



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2016 – 10:33 AM EDT

PDB ID : 5CZP
Title : 70S termination complex containing E. coli RF2
Authors : Hoffer, E.D.; Dunham, C.M.
Deposited on : 2015-07-31
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

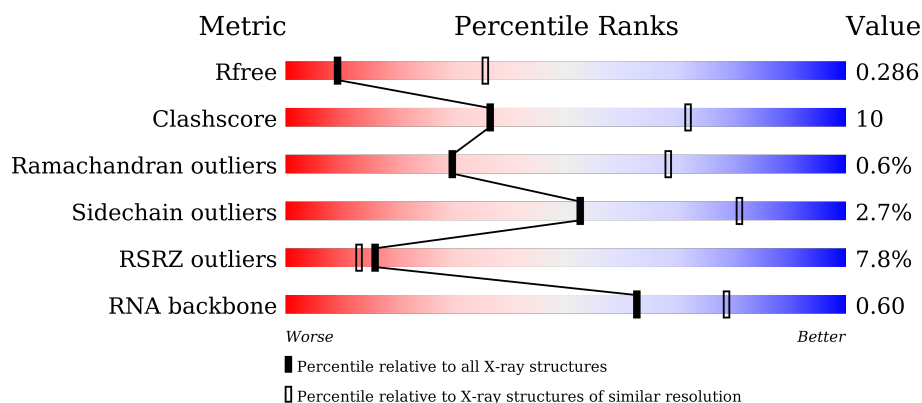
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	RA	2915	<div> <div>4%</div> <div>61% 31% 5% .</div> </div>
1	YA	2915	<div> <div>4%</div> <div>62% 31% 5% .</div> </div>
2	RB	122	<div> <div>2%</div> <div>78% 19% ..</div> </div>
2	YB	122	<div> <div>2%</div> <div>66% 30% ..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	RD	276	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
3	YD	276	<div> <div>%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
4	RE	206	<div> <div>2%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
4	YE	206	<div> <div>2%</div> <div>72%</div> <div>24%</div> <div>...</div> </div>
5	RF	210	<div> <div>%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
5	YF	210	<div> <div>67%</div> <div>28%</div> <div>..</div> </div>
6	RG	182	<div> <div>8%</div> <div>64%</div> <div>35%</div> <div>..</div> </div>
6	YG	182	<div> <div>7%</div> <div>53%</div> <div>41%</div> <div>..</div> </div>
7	RH	180	<div> <div>28%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
7	YH	180	<div> <div>3%</div> <div>61%</div> <div>33%</div> <div>..</div> </div>
8	RI	148	<div> <div>19%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
8	YI	148	<div> <div>7%</div> <div>72%</div> <div>24%</div> <div>..</div> </div>
9	RN	140	<div> <div>8%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
9	YN	140	<div> <div>%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
10	RO	122	<div> <div>%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
10	YO	122	<div> <div>%</div> <div>82%</div> <div>18%</div> <div></div> </div>
11	RP	150	<div> <div>4%</div> <div>74%</div> <div>23%</div> <div>...</div> </div>
11	YP	150	<div> <div>3%</div> <div>73%</div> <div>24%</div> <div>..</div> </div>
12	RQ	141	<div> <div>%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
12	YQ	141	<div> <div>77%</div> <div>20%</div> <div>.</div> </div>
13	RR	118	<div> <div>2%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
13	YR	118	<div> <div>3%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>
14	RS	112	<div> <div>8%</div> <div>78%</div> <div>17%</div> <div>..</div> </div>
14	YS	112	<div> <div>2%</div> <div>67%</div> <div>29%</div> <div>...</div> </div>
15	RT	146	<div> <div>2%</div> <div>63%</div> <div>23%</div> <div>10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	YT	146	
16	RU	118	
16	YU	118	
17	RV	101	
17	YV	101	
18	RW	113	
18	YW	113	
19	RX	96	
19	YX	96	
20	RY	110	
20	YY	110	
21	RZ	206	
21	YZ	206	
22	R0	85	
22	Y0	85	
23	R1	98	
23	Y1	98	
24	R2	72	
24	Y2	72	
25	R3	60	
25	Y3	60	
26	R4	71	
26	Y4	71	
27	R5	60	
27	Y5	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	R6	54	<div>76%</div> <div>74%</div> <div>24%</div> <div>•</div>
28	Y6	54	<div>74%</div> <div>78%</div> <div>20%</div> <div>•</div>
29	R7	49	<div>6%</div> <div>80%</div> <div>16%</div> <div>• •</div>
29	Y7	49	<div>8%</div> <div>80%</div> <div>18%</div> <div>•</div>
30	R8	65	<div>3%</div> <div>69%</div> <div>23%</div> <div>6%</div> <div>•</div>
30	Y8	65	<div>74%</div> <div>22%</div> <div>• •</div>
31	R9	37	<div>54%</div> <div>86%</div> <div>14%</div>
31	Y9	37	<div>51%</div> <div>81%</div> <div>19%</div>
32	QA	1521	<div>2%</div> <div>58%</div> <div>35%</div> <div>6%</div> <div>•</div>
32	XA	1521	<div>2%</div> <div>58%</div> <div>34%</div> <div>6%</div> <div>•</div>
33	QB	256	<div>9%</div> <div>54%</div> <div>32%</div> <div>•</div> <div>10%</div>
33	XB	256	<div>9%</div> <div>52%</div> <div>32%</div> <div>5%</div> <div>•</div> <div>10%</div>
34	QC	239	<div>10%</div> <div>67%</div> <div>18%</div> <div>14%</div>
34	XC	239	<div>8%</div> <div>56%</div> <div>30%</div> <div>14%</div>
35	QD	209	<div>4%</div> <div>67%</div> <div>30%</div> <div>• •</div>
35	XD	209	<div>9%</div> <div>78%</div> <div>20%</div> <div>•</div>
36	QE	162	<div>6%</div> <div>65%</div> <div>25%</div> <div>• •</div> <div>9%</div>
36	XE	162	<div>6%</div> <div>64%</div> <div>27%</div> <div>•</div> <div>9%</div>
37	QF	101	<div>8%</div> <div>77%</div> <div>20%</div> <div>• •</div>
37	XF	101	<div>3%</div> <div>73%</div> <div>23%</div> <div>• • •</div>
38	QG	156	<div>15%</div> <div>71%</div> <div>28%</div> <div>• •</div>
38	XG	156	<div>10%</div> <div>76%</div> <div>21%</div> <div>• •</div>
39	QH	138	<div>10%</div> <div>67%</div> <div>30%</div> <div>• •</div>
39	XH	138	<div>7%</div> <div>75%</div> <div>21%</div> <div>• • •</div>
40	QI	128	<div>23%</div> <div>66%</div> <div>30%</div> <div>• • •</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	XI	128	
41	QJ	105	
41	XJ	105	
42	QK	129	
42	XK	129	
43	QL	132	
43	XL	132	
44	QM	126	
44	XM	126	
45	QN	61	
45	XN	61	
46	QO	89	
46	XO	89	
47	QP	88	
47	XP	88	
48	QQ	105	
48	XQ	105	
49	QR	88	
49	XR	88	
50	QS	93	
50	XS	93	
51	QT	106	
51	XT	106	
52	QU	27	
52	XU	27	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	QV	77	
53	XV	77	
54	QY	380	
54	XY	380	
55	QX	25	
55	XX	25	

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	1614	-	-	-	X
56	MG	QA	1616	-	-	-	X
56	MG	QA	1618	-	-	-	X
56	MG	QA	1619	-	-	-	X
56	MG	QA	1622	-	-	-	X
56	MG	QA	1623	-	-	-	X
56	MG	QA	1625	-	-	-	X
56	MG	QA	1626	-	-	-	X
56	MG	QA	1634	-	-	-	X
56	MG	QA	1638	-	-	-	X
56	MG	QA	1647	-	-	-	X
56	MG	QA	1654	-	-	-	X
56	MG	QA	1658	-	-	-	X
56	MG	QA	1671	-	-	-	X
56	MG	QA	1672	-	-	-	X
56	MG	QA	1680	-	-	-	X
56	MG	QA	1682	-	-	-	X
56	MG	QA	1691	-	-	-	X
56	MG	QA	1704	-	-	-	X
56	MG	QA	1706	-	-	-	X
56	MG	QA	1708	-	-	-	X
56	MG	QA	1711	-	-	-	X
56	MG	QA	1715	-	-	-	X
56	MG	QA	1724	-	-	-	X
56	MG	QA	1731	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1737	-	-	-	X
56	MG	QA	1759	-	-	-	X
56	MG	QA	1771	-	-	-	X
56	MG	QA	1773	-	-	-	X
56	MG	QA	1780	-	-	-	X
56	MG	QA	1802	-	-	-	X
56	MG	QA	1814	-	-	-	X
56	MG	QA	1823	-	-	-	X
56	MG	QA	1828	-	-	-	X
56	MG	QA	1829	-	-	-	X
56	MG	QA	1832	-	-	-	X
56	MG	QA	1835	-	-	-	X
56	MG	QA	1843	-	-	-	X
56	MG	QA	1849	-	-	-	X
56	MG	QA	1854	-	-	-	X
56	MG	QA	1857	-	-	-	X
56	MG	QA	1860	-	-	-	X
56	MG	QA	1872	-	-	-	X
56	MG	QA	1877	-	-	-	X
56	MG	QD	303	-	-	-	X
56	MG	QD	305	-	-	-	X
56	MG	QF	201	-	-	-	X
56	MG	QN	102	-	-	-	X
56	MG	QN	103	-	-	-	X
56	MG	QR	101	-	-	-	X
56	MG	QT	201	-	-	-	X
56	MG	QY	401	-	-	-	X
56	MG	R0	103	-	-	-	X
56	MG	R1	102	-	-	-	X
56	MG	R1	104	-	-	-	X
56	MG	R3	102	-	-	-	X
56	MG	R5	101	-	-	-	X
56	MG	R8	101	-	-	-	X
56	MG	RA	3006	-	-	-	X
56	MG	RA	3014	-	-	-	X
56	MG	RA	3020	-	-	-	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3032	-	-	-	X
56	MG	RA	3040	-	-	-	X
56	MG	RA	3041	-	-	-	X
56	MG	RA	3043	-	-	-	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	3077	-	-	-	X
56	MG	RA	3082	-	-	-	X
56	MG	RA	3088	-	-	-	X
56	MG	RA	3092	-	-	-	X
56	MG	RA	3094	-	-	-	X
56	MG	RA	3098	-	-	-	X
56	MG	RA	3101	-	-	-	X
56	MG	RA	3102	-	-	-	X
56	MG	RA	3109	-	-	-	X
56	MG	RA	3113	-	-	-	X
56	MG	RA	3116	-	-	-	X
56	MG	RA	3117	-	-	-	X
56	MG	RA	3118	-	-	-	X
56	MG	RA	3119	-	-	-	X
56	MG	RA	3121	-	-	-	X
56	MG	RA	3122	-	-	-	X
56	MG	RA	3125	-	-	-	X
56	MG	RA	3128	-	-	-	X
56	MG	RA	3132	-	-	-	X
56	MG	RA	3136	-	-	-	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	3179	-	-	-	X
56	MG	RA	3185	-	-	-	X
56	MG	RA	3186	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3187	-	-	-	X
56	MG	RA	3197	-	-	-	X
56	MG	RA	3205	-	-	-	X
56	MG	RA	3208	-	-	-	X
56	MG	RA	3211	-	-	-	X
56	MG	RA	3217	-	-	-	X
56	MG	RA	3221	-	-	-	X
56	MG	RA	3226	-	-	-	X
56	MG	RA	3230	-	-	-	X
56	MG	RA	3231	-	-	-	X
56	MG	RA	3232	-	-	-	X
56	MG	RA	3234	-	-	-	X
56	MG	RA	3235	-	-	-	X
56	MG	RA	3241	-	-	-	X
56	MG	RA	3248	-	-	-	X
56	MG	RA	3251	-	-	-	X
56	MG	RA	3252	-	-	-	X
56	MG	RA	3265	-	-	-	X
56	MG	RA	3271	-	-	-	X
56	MG	RA	3275	-	-	-	X
56	MG	RA	3279	-	-	-	X
56	MG	RA	3290	-	-	-	X
56	MG	RA	3299	-	-	-	X
56	MG	RA	3300	-	-	-	X
56	MG	RA	3302	-	-	-	X
56	MG	RA	3307	-	-	-	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	3352	-	-	-	X
56	MG	RA	3356	-	-	-	X
56	MG	RA	3359	-	-	-	X
56	MG	RA	3361	-	-	-	X
56	MG	RA	3364	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3366	-	-	-	X
56	MG	RA	3377	-	-	-	X
56	MG	RA	3379	-	-	-	X
56	MG	RA	3381	-	-	-	X
56	MG	RA	3382	-	-	-	X
56	MG	RA	3384	-	-	-	X
56	MG	RA	3385	-	-	-	X
56	MG	RA	3386	-	-	-	X
56	MG	RA	3387	-	-	-	X
56	MG	RA	3390	-	-	-	X
56	MG	RA	3391	-	-	-	X
56	MG	RA	3392	-	-	-	X
56	MG	RA	3394	-	-	-	X
56	MG	RA	3399	-	-	-	X
56	MG	RA	3401	-	-	-	X
56	MG	RA	3402	-	-	-	X
56	MG	RA	3404	-	-	-	X
56	MG	RA	3408	-	-	-	X
56	MG	RA	3409	-	-	-	X
56	MG	RA	3412	-	-	-	X
56	MG	RA	3419	-	-	-	X
56	MG	RA	3421	-	-	-	X
56	MG	RA	3424	-	-	-	X
56	MG	RA	3431	-	-	-	X
56	MG	RA	3436	-	-	-	X
56	MG	RA	3444	-	-	-	X
56	MG	RA	3452	-	-	-	X
56	MG	RA	3458	-	-	-	X
56	MG	RA	3462	-	-	-	X
56	MG	RA	3465	-	-	-	X
56	MG	RA	3466	-	-	-	X
56	MG	RA	3468	-	-	-	X
56	MG	RA	3470	-	-	-	X
56	MG	RA	3471	-	-	-	X
56	MG	RA	3472	-	-	-	X
56	MG	RA	3473	-	-	-	X
56	MG	RA	3476	-	-	-	X
56	MG	RA	3477	-	-	-	X
56	MG	RA	3479	-	-	-	X
56	MG	RA	3483	-	-	-	X
56	MG	RA	3484	-	-	-	X
56	MG	RA	3486	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3491	-	-	-	X
56	MG	RA	3496	-	-	-	X
56	MG	RA	3497	-	-	-	X
56	MG	RA	3501	-	-	-	X
56	MG	RA	3502	-	-	-	X
56	MG	RA	3505	-	-	-	X
56	MG	RA	3512	-	-	-	X
56	MG	RA	3514	-	-	-	X
56	MG	RA	3518	-	-	-	X
56	MG	RA	3521	-	-	-	X
56	MG	RA	3524	-	-	-	X
56	MG	RA	3526	-	-	-	X
56	MG	RA	3533	-	-	-	X
56	MG	RA	3535	-	-	-	X
56	MG	RA	3536	-	-	-	X
56	MG	RA	3537	-	-	-	X
56	MG	RA	3538	-	-	-	X
56	MG	RA	3539	-	-	-	X
56	MG	RA	3551	-	-	-	X
56	MG	RA	3566	-	-	-	X
56	MG	RA	3568	-	-	-	X
56	MG	RA	3572	-	-	-	X
56	MG	RA	3574	-	-	-	X
56	MG	RA	3588	-	-	-	X
56	MG	RA	3598	-	-	-	X
56	MG	RA	3601	-	-	-	X
56	MG	RA	3603	-	-	-	X
56	MG	RA	3607	-	-	-	X
56	MG	RA	3609	-	-	-	X
56	MG	RA	3611	-	-	-	X
56	MG	RA	3614	-	-	-	X
56	MG	RA	3616	-	-	-	X
56	MG	RA	3618	-	-	-	X
56	MG	RA	3623	-	-	-	X
56	MG	RA	3624	-	-	-	X
56	MG	RA	3630	-	-	-	X
56	MG	RA	3631	-	-	-	X
56	MG	RA	3634	-	-	-	X
56	MG	RA	3635	-	-	-	X
56	MG	RA	3638	-	-	-	X
56	MG	RA	3644	-	-	-	X
56	MG	RA	3656	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3659	-	-	-	X
56	MG	RA	3677	-	-	-	X
56	MG	RA	3679	-	-	-	X
56	MG	RA	3684	-	-	-	X
56	MG	RA	3696	-	-	-	X
56	MG	RA	3697	-	-	-	X
56	MG	RA	3707	-	-	-	X
56	MG	RA	3708	-	-	-	X
56	MG	RA	3709	-	-	-	X
56	MG	RA	3712	-	-	-	X
56	MG	RA	3713	-	-	-	X
56	MG	RA	3715	-	-	-	X
56	MG	RA	3717	-	-	-	X
56	MG	RA	3722	-	-	-	X
56	MG	RA	3724	-	-	-	X
56	MG	RA	3727	-	-	-	X
56	MG	RA	3733	-	-	-	X
56	MG	RA	3738	-	-	-	X
56	MG	RA	3742	-	-	-	X
56	MG	RA	3744	-	-	-	X
56	MG	RA	3746	-	-	-	X
56	MG	RA	3751	-	-	-	X
56	MG	RA	3754	-	-	-	X
56	MG	RA	3767	-	-	-	X
56	MG	RA	3770	-	-	-	X
56	MG	RA	3771	-	-	-	X
56	MG	RA	3773	-	-	-	X
56	MG	RA	3774	-	-	-	X
56	MG	RA	3786	-	-	-	X
56	MG	RA	3795	-	-	-	X
56	MG	RA	3803	-	-	-	X
56	MG	RA	3805	-	-	-	X
56	MG	RA	3807	-	-	-	X
56	MG	RA	3809	-	-	-	X
56	MG	RA	3812	-	-	-	X
56	MG	RA	3814	-	-	-	X
56	MG	RA	3821	-	-	-	X
56	MG	RA	3823	-	-	-	X
56	MG	RA	3827	-	-	-	X
56	MG	RA	3829	-	-	-	X
56	MG	RA	3839	-	-	-	X
56	MG	RA	3850	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3854	-	-	-	X
56	MG	RA	3856	-	-	-	X
56	MG	RA	3858	-	-	-	X
56	MG	RA	3862	-	-	-	X
56	MG	RA	3871	-	-	-	X
56	MG	RA	3874	-	-	-	X
56	MG	RA	3875	-	-	-	X
56	MG	RA	3882	-	-	-	X
56	MG	RA	3889	-	-	-	X
56	MG	RA	3892	-	-	-	X
56	MG	RA	3893	-	-	-	X
56	MG	RA	3900	-	-	-	X
56	MG	RA	3902	-	-	-	X
56	MG	RA	3903	-	-	-	X
56	MG	RA	3906	-	-	-	X
56	MG	RA	3911	-	-	-	X
56	MG	RA	3917	-	-	-	X
56	MG	RA	3924	-	-	-	X
56	MG	RA	3928	-	-	-	X
56	MG	RA	3938	-	-	-	X
56	MG	RA	3939	-	-	-	X
56	MG	RA	3941	-	-	-	X
56	MG	RA	3948	-	-	-	X
56	MG	RA	3952	-	-	-	X
56	MG	RA	3953	-	-	-	X
56	MG	RA	3959	-	-	-	X
56	MG	RA	3967	-	-	-	X
56	MG	RA	3969	-	-	-	X
56	MG	RA	3971	-	-	-	X
56	MG	RA	3981	-	-	-	X
56	MG	RA	3986	-	-	-	X
56	MG	RA	3990	-	-	-	X
56	MG	RA	4002	-	-	-	X
56	MG	RA	4003	-	-	-	X
56	MG	RA	4006	-	-	-	X
56	MG	RA	4008	-	-	-	X
56	MG	RA	4009	-	-	-	X
56	MG	RA	4012	-	-	-	X
56	MG	RA	4017	-	-	-	X
56	MG	RA	4018	-	-	-	X
56	MG	RA	4021	-	-	-	X
56	MG	RA	4023	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	4024	-	-	-	X
56	MG	RA	4025	-	-	-	X
56	MG	RA	4026	-	-	-	X
56	MG	RA	4027	-	-	-	X
56	MG	RA	4028	-	-	-	X
56	MG	RA	4030	-	-	-	X
56	MG	RA	4032	-	-	-	X
56	MG	RA	4033	-	-	-	X
56	MG	RA	4034	-	-	-	X
56	MG	RA	4035	-	-	-	X
56	MG	RA	4036	-	-	-	X
56	MG	RA	4037	-	-	-	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	4051	-	-	-	X
56	MG	RA	4052	-	-	-	X
56	MG	RA	4056	-	-	-	X
56	MG	RA	4057	-	-	-	X
56	MG	RA	4058	-	-	-	X
56	MG	RA	4059	-	-	-	X
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	RA	4067	-	-	-	X
56	MG	RA	4068	-	-	-	X
56	MG	RB	201	-	-	-	X
56	MG	RB	209	-	-	-	X
56	MG	RB	225	-	-	-	X
56	MG	RD	302	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RD	303	-	-	-	X
56	MG	RD	305	-	-	-	X
56	MG	RD	306	-	-	-	X
56	MG	RD	308	-	-	-	X
56	MG	RD	309	-	-	-	X
56	MG	RD	312	-	-	-	X
56	MG	RD	313	-	-	-	X
56	MG	RE	302	-	-	-	X
56	MG	RE	306	-	-	-	X
56	MG	RE	307	-	-	-	X
56	MG	RF	301	-	-	-	X
56	MG	RF	303	-	-	-	X
56	MG	RF	304	-	-	-	X
56	MG	RF	305	-	-	-	X
56	MG	RF	306	-	-	-	X
56	MG	RF	308	-	-	-	X
56	MG	RF	309	-	-	-	X
56	MG	RF	311	-	-	-	X
56	MG	RN	201	-	-	-	X
56	MG	RP	201	-	-	-	X
56	MG	RQ	201	-	-	-	X
56	MG	RQ	204	-	-	-	X
56	MG	RR	201	-	-	-	X
56	MG	RR	202	-	-	-	X
56	MG	RU	203	-	-	-	X
56	MG	RV	202	-	-	-	X
56	MG	RV	203	-	-	-	X
56	MG	RX	101	-	-	-	X
56	MG	XA	1609	-	-	-	X
56	MG	XA	1611	-	-	-	X
56	MG	XA	1612	-	-	-	X
56	MG	XA	1616	-	-	-	X
56	MG	XA	1618	-	-	-	X
56	MG	XA	1623	-	-	-	X
56	MG	XA	1627	-	-	-	X
56	MG	XA	1628	-	-	-	X
56	MG	XA	1629	-	-	-	X
56	MG	XA	1631	-	-	-	X
56	MG	XA	1632	-	-	-	X
56	MG	XA	1633	-	-	-	X
56	MG	XA	1637	-	-	-	X
56	MG	XA	1645	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	XA	1658	-	-	-	X
56	MG	XA	1666	-	-	-	X
56	MG	XA	1673	-	-	-	X
56	MG	XA	1683	-	-	-	X
56	MG	XA	1688	-	-	-	X
56	MG	XA	1690	-	-	-	X
56	MG	XA	1696	-	-	-	X
56	MG	XA	1700	-	-	-	X
56	MG	XA	1707	-	-	-	X
56	MG	XA	1720	-	-	-	X
56	MG	XA	1723	-	-	-	X
56	MG	XA	1725	-	-	-	X
56	MG	XA	1727	-	-	-	X
56	MG	XA	1728	-	-	-	X
56	MG	XA	1731	-	-	-	X
56	MG	XA	1737	-	-	-	X
56	MG	XA	1738	-	-	-	X
56	MG	XA	1741	-	-	-	X
56	MG	XA	1744	-	-	-	X
56	MG	XA	1747	-	-	-	X
56	MG	XA	1758	-	-	-	X
56	MG	XA	1759	-	-	-	X
56	MG	XA	1760	-	-	-	X
56	MG	XA	1763	-	-	-	X
56	MG	XA	1770	-	-	-	X
56	MG	XA	1772	-	-	-	X
56	MG	XA	1774	-	-	-	X
56	MG	XA	1776	-	-	-	X
56	MG	XA	1777	-	-	-	X
56	MG	XA	1780	-	-	-	X
56	MG	XA	1781	-	-	-	X
56	MG	XA	1786	-	-	-	X
56	MG	XA	1792	-	-	-	X
56	MG	XA	1793	-	-	-	X
56	MG	XF	202	-	-	-	X
56	MG	XT	201	-	-	-	X
56	MG	Y0	101	-	-	-	X
56	MG	Y6	102	-	-	-	X
56	MG	Y8	101	-	-	-	X
56	MG	YA	3007	-	-	-	X
56	MG	YA	3008	-	-	-	X
56	MG	YA	3011	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3013	-	-	-	X
56	MG	YA	3019	-	-	-	X
56	MG	YA	3020	-	-	-	X
56	MG	YA	3027	-	-	-	X
56	MG	YA	3028	-	-	-	X
56	MG	YA	3030	-	-	-	X
56	MG	YA	3033	-	-	-	X
56	MG	YA	3036	-	-	-	X
56	MG	YA	3049	-	-	-	X
56	MG	YA	3053	-	-	-	X
56	MG	YA	3058	-	-	-	X
56	MG	YA	3071	-	-	-	X
56	MG	YA	3074	-	-	-	X
56	MG	YA	3077	-	-	-	X
56	MG	YA	3088	-	-	-	X
56	MG	YA	3089	-	-	-	X
56	MG	YA	3091	-	-	-	X
56	MG	YA	3092	-	-	-	X
56	MG	YA	3094	-	-	-	X
56	MG	YA	3102	-	-	-	X
56	MG	YA	3104	-	-	-	X
56	MG	YA	3107	-	-	-	X
56	MG	YA	3110	-	-	-	X
56	MG	YA	3112	-	-	-	X
56	MG	YA	3122	-	-	-	X
56	MG	YA	3129	-	-	-	X
56	MG	YA	3131	-	-	-	X
56	MG	YA	3133	-	-	-	X
56	MG	YA	3134	-	-	-	X
56	MG	YA	3146	-	-	-	X
56	MG	YA	3148	-	-	-	X
56	MG	YA	3150	-	-	-	X
56	MG	YA	3152	-	-	-	X
56	MG	YA	3153	-	-	-	X
56	MG	YA	3156	-	-	-	X
56	MG	YA	3166	-	-	-	X
56	MG	YA	3170	-	-	-	X
56	MG	YA	3174	-	-	-	X
56	MG	YA	3183	-	-	-	X
56	MG	YA	3192	-	-	-	X
56	MG	YA	3199	-	-	-	X
56	MG	YA	3201	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3209	-	-	-	X
56	MG	YA	3210	-	-	-	X
56	MG	YA	3216	-	-	-	X
56	MG	YA	3217	-	-	-	X
56	MG	YA	3237	-	-	-	X
56	MG	YA	3240	-	-	-	X
56	MG	YA	3247	-	-	-	X
56	MG	YA	3249	-	-	-	X
56	MG	YA	3268	-	-	-	X
56	MG	YA	3269	-	-	-	X
56	MG	YA	3270	-	-	-	X
56	MG	YA	3272	-	-	-	X
56	MG	YA	3284	-	-	-	X
56	MG	YA	3285	-	-	-	X
56	MG	YA	3291	-	-	-	X
56	MG	YA	3295	-	-	-	X
56	MG	YA	3297	-	-	-	X
56	MG	YA	3299	-	-	-	X
56	MG	YA	3303	-	-	-	X
56	MG	YA	3311	-	-	-	X
56	MG	YA	3314	-	-	-	X
56	MG	YA	3316	-	-	-	X
56	MG	YA	3317	-	-	-	X
56	MG	YA	3318	-	-	-	X
56	MG	YA	3320	-	-	-	X
56	MG	YA	3321	-	-	-	X
56	MG	YA	3323	-	-	-	X
56	MG	YA	3324	-	-	-	X
56	MG	YA	3325	-	-	-	X
56	MG	YA	3326	-	-	-	X
56	MG	YA	3328	-	-	-	X
56	MG	YA	3332	-	-	-	X
56	MG	YA	3335	-	-	-	X
56	MG	YA	3336	-	-	-	X
56	MG	YA	3339	-	-	-	X
56	MG	YA	3343	-	-	-	X
56	MG	YA	3345	-	-	-	X
56	MG	YA	3350	-	-	-	X
56	MG	YA	3351	-	-	-	X
56	MG	YA	3355	-	-	-	X
56	MG	YA	3360	-	-	-	X
56	MG	YA	3361	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3368	-	-	-	X
56	MG	YA	3374	-	-	-	X
56	MG	YA	3377	-	-	-	X
56	MG	YA	3378	-	-	-	X
56	MG	YA	3382	-	-	-	X
56	MG	YA	3384	-	-	-	X
56	MG	YA	3386	-	-	-	X
56	MG	YA	3387	-	-	-	X
56	MG	YA	3388	-	-	-	X
56	MG	YA	3391	-	-	-	X
56	MG	YA	3392	-	-	-	X
56	MG	YA	3397	-	-	-	X
56	MG	YA	3398	-	-	-	X
56	MG	YA	3401	-	-	-	X
56	MG	YA	3404	-	-	-	X
56	MG	YA	3409	-	-	-	X
56	MG	YA	3413	-	-	-	X
56	MG	YA	3415	-	-	-	X
56	MG	YA	3419	-	-	-	X
56	MG	YA	3420	-	-	-	X
56	MG	YA	3421	-	-	-	X
56	MG	YA	3429	-	-	-	X
56	MG	YA	3439	-	-	-	X
56	MG	YA	3440	-	-	-	X
56	MG	YA	3446	-	-	-	X
56	MG	YA	3447	-	-	-	X
56	MG	YA	3449	-	-	-	X
56	MG	YA	3456	-	-	-	X
56	MG	YA	3468	-	-	-	X
56	MG	YA	3474	-	-	-	X
56	MG	YA	3475	-	-	-	X
56	MG	YA	3476	-	-	-	X
56	MG	YA	3485	-	-	-	X
56	MG	YA	3488	-	-	-	X
56	MG	YA	3495	-	-	-	X
56	MG	YA	3499	-	-	-	X
56	MG	YA	3503	-	-	-	X
56	MG	YA	3509	-	-	-	X
56	MG	YA	3511	-	-	-	X
56	MG	YA	3514	-	-	-	X
56	MG	YA	3516	-	-	-	X
56	MG	YA	3517	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3518	-	-	-	X
56	MG	YA	3532	-	-	-	X
56	MG	YA	3538	-	-	-	X
56	MG	YA	3540	-	-	-	X
56	MG	YA	3550	-	-	-	X
56	MG	YA	3552	-	-	-	X
56	MG	YA	3554	-	-	-	X
56	MG	YA	3560	-	-	-	X
56	MG	YA	3570	-	-	-	X
56	MG	YA	3577	-	-	-	X
56	MG	YA	3578	-	-	-	X
56	MG	YA	3579	-	-	-	X
56	MG	YA	3580	-	-	-	X
56	MG	YA	3582	-	-	-	X
56	MG	YA	3587	-	-	-	X
56	MG	YA	3588	-	-	-	X
56	MG	YA	3600	-	-	-	X
56	MG	YA	3601	-	-	-	X
56	MG	YA	3606	-	-	-	X
56	MG	YA	3607	-	-	-	X
56	MG	YA	3610	-	-	-	X
56	MG	YA	3611	-	-	-	X
56	MG	YA	3612	-	-	-	X
56	MG	YA	3613	-	-	-	X
56	MG	YA	3614	-	-	-	X
56	MG	YA	3616	-	-	-	X
56	MG	YA	3621	-	-	-	X
56	MG	YA	3623	-	-	-	X
56	MG	YA	3630	-	-	-	X
56	MG	YA	3632	-	-	-	X
56	MG	YA	3633	-	-	-	X
56	MG	YA	3647	-	-	-	X
56	MG	YA	3648	-	-	-	X
56	MG	YA	3650	-	-	-	X
56	MG	YA	3656	-	-	-	X
56	MG	YA	3658	-	-	-	X
56	MG	YA	3660	-	-	-	X
56	MG	YA	3664	-	-	-	X
56	MG	YA	3665	-	-	-	X
56	MG	YA	3668	-	-	-	X
56	MG	YA	3679	-	-	-	X
56	MG	YA	3681	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YA	3684	-	-	-	X
56	MG	YA	3685	-	-	-	X
56	MG	YA	3689	-	-	-	X
56	MG	YA	3691	-	-	-	X
56	MG	YA	3694	-	-	-	X
56	MG	YA	3699	-	-	-	X
56	MG	YA	3701	-	-	-	X
56	MG	YA	3702	-	-	-	X
56	MG	YA	3704	-	-	-	X
56	MG	YA	3705	-	-	-	X
56	MG	YA	3709	-	-	-	X
56	MG	YA	3710	-	-	-	X
56	MG	YA	3714	-	-	-	X
56	MG	YA	3715	-	-	-	X
56	MG	YA	3724	-	-	-	X
56	MG	YA	3727	-	-	-	X
56	MG	YA	3729	-	-	-	X
56	MG	YA	3733	-	-	-	X
56	MG	YA	3737	-	-	-	X
56	MG	YA	3740	-	-	-	X
56	MG	YA	3744	-	-	-	X
56	MG	YA	3745	-	-	-	X
56	MG	YA	3746	-	-	-	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	3752	-	-	-	X
56	MG	YA	3753	-	-	-	X
56	MG	YA	3754	-	-	-	X
56	MG	YA	3755	-	-	-	X
56	MG	YA	3756	-	-	-	X
56	MG	YB	214	-	-	-	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	301	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	YE	302	-	-	-	X
56	MG	YE	303	-	-	-	X
56	MG	YE	305	-	-	-	X
56	MG	YF	301	-	-	-	X
56	MG	YF	303	-	-	-	X
56	MG	YQ	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 [i](#)

There are 58 unique types of molecules in this entry. The entry contains 296497 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 23S rRNA.

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

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	YI	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			
8	RI	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

Continued on next page...

Continued from previous page...

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Y2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			
24	R2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R4	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

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

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

- Molecule 32 is a RNA chain called 16S rRNA.

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

- Molecule 33 is a protein called 30S ribosomal protein S2.

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

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

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

- Molecule 37 is a protein called 30S ribosomal protein S6.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	XI	126	Total	C	N	O	0	0	0
			966	613	186	167			
40	QI	127	Total	C	N	O	0	0	0
			986	625	193	168			

- Molecule 41 is a protein called 30S ribosomal protein S10.

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

- Molecule 42 is a protein called 30S ribosomal protein S11.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 30S ribosomal protein S12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

- Molecule 48 is a protein called 30S ribosomal protein S17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

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

- Molecule 50 is a protein called 30S ribosomal protein S19.

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

- Molecule 51 is a protein called 30S ribosomal protein S20.

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

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

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

- Molecule 53 is a RNA chain called P-site tRNA fMet.

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

- Molecule 54 is a protein called Peptide chain release factor 2.

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

There are 32 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
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
QY	298	VAL	LEU	conflict	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
XY	298	VAL	LEU	conflict	UNP P07012

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	XX	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			
55	QX	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	280	Total	Mg	0	0
			280	280		
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	756	Total	Mg	0	0
			756	756		
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	4	Total	Mg	0	0
			4	4		
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	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YD	9	Total 9	Mg 9	0	0
56	QV	4	Total 4	Mg 4	0	0
56	RX	1	Total 1	Mg 1	0	0
56	Y8	2	Total 2	Mg 2	0	0
56	YO	2	Total 2	Mg 2	0	0
56	XA	193	Total 193	Mg 193	0	0
56	QI	1	Total 1	Mg 1	0	0
56	RQ	4	Total 4	Mg 4	0	0
56	R0	4	Total 4	Mg 4	0	0
56	XT	1	Total 1	Mg 1	0	0
56	QR	1	Total 1	Mg 1	0	0
56	QL	2	Total 2	Mg 2	0	0
56	RU	3	Total 3	Mg 3	0	0
56	QG	3	Total 3	Mg 3	0	0
56	RO	1	Total 1	Mg 1	0	0
56	XJ	1	Total 1	Mg 1	0	0
56	QO	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	YG	3	Total 3	Mg 3	0	0
56	XY	1	Total 1	Mg 1	0	0
56	YQ	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YN	1	Total 1	Mg 1	0	0
56	XF	3	Total 3	Mg 3	0	0
56	YX	1	Total 1	Mg 1	0	0
56	RR	4	Total 4	Mg 4	0	0
56	RD	14	Total 14	Mg 14	0	0
56	R1	4	Total 4	Mg 4	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	1069	Total 1069	Mg 1069	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

Continued on next page...

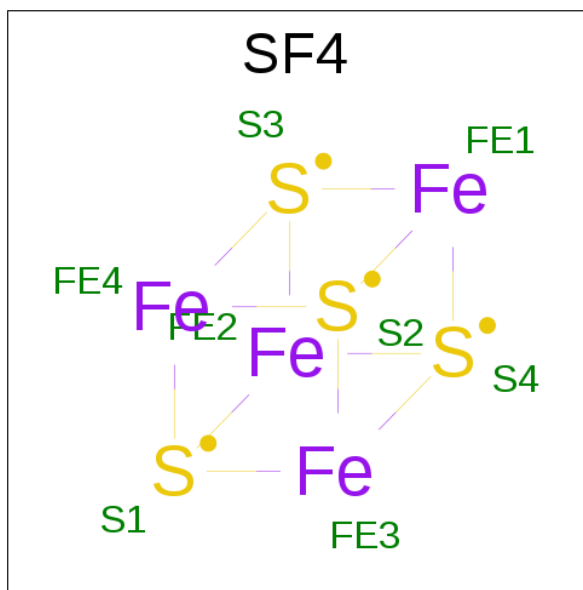
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	R9	2	Total 2	Mg 2	0	0
56	RE	7	Total 7	Mg 7	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	Y6	1	Total 1	Mg 1	0	0
56	YW	2	Total 2	Mg 2	0	0
56	RW	2	Total 2	Mg 2	0	0
56	QY	2	Total 2	Mg 2	0	0
56	XH	1	Total 1	Mg 1	0	0
56	XV	3	Total 3	Mg 3	0	0
56	RB	28	Total 28	Mg 28	0	0
56	YI	1	Total 1	Mg 1	0	0
56	QE	2	Total 2	Mg 2	0	0
56	R5	4	Total 4	Mg 4	0	0
56	R8	1	Total 1	Mg 1	0	0
56	RF	11	Total 11	Mg 11	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: Fe₄S₄).

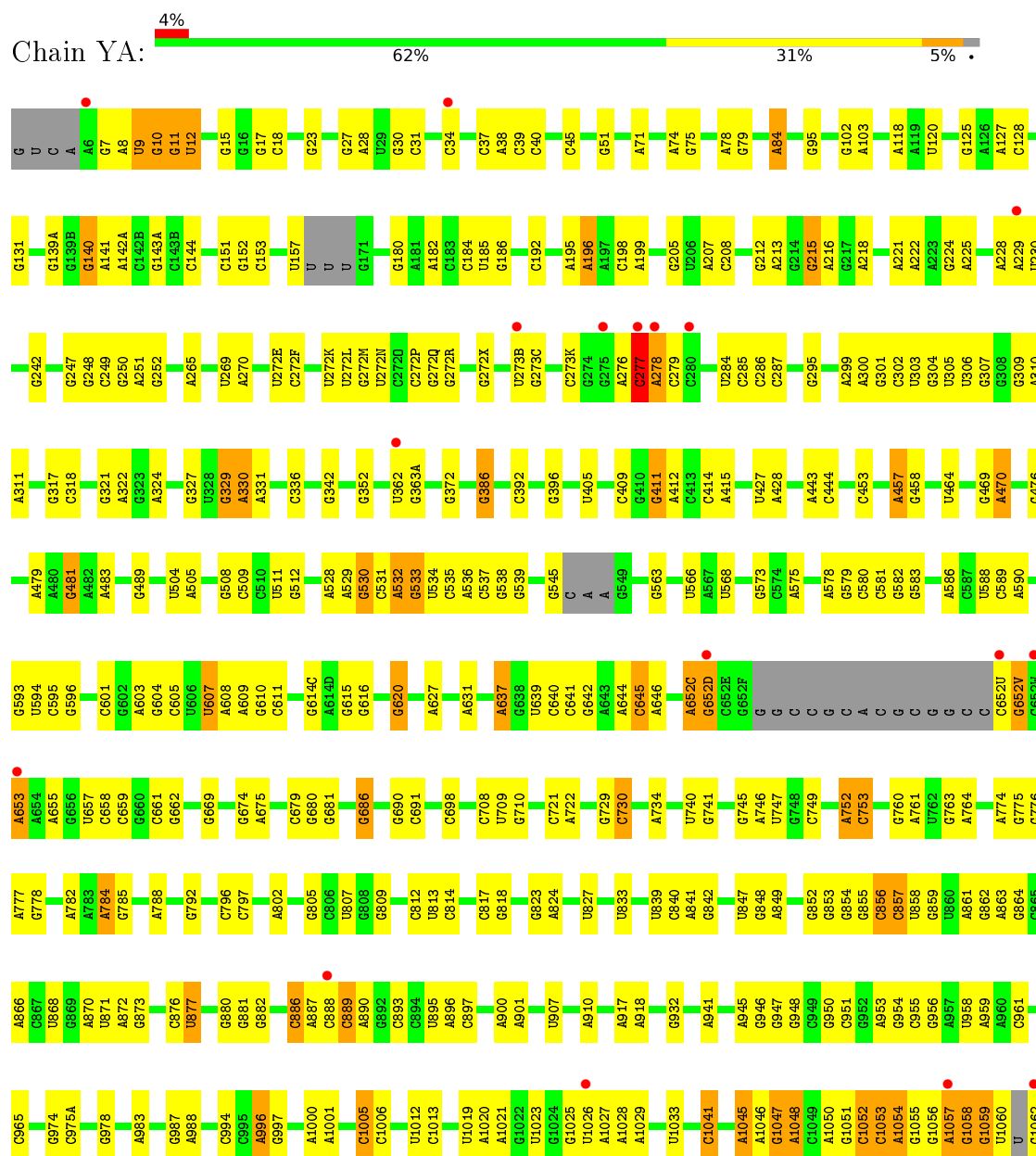


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	XD	1	Total 8	Fe 4	S 4	0	0
58	QD	1	Total 8	Fe 4	S 4	0	0

