98	0.30	6.85	29,29,29,29	0
56	MG	YA	3012	1/1	0.83	0.26	6.78	56,56,56,56	0
56	MG	XA	1608	1/1	0.41	0.47	6.75	76,76,76,76	0
56	MG	RO	201	1/1	0.71	0.56	6.71	93,93,93,93	0
56	MG	QA	1680	1/1	0.46	0.37	6.69	64,64,64,64	0
56	MG	YA	3014	1/1	0.98	0.28	6.64	39,39,39,39	0
56	MG	RA	3811	1/1	0.85	0.24	6.60	55,55,55,55	0
56	MG	RA	4044	1/1	0.97	0.50	6.52	95,95,95,95	0
56	MG	RA	3676	1/1	0.94	0.41	6.48	86,86,86,86	0
56	MG	RA	3030	1/1	0.87	0.72	6.48	113,113,113,113	0
56	MG	RA	3234	1/1	0.85	0.36	6.44	64,64,64,64	0
56	MG	R8	101	1/1	0.77	0.70	6.39	75,75,75,75	0
56	MG	RA	3861	1/1	0.79	0.25	6.34	43,43,43,43	0
56	MG	RA	3216	1/1	0.93	0.31	6.34	77,77,77,77	0
56	MG	YA	3646	1/1	0.77	0.40	6.33	69,69,69,69	0
56	MG	YA	3314	1/1	0.68	0.46	6.26	55,55,55,55	0
56	MG	XA	1757	1/1	0.94	0.27	6.24	30,30,30,30	0
56	MG	YD	309	1/1	0.94	0.32	6.21	14,14,14,14	0
56	MG	RA	4049	1/1	0.85	0.46	6.18	92,92,92,92	0
56	MG	RA	3820	1/1	0.98	0.26	6.16	28,28,28,28	0
56	MG	YA	3038	1/1	0.95	0.27	6.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1672	1/1	0.78	0.50	6.13	45,45,45,45	0
56	MG	QA	1606	1/1	0.87	0.45	6.12	93,93,93,93	0
56	MG	YA	3385	1/1	0.99	0.34	6.12	23,23,23,23	0
56	MG	RA	3073	1/1	0.93	0.33	6.11	64,64,64,64	0
56	MG	YE	304	1/1	0.91	0.29	6.09	51,51,51,51	0
56	MG	QA	1843	1/1	0.67	0.31	6.02	89,89,89,89	0
56	MG	RA	3723	1/1	0.88	0.22	6.00	68,68,68,68	0
56	MG	RA	3701	1/1	0.77	0.50	5.99	64,64,64,64	0
56	MG	QA	1665	1/1	0.79	0.50	5.96	102,102,102,102	0
56	MG	QY	402	1/1	0.48	0.55	5.91	111,111,111,111	0
56	MG	YA	3754	1/1	0.97	0.31	5.89	26,26,26,26	0
56	MG	RA	3773	1/1	0.96	0.24	5.89	25,25,25,25	0
56	MG	YA	3295	1/1	0.86	0.30	5.87	44,44,44,44	0
56	MG	YD	308	1/1	0.99	0.27	5.81	71,71,71,71	0
56	MG	RA	3529	1/1	0.90	0.27	5.78	77,77,77,77	0
56	MG	QA	1714	1/1	0.94	0.28	5.66	42,42,42,42	0
56	MG	RA	3464	1/1	0.92	0.27	5.60	71,71,71,71	0
56	MG	RA	3534	1/1	0.89	0.25	5.58	44,44,44,44	0
56	MG	YA	3387	1/1	0.93	0.39	5.57	37,37,37,37	0
56	MG	RA	4055	1/1	0.73	0.71	5.57	86,86,86,86	0
56	MG	YA	3114	1/1	0.89	0.29	5.54	90,90,90,90	0
56	MG	RA	3938	1/1	0.84	0.59	5.51	100,100,100,100	0
56	MG	YA	3538	1/1	0.92	0.39	5.49	44,44,44,44	0
56	MG	RA	3597	1/1	0.95	0.26	5.40	19,19,19,19	0
56	MG	QA	1710	1/1	0.98	0.29	5.35	28,28,28,28	0
56	MG	YA	3079	1/1	0.94	0.29	5.32	91,91,91,91	0
56	MG	QT	201	1/1	0.66	0.50	5.30	65,65,65,65	0
56	MG	QA	1707	1/1	0.95	0.30	5.29	28,28,28,28	0
56	MG	RE	305	1/1	0.73	0.30	5.27	33,33,33,33	0
56	MG	RA	3351	1/1	0.50	0.63	5.23	70,70,70,70	0
56	MG	RA	3531	1/1	0.81	0.24	5.21	34,34,34,34	0
56	MG	RA	3622	1/1	0.99	0.34	5.19	20,20,20,20	0
56	MG	RA	3119	1/1	0.95	0.45	5.16	74,74,74,74	0
56	MG	RA	3899	1/1	0.96	0.35	5.07	66,66,66,66	0
56	MG	RD	311	1/1	0.78	0.50	5.03	70,70,70,70	0
56	MG	YA	3030	1/1	0.92	0.25	4.96	39,39,39,39	0
56	MG	RV	203	1/1	0.82	0.35	4.94	55,55,55,55	0
56	MG	QA	1625	1/1	0.77	0.31	4.84	61,61,61,61	0
56	MG	RA	3381	1/1	0.93	0.27	4.82	39,39,39,39	0
56	MG	YA	3507	1/1	0.75	0.24	4.76	44,44,44,44	0
56	MG	RA	3905	1/1	0.95	0.42	4.74	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	RA	3299	1/1	0.82	0.38	4.71	96,96,96,96	0
56	MG	RA	3608	1/1	0.80	0.74	4.67	104,104,104,104	0
56	MG	RA	3270	1/1	0.83	0.33	4.56	103,103,103,103	0
56	MG	YA	3202	1/1	0.93	0.28	4.53	38,38,38,38	0
56	MG	RX	101	1/1	0.91	0.35	4.51	51,51,51,51	0
56	MG	YF	303	1/1	0.95	0.26	4.49	85,85,85,85	0
56	MG	RD	307	1/1	0.73	0.37	4.49	83,83,83,83	0
56	MG	RA	3999	1/1	0.96	0.23	4.44	21,21,21,21	0
56	MG	XA	1770	1/1	0.75	0.35	4.39	104,104,104,104	0
56	MG	RB	215	1/1	0.54	0.32	4.37	91,91,91,91	0
56	MG	RA	3902	1/1	0.96	0.27	4.35	49,49,49,49	0
56	MG	XA	1658	1/1	0.84	0.29	4.32	79,79,79,79	0
56	MG	RA	3323	1/1	0.93	0.25	4.31	38,38,38,38	0
56	MG	RA	3610	1/1	0.89	0.25	4.29	67,67,67,67	0
56	MG	RQ	204	1/1	0.88	0.36	4.28	72,72,72,72	0
56	MG	YE	303	1/1	0.59	0.43	4.27	103,103,103,103	0
56	MG	RA	3050	1/1	0.92	0.43	4.19	88,88,88,88	0
56	MG	RA	3506	1/1	0.97	0.22	4.16	26,26,26,26	0
56	MG	XA	1620	1/1	0.68	0.26	4.11	63,63,63,63	0
56	MG	YQ	201	1/1	0.92	0.26	4.07	33,33,33,33	0
56	MG	XA	1756	1/1	0.96	0.29	4.03	27,27,27,27	0
56	MG	YA	3062	1/1	0.89	0.22	4.02	57,57,57,57	0
56	MG	YA	3116	1/1	0.89	0.22	3.99	58,58,58,58	0
56	MG	XA	1762	1/1	0.86	0.26	3.98	48,48,48,48	0
56	MG	QA	1876	1/1	0.77	0.26	3.97	84,84,84,84	0
56	MG	YA	3453	1/1	0.88	0.24	3.96	35,35,35,35	0
56	MG	RA	4042	1/1	0.61	0.36	3.94	80,80,80,80	0
56	MG	YA	3096	1/1	0.92	0.20	3.94	26,26,26,26	0
56	MG	QA	1655	1/1	0.89	0.41	3.84	64,64,64,64	0
56	MG	YA	3093	1/1	0.88	0.23	3.83	18,18,18,18	0
56	MG	RA	3014	1/1	0.96	0.23	3.64	38,38,38,38	0
56	MG	RA	3567	1/1	0.76	0.27	3.59	81,81,81,81	0
56	MG	YR	201	1/1	0.82	0.34	3.59	66,66,66,66	0
56	MG	RA	3708	1/1	0.81	0.34	3.55	54,54,54,54	0
56	MG	YA	3410	1/1	0.97	0.31	3.54	31,31,31,31	0
56	MG	YA	3300	1/1	0.93	0.26	3.52	40,40,40,40	0
56	MG	RA	4001	1/1	0.89	0.33	3.48	58,58,58,58	0
56	MG	RA	3117	1/1	0.92	0.28	3.47	64,64,64,64	0
56	MG	YA	3503	1/1	0.93	0.19	3.46	18,18,18,18	0
56	MG	RA	3168	1/1	0.94	0.20	3.44	71,71,71,71	0
56	MG	QA	1830	1/1	0.24	0.24	3.34	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	4033	1/1	0.95	0.27	3.27	17,17,17,17	0
56	MG	RA	3430	1/1	0.97	0.26	3.26	9,9,9,9	0
56	MG	YA	3582	1/1	0.78	0.52	3.25	101,101,101,101	0
56	MG	RA	3952	1/1	0.93	0.24	3.21	49,49,49,49	0
56	MG	YA	3255	1/1	0.71	0.33	3.20	88,88,88,88	0
57	ZN	Y4	101	1/1	0.14	0.44	3.20	305,305,305,305	0
56	MG	XR	101	1/1	0.79	0.44	3.20	89,89,89,89	0
56	MG	RA	3233	1/1	0.87	0.30	3.16	72,72,72,72	0
56	MG	YA	3452	1/1	0.95	0.21	3.08	46,46,46,46	0
56	MG	QA	1800	1/1	0.97	0.21	3.08	41,41,41,41	0
56	MG	YA	3728	1/1	0.95	0.25	2.99	8,8,8,8	0
56	MG	RA	3064	1/1	0.81	0.20	2.94	54,54,54,54	0
56	MG	RA	3001	1/1	0.88	0.32	2.87	68,68,68,68	0
56	MG	YA	3087	1/1	0.78	0.23	2.85	64,64,64,64	0
56	MG	RA	3328	1/1	0.88	0.21	2.83	34,34,34,34	0
56	MG	YA	3142	1/1	0.92	0.23	2.80	58,58,58,58	0
56	MG	XA	1726	1/1	0.91	0.21	2.73	74,74,74,74	0
56	MG	YA	3460	1/1	0.95	0.21	2.72	28,28,28,28	0
56	MG	RA	3330	1/1	0.80	0.20	2.61	41,41,41,41	0
56	MG	YA	3112	1/1	0.97	0.21	2.60	9,9,9,9	0
56	MG	QL	201	1/1	0.78	0.31	2.55	66,66,66,66	0
56	MG	XA	1761	1/1	0.90	0.21	2.47	38,38,38,38	0
56	MG	YA	3010	1/1	0.95	0.23	2.30	41,41,41,41	0
56	MG	RG	201	1/1	0.25	0.48	2.28	121,121,121,121	0
56	MG	RA	4000	1/1	0.93	0.26	2.24	30,30,30,30	0
56	MG	RE	306	1/1	0.83	0.30	2.23	59,59,59,59	0
56	MG	XA	1768	1/1	0.90	0.24	2.17	45,45,45,45	0
57	ZN	R4	101	1/1	0.73	0.34	2.15	269,269,269,269	0
56	MG	XA	1631	1/1	0.99	0.40	2.11	60,60,60,60	0
56	MG	XA	1730	1/1	0.81	0.18	2.10	47,47,47,47	0
56	MG	RR	3203	1/1	0.68	0.28	2.10	84,84,84,84	0
56	MG	RE	302	1/1	0.45	0.34	2.09	109,109,109,109	0
56	MG	XA	1605	1/1	0.74	0.50	2.07	72,72,72,72	0
56	MG	YA	3141	1/1	0.96	0.20	2.04	23,23,23,23	0
56	MG	RA	4052	1/1	0.66	0.70	2.00	90,90,90,90	0
56	MG	YA	3092	1/1	0.52	0.25	1.92	113,113,113,113	0
56	MG	XA	1689	1/1	0.80	0.26	1.91	64,64,64,64	0
56	MG	RA	3157	1/1	0.86	0.22	1.90	72,72,72,72	0
56	MG	QN	102	1/1	0.66	0.38	1.83	68,68,68,68	0
56	MG	YA	3013	1/1	0.91	0.19	1.74	23,23,23,23	0
56	MG	RA	4021	1/1	0.84	0.30	1.70	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	RA	3716	1/1	0.87	0.21	1.68	52,52,52,52	0
56	MG	YV	201	1/1	0.87	0.27	1.67	44,44,44,44	0
56	MG	RA	3653	1/1	0.80	0.25	1.64	75,75,75,75	0
56	MG	RA	4025	1/1	0.83	0.26	1.64	32,32,32,32	0
56	MG	QA	1618	1/1	0.91	0.23	1.62	96,96,96,96	0
56	MG	YA	3317	1/1	0.95	0.19	1.61	24,24,24,24	0
56	MG	RA	3376	1/1	0.90	0.20	1.40	52,52,52,52	0
56	MG	QD	304	1/1	0.47	0.27	1.39	111,111,111,111	0
56	MG	QF	201	1/1	0.81	0.28	1.38	59,59,59,59	0
56	MG	XL	201	1/1	0.72	0.31	1.33	85,85,85,85	0
56	MG	YA	3747	1/1	0.75	0.43	1.32	108,108,108,108	0
56	MG	YA	3673	1/1	0.99	0.22	1.32	13,13,13,13	0
56	MG	XA	1685	1/1	0.95	0.28	1.28	65,65,65,65	0
56	MG	RA	3507	1/1	0.95	0.19	1.26	109,109,109,109	0
56	MG	QA	1635	1/1	0.84	0.18	1.25	58,58,58,58	0
56	MG	RA	4051	1/1	0.92	0.27	1.23	63,63,63,63	0
56	MG	YB	214	1/1	0.90	0.16	1.20	45,45,45,45	0
56	MG	RB	205	1/1	0.97	0.22	1.15	47,47,47,47	0
56	MG	YA	3001	1/1	0.81	0.33	1.15	90,90,90,90	0
56	MG	RA	3125	1/1	0.98	0.20	1.06	36,36,36,36	0
56	MG	YA	3702	1/1	0.95	0.17	1.06	30,30,30,30	0
56	MG	RA	3670	1/1	0.81	0.23	0.99	80,80,80,80	0
56	MG	QA	1656	1/1	0.81	0.20	0.93	58,58,58,58	0
56	MG	YA	3177	1/1	0.42	0.20	0.83	71,71,71,71	0
56	MG	QA	1771	1/1	0.77	0.15	0.82	57,57,57,57	0
56	MG	RA	3401	1/1	0.85	0.19	0.80	44,44,44,44	0
56	MG	YF	301	1/1	0.85	0.19	0.79	54,54,54,54	0
56	MG	XA	1653	1/1	0.87	0.30	0.77	79,79,79,79	0
56	MG	QA	1678	1/1	0.84	0.22	0.75	80,80,80,80	0
56	MG	QA	1690	1/1	0.80	0.28	0.74	72,72,72,72	0
56	MG	QA	1619	1/1	0.88	0.23	0.72	75,75,75,75	0
56	MG	YA	3306	1/1	0.98	0.17	0.69	9,9,9,9	0
56	MG	RB	206	1/1	0.74	0.18	0.66	74,74,74,74	0
56	MG	RA	3937	1/1	0.83	0.19	0.66	38,38,38,38	0
56	MG	YA	3335	1/1	0.93	0.16	0.64	30,30,30,30	0
56	MG	XA	1635	1/1	0.91	0.20	0.57	29,29,29,29	0
56	MG	XT	201	1/1	0.66	0.29	0.52	65,65,65,65	0
56	MG	QA	1614	1/1	0.86	0.19	0.50	48,48,48,48	0
56	MG	RQ	201	1/1	0.90	0.20	0.44	47,47,47,47	0
56	MG	YA	3153	1/1	0.87	0.20	0.40	37,37,37,37	0
56	MG	QA	1872	1/1	0.87	0.22	0.26	85,85,85,85	0
56	MG	XA	1722	1/1	0.64	0.20	0.25	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	XA	1790	1/1	0.78	0.25	0.24	98,98,98,98	0
56	MG	YA	3746	1/1	0.94	0.19	0.24	35,35,35,35	0
56	MG	RA	4023	1/1	0.95	0.19	0.20	49,49,49,49	0
56	MG	QA	1616	1/1	0.93	0.19	0.12	92,92,92,92	0
56	MG	RD	306	1/1	0.94	0.17	0.09	33,33,33,33	0
56	MG	YA	3117	1/1	0.71	0.16	0.09	42,42,42,42	0
56	MG	RA	3062	1/1	0.14	0.20	-0.03	82,82,82,82	0
56	MG	RA	3304	1/1	0.91	0.18	-0.04	39,39,39,39	0
56	MG	YG	202	1/1	0.89	0.18	-0.05	78,78,78,78	0
56	MG	YA	3187	1/1	0.85	0.23	-0.06	40,40,40,40	0
56	MG	QA	1779	1/1	0.86	0.22	-0.06	80,80,80,80	0
56	MG	QA	1638	1/1	0.97	0.15	-0.15	41,41,41,41	0
56	MG	RA	3726	1/1	0.92	0.16	-0.21	53,53,53,53	0
56	MG	QA	1827	1/1	0.97	0.18	-0.21	52,52,52,52	0
56	MG	YA	3002	1/1	0.94	0.23	-0.25	64,64,64,64	0
56	MG	RA	3758	1/1	0.83	0.16	-0.30	49,49,49,49	0
56	MG	RA	3008	1/1	0.80	0.17	-0.37	46,46,46,46	0
56	MG	RA	3043	1/1	0.94	0.14	-0.39	38,38,38,38	0
56	MG	QA	1634	1/1	0.92	0.18	-0.39	44,44,44,44	0
56	MG	RA	3732	1/1	0.83	0.14	-0.45	54,54,54,54	0
56	MG	RA	3570	1/1	0.89	0.13	-0.51	35,35,35,35	0
56	MG	QA	1658	1/1	0.84	0.15	-0.52	94,94,94,94	0
56	MG	QQ	202	1/1	0.90	0.14	-0.54	68,68,68,68	0
56	MG	RB	219	1/1	0.98	0.14	-0.55	57,57,57,57	0
57	ZN	YY	201	1/1	0.72	0.18	-0.57	221,221,221,221	0
56	MG	QA	1869	1/1	0.68	0.18	-0.66	61,61,61,61	0
57	ZN	RY	201	1/1	0.55	0.21	-0.68	210,210,210,210	0
56	MG	RA	3867	1/1	0.61	0.14	-0.71	63,63,63,63	0
56	MG	XA	1615	1/1	0.84	0.21	-0.77	63,63,63,63	0
56	MG	QR	101	1/1	0.76	0.19	-0.85	71,71,71,71	0
56	MG	RG	204	1/1	0.76	0.19	-0.92	67,67,67,67	0
56	MG	XA	1752	1/1	0.98	0.18	-0.93	51,51,51,51	0
56	MG	RA	3584	1/1	0.91	0.13	-1.00	45,45,45,45	0
56	MG	YA	3736	1/1	0.92	0.15	-1.04	39,39,39,39	0
56	MG	RA	3420	1/1	0.95	0.15	-1.06	19,19,19,19	0
56	MG	QB	301	1/1	0.86	0.13	-1.06	91,91,91,91	0
56	MG	XA	1643	1/1	0.55	0.15	-1.08	80,80,80,80	0
56	MG	RA	3851	1/1	0.59	0.14	-1.08	91,91,91,91	0
56	MG	QA	1650	1/1	0.70	0.14	-1.11	72,72,72,72	0
56	MG	YA	3424	1/1	0.88	0.16	-1.16	27,27,27,27	0
56	MG	RF	309	1/1	0.93	0.14	-1.16	68,68,68,68	0
56	MG	RA	3866	1/1	0.92	0.11	-1.23	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	SF4	QD	302	8/8	0.99	0.15	-1.36	51,57,76,106	0
57	ZN	QN	101	1/1	0.96	0.13	-1.40	105,105,105,105	0
56	MG	YA	3457	1/1	0.95	0.12	-1.41	33,33,33,33	0
56	MG	RA	3532	1/1	0.74	0.12	-1.43	52,52,52,52	0
57	ZN	XN	101	1/1	0.98	0.10	-1.44	94,94,94,94	0
56	MG	YA	3279	1/1	0.93	0.15	-1.48	61,61,61,61	0
56	MG	YA	3190	1/1	0.82	0.12	-1.48	78,78,78,78	0
56	MG	XA	1696	1/1	0.85	0.14	-1.53	67,67,67,67	0
58	SF4	XD	301	8/8	0.99	0.14	-1.55	58,74,100,102	0
56	MG	YG	203	1/1	0.73	0.14	-1.65	54,54,54,54	0
56	MG	QA	1739	1/1	0.73	0.12	-1.66	87,87,87,87	0
57	ZN	Y9	101	1/1	0.97	0.10	-1.72	107,107,107,107	0
56	MG	YA	3023	1/1	0.95	0.13	-1.80	16,16,16,16	0
56	MG	YA	3204	1/1	0.89	0.14	-1.85	42,42,42,42	0
56	MG	RA	3025	1/1	0.97	0.14	-1.96	23,23,23,23	0
56	MG	RA	3032	1/1	0.88	0.14	-2.01	49,49,49,49	0
57	ZN	R9	102	1/1	0.99	0.05	-2.05	92,92,92,92	0
57	ZN	R6	101	1/1	0.92	0.16	-2.10	160,160,160,160	0
56	MG	RA	3131	1/1	0.71	0.09	-2.19	67,67,67,67	0
56	MG	QA	1626	1/1	0.87	0.09	-2.20	78,78,78,78	0
57	ZN	Y5	102	1/1	0.98	0.05	-2.40	119,119,119,119	0
56	MG	YA	3752	1/1	0.95	0.12	-2.50	52,52,52,52	0
56	MG	XK	201	1/1	0.93	0.07	-2.52	53,53,53,53	0
56	MG	RA	3006	1/1	0.79	0.12	-2.75	33,33,33,33	0
57	ZN	R5	102	1/1	0.99	0.03	-2.86	119,119,119,119	0
57	ZN	Y6	101	1/1	0.98	0.17	-3.05	169,169,169,169	0
56	MG	RA	3965	1/1	0.96	0.11	-3.05	45,45,45,45	0
56	MG	YA	3286	1/1	0.92	0.10	-3.05	35,35,35,35	0
56	MG	RA	3049	1/1	0.95	0.12	-3.20	48,48,48,48	0
56	MG	YA	3224	1/1	0.90	0.10	-3.28	66,66,66,66	0
56	MG	YA	3091	1/1	0.95	0.14	-3.38	36,36,36,36	0
56	MG	RA	3395	1/1	0.95	0.09	-3.60	22,22,22,22	0
56	MG	YA	3564	1/1	0.96	0.11	-3.80	42,42,42,42	0
56	MG	YA	3009	1/1	0.98	0.12	-3.87	37,37,37,37	0
56	MG	RA	3964	1/1	0.94	0.10	-4.22	44,44,44,44	0
56	MG	YA	3041	1/1	0.95	0.06	-4.70	35,35,35,35	0
56	MG	XA	1636	1/1	0.87	0.07	-4.84	60,60,60,60	0
56	MG	RA	3513	1/1	0.98	0.11	-4.90	14,14,14,14	0
56	MG	QA	1631	1/1	0.97	0.08	-5.18	34,34,34,34	0
56	MG	RA	3041	1/1	0.96	0.06	-5.71	44,44,44,44	0
56	MG	YA	3106	1/1	0.89	0.10	-7.45	30,30,30,30	0
56	MG	QA	1774	1/1	0.57	0.42	-	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	YA	3559	1/1	0.96	0.40	-	54,54,54,54	0
56	MG	YA	3596	1/1	0.97	0.41	-	39,39,39,39	0
56	MG	RA	3607	1/1	0.75	0.35	-	98,98,98,98	0
56	MG	RA	3713	1/1	0.85	0.45	-	47,47,47,47	0
56	MG	XF	202	1/1	0.72	0.45	-	73,73,73,73	0
56	MG	YA	3530	1/1	0.82	0.69	-	59,59,59,59	0
56	MG	XA	1651	1/1	0.07	0.55	-	90,90,90,90	0
56	MG	RA	3803	1/1	0.88	0.14	-	64,64,64,64	0
56	MG	XE	201	1/1	0.55	0.48	-	79,79,79,79	0
56	MG	XA	1648	1/1	0.48	0.51	-	74,74,74,74	0
56	MG	QA	1673	1/1	0.83	0.41	-	52,52,52,52	0
56	MG	RA	3897	1/1	0.95	0.37	-	61,61,61,61	0
56	MG	RB	226	1/1	0.15	0.66	-	99,99,99,99	0
56	MG	YA	3403	1/1	0.54	0.38	-	59,59,59,59	0
56	MG	YA	3606	1/1	0.98	0.62	-	25,25,25,25	0
56	MG	YA	3399	1/1	0.91	0.62	-	36,36,36,36	0
56	MG	QA	1801	1/1	0.66	0.30	-	78,78,78,78	0
56	MG	RA	3134	1/1	0.60	0.54	-	83,83,83,83	0
56	MG	QA	1846	1/1	0.91	0.57	-	47,47,47,47	0
56	MG	YA	3666	1/1	0.94	0.46	-	36,36,36,36	0
56	MG	QA	1867	1/1	0.16	1.16	-	99,99,99,99	0
56	MG	RA	3166	1/1	0.69	0.99	-	68,68,68,68	0
56	MG	RA	3934	1/1	0.81	0.17	-	62,62,62,62	0
56	MG	YA	3228	1/1	0.67	0.33	-	75,75,75,75	0
56	MG	RA	3484	1/1	0.98	0.46	-	30,30,30,30	0
56	MG	RA	3563	1/1	0.82	0.60	-	66,66,66,66	0
56	MG	YA	3158	1/1	0.85	0.68	-	49,49,49,49	0
56	MG	YA	3280	1/1	0.93	0.33	-	14,14,14,14	0
56	MG	RA	3143	1/1	0.90	0.15	-	72,72,72,72	0
56	MG	RB	210	1/1	0.62	1.00	-	109,109,109,109	0
56	MG	RA	3199	1/1	0.71	0.24	-	68,68,68,68	0
56	MG	RA	3886	1/1	0.92	0.60	-	52,52,52,52	0
56	MG	YA	3733	1/1	0.89	0.25	-	62,62,62,62	0
56	MG	QA	1765	1/1	0.90	0.20	-	83,83,83,83	0
56	MG	YA	3597	1/1	0.83	0.75	-	74,74,74,74	0
56	MG	YA	3576	1/1	0.93	0.35	-	37,37,37,37	0
56	MG	QA	1799	1/1	-0.38	0.83	-	83,83,83,83	0
56	MG	YA	3352	1/1	0.95	0.46	-	11,11,11,11	0
56	MG	QA	1603	1/1	0.77	0.40	-	105,105,105,105	0
56	MG	RA	3858	1/1	0.49	0.71	-	80,80,80,80	0
56	MG	RA	3247	1/1	0.85	0.60	-	88,88,88,88	0
56	MG	YA	3068	1/1	0.89	0.35	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3396	1/1	0.89	0.47	-	58,58,58,58	0
56	MG	RA	3206	1/1	0.79	0.56	-	97,97,97,97	0
56	MG	YA	3227	1/1	0.81	0.46	-	64,64,64,64	0
56	MG	XA	1604	1/1	0.43	0.71	-	99,99,99,99	0
56	MG	YA	3052	1/1	0.74	0.31	-	45,45,45,45	0
56	MG	YA	3588	1/1	0.88	0.18	-	76,76,76,76	0
56	MG	YA	3549	1/1	0.94	0.31	-	34,34,34,34	0
56	MG	XA	1749	1/1	0.84	0.41	-	82,82,82,82	0
56	MG	RA	3918	1/1	0.95	0.52	-	71,71,71,71	0
56	MG	RB	229	1/1	0.44	0.52	-	108,108,108,108	0
56	MG	RA	3920	1/1	0.91	0.50	-	41,41,41,41	0
56	MG	RA	3986	1/1	0.70	0.53	-	79,79,79,79	0
56	MG	YA	3332	1/1	0.96	0.33	-	28,28,28,28	0
56	MG	YA	3511	1/1	0.49	0.60	-	60,60,60,60	0
56	MG	RA	3499	1/1	0.77	0.50	-	77,77,77,77	0
56	MG	RA	3740	1/1	0.36	0.97	-	76,76,76,76	0
56	MG	RA	3558	1/1	0.71	0.56	-	82,82,82,82	0
56	MG	RA	3183	1/1	0.84	0.34	-	81,81,81,81	0
56	MG	YA	3567	1/1	0.86	0.23	-	42,42,42,42	0
56	MG	YA	3185	1/1	0.13	0.86	-	105,105,105,105	0
56	MG	RA	3236	1/1	0.79	0.69	-	69,69,69,69	0
56	MG	RA	3681	1/1	0.21	0.67	-	119,119,119,119	0
56	MG	XA	1711	1/1	0.12	0.61	-	92,92,92,92	0
56	MG	YA	3483	1/1	0.97	0.35	-	26,26,26,26	0
56	MG	RA	3211	1/1	0.79	0.55	-	88,88,88,88	0
56	MG	RA	3111	1/1	0.80	0.25	-	106,106,106,106	0
56	MG	RA	3059	1/1	0.90	0.13	-	76,76,76,76	0
56	MG	RA	3977	1/1	0.40	0.90	-	62,62,62,62	0
56	MG	RA	3276	1/1	0.50	0.64	-	91,91,91,91	0
56	MG	RA	3007	1/1	0.91	0.22	-	61,61,61,61	0
56	MG	RA	3152	1/1	0.74	0.45	-	106,106,106,106	0
56	MG	RA	3724	1/1	0.64	0.26	-	67,67,67,67	0
56	MG	QA	1667	1/1	0.94	0.21	-	67,67,67,67	0
56	MG	YA	3396	1/1	0.00	0.89	-	94,94,94,94	0
56	MG	YA	3085	1/1	0.60	0.28	-	86,86,86,86	0
56	MG	RA	3771	1/1	0.82	0.31	-	45,45,45,45	0
56	MG	RA	3542	1/1	0.60	0.55	-	76,76,76,76	0
56	MG	QA	1818	1/1	0.91	0.23	-	63,63,63,63	0
56	MG	RA	3123	1/1	0.93	0.23	-	30,30,30,30	0
56	MG	YA	3580	1/1	0.92	0.46	-	27,27,27,27	0
56	MG	RA	3172	1/1	0.96	0.51	-	80,80,80,80	0
56	MG	YA	3602	1/1	0.99	0.41	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3535	1/1	0.31	0.98	-	75,75,75,75	0
56	MG	RA	3675	1/1	0.60	0.33	-	75,75,75,75	0
56	MG	QA	1848	1/1	0.47	0.57	-	68,68,68,68	0
56	MG	QA	1764	1/1	0.29	0.34	-	101,101,101,101	0
56	MG	YA	3706	1/1	0.95	0.28	-	79,79,79,79	0
56	MG	YA	3145	1/1	0.96	0.46	-	59,59,59,59	0
56	MG	YA	3162	1/1	0.91	0.15	-	27,27,27,27	0
56	MG	QA	1758	1/1	0.75	0.50	-	76,76,76,76	0
56	MG	XA	1656	1/1	0.81	0.37	-	80,80,80,80	0
56	MG	QY	401	1/1	-0.00	0.42	-	111,111,111,111	0
56	MG	YA	3632	1/1	0.85	0.34	-	62,62,62,62	0
56	MG	RA	3875	1/1	0.48	0.59	-	90,90,90,90	0
56	MG	XA	1638	1/1	0.90	0.07	-	118,118,118,118	0
56	MG	RA	3674	1/1	0.87	0.59	-	77,77,77,77	0
56	MG	RA	3291	1/1	0.71	0.76	-	86,86,86,86	0
56	MG	RA	3601	1/1	0.93	0.79	-	87,87,87,87	0
56	MG	YA	3724	1/1	0.97	0.57	-	51,51,51,51	0
56	MG	YA	3711	1/1	0.92	0.67	-	47,47,47,47	0
56	MG	XA	1702	1/1	0.55	0.38	-	61,61,61,61	0
56	MG	YA	3254	1/1	0.88	0.32	-	67,67,67,67	0
56	MG	QA	1611	1/1	0.43	0.75	-	89,89,89,89	0
56	MG	RA	3819	1/1	0.81	0.23	-	33,33,33,33	0
56	MG	QA	1767	1/1	0.86	0.22	-	90,90,90,90	0
56	MG	RA	3552	1/1	0.85	0.17	-	97,97,97,97	0
56	MG	RA	3995	1/1	0.76	0.38	-	111,111,111,111	0
56	MG	YA	3656	1/1	0.99	0.29	-	34,34,34,34	0
56	MG	RA	3631	1/1	0.68	0.42	-	125,125,125,125	0
56	MG	YA	3519	1/1	0.78	0.44	-	79,79,79,79	0
56	MG	QA	1613	1/1	0.97	0.10	-	97,97,97,97	0
56	MG	QA	1747	1/1	0.65	0.46	-	72,72,72,72	0
56	MG	YA	3579	1/1	0.96	0.56	-	36,36,36,36	0
56	MG	RA	3257	1/1	0.94	0.55	-	100,100,100,100	0
56	MG	RA	3375	1/1	0.51	0.68	-	73,73,73,73	0
56	MG	RA	3827	1/1	0.81	0.34	-	57,57,57,57	0
56	MG	XA	1771	1/1	0.93	0.54	-	62,62,62,62	0
56	MG	YA	3017	1/1	0.82	0.57	-	60,60,60,60	0
56	MG	YA	3430	1/1	0.95	0.20	-	20,20,20,20	0
56	MG	XA	1721	1/1	0.68	0.60	-	86,86,86,86	0
56	MG	RA	3167	1/1	0.90	0.13	-	69,69,69,69	0
56	MG	QA	1750	1/1	0.88	0.35	-	67,67,67,67	0
56	MG	YA	3667	1/1	0.59	0.64	-	90,90,90,90	0
56	MG	YA	3192	1/1	0.88	0.21	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3282	1/1	-0.37	2.52	-	109,109,109,109	0
56	MG	RA	3815	1/1	0.92	0.29	-	68,68,68,68	0
56	MG	YA	3084	1/1	0.87	0.37	-	66,66,66,66	0
56	MG	XA	1661	1/1	0.46	0.34	-	87,87,87,87	0
56	MG	XA	1610	1/1	0.70	0.36	-	79,79,79,79	0
56	MG	QA	1761	1/1	0.80	0.62	-	72,72,72,72	0
56	MG	YA	3448	1/1	0.62	0.32	-	81,81,81,81	0
56	MG	RA	3458	1/1	0.90	0.21	-	74,74,74,74	0
56	MG	RA	3840	1/1	0.46	0.55	-	83,83,83,83	0
56	MG	QA	1817	1/1	0.67	0.35	-	64,64,64,64	0
56	MG	QA	1842	1/1	0.36	0.37	-	84,84,84,84	0
56	MG	YA	3467	1/1	0.52	0.93	-	82,82,82,82	0
56	MG	RA	3412	1/1	0.83	0.48	-	71,71,71,71	0
56	MG	YA	3677	1/1	0.96	0.74	-	42,42,42,42	0
56	MG	RA	3515	1/1	0.76	0.55	-	67,67,67,67	0
56	MG	XA	1780	1/1	0.94	0.62	-	40,40,40,40	0
56	MG	YA	3485	1/1	0.78	0.53	-	77,77,77,77	0
56	MG	RA	3832	1/1	0.84	0.36	-	74,74,74,74	0
56	MG	QA	1802	1/1	0.81	0.65	-	79,79,79,79	0
56	MG	RA	3660	1/1	0.92	0.23	-	46,46,46,46	0
56	MG	RA	3829	1/1	0.77	1.09	-	65,65,65,65	0
56	MG	RD	309	1/1	0.79	0.29	-	78,78,78,78	0
56	MG	RA	3679	1/1	0.89	0.84	-	54,54,54,54	0
56	MG	XA	1601	1/1	0.86	0.23	-	75,75,75,75	0
56	MG	RA	3038	1/1	0.87	0.20	-	63,63,63,63	0
56	MG	RA	3442	1/1	0.99	0.59	-	18,18,18,18	0
56	MG	YA	3261	1/1	0.88	0.24	-	55,55,55,55	0
56	MG	QA	1620	1/1	0.56	0.27	-	75,75,75,75	0
56	MG	RA	3944	1/1	0.96	0.18	-	22,22,22,22	0
56	MG	YA	3042	1/1	0.95	0.19	-	61,61,61,61	0
56	MG	XA	1684	1/1	0.90	0.48	-	40,40,40,40	0
56	MG	YA	3698	1/1	0.78	0.48	-	77,77,77,77	0
56	MG	RA	3477	1/1	0.87	0.39	-	46,46,46,46	0
56	MG	RA	3512	1/1	0.41	0.86	-	80,80,80,80	0
56	MG	RA	3147	1/1	0.98	0.20	-	39,39,39,39	0
56	MG	RA	3790	1/1	0.41	0.50	-	82,82,82,82	0
56	MG	YA	3700	1/1	0.81	0.36	-	71,71,71,71	0
56	MG	XA	1642	1/1	0.96	0.25	-	55,55,55,55	0
56	MG	RA	3314	1/1	0.66	0.65	-	58,58,58,58	0
56	MG	YA	3378	1/1	0.89	0.25	-	53,53,53,53	0
56	MG	QD	303	1/1	0.69	0.47	-	79,79,79,79	0
56	MG	YA	3203	1/1	0.61	0.54	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3870	1/1	0.97	0.44	-	24,24,24,24	0
56	MG	YA	3577	1/1	0.71	0.67	-	53,53,53,53	0
56	MG	YA	3679	1/1	0.84	0.45	-	36,36,36,36	0
56	MG	QA	1875	1/1	0.83	0.42	-	75,75,75,75	0
56	MG	RA	3034	1/1	0.80	0.81	-	100,100,100,100	0
56	MG	XA	1718	1/1	0.15	1.23	-	73,73,73,73	0
56	MG	YA	3309	1/1	0.89	0.37	-	37,37,37,37	0
56	MG	RA	3936	1/1	0.83	1.03	-	74,74,74,74	0
56	MG	RA	3448	1/1	0.64	0.68	-	71,71,71,71	0
56	MG	YA	3137	1/1	0.94	0.34	-	40,40,40,40	0
56	MG	QA	1859	1/1	0.94	0.34	-	50,50,50,50	0
56	MG	RA	3422	1/1	0.43	0.69	-	84,84,84,84	0
56	MG	YA	3274	1/1	0.95	0.39	-	48,48,48,48	0
56	MG	RA	3878	1/1	0.72	0.72	-	81,81,81,81	0
56	MG	RA	3042	1/1	0.77	0.31	-	80,80,80,80	0
56	MG	QA	1612	1/1	-0.13	0.93	-	97,97,97,97	0
56	MG	YA	3296	1/1	0.92	0.58	-	32,32,32,32	0
56	MG	RD	313	1/1	0.38	0.78	-	82,82,82,82	0
56	MG	YA	3613	1/1	0.91	0.65	-	53,53,53,53	0
56	MG	RA	4010	1/1	0.83	0.33	-	76,76,76,76	0
56	MG	RA	3514	1/1	0.77	0.25	-	87,87,87,87	0
56	MG	RA	3765	1/1	0.99	0.57	-	40,40,40,40	0
56	MG	YA	3076	1/1	0.95	0.29	-	4,4,4,4	0
56	MG	XA	1781	1/1	-0.11	0.82	-	110,110,110,110	0
56	MG	RA	3138	1/1	0.73	0.44	-	53,53,53,53	0
56	MG	QA	1605	1/1	0.81	0.29	-	67,67,67,67	0
56	MG	YA	3501	1/1	0.45	0.65	-	115,115,115,115	0
56	MG	RA	3406	1/1	0.81	0.27	-	60,60,60,60	0
56	MG	YA	3461	1/1	0.47	0.91	-	81,81,81,81	0
56	MG	YA	3626	1/1	0.98	0.30	-	25,25,25,25	0
56	MG	XA	1707	1/1	0.87	0.52	-	58,58,58,58	0
56	MG	XA	1782	1/1	0.92	0.20	-	46,46,46,46	0
56	MG	RA	3452	1/1	0.75	0.29	-	78,78,78,78	0
56	MG	XA	1709	1/1	0.51	0.17	-	72,72,72,72	0
56	MG	QA	1657	1/1	0.45	0.57	-	98,98,98,98	0
56	MG	RA	3576	1/1	0.93	0.39	-	43,43,43,43	0
56	MG	RA	3667	1/1	0.67	0.19	-	60,60,60,60	0
56	MG	RA	3181	1/1	0.79	0.29	-	90,90,90,90	0
56	MG	RA	3015	1/1	0.89	0.30	-	72,72,72,72	0
56	MG	QA	1742	1/1	0.90	0.72	-	58,58,58,58	0
56	MG	RA	3079	1/1	0.97	0.38	-	64,64,64,64	0
56	MG	RA	4014	1/1	0.81	0.57	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RB	218	1/1	0.84	0.28	-	79,79,79,79	0
56	MG	RA	3982	1/1	0.61	0.53	-	83,83,83,83	0
56	MG	QA	1809	1/1	0.83	0.26	-	67,67,67,67	0
56	MG	RA	3976	1/1	0.54	0.63	-	81,81,81,81	0
56	MG	RA	3583	1/1	0.62	0.61	-	72,72,72,72	0
56	MG	RA	3432	1/1	0.58	0.43	-	58,58,58,58	0
56	MG	RA	3604	1/1	0.80	0.28	-	91,91,91,91	0
56	MG	QA	1687	1/1	0.79	0.32	-	97,97,97,97	0
56	MG	XA	1694	1/1	0.98	0.34	-	30,30,30,30	0
56	MG	QA	1627	1/1	0.91	0.09	-	42,42,42,42	0
56	MG	YA	3594	1/1	0.90	0.33	-	35,35,35,35	0
56	MG	RA	3662	1/1	0.35	0.96	-	89,89,89,89	0
56	MG	RA	3628	1/1	0.77	0.55	-	65,65,65,65	0
56	MG	RA	3797	1/1	0.74	0.49	-	84,84,84,84	0
56	MG	YA	3459	1/1	0.48	0.38	-	85,85,85,85	0
56	MG	XA	1785	1/1	0.52	0.42	-	81,81,81,81	0
56	MG	XA	1647	1/1	0.21	0.35	-	92,92,92,92	0