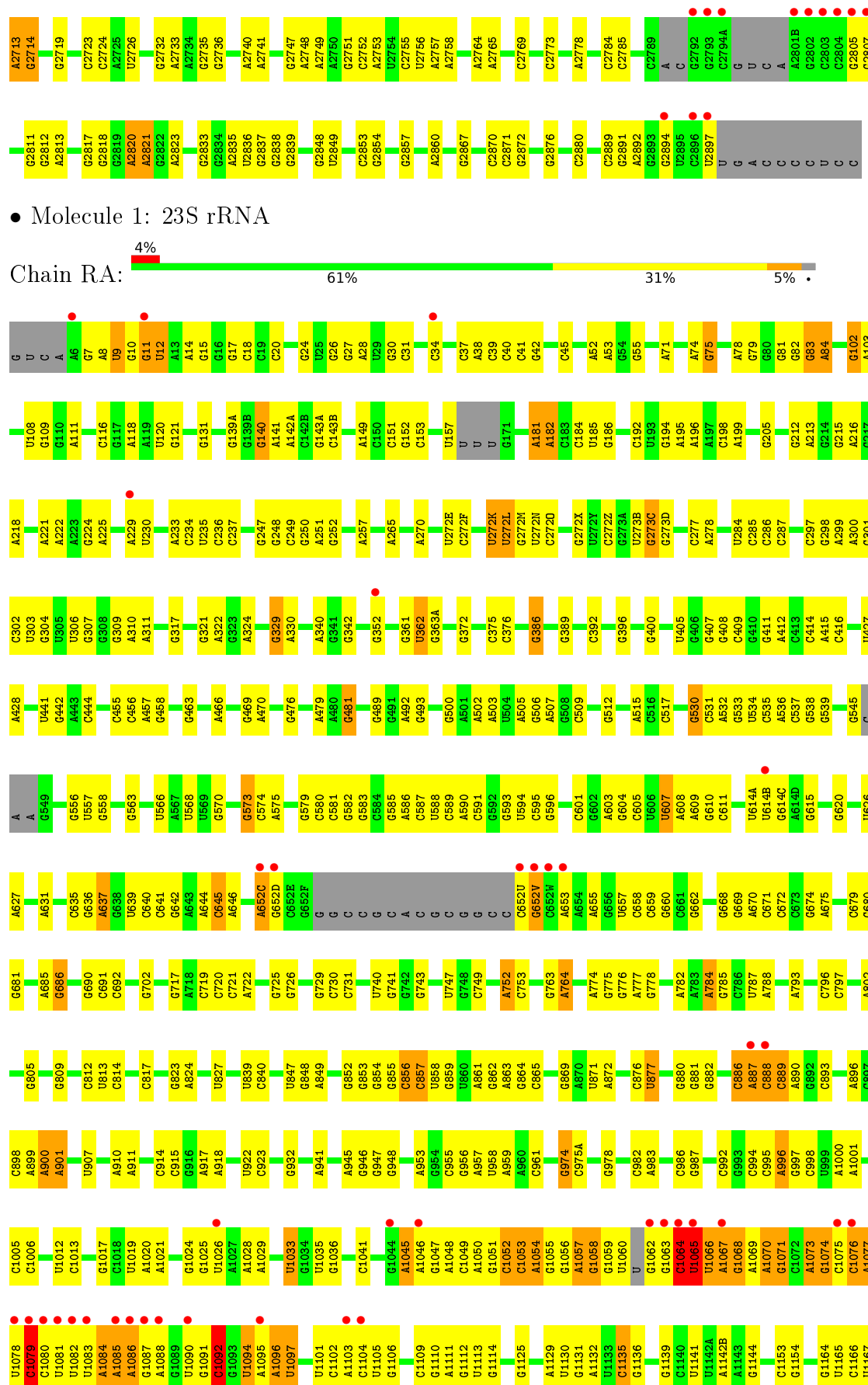
3 Residue-property plots

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: 23S rRNA



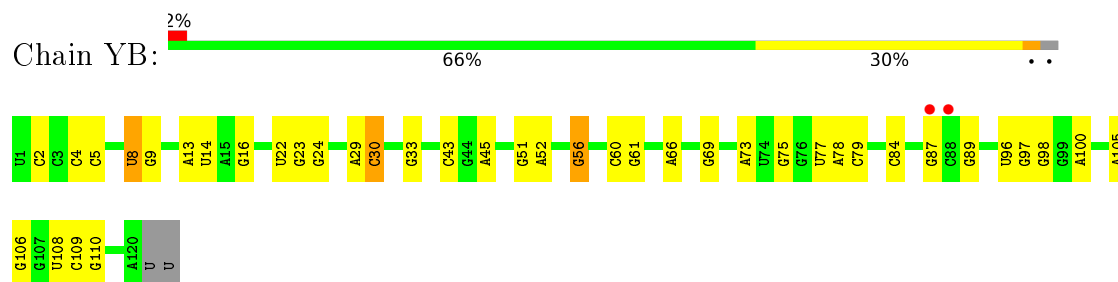
A2602	C2356	A2269	G2165	C2105	G2012	C1866	G1756	A1614	C1509A	C1398	A1278	G1164	G1063
U2603	C2359	G2270	U2166	C2106	A2012	C1876	G1757	G1622	A1509B	C1404	G1279	U1165	U1065
C2604	A2360	G2271	G2167	C2107	A2013	A1877	A1759	U1514	U1514	U1405	C1289	C1166	U1066
U2611	A2361	C2275	C2168	U2109	G2018	G1878	U1762	U1629	U1515	U1406	C1295	U1167	A1067
C2612	C2364	G2279	A2170	C2111	A2019	G1883	G1763	G1630	U1518	C1407	C1296	G1068	
U2615	C2365	C2283	U2172	G2112	U2022	A1884	G1764	U1639	U1519	C1408	C1297	A1069	
C2616	C2366	A2286	A2173	U2113	G2023	A1885	A1773	C1640	G1525	G1410	U1300	G1071	
C2617	G2373	G2287	C2174	A2114	G2024	C1886	C1774	G1645	G1526	U	A	U	G1072
A2629	G2374	A2288	C2175	G2115	C2025	G1889	U1780	C1646	G1529	G1411	A1301	G	A1073
C2630	G2375	G2289	U2180	U2117	C2026	A1900	A1786	G1647	G1530	G1412	A1308	A	C1074
U2635	A2378	U2290	G2181	A2118	A2031	A1906	A1788	C1648	C1530	U1413	G1309	A1182	A1077
C2639	C2379	G2291	G2182	U2119	G2032	G1906	A1786	G1649	C1531	C1414	U1313	G1183	U1078
U2646	G2383	C2292	C2183	G2120	U2033	A1913	A1789	G1650	G1532	C1417	C1314	G1184	C1079
C2640	G2384	C2293	G2186	U2121	U2034	A1914	C1790	G1651	U	U1420	C1315	C1080	C1080
G2642	C2385	C2294	G2187	G2122	G2035	C1914	A1791	C1656	A	G1421	U1316	G1187	U1081
U2646	U2390	G2303	U2188	G2123	C2043	U1915	G1792	C1657	C1536		A1317	U1082	U1082
C2647	U2391	A2304	G2190	U2124	U2047	A1918	C1793	C1658	G1539	G1427	G1318	U1197	U1083
U2648	G2397	C2306	U2191	A2126	U2048	A1919	U1794	A1665	U1540	C1428	U1198	U1198	A1084
C2651	U2406	G2308	G2192	C2128	G2048	C1920	U1795	G1666	G1541	G1429	A1322	A1085	A1085
C2654	C2410	C2312	G2193	C2129	C2055	G1921	U1796	G1667	G1542	C1430	U1323	C1201	A1086
U2659	G2411	U2312	G2194	C2130	G2056	G1929	U1797	A1668	C1543	U1431	A1336	G1206	G1087
C2659	C2412	C2313	G2198	G2131	C2066	U1930	U1798	A1669	U1566	C1432	G1337	G1206	A1088
U2663	G2413	G2314	A2198	U2132	A2060	A1936	C1800	G1674	C1546	G1441	U1340	A1210	U1090
C2669	C2414	C2315	G2206	A2134	A2061	A1937	G1801	U1688	U1578	G1442	A1211	G1212	G1091
U2669	C2420	C2316	G2207	C2135	C2062	A1938	A1802	C1683	C1587	G1443	U1341	G1212	C1092
C2673	A2421	G2317	A2208	U2136	A2063	U1939	C1804	C1684	G1558	G1444	U1352	A1220	U1094
U2679	C2422	C2318	C2209	C2137	C2063	U1946	U1805	C1685	G1560	C1445A	A1353	A1220	A1095
C2680	G2423	G2319	U2218	C2138	C2064	U1946	A1812	G1687	A1566	A1449	A1354	C1230	A1096
U2683	C2424	C2320	G2224	C2139	C2065	C1947	A1812	U1688	A1566	G1450A	G1355	G1231	U1097
C2687	A2425	A2322	A2225	C2140	C2066	G1948	A1815	U1688	A1569	U1453	U1357	G1232	A1098
U2687	G2429	G2325	C2226	G2141	G2069	U1949	G1816	U1693	U1578	G1455	G1358	G1236	G1099
C2689	C2430	C2326	U2233	C2142	G2070	U1951	G1816	G1696	A1579	C1459	A1359	A1248	U1101
U2692	A2435	G2327	G2234	C2145	C2072	U1955	G1823	U1700	A1580	G1459	G1364	U1249	A1102
C2694	C2439	C2329	G2238	G2146	G2073	U1962	C1827	A1701	C1584	C1467	A1365	G1248	A1103
U2695	A2440	G2330	G2239	C2147	U2074	C1962	G1828	A1701	C1584	C1467	G1250	G1248	C1109
C2696	C2443	A2336	U2243	G2149	U2075	U1963	A1829	U1709	A1586	C1471	G1252	G1248	G1110
U2697	C2444	G2337	U2244	U2150	A2077	U1967	C1830	C1710	A1587	A1471	A1253	G1252	A1111
C2699	G2445	C2342	G2245	G2151	C2078	G1967	U1833	C1711	C1588	G1475	G1371	A1254	G1112
U2702	C2446	C2343	U2246	C2152	U2079	G1968	U1834	C1712	C1589	C1476	U1372	U1255	U1113
C2703	G2447	G2344	U2247	G2153	U2086	A1969	G1835	C1712	G1593	A1477	A1379	G1256	G1114
U2709	U2448	C2347	C2248	U2156	G2087	A1970	U1842	U1720	G1594	G1478	G1380	U1263	G1125
C2710	U2449	C2347	C2249	G2157	U2096	A1971	C1843	A1722	A1596	G1479	G1264	G1264	G1126
U2712A	C2452	C2350	G2251	A2158	U2099	U1991	A1847	U1739	C1604	G1482	A1384	A1265	A1129
U2712B	C2453	G2351	U2262	G2159	U2099	G1992	A1848	G1740	C1607	G1482	G1385	G1266	U1130
C2703	A2454	A2352	U2262	C2160	G2100	U1993	A1848	A1741	A1608	C1493	C1386	G1266	U1130
U2709	C2455	C2353	A2266	C2161	G2101	G1997	A1853	G1747B	C1607	U1497	G1387	G1271	C1135
C2710	G2455	G2354	A2267	U2102	G2163	G1997	A1854	U1740	A1609	C1497	G1388	A1272	C1136
U2712A	C2456	C2355	C2267	C2103	C2103	G1998	A1854	G1750	A1610	U1497	G1389	A1273	U1141
C2712B	U2456	C2355	C2268	C2104	C2104	C1999	A1859			A1507	U1396	A1275	U1142A
U2712C	U2457	C2356	C2269	C2105	C2105	C1999	A1859			A1508	U1397	A1276	A1142B



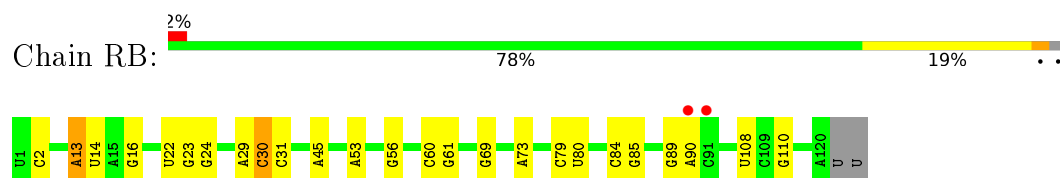
G2802	C2803	A2704	G2804	C2805	G2709	G2710	A2711	U2712A	A2712B	A2713	G2714	C2816	C2817	C2826	G2827	C2828	A2829	G2830	G2831	G2841	G2842	G2843	G2844	G2845	G2846	G2847	A2848	A2849	A2850	G2853	G2854	G2855	G2867	A2868	G2872	G2880	A2883	G2886	A2892	G2893	G2894	G2895	G2896	G2897	U	G	A	C	C	C	C	A	A2801B
C2704	A2705	G2709	G2710	A2711	U2712A	A2712B	A2713	G2714	G2719	U2726	G2727	G2732	A2733	A2734	G2735	G2736	A2740	A2741	C2742	G2747	A2748	A2749	A2750	A2753	U2754	C2755	A2758	A2764	A2765	C2769	A2778	G2779	G2780	A2781	C2785	C2789	A	C	G2792	G2793	G2794	G	U	C	C	A	A2801B						
A2602	G2603	U2604	U2611	C2612	U2615	C2616	C2617	C2626	G2627	C2628	A2629	G2630	G2631	G2641	G2642	G2643	G2644	C2645	U2647	G2648	U2649	U2650	C2651	A2654	A2657	G2663	G2674	G2677	C2678	C2679	C2680	C2683	U2684	U2689	C2691	C2692	A2693	G2694	C2695	U2696	G2697	U2698	C2699	C2703									
G2489	G2490	U2491	C2496	C2502	A2503	U2504	G2505	U2506	C2507	G2513	U2514	C2515	G2516	C2517	A2518	U2519	C2520	G2525	G2529	G2532	U2537	C2538	A2543	G2544	U2547	G2548	G2549	U2554	U2555	A2566	C2567	C2568	A2572	C2573	G2578	G2583	G2584	U2585	U2586	U2587	A2590	C2591	U2592	U2593	C2594								
G2439	C2440	C2441	C2442	C2443	G2444	G2445	G2446	G2447	A2448	U2449	C2452	A2453	G2454	C2455	C2456	C2461	C2462	C2463	C2474	G2475	A2476	C2477	A2478	G2486																													
U2262	G2266	A2267	G2268	A2269	C2275	G2276	G2277	A2278	G2279	G2282	C2283	C2284	C2285	A2286	A2287	G2290	U2291	C2292	G2300	C2301	G2304	A2305	G2308	A2311	U2312	C2317	G2318	G2319	A2320	G2321	A2322	G2325	A2328	G2329	G2330	G2334	G2335	A2336	U2343	U2344	G2345	U2346	C2347	C2348	C2349	C2350							
G2159	G2160	G2161	G2162	C2163	C2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174	C2175	C2176	C2177	C2178	C2179	U2180	G2181	G2182	C2183	G2186	G2187	C2188	U2189	G2190	G2191	G2192	A2198	G2206	G2207	A2208	U2218	G2223	G2224	A2225	U2233	G2234	G2238	G2239	U2243	U2244	U2245	U2246	U2247	C2248	U2249	G2250		
G2002	G2010	A2014	G2019	A2020	A2021	G2022	G2023	G2024	G2025	C2026	A2030	A2031	G2032	A2033	C2043	U2047	G2048	A2051	C2055	A2056	A2059	A2060	U2062	C2063	C2064	C2065	C2066	G2069	G2070	A2071	G2072	C2073	U2074	U2075	U2076	A2077	C2078	U2079	G2080	A2081	A2082	U2086	G2087	G2094	C2095	U2096							
A1853	A1854	U1864	G1865	G1866	A1876	A1877	G1878	A1889	G1899	A1900	G1906	A1914	U1915	A1916	G1929	G1930	G1935	A1936	A1937	A1938	U1939	C1942	G1945	U1946	C1947	G1948	G1949	G1950	U1951	A1952	U1955	C1962	U1963	G1964	C1967	A1970	A1971	A1972	U1991	G1992	U1993	G1997	A2001										
A1741	G1747B	G1756	U1757	G1758	A1762	G1763	G1764	A1773	C1774	U1779	A1780	G1781	C1782	A1783	A1784	A1785	A1786	A1791	U1794	G1795	U1796	C1797	U1798	C1799	G1800	A1801	A1802	A1803	C1804	U1805	G1811	A1812	A1815	G1816	G1817	G1824	C1827	G1828	A1829	C1830	G1831	C1832	G1835	A1847	A1848								
C1582	A1583	A1584	A1586	A1587	C1588	C1589	A1596	A1608	A1609	A1610	A1614	U1629	G1630	C1631A	C1636	A1637	C1638	U1639	C1640	G1647	C1648	G1656	C1657	C1658	U1659	U1514	G1515	G1529	G1530	C1531	C1532	G1533	U	A	C1536	A1542	C1543	C1546	A1558	A1566	A1567	G1568	A1569	U1578	A1579	U1739	G1740						
G1310	U1313	C1314	G1315	U1316	A1317	A1322	U1323	U1340	U1341	U1352	A1353	A1354	G1355	A1359	A1365	A1368	G1377	A1378	A1379	G1380	A1384	G1385	C1386	C1387	G1388	G1389	A1395	U1396	C1404	U1405	A1406	C1407	G1416	C1417	G1418	A1419	U1420	G1421	C1428	G1429	U1430	U1431	C1432	G1444	A1445A								
C1445B	C1446	G1447	G1448	G1449	G1450A	U1453	G1455	G1459	A1460	C1467	A1471	C1474	G1475	C1476	G1482	C1493	U1497	A1507	A1508	C1509A	A1509B	U1514	G1515	G1529	G1530	C1531	C1532	G1533	U	A	C1536	A1542	C1543	C1546	A1558	A1566	A1567	G1568	A1569	U1578	A1579	U1739	G1581										
G1171	G	A	U	G	A	C1178	G1187	U1188	U1198	U1199	C1200	C1201	C1202	G1206	A1210	U1211	G1212	A1220	G1223	A1226	G1236	G1250	C1251	G1252	A1253	G1256	U1263	G1264	A1265	G1266	G1271	A1272	U1273	A1278	G1279	U1292	C1293	G1296	U1300	A1301	A1302												

C C C

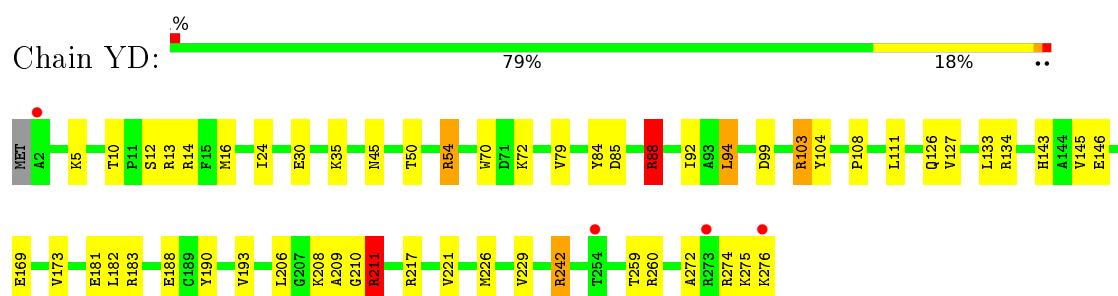
- Molecule 2: 5S rRNA



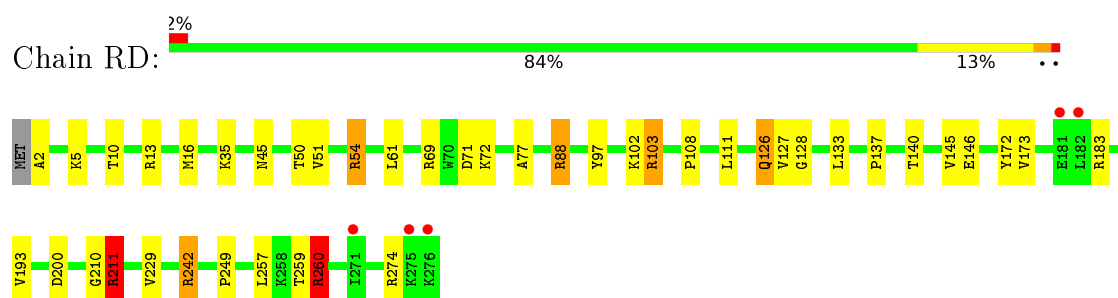
- Molecule 2: 5S rRNA



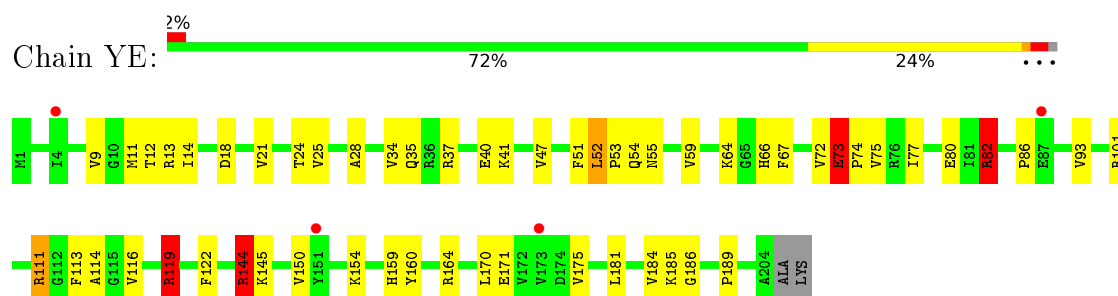
- Molecule 3: 50S ribosomal protein L2



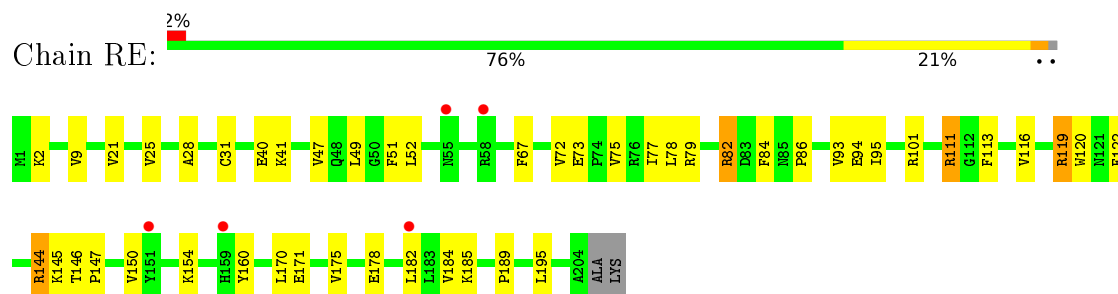
- Molecule 3: 50S ribosomal protein L2



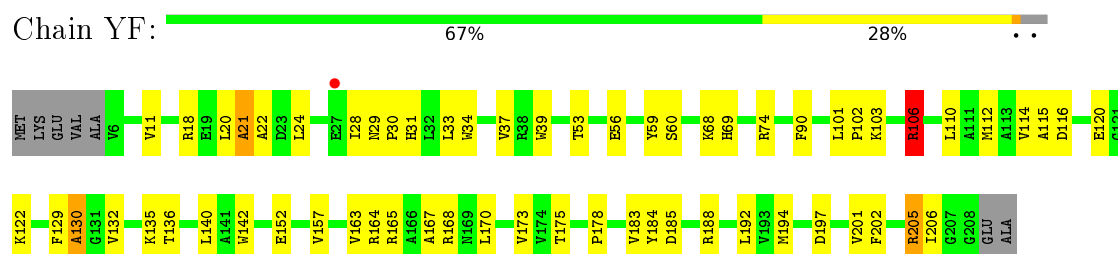
- Molecule 4: 50S ribosomal protein L3



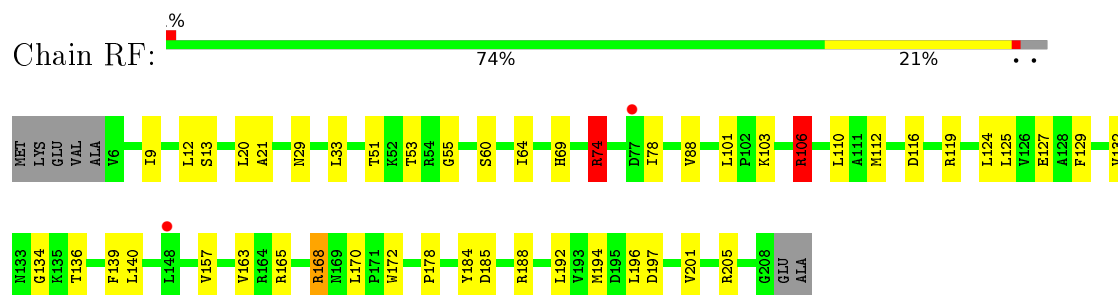
- Molecule 4: 50S ribosomal protein L3



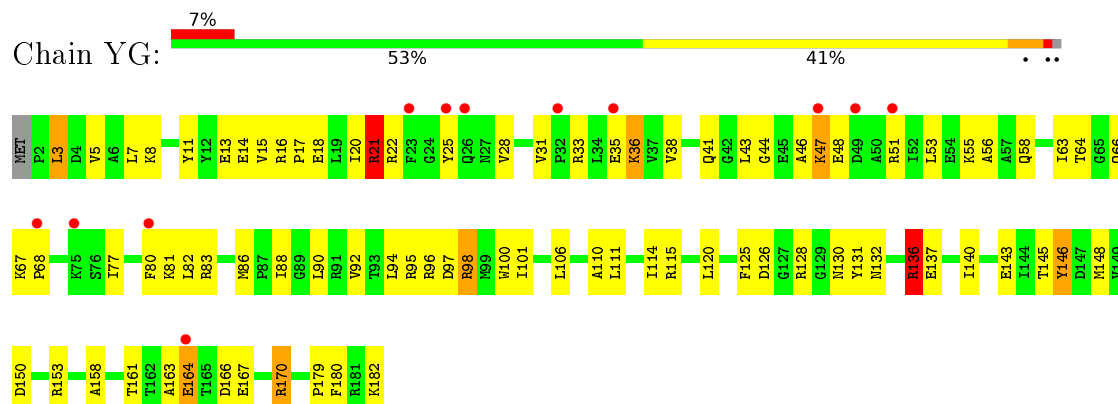
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

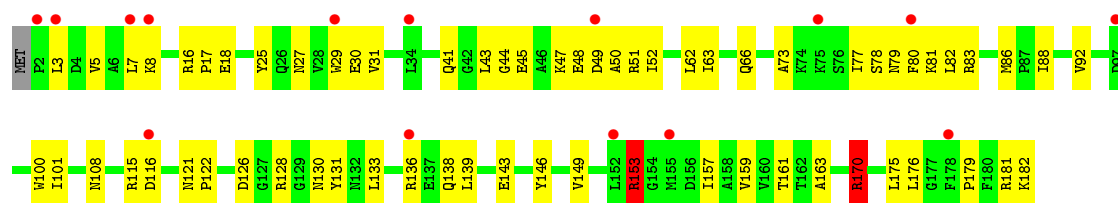


- Molecule 6: 50S ribosomal protein L5

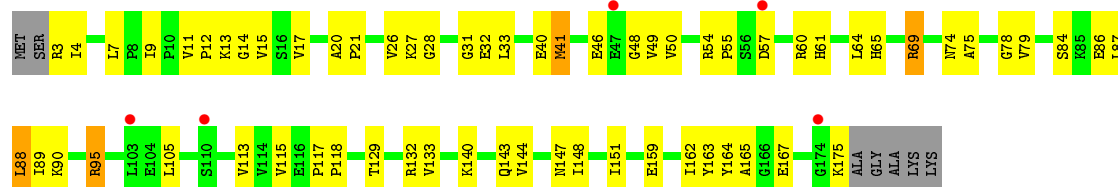


- Molecule 6: 50S ribosomal protein L5

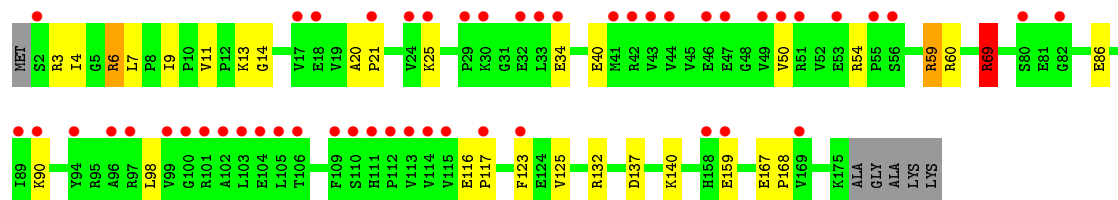
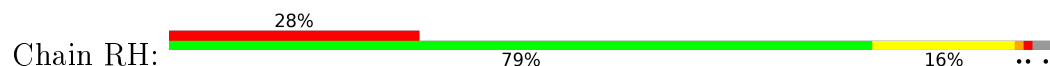




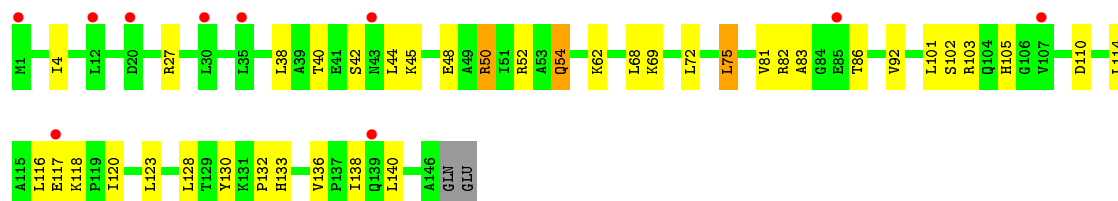
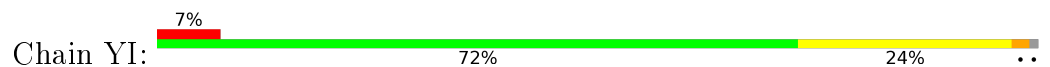
• Molecule 7: 50S ribosomal protein L6



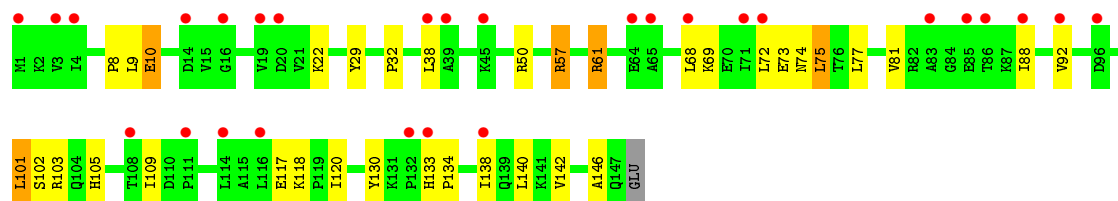
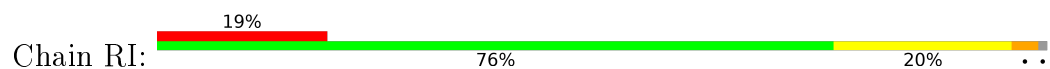
• Molecule 7: 50S ribosomal protein L6



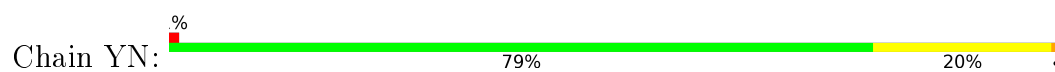
• Molecule 8: 50S ribosomal protein L9



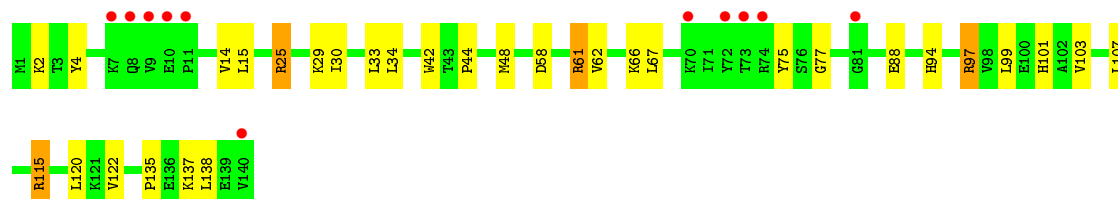
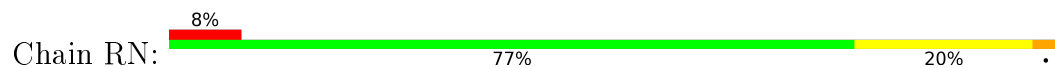
• Molecule 8: 50S ribosomal protein L9



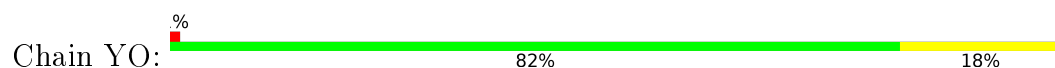
• Molecule 9: 50S ribosomal protein L13



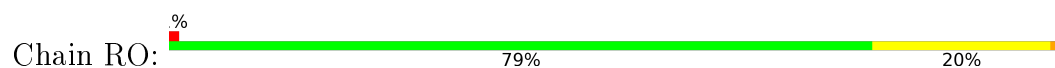
- Molecule 9: 50S ribosomal protein L13



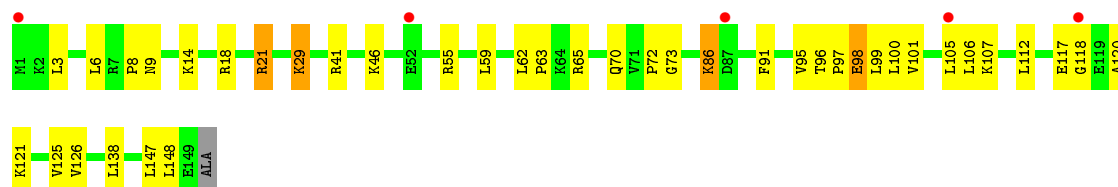
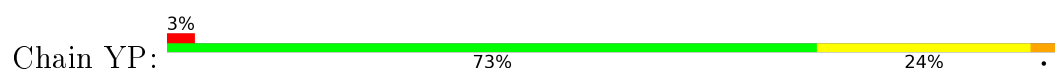
- Molecule 10: 50S ribosomal protein L14



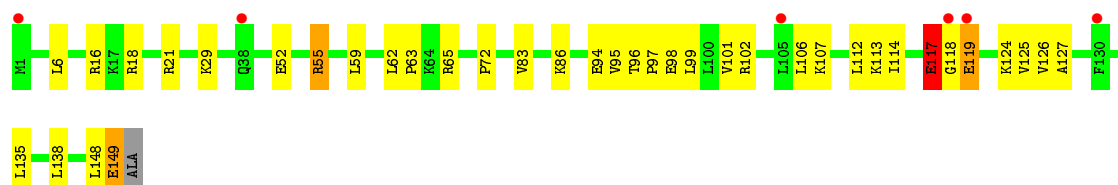
- Molecule 10: 50S ribosomal protein L14




- Molecule 11: 50S ribosomal protein L15

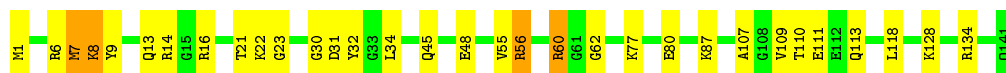


- Molecule 11: 50S ribosomal protein L15




- Molecule 12: 50S ribosomal protein L16

Chain YQ:  77% 20% .




- Molecule 12: 50S ribosomal protein L16

Chain RQ:  78% 19% .




- Molecule 13: 50S ribosomal protein L17

Chain YR:  71% 28% 3% .



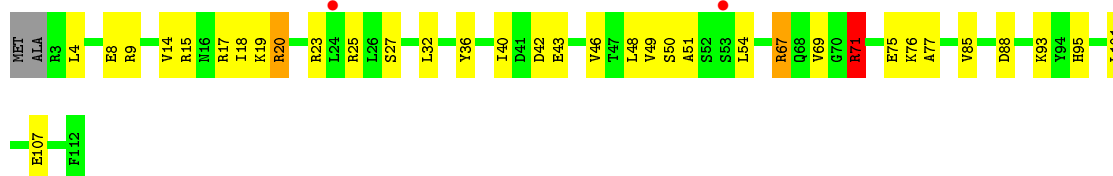
- Molecule 13: 50S ribosomal protein L17

Chain RR:  83% 15% 2% .




- Molecule 14: 50S ribosomal protein L18

Chain YS:  67% 29% 2% ...



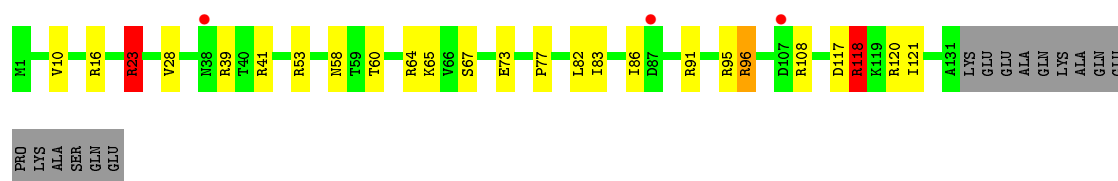
- Molecule 14: 50S ribosomal protein L18

Chain RS:  78% 17% 8% . .

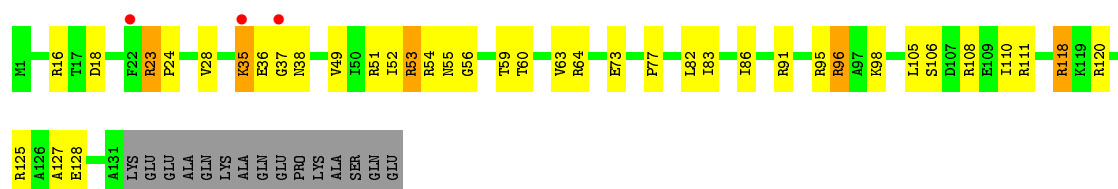


- Molecule 15: 50S ribosomal protein L19

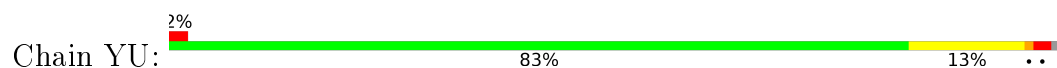
Chain YT:  73% 15% 10% 2% ..



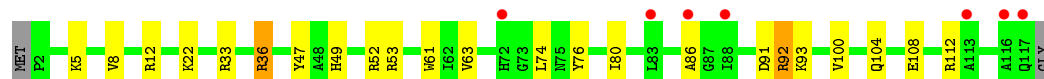
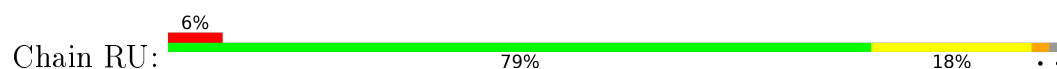
- Molecule 15: 50S ribosomal protein L19



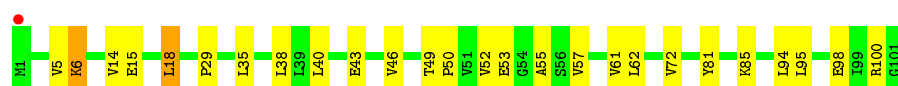
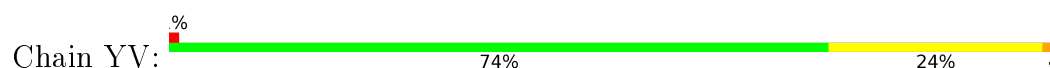
- Molecule 16: 50S ribosomal protein L20



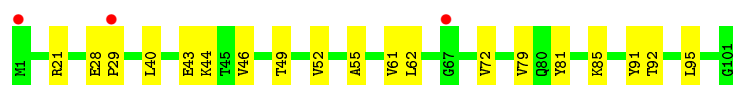
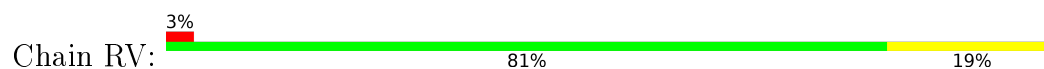
- Molecule 16: 50S ribosomal protein L20



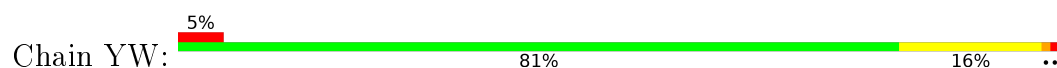
- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21

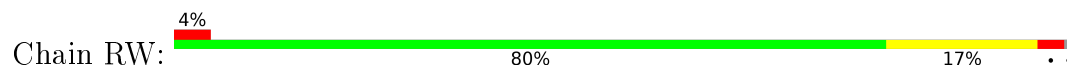


- Molecule 18: 50S ribosomal protein L22

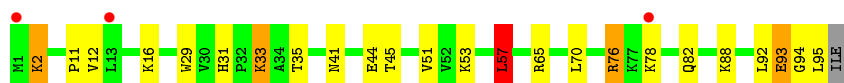
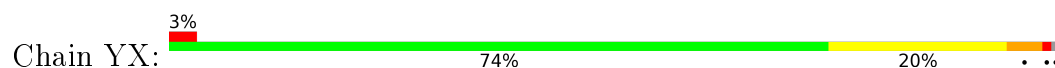




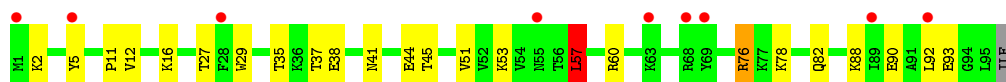
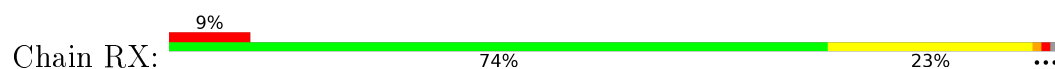
- Molecule 18: 50S ribosomal protein L22



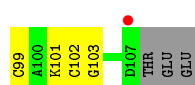
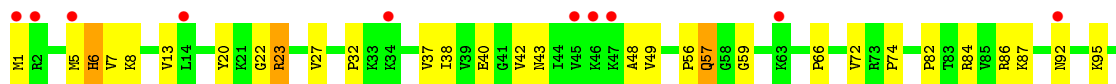
- Molecule 19: 50S ribosomal protein L23



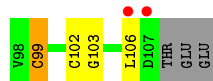
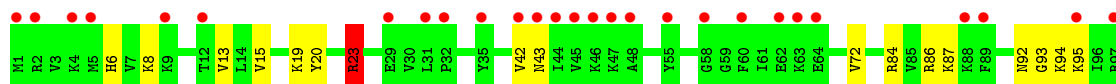
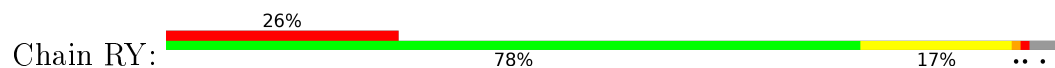
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

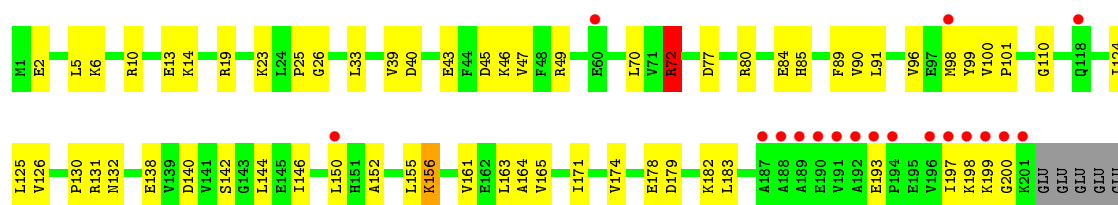


- Molecule 20: 50S ribosomal protein L24

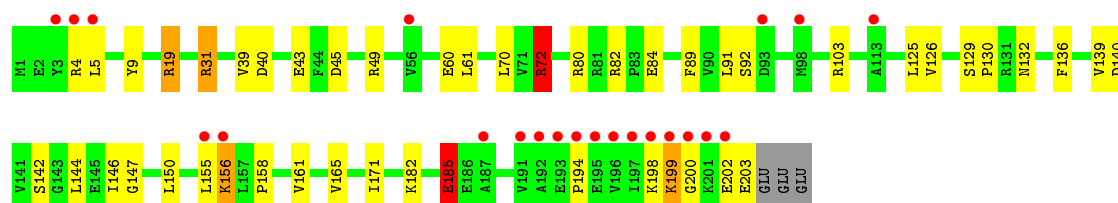
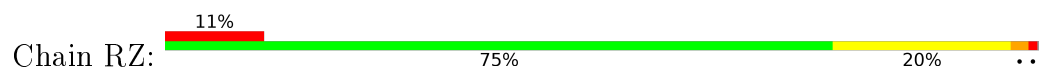


- Molecule 21: 50S ribosomal protein L25

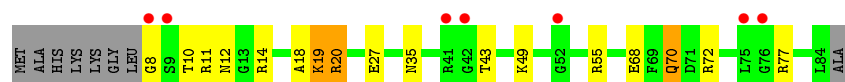
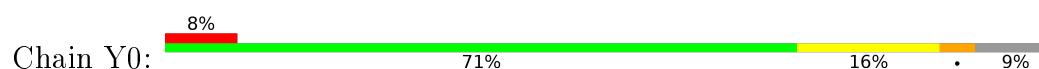




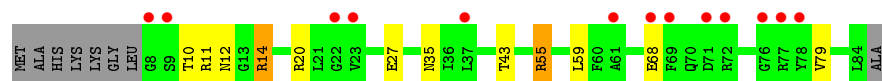
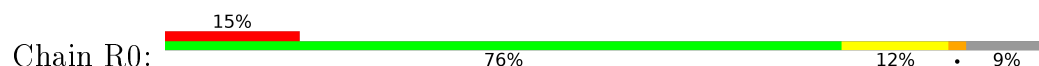
- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27



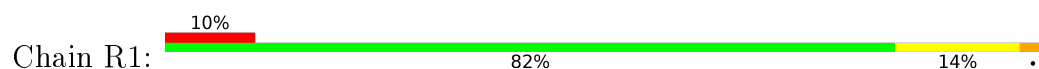
- Molecule 22: 50S ribosomal protein L27



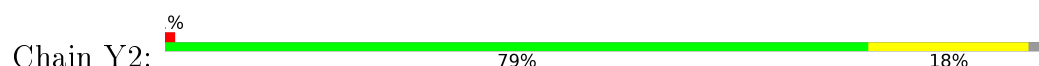
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28

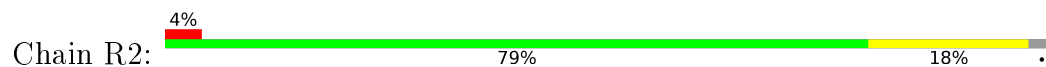


- Molecule 24: 50S ribosomal protein L29

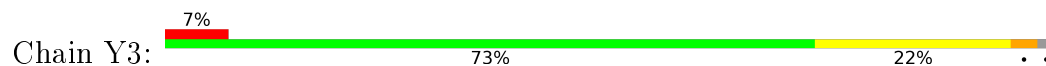




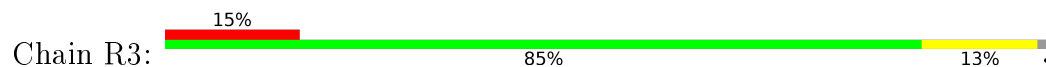
- Molecule 24: 50S ribosomal protein L29



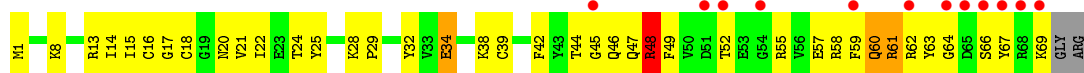
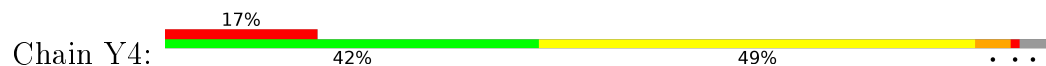
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



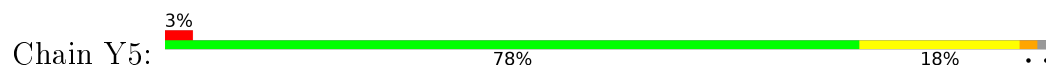
- Molecule 26: 50S ribosomal protein L31