56	MG	YA	3100	1/1	0.64	0.28	-	87,87,87,87	0
56	MG	YA	3406	1/1	0.66	0.44	-	80,80,80,80	0
56	MG	YA	3033	1/1	0.95	0.12	-	13,13,13,13	0
56	MG	RA	3427	1/1	0.69	0.62	-	78,78,78,78	0
56	MG	XA	1621	1/1	0.56	0.59	-	68,68,68,68	0
56	MG	RH	202	1/1	0.40	0.50	-	96,96,96,96	0
56	MG	YA	3277	1/1	0.96	0.47	-	17,17,17,17	0
56	MG	YA	3193	1/1	0.18	0.70	-	101,101,101,101	0
56	MG	RA	3447	1/1	0.88	0.29	-	57,57,57,57	0
56	MG	RA	3505	1/1	0.80	0.26	-	64,64,64,64	0
56	MG	YA	3439	1/1	0.68	0.52	-	80,80,80,80	0
56	MG	RA	3636	1/1	0.34	1.23	-	91,91,91,91	0
56	MG	XA	1683	1/1	0.88	0.79	-	69,69,69,69	0
56	MG	RA	3672	1/1	0.40	0.69	-	75,75,75,75	0
56	MG	R7	102	1/1	0.63	0.52	-	72,72,72,72	0
56	MG	YA	3188	1/1	0.81	0.41	-	94,94,94,94	0
56	MG	QA	1844	1/1	0.89	0.17	-	80,80,80,80	0
56	MG	RA	3445	1/1	0.92	0.26	-	58,58,58,58	0
56	MG	QA	1624	1/1	0.72	0.54	-	73,73,73,73	0
56	MG	YA	3197	1/1	0.84	0.38	-	77,77,77,77	0
56	MG	RA	3956	1/1	0.66	0.33	-	77,77,77,77	0
56	MG	QA	1726	1/1	0.74	0.24	-	81,81,81,81	0
56	MG	RA	3324	1/1	0.97	0.37	-	14,14,14,14	0
56	MG	YA	3291	1/1	0.94	0.48	-	24,24,24,24	0
56	MG	RA	3776	1/1	0.69	0.36	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	XA	1700	1/1	0.76	0.43	-	43,43,43,43	0
56	MG	RA	3377	1/1	0.86	0.47	-	42,42,42,42	0
56	MG	RA	3718	1/1	0.88	0.13	-	62,62,62,62	0
56	MG	YA	3171	1/1	0.67	0.38	-	104,104,104,104	0
56	MG	YA	3561	1/1	0.77	0.35	-	45,45,45,45	0
56	MG	RA	3437	1/1	0.20	0.64	-	77,77,77,77	0
56	MG	YA	3442	1/1	0.84	0.48	-	53,53,53,53	0
56	MG	YA	3526	1/1	0.88	0.43	-	43,43,43,43	0
56	MG	YA	3305	1/1	0.95	0.13	-	19,19,19,19	0
56	MG	YA	3239	1/1	0.83	0.38	-	94,94,94,94	0
56	MG	RA	3650	1/1	0.82	0.41	-	69,69,69,69	0
56	MG	YA	3266	1/1	0.85	0.78	-	70,70,70,70	0
56	MG	YA	3061	1/1	0.60	0.58	-	57,57,57,57	0
56	MG	RA	3094	1/1	0.97	0.87	-	71,71,71,71	0
56	MG	QA	1715	1/1	0.33	0.44	-	77,77,77,77	0
56	MG	QA	1697	1/1	0.54	0.30	-	76,76,76,76	0
56	MG	RA	3612	1/1	0.89	0.76	-	64,64,64,64	0
56	MG	RA	3687	1/1	0.81	0.30	-	57,57,57,57	0
56	MG	YA	3264	1/1	0.86	0.56	-	88,88,88,88	0
56	MG	QA	1824	1/1	0.64	1.30	-	127,127,127,127	0
56	MG	RB	216	1/1	0.76	0.32	-	59,59,59,59	0
56	MG	QA	1743	1/1	0.62	0.33	-	71,71,71,71	0
56	MG	RA	3757	1/1	0.83	0.35	-	70,70,70,70	0
56	MG	QA	1692	1/1	0.90	0.37	-	52,52,52,52	0
56	MG	RA	3645	1/1	0.61	0.54	-	84,84,84,84	0
56	MG	RA	3198	1/1	0.25	1.31	-	84,84,84,84	0
56	MG	QA	1731	1/1	0.71	0.48	-	71,71,71,71	0
56	MG	RA	3722	1/1	0.64	0.36	-	82,82,82,82	0
56	MG	RA	3801	1/1	0.65	0.19	-	74,74,74,74	0
56	MG	YA	3587	1/1	0.97	0.27	-	31,31,31,31	0
56	MG	RA	3201	1/1	0.83	0.34	-	70,70,70,70	0
56	MG	YA	3607	1/1	0.93	0.58	-	53,53,53,53	0
56	MG	RA	3962	1/1	0.65	0.82	-	62,62,62,62	0
56	MG	YA	3020	1/1	0.86	0.26	-	80,80,80,80	0
56	MG	RA	3039	1/1	0.36	0.54	-	76,76,76,76	0
56	MG	RT	202	1/1	0.87	0.30	-	65,65,65,65	0
56	MG	YA	3655	1/1	0.66	0.81	-	86,86,86,86	0
56	MG	YE	307	1/1	0.84	0.24	-	64,64,64,64	0
56	MG	RA	3357	1/1	0.67	0.16	-	61,61,61,61	0
56	MG	RA	3126	1/1	0.50	1.12	-	79,79,79,79	0
56	MG	YA	3071	1/1	0.83	0.43	-	77,77,77,77	0
56	MG	QA	1756	1/1	0.45	0.55	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3719	1/1	0.84	0.39	-	79,79,79,79	0
56	MG	QH	202	1/1	0.79	0.67	-	77,77,77,77	0
56	MG	XA	1787	1/1	0.81	1.38	-	84,84,84,84	0
56	MG	YA	3454	1/1	0.88	1.12	-	52,52,52,52	0
56	MG	RA	3481	1/1	0.21	0.21	-	81,81,81,81	0
56	MG	YN	201	1/1	0.09	0.83	-	87,87,87,87	0
56	MG	QI	201	1/1	0.68	0.55	-	106,106,106,106	0
56	MG	QA	1766	1/1	0.61	0.39	-	71,71,71,71	0
56	MG	R1	103	1/1	0.88	0.30	-	55,55,55,55	0
56	MG	RA	3154	1/1	0.87	0.11	-	88,88,88,88	0
56	MG	RA	3697	1/1	0.88	0.32	-	55,55,55,55	0
56	MG	RA	3640	1/1	0.94	0.14	-	48,48,48,48	0
56	MG	YA	3659	1/1	0.88	0.43	-	29,29,29,29	0
56	MG	YA	3583	1/1	0.95	0.50	-	29,29,29,29	0
56	MG	QA	1860	1/1	0.14	0.63	-	100,100,100,100	0
56	MG	YA	3540	1/1	0.92	0.45	-	27,27,27,27	0
56	MG	RA	3239	1/1	0.37	0.81	-	112,112,112,112	0
56	MG	RA	3609	1/1	0.87	0.27	-	71,71,71,71	0
56	MG	RA	3136	1/1	0.66	0.41	-	84,84,84,84	0
56	MG	RA	3409	1/1	0.95	0.32	-	33,33,33,33	0
56	MG	QA	1789	1/1	-0.04	0.40	-	99,99,99,99	0
56	MG	RA	3862	1/1	0.74	0.41	-	79,79,79,79	0
56	MG	RA	3812	1/1	0.53	0.62	-	106,106,106,106	0
56	MG	YW	202	1/1	0.56	0.24	-	55,55,55,55	0
56	MG	YA	3139	1/1	0.78	0.47	-	66,66,66,66	0
56	MG	XA	1763	1/1	0.89	0.57	-	49,49,49,49	0
56	MG	QA	1834	1/1	0.91	0.35	-	43,43,43,43	0
56	MG	XA	1663	1/1	0.80	0.43	-	107,107,107,107	0
56	MG	YA	3695	1/1	0.61	0.94	-	76,76,76,76	0
56	MG	YA	3045	1/1	0.95	0.46	-	27,27,27,27	0
56	MG	RA	3915	1/1	0.97	0.31	-	41,41,41,41	0
56	MG	RA	3161	1/1	0.82	0.33	-	72,72,72,72	0
56	MG	RA	3746	1/1	-0.06	0.70	-	112,112,112,112	0
56	MG	RA	3044	1/1	0.94	0.32	-	29,29,29,29	0
56	MG	QA	1754	1/1	-0.02	0.82	-	108,108,108,108	0
56	MG	XA	1629	1/1	0.84	0.19	-	51,51,51,51	0
56	MG	YA	3449	1/1	0.19	0.78	-	81,81,81,81	0
56	MG	RA	3599	1/1	0.63	0.26	-	66,66,66,66	0
56	MG	RA	3212	1/1	0.71	0.61	-	95,95,95,95	0
56	MG	YA	3635	1/1	0.77	0.53	-	80,80,80,80	0
56	MG	RA	3150	1/1	0.74	0.16	-	74,74,74,74	0
56	MG	RA	3930	1/1	0.93	0.40	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3176	1/1	0.57	0.45	-	102,102,102,102	0
56	MG	RA	3810	1/1	0.54	0.63	-	75,75,75,75	0
56	MG	RA	3689	1/1	0.88	0.89	-	70,70,70,70	0
56	MG	QA	1641	1/1	0.42	0.65	-	105,105,105,105	0
56	MG	RA	3762	1/1	0.81	0.26	-	76,76,76,76	0
56	MG	YA	3181	1/1	0.87	0.27	-	66,66,66,66	0
56	MG	RA	3085	1/1	0.78	0.45	-	76,76,76,76	0
56	MG	RA	3302	1/1	0.45	0.55	-	92,92,92,92	0
56	MG	XA	1649	1/1	0.30	0.36	-	92,92,92,92	0
56	MG	RA	3657	1/1	0.88	0.52	-	65,65,65,65	0
56	MG	QA	1688	1/1	0.84	0.71	-	62,62,62,62	0
56	MG	YA	3265	1/1	0.75	0.42	-	64,64,64,64	0
56	MG	YA	3555	1/1	0.81	0.63	-	77,77,77,77	0
56	MG	YA	3236	1/1	0.54	0.36	-	106,106,106,106	0
56	MG	YA	3115	1/1	0.78	0.29	-	52,52,52,52	0
56	MG	XA	1654	1/1	0.09	0.90	-	89,89,89,89	0
56	MG	RA	3688	1/1	0.30	0.32	-	90,90,90,90	0
56	MG	RA	3761	1/1	0.99	0.44	-	22,22,22,22	0
56	MG	YA	3110	1/1	0.50	0.47	-	63,63,63,63	0
56	MG	YA	3102	1/1	0.88	0.52	-	60,60,60,60	0
56	MG	RA	4035	1/1	0.45	0.38	-	116,116,116,116	0
56	MG	RA	3856	1/1	0.94	0.30	-	33,33,33,33	0
56	MG	RA	3642	1/1	0.79	0.24	-	70,70,70,70	0
56	MG	RA	3752	1/1	0.14	0.61	-	102,102,102,102	0
56	MG	YA	3167	1/1	0.56	0.87	-	88,88,88,88	0
56	MG	XA	1742	1/1	0.91	0.39	-	52,52,52,52	0
56	MG	QA	1706	1/1	0.97	0.47	-	35,35,35,35	0
56	MG	RA	3789	1/1	0.81	0.33	-	95,95,95,95	0
56	MG	RA	3449	1/1	0.85	0.22	-	45,45,45,45	0
56	MG	XA	1644	1/1	0.87	0.34	-	61,61,61,61	0
56	MG	RA	3997	1/1	0.86	0.30	-	98,98,98,98	0
56	MG	YA	3246	1/1	0.11	0.52	-	118,118,118,118	0
56	MG	YA	3543	1/1	0.94	0.52	-	36,36,36,36	0
56	MG	RA	3341	1/1	0.95	0.52	-	30,30,30,30	0
56	MG	YA	3629	1/1	0.90	0.36	-	44,44,44,44	0
56	MG	YA	3058	1/1	0.85	0.20	-	75,75,75,75	0
56	MG	YA	3039	1/1	0.71	0.59	-	73,73,73,73	0
56	MG	RA	3058	1/1	0.20	1.00	-	88,88,88,88	0
56	MG	RA	3268	1/1	0.86	0.42	-	95,95,95,95	0
56	MG	R0	101	1/1	0.82	0.43	-	94,94,94,94	0
56	MG	YP	201	1/1	0.62	0.56	-	79,79,79,79	0
56	MG	YA	3693	1/1	0.83	0.29	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3313	1/1	0.94	0.40	-	21,21,21,21	0
56	MG	YA	3648	1/1	0.93	0.28	-	40,40,40,40	0
56	MG	RA	3665	1/1	0.81	0.36	-	77,77,77,77	0
56	MG	RA	3246	1/1	0.81	0.77	-	69,69,69,69	0
56	MG	YA	3074	1/1	0.90	0.30	-	63,63,63,63	0
56	MG	RA	3618	1/1	0.85	0.33	-	48,48,48,48	0
56	MG	RA	3824	1/1	0.32	1.39	-	76,76,76,76	0
56	MG	YA	3691	1/1	0.95	0.29	-	38,38,38,38	0
56	MG	RA	3530	1/1	0.69	0.42	-	75,75,75,75	0
56	MG	YA	3031	1/1	0.88	0.38	-	46,46,46,46	0
56	MG	YA	3130	1/1	0.84	0.59	-	65,65,65,65	0
56	MG	YA	3344	1/1	0.42	0.27	-	80,80,80,80	0
56	MG	XA	1678	1/1	0.94	0.61	-	81,81,81,81	0
56	MG	YA	3568	1/1	0.96	0.25	-	19,19,19,19	0
56	MG	RA	3704	1/1	0.62	0.60	-	91,91,91,91	0
56	MG	RA	3035	1/1	0.55	0.47	-	97,97,97,97	0
56	MG	YB	219	1/1	0.94	0.42	-	31,31,31,31	0
56	MG	YA	3653	1/1	0.88	0.54	-	55,55,55,55	0
56	MG	QA	1850	1/1	0.67	0.61	-	51,51,51,51	0
56	MG	RF	304	1/1	0.79	0.17	-	63,63,63,63	0
56	MG	RR	3205	1/1	0.76	0.41	-	60,60,60,60	0
56	MG	YA	3209	1/1	0.86	0.44	-	48,48,48,48	0
56	MG	RA	3825	1/1	-0.00	1.06	-	98,98,98,98	0
56	MG	QA	1785	1/1	0.59	0.51	-	84,84,84,84	0
56	MG	RA	3869	1/1	0.89	1.08	-	77,77,77,77	0
56	MG	RA	3344	1/1	0.97	0.38	-	51,51,51,51	0
56	MG	YA	3504	1/1	0.64	0.28	-	74,74,74,74	0
56	MG	YA	3067	1/1	0.93	1.04	-	53,53,53,53	0
56	MG	XA	1690	1/1	0.92	0.29	-	53,53,53,53	0
56	MG	RA	3763	1/1	0.83	0.47	-	61,61,61,61	0
56	MG	RA	3226	1/1	0.78	0.98	-	104,104,104,104	0
56	MG	RA	3494	1/1	0.94	0.89	-	55,55,55,55	0
56	MG	RA	3917	1/1	0.82	0.57	-	67,67,67,67	0
56	MG	RA	3115	1/1	-0.39	1.51	-	92,92,92,92	0
56	MG	RB	207	1/1	0.88	0.17	-	82,82,82,82	0
56	MG	RA	3093	1/1	0.93	0.12	-	72,72,72,72	0
56	MG	XA	1641	1/1	0.92	0.36	-	61,61,61,61	0
56	MG	YA	3637	1/1	0.13	1.13	-	101,101,101,101	0
56	MG	QA	1760	1/1	0.04	0.95	-	77,77,77,77	0
56	MG	RA	3877	1/1	0.98	0.37	-	23,23,23,23	0
56	MG	RA	3975	1/1	0.93	0.23	-	63,63,63,63	0
56	MG	YA	3680	1/1	0.98	0.73	-	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	R9	101	1/1	0.57	0.42	-	92,92,92,92	0
56	MG	YA	3126	1/1	0.93	0.17	-	91,91,91,91	0
56	MG	QA	1724	1/1	0.79	0.23	-	76,76,76,76	0
56	MG	RA	3760	1/1	0.89	0.16	-	74,74,74,74	0
56	MG	YA	3351	1/1	0.87	0.51	-	51,51,51,51	0
56	MG	RA	3889	1/1	0.91	0.54	-	48,48,48,48	0
56	MG	RA	3848	1/1	0.97	0.68	-	50,50,50,50	0
56	MG	RA	3887	1/1	0.96	0.34	-	53,53,53,53	0
56	MG	YA	3716	1/1	0.85	0.38	-	65,65,65,65	0
56	MG	YE	306	1/1	0.96	0.41	-	13,13,13,13	0
56	MG	Y7	101	1/1	0.89	0.55	-	75,75,75,75	0
56	MG	RA	3428	1/1	0.87	0.29	-	60,60,60,60	0
56	MG	RN	202	1/1	0.59	1.06	-	98,98,98,98	0
56	MG	QA	1644	1/1	0.68	0.53	-	108,108,108,108	0
56	MG	RA	3528	1/1	0.80	0.33	-	76,76,76,76	0
56	MG	YA	3119	1/1	0.61	0.55	-	78,78,78,78	0
56	MG	QA	1755	1/1	0.72	0.39	-	69,69,69,69	0
56	MG	YA	3349	1/1	0.94	0.36	-	49,49,49,49	0
56	MG	YA	3494	1/1	0.98	0.20	-	36,36,36,36	0
56	MG	YA	3040	1/1	0.86	0.19	-	66,66,66,66	0
56	MG	YA	3441	1/1	0.98	0.44	-	34,34,34,34	0
56	MG	RA	3002	1/1	0.93	0.28	-	70,70,70,70	0
56	MG	XA	1735	1/1	0.78	0.75	-	53,53,53,53	0
56	MG	RA	3402	1/1	0.68	0.80	-	71,71,71,71	0
56	MG	RA	3730	1/1	0.76	0.22	-	51,51,51,51	0
56	MG	YA	3595	1/1	0.98	0.51	-	12,12,12,12	0
56	MG	RA	3555	1/1	0.91	1.15	-	68,68,68,68	0
56	MG	YA	3225	1/1	0.85	0.30	-	74,74,74,74	0
56	MG	QA	1643	1/1	0.89	0.67	-	86,86,86,86	0
56	MG	QA	1845	1/1	0.73	0.77	-	77,77,77,77	0
56	MG	RA	3692	1/1	0.86	0.74	-	87,87,87,87	0
56	MG	RA	3382	1/1	0.98	0.31	-	20,20,20,20	0
56	MG	QA	1816	1/1	0.69	0.78	-	76,76,76,76	0
56	MG	QA	1879	1/1	0.75	0.44	-	78,78,78,78	0
56	MG	YA	3497	1/1	0.65	0.41	-	63,63,63,63	0
56	MG	RA	3387	1/1	0.95	0.64	-	50,50,50,50	0
56	MG	QA	1811	1/1	0.63	0.33	-	83,83,83,83	0
56	MG	RA	3686	1/1	0.69	0.37	-	62,62,62,62	0
56	MG	YA	3391	1/1	0.98	0.45	-	18,18,18,18	0
56	MG	YA	3253	1/1	0.21	0.63	-	98,98,98,98	0
56	MG	RA	3339	1/1	0.63	0.46	-	68,68,68,68	0
56	MG	YA	3322	1/1	0.97	0.29	-	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	XA	1751	1/1	0.79	0.43	-	59,59,59,59	0
56	MG	RA	3921	1/1	0.62	2.25	-	88,88,88,88	0
56	MG	YA	3337	1/1	0.94	0.28	-	35,35,35,35	0
56	MG	YA	3725	1/1	0.86	0.40	-	68,68,68,68	0
56	MG	YA	3304	1/1	0.81	0.61	-	56,56,56,56	0
56	MG	YA	3550	1/1	0.74	0.82	-	76,76,76,76	0
56	MG	YA	3523	1/1	0.51	0.28	-	56,56,56,56	0
56	MG	YA	3375	1/1	0.80	0.42	-	55,55,55,55	0
56	MG	YA	3267	1/1	-0.10	1.03	-	100,100,100,100	0
56	MG	YA	3475	1/1	0.72	0.58	-	84,84,84,84	0
56	MG	RA	3076	1/1	0.73	0.68	-	83,83,83,83	0
56	MG	RA	3659	1/1	0.78	0.58	-	62,62,62,62	0
56	MG	RA	3561	1/1	0.88	0.35	-	42,42,42,42	0
56	MG	RA	3816	1/1	0.84	0.55	-	102,102,102,102	0
56	MG	QA	1683	1/1	0.68	0.26	-	112,112,112,112	0
56	MG	YA	3214	1/1	0.46	0.74	-	111,111,111,111	0
56	MG	RA	3180	1/1	0.94	0.34	-	75,75,75,75	0
56	MG	QA	1711	1/1	0.84	0.27	-	63,63,63,63	0
56	MG	YA	3534	1/1	-0.20	0.53	-	124,124,124,124	0
56	MG	YA	3025	1/1	0.82	0.07	-	55,55,55,55	0
56	MG	XA	1625	1/1	0.85	0.70	-	74,74,74,74	0
56	MG	RA	3581	1/1	0.92	0.25	-	75,75,75,75	0
56	MG	RA	3258	1/1	0.66	0.62	-	96,96,96,96	0
56	MG	QA	1797	1/1	0.77	0.38	-	95,95,95,95	0
56	MG	QA	1795	1/1	0.80	0.34	-	61,61,61,61	0
56	MG	QA	1819	1/1	0.32	0.57	-	65,65,65,65	0
56	MG	QA	1636	1/1	0.56	0.30	-	66,66,66,66	0
56	MG	RA	3577	1/1	-0.29	1.14	-	94,94,94,94	0
56	MG	RA	3648	1/1	0.86	0.51	-	82,82,82,82	0
56	MG	RA	3228	1/1	0.75	0.55	-	101,101,101,101	0
56	MG	XA	1676	1/1	0.95	0.30	-	42,42,42,42	0
56	MG	YA	3043	1/1	0.85	0.77	-	62,62,62,62	0
56	MG	RA	3884	1/1	0.89	0.31	-	71,71,71,71	0
56	MG	RA	3744	1/1	0.92	0.43	-	41,41,41,41	0
56	MG	RA	3831	1/1	0.98	0.30	-	65,65,65,65	0
56	MG	RA	3095	1/1	0.87	0.58	-	88,88,88,88	0
56	MG	RA	3066	1/1	0.61	0.54	-	56,56,56,56	0
56	MG	RA	3083	1/1	0.91	0.37	-	80,80,80,80	0
56	MG	YA	3397	1/1	0.87	0.61	-	68,68,68,68	0
56	MG	YA	3663	1/1	0.98	0.71	-	38,38,38,38	0
56	MG	XA	1745	1/1	0.96	0.46	-	44,44,44,44	0
56	MG	RA	3598	1/1	0.83	0.37	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	XA	1765	1/1	0.95	0.55	-	49,49,49,49	0
56	MG	RA	3241	1/1	0.92	0.32	-	108,108,108,108	0
56	MG	YA	3235	1/1	0.84	0.24	-	91,91,91,91	0
56	MG	YA	3445	1/1	0.72	0.66	-	72,72,72,72	0
56	MG	RA	3503	1/1	0.98	0.28	-	21,21,21,21	0
56	MG	QY	403	1/1	0.20	0.81	-	81,81,81,81	0
56	MG	YB	205	1/1	0.54	0.69	-	89,89,89,89	0
56	MG	QA	1684	1/1	0.86	0.50	-	97,97,97,97	0
56	MG	YA	3498	1/1	0.90	0.42	-	64,64,64,64	0
56	MG	RA	3218	1/1	0.89	0.55	-	65,65,65,65	0
56	MG	RA	3568	1/1	0.97	0.35	-	27,27,27,27	0
56	MG	YA	3600	1/1	0.91	0.41	-	51,51,51,51	0
56	MG	RA	3144	1/1	0.76	0.76	-	84,84,84,84	0
56	MG	XA	1728	1/1	0.12	0.94	-	101,101,101,101	0
56	MG	QA	1782	1/1	0.71	0.26	-	69,69,69,69	0
56	MG	XA	1652	1/1	0.31	0.49	-	78,78,78,78	0
56	MG	RA	3160	1/1	0.88	0.94	-	83,83,83,83	0
56	MG	YA	3714	1/1	0.69	0.41	-	80,80,80,80	0
56	MG	XA	1614	1/1	0.96	0.24	-	60,60,60,60	0
56	MG	RA	3578	1/1	0.84	0.50	-	60,60,60,60	0
56	MG	QA	1738	1/1	0.44	0.60	-	98,98,98,98	0
56	MG	RA	3277	1/1	0.37	0.68	-	94,94,94,94	0
56	MG	YA	3281	1/1	0.87	0.93	-	60,60,60,60	0
56	MG	QO	101	1/1	0.46	0.66	-	79,79,79,79	0
56	MG	YA	3365	1/1	0.87	0.41	-	48,48,48,48	0
56	MG	YA	3455	1/1	0.76	0.54	-	79,79,79,79	0
56	MG	RA	3680	1/1	0.92	0.53	-	46,46,46,46	0
56	MG	RB	220	1/1	0.94	0.51	-	47,47,47,47	0
56	MG	YA	3622	1/1	0.91	0.51	-	49,49,49,49	0
56	MG	YA	3237	1/1	0.76	0.68	-	69,69,69,69	0
56	MG	RA	3909	1/1	0.76	0.73	-	73,73,73,73	0
56	MG	QA	1737	1/1	0.69	0.91	-	72,72,72,72	0
56	MG	RA	3575	1/1	0.89	0.38	-	62,62,62,62	0
56	MG	RQ	203	1/1	0.70	0.69	-	82,82,82,82	0
56	MG	RA	3673	1/1	0.97	0.41	-	45,45,45,45	0
56	MG	QA	1791	1/1	0.17	0.83	-	96,96,96,96	0
56	MG	QA	1700	1/1	0.77	0.44	-	66,66,66,66	0
56	MG	RA	4011	1/1	0.77	0.64	-	83,83,83,83	0
56	MG	YA	3258	1/1	0.89	0.36	-	68,68,68,68	0
56	MG	RA	3102	1/1	0.72	0.85	-	107,107,107,107	0
56	MG	YA	3557	1/1	0.72	0.73	-	67,67,67,67	0
56	MG	YA	3731	1/1	0.94	0.30	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1649	1/1	0.93	0.18	-	50,50,50,50	0
56	MG	YA	3333	1/1	0.95	0.64	-	26,26,26,26	0
56	MG	YA	3393	1/1	0.88	0.20	-	66,66,66,66	0
56	MG	RA	3595	1/1	0.74	0.41	-	84,84,84,84	0
56	MG	YA	3318	1/1	0.98	0.41	-	26,26,26,26	0
56	MG	RA	3200	1/1	0.73	0.41	-	99,99,99,99	0
56	MG	QA	1823	1/1	0.49	0.60	-	70,70,70,70	0
56	MG	YA	3437	1/1	0.39	0.84	-	85,85,85,85	0
56	MG	RB	204	1/1	0.93	0.17	-	71,71,71,71	0
56	MG	YA	3386	1/1	0.96	0.55	-	23,23,23,23	0
56	MG	RA	3990	1/1	0.96	0.35	-	109,109,109,109	0
56	MG	YA	3435	1/1	0.91	0.49	-	36,36,36,36	0
56	MG	QA	1825	1/1	0.86	0.39	-	74,74,74,74	0
56	MG	YA	3411	1/1	0.90	0.26	-	83,83,83,83	0
56	MG	XA	1675	1/1	0.32	0.73	-	82,82,82,82	0
56	MG	YA	3370	1/1	0.37	0.30	-	67,67,67,67	0
56	MG	YA	3107	1/1	0.33	0.65	-	80,80,80,80	0
56	MG	RA	3426	1/1	0.74	0.47	-	88,88,88,88	0
56	MG	RA	3139	1/1	0.87	0.28	-	72,72,72,72	0
56	MG	RA	3316	1/1	0.43	0.57	-	84,84,84,84	0
56	MG	YA	3105	1/1	0.86	0.39	-	37,37,37,37	0
56	MG	RA	3253	1/1	0.88	0.29	-	66,66,66,66	0
56	MG	RA	3715	1/1	0.87	0.41	-	76,76,76,76	0
56	MG	YB	215	1/1	0.85	0.22	-	92,92,92,92	0
56	MG	RD	303	1/1	0.89	0.28	-	41,41,41,41	0
56	MG	RA	3404	1/1	0.84	0.24	-	81,81,81,81	0
56	MG	XA	1692	1/1	0.09	0.77	-	75,75,75,75	0
56	MG	RA	3311	1/1	0.55	0.43	-	100,100,100,100	0
56	MG	XA	1723	1/1	0.49	0.28	-	75,75,75,75	0
56	MG	RA	3497	1/1	0.51	0.33	-	82,82,82,82	0
56	MG	RA	3800	1/1	-0.07	0.46	-	102,102,102,102	0
56	MG	XA	1708	1/1	0.73	0.38	-	78,78,78,78	0
56	MG	YB	213	1/1	0.85	0.40	-	57,57,57,57	0
56	MG	YA	3573	1/1	0.91	0.64	-	38,38,38,38	0
56	MG	RV	201	1/1	0.09	0.64	-	110,110,110,110	0
56	MG	XA	1624	1/1	0.52	0.61	-	76,76,76,76	0
56	MG	YB	218	1/1	0.29	0.40	-	80,80,80,80	0
56	MG	YA	3231	1/1	0.91	0.29	-	59,59,59,59	0
56	MG	RA	3545	1/1	0.75	0.51	-	70,70,70,70	0
56	MG	YA	3474	1/1	0.81	0.37	-	72,72,72,72	0
56	MG	YA	3420	1/1	0.92	0.46	-	39,39,39,39	0
56	MG	YA	3687	1/1	0.85	0.21	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1752	1/1	0.83	0.24	-	77,77,77,77	0
56	MG	YA	3072	1/1	0.90	0.37	-	99,99,99,99	0
56	MG	RA	3182	1/1	0.83	0.50	-	85,85,85,85	0
56	MG	YA	3205	1/1	0.81	0.29	-	58,58,58,58	0
56	MG	YA	3471	1/1	0.92	0.61	-	58,58,58,58	0
56	MG	RA	3254	1/1	0.84	0.30	-	92,92,92,92	0
56	MG	RB	202	1/1	0.83	0.14	-	55,55,55,55	0
56	MG	YA	3689	1/1	0.92	0.44	-	67,67,67,67	0
56	MG	YA	3245	1/1	0.93	0.56	-	107,107,107,107	0
56	MG	RG	203	1/1	0.77	0.37	-	79,79,79,79	0
56	MG	YB	203	1/1	0.84	0.14	-	72,72,72,72	0
56	MG	RA	3155	1/1	0.90	0.51	-	78,78,78,78	0
56	MG	RA	3047	1/1	0.96	0.10	-	12,12,12,12	0
56	MG	QA	1829	1/1	-0.01	0.94	-	94,94,94,94	0
56	MG	RA	3959	1/1	0.84	0.26	-	43,43,43,43	0
56	MG	YA	3463	1/1	0.85	0.23	-	47,47,47,47	0
56	MG	RA	3488	1/1	0.68	0.31	-	57,57,57,57	0
56	MG	QA	1862	1/1	0.64	0.50	-	101,101,101,101	0
56	MG	RA	3266	1/1	0.88	0.40	-	74,74,74,74	0
56	MG	RA	3847	1/1	0.61	0.45	-	102,102,102,102	0
56	MG	XA	1607	1/1	0.80	0.38	-	47,47,47,47	0
56	MG	RA	3219	1/1	0.89	0.20	-	66,66,66,66	0
56	MG	RA	3872	1/1	0.75	0.65	-	78,78,78,78	0
56	MG	RA	3439	1/1	0.41	0.71	-	89,89,89,89	0
56	MG	QA	1787	1/1	0.39	0.71	-	76,76,76,76	0
56	MG	YA	3578	1/1	0.40	0.88	-	95,95,95,95	0
56	MG	RA	3945	1/1	0.99	0.47	-	25,25,25,25	0
56	MG	YA	3598	1/1	0.91	0.47	-	49,49,49,49	0
56	MG	RA	3232	1/1	0.89	0.75	-	57,57,57,57	0
56	MG	YA	3601	1/1	0.97	0.60	-	29,29,29,29	0
56	MG	RA	3010	1/1	0.94	0.28	-	50,50,50,50	0
56	MG	RA	3787	1/1	0.14	1.12	-	105,105,105,105	0
56	MG	YA	3221	1/1	0.86	0.34	-	77,77,77,77	0
56	MG	RA	3137	1/1	0.96	0.80	-	97,97,97,97	0
56	MG	XA	1727	1/1	0.47	0.44	-	84,84,84,84	0
56	MG	RA	3777	1/1	0.87	0.45	-	93,93,93,93	0
56	MG	YA	3144	1/1	0.95	0.34	-	57,57,57,57	0
56	MG	RA	3953	1/1	0.58	0.30	-	86,86,86,86	0
56	MG	RA	3100	1/1	-0.13	1.07	-	93,93,93,93	0
56	MG	RA	3252	1/1	0.59	0.59	-	91,91,91,91	0
56	MG	YA	3183	1/1	0.81	0.36	-	47,47,47,47	0
56	MG	RA	3121	1/1	0.88	0.49	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YB	204	1/1	0.75	0.41	-	99,99,99,99	0
56	MG	RA	3998	1/1	0.15	0.88	-	87,87,87,87	0
56	MG	QA	1813	1/1	0.41	0.77	-	83,83,83,83	0
56	MG	RA	3895	1/1	0.95	0.67	-	54,54,54,54	0
56	MG	RA	3399	1/1	0.41	0.77	-	117,117,117,117	0
56	MG	YA	3657	1/1	0.90	0.60	-	34,34,34,34	0
56	MG	RA	3836	1/1	0.74	0.42	-	91,91,91,91	0
56	MG	QA	1630	1/1	0.49	0.64	-	81,81,81,81	0
56	MG	YA	3623	1/1	0.81	0.34	-	54,54,54,54	0
56	MG	RA	3237	1/1	0.48	0.52	-	100,100,100,100	0
56	MG	YA	3218	1/1	0.90	0.36	-	89,89,89,89	0
56	MG	QU	101	1/1	0.14	0.49	-	81,81,81,81	0
56	MG	RA	3764	1/1	0.82	0.48	-	60,60,60,60	0
56	MG	YA	3157	1/1	0.91	0.41	-	44,44,44,44	0
56	MG	RA	3989	1/1	0.95	0.30	-	39,39,39,39	0
56	MG	RA	3911	1/1	0.96	0.30	-	46,46,46,46	0
56	MG	YA	3312	1/1	0.73	0.41	-	73,73,73,73	0
56	MG	RA	3265	1/1	0.87	0.10	-	111,111,111,111	0
56	MG	YA	3108	1/1	0.48	0.48	-	98,98,98,98	0
56	MG	Y5	101	1/1	0.84	0.31	-	63,63,63,63	0
56	MG	QA	1705	1/1	0.85	0.27	-	37,37,37,37	0
56	MG	RA	4056	1/1	0.82	0.73	-	70,70,70,70	0
56	MG	XE	202	1/1	0.86	0.07	-	67,67,67,67	0
56	MG	YB	208	1/1	0.78	0.31	-	81,81,81,81	0
56	MG	RA	3782	1/1	0.03	0.60	-	94,94,94,94	0
56	MG	YA	3699	1/1	0.91	0.67	-	66,66,66,66	0
56	MG	RE	303	1/1	0.97	0.33	-	15,15,15,15	0
56	MG	RA	3641	1/1	0.77	0.57	-	65,65,65,65	0
56	MG	RA	3416	1/1	0.92	0.20	-	60,60,60,60	0
56	MG	YA	3477	1/1	0.78	0.52	-	70,70,70,70	0
56	MG	RA	3845	1/1	0.73	0.58	-	94,94,94,94	0
56	MG	YA	3599	1/1	0.76	0.41	-	70,70,70,70	0
56	MG	YA	3438	1/1	0.96	0.32	-	45,45,45,45	0
56	MG	RA	3972	1/1	0.89	0.43	-	81,81,81,81	0
56	MG	YA	3247	1/1	-0.23	0.92	-	106,106,106,106	0
56	MG	RA	3759	1/1	0.73	0.27	-	67,67,67,67	0
56	MG	QA	1632	1/1	0.77	0.76	-	70,70,70,70	0
56	MG	QA	1780	1/1	0.58	0.26	-	92,92,92,92	0
56	MG	YA	3118	1/1	0.90	0.38	-	91,91,91,91	0
56	MG	RA	3028	1/1	0.64	0.17	-	69,69,69,69	0
56	MG	RA	3319	1/1	0.83	0.71	-	54,54,54,54	0
56	MG	QA	1730	1/1	0.91	0.30	-	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	YD	301	1/1	0.72	0.67	-	60,60,60,60	0
56	MG	RA	3779	1/1	0.90	0.23	-	86,86,86,86	0
56	MG	YA	3495	1/1	0.92	0.56	-	63,63,63,63	0
56	MG	RA	3624	1/1	0.98	0.23	-	38,38,38,38	0
56	MG	R1	101	1/1	0.69	0.65	-	82,82,82,82	0
56	MG	YA	3276	1/1	0.96	0.60	-	67,67,67,67	0
56	MG	XA	1753	1/1	0.53	0.69	-	99,99,99,99	0
56	MG	XA	1660	1/1	0.39	0.39	-	99,99,99,99	0
56	MG	RA	3120	1/1	0.88	0.24	-	63,63,63,63	0
56	MG	RA	3551	1/1	0.91	0.30	-	72,72,72,72	0
56	MG	RA	3842	1/1	0.76	0.40	-	72,72,72,72	0
56	MG	YA	3196	1/1	0.88	0.35	-	109,109,109,109	0
56	MG	QA	1741	1/1	0.76	0.56	-	45,45,45,45	0
56	MG	YA	3722	1/1	0.27	0.49	-	89,89,89,89	0
56	MG	RA	4053	1/1	0.79	0.80	-	74,74,74,74	0
56	MG	RA	3805	1/1	0.79	0.31	-	98,98,98,98	0
56	MG	RA	3224	1/1	0.64	0.55	-	96,96,96,96	0
56	MG	RW	202	1/1	0.69	0.42	-	89,89,89,89	0
56	MG	YA	3036	1/1	0.89	0.31	-	55,55,55,55	0
56	MG	YA	3402	1/1	0.90	0.51	-	32,32,32,32	0
56	MG	YA	3619	1/1	0.96	0.20	-	38,38,38,38	0
56	MG	YA	3201	1/1	0.68	0.33	-	87,87,87,87	0
56	MG	QA	1836	1/1	0.60	0.44	-	89,89,89,89	0
56	MG	QA	1662	1/1	0.68	0.51	-	82,82,82,82	0
56	MG	RA	3943	1/1	0.82	0.33	-	86,86,86,86	0
56	MG	XA	1664	1/1	0.59	0.29	-	67,67,67,67	0
56	MG	RA	3592	1/1	0.83	0.57	-	56,56,56,56	0
56	MG	YA	3446	1/1	0.63	0.61	-	71,71,71,71	0
56	MG	RA	3175	1/1	0.84	0.51	-	70,70,70,70	0
56	MG	Y1	101	1/1	0.53	1.05	-	104,104,104,104	0
56	MG	RA	3361	1/1	0.67	0.34	-	76,76,76,76	0
56	MG	RA	3046	1/1	0.91	0.68	-	68,68,68,68	0
56	MG	YA	3743	1/1	0.97	0.40	-	43,43,43,43	0
56	MG	RA	3784	1/1	0.78	0.31	-	94,94,94,94	0
56	MG	RA	3837	1/1	0.91	0.22	-	59,59,59,59	0
56	MG	RA	3844	1/1	0.87	0.44	-	113,113,113,113	0
56	MG	YA	3565	1/1	0.30	0.78	-	85,85,85,85	0
56	MG	RA	3980	1/1	0.88	0.34	-	49,49,49,49	0
56	MG	YA	3168	1/1	0.86	0.39	-	88,88,88,88	0
56	MG	RA	3127	1/1	0.98	0.42	-	52,52,52,52	0
56	MG	RA	3557	1/1	0.81	0.42	-	63,63,63,63	0
56	MG	RA	3227	1/1	0.73	0.53	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3368	1/1	0.78	1.34	-	76,76,76,76	0
56	MG	RA	3350	1/1	0.89	0.11	-	65,65,65,65	0
56	MG	RA	3646	1/1	0.66	0.69	-	92,92,92,92	0
56	MG	YA	3639	1/1	0.92	0.65	-	74,74,74,74	0
56	MG	XA	1786	1/1	0.77	0.24	-	72,72,72,72	0
56	MG	QA	1781	1/1	0.96	0.42	-	54,54,54,54	0
56	MG	YA	3208	1/1	0.63	1.12	-	60,60,60,60	0
56	MG	RA	3074	1/1	0.85	0.28	-	52,52,52,52	0
56	MG	RA	3961	1/1	0.22	1.07	-	114,114,114,114	0
56	MG	RA	3834	1/1	0.65	0.40	-	80,80,80,80	0
56	MG	YA	3690	1/1	0.95	0.30	-	31,31,31,31	0
56	MG	RA	3446	1/1	0.66	1.11	-	63,63,63,63	0
56	MG	YA	3481	1/1	0.76	0.50	-	77,77,77,77	0
56	MG	XA	1662	1/1	0.57	0.22	-	80,80,80,80	0
56	MG	RA	3373	1/1	0.87	0.53	-	44,44,44,44	0
56	MG	RA	3065	1/1	0.51	0.59	-	89,89,89,89	0
56	MG	YA	3649	1/1	0.84	0.35	-	60,60,60,60	0
56	MG	YA	3674	1/1	0.86	0.59	-	74,74,74,74	0
56	MG	RA	3325	1/1	0.96	0.32	-	42,42,42,42	0
56	MG	YA	3199	1/1	0.93	0.64	-	102,102,102,102	0
56	MG	YA	3643	1/1	0.95	0.63	-	36,36,36,36	0
56	MG	RA	3906	1/1	0.97	0.30	-	20,20,20,20	0
56	MG	QG	201	1/1	0.80	0.88	-	91,91,91,91	0
56	MG	YA	3359	1/1	0.71	0.15	-	72,72,72,72	0
56	MG	YA	3257	1/1	0.87	0.21	-	84,84,84,84	0
56	MG	RA	3883	1/1	0.82	0.34	-	93,93,93,93	0
56	MG	YA	3080	1/1	0.76	0.38	-	80,80,80,80	0
56	MG	QA	1877	1/1	0.90	0.38	-	94,94,94,94	0