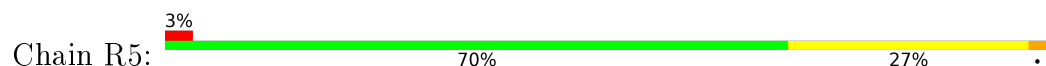
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32

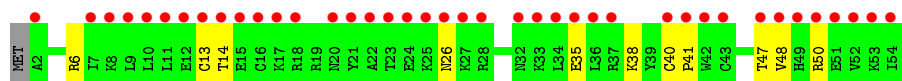
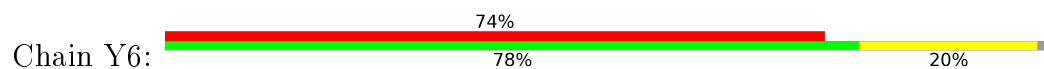


- Molecule 27: 50S ribosomal protein L32

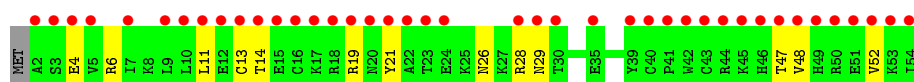
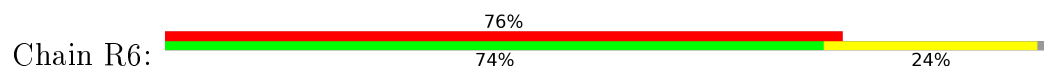




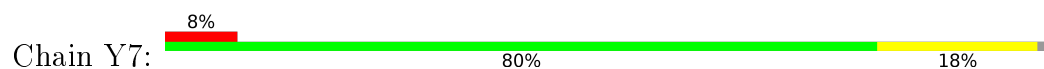
- Molecule 28: 50S ribosomal protein L33



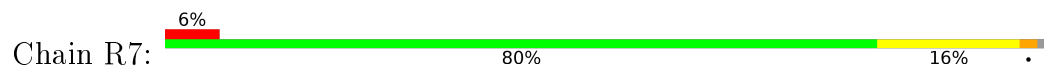
- Molecule 28: 50S ribosomal protein L33



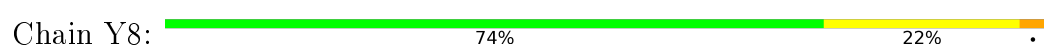
- Molecule 29: 50S ribosomal protein L34



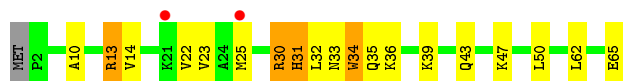
- Molecule 29: 50S ribosomal protein L34



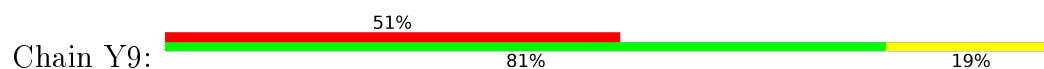
- Molecule 30: 50S ribosomal protein L35

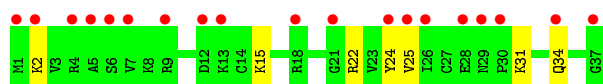


- Molecule 30: 50S ribosomal protein L35

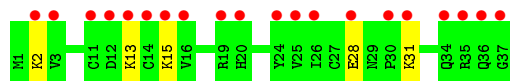
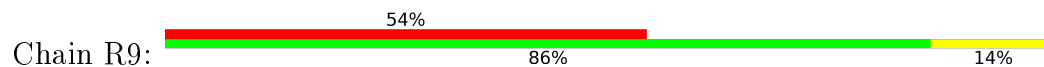


- Molecule 31: 50S ribosomal protein L36

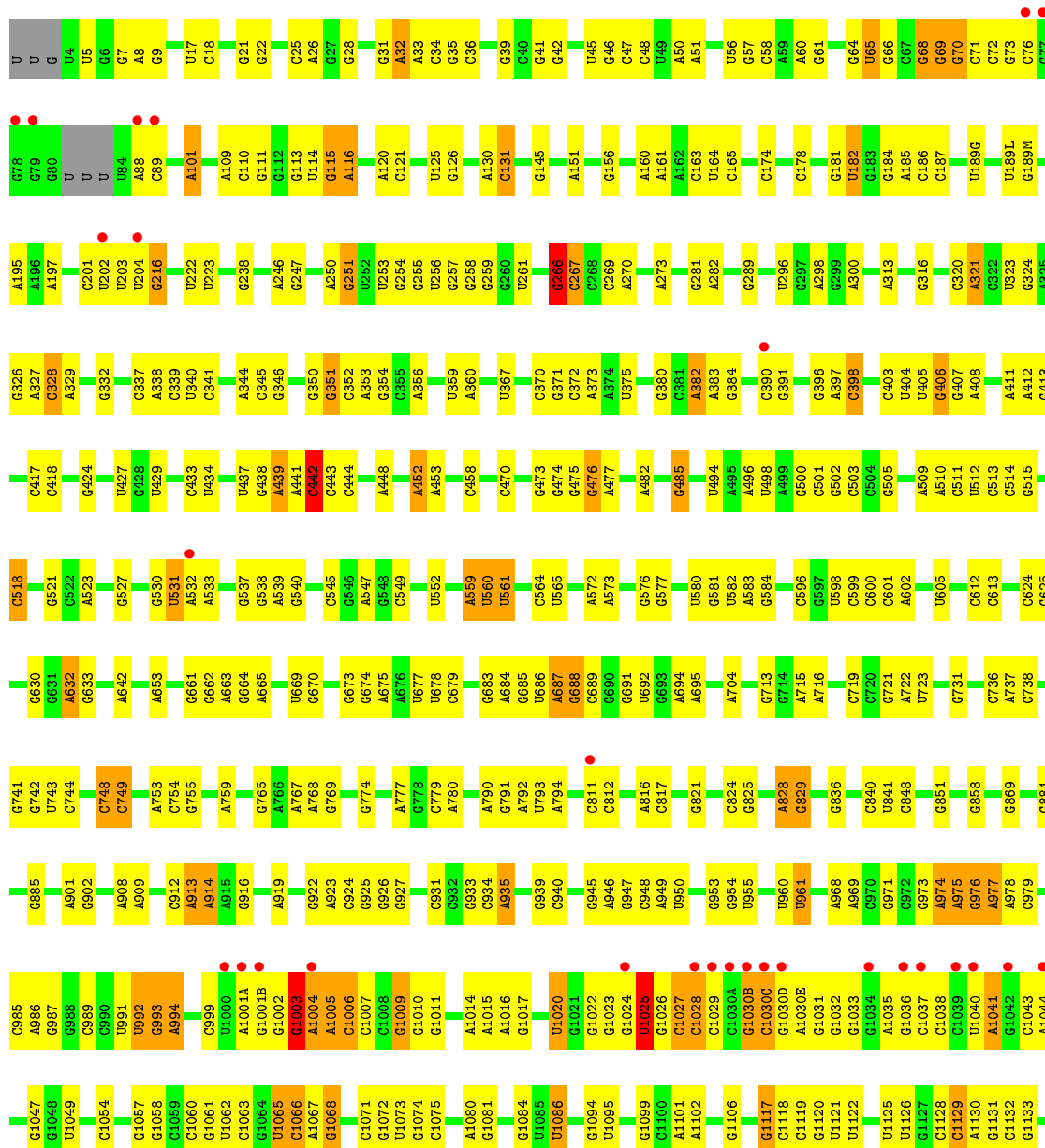




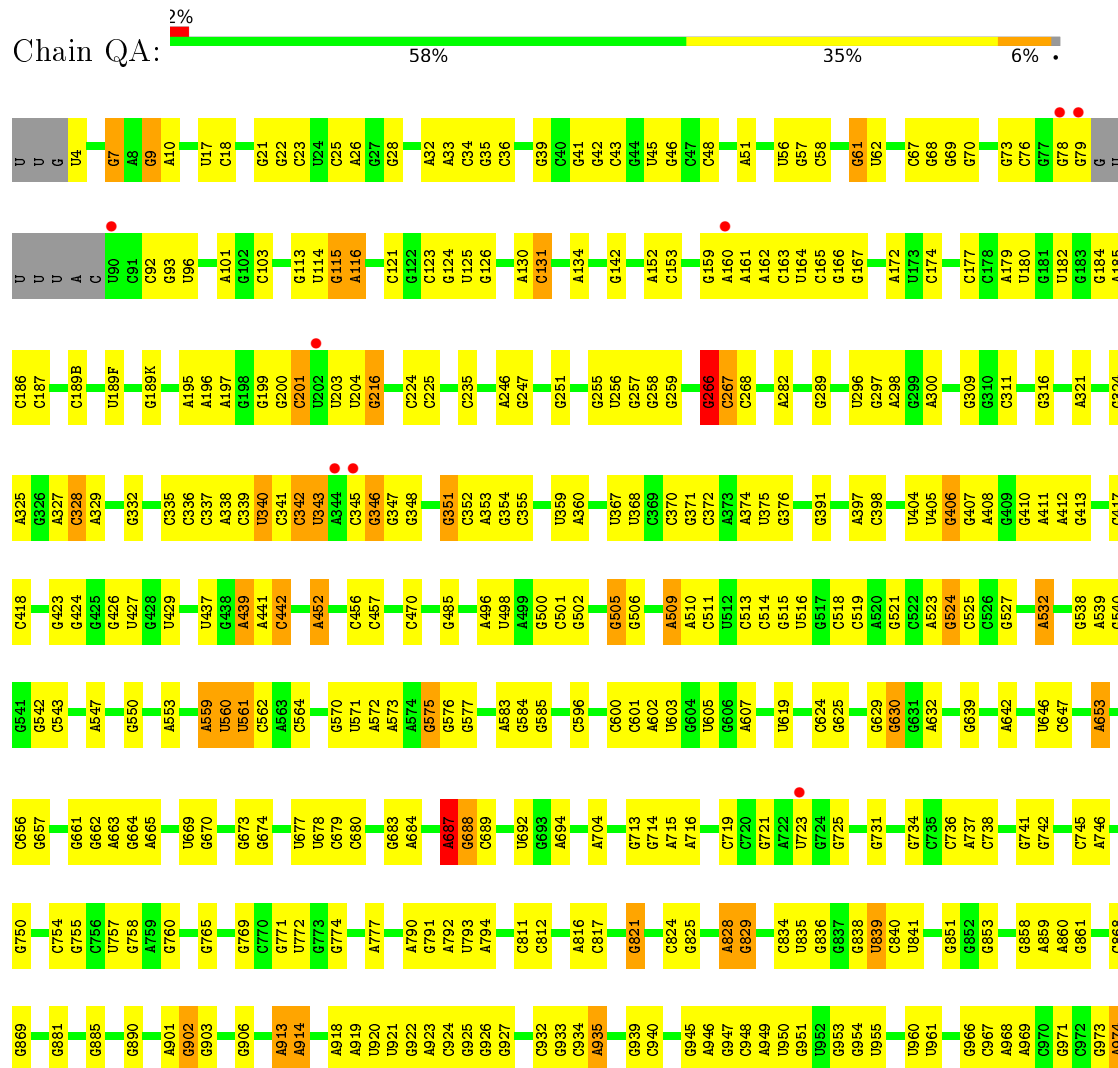
- Molecule 31: 50S ribosomal protein L36

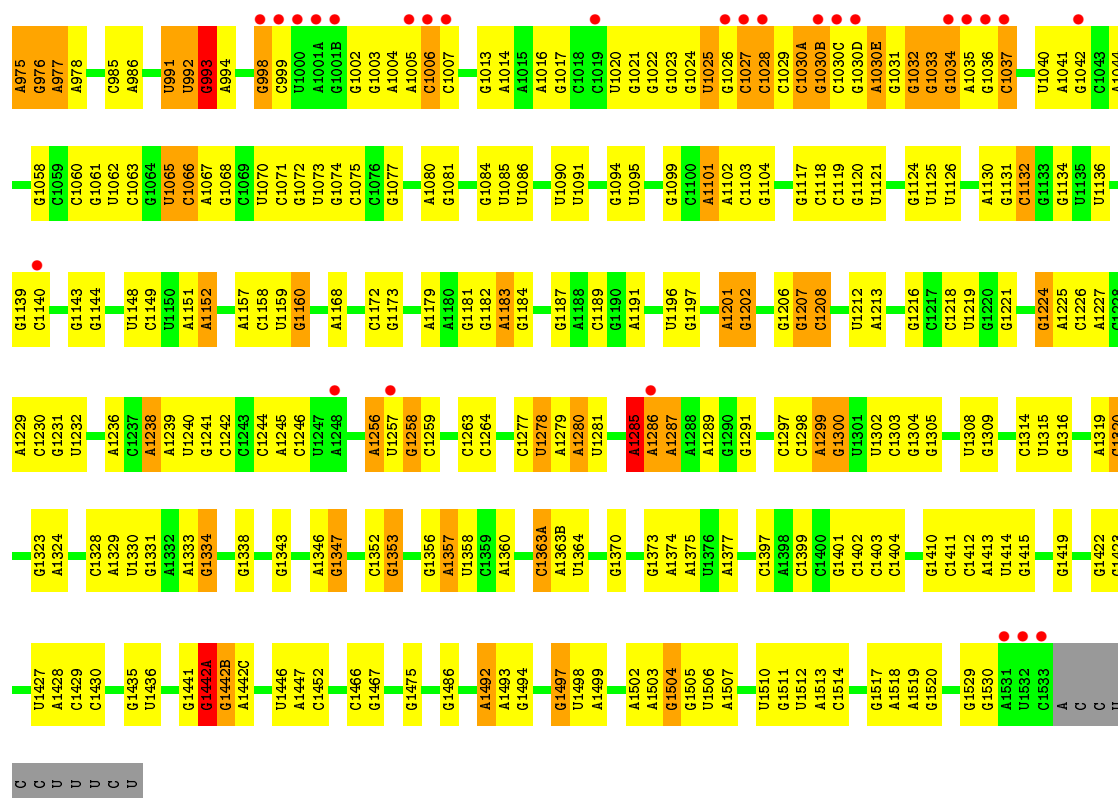


- Molecule 32: 16S rRNA

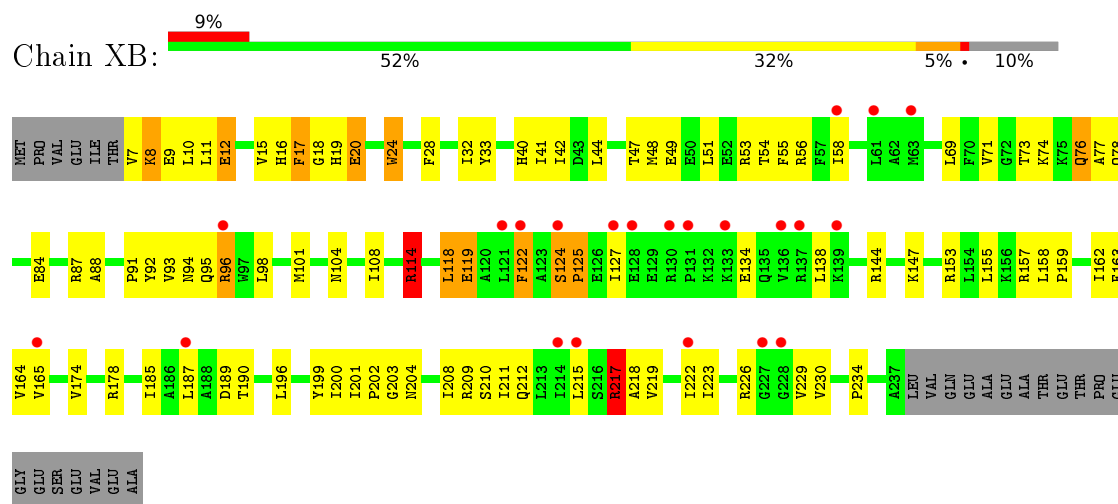


- Molecule 32: 16S rRNA

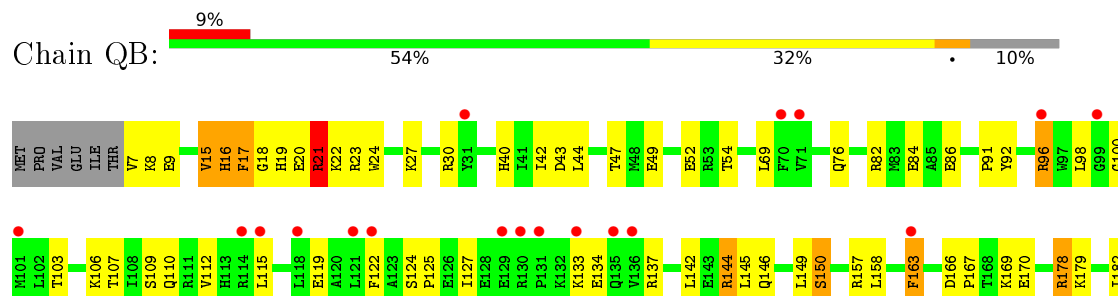


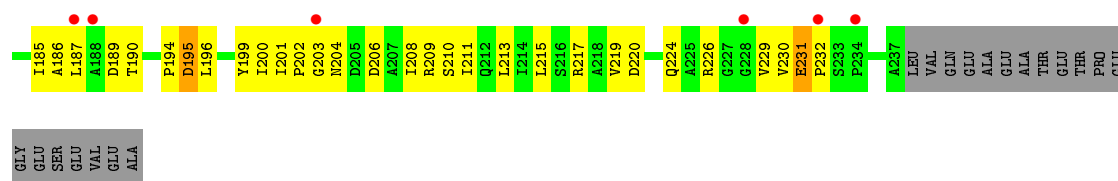


• Molecule 33: 30S ribosomal protein S2

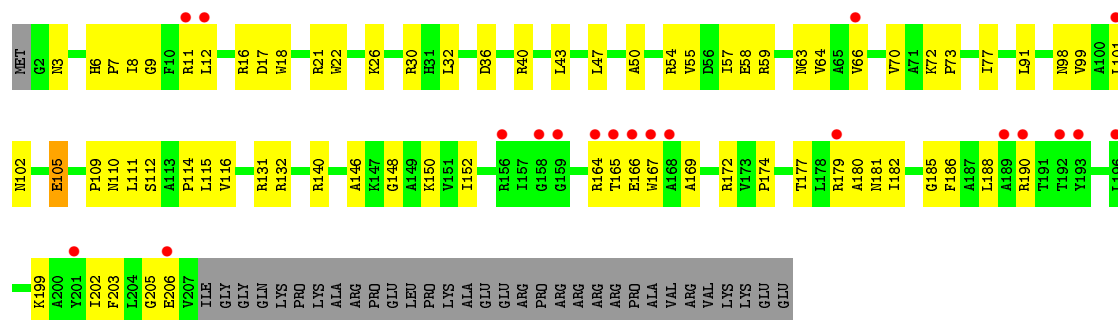


• Molecule 33: 30S ribosomal protein S2

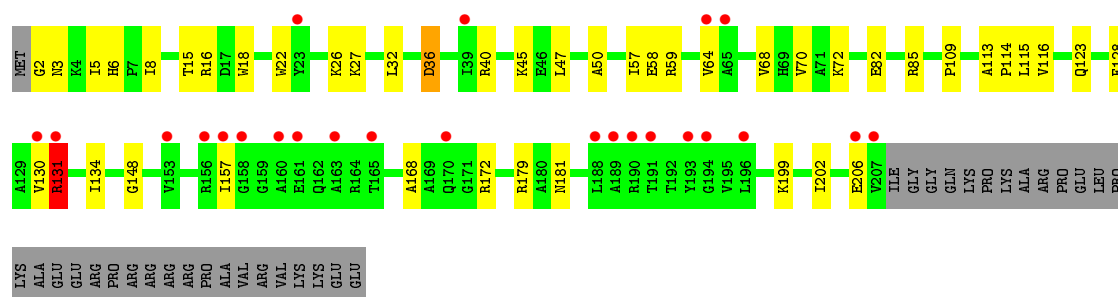




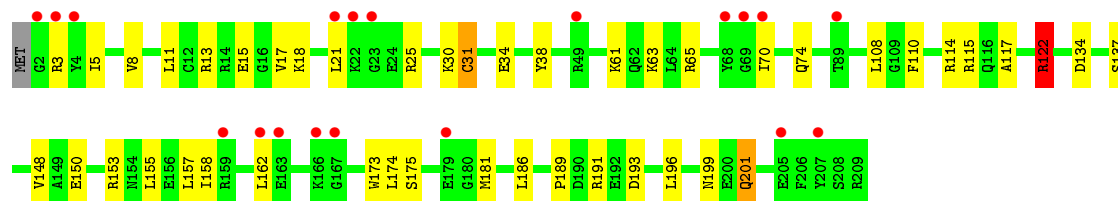
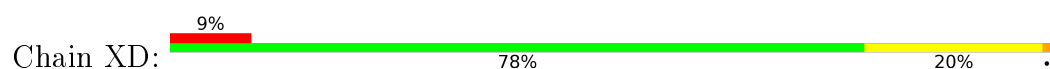
• Molecule 34: 30S ribosomal protein S3



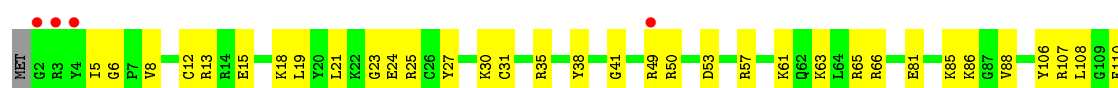
• Molecule 34: 30S ribosomal protein S3

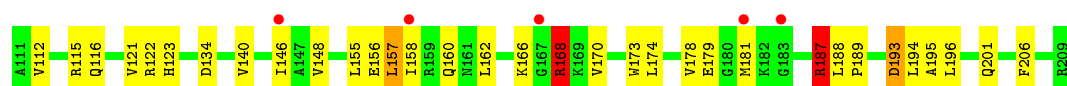


• Molecule 35: 30S ribosomal protein S4

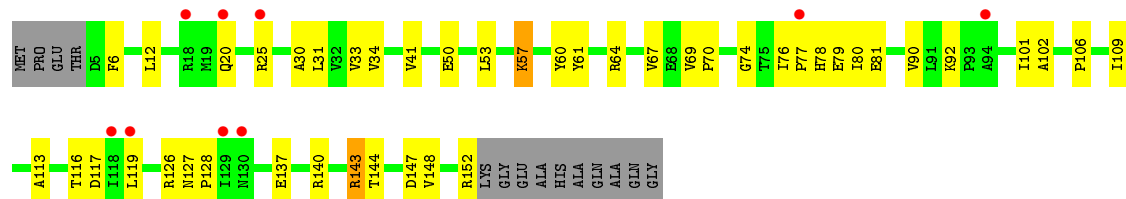


• Molecule 35: 30S ribosomal protein S4

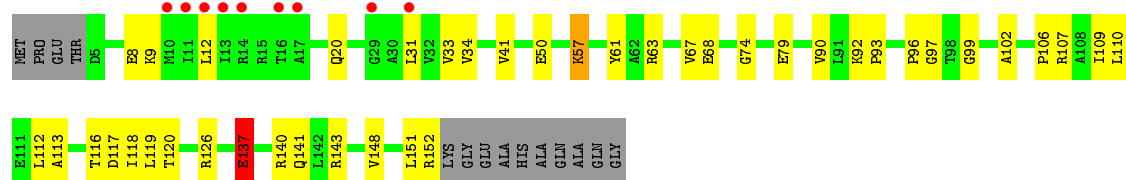




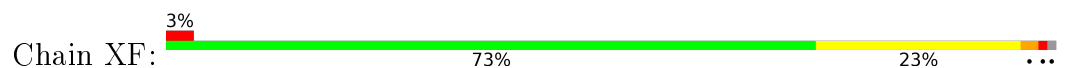
- Molecule 36: 30S ribosomal protein S5



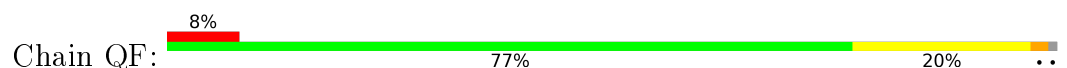
- Molecule 36: 30S ribosomal protein S5



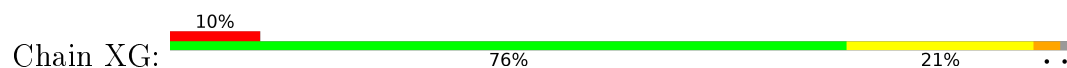
- Molecule 37: 30S ribosomal protein S6



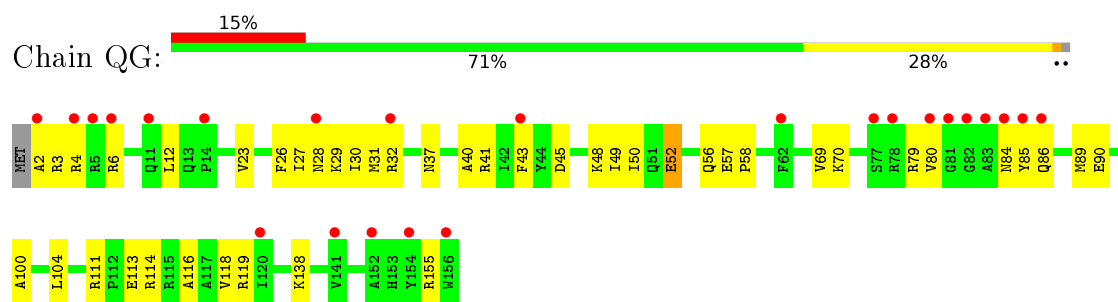
- Molecule 37: 30S ribosomal protein S6



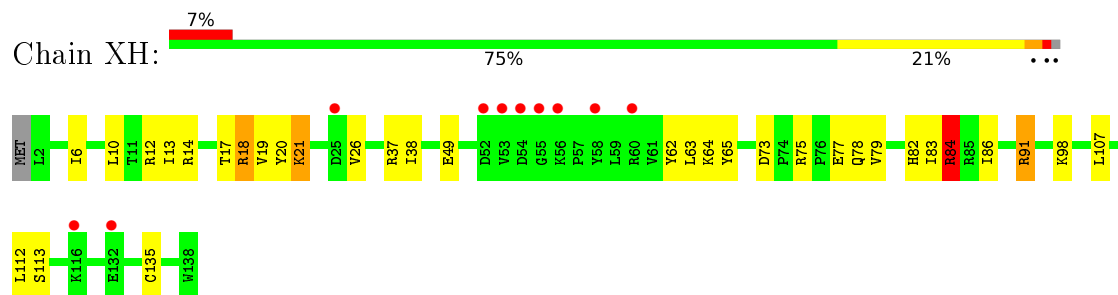
- Molecule 38: 30S ribosomal protein S7



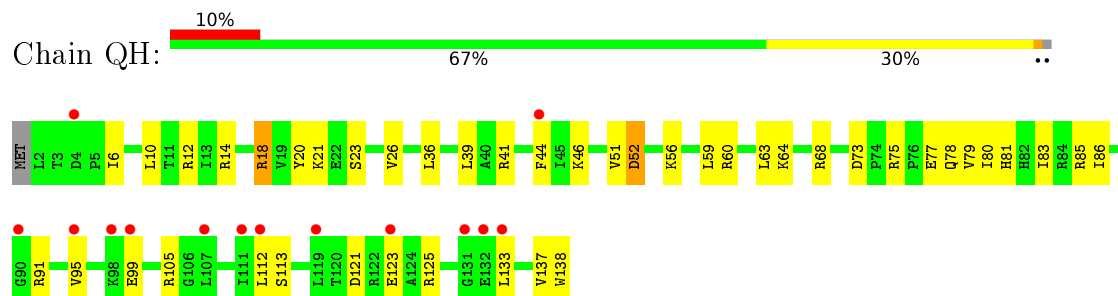
- Molecule 38: 30S ribosomal protein S7



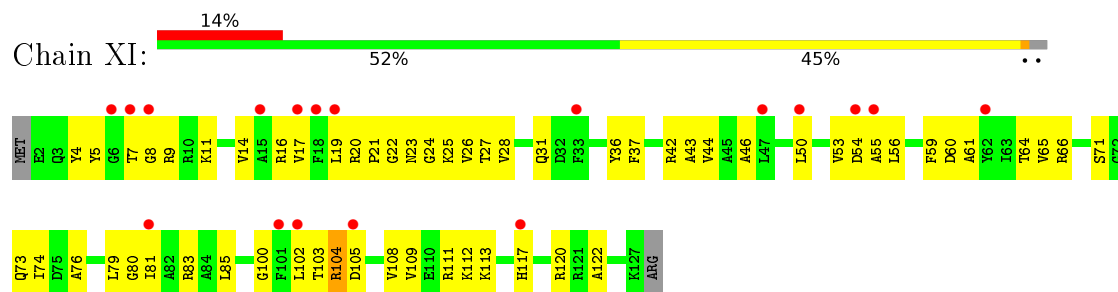
• Molecule 39: 30S ribosomal protein S8



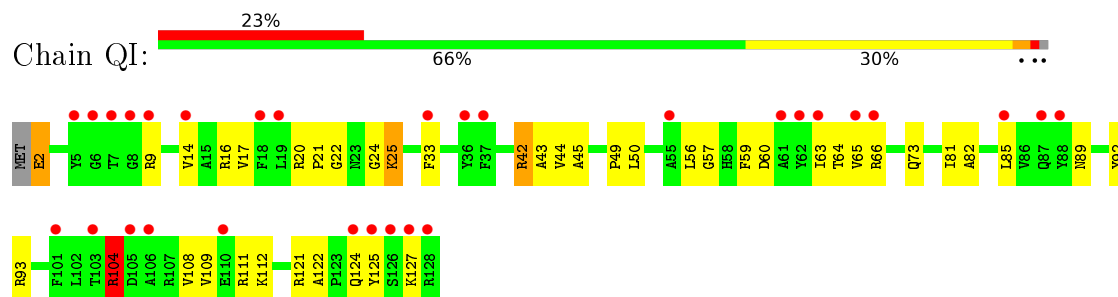
• Molecule 39: 30S ribosomal protein S8



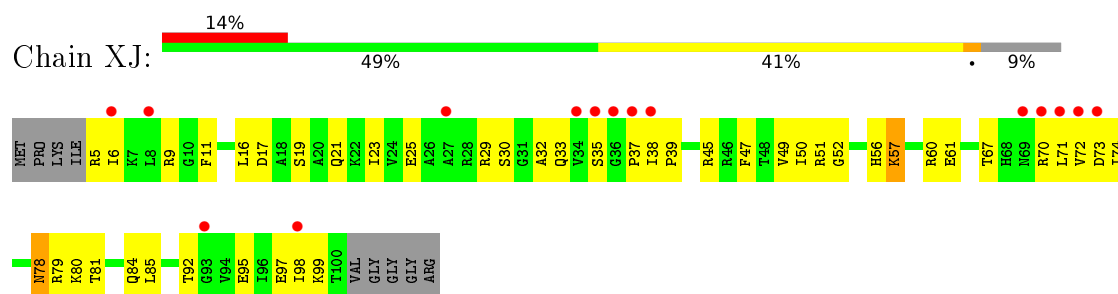
• Molecule 40: 30S ribosomal protein S9



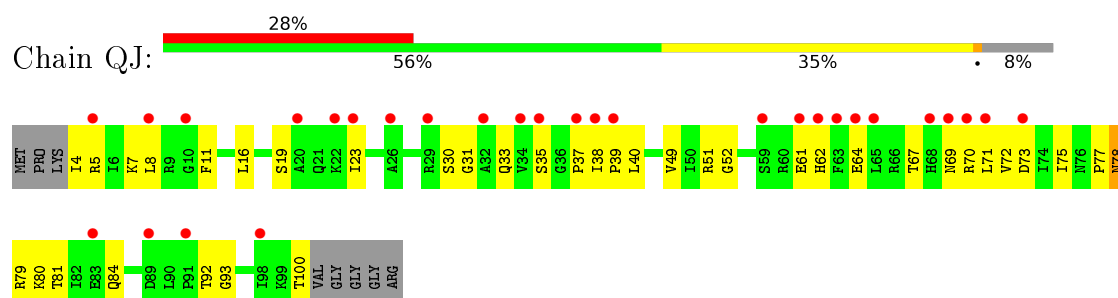
• Molecule 40: 30S ribosomal protein S9



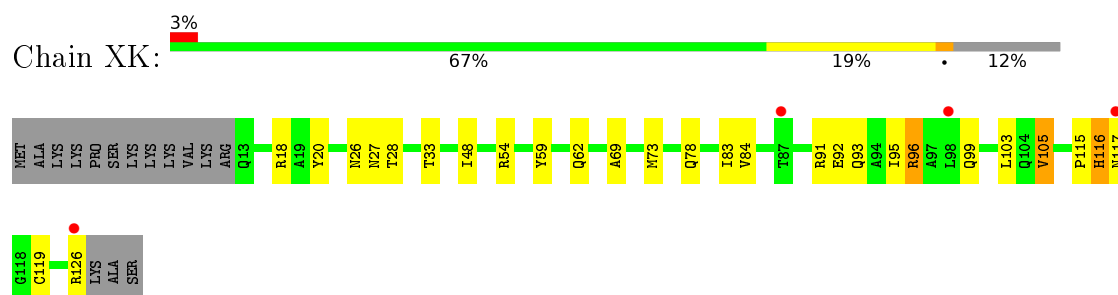
- Molecule 41: 30S ribosomal protein S10



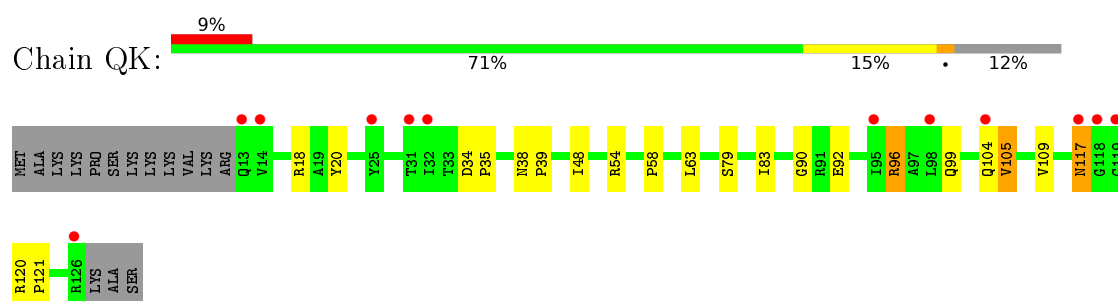
- Molecule 41: 30S ribosomal protein S10



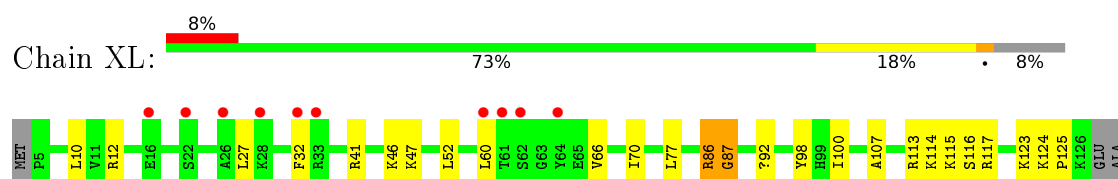
- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11



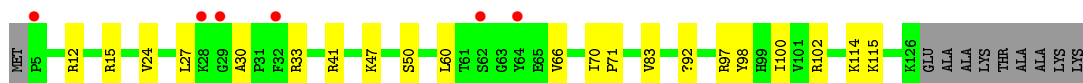
- Molecule 43: 30S ribosomal protein S12



ALA
LYS
THR
ALA
LYS
LYS

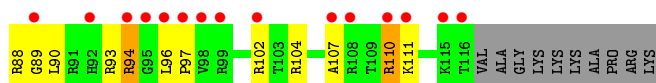
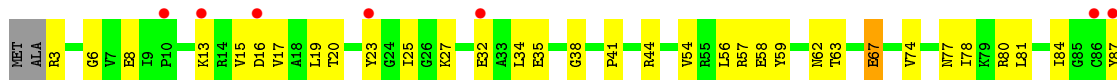
- Molecule 43: 30S ribosomal protein S12

Chain QL: 5% 77% 16% 8%



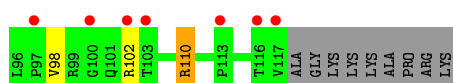
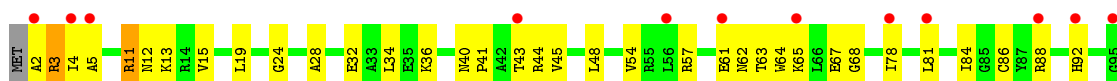
- Molecule 44: 30S ribosomal protein S13

Chain XM: 17% 55% 33% 10%



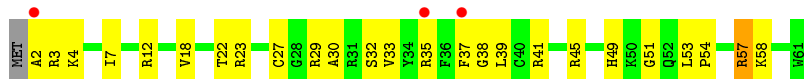
- Molecule 44: 30S ribosomal protein S13

Chain QM: 15% 62% 28% 8%



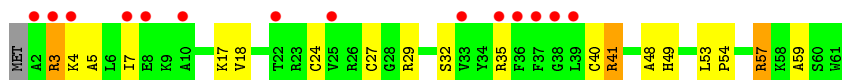
- Molecule 45: 30S ribosomal protein S14 type Z

Chain XN: 5% 57% 39% 2%



- Molecule 45: 30S ribosomal protein S14 type Z

Chain QN: 23% 67% 26% 5%

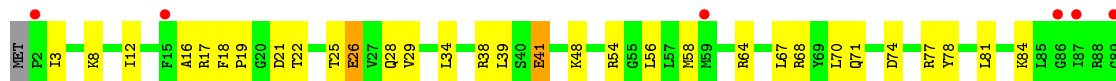


- Molecule 46: 30S ribosomal protein S15

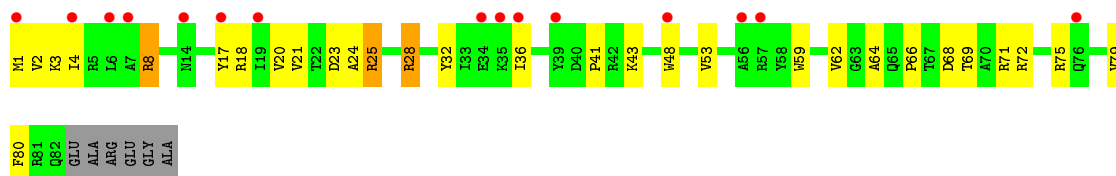
Chain XO: 7% 84% 12% 1%



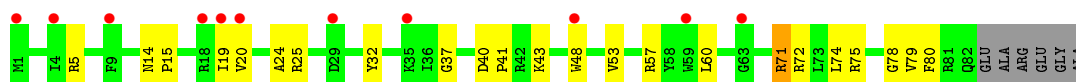
- Molecule 46: 30S ribosomal protein S15



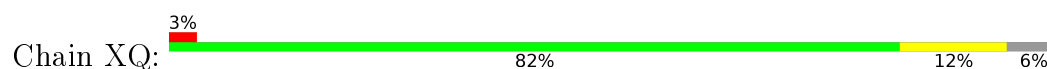
- Molecule 47: 30S ribosomal protein S16



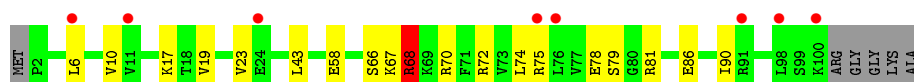
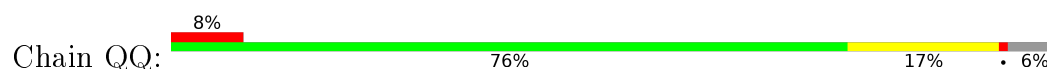
- Molecule 47: 30S ribosomal protein S16



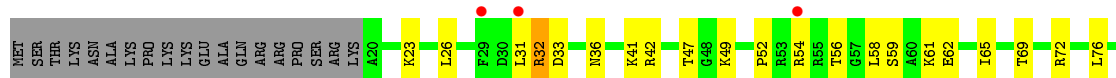
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

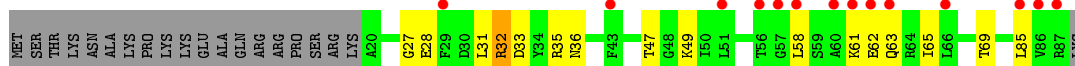


- Molecule 49: 30S ribosomal protein S18

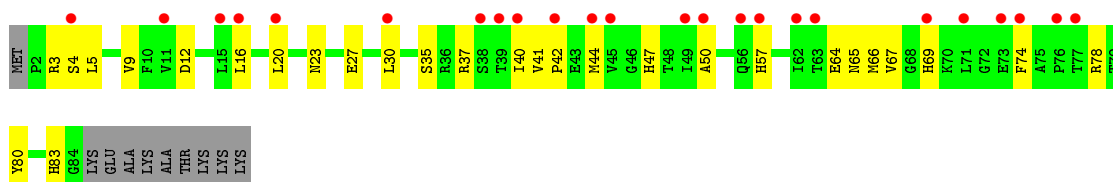




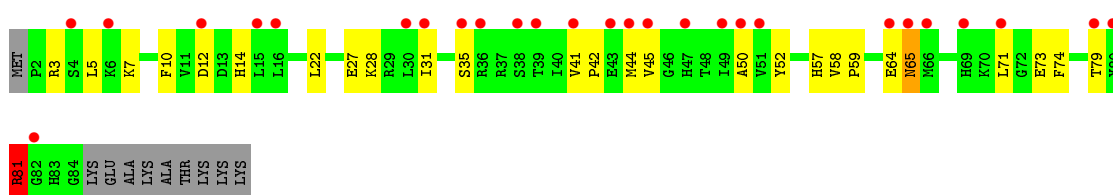
- Molecule 49: 30S ribosomal protein S18



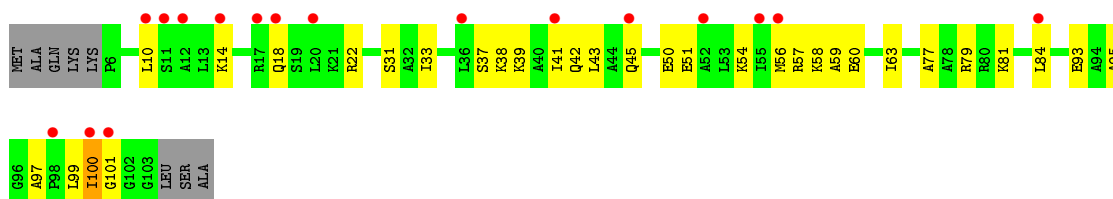
- Molecule 50: 30S ribosomal protein S19



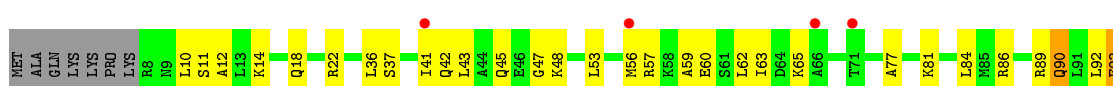
- Molecule 50: 30S ribosomal protein S19

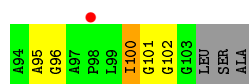


- Molecule 51: 30S ribosomal protein S20

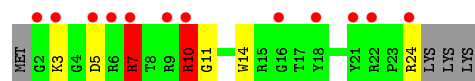


- Molecule 51: 30S ribosomal protein S20

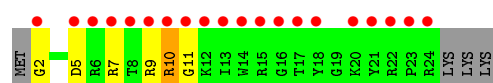
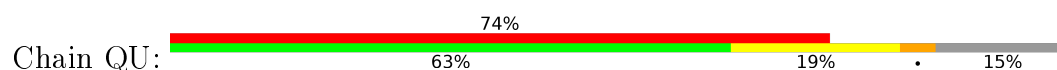




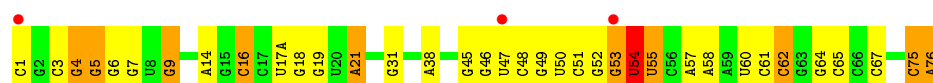
- Molecule 52: 30S ribosomal protein Thx



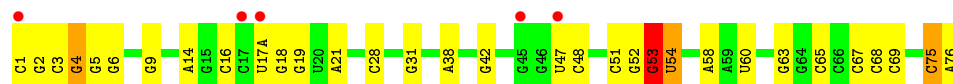
- Molecule 52: 30S ribosomal protein Thx



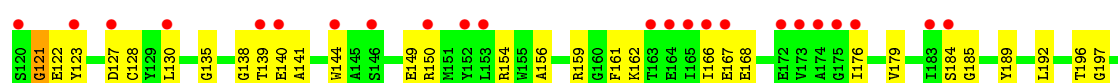
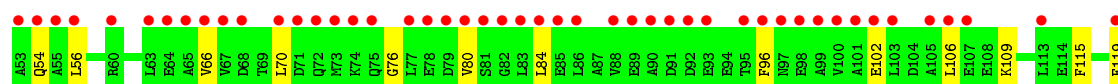
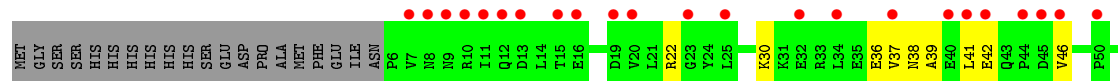
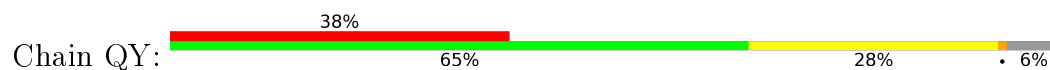
- Molecule 53: P-site tRNA fMet