56	MG	YA	3373	1/1	0.89	0.38	-	41,41,41,41	0
56	MG	YA	3034	1/1	0.85	0.28	-	68,68,68,68	0
56	MG	YA	3658	1/1	0.45	0.27	-	77,77,77,77	0
56	MG	QA	1806	1/1	0.88	0.17	-	73,73,73,73	0
56	MG	RA	3459	1/1	0.65	0.52	-	78,78,78,78	0
56	MG	YB	201	1/1	0.53	0.52	-	89,89,89,89	0
56	MG	QA	1820	1/1	0.75	0.19	-	79,79,79,79	0
56	MG	RA	3821	1/1	0.97	0.48	-	29,29,29,29	0
56	MG	RA	3293	1/1	0.79	0.21	-	128,128,128,128	0
56	MG	RA	3436	1/1	0.75	0.93	-	56,56,56,56	0
56	MG	XA	1659	1/1	0.96	0.14	-	75,75,75,75	0
56	MG	RA	3099	1/1	0.71	0.31	-	102,102,102,102	0
56	MG	YA	3563	1/1	0.94	0.75	-	76,76,76,76	0
56	MG	XA	1704	1/1	0.36	0.32	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1864	1/1	0.75	0.58	-	90,90,90,90	0
56	MG	YA	3531	1/1	0.29	0.32	-	66,66,66,66	0
56	MG	RA	3255	1/1	0.97	0.57	-	100,100,100,100	0
56	MG	YA	3278	1/1	0.91	0.24	-	38,38,38,38	0
56	MG	YA	3088	1/1	0.80	0.32	-	42,42,42,42	0
56	MG	RA	3950	1/1	0.32	0.80	-	87,87,87,87	0
56	MG	RA	3366	1/1	0.67	0.35	-	72,72,72,72	0
56	MG	YA	3121	1/1	0.92	0.70	-	47,47,47,47	0
56	MG	RA	3823	1/1	0.52	0.51	-	97,97,97,97	0
56	MG	YA	3077	1/1	0.91	0.28	-	35,35,35,35	0
56	MG	QA	1749	1/1	0.61	0.94	-	56,56,56,56	0
56	MG	YA	3054	1/1	0.94	0.11	-	27,27,27,27	0
56	MG	XA	1669	1/1	-0.04	0.93	-	103,103,103,103	0
56	MG	YA	3251	1/1	0.76	0.38	-	100,100,100,100	0
56	MG	RA	3310	1/1	0.94	0.59	-	96,96,96,96	0
56	MG	YA	3075	1/1	0.78	0.40	-	43,43,43,43	0
56	MG	YA	3715	1/1	0.72	0.71	-	58,58,58,58	0
56	MG	RA	3186	1/1	0.83	0.33	-	77,77,77,77	0
56	MG	QA	1839	1/1	-0.16	0.48	-	93,93,93,93	0
56	MG	RA	3440	1/1	0.88	0.47	-	57,57,57,57	0
56	MG	YA	3293	1/1	0.84	1.21	-	70,70,70,70	0
56	MG	YA	3018	1/1	0.71	0.44	-	75,75,75,75	0
56	MG	YA	3682	1/1	0.91	0.33	-	37,37,37,37	0
56	MG	RA	3685	1/1	0.85	0.48	-	97,97,97,97	0
56	MG	XA	1729	1/1	0.88	0.24	-	58,58,58,58	0
56	MG	QA	1648	1/1	0.79	0.20	-	67,67,67,67	0
56	MG	RA	3486	1/1	0.88	0.40	-	78,78,78,78	0
56	MG	RA	3876	1/1	0.96	0.69	-	54,54,54,54	0
56	MG	RA	3524	1/1	0.49	0.63	-	71,71,71,71	0
56	MG	XA	1777	1/1	0.86	0.58	-	98,98,98,98	0
56	MG	RA	3924	1/1	0.63	0.48	-	65,65,65,65	0
56	MG	QA	1807	1/1	0.78	0.31	-	65,65,65,65	0
56	MG	YA	3469	1/1	0.85	0.35	-	88,88,88,88	0
56	MG	YA	3638	1/1	0.86	0.33	-	65,65,65,65	0
56	MG	RA	3498	1/1	0.86	0.46	-	58,58,58,58	0
56	MG	RA	3214	1/1	0.91	0.47	-	59,59,59,59	0
56	MG	YA	3066	1/1	0.95	0.28	-	50,50,50,50	0
56	MG	QA	1681	1/1	-0.01	1.05	-	85,85,85,85	0
56	MG	QA	1716	1/1	0.93	0.14	-	81,81,81,81	0
56	MG	QA	1674	1/1	0.35	0.39	-	85,85,85,85	0
56	MG	Y8	102	1/1	0.94	0.48	-	41,41,41,41	0
56	MG	RA	3868	1/1	0.70	0.44	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3143	1/1	0.98	0.10	-	56,56,56,56	0
56	MG	RA	3799	1/1	0.87	0.42	-	54,54,54,54	0
56	MG	YA	3466	1/1	0.53	0.53	-	80,80,80,80	0
56	MG	QE	202	1/1	0.29	0.61	-	91,91,91,91	0
56	MG	QA	1776	1/1	0.71	0.37	-	80,80,80,80	0
56	MG	RB	217	1/1	0.62	0.81	-	94,94,94,94	0
56	MG	XA	1670	1/1	0.95	0.32	-	80,80,80,80	0
56	MG	YA	3409	1/1	0.52	0.28	-	120,120,120,120	0
56	MG	YA	3703	1/1	0.92	0.39	-	35,35,35,35	0
56	MG	XA	1679	1/1	0.95	0.41	-	52,52,52,52	0
56	MG	QA	1663	1/1	0.91	0.20	-	73,73,73,73	0
56	MG	YA	3099	1/1	0.38	0.63	-	106,106,106,106	0
56	MG	RA	3590	1/1	0.17	0.89	-	104,104,104,104	0
56	MG	YA	3696	1/1	0.96	0.38	-	17,17,17,17	0
56	MG	RA	3818	1/1	0.61	0.65	-	67,67,67,67	0
56	MG	YA	3745	1/1	0.71	0.66	-	67,67,67,67	0
56	MG	RA	3060	1/1	0.96	0.14	-	21,21,21,21	0
56	MG	RA	3544	1/1	0.44	0.76	-	78,78,78,78	0
56	MG	RA	3493	1/1	0.93	0.43	-	60,60,60,60	0
56	MG	YA	3356	1/1	0.94	0.36	-	50,50,50,50	0
56	MG	YA	3426	1/1	0.79	0.52	-	50,50,50,50	0
56	MG	RA	3617	1/1	0.49	0.54	-	83,83,83,83	0
56	MG	XA	1776	1/1	0.94	0.56	-	61,61,61,61	0
56	MG	YA	3207	1/1	0.93	0.35	-	70,70,70,70	0
56	MG	RA	3626	1/1	0.81	0.43	-	68,68,68,68	0
56	MG	RA	3202	1/1	0.63	0.62	-	92,92,92,92	0
56	MG	YA	3011	1/1	0.96	0.21	-	40,40,40,40	0
56	MG	RA	3162	1/1	0.59	1.07	-	72,72,72,72	0
56	MG	RA	4012	1/1	0.81	0.79	-	89,89,89,89	0
56	MG	RA	3334	1/1	0.96	0.37	-	46,46,46,46	0
56	MG	RA	3055	1/1	0.83	0.53	-	85,85,85,85	0
56	MG	RA	3768	1/1	0.54	0.85	-	76,76,76,76	0
56	MG	QA	1835	1/1	0.31	0.75	-	89,89,89,89	0
56	MG	RA	3153	1/1	0.94	0.12	-	35,35,35,35	0
56	MG	RQ	202	1/1	0.88	0.34	-	51,51,51,51	0
56	MG	RA	3830	1/1	0.96	0.17	-	66,66,66,66	0
56	MG	RA	3272	1/1	0.59	0.34	-	83,83,83,83	0
56	MG	YA	3229	1/1	0.82	0.34	-	71,71,71,71	0
56	MG	RA	4027	1/1	0.97	0.36	-	39,39,39,39	0
56	MG	QA	1793	1/1	0.59	1.19	-	82,82,82,82	0
56	MG	XA	1741	1/1	0.80	0.23	-	67,67,67,67	0
56	MG	XA	1616	1/1	0.66	1.74	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3083	1/1	0.64	0.44	-	99,99,99,99	0
56	MG	RA	3336	1/1	0.77	0.30	-	66,66,66,66	0
56	MG	RA	3292	1/1	0.97	0.10	-	83,83,83,83	0
56	MG	YA	3717	1/1	0.83	0.41	-	45,45,45,45	0
56	MG	XA	1703	1/1	0.40	0.67	-	60,60,60,60	0
56	MG	XA	1693	1/1	0.43	0.51	-	81,81,81,81	0
56	MG	RA	3369	1/1	0.96	0.58	-	47,47,47,47	0
56	MG	YA	3408	1/1	0.93	0.37	-	17,17,17,17	0
56	MG	YA	3473	1/1	0.64	0.53	-	77,77,77,77	0
56	MG	XA	1606	1/1	0.94	0.12	-	95,95,95,95	0
56	MG	XA	1738	1/1	0.90	0.62	-	58,58,58,58	0
56	MG	RA	3963	1/1	0.55	2.00	-	110,110,110,110	0
56	MG	QV	101	1/1	0.60	0.64	-	118,118,118,118	0
56	MG	XA	1720	1/1	0.88	1.05	-	63,63,63,63	0
56	MG	RA	3521	1/1	0.69	0.40	-	81,81,81,81	0
56	MG	RA	3005	1/1	0.11	1.05	-	99,99,99,99	0
56	MG	QA	1828	1/1	0.97	0.24	-	41,41,41,41	0
56	MG	YA	3053	1/1	0.67	0.51	-	77,77,77,77	0
56	MG	YA	3419	1/1	0.61	0.47	-	66,66,66,66	0
56	MG	XA	1789	1/1	0.69	0.39	-	58,58,58,58	0
56	MG	RA	3081	1/1	0.72	0.54	-	91,91,91,91	0
56	MG	RA	3774	1/1	0.79	0.51	-	59,59,59,59	0
56	MG	YA	3369	1/1	0.48	0.17	-	63,63,63,63	0
56	MG	QA	1792	1/1	0.58	0.58	-	69,69,69,69	0
56	MG	QA	1718	1/1	0.64	0.75	-	82,82,82,82	0
56	MG	RA	3720	1/1	0.97	0.42	-	33,33,33,33	0
56	MG	YA	3738	1/1	0.58	0.54	-	68,68,68,68	0
56	MG	RA	3994	1/1	0.03	0.89	-	88,88,88,88	0
56	MG	QA	1728	1/1	0.49	0.31	-	64,64,64,64	0
56	MG	YA	3215	1/1	0.82	0.19	-	54,54,54,54	0
56	MG	RA	3655	1/1	0.97	0.30	-	25,25,25,25	0
56	MG	XA	1671	1/1	-0.47	1.25	-	108,108,108,108	0
56	MG	QA	1604	1/1	0.82	0.23	-	75,75,75,75	0
56	MG	RA	3654	1/1	0.58	0.47	-	87,87,87,87	0
56	MG	YA	3603	1/1	0.49	0.53	-	100,100,100,100	0
56	MG	RA	3487	1/1	0.96	0.18	-	17,17,17,17	0
56	MG	YA	3545	1/1	0.43	0.43	-	99,99,99,99	0
56	MG	YA	3347	1/1	-0.11	0.26	-	99,99,99,99	0
56	MG	QA	1633	1/1	0.86	0.20	-	95,95,95,95	0
56	MG	RA	3262	1/1	0.93	0.59	-	80,80,80,80	0
56	MG	YA	3630	1/1	0.96	0.50	-	32,32,32,32	0
56	MG	QA	1694	1/1	0.88	0.36	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3189	1/1	0.94	0.28	-	96,96,96,96	0
56	MG	RA	3793	1/1	0.96	0.41	-	38,38,38,38	0
56	MG	YA	3364	1/1	0.79	0.43	-	67,67,67,67	0
56	MG	RA	3164	1/1	0.80	0.47	-	87,87,87,87	0
56	MG	RA	3052	1/1	0.90	0.23	-	85,85,85,85	0
56	MG	RA	3543	1/1	0.96	0.30	-	26,26,26,26	0
56	MG	RA	3403	1/1	0.95	0.35	-	25,25,25,25	0
56	MG	QA	1685	1/1	0.44	0.42	-	91,91,91,91	0
56	MG	YA	3552	1/1	0.82	0.70	-	52,52,52,52	0
56	MG	YA	3621	1/1	0.94	0.34	-	49,49,49,49	0
56	MG	QA	1615	1/1	0.79	0.25	-	107,107,107,107	0
56	MG	RA	3509	1/1	0.95	1.03	-	69,69,69,69	0
56	MG	YA	3675	1/1	0.97	0.30	-	29,29,29,29	0
56	MG	RA	3518	1/1	0.63	0.60	-	82,82,82,82	0
56	MG	QA	1717	1/1	0.96	0.53	-	29,29,29,29	0
56	MG	YA	3737	1/1	0.23	1.27	-	107,107,107,107	0
56	MG	RA	3929	1/1	0.94	0.23	-	65,65,65,65	0
56	MG	RA	3327	1/1	0.69	0.61	-	62,62,62,62	0
56	MG	XA	1665	1/1	0.79	0.29	-	73,73,73,73	0
56	MG	YA	3418	1/1	0.67	0.77	-	56,56,56,56	0
56	MG	RA	3614	1/1	0.97	0.42	-	32,32,32,32	0
56	MG	YA	3633	1/1	0.81	0.69	-	47,47,47,47	0
56	MG	YA	3398	1/1	0.93	0.22	-	25,25,25,25	0
56	MG	QV	102	1/1	0.89	0.38	-	45,45,45,45	0
56	MG	RA	3729	1/1	0.73	0.39	-	59,59,59,59	0
56	MG	QA	1746	1/1	0.72	0.23	-	65,65,65,65	0
56	MG	RA	3067	1/1	0.73	0.39	-	83,83,83,83	0
56	MG	RA	3556	1/1	0.48	0.68	-	75,75,75,75	0
56	MG	QA	1798	1/1	-0.41	1.43	-	119,119,119,119	0
56	MG	QA	1770	1/1	0.75	0.25	-	73,73,73,73	0
56	MG	YA	3665	1/1	0.93	0.38	-	31,31,31,31	0
56	MG	YA	3537	1/1	0.92	0.37	-	57,57,57,57	0
56	MG	RA	3747	1/1	0.36	0.57	-	96,96,96,96	0
56	MG	RF	307	1/1	0.89	0.29	-	65,65,65,65	0
56	MG	YA	3496	1/1	0.97	0.42	-	18,18,18,18	0
56	MG	YA	3560	1/1	0.98	0.21	-	6,6,6,6	0
56	MG	RA	3434	1/1	0.83	0.33	-	61,61,61,61	0
56	MG	RA	3012	1/1	0.92	0.19	-	53,53,53,53	0
56	MG	YA	3325	1/1	0.97	0.33	-	20,20,20,20	0
56	MG	QA	1651	1/1	0.85	0.62	-	89,89,89,89	0
56	MG	YA	3612	1/1	0.99	0.23	-	23,23,23,23	0
56	MG	RA	3942	1/1	0.09	0.90	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3464	1/1	0.56	0.67	-	73,73,73,73	0
56	MG	RA	3835	1/1	0.85	0.73	-	56,56,56,56	0
56	MG	RA	3223	1/1	0.92	0.64	-	63,63,63,63	0
56	MG	YA	3571	1/1	0.98	0.49	-	23,23,23,23	0
56	MG	YA	3104	1/1	0.87	0.55	-	85,85,85,85	0
56	MG	RA	3305	1/1	0.90	0.88	-	98,98,98,98	0
56	MG	YA	3670	1/1	0.97	0.35	-	12,12,12,12	0
56	MG	XA	1609	1/1	0.60	1.30	-	88,88,88,88	0
56	MG	YA	3230	1/1	0.86	0.58	-	57,57,57,57	0
56	MG	YA	3308	1/1	0.29	0.28	-	64,64,64,64	0
56	MG	RA	3133	1/1	0.87	0.29	-	79,79,79,79	0
56	MG	XA	1674	1/1	0.51	0.31	-	73,73,73,73	0
56	MG	YA	3388	1/1	0.95	0.26	-	33,33,33,33	0
56	MG	R4	102	1/1	0.43	0.38	-	88,88,88,88	0
56	MG	YA	3210	1/1	0.87	0.30	-	65,65,65,65	0
56	MG	YA	3631	1/1	0.98	0.12	-	55,55,55,55	0
56	MG	RA	4007	1/1	0.91	0.63	-	49,49,49,49	0
56	MG	RA	3585	1/1	0.83	0.53	-	59,59,59,59	0
56	MG	XA	1691	1/1	0.91	0.43	-	60,60,60,60	0
56	MG	RA	3429	1/1	0.17	0.21	-	89,89,89,89	0
56	MG	QD	301	1/1	0.30	1.54	-	90,90,90,90	0
56	MG	YA	3383	1/1	0.80	0.45	-	70,70,70,70	0
56	MG	XJ	201	1/1	0.50	0.15	-	97,97,97,97	0
56	MG	RA	3916	1/1	0.62	0.70	-	72,72,72,72	0
56	MG	R5	103	1/1	0.93	0.77	-	59,59,59,59	0
56	MG	QA	1878	1/1	0.29	1.20	-	108,108,108,108	0
56	MG	RA	3149	1/1	0.87	0.27	-	39,39,39,39	0
56	MG	YA	3006	1/1	0.96	0.13	-	18,18,18,18	0
56	MG	YA	3558	1/1	0.94	0.27	-	25,25,25,25	0
56	MG	XA	1666	1/1	0.57	0.76	-	63,63,63,63	0
56	MG	RA	3388	1/1	0.92	0.52	-	49,49,49,49	0
56	MG	RA	3108	1/1	0.94	0.54	-	69,69,69,69	0
56	MG	YA	3140	1/1	0.85	0.56	-	65,65,65,65	0
56	MG	YA	3113	1/1	0.99	0.20	-	104,104,104,104	0
56	MG	YA	3701	1/1	0.95	0.56	-	60,60,60,60	0
56	MG	QA	1733	1/1	0.52	0.78	-	60,60,60,60	0
56	MG	XA	1764	1/1	0.83	0.54	-	52,52,52,52	0
56	MG	YA	3500	1/1	0.73	0.96	-	53,53,53,53	0
56	MG	YA	3493	1/1	0.74	0.34	-	74,74,74,74	0
56	MG	QA	1814	1/1	0.29	0.56	-	97,97,97,97	0
56	MG	YA	3200	1/1	0.87	0.33	-	70,70,70,70	0
56	MG	QA	1723	1/1	0.88	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	YA	3506	1/1	0.84	0.35	-	53,53,53,53	0
56	MG	QA	1851	1/1	0.74	0.44	-	94,94,94,94	0
56	MG	RA	3480	1/1	0.95	0.47	-	42,42,42,42	0
56	MG	YA	3509	1/1	0.89	0.27	-	71,71,71,71	0
56	MG	RA	3221	1/1	0.83	0.57	-	63,63,63,63	0
56	MG	RA	3156	1/1	0.88	0.27	-	117,117,117,117	0
56	MG	RB	222	1/1	0.59	0.45	-	94,94,94,94	0
56	MG	YD	310	1/1	0.81	0.44	-	64,64,64,64	0
56	MG	RA	3931	1/1	0.89	0.27	-	73,73,73,73	0
56	MG	RA	3303	1/1	0.75	0.74	-	79,79,79,79	0
56	MG	RH	201	1/1	0.51	0.54	-	88,88,88,88	0
56	MG	QA	1617	1/1	0.94	0.35	-	61,61,61,61	0
56	MG	RA	3009	1/1	0.80	0.30	-	53,53,53,53	0
56	MG	QA	1861	1/1	0.48	0.92	-	75,75,75,75	0
56	MG	RA	3939	1/1	0.91	0.26	-	58,58,58,58	0
56	MG	QA	1679	1/1	0.91	0.20	-	64,64,64,64	0
56	MG	RF	302	1/1	0.57	0.73	-	73,73,73,73	0
56	MG	RA	3560	1/1	0.96	0.61	-	23,23,23,23	0
56	MG	RA	3947	1/1	0.97	0.20	-	20,20,20,20	0
56	MG	RA	3992	1/1	0.79	0.16	-	74,74,74,74	0
56	MG	QA	1664	1/1	0.36	0.90	-	92,92,92,92	0
56	MG	YA	3362	1/1	0.99	0.50	-	18,18,18,18	0
56	MG	RA	3235	1/1	0.94	0.31	-	70,70,70,70	0
56	MG	QA	1784	1/1	0.70	0.47	-	64,64,64,64	0
56	MG	RA	3285	1/1	0.51	0.65	-	85,85,85,85	0
56	MG	RA	3572	1/1	0.91	0.38	-	83,83,83,83	0
56	MG	XA	1602	1/1	0.92	0.28	-	86,86,86,86	0
56	MG	YA	3589	1/1	0.98	0.43	-	31,31,31,31	0
56	MG	QA	1810	1/1	0.86	0.41	-	69,69,69,69	0
56	MG	RA	3069	1/1	0.90	0.29	-	55,55,55,55	0
56	MG	RA	3087	1/1	0.87	0.60	-	99,99,99,99	0
56	MG	RA	3705	1/1	0.89	0.56	-	50,50,50,50	0
56	MG	QA	1670	1/1	0.80	0.52	-	81,81,81,81	0
56	MG	QA	1786	1/1	0.90	0.30	-	54,54,54,54	0
56	MG	RA	3359	1/1	0.97	0.31	-	32,32,32,32	0
56	MG	RA	3176	1/1	0.84	0.69	-	96,96,96,96	0
56	MG	YA	3128	1/1	0.86	0.20	-	26,26,26,26	0
56	MG	YA	3151	1/1	0.97	0.13	-	8,8,8,8	0
56	MG	YA	3476	1/1	0.85	0.54	-	52,52,52,52	0
56	MG	YA	3340	1/1	0.68	0.24	-	59,59,59,59	0
56	MG	XA	1657	1/1	0.87	0.42	-	65,65,65,65	0
56	MG	YA	3249	1/1	0.83	0.54	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3466	1/1	0.69	0.47	-	56,56,56,56	0
56	MG	QA	1607	1/1	0.75	0.23	-	71,71,71,71	0
56	MG	RA	3619	1/1	0.93	0.48	-	27,27,27,27	0
56	MG	YA	3585	1/1	0.92	0.42	-	75,75,75,75	0
56	MG	R3	101	1/1	0.52	1.02	-	95,95,95,95	0
56	MG	YA	3361	1/1	0.92	0.19	-	65,65,65,65	0
56	MG	RB	221	1/1	0.72	0.23	-	64,64,64,64	0
56	MG	XA	1623	1/1	0.67	0.78	-	73,73,73,73	0
56	MG	YA	3166	1/1	0.09	1.14	-	132,132,132,132	0
56	MG	YA	3617	1/1	0.95	0.29	-	17,17,17,17	0
56	MG	RA	3651	1/1	0.89	0.21	-	41,41,41,41	0
56	MG	RA	3879	1/1	0.97	0.35	-	29,29,29,29	0
56	MG	YA	3468	1/1	0.70	0.94	-	58,58,58,58	0
56	MG	YA	3487	1/1	0.94	0.71	-	46,46,46,46	0
56	MG	YA	3132	1/1	0.96	0.58	-	86,86,86,86	0
56	MG	YA	3710	1/1	0.85	0.54	-	61,61,61,61	0
56	MG	RA	3193	1/1	0.37	0.60	-	94,94,94,94	0
56	MG	RA	3734	1/1	0.82	0.59	-	70,70,70,70	0
56	MG	YA	3514	1/1	0.91	0.38	-	62,62,62,62	0
56	MG	YB	207	1/1	0.65	0.47	-	110,110,110,110	0
56	MG	YA	3624	1/1	0.74	0.42	-	71,71,71,71	0
56	MG	YA	3374	1/1	0.97	0.55	-	34,34,34,34	0
56	MG	RA	3140	1/1	0.87	0.78	-	93,93,93,93	0
56	MG	RA	3337	1/1	0.85	0.46	-	81,81,81,81	0
56	MG	YA	3553	1/1	0.82	0.47	-	58,58,58,58	0
56	MG	YA	3367	1/1	0.89	0.15	-	56,56,56,56	0
56	MG	YA	3732	1/1	0.86	1.04	-	73,73,73,73	0
56	MG	RA	3912	1/1	0.71	0.65	-	76,76,76,76	0
56	MG	YG	201	1/1	0.62	1.62	-	116,116,116,116	0
56	MG	YA	3330	1/1	0.66	0.52	-	62,62,62,62	0
56	MG	YA	3297	1/1	0.97	0.49	-	19,19,19,19	0
56	MG	RA	3908	1/1	0.97	0.41	-	22,22,22,22	0
56	MG	QA	1837	1/1	0.48	0.42	-	69,69,69,69	0
56	MG	YA	3064	1/1	0.90	0.41	-	55,55,55,55	0
56	MG	RA	3421	1/1	0.90	0.31	-	42,42,42,42	0
56	MG	RA	3283	1/1	0.54	0.60	-	101,101,101,101	0
56	MG	QA	1838	1/1	0.92	0.28	-	85,85,85,85	0
56	MG	RA	3516	1/1	0.97	0.43	-	13,13,13,13	0
56	MG	YA	3423	1/1	0.89	0.65	-	59,59,59,59	0
56	MG	RZ	301	1/1	0.41	0.33	-	66,66,66,66	0
56	MG	RA	3890	1/1	0.68	0.82	-	57,57,57,57	0
56	MG	YA	3242	1/1	0.82	0.29	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	R5	104	1/1	0.87	0.63	-	67,67,67,67	0
56	MG	YA	3152	1/1	0.96	0.25	-	50,50,50,50	0
56	MG	RA	3208	1/1	0.74	0.35	-	70,70,70,70	0
56	MG	RA	3871	1/1	0.54	0.49	-	77,77,77,77	0
56	MG	XA	1760	1/1	0.82	0.30	-	71,71,71,71	0
56	MG	RA	3833	1/1	0.98	0.40	-	29,29,29,29	0
56	MG	QA	1775	1/1	0.78	0.47	-	72,72,72,72	0
56	MG	RA	3071	1/1	0.93	0.62	-	63,63,63,63	0
56	MG	RA	4002	1/1	0.62	0.31	-	83,83,83,83	0
56	MG	RA	3194	1/1	0.96	0.28	-	67,67,67,67	0
56	MG	YA	3313	1/1	0.91	0.82	-	46,46,46,46	0
56	MG	RA	3322	1/1	0.16	0.88	-	90,90,90,90	0
56	MG	RA	3297	1/1	0.85	0.15	-	39,39,39,39	0
56	MG	RA	3004	1/1	0.96	0.10	-	29,29,29,29	0
56	MG	RF	312	1/1	0.76	0.48	-	62,62,62,62	0
56	MG	RA	3748	1/1	0.84	0.22	-	61,61,61,61	0
56	MG	RA	3269	1/1	0.89	0.28	-	74,74,74,74	0
56	MG	RA	3993	1/1	0.75	0.45	-	86,86,86,86	0
56	MG	YA	3259	1/1	0.86	0.31	-	66,66,66,66	0
56	MG	YA	3709	1/1	0.92	0.86	-	58,58,58,58	0
56	MG	RA	3217	1/1	0.57	0.35	-	88,88,88,88	0
56	MG	RA	3540	1/1	0.74	0.26	-	73,73,73,73	0
56	MG	RA	3174	1/1	0.83	0.29	-	62,62,62,62	0
56	MG	RA	3826	1/1	0.81	0.28	-	62,62,62,62	0
56	MG	YA	3226	1/1	0.78	0.44	-	75,75,75,75	0
56	MG	RA	3970	1/1	0.93	0.37	-	31,31,31,31	0
56	MG	RA	3151	1/1	0.89	0.60	-	59,59,59,59	0
56	MG	RA	3158	1/1	0.85	0.35	-	67,67,67,67	0
56	MG	YA	3741	1/1	0.97	0.29	-	57,57,57,57	0
56	MG	RA	3260	1/1	0.88	0.99	-	71,71,71,71	0
56	MG	QA	1777	1/1	0.92	0.19	-	81,81,81,81	0
56	MG	RA	3791	1/1	0.69	0.31	-	64,64,64,64	0
56	MG	YB	211	1/1	0.59	0.34	-	70,70,70,70	0
56	MG	Y0	101	1/1	0.64	0.85	-	65,65,65,65	0
56	MG	RW	201	1/1	0.87	0.33	-	64,64,64,64	0
56	MG	RA	3173	1/1	0.77	0.35	-	50,50,50,50	0
56	MG	RA	3539	1/1	0.87	0.54	-	39,39,39,39	0
56	MG	YA	3739	1/1	0.98	0.47	-	79,79,79,79	0
56	MG	YA	3316	1/1	0.93	0.47	-	53,53,53,53	0
56	MG	RA	3669	1/1	0.25	0.61	-	81,81,81,81	0
56	MG	QA	1796	1/1	0.63	0.43	-	73,73,73,73	0
56	MG	RA	3788	1/1	0.67	0.10	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3490	1/1	0.66	0.51	-	104,104,104,104	0
56	MG	RA	3456	1/1	0.72	0.21	-	58,58,58,58	0
56	MG	RA	3864	1/1	0.96	0.79	-	76,76,76,76	0
56	MG	QA	1804	1/1	0.69	0.39	-	71,71,71,71	0
56	MG	QA	1735	1/1	0.04	0.69	-	107,107,107,107	0
56	MG	RA	3564	1/1	0.61	0.59	-	101,101,101,101	0
56	MG	RA	3278	1/1	0.84	0.67	-	83,83,83,83	0
56	MG	QA	1769	1/1	0.10	0.54	-	95,95,95,95	0
56	MG	QA	1740	1/1	0.97	0.34	-	55,55,55,55	0
56	MG	YA	3456	1/1	0.61	0.66	-	68,68,68,68	0
56	MG	RA	3345	1/1	0.97	0.46	-	20,20,20,20	0
56	MG	RA	3013	1/1	0.80	0.54	-	71,71,71,71	0
56	MG	RA	3739	1/1	0.90	0.31	-	78,78,78,78	0
56	MG	XA	1713	1/1	0.76	0.24	-	49,49,49,49	0
56	MG	RA	3903	1/1	0.74	0.28	-	57,57,57,57	0
56	MG	RA	3215	1/1	0.83	0.40	-	98,98,98,98	0
56	MG	RA	3635	1/1	0.68	0.30	-	112,112,112,112	0
56	MG	RA	3096	1/1	0.92	0.17	-	48,48,48,48	0
56	MG	YB	209	1/1	0.22	1.01	-	102,102,102,102	0
56	MG	QA	1866	1/1	0.40	1.84	-	89,89,89,89	0
56	MG	RA	3932	1/1	0.94	0.61	-	61,61,61,61	0
56	MG	QA	1608	1/1	0.71	0.68	-	110,110,110,110	0
56	MG	YA	3194	1/1	0.88	0.32	-	70,70,70,70	0
56	MG	YA	3376	1/1	0.90	0.16	-	58,58,58,58	0
56	MG	XA	1667	1/1	0.94	0.32	-	77,77,77,77	0
56	MG	YA	3484	1/1	0.96	0.34	-	21,21,21,21	0
56	MG	RA	3894	1/1	0.96	0.48	-	23,23,23,23	0
56	MG	YA	3431	1/1	0.61	0.59	-	57,57,57,57	0
56	MG	RA	3320	1/1	0.98	0.37	-	14,14,14,14	0
56	MG	YA	3049	1/1	0.93	0.31	-	78,78,78,78	0
56	MG	YA	3284	1/1	0.97	0.23	-	8,8,8,8	0
56	MG	RA	3985	1/1	0.41	0.68	-	81,81,81,81	0
56	MG	RA	3286	1/1	0.93	0.46	-	118,118,118,118	0
56	MG	YA	3647	1/1	0.96	0.49	-	27,27,27,27	0
56	MG	RA	3663	1/1	0.75	0.49	-	77,77,77,77	0
56	MG	YA	3004	1/1	0.96	0.14	-	43,43,43,43	0
56	MG	RA	3574	1/1	0.78	0.34	-	62,62,62,62	0
56	MG	RA	3979	1/1	0.96	0.20	-	37,37,37,37	0
56	MG	QA	1712	1/1	0.61	0.56	-	87,87,87,87	0
56	MG	QA	1659	1/1	0.90	1.38	-	84,84,84,84	0
56	MG	QQ	201	1/1	0.85	0.20	-	71,71,71,71	0
56	MG	RA	3048	1/1	0.67	0.32	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3051	1/1	0.63	0.60	-	83,83,83,83	0
56	MG	RA	3275	1/1	0.71	0.46	-	72,72,72,72	0
56	MG	RA	3192	1/1	0.92	0.75	-	92,92,92,92	0
56	MG	YA	3095	1/1	0.76	0.17	-	68,68,68,68	0
56	MG	RA	3693	1/1	0.80	0.38	-	67,67,67,67	0
56	MG	RT	203	1/1	0.14	0.50	-	88,88,88,88	0
56	MG	YA	3008	1/1	0.91	0.20	-	47,47,47,47	0
56	MG	QA	1689	1/1	0.81	0.50	-	80,80,80,80	0
56	MG	YA	3262	1/1	0.38	0.68	-	88,88,88,88	0
56	MG	RA	3896	1/1	0.75	0.75	-	59,59,59,59	0
56	MG	YA	3211	1/1	0.58	0.53	-	89,89,89,89	0
56	MG	QA	1822	1/1	0.71	0.56	-	65,65,65,65	0
56	MG	YA	3505	1/1	0.70	0.97	-	88,88,88,88	0
56	MG	YA	3263	1/1	0.83	0.58	-	81,81,81,81	0
56	MG	RA	3719	1/1	0.78	0.39	-	55,55,55,55	0
56	MG	RA	3925	1/1	0.88	0.28	-	83,83,83,83	0
56	MG	QA	1609	1/1	0.66	0.60	-	106,106,106,106	0
56	MG	YA	3232	1/1	0.48	0.37	-	104,104,104,104	0
56	MG	QA	1701	1/1	0.88	0.79	-	50,50,50,50	0
56	MG	YA	3292	1/1	0.85	0.75	-	81,81,81,81	0
56	MG	RA	3379	1/1	0.96	0.47	-	44,44,44,44	0
56	MG	YA	3645	1/1	0.89	0.62	-	67,67,67,67	0
56	MG	RA	3935	1/1	-0.02	0.51	-	91,91,91,91	0
56	MG	RA	3666	1/1	0.91	0.98	-	69,69,69,69	0
56	MG	RA	3450	1/1	0.86	1.24	-	53,53,53,53	0
56	MG	RA	3638	1/1	0.73	0.37	-	85,85,85,85	0
56	MG	RA	3949	1/1	0.39	0.67	-	80,80,80,80	0
56	MG	YA	3103	1/1	0.62	0.25	-	63,63,63,63	0
56	MG	QA	1652	1/1	0.32	0.62	-	83,83,83,83	0
56	MG	YI	201	1/1	0.81	0.34	-	110,110,110,110	0
56	MG	RA	3238	1/1	0.95	0.38	-	106,106,106,106	0
56	MG	RA	3694	1/1	0.43	0.53	-	107,107,107,107	0
56	MG	QA	1601	1/1	-0.53	0.53	-	129,129,129,129	0
56	MG	RA	3537	1/1	0.45	0.61	-	93,93,93,93	0
56	MG	RA	3019	1/1	0.83	0.27	-	113,113,113,113	0
56	MG	XA	1714	1/1	0.80	0.20	-	58,58,58,58	0
56	MG	RA	3741	1/1	0.72	0.21	-	61,61,61,61	0
56	MG	RA	3852	1/1	0.96	0.35	-	47,47,47,47	0
56	MG	YA	3357	1/1	0.90	0.30	-	39,39,39,39	0
56	MG	RA	3682	1/1	0.71	0.37	-	81,81,81,81	0
56	MG	QA	1783	1/1	0.54	0.21	-	77,77,77,77	0
56	MG	RA	3700	1/1	0.89	0.23	-	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	RA	3502	1/1	0.98	0.31	-	20,20,20,20	0
56	MG	QA	1653	1/1	0.60	0.42	-	85,85,85,85	0
56	MG	RA	3189	1/1	0.96	0.24	-	39,39,39,39	0
56	MG	YA	3082	1/1	0.93	0.26	-	78,78,78,78	0
56	MG	RA	3171	1/1	0.65	0.51	-	89,89,89,89	0
56	MG	RA	3865	1/1	0.93	0.49	-	51,51,51,51	0
56	MG	RA	3699	1/1	0.41	1.14	-	98,98,98,98	0
56	MG	YQ	202	1/1	0.83	0.37	-	59,59,59,59	0
56	MG	YA	3046	1/1	0.87	0.38	-	75,75,75,75	0
56	MG	RA	3222	1/1	0.84	0.11	-	72,72,72,72	0
56	MG	YA	3355	1/1	0.76	0.11	-	75,75,75,75	0
56	MG	RA	3632	1/1	0.86	0.49	-	55,55,55,55	0
56	MG	RA	3914	1/1	0.92	0.50	-	56,56,56,56	0
56	MG	YA	3451	1/1	0.60	0.37	-	64,64,64,64	0
56	MG	RA	4005	1/1	0.83	0.28	-	58,58,58,58	0
56	MG	YA	3697	1/1	0.92	0.64	-	38,38,38,38	0
56	MG	YA	3191	1/1	0.55	0.14	-	76,76,76,76	0
56	MG	QA	1863	1/1	0.80	0.28	-	80,80,80,80	0
56	MG	YA	3282	1/1	0.97	0.36	-	10,10,10,10	0
56	MG	RA	3627	1/1	0.87	0.62	-	76,76,76,76	0
56	MG	YA	3223	1/1	0.86	0.47	-	91,91,91,91	0
56	MG	XA	1734	1/1	0.89	0.17	-	78,78,78,78	0
56	MG	RA	3370	1/1	0.29	0.99	-	88,88,88,88	0
56	MG	RA	3933	1/1	0.73	0.85	-	76,76,76,76	0
56	MG	YA	3334	1/1	0.97	0.51	-	14,14,14,14	0
56	MG	YA	3640	1/1	0.96	0.56	-	40,40,40,40	0
56	MG	RA	3300	1/1	0.82	1.18	-	68,68,68,68	0
56	MG	YA	3063	1/1	0.92	0.23	-	35,35,35,35	0
56	MG	RA	3417	1/1	0.96	0.12	-	42,42,42,42	0
56	MG	RA	3987	1/1	0.72	0.65	-	80,80,80,80	0
56	MG	RA	3547	1/1	0.45	0.35	-	74,74,74,74	0
56	MG	RA	3742	1/1	0.59	0.60	-	81,81,81,81	0
56	MG	RA	3340	1/1	0.69	0.49	-	52,52,52,52	0
56	MG	YA	3086	1/1	0.02	0.93	-	95,95,95,95	0
56	MG	YA	3533	1/1	0.97	0.22	-	48,48,48,48	0
56	MG	XA	1673	1/1	-0.23	1.71	-	103,103,103,103	0
56	MG	RA	3097	1/1	0.95	0.49	-	93,93,93,93	0
56	MG	QA	1698	1/1	0.48	0.40	-	100,100,100,100	0
56	MG	RA	3579	1/1	0.98	0.30	-	24,24,24,24	0
56	MG	YA	3216	1/1	0.94	0.37	-	25,25,25,25	0
56	MG	RA	3080	1/1	0.82	0.60	-	81,81,81,81	0
56	MG	YA	3147	1/1	0.60	0.40	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	XA	1680	1/1	0.66	0.18	-	77,77,77,77	0
56	MG	YA	3170	1/1	0.79	0.63	-	56,56,56,56	0
56	MG	RA	3086	1/1	0.40	0.77	-	124,124,124,124	0
56	MG	RA	3326	1/1	0.95	0.19	-	20,20,20,20	0
56	MG	R0	102	1/1	0.67	0.21	-	84,84,84,84	0
56	MG	QA	1629	1/1	0.88	0.31	-	51,51,51,51	0
56	MG	XA	1739	1/1	0.92	0.51	-	61,61,61,61	0
56	MG	RA	3755	1/1	0.74	0.56	-	71,71,71,71	0
56	MG	RA	3859	1/1	0.88	0.72	-	72,72,72,72	0
56	MG	RA	4054	1/1	0.39	0.99	-	97,97,97,97	0
56	MG	RA	3569	1/1	0.91	0.46	-	64,64,64,64	0
56	MG	YA	3413	1/1	0.97	0.40	-	36,36,36,36	0
56	MG	QL	202	1/1	0.84	0.11	-	68,68,68,68	0
56	MG	RA	3671	1/1	0.84	0.29	-	71,71,71,71	0
56	MG	YA	3285	1/1	0.95	0.55	-	25,25,25,25	0
56	MG	RA	3893	1/1	0.98	0.62	-	34,34,34,34	0
56	MG	YA	3299	1/1	0.96	0.53	-	10,10,10,10	0
56	MG	YA	3527	1/1	0.91	0.38	-	50,50,50,50	0
56	MG	YA	3395	1/1	0.99	0.41	-	17,17,17,17	0
56	MG	XA	1650	1/1	0.79	0.64	-	84,84,84,84	0
56	MG	RA	3733	1/1	0.27	0.94	-	96,96,96,96	0
56	MG	XA	1783	1/1	0.17	1.23	-	99,99,99,99	0
56	MG	YA	3123	1/1	0.89	0.14	-	86,86,86,86	0
56	MG	RA	3197	1/1	0.31	1.25	-	85,85,85,85	0
56	MG	YA	3019	1/1	0.91	0.34	-	81,81,81,81	0
56	MG	RA	3455	1/1	0.82	0.41	-	48,48,48,48	0
56	MG	QA	1677	1/1	0.21	0.91	-	94,94,94,94	0
56	MG	RA	3661	1/1	0.80	0.32	-	89,89,89,89	0
56	MG	XA	1645	1/1	0.66	0.53	-	93,93,93,93	0
56	MG	QA	1693	1/1	0.09	0.39	-	88,88,88,88	0
56	MG	YA	3081	1/1	0.88	0.53	-	71,71,71,71	0
56	MG	RA	3508	1/1	0.98	0.46	-	42,42,42,42	0
56	MG	YA	3729	1/1	0.79	0.55	-	61,61,61,61	0
56	MG	RA	3103	1/1	0.38	0.50	-	104,104,104,104	0
56	MG	XA	1773	1/1	0.12	0.97	-	96,96,96,96	0
56	MG	RA	3188	1/1	0.91	0.75	-	115,115,115,115	0
56	MG	YA	3525	1/1	0.88	0.54	-	86,86,86,86	0
56	MG	RB	211	1/1	0.21	0.37	-	95,95,95,95	0
56	MG	RA	3969	1/1	0.65	0.45	-	98,98,98,98	0
56	MG	YA	3440	1/1	0.97	0.24	-	29,29,29,29	0