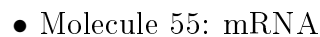


- Molecule 53: P-site tRNA fMet



- Molecule 54: Peptide chain release factor 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.89Å 450.12Å 620.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 3.30 49.92 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.92-3.30) 98.9 (49.92-3.30)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.10.1_2155)	Depositor
R, R_{free}	0.267 , 0.286 0.266 , 0.286	Depositor DCC
R_{free} test set	40126 reflections (4.63%)	DCC
Wilson B-factor (Å ²)	99.5	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	296497	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, MEQ, 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	RA	0.25	0/68901	0.81	30/107544 (0.0%)
1	YA	0.27	0/68901	0.81	39/107544 (0.0%)
2	RB	0.22	0/2876	0.78	0/4486
2	YB	0.23	0/2878	0.79	0/4490
3	RD	0.71	8/2181 (0.4%)	0.69	1/2940 (0.0%)
3	YD	0.75	13/2186 (0.6%)	0.66	0/2944
4	RE	1.10	19/1592 (1.2%)	0.65	0/2149
4	YE	1.36	19/1592 (1.2%)	0.69	3/2149 (0.1%)
5	RF	0.59	2/1619 (0.1%)	0.68	2/2193 (0.1%)
5	YF	0.50	2/1615 (0.1%)	0.62	0/2188
6	RG	0.69	9/1451 (0.6%)	0.59	0/1961
6	YG	0.71	9/1449 (0.6%)	0.56	0/1957
7	RH	0.77	8/1356 (0.6%)	0.56	0/1834
7	YH	0.62	6/1350 (0.4%)	0.59	1/1826 (0.1%)
8	RI	0.84	7/1109 (0.6%)	0.60	0/1512
8	YI	0.55	3/1091 (0.3%)	0.63	2/1490 (0.1%)
9	RN	0.76	6/1148 (0.5%)	0.67	1/1547 (0.1%)
9	YN	0.81	7/1144 (0.6%)	0.57	0/1543
10	RO	0.63	4/943 (0.4%)	0.67	1/1269 (0.1%)
10	YO	0.61	4/943 (0.4%)	0.62	1/1269 (0.1%)
11	RP	0.89	8/1152 (0.7%)	0.71	0/1533
11	YP	0.64	6/1152 (0.5%)	0.61	1/1533 (0.1%)
12	RQ	0.91	12/1143 (1.0%)	0.67	0/1527
12	YQ	0.81	9/1143 (0.8%)	0.60	0/1527
13	RR	0.97	8/982 (0.8%)	0.72	2/1312 (0.2%)
13	YR	0.81	7/982 (0.7%)	0.66	0/1312
14	RS	0.74	4/887 (0.5%)	0.61	0/1180
14	YS	0.87	9/880 (1.0%)	0.63	0/1172
15	RT	0.87	12/1105 (1.1%)	0.66	0/1477
15	YT	0.83	10/1097 (0.9%)	0.63	0/1468
16	RU	0.87	7/977 (0.7%)	0.67	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	YU	0.98	11/977 (1.1%)	0.66	2/1301 (0.2%)
17	RV	0.71	2/786 (0.3%)	0.62	0/1053
17	YV	0.63	0/782	0.63	0/1049
18	RW	0.89	9/897 (1.0%)	0.67	2/1205 (0.2%)
18	YW	0.71	6/897 (0.7%)	0.60	0/1205
19	RX	0.76	4/764 (0.5%)	0.65	1/1025 (0.1%)
19	YX	0.70	3/764 (0.4%)	0.65	1/1025 (0.1%)
20	RY	0.78	4/823 (0.5%)	0.66	0/1099
20	YY	0.49	0/823	0.59	0/1100
21	RZ	0.70	9/1620 (0.6%)	0.58	1/2200 (0.0%)
21	YZ	1.52	14/1590 (0.9%)	0.59	0/2162
22	R0	0.69	2/616 (0.3%)	0.68	1/821 (0.1%)
22	Y0	0.53	2/616 (0.3%)	0.55	0/821
23	R1	0.76	3/761 (0.4%)	0.61	0/1013
23	Y1	0.81	5/766 (0.7%)	0.62	0/1018
24	R2	0.40	0/590	0.55	0/781
24	Y2	0.44	0/594	0.51	0/785
25	R3	0.49	0/474	0.62	0/635
25	Y3	0.66	3/469 (0.6%)	0.62	0/630
26	R4	0.98	5/559 (0.9%)	0.74	0/754
26	Y4	1.29	10/549 (1.8%)	0.71	0/741
27	R5	0.65	2/473 (0.4%)	0.69	0/639
27	Y5	0.77	4/469 (0.9%)	0.58	0/635
28	R6	0.80	1/460 (0.2%)	0.59	0/613
28	Y6	0.56	0/456	0.54	0/608
29	R7	0.67	0/426	0.77	2/561 (0.4%)
29	Y7	0.69	2/426 (0.5%)	0.67	0/561
30	R8	0.83	4/525 (0.8%)	0.65	1/691 (0.1%)
30	Y8	0.82	4/525 (0.8%)	0.64	0/691
31	R9	0.44	0/310	0.58	0/407
31	Y9	0.37	0/310	0.54	0/407
32	QA	0.23	0/35795	0.79	14/55864 (0.0%)
32	XA	0.24	0/35890	0.80	20/56012 (0.0%)
33	QB	0.76	15/1876 (0.8%)	0.63	2/2533 (0.1%)
33	XB	1.13	25/1860 (1.3%)	0.62	0/2518
34	QC	0.51	3/1582 (0.2%)	0.54	0/2137
34	XC	0.60	4/1566 (0.3%)	0.55	0/2119
35	QD	0.63	7/1695 (0.4%)	0.58	0/2274
35	XD	0.58	8/1698 (0.5%)	0.53	0/2277
36	QE	0.62	3/1149 (0.3%)	0.58	0/1548
36	XE	0.77	6/1149 (0.5%)	0.56	0/1548
37	QF	0.63	4/827 (0.5%)	0.58	0/1120
37	XF	0.91	10/829 (1.2%)	0.57	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	QG	0.75	6/1254 (0.5%)	0.50	0/1683
38	XG	1.05	17/1248 (1.4%)	0.57	0/1676
39	QH	0.69	5/1118 (0.4%)	0.55	0/1506
39	XH	0.60	3/1108 (0.3%)	0.57	1/1494 (0.1%)
40	QI	0.82	8/1005 (0.8%)	0.58	0/1351
40	XI	0.49	0/985	0.58	1/1329 (0.1%)
41	QJ	0.52	2/732 (0.3%)	0.58	0/993
41	XJ	0.39	0/723	0.56	0/984
42	QK	0.76	6/849 (0.7%)	0.58	1/1150 (0.1%)
42	XK	0.65	4/848 (0.5%)	0.59	0/1149
43	QL	0.63	2/937 (0.2%)	0.57	1/1260 (0.1%)
43	XL	0.44	0/937	0.62	1/1260 (0.1%)
44	QM	0.69	5/924 (0.5%)	0.59	0/1242
44	XM	0.67	4/905 (0.4%)	0.60	0/1217
45	QN	0.76	4/501 (0.8%)	0.49	0/664
45	XN	1.04	9/501 (1.8%)	0.59	0/664
46	QO	0.81	7/739 (0.9%)	0.56	0/985
46	XO	0.78	7/739 (0.9%)	0.56	0/985
47	QP	0.57	2/697 (0.3%)	0.62	0/939
47	XP	0.94	7/693 (1.0%)	0.59	0/935
48	QQ	0.61	4/836 (0.5%)	0.56	0/1117
48	XQ	0.77	8/836 (1.0%)	0.58	1/1117 (0.1%)
49	QR	0.78	4/560 (0.7%)	0.64	0/746
49	XR	0.56	2/560 (0.4%)	0.57	0/746
50	QS	0.66	4/663 (0.6%)	0.59	0/895
50	XS	0.45	0/660	0.56	0/893
51	QT	0.61	2/734 (0.3%)	0.58	0/969
51	XT	0.53	2/736 (0.3%)	0.51	0/976
52	QU	1.23	7/203 (3.4%)	0.50	0/266
52	XU	1.42	8/203 (3.9%)	0.59	0/266
53	QV	0.36	1/1836 (0.1%)	0.86	9/2859 (0.3%)
53	XV	0.35	1/1836 (0.1%)	0.79	2/2859 (0.1%)
54	QY	0.38	0/2862	0.60	0/3854
54	XY	0.38	1/2862 (0.0%)	0.59	0/3854
55	QX	0.22	0/144	0.72	0/222
55	XX	0.19	0/144	0.70	0/222
All	All	0.47	554/317956 (0.2%)	0.75	148/474813 (0.0%)

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
14	RS	0	1
19	RX	0	1
19	YX	0	1
33	QB	0	1
43	XL	0	1
54	XY	0	1
All	All	0	6

The worst 5 of 554 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	YZ	72	ARG	NE-CZ	-30.04	0.94	1.33
21	YZ	72	ARG	CZ-NH1	-26.71	0.98	1.33
21	YZ	72	ARG	CZ-NH2	-26.64	0.98	1.33
21	YZ	72	ARG	CD-NE	-22.76	1.07	1.46
4	YE	144	ARG	NE-CZ	-22.31	1.04	1.33

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	1064	C	N1-C2-O2	9.58	124.65	118.90
1	RA	1064	C	N1-C2-O2	8.93	124.26	118.90
19	YX	57	LEU	CA-CB-CG	7.78	133.19	115.30
21	RZ	31	ARG	NE-CZ-NH1	-7.56	116.52	120.30
32	QA	639	G	N3-C4-N9	-7.37	121.58	126.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	QB	231	GLU	Peptide
14	RS	58	LEU	Peptide
19	RX	93	GLU	Peptide
43	XL	86	ARG	Peptide
19	YX	93	GLU	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	RA	61758	0	31146	667	0
1	YA	61758	0	31149	669	1
2	RB	2572	0	1305	12	0
2	YB	2573	0	1306	22	0
3	RD	2131	0	2207	48	0
3	YD	2136	0	2218	49	0
4	RE	1559	0	1618	36	0
4	YE	1559	0	1618	58	0
5	RF	1584	0	1625	43	0
5	YF	1580	0	1619	67	0
6	RG	1426	0	1445	61	0
6	YG	1424	0	1441	99	0
7	RH	1330	0	1407	26	0
7	YH	1324	0	1402	56	6
8	RI	1094	0	1127	33	0
8	YI	1076	0	1094	47	0
9	RN	1121	0	1195	27	0
9	YN	1117	0	1184	27	0
10	RO	933	0	996	25	0
10	YO	933	0	996	18	0
11	RP	1135	0	1212	39	0
11	YP	1135	0	1212	42	0
12	RQ	1122	0	1179	26	0
12	YQ	1122	0	1179	27	0
13	RR	968	0	1033	15	0
13	YR	968	0	1033	34	0
14	RS	877	0	938	15	0
14	YS	870	0	923	21	0
15	RT	1091	0	1151	38	0
15	YT	1083	0	1136	32	0
16	RU	959	0	1019	16	0
16	YU	959	0	1019	11	0
17	RV	775	0	841	22	0
17	YV	771	0	830	17	5
18	RW	886	0	940	18	1
18	YW	886	0	940	23	0
19	RX	750	0	814	26	0
19	YX	750	0	814	16	0
20	RY	810	0	892	16	0
20	YY	810	0	887	22	7
21	RZ	1587	0	1598	44	0
21	YZ	1557	0	1564	52	0
22	R0	608	0	622	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Y0	608	0	622	16	0
23	R1	754	0	823	12	0
23	Y1	759	0	837	24	0
24	R2	588	0	643	16	1
24	Y2	592	0	654	7	0
25	R3	469	0	518	8	0
25	Y3	464	0	514	16	0
26	R4	546	0	522	55	0
26	Y4	536	0	514	58	0
27	R5	459	0	476	18	0
27	Y5	455	0	465	10	5
28	R6	453	0	473	9	0
28	Y6	449	0	469	6	0
29	R7	418	0	467	13	0
29	Y7	418	0	467	5	0
30	R8	517	0	582	24	0
30	Y8	517	0	582	20	0
31	R9	307	0	335	6	0
31	Y9	307	0	335	5	0
32	QA	32246	0	16293	408	0
32	XA	32331	0	16339	421	0
33	QB	1842	0	1862	86	0
33	XB	1825	0	1828	88	0
34	QC	1558	0	1557	44	0
34	XC	1542	0	1517	56	0
35	QD	1665	0	1687	71	0
35	XD	1668	0	1703	38	0
36	QE	1133	0	1191	47	0
36	XE	1133	0	1191	31	0
37	QF	814	0	808	18	0
37	XF	816	0	808	24	0
38	QG	1235	0	1249	37	0
38	XG	1229	0	1238	25	0
39	QH	1098	0	1143	42	0
39	XH	1088	0	1126	22	0
40	QI	986	0	990	44	0
40	XI	966	0	953	46	0
41	QJ	719	0	672	33	0
41	XJ	710	0	661	41	0
42	QK	834	0	838	16	0
42	XK	833	0	836	24	0
43	QL	932	0	981	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	XL	932	0	981	22	0
44	QM	914	0	954	53	0
44	XM	895	0	920	50	0
45	QN	492	0	529	20	0
45	XN	492	0	529	23	0
46	QO	728	0	760	27	0
46	XO	728	0	760	6	0
47	QP	681	0	697	20	0
47	XP	677	0	686	28	0
48	QQ	823	0	891	15	0
48	XQ	823	0	891	10	0
49	QR	555	0	618	16	0
49	XR	555	0	618	26	0
50	QS	648	0	658	29	0
50	XS	645	0	635	43	0
51	QT	732	0	809	34	0
51	XT	733	0	795	31	0
52	QU	199	0	208	3	0
52	XU	199	0	208	5	0
53	QV	1644	0	836	30	0
53	XV	1644	0	836	22	0
54	QY	2833	0	2729	96	0
54	XY	2833	0	2728	124	0
55	QX	129	0	64	1	0
55	XX	129	0	65	1	0
56	QA	280	0	0	0	0
56	QB	1	0	0	0	0
56	QD	4	0	0	0	0
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	2	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	QV	4	0	0	0	0
56	QY	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	R0	4	0	0	0	0
56	R1	4	0	0	0	0
56	R3	2	0	0	0	0
56	R4	1	0	0	0	0
56	R5	4	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	1069	0	0	0	0
56	RB	28	0	0	0	0
56	RD	14	0	0	0	0
56	RE	7	0	0	0	0
56	RF	11	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	4	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	193	0	0	0	0
56	XE	2	0	0	0	0
56	XF	3	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	XT	1	0	0	0	0
56	XV	3	0	0	0	0
56	XY	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	2	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YA	756	0	0	0	0
56	YB	19	0	0	0	0
56	YD	9	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	2	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
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
All	All	296497	0	200048	4678	13

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 10.

The worst 5 of 4678 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)
33:XB:114:ARG:NH1	33:XB:118:LEU:HG	1.41	1.36
42:QK:48:ILE:HD12	42:QK:63:LEU:CB	1.60	1.29
7:YH:7:LEU:O	7:YH:69:ARG:NH1	1.63	1.29

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:QK:48:ILE:CD1	42:QK:63:LEU:HB2	1.66	1.25
26:Y4:59:PHE:CE1	50:XS:64:GLU:HB2	1.73	1.23

The worst 5 of 13 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:YH:46:GLU:OE1	20:YY:22:GLY:C[4_445]	0.78	1.42
7:YH:46:GLU:OE1	20:YY:22:GLY:O[4_445]	1.12	1.08
7:YH:46:GLU:OE1	20:YY:23:ARG:N[4_445]	1.56	0.64
17:YV:49:THR:O	27:Y5:60:VAL:O[4_445]	1.77	0.43
17:YV:53:GLU:OE2	27:Y5:59:GLU:CA[4_445]	1.88	0.32

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	RD	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	YD	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	34	71
4	YE	202/206 (98%)	196 (97%)	6 (3%)	0	100	100
5	RF	201/210 (96%)	197 (98%)	4 (2%)	0	100	100
5	YF	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	19	58
6	RG	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	30	68
6	YG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	30	68
7	RH	172/180 (96%)	167 (97%)	5 (3%)	0	100	100
7	YH	171/180 (95%)	165 (96%)	6 (4%)	0	100	100
8	RI	145/148 (98%)	133 (92%)	11 (8%)	1 (1%)	26	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	YI	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
9	RN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	YN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	RO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	YO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
11	RP	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
11	YP	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	26	66
12	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	YQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	RR	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	YR	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	RS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	21	60
14	YS	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	RT	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
15	YT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	RU	114/118 (97%)	114 (100%)	0	0	100	100
16	YU	114/118 (97%)	114 (100%)	0	0	100	100
17	RV	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
17	YV	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
18	RW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	YW	110/113 (97%)	110 (100%)	0	0	100	100
19	RX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	YX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
20	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	RZ	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
21	YZ	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
22	R0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	Y0	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	R1	95/98 (97%)	94 (99%)	0	1 (1%)	17	57
23	Y1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	R2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	Y2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	R4	67/71 (94%)	55 (82%)	6 (9%)	6 (9%)	1	6
26	Y4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	3	21
27	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	R7	46/49 (94%)	46 (100%)	0	0	100	100
29	Y7	46/49 (94%)	46 (100%)	0	0	100	100
30	R8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	Y8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	R9	35/37 (95%)	35 (100%)	0	0	100	100
31	Y9	35/37 (95%)	35 (100%)	0	0	100	100
33	QB	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	5	32
33	XB	229/256 (90%)	205 (90%)	19 (8%)	5 (2%)	8	41
34	QC	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	XC	204/239 (85%)	187 (92%)	17 (8%)	0	100	100
35	QD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
35	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
36	QE	146/162 (90%)	144 (99%)	2 (1%)	0	100	100
36	XE	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
37	QF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	XF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	QG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	XG	153/156 (98%)	148 (97%)	4 (3%)	1 (1%)	26	66
39	QH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	XH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	QI	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	24	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	XI	124/128 (97%)	113 (91%)	8 (6%)	3 (2%)	7	38
41	QJ	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	23
41	XJ	94/105 (90%)	85 (90%)	7 (7%)	2 (2%)	9	42
42	QK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	11	46
42	XK	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	21	60
43	QL	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
43	XL	119/132 (90%)	116 (98%)	3 (2%)	0	100	100
44	QM	114/126 (90%)	105 (92%)	7 (6%)	2 (2%)	11	46
44	XM	112/126 (89%)	105 (94%)	6 (5%)	1 (1%)	21	60
45	QN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	XN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	XO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	QP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
47	XP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
48	QQ	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	19	58
48	XQ	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	QR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	XR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	QS	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
50	XS	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
51	QT	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	9	42
51	XT	96/106 (91%)	88 (92%)	6 (6%)	2 (2%)	9	42
52	QU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	XU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	3	20
54	QY	354/380 (93%)	309 (87%)	37 (10%)	8 (2%)	8	39
54	XY	354/380 (93%)	309 (87%)	36 (10%)	9 (2%)	7	37
All	All	12148/12888 (94%)	11573 (95%)	504 (4%)	71 (1%)	30	68

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	Y1	3	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	XB	17	PHE
33	XB	20	GLU
33	XB	124	SER
40	XI	44	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	RD	214/218 (98%)	209 (98%)	5 (2%)	58	83
3	YD	215/218 (99%)	209 (97%)	6 (3%)	51	80
4	RE	164/166 (99%)	163 (99%)	1 (1%)	90	95
4	YE	164/166 (99%)	159 (97%)	5 (3%)	48	79
5	RF	160/166 (96%)	152 (95%)	8 (5%)	30	68
5	YF	159/166 (96%)	154 (97%)	5 (3%)	47	79
6	RG	144/156 (92%)	139 (96%)	5 (4%)	43	77
6	YG	142/156 (91%)	133 (94%)	9 (6%)	22	60
7	RH	144/148 (97%)	142 (99%)	2 (1%)	74	88
7	YH	143/148 (97%)	140 (98%)	3 (2%)	61	84
8	RI	111/124 (90%)	105 (95%)	6 (5%)	27	66
8	YI	108/124 (87%)	108 (100%)	0	100	100
9	RN	119/119 (100%)	115 (97%)	4 (3%)	44	77
9	YN	118/119 (99%)	115 (98%)	3 (2%)	55	82
10	RO	100/100 (100%)	100 (100%)	0	100	100
10	YO	100/100 (100%)	100 (100%)	0	100	100
11	RP	115/116 (99%)	112 (97%)	3 (3%)	54	81
11	YP	115/116 (99%)	113 (98%)	2 (2%)	68	86
12	RQ	111/111 (100%)	107 (96%)	4 (4%)	42	76
12	YQ	111/111 (100%)	106 (96%)	5 (4%)	34	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	RR	101/101 (100%)	99 (98%)	2 (2%)	63	84
13	YR	101/101 (100%)	101 (100%)	0	100	100
14	RS	87/88 (99%)	84 (97%)	3 (3%)	44	77
14	YS	85/88 (97%)	82 (96%)	3 (4%)	43	77
15	RT	115/127 (91%)	110 (96%)	5 (4%)	35	72
15	YT	113/127 (89%)	110 (97%)	3 (3%)	52	81
16	RU	93/94 (99%)	90 (97%)	3 (3%)	46	79
16	YU	93/94 (99%)	89 (96%)	4 (4%)	35	72
17	RV	81/82 (99%)	80 (99%)	1 (1%)	78	90
17	YV	80/82 (98%)	78 (98%)	2 (2%)	55	82
18	RW	90/92 (98%)	86 (96%)	4 (4%)	35	72
18	YW	90/92 (98%)	88 (98%)	2 (2%)	60	84
19	RX	77/78 (99%)	76 (99%)	1 (1%)	76	89
19	YX	77/78 (99%)	74 (96%)	3 (4%)	39	75
20	RY	86/91 (94%)	83 (96%)	3 (4%)	43	77
20	YY	86/91 (94%)	82 (95%)	4 (5%)	32	70
21	RZ	169/179 (94%)	165 (98%)	4 (2%)	57	83
21	YZ	165/179 (92%)	159 (96%)	6 (4%)	42	76
22	R0	61/67 (91%)	59 (97%)	2 (3%)	45	78
22	Y0	61/67 (91%)	56 (92%)	5 (8%)	14	48
23	R1	79/83 (95%)	77 (98%)	2 (2%)	55	82
23	Y1	81/83 (98%)	79 (98%)	2 (2%)	55	82
24	R2	65/67 (97%)	63 (97%)	2 (3%)	47	79
24	Y2	66/67 (98%)	64 (97%)	2 (3%)	48	79
25	R3	51/52 (98%)	51 (100%)	0	100	100
25	Y3	50/52 (96%)	47 (94%)	3 (6%)	24	62
26	R4	58/63 (92%)	55 (95%)	3 (5%)	29	67
26	Y4	54/63 (86%)	47 (87%)	7 (13%)	5	22
27	R5	51/52 (98%)	50 (98%)	1 (2%)	63	84
27	Y5	50/52 (96%)	49 (98%)	1 (2%)	63	84
28	R6	51/52 (98%)	50 (98%)	1 (2%)	63	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	Y6	50/52 (96%)	50 (100%)	0	100	100
29	R7	41/42 (98%)	41 (100%)	0	100	100
29	Y7	41/42 (98%)	41 (100%)	0	100	100
30	R8	54/55 (98%)	52 (96%)	2 (4%)	41	76
30	Y8	54/55 (98%)	52 (96%)	2 (4%)	41	76
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
33	QB	191/220 (87%)	182 (95%)	9 (5%)	32	70
33	XB	187/220 (85%)	176 (94%)	11 (6%)	24	63
34	QC	144/188 (77%)	141 (98%)	3 (2%)	61	84
34	XC	140/188 (74%)	135 (96%)	5 (4%)	42	76
35	QD	171/181 (94%)	166 (97%)	5 (3%)	50	80
35	XD	172/181 (95%)	168 (98%)	4 (2%)	58	83
36	QE	114/123 (93%)	112 (98%)	2 (2%)	66	85
36	XE	114/123 (93%)	113 (99%)	1 (1%)	84	92
37	QF	85/90 (94%)	83 (98%)	2 (2%)	57	83
37	XF	85/90 (94%)	83 (98%)	2 (2%)	57	83
38	QG	120/127 (94%)	117 (98%)	3 (2%)	55	82
38	XG	119/127 (94%)	116 (98%)	3 (2%)	55	82
39	QH	116/119 (98%)	114 (98%)	2 (2%)	68	86
39	XH	114/119 (96%)	109 (96%)	5 (4%)	35	72
40	QI	91/99 (92%)	85 (93%)	6 (7%)	21	59
40	XI	88/99 (89%)	86 (98%)	2 (2%)	58	83
41	QJ	68/92 (74%)	67 (98%)	1 (2%)	72	88
41	XJ	68/92 (74%)	67 (98%)	1 (2%)	72	88
42	QK	83/99 (84%)	82 (99%)	1 (1%)	78	90
42	XK	83/99 (84%)	81 (98%)	2 (2%)	57	83
43	QL	96/108 (89%)	95 (99%)	1 (1%)	82	91
43	XL	96/108 (89%)	95 (99%)	1 (1%)	82	91
44	QM	90/101 (89%)	86 (96%)	4 (4%)	35	72
44	XM	87/101 (86%)	85 (98%)	2 (2%)	58	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	QN	49/50 (98%)	46 (94%)	3 (6%)	23	62
45	XN	49/50 (98%)	48 (98%)	1 (2%)	63	84
46	QO	78/80 (98%)	76 (97%)	2 (3%)	54	81
46	XO	78/80 (98%)	75 (96%)	3 (4%)	40	75
47	QP	69/74 (93%)	69 (100%)	0	100	100
47	XP	68/74 (92%)	66 (97%)	2 (3%)	50	80
48	QQ	94/97 (97%)	93 (99%)	1 (1%)	80	90
48	XQ	94/97 (97%)	94 (100%)	0	100	100
49	QR	59/77 (77%)	58 (98%)	1 (2%)	68	86
49	XR	59/77 (77%)	58 (98%)	1 (2%)	68	86
50	QS	68/80 (85%)	65 (96%)	3 (4%)	35	72
50	XS	67/80 (84%)	67 (100%)	0	100	100
51	QT	71/82 (87%)	70 (99%)	1 (1%)	74	88
51	XT	70/82 (85%)	70 (100%)	0	100	100
52	QU	18/22 (82%)	17 (94%)	1 (6%)	26	65
52	XU	18/22 (82%)	16 (89%)	2 (11%)	8	31
54	QY	303/323 (94%)	301 (99%)	2 (1%)	88	94
54	XY	303/323 (94%)	301 (99%)	2 (1%)	88	94
All	All	9969/10710 (93%)	9702 (97%)	267 (3%)	52	81

5 of 267 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	XJ	57	LYS
35	QD	168	ARG
21	RZ	72	ARG
44	XM	94	ARG
33	QB	21	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
50	QS	57	HIS
50	QS	65	ASN
54	XY	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	QG	56	GLN
54	QY	308	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2855/2915 (97%)	427 (14%)	21 (0%)
1	YA	2855/2915 (97%)	430 (15%)	24 (0%)
2	RB	119/122 (97%)	10 (8%)	0
2	YB	119/122 (97%)	12 (10%)	0
32	QA	1494/1521 (98%)	220 (14%)	14 (0%)
32	XA	1498/1521 (98%)	232 (15%)	18 (1%)
53	QV	76/77 (98%)	19 (25%)	1 (1%)
53	XV	76/77 (98%)	18 (23%)	1 (1%)
55	QX	5/25 (20%)	1 (20%)	0
55	XX	5/25 (20%)	1 (20%)	0
All	All	9102/9320 (97%)	1370 (15%)	79 (0%)

5 of 1370 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	YA	10	G
1	YA	11	G
1	YA	12	U
1	YA	15	G
1	YA	34	C

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	XA	991	U
32	QA	509	A
1	RA	2171	A
32	XA	992	U
32	XA	1256	A

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

50 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$
32	2MG	QA	1207	32	18,26,27	1.21	2 (11%)	21,38,41	2.34	7 (33%)
32	5MC	QA	1400	32	14,22,23	1.32	1 (7%)	17,32,35	0.92	1 (5%)
32	4OC	QA	1402	32	15,23,24	0.56	0	21,32,35	1.80	3 (14%)
32	5MC	QA	1404	32	14,22,23	1.32	1 (7%)	17,32,35	0.95	1 (5%)
32	5MC	QA	1407	32	14,22,23	1.32	1 (7%)	17,32,35	1.01	1 (5%)
32	UR3	QA	1498	32	13,22,23	0.70	0	18,32,35	0.69	0
32	MA6	QA	1518	32	18,26,27	0.98	1 (5%)	15,38,41	2.31	3 (20%)
32	MA6	QA	1519	32	18,26,27	1.01	1 (5%)	15,38,41	2.09	2 (13%)
32	PSU	QA	516	32,56	15,21,22	1.30	2 (13%)	16,30,33	2.13	3 (18%)
32	7MG	QA	527	32,56	20,26,27	1.48	2 (10%)	23,39,42	3.27	5 (21%)
32	M2G	QA	966	32	18,27,28	1.38	3 (16%)	22,40,43	1.82	4 (18%)
32	5MC	QA	967	32	14,22,23	1.35	1 (7%)	17,32,35	0.81	1 (5%)
43	0TD	QL	92	43	4,9,10	4.32	3 (75%)	4,11,13	5.62	4 (100%)
54	MEQ	QY	252	54	7,9,10	0.76	0	8,10,12	0.76	0
1	PSU	RA	1911	1	15,21,22	1.33	1 (6%)	16,30,33	2.21	4 (25%)
1	5MU	RA	1915	1,56	13,22,23	0.54	0	16,32,35	2.82	2 (12%)
1	PSU	RA	1917	1	15,21,22	1.31	1 (6%)	16,30,33	2.33	4 (25%)
1	4OC	RA	1920	1	15,22,24	0.51	0	20,31,35	1.46	2 (10%)
1	5MU	RA	1939	1	13,22,23	0.59	0	16,32,35	2.52	2 (12%)
1	5MC	RA	1942	1	14,22,23	1.29	1 (7%)	17,32,35	0.94	1 (5%)
1	5MC	RA	1962	1,56	14,22,23	1.31	1 (7%)	17,32,35	0.94	1 (5%)
1	OMG	RA	2251	1,56,53	18,26,27	1.15	2 (11%)	21,38,41	1.87	4 (19%)
1	2MA	RA	2503	1,56	17,25,26	1.62	3 (17%)	18,37,40	2.91	1 (5%)
1	2MU	RA	2552	1,56	14,22,24	0.81	0	19,31,36	1.64	1 (5%)
1	PSU	RA	2605	1	15,21,22	1.45	1 (6%)	16,30,33	2.31	4 (25%)
32	2MG	XA	1207	32	18,26,27	1.22	2 (11%)	21,38,41	2.25	6 (28%)
32	5MC	XA	1400	32	14,22,23	1.34	1 (7%)	17,32,35	0.86	1 (5%)
32	4OC	XA	1402	32	15,23,24	0.57	0	21,32,35	1.82	3 (14%)
32	5MC	XA	1404	32	14,22,23	1.28	1 (7%)	17,32,35	0.99	1 (5%)
32	5MC	XA	1407	32	14,22,23	1.27	1 (7%)	17,32,35	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	XA	1498	32,56	13,22,23	0.75	1 (7%)	18,32,35	0.73	0
32	MA6	XA	1518	32	18,26,27	0.95	1 (5%)	15,38,41	2.21	3 (20%)
32	MA6	XA	1519	32	18,26,27	0.97	1 (5%)	15,38,41	2.25	3 (20%)
32	PSU	XA	516	32	15,21,22	1.25	1 (6%)	16,30,33	2.13	3 (18%)
32	7MG	XA	527	32,56	20,26,27	1.46	2 (10%)	23,39,42	3.23	5 (21%)
32	M2G	XA	966	32	18,27,28	1.42	3 (16%)	22,40,43	1.86	4 (18%)
32	5MC	XA	967	32	14,22,23	1.36	1 (7%)	17,32,35	0.85	1 (5%)
43	0TD	XL	92	43	4,9,10	3.07	1 (25%)	4,11,13	2.53	1 (25%)
54	MEQ	XY	252	54	7,9,10	0.83	0	8,10,12	0.74	0
1	PSU	YA	1911	1	15,21,22	1.32	1 (6%)	16,30,33	2.22	4 (25%)
1	5MU	YA	1915	1	13,22,23	0.53	0	16,32,35	2.91	3 (18%)
1	PSU	YA	1917	1	15,21,22	1.29	1 (6%)	16,30,33	2.28	4 (25%)
1	4OC	YA	1920	1	15,22,24	0.62	0	20,31,35	1.24	2 (10%)
1	5MU	YA	1939	1,56	13,22,23	0.63	0	16,32,35	2.56	2 (12%)
1	5MC	YA	1942	1	14,22,23	1.27	1 (7%)	17,32,35	1.00	1 (5%)
1	5MC	YA	1962	1,56	14,22,23	1.30	1 (7%)	17,32,35	0.94	1 (5%)
1	OMG	YA	2251	1,56,53	18,26,27	1.17	2 (11%)	21,38,41	1.83	4 (19%)
1	2MA	YA	2503	1,56	17,25,26	1.61	3 (17%)	18,37,40	3.01	1 (5%)
1	2MU	YA	2552	1,56	14,22,24	0.82	0	19,31,36	1.63	1 (5%)
1	PSU	YA	2605	1	15,21,22	1.41	1 (6%)	16,30,33	2.32	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
32	2MG	QA	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	QA	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	QA	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	QA	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	QA	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	QA	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	QA	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	QA	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	QA	516	32,56	-	0/7/25/26	0/2/2/2
32	7MG	QA	527	32,56	-	0/7/37/38	0/3/3/3
32	M2G	QA	966	32	-	0/7/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	QA	967	32	-	0/3/25/26	0/2/2/2
43	0TD	QL	92	43	-	0/2/12/14	0/0/0/0
54	MEQ	QY	252	54	-	0/7/9/11	0/0/0/0
1	PSU	RA	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	RA	1915	1,56	-	0/3/25/26	0/2/2/2
1	PSU	RA	1917	1	-	0/7/25/26	0/2/2/2
1	4OC	RA	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	RA	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	RA	1942	1	-	0/3/25/26	0/2/2/2
1	5MC	RA	1962	1,56	-	0/3/25/26	0/2/2/2
1	OMG	RA	2251	1,56,53	-	0/5/27/28	0/3/3/3
1	2MA	RA	2503	1,56	-	0/3/25/26	0/3/3/3
1	2MU	RA	2552	1,56	-	0/5/27/28	0/2/2/2
1	PSU	RA	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	XA	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	XA	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	XA	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	XA	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	XA	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	XA	1498	32,56	-	0/3/25/26	0/2/2/2
32	MA6	XA	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	XA	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	XA	516	32	-	0/7/25/26	0/2/2/2
32	7MG	XA	527	32,56	-	0/7/37/38	0/3/3/3
32	M2G	XA	966	32	-	0/7/29/30	0/3/3/3
32	5MC	XA	967	32	-	0/3/25/26	0/2/2/2
43	0TD	XL	92	43	-	0/2/12/14	0/0/0/0
54	MEQ	XY	252	54	-	0/7/9/11	0/0/0/0
1	PSU	YA	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	YA	1915	1	-	0/3/25/26	0/2/2/2
1	PSU	YA	1917	1	-	0/7/25/26	0/2/2/2
1	4OC	YA	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	YA	1939	1,56	-	0/3/25/26	0/2/2/2
1	5MC	YA	1942	1	-	0/3/25/26	0/2/2/2
1	5MC	YA	1962	1,56	-	0/3/25/26	0/2/2/2
1	OMG	YA	2251	1,56,53	-	0/5/27/28	0/3/3/3
1	2MA	YA	2503	1,56	-	0/3/25/26	0/3/3/3
1	2MU	YA	2552	1,56	-	0/5/27/28	0/2/2/2
1	PSU	YA	2605	1	-	0/7/25/26	0/2/2/2

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	QL	92	0TD	CB-SB	-7.55	1.64	1.84
43	XL	92	0TD	CB-SB	-5.77	1.69	1.84
1	RA	2605	PSU	C5-C1'	-4.54	1.48	1.52
1	YA	2605	PSU	C5-C1'	-4.36	1.48	1.52
1	RA	1911	PSU	C5-C1'	-4.04	1.48	1.52

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	QA	527	7MG	C5-C4-N3	-8.94	117.64	126.74
32	XA	527	7MG	C5-C4-N3	-8.70	117.88	126.74
43	QL	92	0TD	CB-CA-N	-8.36	93.10	109.83
1	YA	1915	5MU	C5-C4-N3	-8.24	118.43	125.35
1	RA	1915	5MU	C5-C4-N3	-7.99	118.64	125.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	QA	1207	2MG	2	0
32	QA	1402	4OC	1	0
32	QA	1498	UR3	1	0
32	QA	1518	MA6	1	0
32	QA	1519	MA6	1	0
32	QA	516	PSU	1	0
32	QA	966	M2G	1	0
32	QA	967	5MC	1	0
43	QL	92	0TD	1	0
1	RA	1939	5MU	1	0
1	RA	1942	5MC	1	0
1	RA	1962	5MC	1	0
1	RA	2503	2MA	1	0
32	XA	1207	2MG	1	0
32	XA	1402	4OC	1	0
32	XA	1518	MA6	1	0
43	XL	92	0TD	1	0
1	YA	1920	4OC	2	0
1	YA	1939	5MU	1	0
1	YA	1962	5MC	1	0
1	YA	2251	OMG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	YA	2503	2MA	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2534 ligands modelled in this entry, 2532 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	35	0,12,12	0.00	-	0,24,24	0.00	-
58	SF4	XD	301	35	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	35	-	0/0/48/48	0/6/5/5
58	SF4	XD	301	35	-	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	RA	2856/2915 (97%)	0.33	130 (4%) 36 30	76, 86, 96, 102	0
1	YA	2856/2915 (97%)	0.44	117 (4%) 41 34	71, 83, 96, 100	0
2	RB	120/122 (98%)	-0.10	2 (1%) 73 67	84, 90, 93, 96	0
2	YB	120/122 (98%)	-0.17	2 (1%) 73 67	80, 87, 91, 94	0
3	RD	275/276 (99%)	0.47	5 (1%) 71 65	77, 85, 89, 96	0
3	YD	275/276 (99%)	0.50	4 (1%) 76 71	76, 83, 89, 90	0
4	RE	204/206 (99%)	0.50	5 (2%) 61 54	78, 86, 91, 93	0
4	YE	204/206 (99%)	0.54	4 (1%) 68 62	77, 86, 90, 94	0
5	RF	203/210 (96%)	0.32	2 (0%) 84 80	81, 87, 92, 95	0
5	YF	203/210 (96%)	0.34	1 (0%) 91 90	76, 85, 91, 94	0
6	RG	181/182 (99%)	0.48	15 (8%) 14 11	87, 91, 94, 97	0
6	YG	181/182 (99%)	0.32	12 (6%) 22 17	85, 89, 93, 95	0
7	RH	174/180 (96%)	1.30	50 (28%) 1 1	86, 92, 95, 97	0
7	YH	173/180 (96%)	0.32	5 (2%) 55 49	82, 88, 92, 95	0
8	RI	147/148 (99%)	0.91	28 (19%) 2 1	85, 91, 94, 97	0
8	YI	146/148 (98%)	0.53	10 (6%) 20 17	84, 90, 94, 96	0
9	RN	140/140 (100%)	0.63	11 (7%) 15 12	83, 88, 92, 96	0
9	YN	140/140 (100%)	0.53	1 (0%) 89 86	80, 86, 91, 94	0
10	RO	122/122 (100%)	0.45	1 (0%) 87 84	79, 85, 90, 91	0
10	YO	122/122 (100%)	0.42	1 (0%) 87 84	78, 85, 89, 92	0
11	RP	149/150 (99%)	0.77	6 (4%) 42 34	78, 88, 92, 95	0
11	YP	149/150 (99%)	0.62	5 (3%) 49 42	77, 85, 90, 94	0
12	RQ	141/141 (100%)	0.26	2 (1%) 78 73	82, 87, 91, 93	0
12	YQ	141/141 (100%)	0.36	0 100 100	77, 85, 89, 91	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	RR	118/118 (100%)	0.47	2 (1%) 73 67	81, 86, 89, 91	0
13	YR	118/118 (100%)	0.52	3 (2%) 61 54	80, 85, 89, 92	0
14	RS	110/112 (98%)	0.56	9 (8%) 14 11	84, 89, 93, 95	0
14	YS	110/112 (98%)	0.46	2 (1%) 71 65	82, 88, 91, 94	0
15	RT	131/146 (89%)	0.29	3 (2%) 64 57	82, 87, 91, 95	0
15	YT	131/146 (89%)	0.34	3 (2%) 64 57	82, 86, 92, 95	0
16	RU	116/118 (98%)	0.44	7 (6%) 25 20	82, 87, 92, 93	0
16	YU	116/118 (98%)	0.45	2 (1%) 73 67	78, 84, 90, 91	0
17	RV	101/101 (100%)	0.21	3 (2%) 54 47	81, 89, 92, 95	0
17	YV	101/101 (100%)	0.50	1 (0%) 84 80	80, 86, 91, 93	0
18	RW	112/113 (99%)	0.61	4 (3%) 46 39	80, 85, 90, 95	0
18	YW	112/113 (99%)	0.59	6 (5%) 29 24	78, 84, 90, 95	0
19	RX	95/96 (98%)	0.70	9 (9%) 10 9	83, 87, 90, 93	0
19	YX	95/96 (98%)	0.44	3 (3%) 51 44	79, 84, 89, 94	0
20	RY	107/110 (97%)	1.49	29 (27%) 1 1	85, 90, 93, 100	0
20	YY	107/110 (97%)	0.73	11 (10%) 9 7	82, 88, 92, 98	0
21	RZ	203/206 (98%)	0.92	22 (10%) 8 6	87, 90, 94, 99	0
21	YZ	201/206 (97%)	0.50	18 (8%) 12 9	83, 89, 94, 96	0
22	R0	77/85 (90%)	1.16	13 (16%) 2 2	83, 87, 90, 95	0
22	Y0	77/85 (90%)	0.72	7 (9%) 11 9	80, 85, 90, 95	0
23	R1	97/98 (98%)	0.78	10 (10%) 9 7	82, 86, 92, 94	0
23	Y1	97/98 (98%)	0.81	6 (6%) 24 19	78, 85, 91, 94	0
24	R2	70/72 (97%)	0.38	3 (4%) 39 32	83, 89, 92, 94	0
24	Y2	70/72 (97%)	0.40	1 (1%) 78 73	79, 86, 90, 97	0
25	R3	59/60 (98%)	1.13	9 (15%) 3 2	82, 88, 93, 98	0
25	Y3	59/60 (98%)	0.87	4 (6%) 20 17	79, 85, 91, 95	0
26	R4	69/71 (97%)	1.27	18 (26%) 1 1	89, 93, 96, 97	0
26	Y4	69/71 (97%)	0.70	12 (17%) 2 2	87, 92, 96, 97	0
27	R5	59/60 (98%)	0.41	2 (3%) 49 42	78, 86, 92, 95	0
27	Y5	59/60 (98%)	0.38	2 (3%) 49 42	78, 85, 92, 97	0
28	R6	53/54 (98%)	3.35	41 (77%) 0 0	89, 93, 96, 100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y6	53/54 (98%)	3.02	40 (75%) 0 0	88, 92, 95, 97	0
29	R7	48/49 (97%)	0.74	3 (6%) 23 19	79, 84, 91, 93	0
29	Y7	48/49 (97%)	1.05	4 (8%) 14 11	76, 81, 88, 93	0
30	R8	64/65 (98%)	0.78	2 (3%) 52 46	81, 86, 90, 91	0
30	Y8	64/65 (98%)	0.64	0 100 100	76, 83, 89, 90	0
31	R9	37/37 (100%)	2.40	20 (54%) 0 0	88, 90, 94, 97	0
31	Y9	37/37 (100%)	2.14	19 (51%) 0 0	84, 89, 91, 91	0
32	QA	1488/1521 (97%)	0.10	35 (2%) 62 55	83, 90, 96, 103	0
32	XA	1492/1521 (98%)	0.10	37 (2%) 61 54	78, 90, 96, 101	0
33	QB	231/256 (90%)	0.62	24 (10%) 8 7	88, 92, 95, 97	0
33	XB	231/256 (90%)	0.46	22 (9%) 10 9	87, 91, 95, 98	0
34	QC	206/239 (86%)	0.58	24 (11%) 6 5	88, 91, 94, 96	0
34	XC	206/239 (86%)	0.58	20 (9%) 10 9	87, 90, 93, 96	0
35	QD	208/209 (99%)	0.34	9 (4%) 39 32	85, 89, 93, 97	0
35	XD	208/209 (99%)	0.52	19 (9%) 11 9	85, 90, 94, 97	0
36	QE	148/162 (91%)	0.38	9 (6%) 25 20	85, 90, 93, 95	0
36	XE	148/162 (91%)	0.52	9 (6%) 25 20	85, 88, 92, 94	0
37	QF	100/101 (99%)	0.32	8 (8%) 15 12	87, 90, 93, 95	0
37	XF	100/101 (99%)	0.16	3 (3%) 54 47	83, 89, 93, 95	0
38	QG	155/156 (99%)	0.90	24 (15%) 3 2	88, 91, 94, 96	0
38	XG	155/156 (99%)	0.66	15 (9%) 10 9	87, 91, 95, 96	0
39	QH	137/138 (99%)	0.63	14 (10%) 9 7	86, 89, 92, 94	0
39	XH	137/138 (99%)	0.62	10 (7%) 18 15	82, 89, 92, 94	0
40	QI	127/128 (99%)	1.33	30 (23%) 1 1	86, 92, 95, 96	0
40	XI	126/128 (98%)	0.89	18 (14%) 4 3	85, 92, 95, 98	0
41	QJ	97/105 (92%)	1.33	29 (29%) 1 1	86, 92, 95, 97	0
41	XJ	96/105 (91%)	0.96	15 (15%) 3 2	87, 91, 94, 96	0
42	QK	114/129 (88%)	0.75	12 (10%) 8 7	86, 90, 93, 94	0
42	XK	114/129 (88%)	0.51	4 (3%) 48 40	82, 88, 92, 95	0
43	QL	121/132 (91%)	0.51	6 (4%) 32 26	81, 87, 90, 92	0
43	XL	121/132 (91%)	0.66	10 (8%) 14 11	83, 87, 91, 93	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	QM	116/126 (92%)	0.76	19 (16%) 2 2	88, 92, 95, 97	0
44	XM	114/126 (90%)	0.97	22 (19%) 2 1	87, 91, 94, 95	0
45	QN	60/61 (98%)	1.46	14 (23%) 1 1	87, 91, 94, 95	0
45	XN	60/61 (98%)	0.51	3 (5%) 32 26	88, 90, 93, 95	0
46	QO	88/89 (98%)	0.50	6 (6%) 20 17	86, 89, 93, 94	0
46	XO	88/89 (98%)	0.59	6 (6%) 20 17	84, 89, 92, 94	0
47	QP	82/88 (93%)	1.02	11 (13%) 4 3	84, 89, 91, 93	0
47	XP	82/88 (93%)	0.96	15 (18%) 2 1	86, 90, 92, 95	0
48	QQ	99/105 (94%)	0.70	8 (8%) 15 11	85, 89, 93, 95	0
48	XQ	99/105 (94%)	0.44	3 (3%) 54 47	85, 88, 91, 93	0
49	QR	68/88 (77%)	1.23	14 (20%) 1 1	87, 90, 94, 96	0
49	XR	68/88 (77%)	0.67	3 (4%) 38 31	83, 89, 92, 93	0
50	QS	83/93 (89%)	1.55	27 (32%) 1 1	88, 92, 95, 97	0
50	XS	83/93 (89%)	1.50	24 (28%) 1 1	89, 92, 94, 96	0
51	QT	96/106 (90%)	0.65	5 (5%) 31 25	84, 89, 91, 93	0
51	XT	98/106 (92%)	1.18	17 (17%) 2 2	86, 90, 93, 94	0
52	QU	23/27 (85%)	3.02	20 (86%) 0 0	88, 92, 94, 95	0
52	XU	23/27 (85%)	2.17	12 (52%) 0 0	89, 91, 93, 93	0
53	QV	77/77 (100%)	0.22	3 (3%) 43 36	85, 91, 96, 98	0
53	XV	77/77 (100%)	0.41	5 (6%) 22 18	83, 90, 96, 100	0
54	QY	356/380 (93%)	1.86	144 (40%) 0 0	86, 92, 96, 99	0
54	XY	356/380 (93%)	1.63	119 (33%) 0 1	84, 91, 96, 99	0
55	QX	6/25 (24%)	0.64	0 100 100	87, 90, 91, 92	0
55	XX	6/25 (24%)	0.63	0 100 100	85, 88, 91, 91	0
All	All	21446/22208 (96%)	0.54	1678 (7%) 16 13	71, 88, 95, 103	0