56	MG	YA	3161	1/1	0.78	0.52	-	76,76,76,76	0
56	MG	RB	228	1/1	0.61	0.56	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3639	1/1	0.70	1.07	-	65,65,65,65	0
56	MG	YA	3125	1/1	0.96	0.37	-	58,58,58,58	0
56	MG	RA	3104	1/1	0.69	0.48	-	57,57,57,57	0
56	MG	QA	1808	1/1	0.80	0.48	-	54,54,54,54	0
56	MG	RA	3309	1/1	0.57	0.58	-	63,63,63,63	0
56	MG	RA	3329	1/1	0.84	0.28	-	86,86,86,86	0
56	MG	RA	3644	1/1	-0.05	1.01	-	84,84,84,84	0
56	MG	YA	3488	1/1	0.54	0.38	-	105,105,105,105	0
56	MG	YA	3735	1/1	0.89	0.56	-	71,71,71,71	0
56	MG	YA	3429	1/1	0.90	0.29	-	67,67,67,67	0
56	MG	QA	1639	1/1	0.85	0.20	-	79,79,79,79	0
56	MG	YA	3138	1/1	0.95	0.23	-	61,61,61,61	0
56	MG	RA	3698	1/1	0.97	0.13	-	73,73,73,73	0
56	MG	YA	3541	1/1	0.89	0.41	-	20,20,20,20	0
56	MG	R9	103	1/1	0.91	0.23	-	67,67,67,67	0
56	MG	YA	3529	1/1	0.60	0.71	-	73,73,73,73	0
56	MG	RA	3473	1/1	0.99	0.37	-	26,26,26,26	0
56	MG	QA	1871	1/1	0.09	2.62	-	100,100,100,100	0
56	MG	RA	3756	1/1	0.82	0.48	-	83,83,83,83	0
56	MG	RA	3245	1/1	0.72	0.47	-	81,81,81,81	0
56	MG	RA	3290	1/1	0.80	0.35	-	74,74,74,74	0
56	MG	YA	3059	1/1	0.65	0.63	-	79,79,79,79	0
56	MG	YB	212	1/1	0.94	0.50	-	57,57,57,57	0
56	MG	QA	1702	1/1	0.86	0.35	-	64,64,64,64	0
56	MG	QG	202	1/1	0.79	0.31	-	92,92,92,92	0
56	MG	RA	3991	1/1	0.71	0.59	-	73,73,73,73	0
56	MG	RA	3397	1/1	0.82	0.44	-	65,65,65,65	0
56	MG	RF	311	1/1	0.74	0.62	-	74,74,74,74	0
56	MG	YA	3028	1/1	0.86	0.31	-	51,51,51,51	0
56	MG	YA	3590	1/1	0.98	0.68	-	41,41,41,41	0
56	MG	RA	3702	1/1	0.81	0.96	-	67,67,67,67	0
56	MG	XA	1677	1/1	0.87	0.26	-	71,71,71,71	0
56	MG	QA	1831	1/1	0.54	0.40	-	93,93,93,93	0
56	MG	QA	1853	1/1	0.65	0.63	-	107,107,107,107	0
56	MG	RA	3479	1/1	0.91	0.33	-	19,19,19,19	0
56	MG	YA	3220	1/1	0.79	0.30	-	87,87,87,87	0
56	MG	YA	3671	1/1	0.90	0.47	-	37,37,37,37	0
56	MG	XA	1637	1/1	0.36	0.69	-	89,89,89,89	0
56	MG	RA	3880	1/1	0.80	0.48	-	54,54,54,54	0
56	MG	YA	3307	1/1	0.77	0.34	-	73,73,73,73	0
56	MG	XA	1612	1/1	0.97	0.09	-	41,41,41,41	0
56	MG	XA	1747	1/1	0.88	0.51	-	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	QM	201	1/1	0.31	0.63	-	85,85,85,85	0
56	MG	RA	3904	1/1	0.98	0.29	-	24,24,24,24	0
56	MG	RA	3588	1/1	0.84	0.48	-	63,63,63,63	0
56	MG	RA	3527	1/1	0.79	0.77	-	67,67,67,67	0
56	MG	YA	3486	1/1	0.96	0.55	-	30,30,30,30	0
56	MG	YA	3458	1/1	0.92	0.31	-	46,46,46,46	0
56	MG	YA	3642	1/1	0.97	0.69	-	58,58,58,58	0
56	MG	RA	3984	1/1	0.94	0.38	-	41,41,41,41	0
56	MG	RA	3090	1/1	0.31	0.43	-	93,93,93,93	0
56	MG	RA	3474	1/1	0.99	0.28	-	45,45,45,45	0
56	MG	XA	1748	1/1	0.76	0.46	-	60,60,60,60	0
56	MG	RA	3033	1/1	0.87	0.26	-	91,91,91,91	0
56	MG	QA	1772	1/1	0.75	0.99	-	79,79,79,79	0
56	MG	RA	3967	1/1	0.59	0.57	-	61,61,61,61	0
56	MG	RA	3620	1/1	0.41	0.59	-	90,90,90,90	0
56	MG	YA	3650	1/1	0.92	0.61	-	48,48,48,48	0
56	MG	YA	3320	1/1	0.98	0.36	-	26,26,26,26	0
56	MG	YA	3234	1/1	0.72	0.53	-	76,76,76,76	0
56	MG	XA	1750	1/1	0.89	0.28	-	87,87,87,87	0
56	MG	RA	3352	1/1	0.92	0.57	-	65,65,65,65	0
56	MG	RA	3031	1/1	0.59	0.39	-	75,75,75,75	0
56	MG	RA	3983	1/1	0.56	0.70	-	84,84,84,84	0
56	MG	RB	212	1/1	0.85	0.17	-	74,74,74,74	0
56	MG	RA	3280	1/1	0.89	0.23	-	78,78,78,78	0
56	MG	YT	201	1/1	0.74	0.43	-	57,57,57,57	0
56	MG	RA	3113	1/1	0.93	0.58	-	65,65,65,65	0
56	MG	RA	3546	1/1	0.55	0.44	-	111,111,111,111	0
56	MG	YA	3384	1/1	0.93	0.55	-	38,38,38,38	0
56	MG	YA	3436	1/1	0.91	0.38	-	51,51,51,51	0
56	MG	RA	3405	1/1	0.88	0.56	-	32,32,32,32	0
56	MG	RA	3020	1/1	0.99	0.45	-	89,89,89,89	0
56	MG	QA	1640	1/1	0.77	0.73	-	75,75,75,75	0
56	MG	RA	3885	1/1	0.97	0.52	-	66,66,66,66	0
56	MG	RA	3603	1/1	0.28	0.50	-	101,101,101,101	0
56	MG	YA	3122	1/1	0.92	0.51	-	60,60,60,60	0
56	MG	QA	1873	1/1	0.46	0.60	-	70,70,70,70	0
56	MG	YA	3165	1/1	0.29	0.51	-	73,73,73,73	0
56	MG	QE	201	1/1	0.68	0.17	-	84,84,84,84	0
56	MG	RA	3971	1/1	0.97	0.38	-	19,19,19,19	0
56	MG	RA	3191	1/1	0.92	0.13	-	69,69,69,69	0
56	MG	RA	3296	1/1	0.62	0.43	-	102,102,102,102	0
56	MG	RA	3863	1/1	0.73	1.26	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3738	1/1	0.95	0.40	-	53,53,53,53	0
56	MG	RA	3850	1/1	0.97	0.31	-	43,43,43,43	0
56	MG	YA	3516	1/1	0.84	0.60	-	78,78,78,78	0
56	MG	RB	224	1/1	0.60	0.65	-	78,78,78,78	0
56	MG	XA	1744	1/1	0.91	0.59	-	59,59,59,59	0
56	MG	RA	3841	1/1	0.81	0.44	-	64,64,64,64	0
56	MG	QA	1691	1/1	-0.06	0.46	-	104,104,104,104	0
56	MG	YA	3238	1/1	0.89	0.32	-	91,91,91,91	0
56	MG	RA	3413	1/1	0.97	0.39	-	34,34,34,34	0
56	MG	RA	3356	1/1	0.90	0.11	-	23,23,23,23	0
56	MG	XA	1731	1/1	0.85	0.26	-	65,65,65,65	0
56	MG	YA	3269	1/1	0.75	0.54	-	78,78,78,78	0
56	MG	YA	3101	1/1	0.83	0.35	-	70,70,70,70	0
56	MG	YA	3005	1/1	0.95	0.29	-	63,63,63,63	0
56	MG	YA	3676	1/1	0.55	0.84	-	73,73,73,73	0
56	MG	RA	3106	1/1	0.96	0.26	-	102,102,102,102	0
56	MG	RA	3690	1/1	0.83	0.99	-	74,74,74,74	0
56	MG	RA	3371	1/1	0.88	0.54	-	75,75,75,75	0
56	MG	YA	3163	1/1	0.89	0.19	-	52,52,52,52	0
56	MG	QA	1762	1/1	-0.08	1.11	-	93,93,93,93	0
56	MG	XA	1639	1/1	0.52	0.52	-	98,98,98,98	0
56	MG	YA	3050	1/1	0.83	0.19	-	85,85,85,85	0
56	MG	YA	3343	1/1	0.96	0.40	-	21,21,21,21	0
56	MG	YA	3450	1/1	0.48	0.70	-	79,79,79,79	0
56	MG	YA	3470	1/1	0.83	0.31	-	59,59,59,59	0
56	MG	YA	3502	1/1	0.67	0.44	-	79,79,79,79	0
56	MG	RB	213	1/1	0.89	0.61	-	58,58,58,58	0
56	MG	QA	1695	1/1	0.82	0.47	-	48,48,48,48	0
56	MG	YA	3150	1/1	0.54	0.82	-	84,84,84,84	0
56	MG	YA	3289	1/1	0.96	0.24	-	38,38,38,38	0
56	MG	YE	301	1/1	0.34	0.49	-	95,95,95,95	0
56	MG	RA	3145	1/1	0.93	0.16	-	43,43,43,43	0
56	MG	QA	1699	1/1	0.76	0.57	-	65,65,65,65	0
56	MG	RA	3727	1/1	-0.47	0.55	-	108,108,108,108	0
56	MG	YA	3539	1/1	0.97	0.30	-	18,18,18,18	0
56	MG	RA	3954	1/1	0.36	0.63	-	77,77,77,77	0
56	MG	RA	3343	1/1	0.90	0.16	-	68,68,68,68	0
56	MG	RA	3263	1/1	0.69	0.23	-	67,67,67,67	0
56	MG	RA	3786	1/1	0.31	0.66	-	87,87,87,87	0
56	MG	YA	3428	1/1	0.82	0.32	-	44,44,44,44	0
56	MG	YA	3726	1/1	0.38	0.80	-	81,81,81,81	0
56	MG	XA	1634	1/1	0.18	0.46	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1669	1/1	0.71	1.07	-	71,71,71,71	0
56	MG	YA	3070	1/1	0.70	0.42	-	62,62,62,62	0
56	MG	RB	201	1/1	0.94	0.19	-	72,72,72,72	0
56	MG	XA	1603	1/1	0.52	0.87	-	76,76,76,76	0
56	MG	YA	3174	1/1	0.21	0.99	-	95,95,95,95	0
56	MG	RA	3129	1/1	0.83	0.25	-	45,45,45,45	0
56	MG	QA	1720	1/1	-0.02	0.88	-	97,97,97,97	0
56	MG	QA	1794	1/1	0.60	0.46	-	79,79,79,79	0
56	MG	QA	1628	1/1	0.80	0.27	-	49,49,49,49	0
56	MG	RA	3652	1/1	0.69	0.62	-	88,88,88,88	0
56	MG	RA	3492	1/1	0.93	0.41	-	68,68,68,68	0
56	MG	RA	3957	1/1	0.81	0.32	-	66,66,66,66	0
56	MG	RA	3057	1/1	0.63	0.52	-	93,93,93,93	0
56	MG	YO	201	1/1	0.76	0.35	-	78,78,78,78	0
56	MG	RA	3089	1/1	0.92	0.07	-	67,67,67,67	0
56	MG	YA	3609	1/1	0.92	0.26	-	51,51,51,51	0
56	MG	YA	3508	1/1	0.79	0.37	-	102,102,102,102	0
56	MG	YA	3007	1/1	0.93	0.25	-	63,63,63,63	0
56	MG	RA	3061	1/1	0.62	0.23	-	84,84,84,84	0
56	MG	YA	3414	1/1	0.66	0.68	-	83,83,83,83	0
56	MG	XA	1697	1/1	0.66	0.81	-	70,70,70,70	0
56	MG	YA	3405	1/1	0.84	0.42	-	86,86,86,86	0
56	MG	YA	3027	1/1	0.73	0.49	-	45,45,45,45	0
56	MG	RA	3018	1/1	0.85	0.32	-	89,89,89,89	0
56	MG	RA	3580	1/1	0.53	0.65	-	112,112,112,112	0
56	MG	RA	3063	1/1	0.95	0.30	-	41,41,41,41	0
56	MG	RA	3533	1/1	0.80	0.26	-	49,49,49,49	0
56	MG	XA	1733	1/1	0.90	0.25	-	72,72,72,72	0
56	MG	YA	3368	1/1	0.80	0.45	-	62,62,62,62	0
56	MG	RP	202	1/1	0.73	0.22	-	78,78,78,78	0
56	MG	YA	3447	1/1	0.84	0.59	-	68,68,68,68	0
56	MG	RA	3647	1/1	0.89	0.29	-	88,88,88,88	0
56	MG	RA	3946	1/1	0.96	0.15	-	18,18,18,18	0
56	MG	YA	3184	1/1	0.60	0.43	-	80,80,80,80	0
56	MG	YA	3686	1/1	0.99	0.35	-	15,15,15,15	0
56	MG	RA	3307	1/1	0.96	0.45	-	76,76,76,76	0
56	MG	XA	1766	1/1	0.97	0.72	-	52,52,52,52	0
56	MG	QA	1676	1/1	0.72	0.61	-	88,88,88,88	0
56	MG	XA	1710	1/1	0.85	0.35	-	66,66,66,66	0
56	MG	RA	4019	1/1	0.79	0.68	-	87,87,87,87	0
56	MG	RA	3860	1/1	0.94	0.48	-	25,25,25,25	0
56	MG	YA	3661	1/1	0.88	0.61	-	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	RA	3541	1/1	0.68	0.87	-	74,74,74,74	0
56	MG	YA	3427	1/1	-0.06	1.07	-	75,75,75,75	0
56	MG	QA	1671	1/1	0.94	0.16	-	64,64,64,64	0
56	MG	RA	3519	1/1	0.58	0.44	-	82,82,82,82	0
56	MG	RA	3213	1/1	0.92	0.31	-	105,105,105,105	0
56	MG	RA	3179	1/1	0.44	0.84	-	77,77,77,77	0
56	MG	RA	3796	1/1	0.47	0.94	-	67,67,67,67	0
56	MG	RA	3244	1/1	0.90	0.08	-	71,71,71,71	0
56	MG	RA	3960	1/1	0.75	0.69	-	89,89,89,89	0
56	MG	RA	3261	1/1	0.16	0.49	-	82,82,82,82	0
56	MG	YA	3723	1/1	0.77	0.37	-	67,67,67,67	0
56	MG	YA	3172	1/1	0.83	0.28	-	69,69,69,69	0
56	MG	RA	3898	1/1	0.86	0.32	-	48,48,48,48	0
56	MG	YB	202	1/1	0.89	0.17	-	56,56,56,56	0
56	MG	RA	3107	1/1	0.80	0.53	-	109,109,109,109	0
56	MG	RA	3091	1/1	0.86	1.44	-	104,104,104,104	0
56	MG	YA	3517	1/1	0.78	0.41	-	92,92,92,92	0
56	MG	YA	3134	1/1	0.76	0.45	-	89,89,89,89	0
56	MG	RA	3596	1/1	0.71	0.42	-	83,83,83,83	0
56	MG	RD	310	1/1	0.53	0.41	-	94,94,94,94	0
56	MG	XA	1705	1/1	0.74	0.26	-	67,67,67,67	0
56	MG	YA	3198	1/1	0.72	0.60	-	80,80,80,80	0
56	MG	YF	302	1/1	0.39	0.53	-	85,85,85,85	0
56	MG	YA	3417	1/1	0.14	0.70	-	106,106,106,106	0
56	MG	RA	3728	1/1	0.90	0.32	-	74,74,74,74	0
56	MG	YA	3421	1/1	0.30	1.11	-	75,75,75,75	0
56	MG	YA	3270	1/1	0.57	0.45	-	83,83,83,83	0
56	MG	RA	3248	1/1	0.86	0.34	-	56,56,56,56	0
56	MG	RA	3003	1/1	0.73	0.40	-	73,73,73,73	0
56	MG	QA	1642	1/1	0.43	0.66	-	83,83,83,83	0
56	MG	RA	3554	1/1	0.87	0.51	-	55,55,55,55	0
56	MG	QH	201	1/1	0.54	0.49	-	76,76,76,76	0
56	MG	RA	3817	1/1	0.50	0.81	-	76,76,76,76	0
56	MG	RA	3036	1/1	0.59	0.41	-	69,69,69,69	0
56	MG	RA	3562	1/1	0.92	0.16	-	59,59,59,59	0
56	MG	RA	3124	1/1	0.78	0.19	-	46,46,46,46	0
56	MG	RA	3522	1/1	0.85	0.29	-	55,55,55,55	0
56	MG	RA	3593	1/1	0.90	0.56	-	66,66,66,66	0
56	MG	RA	3347	1/1	0.95	0.47	-	23,23,23,23	0
56	MG	YA	3160	1/1	0.87	0.47	-	67,67,67,67	0
56	MG	RA	3926	1/1	0.69	0.50	-	83,83,83,83	0
56	MG	RA	3279	1/1	0.28	0.57	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3958	1/1	0.60	0.54	-	104,104,104,104	0
56	MG	RA	3996	1/1	0.87	0.86	-	73,73,73,73	0
56	MG	YD	302	1/1	0.81	0.38	-	71,71,71,71	0
56	MG	YA	3180	1/1	0.85	0.41	-	43,43,43,43	0
56	MG	RA	3308	1/1	0.91	0.50	-	64,64,64,64	0
56	MG	RB	227	1/1	0.67	0.53	-	74,74,74,74	0
56	MG	QA	1826	1/1	-0.17	0.47	-	74,74,74,74	0
56	MG	YA	3233	1/1	0.41	0.47	-	95,95,95,95	0
56	MG	RA	4013	1/1	0.83	0.42	-	76,76,76,76	0
56	MG	RA	3392	1/1	0.86	0.27	-	28,28,28,28	0
56	MG	RA	3749	1/1	0.87	0.31	-	63,63,63,63	0
56	MG	RA	3625	1/1	0.47	0.67	-	91,91,91,91	0
56	MG	YB	210	1/1	0.94	0.40	-	57,57,57,57	0
56	MG	QA	1660	1/1	0.66	0.19	-	77,77,77,77	0
56	MG	YA	3510	1/1	0.64	0.61	-	80,80,80,80	0
56	MG	RA	3068	1/1	0.61	0.49	-	79,79,79,79	0
56	MG	QA	1666	1/1	0.69	0.22	-	74,74,74,74	0
56	MG	YA	3311	1/1	0.20	1.31	-	94,94,94,94	0
56	MG	QA	1849	1/1	0.85	0.69	-	81,81,81,81	0
56	MG	YA	3512	1/1	0.80	0.48	-	62,62,62,62	0
56	MG	YA	3547	1/1	0.67	0.41	-	80,80,80,80	0
56	MG	YA	3175	1/1	0.90	0.48	-	123,123,123,123	0
56	MG	QA	1686	1/1	-0.13	1.02	-	103,103,103,103	0
56	MG	RA	3287	1/1	0.94	0.16	-	83,83,83,83	0
56	MG	XA	1754	1/1	0.83	0.57	-	86,86,86,86	0
56	MG	YA	3608	1/1	0.95	0.64	-	44,44,44,44	0
56	MG	QA	1736	1/1	0.29	0.81	-	86,86,86,86	0
56	MG	RA	3941	1/1	0.93	0.14	-	69,69,69,69	0
56	MG	RR	3204	1/1	0.63	0.50	-	83,83,83,83	0
56	MG	XA	1717	1/1	0.93	0.49	-	59,59,59,59	0
56	MG	RA	3424	1/1	0.91	0.35	-	80,80,80,80	0
56	MG	RA	3913	1/1	0.87	0.43	-	43,43,43,43	0
56	MG	YA	3528	1/1	0.37	0.63	-	104,104,104,104	0
56	MG	RA	3736	1/1	0.78	0.37	-	74,74,74,74	0
56	MG	RA	3394	1/1	0.99	0.45	-	31,31,31,31	0
56	MG	RA	3110	1/1	0.96	0.21	-	70,70,70,70	0
56	MG	YA	3524	1/1	0.45	0.38	-	96,96,96,96	0
56	MG	RA	3948	1/1	0.49	0.57	-	89,89,89,89	0
56	MG	QA	1675	1/1	0.56	1.02	-	94,94,94,94	0
56	MG	YA	3465	1/1	0.17	0.79	-	82,82,82,82	0
56	MG	YA	3111	1/1	0.68	0.57	-	58,58,58,58	0
56	MG	YA	3432	1/1	0.67	0.47	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3843	1/1	0.79	0.29	-	72,72,72,72	0
56	MG	QA	1708	1/1	0.70	0.17	-	77,77,77,77	0
56	MG	YA	3016	1/1	0.99	0.16	-	29,29,29,29	0
56	MG	RA	3605	1/1	0.88	0.33	-	70,70,70,70	0