The worst 5 of 1678 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	R6	20	ASN	11.6
21	YZ	192	ALA	10.7
20	YY	1	MET	9.1
31	R9	37	GLY	8.8
25	R3	60	GLU	8.8

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	UR3	XA	1498	21/22	0.96	0.22	-	74,83,87,88	0
1	5MC	RA	1942	21/22	0.94	0.23	-	81,85,88,90	0
1	5MC	YA	1942	21/22	0.93	0.23	-	76,81,87,88	0
43	0TD	XL	92	10/11	0.95	0.26	-	85,89,93,95	0
32	2MG	QA	1207	24/25	0.92	0.19	-	89,91,96,97	0
1	5MU	YA	1915	21/22	0.86	0.21	-	85,89,92,95	0
32	5MC	XA	1407	21/22	0.94	0.22	-	81,84,89,91	0
1	PSU	RA	1917	20/21	0.92	0.16	-	84,87,91,91	0
32	MA6	QA	1519	24/25	0.94	0.28	-	82,85,85,87	0
1	2MU	RA	2552	21/23	0.95	0.27	-	75,82,84,87	0
1	4OC	YA	1920	21/23	0.94	0.23	-	81,83,85,87	0
32	5MC	XA	1400	21/22	0.95	0.21	-	78,85,86,88	0
54	MEQ	XY	252	10/11	0.94	0.33	-	86,87,91,91	0
32	PSU	XA	516	20/21	0.91	0.16	-	89,90,93,94	0
32	M2G	XA	966	25/26	0.92	0.19	-	83,87,94,94	0
1	PSU	YA	1911	20/21	0.95	0.18	-	79,85,88,90	0
1	5MU	YA	1939	21/22	0.95	0.27	-	72,77,82,84	0
1	2MA	RA	2503	23/24	0.95	0.25	-	75,81,83,84	0
32	5MC	XA	1404	21/22	0.96	0.18	-	79,84,85,87	0
1	2MU	YA	2552	21/23	0.93	0.29	-	74,78,86,87	0
1	4OC	RA	1920	21/23	0.93	0.20	-	83,85,89,92	0
43	0TD	QL	92	10/11	0.94	0.20	-	87,90,94,95	0
32	MA6	QA	1518	24/25	0.93	0.27	-	82,86,88,89	0
32	5MC	QA	967	21/22	0.94	0.20	-	83,87,90,93	0
54	MEQ	QY	252	10/11	0.93	0.32	-	85,87,90,90	0
32	4OC	XA	1402	22/23	0.90	0.28	-	83,85,87,89	0
32	PSU	QA	516	20/21	0.90	0.15	-	87,89,91,91	0
1	5MC	YA	1962	21/22	0.96	0.19	-	73,81,85,85	0
32	4OC	QA	1402	22/23	0.89	0.24	-	84,87,89,90	0
1	PSU	RA	1911	20/21	0.95	0.14	-	82,85,88,89	0
32	5MC	QA	1404	21/22	0.94	0.20	-	83,86,88,88	0
32	2MG	XA	1207	24/25	0.90	0.22	-	88,90,95,97	0
32	MA6	XA	1518	24/25	0.96	0.29	-	70,82,82,83	0
1	2MA	YA	2503	23/24	0.94	0.29	-	72,78,79,81	0
1	PSU	YA	2605	20/21	0.94	0.28	-	69,77,81,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	7MG	XA	527	24/25	0.93	0.24	-	83,86,87,88	0
32	M2G	QA	966	25/26	0.93	0.18	-	85,87,91,93	0
32	MA6	XA	1519	24/25	0.96	0.27	-	76,83,84,86	0
1	5MU	RA	1939	21/22	0.95	0.23	-	76,82,84,85	0
1	PSU	RA	2605	20/21	0.93	0.25	-	72,79,84,84	0
1	PSU	YA	1917	20/21	0.93	0.18	-	81,86,88,89	0
32	5MC	QA	1400	21/22	0.94	0.24	-	85,89,90,90	0
32	UR3	QA	1498	21/22	0.90	0.27	-	80,84,87,92	0
32	5MC	QA	1407	21/22	0.96	0.16	-	80,83,85,86	0
1	5MC	RA	1962	21/22	0.94	0.18	-	76,84,87,87	0
32	5MC	XA	967	21/22	0.93	0.25	-	87,88,89,89	0
1	5MU	RA	1915	21/22	0.89	0.13	-	84,89,93,97	0
32	7MG	QA	527	24/25	0.93	0.21	-	85,87,87,88	0
1	OMG	YA	2251	24/25	0.97	0.28	-	72,78,83,84	0
1	OMG	RA	2251	24/25	0.95	0.27	-	80,83,85,85	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3324	1/1	0.92	1.09	154.64	62,62,62,62	0
56	MG	XA	1781	1/1	0.84	1.36	87.52	79,79,79,79	0
56	MG	YA	3360	1/1	0.94	1.11	82.31	62,62,62,62	0
56	MG	YA	3343	1/1	0.94	0.83	71.35	62,62,62,62	0
56	MG	YA	3247	1/1	0.40	0.74	65.95	80,80,80,80	0
56	MG	RA	3444	1/1	0.90	1.29	64.47	62,62,62,62	0
56	MG	RA	3122	1/1	0.43	1.93	64.04	102,102,102,102	0
56	MG	RA	3854	1/1	0.61	1.73	63.73	87,87,87,87	0
56	MG	YA	3102	1/1	0.55	1.80	60.80	101,101,101,101	0
56	MG	YA	3295	1/1	0.80	1.09	59.63	62,62,62,62	0
56	MG	YA	3131	1/1	0.60	1.26	58.98	105,105,105,105	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3697	1/1	0.72	2.04	58.95	101,101,101,101	0
56	MG	YA	3582	1/1	0.74	1.24	57.95	74,74,74,74	0
56	MG	QA	1704	1/1	0.24	0.78	57.72	89,89,89,89	0
56	MG	YA	3058	1/1	0.40	1.08	55.29	93,93,93,93	0
56	MG	QA	1771	1/1	-0.14	1.08	55.04	93,93,93,93	0
56	MG	XA	1780	1/1	0.51	1.11	52.98	74,74,74,74	0
56	MG	YA	3710	1/1	0.25	1.19	50.96	80,80,80,80	0
56	MG	RA	3588	1/1	0.79	1.02	50.37	76,76,76,76	0
56	MG	YA	3374	1/1	0.76	0.98	49.44	75,75,75,75	0
56	MG	RA	3394	1/1	0.97	0.91	47.40	62,62,62,62	0
56	MG	XA	1623	1/1	-0.04	0.50	47.17	83,83,83,83	0
56	MG	RA	3754	1/1	0.88	0.82	46.82	62,62,62,62	0
56	MG	RA	3029	1/1	0.69	1.46	46.68	104,104,104,104	0
56	MG	YA	3320	1/1	0.26	1.08	44.91	87,87,87,87	0
56	MG	RA	3205	1/1	0.23	1.13	44.88	87,87,87,87	0
56	MG	RA	3631	1/1	0.32	1.07	43.28	94,94,94,94	0
56	MG	YA	3745	1/1	0.82	0.96	42.51	104,104,104,104	0
56	MG	RA	3773	1/1	0.97	0.76	42.15	70,70,70,70	0
56	MG	RA	3829	1/1	-0.04	1.51	42.13	96,96,96,96	0
56	MG	RA	3221	1/1	0.83	1.14	41.66	92,92,92,92	0
56	MG	RA	3141	1/1	0.65	1.21	41.13	92,92,92,92	0
56	MG	YA	3166	1/1	0.72	0.96	40.74	109,109,109,109	0
56	MG	YA	3705	1/1	0.38	1.20	40.41	78,78,78,78	0
56	MG	YA	3419	1/1	0.87	0.74	39.71	77,77,77,77	0
56	MG	RA	3882	1/1	0.77	1.20	39.12	87,87,87,87	0
56	MG	RA	3751	1/1	0.49	1.29	38.87	83,83,83,83	0
56	MG	YA	3401	1/1	0.94	0.69	38.86	62,62,62,62	0
56	MG	YA	3409	1/1	0.42	1.29	38.17	95,95,95,95	0
56	MG	RA	3537	1/1	-0.03	1.01	37.60	84,84,84,84	0
56	MG	YA	3647	1/1	0.74	1.16	37.47	62,62,62,62	0
56	MG	RA	3116	1/1	0.63	1.16	37.42	104,104,104,104	0
56	MG	RA	3094	1/1	0.86	1.24	35.97	85,85,85,85	0
56	MG	YD	303	1/1	0.78	1.07	35.16	84,84,84,84	0
56	MG	RA	3850	1/1	0.44	0.56	35.15	72,72,72,72	0
56	MG	RA	3572	1/1	0.36	0.56	35.03	81,81,81,81	0
56	MG	QA	1780	1/1	0.33	1.33	34.95	80,80,80,80	0
56	MG	YA	3316	1/1	0.83	0.62	34.86	62,62,62,62	0
56	MG	RA	3738	1/1	0.40	0.61	34.81	93,93,93,93	0
56	MG	YA	3630	1/1	0.89	0.86	34.59	66,66,66,66	0
56	MG	RA	3436	1/1	0.80	1.11	34.43	63,63,63,63	0
56	MG	RA	3088	1/1	0.82	1.03	34.14	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3486	1/1	0.47	0.78	33.57	83,83,83,83	0
56	MG	RA	3118	1/1	0.80	0.72	33.04	96,96,96,96	0
56	MG	XA	1611	1/1	0.75	0.65	32.98	81,81,81,81	0
56	MG	YA	3314	1/1	0.66	0.60	31.85	69,69,69,69	0
56	MG	YA	3518	1/1	0.13	0.88	31.84	70,70,70,70	0
56	MG	YA	3694	1/1	0.23	0.89	31.80	82,82,82,82	0
56	MG	RA	3101	1/1	0.69	0.82	31.60	95,95,95,95	0
56	MG	QA	1625	1/1	0.71	0.53	31.18	88,88,88,88	0
56	MG	RA	3142	1/1	0.39	0.49	31.13	85,85,85,85	0
56	MG	YA	3633	1/1	0.23	1.20	30.47	95,95,95,95	0
56	MG	QA	1614	1/1	0.78	0.80	30.42	85,85,85,85	0
56	MG	RA	3408	1/1	0.96	0.76	30.36	62,62,62,62	0
56	MG	RA	3208	1/1	0.59	0.68	30.23	89,89,89,89	0
56	MG	YA	3509	1/1	-0.35	0.79	30.11	97,97,97,97	0
56	MG	XA	1627	1/1	0.74	0.97	30.10	80,80,80,80	0
56	MG	YA	3747	1/1	0.74	1.25	29.96	98,98,98,98	0
56	MG	RA	3889	1/1	0.88	0.66	29.90	62,62,62,62	0
56	MG	YA	3350	1/1	0.79	0.58	29.33	76,76,76,76	0
56	MG	RA	3677	1/1	-0.04	1.12	28.86	86,86,86,86	0
56	MG	YA	3476	1/1	0.93	0.93	28.80	62,62,62,62	0
56	MG	RA	3634	1/1	0.60	0.61	28.68	79,79,79,79	0
56	MG	YA	3648	1/1	0.84	0.63	28.66	62,62,62,62	0
56	MG	RA	3903	1/1	0.95	0.47	28.50	79,79,79,79	0
56	MG	RA	3470	1/1	0.95	0.80	28.47	62,62,62,62	0
56	MG	QA	1849	1/1	0.51	1.44	28.34	76,76,76,76	0
56	MG	RA	3302	1/1	0.91	0.77	28.10	91,91,91,91	0
56	MG	RA	3163	1/1	0.85	1.46	27.99	88,88,88,88	0
56	MG	RA	3603	1/1	0.17	1.55	27.87	90,90,90,90	0
56	MG	RA	3132	1/1	0.71	0.39	27.65	95,95,95,95	0
56	MG	RA	3364	1/1	0.70	0.95	27.27	74,74,74,74	0
56	MG	YA	3391	1/1	0.93	0.79	26.90	62,62,62,62	0
56	MG	RA	3027	1/1	0.15	0.84	26.83	112,112,112,112	0
56	MG	RA	3924	1/1	0.47	0.66	26.76	89,89,89,89	0
56	MG	XA	1645	1/1	0.97	0.64	26.66	82,82,82,82	0
56	MG	RA	3252	1/1	0.95	0.68	26.56	89,89,89,89	0
56	MG	YA	3611	1/1	0.95	1.04	26.52	62,62,62,62	0
56	MG	QA	1814	1/1	0.72	0.89	25.95	89,89,89,89	0
56	MG	RA	3392	1/1	0.87	0.80	25.93	62,62,62,62	0
56	MG	RA	3290	1/1	0.69	1.46	25.71	99,99,99,99	0
56	MG	RA	3412	1/1	0.90	0.46	25.59	62,62,62,62	0
56	MG	RA	3839	1/1	0.94	0.86	25.57	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3419	1/1	0.92	0.78	25.48	62,62,62,62	0
56	MG	RA	3941	1/1	0.23	0.78	25.44	87,87,87,87	0
56	MG	RB	201	1/1	0.78	0.76	25.27	104,104,104,104	0
56	MG	YA	3650	1/1	0.67	0.90	25.08	76,76,76,76	0
56	MG	RA	3917	1/1	0.54	0.49	24.90	92,92,92,92	0
56	MG	YA	3552	1/1	0.78	0.68	24.88	65,65,65,65	0
56	MG	RA	3022	1/1	0.72	0.85	24.82	98,98,98,98	0
56	MG	RA	3616	1/1	0.89	0.86	24.52	62,62,62,62	0
56	MG	RD	313	1/1	0.75	0.86	24.48	84,84,84,84	0
56	MG	YA	3088	1/1	0.84	0.97	24.43	90,90,90,90	0
56	MG	YA	3570	1/1	0.92	0.77	24.42	62,62,62,62	0
56	MG	YF	303	1/1	0.80	0.97	24.33	108,108,108,108	0
56	MG	YA	3323	1/1	0.75	0.64	24.30	62,62,62,62	0
56	MG	YA	3681	1/1	0.89	0.62	24.28	62,62,62,62	0
56	MG	RA	3384	1/1	0.91	0.62	24.21	67,67,67,67	0
56	MG	YA	3030	1/1	0.26	0.59	24.21	88,88,88,88	0
56	MG	QA	1854	1/1	0.23	0.97	24.13	94,94,94,94	0
56	MG	YA	3355	1/1	0.92	0.97	23.99	62,62,62,62	0
56	MG	YA	3387	1/1	0.78	0.71	23.99	62,62,62,62	0
56	MG	RA	3165	1/1	0.79	1.06	23.90	103,103,103,103	0
56	MG	RP	201	1/1	0.48	1.10	23.88	86,86,86,86	0
56	MG	YA	3378	1/1	0.89	0.65	23.47	62,62,62,62	0
56	MG	RA	4044	1/1	0.75	1.12	23.40	106,106,106,106	0
56	MG	RA	3483	1/1	0.84	0.66	23.28	62,62,62,62	0
56	MG	QA	1724	1/1	0.47	1.89	23.12	85,85,85,85	0
56	MG	RA	3805	1/1	0.71	0.61	23.10	97,97,97,97	0
56	MG	RA	3521	1/1	0.68	0.47	23.10	69,69,69,69	0
56	MG	RA	4012	1/1	0.72	2.56	23.06	103,103,103,103	0
56	MG	RA	3512	1/1	-0.35	0.93	22.61	94,94,94,94	0
56	MG	RA	3696	1/1	0.58	0.92	22.54	82,82,82,82	0
56	MG	RA	3893	1/1	0.81	0.59	22.49	76,76,76,76	0
56	MG	RA	3113	1/1	0.47	1.02	22.48	90,90,90,90	0
56	MG	XA	1612	1/1	0.64	0.51	22.47	84,84,84,84	0
56	MG	YA	3724	1/1	0.41	0.53	22.47	71,71,71,71	0
56	MG	RA	3497	1/1	0.93	0.70	22.39	62,62,62,62	0
56	MG	RA	3611	1/1	0.49	0.50	22.39	95,95,95,95	0
56	MG	RA	3226	1/1	0.83	0.81	22.34	113,113,113,113	0
56	MG	RA	4062	1/1	0.57	1.38	22.16	98,98,98,98	0
56	MG	RA	3624	1/1	0.81	0.81	22.16	75,75,75,75	0
56	MG	YA	3183	1/1	0.53	0.66	21.97	88,88,88,88	0
56	MG	YA	3514	1/1	0.91	0.62	21.80	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3708	1/1	0.72	0.98	21.60	77,77,77,77	0
56	MG	YA	3027	1/1	0.23	0.92	21.22	83,83,83,83	0
56	MG	RA	3742	1/1	0.59	0.35	21.18	88,88,88,88	0
56	MG	YA	3623	1/1	0.82	0.55	21.11	65,65,65,65	0
56	MG	RA	3366	1/1	0.76	0.41	21.03	71,71,71,71	0
56	MG	RA	3186	1/1	0.86	0.93	21.02	98,98,98,98	0
56	MG	RA	3077	1/1	0.62	0.53	20.65	80,80,80,80	0
56	MG	RA	3713	1/1	0.74	1.84	20.61	89,89,89,89	0
56	MG	YA	3456	1/1	0.47	0.77	20.39	84,84,84,84	0
56	MG	RD	303	1/1	0.72	1.20	20.39	88,88,88,88	0
56	MG	YA	3170	1/1	0.06	0.52	20.37	92,92,92,92	0
56	MG	Y0	101	1/1	-0.08	1.09	20.33	78,78,78,78	0
56	MG	RA	3484	1/1	0.93	0.84	20.23	62,62,62,62	0
56	MG	RA	4060	1/1	0.84	1.10	20.11	109,109,109,109	0
56	MG	YA	3715	1/1	0.78	0.42	19.97	83,83,83,83	0
56	MG	RA	3618	1/1	0.15	0.82	19.79	88,88,88,88	0
56	MG	RA	3786	1/1	0.85	0.69	19.72	89,89,89,89	0
56	MG	YA	3270	1/1	0.42	0.90	19.69	79,79,79,79	0
56	MG	YA	3328	1/1	0.87	0.59	19.69	62,62,62,62	0
56	MG	XA	1658	1/1	0.42	0.67	19.61	86,86,86,86	0
56	MG	RA	3767	1/1	0.47	0.91	19.52	63,63,63,63	0
56	MG	RA	3707	1/1	0.67	0.46	19.39	73,73,73,73	0
56	MG	RA	4049	1/1	0.93	0.94	19.38	99,99,99,99	0
56	MG	RA	3185	1/1	0.87	0.73	19.25	85,85,85,85	0
56	MG	QA	1711	1/1	0.86	0.50	19.24	78,78,78,78	0
56	MG	RA	3458	1/1	0.27	0.90	19.24	84,84,84,84	0
56	MG	RA	3536	1/1	0.38	0.66	19.23	86,86,86,86	0
56	MG	RA	3332	1/1	0.48	0.52	19.17	93,93,93,93	0
56	MG	YA	3033	1/1	0.03	0.52	19.11	99,99,99,99	0
56	MG	YA	3361	1/1	0.45	0.63	18.90	88,88,88,88	0
56	MG	YA	3269	1/1	0.46	0.54	18.84	75,75,75,75	0
56	MG	YA	3475	1/1	0.72	0.56	18.76	65,65,65,65	0
56	MG	RA	3858	1/1	0.96	0.54	18.73	70,70,70,70	0
56	MG	RA	3526	1/1	0.07	0.84	18.67	89,89,89,89	0
56	MG	RA	3117	1/1	0.76	0.66	18.64	96,96,96,96	0
56	MG	XA	1738	1/1	0.85	0.61	18.60	64,64,64,64	0
56	MG	RA	3468	1/1	0.91	0.46	18.46	63,63,63,63	0
56	MG	RA	3348	1/1	0.95	0.59	18.38	74,74,74,74	0
56	MG	YA	3614	1/1	0.94	0.53	18.35	68,68,68,68	0
56	MG	YA	3291	1/1	0.25	0.84	18.29	88,88,88,88	0
56	MG	RA	3524	1/1	0.42	0.69	18.22	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YW	201	1/1	0.59	0.94	18.19	98,98,98,98	0
56	MG	YA	3091	1/1	0.76	0.47	18.15	76,76,76,76	0
56	MG	RA	3939	1/1	0.42	2.08	18.14	95,95,95,95	0
56	MG	RE	302	1/1	0.45	0.95	18.08	97,97,97,97	0
56	MG	YA	3192	1/1	0.42	0.44	18.05	74,74,74,74	0
56	MG	RA	3952	1/1	0.18	0.52	18.03	96,96,96,96	0
56	MG	YA	3612	1/1	0.95	0.59	18.01	64,64,64,64	0
56	MG	RA	3241	1/1	0.79	0.62	18.00	91,91,91,91	0
56	MG	RA	3948	1/1	0.72	0.58	17.98	64,64,64,64	0
56	MG	RA	3187	1/1	0.49	0.57	17.95	90,90,90,90	0
56	MG	RA	3568	1/1	0.27	0.54	17.91	89,89,89,89	0
56	MG	RA	3197	1/1	0.23	0.56	17.89	100,100,100,100	0
56	MG	RA	3574	1/1	0.84	1.32	17.83	90,90,90,90	0
56	MG	RR	201	1/1	0.36	0.77	17.76	98,98,98,98	0
56	MG	YA	3249	1/1	0.45	0.69	17.72	94,94,94,94	0
56	MG	XA	1720	1/1	0.46	0.65	17.71	96,96,96,96	0
56	MG	QA	1860	1/1	0.13	0.83	17.69	92,92,92,92	0
56	MG	RA	4030	1/1	0.85	1.21	17.55	103,103,103,103	0
56	MG	RA	3496	1/1	0.95	0.70	17.33	63,63,63,63	0
56	MG	RF	303	1/1	0.39	1.36	17.30	98,98,98,98	0
56	MG	XA	1725	1/1	0.75	0.50	17.04	85,85,85,85	0
56	MG	XA	1774	1/1	0.94	0.65	17.03	80,80,80,80	0
56	MG	RA	3121	1/1	0.66	0.95	17.02	100,100,100,100	0
56	MG	YA	3709	1/1	0.69	0.43	16.99	71,71,71,71	0
56	MG	RA	3386	1/1	0.85	0.71	16.97	76,76,76,76	0
56	MG	RA	3082	1/1	0.84	0.95	16.97	100,100,100,100	0
56	MG	RA	3109	1/1	0.41	0.72	16.88	97,97,97,97	0
56	MG	RA	3045	1/1	0.72	0.89	16.77	86,86,86,86	0
56	MG	RA	3125	1/1	0.94	0.52	16.75	93,93,93,93	0
56	MG	XA	1673	1/1	0.59	0.46	16.64	89,89,89,89	0
56	MG	RA	3659	1/1	0.84	0.76	16.52	95,95,95,95	0
56	MG	YA	3107	1/1	0.81	0.43	16.39	74,74,74,74	0
56	MG	YA	3134	1/1	0.72	0.62	16.29	73,73,73,73	0
56	MG	XA	1786	1/1	0.54	0.71	16.27	89,89,89,89	0
56	MG	R5	101	1/1	0.77	1.50	16.13	105,105,105,105	0
56	MG	RA	3856	1/1	0.81	0.54	16.13	77,77,77,77	0
56	MG	YA	3112	1/1	0.02	0.72	16.09	85,85,85,85	0
56	MG	RA	3098	1/1	0.62	0.54	16.03	68,68,68,68	0
56	MG	YA	3272	1/1	0.90	0.76	15.98	77,77,77,77	0
56	MG	YD	305	1/1	0.58	0.70	15.95	92,92,92,92	0
56	MG	RA	4052	1/1	0.83	1.03	15.92	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	YA	3753	1/1	0.82	1.13	15.76	81,81,81,81	0
56	MG	RA	4034	1/1	0.81	0.97	15.70	88,88,88,88	0
56	MG	RA	3566	1/1	0.68	0.56	15.67	67,67,67,67	0
56	MG	RA	4065	1/1	0.17	1.02	15.63	91,91,91,91	0
56	MG	RA	3476	1/1	0.88	0.72	15.61	78,78,78,78	0
56	MG	YA	3468	1/1	0.86	0.59	15.54	62,62,62,62	0
56	MG	RA	3409	1/1	0.81	0.45	15.52	65,65,65,65	0
56	MG	RA	3265	1/1	0.81	0.77	15.50	94,94,94,94	0
56	MG	YA	3074	1/1	0.64	0.65	15.50	68,68,68,68	0
56	MG	RA	3356	1/1	0.97	0.82	15.46	78,78,78,78	0
56	MG	YA	3325	1/1	0.96	0.51	15.45	62,62,62,62	0
56	MG	QA	1715	1/1	0.90	0.52	15.43	71,71,71,71	0
56	MG	QA	1654	1/1	0.59	0.43	15.41	77,77,77,77	0
56	MG	YA	3656	1/1	0.95	0.43	15.40	78,78,78,78	0
56	MG	YA	3660	1/1	0.67	0.61	15.31	69,69,69,69	0
56	MG	RA	4051	1/1	0.92	0.72	15.29	105,105,105,105	0
56	MG	RA	4043	1/1	0.64	1.09	15.28	92,92,92,92	0
56	MG	YA	3129	1/1	0.71	0.47	15.26	77,77,77,77	0
56	MG	YA	3668	1/1	0.93	0.74	15.25	62,62,62,62	0
56	MG	XA	1747	1/1	0.94	0.67	15.25	63,63,63,63	0
56	MG	RA	3712	1/1	0.66	0.78	15.15	83,83,83,83	0
56	MG	RA	3385	1/1	0.97	1.01	15.13	62,62,62,62	0
56	MG	YA	3750	1/1	0.88	0.98	15.09	92,92,92,92	0
56	MG	YA	3388	1/1	0.90	0.54	15.05	62,62,62,62	0
56	MG	YA	3440	1/1	0.92	0.55	15.03	64,64,64,64	0
56	MG	RA	3814	1/1	0.93	0.49	14.98	73,73,73,73	0
56	MG	RD	302	1/1	0.82	0.82	14.96	71,71,71,71	0
56	MG	RF	306	1/1	0.67	1.38	14.91	106,106,106,106	0
56	MG	RA	3401	1/1	0.73	0.70	14.86	62,62,62,62	0
56	MG	RA	4026	1/1	0.89	0.69	14.82	105,105,105,105	0
56	MG	RA	4024	1/1	0.56	1.50	14.78	98,98,98,98	0
56	MG	YA	3447	1/1	0.26	0.56	14.74	80,80,80,80	0
56	MG	RA	4064	1/1	0.81	1.09	14.73	84,84,84,84	0
56	MG	YA	3122	1/1	0.79	0.55	14.70	82,82,82,82	0
56	MG	RA	3466	1/1	0.85	0.70	14.70	62,62,62,62	0
56	MG	YA	3733	1/1	0.91	0.82	14.67	89,89,89,89	0
56	MG	QA	1857	1/1	0.81	0.34	14.63	83,83,83,83	0
56	MG	RV	203	1/1	0.70	0.76	14.54	83,83,83,83	0
56	MG	RA	3502	1/1	0.92	1.11	14.50	64,64,64,64	0
56	MG	RA	3462	1/1	0.61	0.75	14.47	86,86,86,86	0
56	MG	RA	3279	1/1	0.59	0.71	14.42	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XA	1633	1/1	0.59	0.80	14.30	66,66,66,66	0
56	MG	XA	1744	1/1	0.84	0.91	14.27	63,63,63,63	0
56	MG	RA	4063	1/1	0.75	1.57	14.22	100,100,100,100	0
56	MG	RA	4028	1/1	0.55	1.02	14.19	108,108,108,108	0
56	MG	YA	3421	1/1	0.26	0.54	14.18	82,82,82,82	0
56	MG	RA	4048	1/1	0.70	1.12	14.17	103,103,103,103	0
56	MG	RA	3119	1/1	0.92	1.27	14.16	94,94,94,94	0
56	MG	RA	3827	1/1	0.32	0.69	14.13	81,81,81,81	0
56	MG	YA	3077	1/1	0.84	0.80	14.09	107,107,107,107	0
56	MG	YA	3495	1/1	0.61	0.69	14.04	77,77,77,77	0
56	MG	RA	3551	1/1	0.46	0.46	13.96	79,79,79,79	0
56	MG	YA	3485	1/1	0.91	0.56	13.96	62,62,62,62	0
56	MG	YA	3377	1/1	0.94	0.52	13.90	62,62,62,62	0
56	MG	YA	3299	1/1	0.36	0.49	13.88	64,64,64,64	0
56	MG	RA	3404	1/1	0.92	0.48	13.83	71,71,71,71	0
56	MG	RA	3251	1/1	0.17	0.88	13.81	82,82,82,82	0
56	MG	RA	4058	1/1	0.09	0.92	13.81	96,96,96,96	0
56	MG	XA	1760	1/1	0.88	0.49	13.78	67,67,67,67	0
56	MG	RA	3727	1/1	0.35	0.55	13.74	78,78,78,78	0
56	MG	YA	3744	1/1	0.90	0.85	13.72	98,98,98,98	0
56	MG	RA	3990	1/1	0.65	0.73	13.68	68,68,68,68	0
56	MG	YA	3540	1/1	0.83	0.59	13.61	82,82,82,82	0
56	MG	YA	3511	1/1	0.85	0.56	13.60	62,62,62,62	0
56	MG	RA	3871	1/1	0.93	0.66	13.56	62,62,62,62	0
56	MG	QA	1623	1/1	0.79	0.33	13.45	86,86,86,86	0
56	MG	QA	1731	1/1	0.87	0.62	13.42	76,76,76,76	0
56	MG	RA	3379	1/1	0.75	0.52	13.40	62,62,62,62	0
56	MG	RA	3021	1/1	0.81	0.95	13.33	103,103,103,103	0
56	MG	RA	3465	1/1	0.73	0.46	13.32	69,69,69,69	0
56	MG	YA	3632	1/1	0.82	0.56	13.29	67,67,67,67	0
56	MG	RA	3323	1/1	0.63	0.44	13.22	69,69,69,69	0
56	MG	RA	3020	1/1	0.87	0.72	13.21	95,95,95,95	0
56	MG	RA	3911	1/1	0.93	0.44	13.15	71,71,71,71	0
56	MG	RA	3359	1/1	0.65	0.58	13.13	89,89,89,89	0
56	MG	RA	4041	1/1	0.87	0.76	13.12	109,109,109,109	0
56	MG	YA	3752	1/1	0.34	1.10	13.06	100,100,100,100	0
56	MG	RF	305	1/1	0.80	0.93	13.01	101,101,101,101	0
56	MG	RA	3902	1/1	0.90	0.58	13.01	62,62,62,62	0
56	MG	YA	3020	1/1	0.85	0.59	12.91	96,96,96,96	0
56	MG	YA	3398	1/1	0.93	0.84	12.76	63,63,63,63	0
56	MG	RA	3823	1/1	0.72	0.56	12.73	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3424	1/1	0.98	0.54	12.70	62,62,62,62	0
56	MG	XA	1777	1/1	0.91	0.45	12.70	74,74,74,74	0
56	MG	YA	3499	1/1	0.78	0.42	12.69	65,65,65,65	0
56	MG	RA	3179	1/1	0.07	0.99	12.68	105,105,105,105	0
56	MG	YD	309	1/1	0.52	0.69	12.65	62,62,62,62	0
56	MG	RA	3387	1/1	0.96	0.48	12.64	75,75,75,75	0
56	MG	YA	3209	1/1	0.53	0.84	12.63	85,85,85,85	0
56	MG	YA	3413	1/1	0.66	0.80	12.63	85,85,85,85	0
56	MG	YA	3699	1/1	0.71	0.50	12.62	77,77,77,77	0
56	MG	RA	3146	1/1	0.57	0.37	12.58	68,68,68,68	0
56	MG	R0	103	1/1	0.45	0.82	12.52	70,70,70,70	0
56	MG	YA	3351	1/1	0.69	0.55	12.49	68,68,68,68	0
56	MG	YA	3156	1/1	0.73	0.47	12.39	103,103,103,103	0
56	MG	RA	3967	1/1	0.77	0.48	12.39	97,97,97,97	0
56	MG	QA	1828	1/1	0.45	0.55	12.39	86,86,86,86	0
56	MG	YA	3318	1/1	0.95	0.48	12.34	62,62,62,62	0
56	MG	RA	4003	1/1	0.36	0.81	12.34	92,92,92,92	0
56	MG	QA	1872	1/1	0.67	0.85	12.26	70,70,70,70	0
56	MG	RA	3452	1/1	0.93	0.60	12.24	62,62,62,62	0
56	MG	YA	3664	1/1	0.98	0.65	12.03	72,72,72,72	0
56	MG	RA	3684	1/1	0.17	0.52	11.98	93,93,93,93	0
56	MG	XA	1690	1/1	0.29	0.79	11.92	94,94,94,94	0
56	MG	XA	1696	1/1	0.75	0.90	11.90	67,67,67,67	0
56	MG	RA	3006	1/1	0.95	0.35	11.79	73,73,73,73	0
56	MG	RA	3771	1/1	0.99	0.61	11.70	72,72,72,72	0
56	MG	YA	3532	1/1	0.90	0.47	11.65	84,84,84,84	0
56	MG	RA	3679	1/1	0.77	0.40	11.62	72,72,72,72	0
56	MG	YA	3684	1/1	0.85	0.52	11.59	63,63,63,63	0
56	MG	YA	3691	1/1	0.69	0.49	11.52	82,82,82,82	0
56	MG	RA	3744	1/1	0.82	0.58	11.51	73,73,73,73	0
56	MG	YA	3321	1/1	0.88	0.51	11.42	62,62,62,62	0
56	MG	YA	3152	1/1	0.10	1.07	11.39	83,83,83,83	0
56	MG	RA	3539	1/1	0.87	0.45	11.38	98,98,98,98	0
56	MG	YA	3749	1/1	0.65	0.99	11.34	90,90,90,90	0
56	MG	YA	3240	1/1	0.62	0.47	11.29	93,93,93,93	0
56	MG	RA	4045	1/1	0.93	0.72	11.24	101,101,101,101	0
56	MG	YA	3336	1/1	0.69	0.75	11.24	62,62,62,62	0
56	MG	RA	3231	1/1	0.87	0.82	11.17	89,89,89,89	0
56	MG	YA	3679	1/1	0.89	0.58	11.17	65,65,65,65	0
56	MG	YA	3600	1/1	0.80	0.68	11.17	65,65,65,65	0
56	MG	XA	1683	1/1	0.42	0.56	11.08	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3638	1/1	0.87	0.88	11.08	85,85,85,85	0
56	MG	RA	3535	1/1	0.41	0.57	11.07	97,97,97,97	0
56	MG	RA	3607	1/1	0.92	0.92	11.05	91,91,91,91	0
56	MG	YD	308	1/1	0.94	0.61	11.04	97,97,97,97	0
56	MG	QA	1682	1/1	0.09	0.53	10.99	87,87,87,87	0
56	MG	RA	3248	1/1	0.65	0.58	10.95	89,89,89,89	0
56	MG	RA	3900	1/1	0.39	0.59	10.92	92,92,92,92	0
56	MG	XA	1629	1/1	0.69	0.42	10.92	68,68,68,68	0
56	MG	RV	202	1/1	0.38	0.47	10.82	86,86,86,86	0
56	MG	YA	3216	1/1	0.50	0.47	10.71	80,80,80,80	0
56	MG	RA	4035	1/1	0.77	1.19	10.71	90,90,90,90	0
56	MG	RA	4059	1/1	0.91	0.84	10.67	98,98,98,98	0
56	MG	YA	3658	1/1	0.59	0.70	10.65	87,87,87,87	0
56	MG	YA	3577	1/1	0.94	0.65	10.65	62,62,62,62	0
56	MG	RA	3501	1/1	0.88	0.84	10.63	63,63,63,63	0
56	MG	RA	3377	1/1	0.80	0.32	10.63	69,69,69,69	0
56	MG	YA	3013	1/1	0.50	0.55	10.62	72,72,72,72	0
56	MG	RA	3623	1/1	0.93	0.70	10.62	65,65,65,65	0
56	MG	QA	1680	1/1	0.37	0.52	10.61	84,84,84,84	0
56	MG	YA	3579	1/1	0.91	0.69	10.60	62,62,62,62	0
56	MG	YA	3665	1/1	0.96	0.49	10.52	63,63,63,63	0
56	MG	RA	4066	1/1	0.80	0.77	10.48	86,86,86,86	0
56	MG	RA	3232	1/1	0.90	0.82	10.48	100,100,100,100	0
56	MG	YA	3011	1/1	0.76	0.42	10.41	70,70,70,70	0
56	MG	RA	3421	1/1	0.90	0.52	10.25	62,62,62,62	0
56	MG	RA	4057	1/1	0.14	1.28	10.24	97,97,97,97	0
56	MG	RA	4017	1/1	0.80	0.97	10.13	92,92,92,92	0
56	MG	RA	3361	1/1	0.79	0.48	10.12	82,82,82,82	0
56	MG	YA	3701	1/1	0.83	0.62	10.11	62,62,62,62	0
56	MG	YA	3740	1/1	0.84	0.86	10.10	96,96,96,96	0
56	MG	RA	3812	1/1	0.57	0.38	10.02	76,76,76,76	0
56	MG	RA	3391	1/1	0.98	0.42	10.02	74,74,74,74	0
56	MG	RA	3275	1/1	0.64	0.56	10.01	110,110,110,110	0
56	MG	YA	3397	1/1	0.27	0.65	9.99	75,75,75,75	0
56	MG	RA	3330	1/1	0.83	0.41	9.97	68,68,68,68	0
56	MG	YA	3110	1/1	0.80	0.45	9.93	62,62,62,62	0
56	MG	RA	3170	1/1	0.71	0.38	9.90	86,86,86,86	0
56	MG	QA	1626	1/1	0.80	0.33	9.88	87,87,87,87	0
56	MG	YA	3415	1/1	0.86	0.79	9.80	68,68,68,68	0
56	MG	RA	4023	1/1	0.92	0.66	9.76	101,101,101,101	0
56	MG	YA	3368	1/1	0.89	0.63	9.73	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3049	1/1	0.67	0.49	9.71	85,85,85,85	0
56	MG	RA	3953	1/1	0.92	0.33	9.71	81,81,81,81	0
56	MG	YA	3335	1/1	0.88	0.67	9.66	62,62,62,62	0
56	MG	RA	3307	1/1	0.76	1.83	9.65	99,99,99,99	0
56	MG	RF	301	1/1	-0.24	0.83	9.61	99,99,99,99	0
56	MG	RA	4036	1/1	0.90	1.05	9.61	99,99,99,99	0
56	MG	RA	3382	1/1	0.89	0.52	9.59	76,76,76,76	0
56	MG	YA	3268	1/1	0.91	0.62	9.57	83,83,83,83	0
56	MG	RN	201	1/1	0.45	1.15	9.57	91,91,91,91	0
56	MG	RA	4037	1/1	0.73	0.69	9.54	95,95,95,95	0
56	MG	XA	1707	1/1	0.79	0.27	9.40	80,80,80,80	0
56	MG	QA	1843	1/1	0.82	0.50	9.34	68,68,68,68	0
56	MG	RA	3538	1/1	0.49	0.89	9.33	95,95,95,95	0
56	MG	QA	1835	1/1	0.53	0.52	9.33	72,72,72,72	0
56	MG	RA	3390	1/1	0.93	0.42	9.24	65,65,65,65	0
56	MG	XA	1616	1/1	0.56	0.43	9.21	81,81,81,81	0
56	MG	YA	3449	1/1	0.87	0.46	9.19	66,66,66,66	0
56	MG	YA	3446	1/1	0.42	0.64	9.17	89,89,89,89	0
56	MG	RA	3630	1/1	0.49	0.58	9.16	68,68,68,68	0
56	MG	RA	3148	1/1	0.47	0.47	9.09	81,81,81,81	0
56	MG	QN	103	1/1	0.75	1.01	9.05	81,81,81,81	0
56	MG	YA	3751	1/1	0.76	0.71	8.98	102,102,102,102	0
56	MG	RA	3168	1/1	0.80	0.51	8.91	91,91,91,91	0
56	MG	RD	305	1/1	0.83	0.84	8.90	102,102,102,102	0
56	MG	YA	3737	1/1	0.96	0.61	8.88	63,63,63,63	0
56	MG	YT	202	1/1	0.47	0.90	8.87	80,80,80,80	0
56	MG	RA	4032	1/1	0.67	0.87	8.86	89,89,89,89	0
56	MG	RA	3795	1/1	0.80	0.60	8.84	75,75,75,75	0
56	MG	RA	3533	1/1	0.68	0.35	8.83	89,89,89,89	0
56	MG	QA	1877	1/1	0.30	0.70	8.83	92,92,92,92	0
56	MG	YA	3326	1/1	0.95	0.46	8.78	65,65,65,65	0
56	MG	RA	3471	1/1	0.96	0.64	8.78	74,74,74,74	0
56	MG	RA	3040	1/1	0.36	0.71	8.78	97,97,97,97	0
56	MG	RA	3892	1/1	0.65	0.49	8.77	78,78,78,78	0
56	MG	RA	3321	1/1	0.97	0.50	8.77	63,63,63,63	0
56	MG	YD	304	1/1	0.97	0.55	8.76	104,104,104,104	0
56	MG	RA	3518	1/1	0.56	0.57	8.75	96,96,96,96	0
56	MG	RA	3342	1/1	0.66	0.45	8.73	79,79,79,79	0
56	MG	XA	1700	1/1	0.97	0.55	8.68	65,65,65,65	0
56	MG	YA	3488	1/1	0.76	0.46	8.67	77,77,77,77	0
56	MG	RA	3023	1/1	0.79	0.36	8.60	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3754	1/1	0.88	0.42	8.51	84,84,84,84	0
56	MG	XA	1776	1/1	0.91	0.32	8.37	80,80,80,80	0
56	MG	YA	3538	1/1	0.92	0.44	8.32	64,64,64,64	0
56	MG	YA	3284	1/1	0.77	0.51	8.32	63,63,63,63	0
56	MG	YA	3606	1/1	0.96	0.50	8.25	62,62,62,62	0
56	MG	RA	3070	1/1	0.84	0.76	8.19	85,85,85,85	0
56	MG	RA	3300	1/1	0.55	0.65	8.15	100,100,100,100	0
56	MG	RA	3715	1/1	0.96	0.46	8.05	65,65,65,65	0
56	MG	RD	309	1/1	0.79	0.64	8.03	100,100,100,100	0
56	MG	R1	102	1/1	0.31	0.92	8.02	83,83,83,83	0
56	MG	RF	309	1/1	-0.42	0.84	8.01	103,103,103,103	0
56	MG	RA	3479	1/1	0.84	0.39	7.99	80,80,80,80	0
56	MG	RA	3073	1/1	0.92	0.67	7.99	96,96,96,96	0
56	MG	RA	3807	1/1	0.59	0.60	7.97	91,91,91,91	0
56	MG	YA	3621	1/1	0.97	0.53	7.86	62,62,62,62	0
56	MG	YA	3146	1/1	0.59	0.50	7.86	83,83,83,83	0
56	MG	XA	1759	1/1	0.89	0.45	7.86	68,68,68,68	0
56	MG	YE	302	1/1	0.73	0.69	7.85	95,95,95,95	0
56	MG	RA	4025	1/1	0.68	0.82	7.82	97,97,97,97	0