56	MG	YA	3078	1/1	0.83	0.34	-	60,60,60,60	0
56	MG	YA	3248	1/1	0.69	0.42	-	105,105,105,105	0
56	MG	RA	3431	1/1	0.67	0.39	-	88,88,88,88	0
56	MG	QA	1815	1/1	0.86	0.33	-	65,65,65,65	0
56	MG	QA	1865	1/1	0.59	0.77	-	75,75,75,75	0
56	MG	RA	4026	1/1	0.85	0.48	-	71,71,71,71	0
56	MG	QA	1854	1/1	0.62	0.34	-	67,67,67,67	0
56	MG	YB	216	1/1	0.97	0.40	-	45,45,45,45	0
56	MG	RA	3331	1/1	0.74	0.76	-	73,73,73,73	0
56	MG	RA	3011	1/1	0.33	0.58	-	84,84,84,84	0
56	MG	XF	201	1/1	0.89	0.21	-	39,39,39,39	0
56	MG	QA	1874	1/1	0.84	0.37	-	74,74,74,74	0
56	MG	RA	3854	1/1	0.95	0.28	-	47,47,47,47	0
56	MG	RA	3754	1/1	0.36	0.83	-	92,92,92,92	0
56	MG	RA	3078	1/1	0.60	0.89	-	70,70,70,70	0
56	MG	RA	3795	1/1	0.84	0.55	-	75,75,75,75	0
56	MG	XA	1681	1/1	0.87	0.29	-	106,106,106,106	0
56	MG	QA	1646	1/1	0.78	0.59	-	46,46,46,46	0
56	MG	YA	3044	1/1	0.93	0.19	-	35,35,35,35	0
56	MG	RA	3338	1/1	0.96	0.67	-	38,38,38,38	0
56	MG	QA	1759	1/1	0.69	0.15	-	78,78,78,78	0
56	MG	RA	3362	1/1	0.74	0.33	-	93,93,93,93	0
56	MG	RA	3105	1/1	0.46	0.58	-	71,71,71,71	0
56	MG	RT	201	1/1	0.64	0.98	-	77,77,77,77	0
56	MG	XA	1716	1/1	0.65	0.29	-	57,57,57,57	0
56	MG	YA	3628	1/1	0.50	0.46	-	105,105,105,105	0
56	MG	QL	203	1/1	0.59	0.22	-	60,60,60,60	0
56	MG	YA	3379	1/1	0.62	0.34	-	70,70,70,70	0
56	MG	YA	3720	1/1	0.92	0.50	-	83,83,83,83	0
56	MG	RA	3024	1/1	0.84	0.44	-	74,74,74,74	0
56	MG	YA	3178	1/1	0.78	0.89	-	62,62,62,62	0
56	MG	RA	3710	1/1	0.70	0.84	-	70,70,70,70	0
56	MG	RA	3919	1/1	0.85	0.55	-	47,47,47,47	0
56	MG	YA	3492	1/1	0.83	0.57	-	63,63,63,63	0
56	MG	RA	3195	1/1	0.56	0.56	-	115,115,115,115	0
56	MG	RA	4008	1/1	0.61	0.36	-	86,86,86,86	0
56	MG	RA	3668	1/1	0.92	0.33	-	49,49,49,49	0
56	MG	YA	3127	1/1	0.88	0.29	-	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	XA	1732	1/1	0.88	0.67	-	44,44,44,44	0
56	MG	RA	3410	1/1	0.81	0.12	-	76,76,76,76	0
56	MG	RA	3781	1/1	0.66	0.39	-	60,60,60,60	0
56	MG	QA	1704	1/1	0.72	0.81	-	74,74,74,74	0
56	MG	RB	208	1/1	0.31	0.31	-	90,90,90,90	0
56	MG	YA	3222	1/1	0.64	0.54	-	71,71,71,71	0
56	MG	RA	3526	1/1	0.92	0.59	-	51,51,51,51	0
56	MG	XA	1640	1/1	0.98	0.15	-	66,66,66,66	0
56	MG	QA	1745	1/1	0.23	0.80	-	98,98,98,98	0
56	MG	YT	203	1/1	0.54	0.35	-	78,78,78,78	0
56	MG	QA	1805	1/1	0.48	0.22	-	76,76,76,76	0
56	MG	RA	3907	1/1	0.88	0.61	-	78,78,78,78	0
56	MG	RA	3444	1/1	0.90	0.96	-	83,83,83,83	0
56	MG	RA	3037	1/1	0.90	0.37	-	88,88,88,88	0
56	MG	YA	3681	1/1	0.96	0.76	-	38,38,38,38	0
56	MG	XA	1701	1/1	0.94	0.43	-	51,51,51,51	0
56	MG	XA	1686	1/1	0.78	0.26	-	68,68,68,68	0
56	MG	RA	3973	1/1	0.72	0.57	-	84,84,84,84	0
56	MG	YA	3513	1/1	0.91	0.28	-	80,80,80,80	0
56	MG	YA	3372	1/1	0.89	0.29	-	49,49,49,49	0
56	MG	RA	3611	1/1	0.76	0.29	-	80,80,80,80	0
56	MG	XA	1688	1/1	0.81	0.28	-	56,56,56,56	0
56	MG	RA	3780	1/1	0.83	0.94	-	74,74,74,74	0
56	MG	YA	3037	1/1	-0.20	0.92	-	88,88,88,88	0
56	MG	RN	203	1/1	0.77	0.33	-	86,86,86,86	0
56	MG	XA	1633	1/1	0.98	0.34	-	51,51,51,51	0
56	MG	RA	3242	1/1	0.93	0.31	-	54,54,54,54	0
56	MG	RA	4004	1/1	0.55	0.42	-	93,93,93,93	0
56	MG	YD	307	1/1	0.78	0.68	-	64,64,64,64	0
56	MG	YA	3336	1/1	0.65	0.41	-	71,71,71,71	0
56	MG	RA	3294	1/1	0.93	0.28	-	61,61,61,61	0
56	MG	YA	3146	1/1	0.85	0.13	-	60,60,60,60	0
56	MG	RA	3433	1/1	0.81	0.38	-	66,66,66,66	0
56	MG	RA	3839	1/1	0.58	0.66	-	72,72,72,72	0
56	MG	QA	1602	1/1	0.48	0.15	-	95,95,95,95	0
56	MG	RA	3731	1/1	0.81	0.40	-	83,83,83,83	0
56	MG	RA	3725	1/1	0.63	0.47	-	80,80,80,80	0
56	MG	XA	1646	1/1	0.89	0.56	-	63,63,63,63	0
56	MG	YA	3024	1/1	0.83	0.88	-	59,59,59,59	0
56	MG	YA	3057	1/1	-0.03	0.73	-	99,99,99,99	0
56	MG	QA	1790	1/1	0.93	0.84	-	56,56,56,56	0
56	MG	R7	101	1/1	0.82	0.44	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	QA	1763	1/1	0.17	1.00	-	100,100,100,100	0
56	MG	YA	3026	1/1	0.68	0.24	-	93,93,93,93	0
56	MG	RA	3243	1/1	0.83	0.30	-	73,73,73,73	0
56	MG	RA	3460	1/1	0.95	0.86	-	51,51,51,51	0
56	MG	YA	3350	1/1	0.90	0.25	-	23,23,23,23	0
56	MG	RA	3510	1/1	0.76	0.21	-	38,38,38,38	0
56	MG	XA	1618	1/1	0.43	0.74	-	72,72,72,72	0
56	MG	YA	3566	1/1	0.76	0.20	-	60,60,60,60	0
56	MG	XA	1613	1/1	0.91	0.12	-	51,51,51,51	0
56	MG	RA	3591	1/1	0.69	0.56	-	77,77,77,77	0
56	MG	RA	3594	1/1	0.95	0.21	-	67,67,67,67	0
56	MG	YA	3148	1/1	0.25	0.77	-	92,92,92,92	0
56	MG	RA	3026	1/1	0.93	0.72	-	72,72,72,72	0
56	MG	RU	202	1/1	0.82	0.30	-	78,78,78,78	0
56	MG	QA	1856	1/1	-0.05	1.28	-	89,89,89,89	0
56	MG	RA	3098	1/1	0.95	0.19	-	12,12,12,12	0
56	MG	RA	3974	1/1	0.62	1.33	-	70,70,70,70	0
56	MG	YA	3422	1/1	0.70	0.80	-	122,122,122,122	0
56	MG	YA	3260	1/1	0.72	0.45	-	71,71,71,71	0
56	MG	XA	1724	1/1	0.85	0.37	-	65,65,65,65	0
56	MG	RA	3453	1/1	0.90	0.25	-	64,64,64,64	0
56	MG	YA	3366	1/1	0.93	0.67	-	59,59,59,59	0
56	MG	RA	3955	1/1	0.80	0.27	-	74,74,74,74	0
56	MG	YA	3532	1/1	0.81	0.92	-	60,60,60,60	0
56	MG	YA	3206	1/1	0.66	0.45	-	100,100,100,100	0
56	MG	RA	3414	1/1	0.94	0.35	-	34,34,34,34	0
56	MG	RA	3130	1/1	0.87	0.06	-	69,69,69,69	0
56	MG	RA	3441	1/1	0.69	0.69	-	61,61,61,61	0
56	MG	RA	3928	1/1	0.93	0.36	-	59,59,59,59	0
56	MG	YA	3003	1/1	0.38	0.93	-	106,106,106,106	0
56	MG	RA	3205	1/1	0.62	0.45	-	76,76,76,76	0
56	MG	RA	3438	1/1	0.83	0.17	-	71,71,71,71	0
56	MG	QA	1773	1/1	0.91	0.31	-	71,71,71,71	0
56	MG	XA	1755	1/1	0.97	0.58	-	43,43,43,43	0
56	MG	YA	3069	1/1	0.32	0.79	-	78,78,78,78	0
56	MG	RA	3751	1/1	0.48	0.31	-	51,51,51,51	0
56	MG	RA	3548	1/1	0.92	0.43	-	38,38,38,38	0
56	MG	YB	206	1/1	0.42	0.63	-	99,99,99,99	0
56	MG	RE	304	1/1	0.29	0.73	-	75,75,75,75	0
56	MG	QA	1788	1/1	0.32	0.66	-	81,81,81,81	0
56	MG	YA	3241	1/1	0.47	0.49	-	85,85,85,85	0
56	MG	RB	223	1/1	0.63	0.94	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3593	1/1	0.93	0.50	-	28,28,28,28	0
56	MG	RA	3259	1/1	0.76	0.30	-	87,87,87,87	0
56	MG	RA	3846	1/1	0.71	0.72	-	80,80,80,80	0
56	MG	XA	1769	1/1	0.73	0.73	-	64,64,64,64	0
56	MG	QA	1732	1/1	0.67	0.42	-	96,96,96,96	0
56	MG	RA	3203	1/1	0.41	0.71	-	97,97,97,97	0
56	MG	RA	3159	1/1	0.87	0.41	-	107,107,107,107	0
56	MG	RA	3468	1/1	0.92	0.19	-	40,40,40,40	0
56	MG	RA	3586	1/1	0.77	0.50	-	73,73,73,73	0
56	MG	YA	3283	1/1	0.95	0.26	-	36,36,36,36	0
56	MG	RA	3053	1/1	0.84	0.43	-	89,89,89,89	0
56	MG	YA	3217	1/1	0.89	0.21	-	75,75,75,75	0
56	MG	RA	3778	1/1	0.95	0.68	-	41,41,41,41	0
56	MG	RA	3251	1/1	0.71	0.49	-	69,69,69,69	0
56	MG	RA	3072	1/1	0.94	0.94	-	93,93,93,93	0
56	MG	XA	1655	1/1	0.69	0.55	-	84,84,84,84	0
56	MG	RA	3284	1/1	0.90	0.35	-	97,97,97,97	0
56	MG	XA	1759	1/1	0.90	0.31	-	56,56,56,56	0
56	MG	RA	3709	1/1	0.90	0.20	-	75,75,75,75	0
56	MG	RA	3491	1/1	0.54	0.82	-	81,81,81,81	0
56	MG	RB	203	1/1	0.56	0.48	-	106,106,106,106	0
56	MG	RA	3209	1/1	0.91	1.06	-	100,100,100,100	0
56	MG	YA	3268	1/1	0.93	0.40	-	73,73,73,73	0
56	MG	RA	3616	1/1	0.96	0.36	-	33,33,33,33	0
56	MG	RA	3367	1/1	0.30	0.63	-	74,74,74,74	0
56	MG	RU	201	1/1	0.89	0.38	-	70,70,70,70	0
56	MG	RA	3288	1/1	0.73	0.33	-	95,95,95,95	0
56	MG	QA	1725	1/1	0.23	0.63	-	90,90,90,90	0
56	MG	RA	3267	1/1	0.94	0.26	-	47,47,47,47	0
56	MG	RV	204	1/1	0.33	0.51	-	70,70,70,70	0
56	MG	YA	3684	1/1	0.94	0.57	-	39,39,39,39	0
56	MG	YA	3462	1/1	0.34	0.74	-	75,75,75,75	0
56	MG	YA	3310	1/1	0.97	0.48	-	38,38,38,38	0
56	MG	RA	3489	1/1	0.77	0.85	-	50,50,50,50	0
56	MG	RA	3112	1/1	0.51	0.52	-	117,117,117,117	0
56	MG	RA	3656	1/1	0.85	0.56	-	44,44,44,44	0
56	MG	QA	1840	1/1	0.67	0.57	-	89,89,89,89	0
56	MG	YA	3382	1/1	0.97	0.26	-	29,29,29,29	0
56	MG	QA	1668	1/1	0.20	0.69	-	102,102,102,102	0
56	MG	XA	1712	1/1	0.83	0.31	-	61,61,61,61	0
56	MG	XA	1668	1/1	0.27	0.69	-	87,87,87,87	0
56	MG	RA	3190	1/1	0.81	0.31	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QA	1751	1/1	0.75	0.31	-	83,83,83,83	0
56	MG	YA	3301	1/1	0.87	0.22	-	42,42,42,42	0
56	MG	RA	3691	1/1	0.62	0.47	-	64,64,64,64	0
56	MG	RA	3273	1/1	0.90	0.57	-	76,76,76,76	0
56	MG	RA	3281	1/1	0.86	1.19	-	85,85,85,85	0
56	MG	RA	3703	1/1	0.69	0.72	-	71,71,71,71	0
56	MG	RA	3295	1/1	0.91	0.15	-	73,73,73,73	0
56	MG	RA	3717	1/1	0.93	0.46	-	38,38,38,38	0
56	MG	QA	1709	1/1	0.84	0.46	-	53,53,53,53	0
56	MG	RA	3169	1/1	0.88	0.17	-	82,82,82,82	0
56	MG	RA	3792	1/1	0.98	0.41	-	35,35,35,35	0
56	MG	XA	1715	1/1	0.68	0.62	-	55,55,55,55	0
56	MG	RA	3084	1/1	0.88	0.48	-	79,79,79,79	0
56	MG	QA	1637	1/1	0.62	0.72	-	93,93,93,93	0
56	MG	RA	3775	1/1	0.84	0.41	-	56,56,56,56	0
56	MG	RA	3589	1/1	0.49	0.62	-	100,100,100,100	0
56	MG	R0	104	1/1	0.48	0.46	-	90,90,90,90	0
56	MG	YA	3415	1/1	0.13	0.98	-	84,84,84,84	0
56	MG	YA	3742	1/1	0.89	0.39	-	36,36,36,36	0
56	MG	YA	3290	1/1	0.94	0.43	-	47,47,47,47	0
56	MG	RA	3582	1/1	0.87	0.76	-	72,72,72,72	0
56	MG	QA	1868	1/1	0.95	0.68	-	58,58,58,58	0
56	MG	XA	1725	1/1	0.48	0.69	-	87,87,87,87	0
56	MG	YA	3182	1/1	0.89	0.24	-	68,68,68,68	0
56	MG	YA	3098	1/1	0.88	0.13	-	49,49,49,49	0
56	MG	XA	1698	1/1	0.73	0.41	-	66,66,66,66	0
56	MG	RA	3372	1/1	0.76	0.58	-	61,61,61,61	0
56	MG	YA	3641	1/1	0.61	0.83	-	86,86,86,86	0
56	MG	RA	3016	1/1	0.78	0.83	-	77,77,77,77	0
56	MG	YA	3644	1/1	0.93	0.66	-	57,57,57,57	0
56	MG	RA	3882	1/1	0.43	0.70	-	77,77,77,77	0
56	MG	RA	3981	1/1	0.92	0.09	-	69,69,69,69	0
56	MG	QA	1727	1/1	-0.11	0.78	-	100,100,100,100	0
56	MG	QA	1803	1/1	0.88	0.51	-	49,49,49,49	0
56	MG	QA	1744	1/1	0.85	0.67	-	65,65,65,65	0
56	MG	YA	3482	1/1	0.91	0.39	-	65,65,65,65	0
56	MG	QG	203	1/1	0.33	1.46	-	100,100,100,100	0
56	MG	RA	3566	1/1	0.92	0.24	-	57,57,57,57	0
56	MG	RA	3054	1/1	0.86	0.34	-	78,78,78,78	0
56	MG	XH	201	1/1	0.47	0.61	-	78,78,78,78	0
56	MG	RA	3684	1/1	0.67	0.50	-	71,71,71,71	0
56	MG	RA	3767	1/1	0.86	0.37	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3317	1/1	0.76	0.33	-	73,73,73,73	0
56	MG	YA	3740	1/1	0.83	0.38	-	52,52,52,52	0
56	MG	YA	3345	1/1	0.95	0.43	-	39,39,39,39	0
56	MG	RA	3249	1/1	0.53	0.73	-	94,94,94,94	0
56	MG	YA	3129	1/1	0.78	0.33	-	31,31,31,31	0
56	MG	QA	1753	1/1	0.35	0.47	-	71,71,71,71	0
56	MG	RA	3462	1/1	0.89	0.44	-	52,52,52,52	0
56	MG	RA	3922	1/1	0.81	0.44	-	70,70,70,70	0
56	MG	RA	3271	1/1	0.35	0.48	-	93,93,93,93	0
56	MG	YA	3047	1/1	0.96	0.11	-	44,44,44,44	0
56	MG	RA	3664	1/1	0.96	0.24	-	48,48,48,48	0
56	MG	RA	3346	1/1	0.85	0.82	-	72,72,72,72	0
56	MG	YA	3546	1/1	0.87	0.53	-	47,47,47,47	0
56	MG	RA	3318	1/1	0.99	0.32	-	19,19,19,19	0
56	MG	YA	3120	1/1	0.83	0.52	-	72,72,72,72	0
56	MG	RA	3807	1/1	0.51	0.62	-	70,70,70,70	0
56	MG	YA	3721	1/1	0.83	0.55	-	65,65,65,65	0
56	MG	YA	3562	1/1	0.93	0.32	-	70,70,70,70	0
56	MG	YA	3065	1/1	0.74	0.70	-	88,88,88,88	0
56	MG	RA	3735	1/1	0.78	0.62	-	66,66,66,66	0
56	MG	YA	3570	1/1	0.84	0.52	-	59,59,59,59	0
56	MG	QA	1748	1/1	0.29	0.54	-	92,92,92,92	0
56	MG	RA	3677	1/1	0.92	1.04	-	61,61,61,61	0
56	MG	YA	3244	1/1	0.91	0.66	-	39,39,39,39	0
56	MG	RA	3559	1/1	0.62	0.37	-	97,97,97,97	0
56	MG	YA	3360	1/1	0.92	0.73	-	53,53,53,53	0
56	MG	QA	1857	1/1	0.71	0.71	-	71,71,71,71	0
56	MG	YA	3341	1/1	0.94	0.50	-	42,42,42,42	0
56	MG	RA	3017	1/1	0.91	0.59	-	68,68,68,68	0
56	MG	RA	3549	1/1	-0.17	1.05	-	78,78,78,78	0
56	MG	YA	3164	1/1	0.24	0.87	-	87,87,87,87	0
56	MG	XA	1619	1/1	0.70	0.12	-	74,74,74,74	0
56	MG	RA	3114	1/1	0.85	0.32	-	91,91,91,91	0
56	MG	YA	3048	1/1	0.97	0.26	-	57,57,57,57	0
56	MG	RA	3056	1/1	0.95	0.57	-	70,70,70,70	0
56	MG	QA	1713	1/1	0.77	0.43	-	79,79,79,79	0
56	MG	RB	214	1/1	0.91	0.49	-	44,44,44,44	0
56	MG	QA	1696	1/1	0.65	0.35	-	73,73,73,73	0
56	MG	YA	3392	1/1	0.91	0.56	-	54,54,54,54	0
56	MG	RA	3364	1/1	0.59	0.39	-	96,96,96,96	0
56	MG	RG	202	1/1	0.86	0.09	-	85,85,85,85	0
56	MG	RA	3463	1/1	0.60	0.50	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3315	1/1	0.81	0.79	-	62,62,62,62	0
56	MG	YA	3572	1/1	0.97	0.25	-	28,28,28,28	0
56	MG	RA	3256	1/1	0.67	0.40	-	103,103,103,103	0
56	MG	RA	3187	1/1	0.73	0.53	-	106,106,106,106	0
56	MG	RA	3798	1/1	0.44	1.16	-	99,99,99,99	0
56	MG	RA	3425	1/1	0.46	0.49	-	94,94,94,94	0
56	MG	RA	3415	1/1	0.95	0.54	-	42,42,42,42	0
56	MG	QA	1832	1/1	0.53	0.63	-	92,92,92,92	0
56	MG	RA	3354	1/1	0.89	0.18	-	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.