56	MG	YA	3748	1/1	0.92	0.64	7.81	93,93,93,93	0
56	MG	RA	3477	1/1	0.81	0.50	7.79	63,63,63,63	0
56	MG	YB	217	1/1	0.84	0.33	7.78	84,84,84,84	0
56	MG	RF	311	1/1	0.17	0.69	7.68	94,94,94,94	0
56	MG	QA	1708	1/1	0.82	0.44	7.64	69,69,69,69	0
56	MG	YA	3153	1/1	0.72	0.51	7.64	68,68,68,68	0
56	MG	RA	3050	1/1	0.41	0.77	7.58	89,89,89,89	0
56	MG	YA	3610	1/1	0.81	0.55	7.57	64,64,64,64	0
56	MG	RF	308	1/1	0.45	0.79	7.56	92,92,92,92	0
56	MG	YA	3392	1/1	0.94	0.65	7.48	62,62,62,62	0
56	MG	RA	4061	1/1	0.46	0.65	7.47	105,105,105,105	0
56	MG	YA	3580	1/1	0.70	0.51	7.44	70,70,70,70	0
56	MG	YA	3237	1/1	0.84	0.90	7.42	95,95,95,95	0
56	MG	RA	3862	1/1	0.56	0.38	7.42	75,75,75,75	0
56	MG	YA	3217	1/1	0.84	0.34	7.38	98,98,98,98	0
56	MG	RA	3178	1/1	0.81	0.44	7.33	107,107,107,107	0
56	MG	YA	3028	1/1	0.75	0.41	7.27	85,85,85,85	0
56	MG	YA	3613	1/1	0.83	0.40	7.19	75,75,75,75	0
56	MG	YA	3439	1/1	0.60	0.90	7.13	88,88,88,88	0
56	MG	RA	3821	1/1	0.96	0.34	7.05	76,76,76,76	0
56	MG	XA	1763	1/1	0.80	0.41	7.05	70,70,70,70	0
56	MG	RA	3724	1/1	0.86	0.25	6.98	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	RA	3874	1/1	0.92	0.51	6.96	63,63,63,63	0
56	MG	YA	3702	1/1	0.95	0.44	6.95	66,66,66,66	0
56	MG	QF	201	1/1	0.90	0.45	6.93	75,75,75,75	0
56	MG	YA	3384	1/1	0.87	0.60	6.92	64,64,64,64	0
56	MG	QA	1773	1/1	0.71	0.27	6.91	78,78,78,78	0
56	MG	RA	3491	1/1	0.78	0.28	6.87	85,85,85,85	0
56	MG	RA	3230	1/1	0.85	0.58	6.86	106,106,106,106	0
56	MG	RA	3349	1/1	0.73	0.38	6.80	68,68,68,68	0
56	MG	RA	3335	1/1	0.78	0.33	6.78	75,75,75,75	0
56	MG	RA	3969	1/1	0.57	0.52	6.75	97,97,97,97	0
56	MG	QA	1737	1/1	0.61	0.47	6.71	88,88,88,88	0
56	MG	RE	307	1/1	0.47	0.59	6.65	86,86,86,86	0
56	MG	RA	3136	1/1	0.97	0.47	6.59	94,94,94,94	0
56	MG	RA	3299	1/1	0.66	0.45	6.58	68,68,68,68	0
56	MG	RA	3809	1/1	0.55	0.54	6.57	89,89,89,89	0
56	MG	YA	3382	1/1	0.97	0.63	6.53	62,62,62,62	0
56	MG	YA	3104	1/1	0.72	0.28	6.50	69,69,69,69	0
56	MG	YA	3404	1/1	0.93	0.60	6.48	62,62,62,62	0
56	MG	RA	3928	1/1	0.86	0.43	6.47	90,90,90,90	0
56	MG	YA	3210	1/1	0.85	0.39	6.43	70,70,70,70	0
56	MG	YA	3311	1/1	0.22	0.86	6.41	73,73,73,73	0
56	MG	YA	3588	1/1	0.90	0.42	6.40	64,64,64,64	0
56	MG	RA	3609	1/1	0.15	1.11	6.38	90,90,90,90	0
56	MG	RA	3472	1/1	0.96	0.48	6.29	78,78,78,78	0
56	MG	YA	3550	1/1	0.86	0.39	6.22	80,80,80,80	0
56	MG	XA	1737	1/1	0.92	0.29	6.22	78,78,78,78	0
56	MG	RA	3717	1/1	0.65	0.40	6.20	65,65,65,65	0
56	MG	RA	4033	1/1	0.88	0.68	6.18	96,96,96,96	0
56	MG	RA	3128	1/1	0.89	0.41	6.15	85,85,85,85	0
56	MG	YA	3386	1/1	0.75	0.40	6.09	82,82,82,82	0
56	MG	RA	3875	1/1	0.87	0.65	6.06	62,62,62,62	0
56	MG	YA	3516	1/1	0.74	1.26	6.05	85,85,85,85	0
56	MG	YA	3345	1/1	0.95	0.35	5.97	62,62,62,62	0
56	MG	YA	3587	1/1	0.82	0.39	5.88	68,68,68,68	0
56	MG	RA	3635	1/1	0.63	0.41	5.84	96,96,96,96	0
56	MG	QA	1832	1/1	0.17	0.40	5.83	84,84,84,84	0
56	MG	RA	3938	1/1	0.65	0.39	5.80	78,78,78,78	0
56	MG	XA	1770	1/1	0.88	0.51	5.79	87,87,87,87	0
56	MG	YA	3201	1/1	0.36	0.29	5.76	90,90,90,90	0
56	MG	RA	4047	1/1	0.39	0.70	5.74	97,97,97,97	0
56	MG	RA	3644	1/1	0.51	0.56	5.73	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	RA	3315	1/1	0.91	0.32	5.71	82,82,82,82	0
56	MG	YA	3019	1/1	0.58	0.57	5.68	102,102,102,102	0
56	MG	YA	3317	1/1	0.77	0.69	5.66	69,69,69,69	0
56	MG	YA	3285	1/1	0.93	0.33	5.63	76,76,76,76	0
56	MG	RA	3803	1/1	0.73	1.18	5.63	101,101,101,101	0
56	MG	RA	3746	1/1	0.89	0.47	5.59	62,62,62,62	0
56	MG	QA	1706	1/1	0.70	0.34	5.58	76,76,76,76	0
56	MG	QA	1829	1/1	0.86	0.32	5.51	81,81,81,81	0
56	MG	RA	3399	1/1	0.91	0.53	5.51	62,62,62,62	0
56	MG	YA	3474	1/1	0.26	0.44	5.50	78,78,78,78	0
56	MG	RD	308	1/1	0.09	0.60	5.50	83,83,83,83	0
56	MG	R3	102	1/1	0.01	0.87	5.45	102,102,102,102	0
56	MG	XA	1741	1/1	0.87	0.34	5.43	78,78,78,78	0
56	MG	YA	3503	1/1	0.63	0.28	5.41	67,67,67,67	0
56	MG	YA	3092	1/1	0.56	0.42	5.39	85,85,85,85	0
56	MG	RA	3770	1/1	0.95	0.44	5.33	66,66,66,66	0
56	MG	YA	3714	1/1	0.13	0.63	5.30	85,85,85,85	0
56	MG	RA	4002	1/1	0.92	0.42	5.24	74,74,74,74	0
56	MG	RA	3177	1/1	0.50	0.53	5.24	83,83,83,83	0
56	MG	RA	3381	1/1	0.83	0.41	5.23	64,64,64,64	0
56	MG	XA	1637	1/1	0.54	0.19	5.21	86,86,86,86	0
56	MG	QA	1638	1/1	0.94	0.25	5.15	75,75,75,75	0
56	MG	QA	1622	1/1	0.79	0.48	5.15	89,89,89,89	0
56	MG	RA	4027	1/1	0.88	0.59	5.14	88,88,88,88	0
56	MG	YA	3303	1/1	0.90	0.36	5.13	62,62,62,62	0
56	MG	YD	306	1/1	0.93	0.50	5.12	81,81,81,81	0
56	MG	YA	3036	1/1	0.87	0.33	5.10	76,76,76,76	0
56	MG	RA	4021	1/1	0.77	0.63	5.07	78,78,78,78	0
56	MG	YF	301	1/1	-0.11	0.45	5.05	94,94,94,94	0
56	MG	R8	101	1/1	0.21	0.87	5.04	90,90,90,90	0
56	MG	YA	3560	1/1	0.88	0.26	5.03	64,64,64,64	0
56	MG	XA	1631	1/1	0.64	0.47	5.00	88,88,88,88	0
56	MG	XT	201	1/1	0.50	0.66	4.94	93,93,93,93	0
56	MG	RU	203	1/1	0.89	0.39	4.89	81,81,81,81	0
56	MG	RA	3774	1/1	0.98	0.32	4.89	64,64,64,64	0
56	MG	RA	3959	1/1	-0.25	0.92	4.85	97,97,97,97	0
56	MG	RA	4056	1/1	0.94	0.79	4.81	112,112,112,112	0
56	MG	R1	104	1/1	0.47	0.68	4.77	88,88,88,88	0
56	MG	RA	3234	1/1	0.70	0.51	4.75	101,101,101,101	0
56	MG	RA	3431	1/1	0.84	0.48	4.74	63,63,63,63	0
56	MG	QA	1634	1/1	0.88	0.28	4.73	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1671	1/1	0.97	0.37	4.73	85,85,85,85	0
56	MG	RA	3733	1/1	0.91	0.27	4.67	79,79,79,79	0
56	MG	XA	1728	1/1	-0.32	0.41	4.66	84,84,84,84	0
56	MG	YA	3007	1/1	0.69	0.35	4.66	69,69,69,69	0
56	MG	YA	3339	1/1	0.93	0.36	4.62	62,62,62,62	0
56	MG	QA	1759	1/1	0.45	0.75	4.62	77,77,77,77	0
56	MG	RA	3514	1/1	0.76	0.34	4.57	63,63,63,63	0
56	MG	RA	4042	1/1	0.55	0.55	4.54	81,81,81,81	0
56	MG	RA	3102	1/1	0.80	0.83	4.51	88,88,88,88	0
56	MG	RA	3217	1/1	0.92	0.53	4.51	97,97,97,97	0
56	MG	RA	4046	1/1	0.68	0.53	4.46	91,91,91,91	0
56	MG	QA	1616	1/1	0.89	0.30	4.45	101,101,101,101	0
56	MG	RA	3614	1/1	0.80	0.37	4.44	68,68,68,68	0
56	MG	RA	3709	1/1	0.30	0.57	4.43	91,91,91,91	0
56	MG	XF	202	1/1	0.62	0.63	4.42	96,96,96,96	0
56	MG	RA	3352	1/1	-0.12	0.79	4.42	97,97,97,97	0
56	MG	YA	3517	1/1	0.90	0.51	4.42	97,97,97,97	0
56	MG	YA	3607	1/1	0.97	0.34	4.37	65,65,65,65	0
56	MG	YA	3729	1/1	0.93	0.50	4.30	69,69,69,69	0
56	MG	YA	3071	1/1	0.99	0.44	4.22	90,90,90,90	0
56	MG	XA	1628	1/1	0.78	0.27	4.20	79,79,79,79	0
56	MG	QA	1802	1/1	0.91	0.24	4.19	82,82,82,82	0
56	MG	QA	1647	1/1	0.31	0.25	4.17	101,101,101,101	0
56	MG	RA	3333	1/1	0.91	0.46	4.15	64,64,64,64	0
56	MG	RA	3235	1/1	0.57	0.55	4.15	93,93,93,93	0
56	MG	QY	401	1/1	0.31	0.68	4.13	90,90,90,90	0
56	MG	RB	209	1/1	0.38	0.29	4.13	76,76,76,76	0
56	MG	XA	1772	1/1	0.91	0.33	4.12	76,76,76,76	0
56	MG	RA	4050	1/1	0.68	0.38	4.11	98,98,98,98	0
56	MG	YA	3148	1/1	0.81	0.34	4.09	63,63,63,63	0
56	MG	RA	4009	1/1	0.70	0.54	4.01	84,84,84,84	0
56	MG	XA	1792	1/1	0.53	0.59	4.00	95,95,95,95	0
56	MG	QD	303	1/1	0.54	0.55	3.99	94,94,94,94	0
56	MG	YX	101	1/1	0.80	0.41	3.97	69,69,69,69	0
56	MG	RA	3598	1/1	0.94	0.37	3.95	69,69,69,69	0
56	MG	YE	305	1/1	0.51	0.40	3.91	82,82,82,82	0
56	MG	XA	1609	1/1	0.78	0.26	3.87	87,87,87,87	0
56	MG	RA	3473	1/1	0.73	0.25	3.84	80,80,80,80	0
56	MG	Y8	101	1/1	0.77	0.79	3.84	72,72,72,72	0
56	MG	RR	202	1/1	-0.01	0.60	3.81	87,87,87,87	0
56	MG	QA	1619	1/1	0.91	0.37	3.77	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	4040	1/1	0.88	0.57	3.76	99,99,99,99	0
56	MG	YA	3133	1/1	0.92	1.09	3.70	87,87,87,87	0
56	MG	RA	3971	1/1	0.94	0.47	3.69	63,63,63,63	0
56	MG	QA	1658	1/1	0.79	0.30	3.66	88,88,88,88	0
56	MG	RA	3656	1/1	0.96	0.36	3.65	74,74,74,74	0
56	MG	RA	3328	1/1	0.69	0.29	3.64	73,73,73,73	0
56	MG	YA	3755	1/1	0.96	0.36	3.64	74,74,74,74	0
56	MG	YA	3199	1/1	0.93	0.34	3.63	71,71,71,71	0
56	MG	RA	4008	1/1	0.59	0.48	3.63	92,92,92,92	0
56	MG	XA	1688	1/1	0.84	0.43	3.62	97,97,97,97	0
56	MG	YA	3746	1/1	0.90	0.42	3.60	85,85,85,85	0
56	MG	YA	3578	1/1	0.87	0.62	3.60	101,101,101,101	0
56	MG	XA	1793	1/1	0.54	0.59	3.60	94,94,94,94	0
56	MG	RA	3092	1/1	0.86	0.39	3.55	91,91,91,91	0
56	MG	RE	306	1/1	0.42	0.41	3.53	63,63,63,63	0
56	MG	RA	3041	1/1	0.80	0.20	3.51	70,70,70,70	0
56	MG	YA	3601	1/1	0.98	0.36	3.51	62,62,62,62	0
56	MG	QN	102	1/1	0.00	0.88	3.38	90,90,90,90	0
56	MG	XA	1731	1/1	0.70	0.24	3.37	82,82,82,82	0
56	MG	QA	1672	1/1	0.72	0.55	3.32	85,85,85,85	0
56	MG	RB	225	1/1	0.60	0.34	3.32	80,80,80,80	0
56	MG	XA	1758	1/1	0.91	0.42	3.31	68,68,68,68	0
56	MG	YA	3616	1/1	0.84	0.34	3.31	65,65,65,65	0
56	MG	XA	1666	1/1	0.87	0.31	3.30	92,92,92,92	0
56	MG	YA	3332	1/1	0.59	0.28	3.27	62,62,62,62	0
56	MG	RD	306	1/1	0.81	0.52	3.20	84,84,84,84	0
56	MG	QA	1618	1/1	0.88	0.21	3.20	101,101,101,101	0
56	MG	YA	3704	1/1	0.81	0.36	3.14	66,66,66,66	0
56	MG	RA	3271	1/1	0.86	0.38	3.13	97,97,97,97	0
56	MG	YA	3297	1/1	0.26	0.35	3.13	70,70,70,70	0
56	MG	YE	301	1/1	0.53	0.50	3.11	66,66,66,66	0
56	MG	RA	3043	1/1	0.70	0.23	3.09	67,67,67,67	0
56	MG	RA	3064	1/1	0.86	0.27	3.09	81,81,81,81	0
56	MG	QT	201	1/1	0.77	0.54	3.09	77,77,77,77	0
56	MG	RF	304	1/1	0.88	0.40	3.09	74,74,74,74	0
56	MG	YA	3554	1/1	0.79	0.32	3.03	79,79,79,79	0
56	MG	RA	3030	1/1	0.89	0.74	3.03	94,94,94,94	0
56	MG	YE	303	1/1	0.26	0.44	2.99	93,93,93,93	0
56	MG	RA	3014	1/1	0.95	0.31	2.96	68,68,68,68	0
56	MG	QA	1823	1/1	0.53	0.66	2.95	94,94,94,94	0
56	MG	RA	3402	1/1	0.61	0.33	2.93	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3986	1/1	0.82	0.56	2.93	79,79,79,79	0
56	MG	YA	3429	1/1	0.81	0.41	2.89	73,73,73,73	0
56	MG	YQ	201	1/1	0.53	0.34	2.88	69,69,69,69	0
56	MG	YA	3756	1/1	0.39	0.72	2.84	96,96,96,96	0
56	MG	YA	3174	1/1	0.80	0.21	2.84	78,78,78,78	0
56	MG	YA	3008	1/1	0.69	0.65	2.81	66,66,66,66	0
56	MG	YA	3689	1/1	0.78	0.32	2.80	78,78,78,78	0
56	MG	QA	1610	1/1	0.83	0.27	2.80	93,93,93,93	0
56	MG	QD	305	1/1	0.55	0.32	2.76	99,99,99,99	0
56	MG	RD	312	1/1	0.55	0.51	2.72	90,90,90,90	0
56	MG	RX	101	1/1	0.82	0.41	2.60	78,78,78,78	0
56	MG	RA	3601	1/1	0.65	0.49	2.60	83,83,83,83	0
56	MG	RQ	201	1/1	0.47	0.39	2.57	87,87,87,87	0
56	MG	YA	3089	1/1	0.83	0.29	2.56	80,80,80,80	0
56	MG	YB	214	1/1	0.82	0.25	2.52	78,78,78,78	0
56	MG	XA	1618	1/1	0.86	0.30	2.51	81,81,81,81	0
56	MG	RA	3032	1/1	0.51	0.29	2.50	92,92,92,92	0
56	MG	XA	1723	1/1	0.48	0.28	2.46	91,91,91,91	0
56	MG	RA	4068	1/1	0.58	0.58	2.36	91,91,91,91	0
56	MG	RQ	204	1/1	0.72	0.65	2.29	89,89,89,89	0
56	MG	RA	4018	1/1	0.92	0.38	2.28	106,106,106,106	0
56	MG	XA	1727	1/1	0.86	0.23	2.23	79,79,79,79	0
56	MG	QA	1606	1/1	0.68	0.20	2.23	88,88,88,88	0
57	ZN	Y4	101	1/1	0.56	0.40	2.20	176,176,176,176	0
56	MG	YA	3053	1/1	0.82	0.23	2.19	62,62,62,62	0
56	MG	YA	3420	1/1	0.89	0.30	2.18	68,68,68,68	0
56	MG	RA	4006	1/1	0.86	0.30	2.15	74,74,74,74	0
56	MG	RA	3906	1/1	0.93	0.42	2.15	62,62,62,62	0
56	MG	YA	3094	1/1	0.21	0.25	2.14	77,77,77,77	0
56	MG	RA	3505	1/1	0.79	0.31	2.13	68,68,68,68	0
56	MG	YA	3727	1/1	0.94	0.36	2.12	62,62,62,62	0
56	MG	RA	3211	1/1	0.89	0.29	2.10	78,78,78,78	0
56	MG	XA	1632	1/1	0.97	0.58	2.09	84,84,84,84	0
56	MG	YA	3685	1/1	0.49	0.60	2.07	87,87,87,87	0
56	MG	RA	3981	1/1	0.96	0.23	2.01	78,78,78,78	0
57	ZN	R4	101	1/1	0.65	0.51	1.95	177,177,177,177	0
56	MG	QA	1621	1/1	0.64	0.28	1.93	85,85,85,85	0
56	MG	YA	3060	1/1	0.79	0.34	1.92	68,68,68,68	0
56	MG	YA	3407	1/1	0.91	0.33	1.90	62,62,62,62	0
56	MG	YA	3039	1/1	0.87	0.19	1.87	67,67,67,67	0
56	MG	QA	1635	1/1	0.41	0.19	1.86	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	4001	1/1	0.73	0.34	1.85	62,62,62,62	0
56	MG	RA	4067	1/1	0.98	0.41	1.83	72,72,72,72	0
56	MG	RA	3625	1/1	0.83	0.30	1.83	73,73,73,73	0
56	MG	XF	201	1/1	0.54	0.29	1.81	68,68,68,68	0
56	MG	YA	3252	1/1	0.67	0.24	1.72	96,96,96,96	0
56	MG	RA	3571	1/1	0.83	0.17	1.69	74,74,74,74	0
56	MG	YA	3669	1/1	0.89	0.37	1.65	65,65,65,65	0
56	MG	QB	301	1/1	0.60	0.35	1.65	81,81,81,81	0
56	MG	QA	1645	1/1	0.80	0.25	1.62	76,76,76,76	0
56	MG	QA	1656	1/1	0.74	0.25	1.59	78,78,78,78	0
56	MG	YA	3012	1/1	0.82	0.26	1.59	70,70,70,70	0
56	MG	YA	3221	1/1	0.87	0.17	1.58	80,80,80,80	0
56	MG	YA	3281	1/1	0.58	0.33	1.57	62,62,62,62	0
56	MG	RA	4029	1/1	0.66	0.36	1.56	62,62,62,62	0
56	MG	YA	3139	1/1	0.85	0.30	1.53	63,63,63,63	0
56	MG	XA	1697	1/1	0.08	0.21	1.48	87,87,87,87	0
56	MG	YA	3150	1/1	0.86	0.40	1.43	79,79,79,79	0
56	MG	RA	3157	1/1	0.80	0.24	1.37	84,84,84,84	0
56	MG	QA	1717	1/1	0.92	0.17	1.36	92,92,92,92	0
56	MG	RB	206	1/1	0.76	0.15	1.31	80,80,80,80	0
56	MG	XL	201	1/1	0.70	0.40	1.31	82,82,82,82	0
56	MG	RA	3396	1/1	0.77	0.25	1.29	67,67,67,67	0
56	MG	RA	3722	1/1	0.80	0.42	1.25	83,83,83,83	0
56	MG	RA	3867	1/1	0.88	0.15	1.24	81,81,81,81	0
56	MG	QQ	202	1/1	0.84	0.24	1.17	92,92,92,92	0
56	MG	QA	1620	1/1	0.90	0.20	1.11	69,69,69,69	0
56	MG	RA	3532	1/1	0.78	0.27	1.07	63,63,63,63	0
56	MG	RB	205	1/1	0.70	0.21	1.01	92,92,92,92	0
56	MG	RA	4004	1/1	0.87	0.34	0.97	64,64,64,64	0
56	MG	QA	1691	1/1	0.76	0.41	0.94	96,96,96,96	0
56	MG	RA	3084	1/1	0.91	0.26	0.89	76,76,76,76	0
56	MG	YA	3111	1/1	0.92	0.26	0.86	88,88,88,88	0
56	MG	RB	219	1/1	0.93	0.21	0.84	73,73,73,73	0
56	MG	QR	101	1/1	0.60	0.41	0.82	93,93,93,93	0
56	MG	YA	3730	1/1	0.92	0.28	0.80	80,80,80,80	0
56	MG	XA	1753	1/1	0.94	0.25	0.78	81,81,81,81	0
56	MG	RG	201	1/1	0.81	0.33	0.73	89,89,89,89	0
56	MG	QA	1655	1/1	0.82	0.31	0.71	93,93,93,93	0
56	MG	RE	303	1/1	0.45	0.39	0.71	102,102,102,102	0
56	MG	QA	1742	1/1	0.83	0.18	0.69	92,92,92,92	0
56	MG	YA	3725	1/1	0.85	0.35	0.69	62,62,62,62	0
56	MG	RA	3131	1/1	0.38	0.14	0.68	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3337	1/1	0.92	0.26	0.67	76,76,76,76	0
56	MG	RA	3075	1/1	0.78	0.24	0.67	76,76,76,76	0
56	MG	RA	3585	1/1	0.57	0.21	0.59	77,77,77,77	0
56	MG	RA	3530	1/1	0.93	0.30	0.59	62,62,62,62	0
56	MG	RA	3508	1/1	0.93	0.19	0.56	89,89,89,89	0
56	MG	RA	3305	1/1	0.71	0.29	0.55	73,73,73,73	0
56	MG	YA	3565	1/1	0.91	0.39	0.54	64,64,64,64	0
56	MG	QA	1665	1/1	0.86	0.29	0.50	95,95,95,95	0
56	MG	YA	3448	1/1	0.72	0.17	0.47	80,80,80,80	0
56	MG	YA	3535	1/1	0.92	0.28	0.47	69,69,69,69	0
56	MG	RA	3784	1/1	0.95	0.24	0.46	88,88,88,88	0
56	MG	XA	1764	1/1	0.90	0.23	0.41	73,73,73,73	0
56	MG	Y6	102	1/1	0.56	0.48	0.40	102,102,102,102	0
56	MG	YG	202	1/1	0.86	0.20	0.31	92,92,92,92	0
56	MG	QA	1781	1/1	0.88	0.28	0.26	95,95,95,95	0
56	MG	RA	3312	1/1	0.39	0.34	0.20	96,96,96,96	0
56	MG	RA	3852	1/1	0.74	0.20	0.19	90,90,90,90	0
56	MG	Y1	101	1/1	0.73	0.31	0.12	62,62,62,62	0
56	MG	XA	1659	1/1	0.73	0.21	0.06	88,88,88,88	0
56	MG	QA	1770	1/1	0.85	0.15	0.04	91,91,91,91	0
56	MG	RA	3326	1/1	0.94	0.29	0.03	63,63,63,63	0
56	MG	YA	3085	1/1	0.82	0.18	-0.01	85,85,85,85	0
56	MG	RA	4039	1/1	0.91	0.23	-0.02	92,92,92,92	0
56	MG	RB	215	1/1	0.54	0.18	-0.03	81,81,81,81	0
57	ZN	RY	201	1/1	0.84	0.24	-0.04	158,158,158,158	0
56	MG	RA	3654	1/1	0.91	0.19	-0.05	71,71,71,71	0
56	MG	RA	3025	1/1	0.72	0.21	-0.07	69,69,69,69	0
56	MG	RA	3455	1/1	0.85	0.22	-0.09	81,81,81,81	0
56	MG	XA	1654	1/1	0.81	0.28	-0.11	87,87,87,87	0
57	ZN	YY	201	1/1	0.56	0.23	-0.13	167,167,167,167	0
56	MG	QA	1874	1/1	0.67	0.23	-0.15	93,93,93,93	0
56	MG	RA	3901	1/1	0.91	0.24	-0.18	71,71,71,71	0
56	MG	YE	304	1/1	0.77	0.29	-0.22	71,71,71,71	0
56	MG	RA	3008	1/1	0.17	0.22	-0.23	83,83,83,83	0
56	MG	YA	3151	1/1	0.92	0.23	-0.24	87,87,87,87	0
56	MG	YA	3283	1/1	0.62	0.14	-0.31	74,74,74,74	0
56	MG	YA	3115	1/1	0.72	0.17	-0.51	77,77,77,77	0
56	MG	RD	307	1/1	0.81	0.26	-0.54	72,72,72,72	0
56	MG	RA	4038	1/1	0.63	0.23	-0.57	75,75,75,75	0
56	MG	QV	101	1/1	0.69	0.17	-0.62	86,86,86,86	0
58	SF4	QD	302	8/8	0.99	0.17	-0.64	71,79,94,101	0
56	MG	RA	3702	1/1	0.94	0.20	-0.64	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3357	1/1	0.95	0.21	-0.84	62,62,62,62	0
56	MG	YA	3453	1/1	0.87	0.17	-0.85	79,79,79,79	0
56	MG	RA	3062	1/1	0.68	0.13	-0.88	84,84,84,84	0
56	MG	YF	302	1/1	0.62	0.24	-0.95	75,75,75,75	0
58	SF4	XD	301	8/8	0.98	0.15	-0.97	65,79,98,112	0
56	MG	XA	1636	1/1	0.74	0.22	-0.98	68,68,68,68	0
56	MG	XK	201	1/1	0.75	0.18	-1.05	87,87,87,87	0
56	MG	RA	3868	1/1	0.82	0.14	-1.06	83,83,83,83	0
57	ZN	XN	101	1/1	0.98	0.13	-1.09	91,91,91,91	0
56	MG	XA	1644	1/1	0.88	0.13	-1.12	94,94,94,94	0
56	MG	QA	1631	1/1	0.87	0.17	-1.13	73,73,73,73	0
56	MG	RG	204	1/1	0.24	0.18	-1.17	84,84,84,84	0
56	MG	YG	203	1/1	0.65	0.15	-1.17	91,91,91,91	0
56	MG	RA	3671	1/1	0.86	0.12	-1.23	79,79,79,79	0
56	MG	YA	3021	1/1	0.86	0.20	-1.32	66,66,66,66	0
57	ZN	Y6	101	1/1	0.82	0.37	-1.34	156,156,156,156	0
57	ZN	R6	101	1/1	0.80	0.32	-1.43	159,159,159,159	0
56	MG	QA	1845	1/1	0.60	0.12	-1.44	79,79,79,79	0
57	ZN	QN	101	1/1	0.96	0.12	-1.48	110,110,110,110	0
56	MG	RA	3965	1/1	0.81	0.18	-1.50	73,73,73,73	0
56	MG	YA	3430	1/1	0.94	0.27	-1.58	80,80,80,80	0
57	ZN	R9	102	1/1	0.94	0.10	-1.59	125,125,125,125	0
57	ZN	R5	103	1/1	0.88	0.04	-1.59	135,135,135,135	0
57	ZN	Y9	101	1/1	0.94	0.06	-1.67	116,116,116,116	0
57	ZN	Y5	102	1/1	0.89	0.06	-1.73	144,144,144,144	0
56	MG	QA	1871	1/1	0.58	0.12	-1.82	77,77,77,77	0
56	MG	RA	3966	1/1	0.88	0.20	-1.98	71,71,71,71	0
56	MG	XA	1621	1/1	0.70	0.13	-2.09	83,83,83,83	0
56	MG	YA	3184	1/1	0.91	0.15	-2.24	78,78,78,78	0
56	MG	XV	101	1/1	0.79	0.11	-2.60	87,87,87,87	0
56	MG	QA	1650	1/1	0.96	0.08	-3.90	93,93,93,93	0
56	MG	YA	3187	1/1	0.95	0.07	-5.88	89,89,89,89	0
56	MG	RA	3562	1/1	0.61	0.69	-	82,82,82,82	0
56	MG	YA	3241	1/1	0.89	0.65	-	91,91,91,91	0
56	MG	RA	3678	1/1	0.82	0.87	-	78,78,78,78	0
56	MG	YA	3670	1/1	0.64	0.55	-	85,85,85,85	0
56	MG	RA	3848	1/1	0.02	1.03	-	91,91,91,91	0
56	MG	QA	1840	1/1	0.25	0.60	-	88,88,88,88	0
56	MG	XA	1625	1/1	0.54	0.77	-	90,90,90,90	0
56	MG	RA	4005	1/1	0.83	0.21	-	80,80,80,80	0
56	MG	RA	3681	1/1	0.71	0.88	-	72,72,72,72	0
56	MG	RA	3266	1/1	0.80	0.13	-	106,106,106,106	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3273	1/1	0.82	0.36	-	84,84,84,84	0
56	MG	RB	208	1/1	0.30	0.34	-	95,95,95,95	0
56	MG	YA	3399	1/1	0.46	0.80	-	76,76,76,76	0
56	MG	RA	3346	1/1	0.85	0.62	-	83,83,83,83	0
56	MG	RD	304	1/1	0.48	0.52	-	75,75,75,75	0
56	MG	XA	1716	1/1	0.63	0.56	-	79,79,79,79	0
56	MG	YA	3417	1/1	0.83	0.68	-	69,69,69,69	0
56	MG	XA	1619	1/1	0.46	0.82	-	76,76,76,76	0
56	MG	YB	207	1/1	0.94	0.35	-	97,97,97,97	0
56	MG	YA	3334	1/1	0.80	0.57	-	66,66,66,66	0
56	MG	QA	1782	1/1	0.55	0.28	-	98,98,98,98	0
56	MG	RA	3292	1/1	0.79	0.66	-	93,93,93,93	0
56	MG	RA	4020	1/1	0.71	0.45	-	91,91,91,91	0
56	MG	YA	3348	1/1	0.77	0.59	-	88,88,88,88	0
56	MG	XA	1694	1/1	0.76	0.37	-	77,77,77,77	0
56	MG	QA	1727	1/1	0.65	0.47	-	86,86,86,86	0
56	MG	RA	3222	1/1	0.76	0.64	-	88,88,88,88	0
56	MG	RA	3842	1/1	0.87	0.68	-	75,75,75,75	0
56	MG	RA	3220	1/1	0.95	0.29	-	82,82,82,82	0
56	MG	QA	1769	1/1	-0.54	1.08	-	99,99,99,99	0
56	MG	RA	3055	1/1	0.89	0.94	-	112,112,112,112	0
56	MG	YA	3016	1/1	0.47	0.63	-	89,89,89,89	0
56	MG	QA	1661	1/1	0.58	0.90	-	85,85,85,85	0
56	MG	RA	3374	1/1	0.54	0.75	-	72,72,72,72	0
56	MG	RA	3553	1/1	0.70	0.23	-	100,100,100,100	0
56	MG	YA	3687	1/1	0.62	0.72	-	62,62,62,62	0
56	MG	YA	3403	1/1	0.20	0.35	-	81,81,81,81	0
56	MG	RA	3993	1/1	0.48	0.83	-	85,85,85,85	0
56	MG	RA	3622	1/1	0.78	0.43	-	87,87,87,87	0
56	MG	XA	1657	1/1	0.25	0.97	-	91,91,91,91	0
56	MG	RA	3420	1/1	0.93	0.64	-	62,62,62,62	0
56	MG	XA	1742	1/1	0.56	0.42	-	78,78,78,78	0
56	MG	QA	1690	1/1	0.43	0.32	-	68,68,68,68	0
56	MG	YA	3465	1/1	0.44	0.58	-	85,85,85,85	0
56	MG	QA	1818	1/1	-0.00	0.58	-	93,93,93,93	0
56	MG	YA	3657	1/1	0.81	0.67	-	81,81,81,81	0
56	MG	RA	3887	1/1	0.52	0.57	-	91,91,91,91	0
56	MG	RA	3324	1/1	0.85	0.65	-	62,62,62,62	0
56	MG	RA	3564	1/1	0.33	0.76	-	91,91,91,91	0
56	MG	YA	3287	1/1	0.93	0.52	-	78,78,78,78	0
56	MG	RA	3797	1/1	0.01	0.44	-	109,109,109,109	0
56	MG	QA	1644	1/1	0.82	0.39	-	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3219	1/1	0.36	0.60	-	95,95,95,95	0
56	MG	YA	3472	1/1	0.59	0.66	-	82,82,82,82	0
56	MG	RA	3528	1/1	0.37	1.11	-	81,81,81,81	0
56	MG	YA	3742	1/1	0.85	0.27	-	85,85,85,85	0
56	MG	RA	3437	1/1	0.35	1.16	-	77,77,77,77	0
56	MG	RA	3570	1/1	0.79	0.57	-	71,71,71,71	0
56	MG	YA	3507	1/1	0.20	0.79	-	80,80,80,80	0
56	MG	YA	3274	1/1	0.93	0.85	-	62,62,62,62	0
56	MG	RA	3256	1/1	0.84	0.88	-	96,96,96,96	0
56	MG	RA	3227	1/1	0.20	1.13	-	103,103,103,103	0
56	MG	RA	3072	1/1	0.86	1.18	-	110,110,110,110	0
56	MG	RD	301	1/1	0.81	1.08	-	93,93,93,93	0
56	MG	YA	3347	1/1	0.86	0.23	-	79,79,79,79	0
56	MG	RA	3670	1/1	-0.72	1.68	-	103,103,103,103	0
56	MG	QA	1746	1/1	0.68	0.42	-	80,80,80,80	0
56	MG	RA	3400	1/1	0.07	0.79	-	101,101,101,101	0
56	MG	QA	1851	1/1	0.79	0.67	-	78,78,78,78	0
56	MG	YA	3090	1/1	0.26	0.32	-	100,100,100,100	0
56	MG	YA	3005	1/1	0.73	0.42	-	85,85,85,85	0
56	MG	RA	3563	1/1	0.45	0.37	-	87,87,87,87	0
56	MG	QA	1744	1/1	0.93	0.38	-	77,77,77,77	0
56	MG	YA	3246	1/1	0.76	0.57	-	81,81,81,81	0
56	MG	YA	3052	1/1	0.94	0.10	-	80,80,80,80	0
56	MG	YA	3576	1/1	0.85	0.76	-	74,74,74,74	0
56	MG	YA	3383	1/1	0.94	0.61	-	63,63,63,63	0
56	MG	RA	3130	1/1	0.84	0.17	-	85,85,85,85	0
56	MG	QA	1743	1/1	0.86	0.27	-	71,71,71,71	0
56	MG	RW	201	1/1	0.45	0.54	-	83,83,83,83	0
56	MG	YV	201	1/1	0.47	0.54	-	84,84,84,84	0
56	MG	YA	3307	1/1	0.68	0.71	-	71,71,71,71	0
56	MG	RA	3443	1/1	0.94	0.99	-	62,62,62,62	0
56	MG	RA	3613	1/1	0.56	1.04	-	75,75,75,75	0
56	MG	YA	3605	1/1	0.84	0.33	-	84,84,84,84	0
56	MG	YA	3549	1/1	0.15	0.71	-	90,90,90,90	0
56	MG	RA	3645	1/1	0.70	0.74	-	85,85,85,85	0
56	MG	YA	3534	1/1	0.53	0.34	-	85,85,85,85	0
56	MG	QA	1880	1/1	0.64	0.39	-	102,102,102,102	0
56	MG	QA	1681	1/1	0.26	1.12	-	92,92,92,92	0
56	MG	RA	3144	1/1	0.77	0.69	-	86,86,86,86	0
56	MG	YA	3666	1/1	0.77	0.45	-	63,63,63,63	0
56	MG	YA	3003	1/1	0.93	0.68	-	70,70,70,70	0
56	MG	RA	3378	1/1	0.82	0.54	-	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3536	1/1	0.93	0.47	-	63,63,63,63	0
56	MG	RA	3581	1/1	0.63	0.69	-	97,97,97,97	0
56	MG	RA	3034	1/1	0.87	0.69	-	97,97,97,97	0
56	MG	YA	3176	1/1	0.82	0.34	-	78,78,78,78	0
56	MG	RA	3704	1/1	0.70	0.56	-	82,82,82,82	0
56	MG	QA	1786	1/1	0.55	0.58	-	80,80,80,80	0
56	MG	YD	302	1/1	0.80	0.84	-	81,81,81,81	0
56	MG	RA	3257	1/1	0.78	0.52	-	100,100,100,100	0
56	MG	RA	3510	1/1	0.91	0.98	-	71,71,71,71	0
56	MG	YA	3707	1/1	0.74	0.56	-	82,82,82,82	0
56	MG	XY	401	1/1	-0.02	1.97	-	97,97,97,97	0
56	MG	R0	101	1/1	0.84	0.74	-	77,77,77,77	0
56	MG	QA	1808	1/1	0.24	0.39	-	74,74,74,74	0
56	MG	XH	201	1/1	-0.10	0.60	-	99,99,99,99	0
56	MG	RA	3273	1/1	0.41	1.22	-	99,99,99,99	0
56	MG	XA	1669	1/1	0.18	0.62	-	106,106,106,106	0
56	MG	QA	1637	1/1	0.29	0.82	-	85,85,85,85	0
56	MG	RA	3869	1/1	0.40	0.93	-	88,88,88,88	0
56	MG	XA	1736	1/1	0.88	0.87	-	70,70,70,70	0
56	MG	YA	3341	1/1	0.40	0.37	-	91,91,91,91	0
56	MG	RA	3788	1/1	0.64	0.55	-	90,90,90,90	0
56	MG	RA	3647	1/1	0.64	1.10	-	102,102,102,102	0
56	MG	YA	3477	1/1	0.60	0.59	-	77,77,77,77	0
56	MG	RA	3904	1/1	0.22	0.66	-	80,80,80,80	0
56	MG	RA	3925	1/1	0.20	0.33	-	95,95,95,95	0
56	MG	RA	3600	1/1	0.11	0.94	-	94,94,94,94	0
56	MG	YA	3690	1/1	0.74	0.47	-	78,78,78,78	0
56	MG	RA	3016	1/1	0.60	0.86	-	109,109,109,109	0
56	MG	QA	1739	1/1	0.61	0.56	-	80,80,80,80	0
56	MG	QA	1765	1/1	0.40	0.93	-	80,80,80,80	0
56	MG	RA	3370	1/1	0.76	0.75	-	78,78,78,78	0
56	MG	YA	3081	1/1	0.84	0.41	-	81,81,81,81	0
56	MG	RA	3547	1/1	-0.09	0.61	-	99,99,99,99	0
56	MG	RA	3988	1/1	0.58	0.72	-	86,86,86,86	0
56	MG	XA	1749	1/1	0.09	1.00	-	98,98,98,98	0
56	MG	QA	1785	1/1	0.94	0.15	-	95,95,95,95	0
56	MG	QA	1766	1/1	0.89	0.10	-	96,96,96,96	0
56	MG	YA	3159	1/1	0.85	0.14	-	76,76,76,76	0
56	MG	RA	3692	1/1	0.82	0.59	-	84,84,84,84	0
56	MG	RA	3042	1/1	-0.06	0.75	-	92,92,92,92	0
56	MG	RA	3710	1/1	0.75	0.41	-	98,98,98,98	0
56	MG	YA	3034	1/1	0.86	0.28	-	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3051	1/1	0.70	0.42	-	82,82,82,82	0
56	MG	YA	3394	1/1	0.23	0.93	-	75,75,75,75	0
56	MG	QA	1627	1/1	0.84	0.10	-	79,79,79,79	0
56	MG	YA	3508	1/1	0.52	0.39	-	83,83,83,83	0
56	MG	RA	3732	1/1	0.69	0.79	-	85,85,85,85	0
56	MG	YA	3424	1/1	0.89	0.46	-	70,70,70,70	0
56	MG	RU	202	1/1	0.29	0.68	-	94,94,94,94	0
56	MG	QA	1679	1/1	0.46	0.80	-	87,87,87,87	0
56	MG	RA	3426	1/1	0.39	0.32	-	79,79,79,79	0
56	MG	XA	1718	1/1	0.88	0.59	-	78,78,78,78	0
56	MG	QA	1718	1/1	0.85	0.33	-	94,94,94,94	0
56	MG	RA	3940	1/1	0.56	0.79	-	90,90,90,90	0
56	MG	RA	3071	1/1	0.88	0.80	-	86,86,86,86	0
56	MG	RA	3363	1/1	0.87	0.15	-	91,91,91,91	0
56	MG	RA	3036	1/1	0.02	0.85	-	94,94,94,94	0
56	MG	XE	201	1/1	-0.13	1.00	-	93,93,93,93	0
56	MG	QA	1667	1/1	0.91	0.20	-	92,92,92,92	0
56	MG	YA	3617	1/1	0.83	0.51	-	74,74,74,74	0
56	MG	RA	3687	1/1	0.44	0.36	-	86,86,86,86	0
56	MG	RB	226	1/1	0.50	0.40	-	98,98,98,98	0
56	MG	QA	1693	1/1	0.86	0.60	-	87,87,87,87	0
56	MG	RA	3096	1/1	0.82	0.29	-	83,83,83,83	0
56	MG	YA	3188	1/1	0.31	0.28	-	92,92,92,92	0
56	MG	QA	1747	1/1	0.58	1.23	-	81,81,81,81	0
56	MG	YA	3677	1/1	0.89	1.45	-	79,79,79,79	0
56	MG	YA	3189	1/1	0.81	0.32	-	83,83,83,83	0
56	MG	YA	3057	1/1	0.40	0.69	-	90,90,90,90	0
56	MG	RA	3664	1/1	0.85	0.36	-	91,91,91,91	0
56	MG	RE	304	1/1	0.93	0.76	-	62,62,62,62	0
56	MG	RA	3888	1/1	0.52	0.74	-	89,89,89,89	0
56	MG	RA	3475	1/1	0.85	0.30	-	82,82,82,82	0
56	MG	QA	1695	1/1	0.83	0.46	-	93,93,93,93	0
56	MG	YA	3584	1/1	0.85	0.44	-	77,77,77,77	0
56	MG	RN	203	1/1	0.75	0.95	-	90,90,90,90	0
56	MG	YA	3228	1/1	0.40	1.01	-	73,73,73,73	0
56	MG	RA	3637	1/1	0.52	0.73	-	85,85,85,85	0
56	MG	QA	1864	1/1	0.72	0.40	-	97,97,97,97	0
56	MG	XA	1713	1/1	0.62	0.34	-	74,74,74,74	0
56	MG	YA	3490	1/1	0.95	0.24	-	67,67,67,67	0
56	MG	YA	3097	1/1	0.69	0.39	-	96,96,96,96	0
56	MG	YA	3544	1/1	0.58	0.47	-	63,63,63,63	0
56	MG	XA	1762	1/1	0.85	0.29	-	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1809	1/1	0.57	0.47	-	86,86,86,86	0
56	MG	RA	3044	1/1	0.68	0.39	-	82,82,82,82	0
56	MG	YA	3244	1/1	0.16	1.19	-	97,97,97,97	0
56	MG	Y8	102	1/1	0.79	0.61	-	68,68,68,68	0
56	MG	XA	1655	1/1	0.61	0.49	-	82,82,82,82	0
56	MG	YA	3059	1/1	-0.06	1.01	-	86,86,86,86	0
56	MG	YA	3095	1/1	0.77	0.54	-	64,64,64,64	0
56	MG	RA	3123	1/1	0.36	0.37	-	80,80,80,80	0
56	MG	QA	1719	1/1	0.54	1.13	-	73,73,73,73	0
56	MG	RA	3316	1/1	0.06	0.81	-	93,93,93,93	0
56	MG	RA	3049	1/1	0.85	0.17	-	80,80,80,80	0
56	MG	RA	3639	1/1	0.65	0.57	-	82,82,82,82	0
56	MG	YA	3158	1/1	0.82	0.43	-	84,84,84,84	0
56	MG	RA	3819	1/1	0.09	0.92	-	90,90,90,90	0
56	MG	RA	3555	1/1	0.61	0.52	-	80,80,80,80	0
56	MG	YA	3227	1/1	0.27	1.11	-	87,87,87,87	0
56	MG	RA	3005	1/1	0.66	0.74	-	91,91,91,91	0
56	MG	RA	3779	1/1	0.94	1.32	-	71,71,71,71	0
56	MG	RA	3108	1/1	0.71	0.85	-	89,89,89,89	0
56	MG	RA	3430	1/1	0.67	0.31	-	93,93,93,93	0
56	MG	RA	3028	1/1	0.87	0.15	-	84,84,84,84	0
56	MG	RA	3810	1/1	0.66	0.78	-	79,79,79,79	0
56	MG	QA	1831	1/1	0.23	0.82	-	99,99,99,99	0
56	MG	XA	1660	1/1	0.90	0.23	-	91,91,91,91	0
56	MG	YA	3655	1/1	0.82	0.53	-	62,62,62,62	0
56	MG	RA	4015	1/1	0.80	0.71	-	93,93,93,93	0
56	MG	RA	3202	1/1	0.77	0.40	-	87,87,87,87	0
56	MG	RR	204	1/1	0.54	0.51	-	75,75,75,75	0
56	MG	RA	3682	1/1	0.30	0.44	-	104,104,104,104	0
56	MG	RA	3749	1/1	0.72	0.21	-	70,70,70,70	0
56	MG	RA	3689	1/1	0.51	0.22	-	85,85,85,85	0
56	MG	RA	3329	1/1	0.86	0.29	-	94,94,94,94	0
56	MG	RA	3626	1/1	0.66	0.50	-	72,72,72,72	0
56	MG	YA	3628	1/1	0.47	0.34	-	87,87,87,87	0
56	MG	RA	3705	1/1	0.40	0.59	-	89,89,89,89	0
56	MG	YA	3581	1/1	0.34	0.58	-	80,80,80,80	0
56	MG	YA	3126	1/1	0.88	0.19	-	65,65,65,65	0
56	MG	RA	3282	1/1	0.79	0.98	-	102,102,102,102	0
56	MG	RA	4013	1/1	0.71	0.40	-	77,77,77,77	0
56	MG	RA	3228	1/1	0.42	0.56	-	104,104,104,104	0
56	MG	YA	3137	1/1	0.54	0.59	-	81,81,81,81	0
56	MG	RA	3576	1/1	0.61	0.51	-	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3515	1/1	0.62	1.06	-	69,69,69,69	0
56	MG	RA	3103	1/1	0.55	0.48	-	101,101,101,101	0
56	MG	QA	1677	1/1	0.56	0.49	-	89,89,89,89	0
56	MG	YA	3526	1/1	0.83	0.68	-	65,65,65,65	0
56	MG	QA	1858	1/1	0.20	0.82	-	86,86,86,86	0
56	MG	RA	3229	1/1	0.52	0.82	-	104,104,104,104	0
56	MG	YA	3162	1/1	0.77	0.50	-	96,96,96,96	0
56	MG	YA	3292	1/1	0.49	0.50	-	74,74,74,74	0
56	MG	RA	4031	1/1	0.37	0.50	-	108,108,108,108	0
56	MG	RA	3520	1/1	0.53	0.53	-	91,91,91,91	0
56	MG	RA	3556	1/1	0.69	1.66	-	83,83,83,83	0
56	MG	YA	3555	1/1	0.83	0.39	-	64,64,64,64	0
56	MG	YA	3172	1/1	0.78	0.28	-	101,101,101,101	0
56	MG	QA	1673	1/1	0.59	0.71	-	75,75,75,75	0
56	MG	YA	3063	1/1	0.73	0.65	-	92,92,92,92	0
56	MG	YA	3369	1/1	0.85	0.32	-	72,72,72,72	0
56	MG	YA	3218	1/1	0.24	0.55	-	82,82,82,82	0
56	MG	QA	1774	1/1	0.58	1.10	-	84,84,84,84	0
56	MG	YA	3569	1/1	0.58	0.98	-	67,67,67,67	0
56	MG	RA	3019	1/1	0.85	0.40	-	108,108,108,108	0
56	MG	YB	212	1/1	0.75	0.54	-	79,79,79,79	0
56	MG	RA	3093	1/1	0.93	0.17	-	97,97,97,97	0
56	MG	RA	3276	1/1	0.69	0.77	-	95,95,95,95	0
56	MG	RA	3507	1/1	0.92	0.33	-	75,75,75,75	0
56	MG	RA	3832	1/1	0.91	0.33	-	84,84,84,84	0
56	MG	RA	3517	1/1	0.85	0.94	-	62,62,62,62	0
56	MG	RA	3053	1/1	0.47	0.54	-	98,98,98,98	0
56	MG	RA	3494	1/1	0.73	0.47	-	81,81,81,81	0
56	MG	RA	3095	1/1	0.87	0.49	-	92,92,92,92	0
56	MG	YA	3673	1/1	0.81	1.15	-	66,66,66,66	0
56	MG	RA	3685	1/1	0.60	0.57	-	80,80,80,80	0
56	MG	RA	3107	1/1	0.91	0.96	-	90,90,90,90	0
56	MG	YA	3042	1/1	0.81	0.24	-	76,76,76,76	0
56	MG	YA	3194	1/1	0.67	0.53	-	89,89,89,89	0
56	MG	RA	3886	1/1	0.03	0.56	-	97,97,97,97	0
56	MG	QA	1684	1/1	0.75	1.17	-	97,97,97,97	0
56	MG	YA	3105	1/1	0.57	0.60	-	81,81,81,81	0
56	MG	YA	3319	1/1	0.95	0.62	-	62,62,62,62	0
56	MG	QL	201	1/1	0.55	0.19	-	87,87,87,87	0
56	MG	RA	3905	1/1	0.98	0.63	-	63,63,63,63	0
56	MG	RA	3294	1/1	0.73	0.49	-	108,108,108,108	0
56	MG	QA	1812	1/1	0.77	0.37	-	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3200	1/1	0.73	0.39	-	85,85,85,85	0
56	MG	RA	3792	1/1	0.87	0.48	-	87,87,87,87	0
56	MG	XA	1714	1/1	0.63	0.42	-	76,76,76,76	0
56	MG	RA	3929	1/1	0.81	0.44	-	85,85,85,85	0
56	MG	R5	104	1/1	0.39	1.34	-	97,97,97,97	0
56	MG	Y5	101	1/1	0.59	0.57	-	91,91,91,91	0
56	MG	XA	1746	1/1	0.87	0.62	-	62,62,62,62	0
56	MG	RA	3515	1/1	0.76	0.38	-	90,90,90,90	0
56	MG	QA	1839	1/1	0.75	0.57	-	79,79,79,79	0
56	MG	RA	3403	1/1	0.82	1.01	-	87,87,87,87	0
56	MG	YA	3233	1/1	0.13	0.44	-	96,96,96,96	0
56	MG	YA	3055	1/1	0.27	0.37	-	88,88,88,88	0
56	MG	RA	3750	1/1	0.72	0.61	-	83,83,83,83	0
56	MG	YA	3594	1/1	0.77	0.70	-	70,70,70,70	0
56	MG	YA	3010	1/1	0.82	0.43	-	84,84,84,84	0
56	MG	RA	3270	1/1	0.97	0.57	-	95,95,95,95	0
56	MG	QA	1712	1/1	0.71	0.48	-	75,75,75,75	0
56	MG	RA	3936	1/1	0.67	0.36	-	82,82,82,82	0
56	MG	RA	3158	1/1	0.89	0.18	-	81,81,81,81	0
56	MG	QA	1767	1/1	0.83	0.38	-	88,88,88,88	0
56	MG	QA	1762	1/1	0.61	0.69	-	80,80,80,80	0
56	MG	YA	3130	1/1	0.64	0.86	-	90,90,90,90	0
56	MG	YA	3548	1/1	0.40	0.86	-	66,66,66,66	0
56	MG	RA	3765	1/1	0.83	0.28	-	91,91,91,91	0
56	MG	YA	3375	1/1	0.85	0.33	-	80,80,80,80	0
56	MG	RA	3156	1/1	0.32	0.59	-	105,105,105,105	0
56	MG	YA	3464	1/1	0.40	1.57	-	79,79,79,79	0
56	MG	RA	3322	1/1	0.40	0.79	-	93,93,93,93	0
56	MG	QA	1796	1/1	0.78	0.54	-	90,90,90,90	0
56	MG	RA	3407	1/1	0.63	0.60	-	95,95,95,95	0
56	MG	RA	3935	1/1	0.60	0.60	-	90,90,90,90	0
56	MG	RA	3806	1/1	0.30	0.73	-	90,90,90,90	0
56	MG	YA	3659	1/1	0.76	1.06	-	65,65,65,65	0
56	MG	RA	3802	1/1	0.64	0.48	-	85,85,85,85	0
56	MG	YA	3243	1/1	0.76	1.34	-	90,90,90,90	0
56	MG	RA	3881	1/1	0.86	0.29	-	80,80,80,80	0
56	MG	QA	1806	1/1	0.62	0.55	-	79,79,79,79	0
56	MG	YA	3711	1/1	0.84	0.30	-	83,83,83,83	0
56	MG	YA	3367	1/1	0.13	0.27	-	76,76,76,76	0
56	MG	XA	1705	1/1	0.71	0.27	-	84,84,84,84	0
56	MG	RA	3759	1/1	0.90	0.23	-	73,73,73,73	0
56	MG	YA	3720	1/1	0.55	0.44	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3930	1/1	0.93	0.28	-	73,73,73,73	0
56	MG	YA	3619	1/1	0.64	0.59	-	65,65,65,65	0
56	MG	RA	3785	1/1	0.89	0.22	-	83,83,83,83	0
56	MG	RA	3180	1/1	0.58	1.07	-	80,80,80,80	0
56	MG	XA	1734	1/1	0.79	0.36	-	89,89,89,89	0
56	MG	YA	3222	1/1	0.00	0.74	-	88,88,88,88	0
56	MG	RA	3239	1/1	0.73	0.64	-	106,106,106,106	0
56	MG	RA	3367	1/1	0.46	0.54	-	80,80,80,80	0
56	MG	YA	3047	1/1	0.70	0.41	-	86,86,86,86	0
56	MG	YA	3680	1/1	0.90	0.79	-	62,62,62,62	0
56	MG	RA	3578	1/1	-0.01	0.89	-	90,90,90,90	0
56	MG	RA	3554	1/1	0.78	0.56	-	74,74,74,74	0
56	MG	YA	3022	1/1	0.64	1.80	-	91,91,91,91	0
56	MG	YA	3376	1/1	0.67	0.41	-	84,84,84,84	0
56	MG	RA	3464	1/1	0.70	0.40	-	90,90,90,90	0
56	MG	YA	3245	1/1	0.53	0.41	-	88,88,88,88	0
56	MG	XA	1677	1/1	0.90	0.33	-	63,63,63,63	0
56	MG	RA	3337	1/1	0.48	0.69	-	92,92,92,92	0
56	MG	YA	3353	1/1	0.79	0.54	-	68,68,68,68	0
56	MG	QA	1837	1/1	0.48	0.75	-	87,87,87,87	0
56	MG	QA	1738	1/1	0.05	0.78	-	101,101,101,101	0
56	MG	RD	314	1/1	0.39	0.81	-	80,80,80,80	0
56	MG	RW	202	1/1	0.62	0.47	-	99,99,99,99	0
56	MG	RA	3769	1/1	0.47	0.51	-	85,85,85,85	0
56	MG	RA	3662	1/1	0.41	0.55	-	94,94,94,94	0
56	MG	RA	3513	1/1	0.04	1.32	-	87,87,87,87	0
56	MG	QA	1696	1/1	0.34	0.82	-	71,71,71,71	0
56	MG	RA	3368	1/1	-0.01	0.68	-	90,90,90,90	0
56	MG	RA	3063	1/1	0.91	0.31	-	83,83,83,83	0
56	MG	XA	1719	1/1	0.77	0.45	-	78,78,78,78	0
56	MG	QA	1817	1/1	0.63	0.47	-	85,85,85,85	0
56	MG	RA	3523	1/1	0.73	0.43	-	94,94,94,94	0
56	MG	YA	3688	1/1	0.68	0.41	-	72,72,72,72	0
56	MG	RA	3245	1/1	0.73	0.11	-	86,86,86,86	0
56	MG	YA	3545	1/1	0.87	0.56	-	82,82,82,82	0
56	MG	RA	3155	1/1	0.67	0.55	-	95,95,95,95	0
56	MG	QA	1810	1/1	0.81	0.68	-	81,81,81,81	0
56	MG	YA	3333	1/1	0.53	0.45	-	85,85,85,85	0
56	MG	RA	3914	1/1	0.91	0.56	-	70,70,70,70	0
56	MG	RA	3860	1/1	0.72	1.50	-	85,85,85,85	0
56	MG	RA	3970	1/1	0.66	0.56	-	96,96,96,96	0
56	MG	RA	3393	1/1	0.94	0.35	-	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3106	1/1	0.60	0.44	-	92,92,92,92	0
56	MG	YA	3214	1/1	0.88	0.41	-	76,76,76,76	0
56	MG	RA	3395	1/1	0.95	0.60	-	62,62,62,62	0
56	MG	XA	1769	1/1	0.97	0.57	-	77,77,77,77	0
56	MG	QA	1733	1/1	-0.47	0.76	-	94,94,94,94	0
56	MG	RA	3190	1/1	0.91	0.31	-	69,69,69,69	0
56	MG	RA	3188	1/1	0.79	0.56	-	104,104,104,104	0
56	MG	QA	1652	1/1	0.64	0.27	-	83,83,83,83	0
56	MG	YA	3500	1/1	0.80	1.03	-	84,84,84,84	0
56	MG	YA	3254	1/1	0.88	0.40	-	87,87,87,87	0
56	MG	XA	1791	1/1	0.90	0.11	-	74,74,74,74	0
56	MG	YA	3231	1/1	0.40	0.85	-	93,93,93,93	0
56	MG	QA	1607	1/1	0.88	0.28	-	91,91,91,91	0
56	MG	XA	1703	1/1	0.69	0.47	-	82,82,82,82	0
56	MG	XA	1678	1/1	0.86	0.30	-	72,72,72,72	0
56	MG	YA	3414	1/1	0.33	0.71	-	92,92,92,92	0
56	MG	YA	3177	1/1	0.11	0.61	-	95,95,95,95	0
56	MG	RA	3438	1/1	0.15	0.83	-	91,91,91,91	0
56	MG	QA	1613	1/1	0.92	0.15	-	98,98,98,98	0
56	MG	YB	205	1/1	-0.13	0.92	-	93,93,93,93	0
56	MG	YA	3667	1/1	0.91	0.67	-	65,65,65,65	0
56	MG	QA	1772	1/1	0.72	0.37	-	96,96,96,96	0
56	MG	RA	3435	1/1	0.13	0.69	-	75,75,75,75	0
56	MG	QA	1642	1/1	0.25	1.32	-	101,101,101,101	0
56	MG	QA	1683	1/1	0.77	0.28	-	95,95,95,95	0
56	MG	QA	1842	1/1	0.34	0.78	-	95,95,95,95	0
56	MG	XA	1785	1/1	0.83	0.89	-	82,82,82,82	0
56	MG	YA	3497	1/1	0.32	0.58	-	95,95,95,95	0
56	MG	XA	1684	1/1	0.72	1.05	-	70,70,70,70	0
56	MG	RA	3589	1/1	0.79	0.35	-	94,94,94,94	0
56	MG	RA	3548	1/1	-0.37	0.94	-	109,109,109,109	0
56	MG	QA	1867	1/1	0.34	0.74	-	96,96,96,96	0
56	MG	RA	3350	1/1	0.69	0.26	-	74,74,74,74	0
56	MG	RA	3962	1/1	0.25	1.20	-	95,95,95,95	0
56	MG	YB	210	1/1	0.66	0.82	-	88,88,88,88	0
56	MG	YA	3437	1/1	0.75	0.50	-	62,62,62,62	0
56	MG	RA	3463	1/1	0.84	0.55	-	69,69,69,69	0
56	MG	QA	1869	1/1	0.01	1.39	-	105,105,105,105	0
56	MG	XA	1676	1/1	0.43	0.83	-	98,98,98,98	0
56	MG	YA	3340	1/1	0.93	0.56	-	62,62,62,62	0
56	MG	YA	3686	1/1	0.83	0.46	-	77,77,77,77	0
56	MG	RA	3285	1/1	0.84	0.69	-	108,108,108,108	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YB	218	1/1	0.43	0.31	-	85,85,85,85	0
56	MG	RA	3311	1/1	0.71	0.51	-	83,83,83,83	0
56	MG	YA	3410	1/1	0.94	0.59	-	68,68,68,68	0
56	MG	XA	1626	1/1	0.76	0.66	-	78,78,78,78	0
56	MG	RA	3176	1/1	0.36	1.02	-	102,102,102,102	0
56	MG	RA	3423	1/1	0.54	0.59	-	92,92,92,92	0
56	MG	RB	227	1/1	-0.20	0.37	-	88,88,88,88	0
56	MG	RA	3956	1/1	0.94	0.29	-	80,80,80,80	0
56	MG	YA	3213	1/1	0.94	0.52	-	63,63,63,63	0
56	MG	RA	3345	1/1	0.89	0.66	-	62,62,62,62	0
56	MG	YA	3678	1/1	0.76	0.51	-	62,62,62,62	0
56	MG	RA	3124	1/1	0.59	0.47	-	73,73,73,73	0
56	MG	YA	3298	1/1	0.80	0.24	-	82,82,82,82	0
56	MG	XA	1687	1/1	0.52	0.34	-	90,90,90,90	0
56	MG	QA	1676	1/1	0.54	0.88	-	97,97,97,97	0
56	MG	YA	3096	1/1	0.49	0.19	-	87,87,87,87	0
56	MG	RA	3972	1/1	0.95	0.74	-	62,62,62,62	0
56	MG	RA	3261	1/1	0.77	1.23	-	87,87,87,87	0
56	MG	YA	3381	1/1	0.48	0.67	-	70,70,70,70	0
56	MG	RA	3811	1/1	0.78	0.88	-	85,85,85,85	0
56	MG	RA	3024	1/1	0.71	0.68	-	105,105,105,105	0
56	MG	RA	3909	1/1	0.82	0.67	-	62,62,62,62	0
56	MG	RA	3263	1/1	0.82	0.64	-	93,93,93,93	0
56	MG	RA	3193	1/1	0.39	0.69	-	103,103,103,103	0
56	MG	YA	3248	1/1	0.57	0.54	-	88,88,88,88	0
56	MG	YA	3732	1/1	0.83	0.26	-	86,86,86,86	0
56	MG	YA	3257	1/1	0.71	0.49	-	89,89,89,89	0
56	MG	YD	301	1/1	0.63	0.43	-	66,66,66,66	0
56	MG	RA	3371	1/1	-0.32	1.55	-	97,97,97,97	0
56	MG	QA	1611	1/1	0.24	1.17	-	80,80,80,80	0
56	MG	RA	3897	1/1	0.71	0.60	-	72,72,72,72	0
56	MG	RA	3058	1/1	0.34	0.77	-	89,89,89,89	0
56	MG	RA	3688	1/1	0.64	0.71	-	79,79,79,79	0
56	MG	YA	3198	1/1	0.41	0.35	-	88,88,88,88	0
56	MG	YA	3741	1/1	0.59	0.60	-	96,96,96,96	0
56	MG	YA	3114	1/1	0.61	0.76	-	90,90,90,90	0
56	MG	QO	101	1/1	0.82	0.29	-	86,86,86,86	0
56	MG	RA	3327	1/1	0.72	0.56	-	69,69,69,69	0
56	MG	RA	3233	1/1	0.92	0.80	-	96,96,96,96	0
56	MG	YA	3024	1/1	0.70	0.24	-	91,91,91,91	0
56	MG	YB	213	1/1	0.76	0.53	-	81,81,81,81	0
56	MG	RA	3652	1/1	0.83	0.16	-	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3602	1/1	0.82	1.45	-	75,75,75,75	0
56	MG	RA	3847	1/1	0.66	0.62	-	103,103,103,103	0
56	MG	YA	3529	1/1	0.48	0.61	-	72,72,72,72	0
56	MG	XA	1656	1/1	0.48	0.55	-	85,85,85,85	0
56	MG	YA	3483	1/1	0.74	0.62	-	88,88,88,88	0
56	MG	QA	1850	1/1	0.88	0.37	-	78,78,78,78	0
56	MG	YA	3547	1/1	0.41	0.65	-	88,88,88,88	0
56	MG	YA	3286	1/1	0.81	0.28	-	80,80,80,80	0
56	MG	QV	103	1/1	0.72	0.48	-	86,86,86,86	0
56	MG	YA	3731	1/1	0.80	1.43	-	78,78,78,78	0
56	MG	RA	3798	1/1	0.22	0.74	-	93,93,93,93	0
56	MG	YA	3645	1/1	0.78	0.39	-	88,88,88,88	0
56	MG	RA	3199	1/1	0.66	0.64	-	81,81,81,81	0
56	MG	XA	1693	1/1	0.74	0.54	-	95,95,95,95	0
56	MG	RA	3216	1/1	0.74	0.74	-	104,104,104,104	0
56	MG	RA	3954	1/1	0.79	0.26	-	82,82,82,82	0
56	MG	RA	3636	1/1	0.39	0.19	-	94,94,94,94	0
56	MG	RA	3737	1/1	-0.24	1.18	-	84,84,84,84	0
56	MG	YA	3041	1/1	0.07	0.89	-	96,96,96,96	0
56	MG	RA	3090	1/1	0.28	0.71	-	84,84,84,84	0
56	MG	QA	1685	1/1	0.38	0.30	-	89,89,89,89	0
56	MG	RA	3663	1/1	0.43	1.20	-	103,103,103,103	0
56	MG	RA	3800	1/1	0.61	0.40	-	93,93,93,93	0
56	MG	QA	1863	1/1	0.84	0.50	-	81,81,81,81	0
56	MG	YA	3400	1/1	0.88	0.40	-	75,75,75,75	0
56	MG	RH	202	1/1	0.71	0.22	-	95,95,95,95	0
56	MG	YA	3603	1/1	0.16	1.23	-	82,82,82,82	0
56	MG	RA	3111	1/1	0.27	0.43	-	100,100,100,100	0
56	MG	RA	3782	1/1	0.63	0.90	-	99,99,99,99	0
56	MG	QA	1692	1/1	0.83	0.57	-	98,98,98,98	0
56	MG	RA	3859	1/1	0.51	1.25	-	89,89,89,89	0
56	MG	YA	3206	1/1	0.67	0.56	-	73,73,73,73	0
56	MG	RA	3133	1/1	0.75	0.57	-	85,85,85,85	0
56	MG	YA	3165	1/1	0.85	0.46	-	100,100,100,100	0
56	MG	QA	1628	1/1	0.47	0.38	-	77,77,77,77	0
56	MG	QA	1749	1/1	0.58	0.50	-	83,83,83,83	0
56	MG	YA	3179	1/1	0.51	0.59	-	102,102,102,102	0
56	MG	YA	3366	1/1	0.83	0.12	-	95,95,95,95	0
56	MG	RA	3052	1/1	0.70	0.44	-	95,95,95,95	0
56	MG	RA	3853	1/1	0.83	0.56	-	90,90,90,90	0
56	MG	QA	1674	1/1	0.53	0.35	-	94,94,94,94	0
56	MG	RA	3540	1/1	0.65	0.53	-	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3619	1/1	0.90	0.43	-	67,67,67,67	0
56	MG	RV	204	1/1	0.49	0.34	-	79,79,79,79	0
56	MG	QG	201	1/1	0.08	0.87	-	101,101,101,101	0
56	MG	RA	3908	1/1	0.76	0.74	-	92,92,92,92	0
56	MG	YA	3642	1/1	0.55	0.74	-	69,69,69,69	0
56	MG	YA	3533	1/1	0.86	0.45	-	76,76,76,76	0
56	MG	YA	3652	1/1	0.89	0.49	-	79,79,79,79	0
56	MG	RA	3319	1/1	0.90	0.80	-	69,69,69,69	0
56	MG	QA	1853	1/1	0.21	0.76	-	89,89,89,89	0
56	MG	YA	3498	1/1	0.64	0.22	-	89,89,89,89	0
56	MG	QH	201	1/1	0.13	0.51	-	87,87,87,87	0
56	MG	YA	3644	1/1	0.70	0.50	-	75,75,75,75	0
56	MG	QA	1669	1/1	0.61	0.78	-	81,81,81,81	0
56	MG	YA	3140	1/1	0.84	0.36	-	79,79,79,79	0
56	MG	RB	212	1/1	0.59	0.67	-	85,85,85,85	0
56	MG	RA	4022	1/1	0.83	0.47	-	77,77,77,77	0
56	MG	RA	3059	1/1	0.85	0.16	-	84,84,84,84	0
56	MG	QA	1640	1/1	0.20	0.71	-	99,99,99,99	0
56	MG	RA	3120	1/1	0.47	0.54	-	83,83,83,83	0
56	MG	RA	3831	1/1	0.86	0.23	-	90,90,90,90	0
56	MG	RA	3668	1/1	0.80	0.48	-	80,80,80,80	0
56	MG	RA	3985	1/1	0.89	0.53	-	70,70,70,70	0
56	MG	RA	3910	1/1	0.67	0.50	-	83,83,83,83	0
56	MG	RA	3196	1/1	0.00	0.51	-	114,114,114,114	0
56	MG	YA	3181	1/1	0.62	0.54	-	93,93,93,93	0
56	MG	R0	102	1/1	0.31	0.57	-	88,88,88,88	0
56	MG	YA	3624	1/1	0.60	0.45	-	92,92,92,92	0
56	MG	YA	3363	1/1	0.86	0.60	-	75,75,75,75	0
56	MG	RA	3799	1/1	0.75	1.02	-	82,82,82,82	0
56	MG	YA	3304	1/1	0.73	0.34	-	82,82,82,82	0
56	MG	QA	1688	1/1	0.77	1.07	-	81,81,81,81	0
56	MG	RA	3851	1/1	0.96	0.39	-	73,73,73,73	0
56	MG	YA	3726	1/1	0.95	0.74	-	85,85,85,85	0
56	MG	YA	3017	1/1	0.18	0.63	-	91,91,91,91	0
56	MG	YA	3344	1/1	0.22	0.20	-	90,90,90,90	0
56	MG	YA	3455	1/1	0.56	0.45	-	86,86,86,86	0
56	MG	RA	3641	1/1	0.77	0.33	-	79,79,79,79	0
56	MG	RA	3978	1/1	0.50	0.85	-	75,75,75,75	0
56	MG	YA	3408	1/1	0.25	0.81	-	90,90,90,90	0
56	MG	XA	1773	1/1	0.76	0.90	-	79,79,79,79	0
56	MG	YB	202	1/1	0.92	0.14	-	72,72,72,72	0
56	MG	YP	201	1/1	0.62	0.29	-	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3793	1/1	0.84	0.57	-	71,71,71,71	0
56	MG	YA	3433	1/1	-0.37	0.75	-	97,97,97,97	0
56	MG	RA	3529	1/1	0.52	0.54	-	90,90,90,90	0
56	MG	QD	301	1/1	0.33	1.26	-	94,94,94,94	0
56	MG	YA	3637	1/1	0.65	0.55	-	85,85,85,85	0
56	MG	QA	1848	1/1	0.51	0.81	-	81,81,81,81	0
56	MG	QA	1723	1/1	0.66	0.68	-	86,86,86,86	0
56	MG	RA	3703	1/1	0.30	0.49	-	95,95,95,95	0
56	MG	RA	3926	1/1	0.64	0.46	-	78,78,78,78	0
56	MG	YA	3635	1/1	0.48	0.85	-	83,83,83,83	0
56	MG	YA	3674	1/1	0.89	0.70	-	77,77,77,77	0
56	MG	RA	3219	1/1	0.37	1.35	-	88,88,88,88	0
56	MG	RE	305	1/1	0.42	0.55	-	92,92,92,92	0
56	MG	RA	3983	1/1	0.80	0.39	-	91,91,91,91	0
56	MG	RA	3418	1/1	0.96	0.17	-	64,64,64,64	0
56	MG	YD	307	1/1	0.73	0.52	-	79,79,79,79	0
56	MG	RA	3745	1/1	0.74	0.61	-	73,73,73,73	0
56	MG	YA	3359	1/1	0.92	1.02	-	62,62,62,62	0
56	MG	RA	3686	1/1	0.34	0.74	-	97,97,97,97	0
56	MG	YA	3649	1/1	0.51	0.82	-	79,79,79,79	0
56	MG	YA	3075	1/1	0.29	1.78	-	89,89,89,89	0
56	MG	RB	207	1/1	0.72	0.23	-	93,93,93,93	0
56	MG	RA	3873	1/1	0.57	0.40	-	77,77,77,77	0
56	MG	RA	3621	1/1	0.66	0.54	-	95,95,95,95	0
56	MG	YA	3467	1/1	0.71	0.79	-	76,76,76,76	0
56	MG	YA	3352	1/1	0.29	0.13	-	88,88,88,88	0
56	MG	RA	3747	1/1	0.38	1.50	-	93,93,93,93	0
56	MG	RA	3522	1/1	0.33	0.35	-	84,84,84,84	0
56	MG	YA	3250	1/1	0.29	0.37	-	103,103,103,103	0
56	MG	RA	3927	1/1	0.10	0.96	-	91,91,91,91	0
56	MG	QA	1787	1/1	0.59	0.40	-	89,89,89,89	0
56	MG	YA	3643	1/1	0.82	0.30	-	79,79,79,79	0
56	MG	YA	3441	1/1	0.60	0.58	-	80,80,80,80	0
56	MG	RA	3415	1/1	0.81	0.42	-	62,62,62,62	0
56	MG	QA	1736	1/1	-0.11	1.42	-	82,82,82,82	0
56	MG	RA	3289	1/1	0.81	0.40	-	99,99,99,99	0
56	MG	RA	3919	1/1	0.62	0.85	-	83,83,83,83	0
56	MG	RA	3127	1/1	0.93	0.50	-	81,81,81,81	0
56	MG	RA	3726	1/1	0.82	0.50	-	74,74,74,74	0
56	MG	YA	3512	1/1	0.90	0.26	-	74,74,74,74	0
56	MG	RA	3447	1/1	0.51	0.62	-	78,78,78,78	0
56	MG	QA	1697	1/1	0.17	0.69	-	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3844	1/1	0.46	0.47	-	100,100,100,100	0
56	MG	RA	3674	1/1	0.84	0.84	-	70,70,70,70	0
56	MG	QA	1833	1/1	0.55	0.38	-	106,106,106,106	0
56	MG	YA	3253	1/1	0.86	0.62	-	87,87,87,87	0
56	MG	RA	3336	1/1	0.62	0.46	-	86,86,86,86	0
56	MG	RA	3898	1/1	0.70	0.44	-	85,85,85,85	0
56	MG	RB	204	1/1	0.34	0.25	-	85,85,85,85	0
56	MG	RA	3360	1/1	0.92	0.54	-	68,68,68,68	0
56	MG	XA	1701	1/1	0.36	0.45	-	74,74,74,74	0
56	MG	RA	3591	1/1	0.88	0.70	-	92,92,92,92	0
56	MG	RA	4007	1/1	0.71	0.44	-	76,76,76,76	0
56	MG	XA	1765	1/1	0.63	1.09	-	77,77,77,77	0
56	MG	QA	1740	1/1	0.78	0.65	-	69,69,69,69	0
56	MG	RA	3086	1/1	0.61	1.22	-	111,111,111,111	0
56	MG	RB	203	1/1	-0.22	0.93	-	102,102,102,102	0
56	MG	RN	202	1/1	-0.27	2.06	-	102,102,102,102	0
56	MG	YA	3373	1/1	0.72	0.19	-	71,71,71,71	0
56	MG	RA	3632	1/1	0.65	0.90	-	88,88,88,88	0
56	MG	YA	3305	1/1	0.63	0.25	-	69,69,69,69	0
56	MG	YA	3531	1/1	0.25	1.31	-	80,80,80,80	0
56	MG	YA	3267	1/1	-0.52	1.71	-	102,102,102,102	0
56	MG	YA	3207	1/1	0.95	0.29	-	87,87,87,87	0
56	MG	QA	1748	1/1	-0.14	1.50	-	98,98,98,98	0
56	MG	RA	3999	1/1	0.18	0.43	-	98,98,98,98	0
56	MG	RA	3660	1/1	0.67	0.82	-	77,77,77,77	0
56	MG	RA	3247	1/1	0.18	0.86	-	89,89,89,89	0
56	MG	YA	3157	1/1	0.38	0.79	-	66,66,66,66	0
56	MG	RA	3429	1/1	0.79	0.25	-	98,98,98,98	0
56	MG	R1	101	1/1	0.42	0.65	-	89,89,89,89	0
56	MG	RA	3140	1/1	0.85	1.04	-	97,97,97,97	0
56	MG	RA	3828	1/1	0.13	0.49	-	84,84,84,84	0
56	MG	RA	3015	1/1	0.82	0.53	-	84,84,84,84	0
56	MG	YT	201	1/1	0.78	0.74	-	85,85,85,85	0
56	MG	RA	3171	1/1	-0.40	0.93	-	92,92,92,92	0
56	MG	QA	1838	1/1	0.24	0.51	-	87,87,87,87	0
56	MG	RA	3209	1/1	0.72	0.38	-	88,88,88,88	0
56	MG	RA	3787	1/1	0.16	0.79	-	88,88,88,88	0
56	MG	XA	1650	1/1	0.62	0.30	-	87,87,87,87	0
56	MG	RA	3398	1/1	0.23	0.73	-	80,80,80,80	0
56	MG	YE	307	1/1	0.90	0.35	-	85,85,85,85	0
56	MG	YA	3438	1/1	0.73	0.55	-	80,80,80,80	0
56	MG	YA	3713	1/1	0.50	0.63	-	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3763	1/1	0.65	0.27	-	77,77,77,77	0
56	MG	RA	3943	1/1	0.35	0.63	-	91,91,91,91	0
56	MG	RA	3287	1/1	0.91	0.60	-	102,102,102,102	0
56	MG	RA	3720	1/1	0.84	0.44	-	73,73,73,73	0
56	MG	RA	3734	1/1	0.43	0.59	-	85,85,85,85	0
56	MG	QA	1868	1/1	0.52	1.40	-	82,82,82,82	0
56	MG	YA	3023	1/1	0.92	0.17	-	80,80,80,80	0
56	MG	RA	3461	1/1	0.78	1.48	-	84,84,84,84	0
56	MG	RA	3478	1/1	0.77	0.68	-	78,78,78,78	0
56	MG	RA	4069	1/1	-0.29	1.52	-	86,86,86,86	0
56	MG	RA	3355	1/1	0.97	0.07	-	88,88,88,88	0
56	MG	QA	1797	1/1	0.82	0.51	-	75,75,75,75	0
56	MG	YA	3136	1/1	0.94	0.33	-	65,65,65,65	0
56	MG	RA	3268	1/1	0.96	0.32	-	79,79,79,79	0
56	MG	YA	3454	1/1	0.79	0.36	-	94,94,94,94	0
56	MG	YA	3117	1/1	0.79	0.45	-	87,87,87,87	0
56	MG	RA	3573	1/1	0.71	0.53	-	88,88,88,88	0
56	MG	XA	1708	1/1	0.85	0.82	-	75,75,75,75	0
56	MG	YA	3638	1/1	0.62	0.85	-	64,64,64,64	0
56	MG	YA	3255	1/1	0.65	0.46	-	81,81,81,81	0
56	MG	YA	3682	1/1	0.90	0.41	-	62,62,62,62	0
56	MG	YA	3501	1/1	0.55	1.03	-	74,74,74,74	0
56	MG	RA	3582	1/1	0.39	0.77	-	87,87,87,87	0
56	MG	QA	1710	1/1	0.70	0.64	-	74,74,74,74	0
56	MG	YA	3196	1/1	0.54	0.70	-	91,91,91,91	0
56	MG	QA	1699	1/1	0.84	0.20	-	89,89,89,89	0
56	MG	RA	3946	1/1	0.90	0.86	-	67,67,67,67	0
56	MG	QA	1859	1/1	0.37	0.81	-	85,85,85,85	0
56	MG	YA	3661	1/1	0.91	0.62	-	73,73,73,73	0
56	MG	XA	1751	1/1	0.87	0.23	-	87,87,87,87	0
56	MG	XA	1754	1/1	-0.15	1.24	-	88,88,88,88	0
56	MG	YA	3494	1/1	0.94	0.41	-	64,64,64,64	0
56	MG	XF	203	1/1	0.21	2.52	-	103,103,103,103	0
56	MG	YA	3543	1/1	0.80	0.34	-	80,80,80,80	0
56	MG	RA	3262	1/1	0.76	0.18	-	83,83,83,83	0
56	MG	YA	3651	1/1	0.70	0.64	-	78,78,78,78	0
56	MG	YA	3167	1/1	0.10	1.03	-	87,87,87,87	0
56	MG	RA	3039	1/1	-0.09	1.09	-	97,97,97,97	0
56	MG	QA	1745	1/1	-0.04	0.89	-	82,82,82,82	0
56	MG	RA	3481	1/1	0.73	0.67	-	71,71,71,71	0
56	MG	RA	3516	1/1	0.94	0.49	-	84,84,84,84	0
56	MG	XA	1771	1/1	0.80	0.95	-	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1789	1/1	0.77	0.37	-	85,85,85,85	0
56	MG	RA	3752	1/1	0.71	0.58	-	85,85,85,85	0
56	MG	RA	3249	1/1	0.81	0.46	-	99,99,99,99	0
56	MG	RA	4010	1/1	0.31	1.61	-	79,79,79,79	0
56	MG	RA	3388	1/1	0.73	0.75	-	96,96,96,96	0
56	MG	RA	3552	1/1	0.47	0.73	-	93,93,93,93	0
56	MG	YA	3459	1/1	0.85	0.29	-	63,63,63,63	0
56	MG	RA	3657	1/1	0.83	1.07	-	70,70,70,70	0
56	MG	YA	3211	1/1	0.04	1.03	-	98,98,98,98	0
56	MG	RA	3825	1/1	0.23	0.83	-	85,85,85,85	0
56	MG	RA	3320	1/1	0.92	0.57	-	62,62,62,62	0
56	MG	RA	3149	1/1	0.62	0.59	-	73,73,73,73	0
56	MG	QA	1820	1/1	0.67	0.41	-	76,76,76,76	0
56	MG	QA	1663	1/1	0.87	0.23	-	90,90,90,90	0
56	MG	YA	3418	1/1	0.72	0.69	-	90,90,90,90	0
56	MG	RA	3698	1/1	0.69	0.53	-	87,87,87,87	0
56	MG	RA	3383	1/1	0.90	0.35	-	63,63,63,63	0
56	MG	RQ	203	1/1	0.29	0.84	-	96,96,96,96	0
56	MG	XA	1674	1/1	-0.17	1.36	-	94,94,94,94	0
56	MG	QA	1603	1/1	0.74	0.46	-	86,86,86,86	0
56	MG	YB	206	1/1	0.13	0.86	-	89,89,89,89	0
56	MG	XA	1706	1/1	0.81	0.14	-	78,78,78,78	0
56	MG	RA	3162	1/1	0.92	0.70	-	83,83,83,83	0
56	MG	QA	1856	1/1	0.65	0.57	-	94,94,94,94	0
56	MG	YA	3521	1/1	0.54	0.53	-	97,97,97,97	0
56	MG	QA	1873	1/1	-0.34	1.75	-	91,91,91,91	0
56	MG	XA	1682	1/1	0.57	0.71	-	83,83,83,83	0
56	MG	YA	3076	1/1	0.67	0.52	-	92,92,92,92	0
56	MG	XA	1607	1/1	0.81	0.28	-	95,95,95,95	0
56	MG	YA	3180	1/1	0.71	0.28	-	73,73,73,73	0
56	MG	RA	3605	1/1	0.80	0.58	-	90,90,90,90	0
56	MG	QA	1728	1/1	0.20	0.35	-	80,80,80,80	0
56	MG	YA	3357	1/1	0.79	1.26	-	78,78,78,78	0
56	MG	YA	3123	1/1	0.63	0.70	-	105,105,105,105	0
56	MG	QA	1753	1/1	0.39	0.61	-	87,87,87,87	0
56	MG	YA	3026	1/1	0.57	0.54	-	84,84,84,84	0
56	MG	YA	3238	1/1	0.74	0.45	-	100,100,100,100	0
56	MG	RA	3013	1/1	0.42	0.68	-	83,83,83,83	0
56	MG	RA	3106	1/1	0.16	0.56	-	107,107,107,107	0
56	MG	RA	3002	1/1	0.83	0.34	-	67,67,67,67	0
56	MG	RA	3139	1/1	0.81	0.45	-	89,89,89,89	0
56	MG	RA	3160	1/1	0.81	0.94	-	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3239	1/1	0.80	0.53	-	98,98,98,98	0
56	MG	YA	3109	1/1	0.28	0.62	-	85,85,85,85	0
56	MG	RA	3776	1/1	0.62	0.69	-	86,86,86,86	0
56	MG	RA	3723	1/1	0.50	0.38	-	79,79,79,79	0
56	MG	RA	3973	1/1	0.88	0.82	-	99,99,99,99	0
56	MG	YA	3346	1/1	0.74	0.52	-	79,79,79,79	0
56	MG	YA	3640	1/1	0.62	1.02	-	70,70,70,70	0
56	MG	QA	1726	1/1	0.84	0.53	-	88,88,88,88	0
56	MG	RA	3731	1/1	0.97	0.31	-	74,74,74,74	0
56	MG	RA	3976	1/1	0.83	0.34	-	76,76,76,76	0
56	MG	YA	3426	1/1	0.85	0.33	-	72,72,72,72	0
56	MG	RA	3365	1/1	0.15	0.61	-	88,88,88,88	0
56	MG	YA	3700	1/1	0.96	0.43	-	64,64,64,64	0
56	MG	YA	3492	1/1	0.97	0.81	-	62,62,62,62	0
56	MG	YA	3205	1/1	0.01	2.40	-	86,86,86,86	0
56	MG	RA	3277	1/1	0.89	0.34	-	85,85,85,85	0
56	MG	R5	102	1/1	-0.15	0.53	-	97,97,97,97	0
56	MG	R9	103	1/1	0.70	0.47	-	93,93,93,93	0
56	MG	YA	3312	1/1	0.14	1.26	-	80,80,80,80	0
56	MG	YA	3014	1/1	0.95	0.19	-	82,82,82,82	0
56	MG	RA	3762	1/1	0.98	0.58	-	65,65,65,65	0
56	MG	RA	3425	1/1	0.08	1.09	-	91,91,91,91	0
56	MG	RA	3099	1/1	0.28	0.66	-	94,94,94,94	0
56	MG	RB	224	1/1	0.42	0.86	-	86,86,86,86	0
56	MG	RA	3545	1/1	0.84	0.34	-	85,85,85,85	0
56	MG	XA	1651	1/1	0.31	1.56	-	96,96,96,96	0
56	MG	RA	4000	1/1	0.48	0.64	-	95,95,95,95	0
56	MG	RA	3428	1/1	0.24	0.81	-	92,92,92,92	0
56	MG	YG	201	1/1	-0.61	2.04	-	103,103,103,103	0
56	MG	QA	1778	1/1	0.38	0.67	-	88,88,88,88	0
56	MG	YA	3460	1/1	0.69	0.38	-	85,85,85,85	0
56	MG	QA	1790	1/1	0.77	0.40	-	81,81,81,81	0
56	MG	YA	3329	1/1	0.93	0.46	-	62,62,62,62	0
56	MG	XA	1743	1/1	0.52	0.54	-	89,89,89,89	0
56	MG	YA	3164	1/1	0.04	1.20	-	98,98,98,98	0
56	MG	RA	4054	1/1	0.17	1.94	-	91,91,91,91	0
56	MG	RA	3173	1/1	0.65	0.54	-	90,90,90,90	0
56	MG	YI	201	1/1	0.07	0.36	-	94,94,94,94	0
56	MG	YA	3308	1/1	-0.13	1.09	-	92,92,92,92	0
56	MG	RA	3201	1/1	0.84	0.54	-	96,96,96,96	0
56	MG	RA	3215	1/1	0.47	0.75	-	90,90,90,90	0
56	MG	YA	3537	1/1	0.94	0.50	-	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3083	1/1	0.39	0.32	-	90,90,90,90	0
56	MG	YA	3002	1/1	0.93	0.19	-	75,75,75,75	0
56	MG	QA	1678	1/1	0.81	0.32	-	93,93,93,93	0
56	MG	YA	3356	1/1	0.00	0.28	-	85,85,85,85	0
56	MG	RA	3546	1/1	0.37	0.56	-	95,95,95,95	0
56	MG	RA	3413	1/1	0.74	0.52	-	83,83,83,83	0
56	MG	RA	3397	1/1	0.37	0.69	-	76,76,76,76	0
56	MG	XA	1735	1/1	0.78	0.24	-	83,83,83,83	0
56	MG	YA	3557	1/1	0.74	0.58	-	66,66,66,66	0
56	MG	RA	3739	1/1	0.90	0.40	-	69,69,69,69	0
56	MG	QA	1878	1/1	0.92	0.21	-	98,98,98,98	0
56	MG	RA	3838	1/1	0.73	0.54	-	77,77,77,77	0
56	MG	QA	1722	1/1	-0.51	0.98	-	93,93,93,93	0
56	MG	QI	201	1/1	0.38	1.13	-	100,100,100,100	0
56	MG	YA	3568	1/1	0.93	0.45	-	63,63,63,63	0
56	MG	RB	221	1/1	0.83	0.23	-	84,84,84,84	0
56	MG	QA	1841	1/1	0.46	0.37	-	94,94,94,94	0
56	MG	RA	3933	1/1	0.76	0.61	-	84,84,84,84	0
56	MG	RA	3878	1/1	0.94	0.37	-	62,62,62,62	0
56	MG	YA	3567	1/1	0.94	0.65	-	62,62,62,62	0
56	MG	RA	3543	1/1	0.61	0.41	-	83,83,83,83	0
56	MG	QA	1757	1/1	-0.10	0.58	-	102,102,102,102	0
56	MG	RA	3912	1/1	0.89	0.27	-	78,78,78,78	0
56	MG	RA	3789	1/1	0.70	0.23	-	80,80,80,80	0
56	MG	YA	3362	1/1	0.84	0.64	-	70,70,70,70	0
56	MG	QA	1807	1/1	0.26	0.56	-	95,95,95,95	0
56	MG	YA	3108	1/1	0.29	0.62	-	90,90,90,90	0
56	MG	RA	3620	1/1	0.97	0.81	-	81,81,81,81	0
56	MG	RA	3214	1/1	0.95	0.33	-	86,86,86,86	0
56	MG	RA	3204	1/1	0.68	0.61	-	103,103,103,103	0
56	MG	Y1	102	1/1	0.67	0.36	-	87,87,87,87	0
56	MG	RA	3989	1/1	0.70	0.75	-	84,84,84,84	0
56	MG	RA	3417	1/1	0.61	0.30	-	89,89,89,89	0
56	MG	RA	3078	1/1	0.85	0.85	-	90,90,90,90	0
56	MG	RA	3097	1/1	0.67	1.29	-	90,90,90,90	0
56	MG	QA	1756	1/1	0.72	0.75	-	80,80,80,80	0
56	MG	QA	1617	1/1	0.81	0.34	-	98,98,98,98	0
56	MG	RA	3068	1/1	0.80	0.48	-	91,91,91,91	0
56	MG	RA	3775	1/1	0.37	1.33	-	94,94,94,94	0
56	MG	RA	3594	1/1	0.95	0.50	-	80,80,80,80	0
56	MG	RA	3459	1/1	0.66	0.38	-	88,88,88,88	0
56	MG	YA	3235	1/1	0.79	0.45	-	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1630	1/1	0.38	1.44	-	79,79,79,79	0
56	MG	QA	1720	1/1	0.70	0.87	-	85,85,85,85	0
56	MG	YA	3190	1/1	0.48	0.69	-	92,92,92,92	0
56	MG	RA	3456	1/1	0.46	0.45	-	71,71,71,71	0
56	MG	RA	3410	1/1	0.90	0.69	-	70,70,70,70	0
56	MG	YA	3006	1/1	0.50	0.62	-	82,82,82,82	0
56	MG	YA	3195	1/1	0.68	0.31	-	89,89,89,89	0
56	MG	YA	3313	1/1	0.49	0.67	-	89,89,89,89	0
56	MG	RA	3741	1/1	0.39	0.80	-	92,92,92,92	0
56	MG	XA	1614	1/1	0.81	0.19	-	77,77,77,77	0
56	MG	YA	3590	1/1	0.90	0.38	-	65,65,65,65	0
56	MG	RA	3509	1/1	0.81	0.46	-	81,81,81,81	0
56	MG	RA	3955	1/1	0.39	0.88	-	90,90,90,90	0
56	MG	YA	3541	1/1	0.25	0.43	-	94,94,94,94	0
56	MG	YA	3154	1/1	0.79	0.52	-	81,81,81,81	0
56	MG	XA	1691	1/1	0.25	0.40	-	84,84,84,84	0
56	MG	RA	3284	1/1	0.66	0.69	-	87,87,87,87	0
56	MG	RA	3586	1/1	0.41	0.68	-	76,76,76,76	0
56	MG	XA	1782	1/1	0.39	1.41	-	79,79,79,79	0
56	MG	RA	3167	1/1	0.74	0.26	-	84,84,84,84	0
56	MG	RA	3597	1/1	0.57	0.74	-	89,89,89,89	0
56	MG	RA	3503	1/1	0.95	0.47	-	65,65,65,65	0
56	MG	YA	3489	1/1	0.56	0.40	-	77,77,77,77	0
56	MG	QA	1826	1/1	0.88	0.98	-	110,110,110,110	0
56	MG	YA	3618	1/1	0.79	0.80	-	82,82,82,82	0
56	MG	RA	3339	1/1	0.76	0.74	-	86,86,86,86	0
56	MG	YA	3251	1/1	0.71	0.49	-	93,93,93,93	0
56	MG	RA	3549	1/1	0.94	0.44	-	76,76,76,76	0
56	MG	YA	3458	1/1	-0.04	1.00	-	88,88,88,88	0
56	MG	YA	3009	1/1	0.93	0.22	-	70,70,70,70	0
56	MG	YA	3739	1/1	0.25	0.77	-	75,75,75,75	0
56	MG	YA	3722	1/1	0.28	0.89	-	93,93,93,93	0
56	MG	XA	1722	1/1	0.56	0.68	-	88,88,88,88	0
56	MG	RA	3913	1/1	0.71	0.73	-	94,94,94,94	0
56	MG	RA	3259	1/1	0.56	0.74	-	86,86,86,86	0
56	MG	QA	1725	1/1	0.84	0.40	-	76,76,76,76	0
56	MG	YW	202	1/1	0.65	0.41	-	81,81,81,81	0
56	MG	YA	3743	1/1	0.87	0.42	-	63,63,63,63	0
56	MG	RA	3313	1/1	0.91	0.72	-	63,63,63,63	0
56	MG	YA	3038	1/1	0.92	0.48	-	77,77,77,77	0
56	MG	RF	310	1/1	0.66	0.68	-	78,78,78,78	0
56	MG	YA	3574	1/1	0.31	0.82	-	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3223	1/1	0.59	0.44	-	65,65,65,65	0
56	MG	RA	3690	1/1	0.07	0.84	-	90,90,90,90	0
56	MG	YA	3276	1/1	0.51	0.32	-	77,77,77,77	0
56	MG	YA	3639	1/1	0.89	0.77	-	65,65,65,65	0
56	MG	QA	1709	1/1	0.80	0.22	-	90,90,90,90	0
56	MG	RA	3884	1/1	0.87	0.29	-	96,96,96,96	0
56	MG	RA	3876	1/1	0.19	0.90	-	92,92,92,92	0
56	MG	YA	3592	1/1	0.81	0.32	-	78,78,78,78	0
56	MG	YA	3119	1/1	0.53	0.74	-	68,68,68,68	0
56	MG	RA	3633	1/1	0.64	0.45	-	93,93,93,93	0
56	MG	YA	3502	1/1	0.84	0.29	-	71,71,71,71	0
56	MG	QA	1794	1/1	0.29	0.79	-	72,72,72,72	0
56	MG	RA	3836	1/1	0.68	0.50	-	73,73,73,73	0
56	MG	RA	4014	1/1	0.87	0.32	-	79,79,79,79	0
56	MG	YA	3260	1/1	0.88	0.56	-	95,95,95,95	0
56	MG	R3	101	1/1	-0.07	1.30	-	87,87,87,87	0
56	MG	XA	1710	1/1	0.39	0.33	-	78,78,78,78	0
56	MG	RZ	301	1/1	0.56	0.73	-	87,87,87,87	0
56	MG	YA	3482	1/1	0.94	0.85	-	62,62,62,62	0
56	MG	RV	201	1/1	0.36	0.30	-	100,100,100,100	0
56	MG	XA	1755	1/1	0.60	0.75	-	87,87,87,87	0
56	MG	YA	3505	1/1	0.24	0.76	-	88,88,88,88	0
56	MG	QA	1729	1/1	0.58	0.68	-	87,87,87,87	0
56	MG	YA	3068	1/1	0.82	0.40	-	79,79,79,79	0
56	MG	YA	3436	1/1	0.84	0.50	-	65,65,65,65	0
56	MG	RA	3067	1/1	-0.21	1.47	-	100,100,100,100	0
56	MG	YA	3434	1/1	0.93	0.45	-	72,72,72,72	0
56	MG	YA	3525	1/1	0.02	1.06	-	88,88,88,88	0
56	MG	RA	3683	1/1	0.69	0.32	-	85,85,85,85	0
56	MG	YA	3100	1/1	0.90	0.33	-	78,78,78,78	0
56	MG	RA	3445	1/1	0.45	0.95	-	81,81,81,81	0
56	MG	RA	3796	1/1	0.65	0.57	-	90,90,90,90	0
56	MG	QA	1846	1/1	0.65	0.28	-	92,92,92,92	0
56	MG	RA	3066	1/1	0.12	0.78	-	104,104,104,104	0
56	MG	YA	3315	1/1	0.97	0.41	-	64,64,64,64	0
56	MG	YA	3191	1/1	0.78	0.46	-	86,86,86,86	0
56	MG	YA	3626	1/1	0.93	0.70	-	62,62,62,62	0
56	MG	RB	218	1/1	0.67	0.49	-	86,86,86,86	0
56	MG	QA	1844	1/1	0.82	0.32	-	100,100,100,100	0
56	MG	YA	3695	1/1	-0.31	1.27	-	88,88,88,88	0
56	MG	QM	201	1/1	0.53	0.29	-	91,91,91,91	0
56	MG	RA	3676	1/1	0.33	0.29	-	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3462	1/1	0.31	0.86	-	97,97,97,97	0
56	MG	XA	1698	1/1	-0.09	1.09	-	87,87,87,87	0
56	MG	YA	3301	1/1	0.70	0.83	-	74,74,74,74	0
56	MG	YN	201	1/1	0.38	1.56	-	90,90,90,90	0
56	MG	QA	1775	1/1	0.71	0.44	-	91,91,91,91	0
56	MG	RA	3174	1/1	0.28	1.00	-	85,85,85,85	0
56	MG	YA	3103	1/1	0.90	0.32	-	67,67,67,67	0
56	MG	YA	3395	1/1	0.90	0.29	-	63,63,63,63	0
56	MG	RA	3007	1/1	0.59	0.39	-	75,75,75,75	0
56	MG	YA	3563	1/1	0.73	0.27	-	72,72,72,72	0
56	MG	YA	3372	1/1	0.84	0.46	-	69,69,69,69	0
56	MG	XA	1606	1/1	0.81	0.32	-	90,90,90,90	0
56	MG	RA	3495	1/1	0.20	0.84	-	83,83,83,83	0
56	MG	XA	1783	1/1	0.50	0.47	-	97,97,97,97	0
56	MG	RB	202	1/1	0.93	0.26	-	80,80,80,80	0
56	MG	YA	3045	1/1	0.84	0.26	-	64,64,64,64	0
56	MG	YA	3428	1/1	0.47	0.56	-	104,104,104,104	0
56	MG	QA	1862	1/1	0.13	0.67	-	82,82,82,82	0
56	MG	RA	3369	1/1	0.68	1.87	-	79,79,79,79	0
56	MG	RA	3711	1/1	0.57	0.89	-	88,88,88,88	0
56	MG	RA	3453	1/1	0.46	0.30	-	82,82,82,82	0
56	MG	YA	3698	1/1	0.76	0.80	-	76,76,76,76	0
56	MG	QA	1821	1/1	0.39	0.78	-	89,89,89,89	0
56	MG	RB	211	1/1	0.24	0.45	-	89,89,89,89	0
56	MG	RA	3583	1/1	0.59	0.95	-	79,79,79,79	0
56	MG	YA	3469	1/1	0.19	0.62	-	91,91,91,91	0
56	MG	YA	3634	1/1	0.84	0.40	-	86,86,86,86	0
56	MG	YA	3264	1/1	0.65	0.34	-	93,93,93,93	0
56	MG	XA	1667	1/1	0.66	1.22	-	83,83,83,83	0
56	MG	XA	1778	1/1	0.75	0.85	-	70,70,70,70	0
56	MG	YA	3282	1/1	0.90	0.64	-	62,62,62,62	0
56	MG	RB	228	1/1	0.74	0.70	-	92,92,92,92	0
56	MG	YA	3093	1/1	0.70	0.37	-	86,86,86,86	0
56	MG	RA	3065	1/1	0.66	0.45	-	92,92,92,92	0
56	MG	YB	215	1/1	0.77	0.23	-	79,79,79,79	0
56	MG	YA	3101	1/1	0.62	0.38	-	92,92,92,92	0
56	MG	RA	3304	1/1	0.82	0.68	-	76,76,76,76	0
56	MG	RA	3968	1/1	-0.01	0.98	-	84,84,84,84	0
56	MG	RA	3296	1/1	0.13	0.69	-	91,91,91,91	0
56	MG	YA	3523	1/1	0.66	0.69	-	72,72,72,72	0
56	MG	RA	3074	1/1	0.65	0.44	-	69,69,69,69	0
56	MG	RA	3627	1/1	0.72	0.37	-	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3539	1/1	0.91	0.75	-	72,72,72,72	0
56	MG	RA	3375	1/1	0.46	0.53	-	98,98,98,98	0
56	MG	XA	1702	1/1	0.51	0.54	-	75,75,75,75	0
56	MG	YA	3132	1/1	0.70	0.38	-	93,93,93,93	0
56	MG	RA	3653	1/1	-0.03	1.12	-	100,100,100,100	0
56	MG	YA	3161	1/1	-0.10	1.02	-	91,91,91,91	0
56	MG	YA	3265	1/1	0.55	0.54	-	77,77,77,77	0
56	MG	XA	1732	1/1	0.94	0.53	-	87,87,87,87	0
56	MG	YA	3354	1/1	0.66	0.52	-	84,84,84,84	0
56	MG	XA	1642	1/1	0.88	0.61	-	84,84,84,84	0
56	MG	RA	3089	1/1	0.87	0.14	-	91,91,91,91	0
56	MG	QA	1609	1/1	0.72	0.20	-	95,95,95,95	0
56	MG	YA	3263	1/1	0.74	0.52	-	70,70,70,70	0
56	MG	YA	3149	1/1	0.91	0.86	-	95,95,95,95	0
56	MG	RA	3493	1/1	0.91	0.59	-	70,70,70,70	0
56	MG	YA	3735	1/1	0.56	0.59	-	85,85,85,85	0
56	MG	RA	3977	1/1	0.45	0.43	-	89,89,89,89	0
56	MG	R4	102	1/1	-0.26	0.53	-	97,97,97,97	0
56	MG	YA	3675	1/1	0.79	0.64	-	68,68,68,68	0
56	MG	RA	3778	1/1	0.16	0.48	-	105,105,105,105	0
56	MG	RA	3184	1/1	0.43	0.32	-	92,92,92,92	0
56	MG	QA	1633	1/1	0.82	0.15	-	84,84,84,84	0
56	MG	RA	3669	1/1	0.75	0.56	-	68,68,68,68	0
56	MG	RA	3840	1/1	0.21	1.97	-	97,97,97,97	0
56	MG	QA	1601	1/1	0.65	0.39	-	101,101,101,101	0
56	MG	YA	3723	1/1	0.12	1.35	-	89,89,89,89	0
56	MG	YA	3178	1/1	0.58	0.61	-	78,78,78,78	0
56	MG	QA	1784	1/1	0.52	0.36	-	96,96,96,96	0
56	MG	RA	3693	1/1	0.19	1.00	-	102,102,102,102	0
56	MG	QA	1750	1/1	0.84	0.24	-	69,69,69,69	0
56	MG	QA	1836	1/1	0.78	0.42	-	77,77,77,77	0
56	MG	YA	3370	1/1	0.84	0.41	-	66,66,66,66	0
56	MG	YA	3310	1/1	0.63	2.02	-	80,80,80,80	0
56	MG	QA	1761	1/1	0.93	0.14	-	88,88,88,88	0
56	MG	QA	1660	1/1	0.49	0.16	-	81,81,81,81	0
56	MG	YA	3072	1/1	0.89	0.52	-	100,100,100,100	0
56	MG	QA	1791	1/1	0.80	0.27	-	89,89,89,89	0
56	MG	RA	3112	1/1	0.49	0.76	-	96,96,96,96	0
56	MG	RA	3175	1/1	0.94	0.68	-	78,78,78,78	0
56	MG	YA	3416	1/1	0.75	0.46	-	75,75,75,75	0
56	MG	RA	3115	1/1	0.24	0.41	-	78,78,78,78	0
56	MG	RA	3110	1/1	0.84	0.75	-	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1643	1/1	0.57	0.70	-	86,86,86,86	0
56	MG	YA	3379	1/1	0.94	0.27	-	73,73,73,73	0
56	MG	QA	1798	1/1	0.89	0.20	-	89,89,89,89	0
56	MG	YA	3524	1/1	0.14	0.84	-	85,85,85,85	0
56	MG	RA	3544	1/1	0.84	0.39	-	65,65,65,65	0
56	MG	RA	3781	1/1	0.64	0.71	-	90,90,90,90	0
56	MG	QA	1876	1/1	0.88	0.28	-	80,80,80,80	0
56	MG	YA	3546	1/1	0.84	0.77	-	75,75,75,75	0
56	MG	YO	202	1/1	0.48	0.20	-	81,81,81,81	0
56	MG	RA	3666	1/1	0.65	0.56	-	80,80,80,80	0
56	MG	QA	1852	1/1	-0.10	1.02	-	84,84,84,84	0
56	MG	YA	3258	1/1	0.27	0.71	-	86,86,86,86	0
56	MG	RR	203	1/1	0.09	0.46	-	81,81,81,81	0
56	MG	XA	1712	1/1	-0.11	0.72	-	96,96,96,96	0
56	MG	YA	3050	1/1	0.05	0.68	-	92,92,92,92	0
56	MG	QA	1865	1/1	0.68	0.81	-	98,98,98,98	0
56	MG	RA	3694	1/1	0.45	0.50	-	93,93,93,93	0
56	MG	XA	1775	1/1	0.33	0.72	-	98,98,98,98	0
56	MG	RA	3341	1/1	0.76	0.82	-	73,73,73,73	0
56	MG	YA	3393	1/1	0.52	0.60	-	89,89,89,89	0
56	MG	YA	3256	1/1	0.88	0.21	-	85,85,85,85	0
56	MG	RA	3835	1/1	0.61	0.53	-	89,89,89,89	0
56	MG	RB	223	1/1	0.62	1.10	-	96,96,96,96	0
56	MG	RA	3994	1/1	0.45	0.17	-	91,91,91,91	0
56	MG	RA	3137	1/1	0.32	1.17	-	102,102,102,102	0
56	MG	RA	3343	1/1	0.80	0.29	-	80,80,80,80	0
56	MG	RA	3246	1/1	0.34	0.75	-	84,84,84,84	0
56	MG	YA	3070	1/1	0.06	0.72	-	99,99,99,99	0
56	MG	XA	1788	1/1	0.37	0.67	-	95,95,95,95	0
56	MG	RA	3841	1/1	0.20	0.95	-	91,91,91,91	0
56	MG	RA	3877	1/1	0.87	0.88	-	74,74,74,74	0
56	MG	YA	3078	1/1	-0.24	0.65	-	97,97,97,97	0
56	MG	RA	3834	1/1	0.87	0.91	-	63,63,63,63	0
56	MG	RA	3964	1/1	0.40	2.04	-	104,104,104,104	0
56	MG	YA	3087	1/1	0.98	0.36	-	100,100,100,100	0
56	MG	RA	3210	1/1	0.77	2.13	-	110,110,110,110	0
56	MG	XA	1752	1/1	0.87	0.59	-	81,81,81,81	0
56	MG	YA	3046	1/1	0.87	0.32	-	82,82,82,82	0
56	MG	RA	3490	1/1	0.87	0.52	-	67,67,67,67	0
56	MG	RA	3060	1/1	0.96	0.22	-	83,83,83,83	0
56	MG	RA	3991	1/1	0.49	0.63	-	75,75,75,75	0
56	MG	RA	3291	1/1	0.73	0.38	-	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1636	1/1	0.16	0.55	-	90,90,90,90	0
56	MG	XA	1649	1/1	0.62	0.46	-	94,94,94,94	0
56	MG	YA	3452	1/1	0.19	0.88	-	84,84,84,84	0
56	MG	QA	1735	1/1	0.37	0.58	-	93,93,93,93	0
56	MG	YA	3734	1/1	0.70	0.42	-	83,83,83,83	0
56	MG	YA	3145	1/1	0.86	0.25	-	88,88,88,88	0
56	MG	RA	3916	1/1	0.93	0.32	-	71,71,71,71	0
56	MG	YA	3185	1/1	0.23	0.67	-	99,99,99,99	0
56	MG	YA	3342	1/1	0.86	0.68	-	62,62,62,62	0
56	MG	YA	3029	1/1	0.87	0.62	-	62,62,62,62	0
56	MG	YA	3271	1/1	0.90	0.90	-	67,67,67,67	0
56	MG	XA	1686	1/1	0.32	0.65	-	96,96,96,96	0
56	MG	RA	3768	1/1	0.83	0.53	-	74,74,74,74	0
56	MG	RA	3434	1/1	0.28	0.60	-	85,85,85,85	0
56	MG	RA	3317	1/1	0.67	0.46	-	82,82,82,82	0
56	MG	RA	3254	1/1	0.58	0.44	-	105,105,105,105	0
56	MG	YA	3048	1/1	0.79	0.32	-	98,98,98,98	0
56	MG	XA	1630	1/1	0.89	0.20	-	64,64,64,64	0
56	MG	QA	1668	1/1	-0.01	0.85	-	92,92,92,92	0
56	MG	YA	3703	1/1	0.86	0.44	-	90,90,90,90	0
56	MG	YA	3300	1/1	0.65	0.47	-	91,91,91,91	0
56	MG	YA	3593	1/1	0.81	0.60	-	87,87,87,87	0
56	MG	RB	214	1/1	0.60	0.64	-	67,67,67,67	0
56	MG	RA	3560	1/1	0.48	0.56	-	97,97,97,97	0
56	MG	RA	3756	1/1	0.70	0.53	-	73,73,73,73	0
56	MG	RA	3017	1/1	0.96	0.90	-	82,82,82,82	0
56	MG	XA	1704	1/1	0.57	0.51	-	90,90,90,90	0
56	MG	RA	3303	1/1	0.39	0.56	-	92,92,92,92	0
56	MG	YB	201	1/1	0.44	0.63	-	103,103,103,103	0
56	MG	YA	3506	1/1	0.06	1.07	-	95,95,95,95	0
56	MG	RG	202	1/1	0.86	0.07	-	86,86,86,86	0
56	MG	QA	1795	1/1	-0.18	1.27	-	97,97,97,97	0
56	MG	RA	3306	1/1	0.68	1.03	-	97,97,97,97	0
56	MG	RA	3080	1/1	0.92	0.83	-	98,98,98,98	0
56	MG	RA	3922	1/1	0.64	0.64	-	80,80,80,80	0
56	MG	RA	3718	1/1	0.83	0.84	-	65,65,65,65	0
56	MG	YA	3405	1/1	0.87	0.52	-	71,71,71,71	0
56	MG	RA	3047	1/1	0.38	0.34	-	66,66,66,66	0
56	MG	RA	3446	1/1	0.48	1.01	-	77,77,77,77	0
56	MG	RA	3244	1/1	0.08	1.24	-	98,98,98,98	0
56	MG	RA	3557	1/1	0.49	0.40	-	94,94,94,94	0
56	MG	RA	3777	1/1	0.80	0.34	-	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3163	1/1	-0.24	2.13	-	99,99,99,99	0
56	MG	RA	3592	1/1	0.47	0.67	-	93,93,93,93	0
56	MG	RA	3987	1/1	0.85	0.79	-	79,79,79,79	0
56	MG	YA	3585	1/1	0.92	0.64	-	64,64,64,64	0
56	MG	RA	3448	1/1	0.08	1.18	-	87,87,87,87	0
56	MG	YA	3296	1/1	0.87	0.63	-	62,62,62,62	0
56	MG	QA	1666	1/1	0.65	0.42	-	96,96,96,96	0
56	MG	YA	3496	1/1	0.34	1.39	-	85,85,85,85	0
56	MG	YA	3018	1/1	0.67	0.41	-	97,97,97,97	0
56	MG	RA	3755	1/1	0.79	1.16	-	100,100,100,100	0
56	MG	YA	3559	1/1	0.88	0.33	-	80,80,80,80	0
56	MG	RA	3372	1/1	0.91	0.23	-	87,87,87,87	0
56	MG	QA	1714	1/1	0.63	0.57	-	82,82,82,82	0
56	MG	RA	3260	1/1	0.93	0.16	-	99,99,99,99	0
56	MG	YA	3171	1/1	0.52	0.55	-	90,90,90,90	0
56	MG	YA	3065	1/1	0.94	0.85	-	86,86,86,86	0
56	MG	RA	3189	1/1	0.43	1.91	-	109,109,109,109	0
56	MG	RA	3338	1/1	0.79	0.74	-	62,62,62,62	0
56	MG	YA	3380	1/1	0.82	0.47	-	83,83,83,83	0
56	MG	R0	104	1/1	0.76	0.49	-	86,86,86,86	0
56	MG	XA	1739	1/1	0.86	0.73	-	82,82,82,82	0
56	MG	RA	3325	1/1	0.93	0.33	-	77,77,77,77	0
56	MG	XE	202	1/1	0.71	0.14	-	94,94,94,94	0
56	MG	RA	3843	1/1	0.43	0.67	-	88,88,88,88	0
56	MG	YA	3015	1/1	0.73	0.80	-	89,89,89,89	0
56	MG	YA	3142	1/1	0.88	0.64	-	76,76,76,76	0
56	MG	YA	3203	1/1	0.57	0.63	-	93,93,93,93	0
56	MG	RA	3258	1/1	0.84	0.49	-	102,102,102,102	0
56	MG	YA	3493	1/1	0.14	0.84	-	86,86,86,86	0
56	MG	XA	1789	1/1	0.83	0.69	-	81,81,81,81	0
56	MG	YA	3510	1/1	0.83	0.46	-	77,77,77,77	0
56	MG	XA	1641	1/1	0.90	0.24	-	77,77,77,77	0
56	MG	RA	3213	1/1	0.03	0.73	-	112,112,112,112	0
56	MG	RA	3485	1/1	0.90	0.56	-	70,70,70,70	0
56	MG	QA	1847	1/1	0.09	1.28	-	94,94,94,94	0
56	MG	YA	3098	1/1	0.78	0.36	-	95,95,95,95	0
56	MG	YA	3080	1/1	0.92	0.33	-	84,84,84,84	0
56	MG	RA	3154	1/1	0.57	0.34	-	85,85,85,85	0
56	MG	RA	3487	1/1	0.37	0.74	-	83,83,83,83	0
56	MG	YA	3406	1/1	0.72	0.42	-	95,95,95,95	0
56	MG	RA	3629	1/1	-0.13	0.85	-	88,88,88,88	0
56	MG	YA	3718	1/1	0.68	0.42	-	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3480	1/1	0.84	0.47	-	62,62,62,62	0
56	MG	RA	3012	1/1	0.73	0.52	-	84,84,84,84	0
56	MG	YA	3236	1/1	0.64	0.49	-	80,80,80,80	0
56	MG	RA	3885	1/1	-0.09	0.46	-	98,98,98,98	0
56	MG	YA	3629	1/1	0.43	0.81	-	80,80,80,80	0
56	MG	YA	3427	1/1	0.20	0.58	-	88,88,88,88	0
56	MG	QA	1602	1/1	0.86	0.17	-	88,88,88,88	0
56	MG	RA	3541	1/1	0.74	0.40	-	87,87,87,87	0
56	MG	RA	3700	1/1	0.26	0.89	-	104,104,104,104	0
56	MG	RA	3048	1/1	0.72	0.25	-	88,88,88,88	0
56	MG	YA	3066	1/1	0.92	0.60	-	78,78,78,78	0
56	MG	RA	3272	1/1	0.68	0.65	-	90,90,90,90	0
56	MG	RA	3577	1/1	0.93	0.32	-	69,69,69,69	0
56	MG	RA	3599	1/1	0.71	0.62	-	99,99,99,99	0
56	MG	YA	3471	1/1	0.03	0.98	-	99,99,99,99	0
56	MG	QA	1800	1/1	0.68	0.56	-	85,85,85,85	0
56	MG	QA	1702	1/1	0.44	0.90	-	86,86,86,86	0
56	MG	RA	3203	1/1	0.47	0.99	-	98,98,98,98	0
56	MG	RA	3243	1/1	0.84	0.84	-	103,103,103,103	0
56	MG	XA	1695	1/1	0.94	0.54	-	73,73,73,73	0
56	MG	QA	1870	1/1	0.79	0.90	-	81,81,81,81	0
56	MG	RA	3433	1/1	0.32	0.91	-	90,90,90,90	0
56	MG	RA	3145	1/1	0.67	0.46	-	71,71,71,71	0
56	MG	RA	3310	1/1	0.54	0.56	-	93,93,93,93	0
56	MG	YA	3573	1/1	0.85	0.83	-	64,64,64,64	0
56	MG	XA	1750	1/1	0.71	0.91	-	85,85,85,85	0
56	MG	RA	3238	1/1	0.43	0.46	-	109,109,109,109	0
56	MG	QA	1763	1/1	0.84	0.35	-	84,84,84,84	0
56	MG	YA	3025	1/1	0.25	0.88	-	74,74,74,74	0
56	MG	QA	1615	1/1	0.57	0.34	-	93,93,93,93	0
56	MG	YA	3082	1/1	0.66	1.12	-	108,108,108,108	0
56	MG	RA	3820	1/1	0.85	0.42	-	76,76,76,76	0
56	MG	RA	3957	1/1	0.31	0.51	-	79,79,79,79	0
56	MG	R5	105	1/1	-0.23	1.68	-	95,95,95,95	0
56	MG	YA	3676	1/1	0.95	0.94	-	63,63,63,63	0
56	MG	QL	202	1/1	0.12	0.45	-	82,82,82,82	0
56	MG	RA	3525	1/1	0.06	0.98	-	92,92,92,92	0
56	MG	RA	3992	1/1	0.88	0.50	-	101,101,101,101	0
56	MG	XA	1639	1/1	0.84	0.21	-	86,86,86,86	0
56	MG	YA	3625	1/1	0.76	0.53	-	86,86,86,86	0
56	MG	YA	3266	1/1	0.91	0.36	-	91,91,91,91	0
56	MG	RA	3575	1/1	0.82	0.43	-	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3589	1/1	0.87	0.40	-	62,62,62,62	0
56	MG	RA	3442	1/1	0.74	0.89	-	82,82,82,82	0
56	MG	XA	1652	1/1	0.09	0.67	-	92,92,92,92	0
56	MG	QA	1700	1/1	-0.14	0.99	-	94,94,94,94	0
56	MG	RA	3896	1/1	0.80	1.22	-	72,72,72,72	0
56	MG	RA	3714	1/1	0.84	0.57	-	63,63,63,63	0
56	MG	YA	3064	1/1	0.28	0.52	-	86,86,86,86	0
56	MG	YA	3043	1/1	0.50	0.57	-	63,63,63,63	0
56	MG	YA	3212	1/1	0.93	0.24	-	87,87,87,87	0
56	MG	RA	3649	1/1	0.31	0.48	-	94,94,94,94	0
56	MG	QA	1760	1/1	0.65	0.59	-	97,97,97,97	0
56	MG	RH	201	1/1	-0.49	0.82	-	89,89,89,89	0
56	MG	RA	3083	1/1	0.87	0.70	-	95,95,95,95	0
56	MG	RA	3963	1/1	0.30	0.71	-	88,88,88,88	0
56	MG	RA	3923	1/1	0.89	0.31	-	74,74,74,74	0
56	MG	QA	1608	1/1	0.79	0.33	-	107,107,107,107	0
56	MG	RA	3757	1/1	0.72	0.33	-	98,98,98,98	0
56	MG	XA	1664	1/1	0.67	0.50	-	102,102,102,102	0
56	MG	YA	3327	1/1	0.01	1.00	-	85,85,85,85	0
56	MG	QA	1698	1/1	0.33	0.73	-	97,97,97,97	0
56	MG	YA	3423	1/1	0.78	0.34	-	83,83,83,83	0
56	MG	RA	3308	1/1	0.86	0.83	-	94,94,94,94	0
56	MG	RA	3297	1/1	0.82	0.33	-	102,102,102,102	0
56	MG	RU	201	1/1	0.76	0.34	-	85,85,85,85	0
56	MG	RA	3286	1/1	0.59	0.79	-	100,100,100,100	0
56	MG	RA	3595	1/1	0.65	0.54	-	91,91,91,91	0
56	MG	YA	3138	1/1	0.89	0.27	-	72,72,72,72	0
56	MG	RA	3129	1/1	0.79	0.38	-	91,91,91,91	0
56	MG	YA	3598	1/1	0.92	0.53	-	62,62,62,62	0
56	MG	XA	1699	1/1	0.55	0.55	-	82,82,82,82	0
56	MG	RA	3331	1/1	0.92	0.92	-	75,75,75,75	0
56	MG	YA	3479	1/1	0.94	0.48	-	62,62,62,62	0
56	MG	YA	3215	1/1	0.86	0.32	-	86,86,86,86	0
56	MG	RA	3069	1/1	0.84	0.37	-	70,70,70,70	0
56	MG	RA	3617	1/1	0.93	0.52	-	62,62,62,62	0
56	MG	RA	3482	1/1	-0.27	0.33	-	100,100,100,100	0
56	MG	XA	1745	1/1	0.45	0.91	-	71,71,71,71	0
56	MG	RA	3194	1/1	0.58	0.67	-	99,99,99,99	0
56	MG	YA	3444	1/1	0.63	0.35	-	97,97,97,97	0
56	MG	XA	1617	1/1	-0.45	1.67	-	100,100,100,100	0
56	MG	RA	3915	1/1	0.69	0.74	-	73,73,73,73	0
56	MG	RT	202	1/1	0.18	0.81	-	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3542	1/1	0.61	0.81	-	71,71,71,71	0
56	MG	YA	3653	1/1	0.82	0.84	-	64,64,64,64	0
56	MG	RA	3550	1/1	0.59	0.48	-	88,88,88,88	0
56	MG	XA	1613	1/1	0.92	0.09	-	73,73,73,73	0
56	MG	XA	1730	1/1	0.75	0.46	-	88,88,88,88	0
56	MG	XA	1670	1/1	0.80	0.34	-	89,89,89,89	0
56	MG	RA	3736	1/1	0.72	0.70	-	85,85,85,85	0
56	MG	YA	3182	1/1	0.58	0.63	-	103,103,103,103	0
56	MG	YA	3736	1/1	0.64	0.76	-	115,115,115,115	0
56	MG	YA	3470	1/1	0.67	0.51	-	74,74,74,74	0
56	MG	YA	3528	1/1	0.79	1.36	-	72,72,72,72	0
56	MG	R1	103	1/1	0.70	0.69	-	76,76,76,76	0
56	MG	QA	1783	1/1	0.88	0.51	-	63,63,63,63	0
56	MG	YA	3461	1/1	-0.20	0.91	-	87,87,87,87	0
56	MG	RA	4055	1/1	0.79	0.60	-	95,95,95,95	0
56	MG	XA	1680	1/1	0.79	0.76	-	80,80,80,80	0
56	MG	QA	1705	1/1	-0.02	1.00	-	95,95,95,95	0
56	MG	RA	3432	1/1	0.29	0.74	-	77,77,77,77	0
56	MG	YA	3193	1/1	0.37	0.47	-	85,85,85,85	0
56	MG	RD	310	1/1	0.24	0.92	-	86,86,86,86	0
56	MG	YA	3322	1/1	0.89	0.42	-	64,64,64,64	0
56	MG	RA	3153	1/1	0.83	0.48	-	90,90,90,90	0
56	MG	XA	1602	1/1	0.25	1.02	-	88,88,88,88	0
56	MG	YA	3473	1/1	0.40	0.44	-	82,82,82,82	0
56	MG	YA	3349	1/1	0.74	0.58	-	62,62,62,62	0
56	MG	RA	3740	1/1	0.91	0.46	-	85,85,85,85	0
56	MG	RA	3813	1/1	0.28	1.07	-	107,107,107,107	0
56	MG	RA	3504	1/1	0.94	0.40	-	62,62,62,62	0
56	MG	RB	217	1/1	0.38	0.48	-	87,87,87,87	0
56	MG	YA	3728	1/1	0.70	0.51	-	89,89,89,89	0
56	MG	YA	3556	1/1	0.35	0.55	-	73,73,73,73	0
56	MG	YA	3487	1/1	0.74	0.36	-	84,84,84,84	0
56	MG	YA	3230	1/1	0.15	0.50	-	92,92,92,92	0
56	MG	YA	3116	1/1	0.72	0.67	-	95,95,95,95	0
56	MG	XA	1624	1/1	0.29	0.89	-	85,85,85,85	0
56	MG	RA	3748	1/1	-0.26	0.49	-	86,86,86,86	0
56	MG	QA	1716	1/1	0.84	0.55	-	75,75,75,75	0
56	MG	RA	3406	1/1	0.91	0.75	-	68,68,68,68	0
56	MG	RA	3701	1/1	0.75	0.42	-	64,64,64,64	0
56	MG	QA	1816	1/1	-0.09	0.56	-	98,98,98,98	0
56	MG	RA	3236	1/1	0.46	1.08	-	97,97,97,97	0
56	MG	RA	3997	1/1	0.39	0.52	-	106,106,106,106	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3427	1/1	0.18	0.46	-	90,90,90,90	0
56	MG	QA	1776	1/1	0.81	0.42	-	83,83,83,83	0
56	MG	RA	3680	1/1	0.82	1.04	-	69,69,69,69	0
56	MG	RA	3460	1/1	0.87	0.49	-	79,79,79,79	0
56	MG	RA	3861	1/1	0.95	0.92	-	62,62,62,62	0
56	MG	RA	3758	1/1	0.46	0.69	-	93,93,93,93	0
56	MG	RA	3506	1/1	0.71	0.35	-	70,70,70,70	0
56	MG	RA	3895	1/1	0.92	0.84	-	63,63,63,63	0
56	MG	RA	3138	1/1	0.12	0.50	-	79,79,79,79	0
56	MG	RA	3561	1/1	0.91	1.16	-	62,62,62,62	0
56	MG	RA	3815	1/1	0.85	1.16	-	99,99,99,99	0
56	MG	YA	3306	1/1	-0.05	0.99	-	87,87,87,87	0
56	MG	QY	402	1/1	-0.12	1.12	-	92,92,92,92	0
56	MG	YA	3604	1/1	0.78	0.86	-	66,66,66,66	0
56	MG	RA	3658	1/1	0.43	0.45	-	90,90,90,90	0
56	MG	RA	3918	1/1	0.34	0.95	-	93,93,93,93	0
56	MG	RA	3269	1/1	0.86	0.32	-	90,90,90,90	0
56	MG	YA	3186	1/1	0.09	0.40	-	106,106,106,106	0
56	MG	YA	3597	1/1	0.89	0.95	-	71,71,71,71	0
56	MG	XA	1661	1/1	0.72	0.55	-	95,95,95,95	0
56	MG	RA	3808	1/1	0.21	0.75	-	85,85,85,85	0
56	MG	YA	3445	1/1	0.67	0.58	-	94,94,94,94	0
56	MG	RA	3974	1/1	0.83	0.31	-	88,88,88,88	0
56	MG	XA	1721	1/1	0.80	1.30	-	78,78,78,78	0
56	MG	XA	1646	1/1	0.55	0.58	-	104,104,104,104	0
56	MG	RA	3818	1/1	0.65	0.96	-	92,92,92,92	0
56	MG	YB	216	1/1	0.44	0.39	-	66,66,66,66	0
56	MG	YA	3290	1/1	0.73	0.88	-	91,91,91,91	0
56	MG	RA	3223	1/1	0.93	0.06	-	77,77,77,77	0
56	MG	YA	3128	1/1	0.71	0.57	-	82,82,82,82	0
56	MG	RA	3009	1/1	0.96	0.20	-	73,73,73,73	0
56	MG	YA	3457	1/1	0.12	0.63	-	87,87,87,87	0
56	MG	RA	3932	1/1	0.76	0.75	-	88,88,88,88	0
56	MG	QA	1866	1/1	0.41	0.77	-	90,90,90,90	0
56	MG	RA	3650	1/1	0.84	0.29	-	76,76,76,76	0
56	MG	YA	3037	1/1	0.89	0.29	-	84,84,84,84	0
56	MG	QA	1741	1/1	0.59	0.59	-	97,97,97,97	0
56	MG	RA	3606	1/1	0.20	0.64	-	87,87,87,87	0
56	MG	QA	1777	1/1	0.88	0.53	-	83,83,83,83	0
56	MG	RA	3665	1/1	0.86	0.28	-	62,62,62,62	0
56	MG	XA	1635	1/1	0.81	0.33	-	70,70,70,70	0
56	MG	YA	3293	1/1	0.71	1.28	-	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3278	1/1	0.34	0.97	-	89,89,89,89	0
56	MG	YA	3627	1/1	0.86	0.31	-	82,82,82,82	0
56	MG	RA	3979	1/1	0.80	0.78	-	70,70,70,70	0
56	MG	RB	210	1/1	0.88	0.75	-	96,96,96,96	0
56	MG	YB	209	1/1	0.47	0.53	-	102,102,102,102	0
56	MG	QA	1779	1/1	0.99	0.07	-	91,91,91,91	0
56	MG	QA	1751	1/1	0.36	1.18	-	78,78,78,78	0
56	MG	RA	4019	1/1	0.22	1.37	-	103,103,103,103	0
56	MG	RA	3899	1/1	0.29	0.87	-	93,93,93,93	0
56	MG	QA	1662	1/1	0.80	0.32	-	90,90,90,90	0
56	MG	RA	3449	1/1	0.72	0.51	-	83,83,83,83	0
56	MG	YA	3478	1/1	0.73	0.57	-	62,62,62,62	0
56	MG	YA	3062	1/1	0.67	0.40	-	84,84,84,84	0
56	MG	YA	3412	1/1	0.65	0.43	-	90,90,90,90	0
56	MG	QA	1686	1/1	0.46	0.73	-	89,89,89,89	0
56	MG	YA	3004	1/1	0.91	0.24	-	63,63,63,63	0
56	MG	RA	3947	1/1	0.83	0.40	-	63,63,63,63	0
56	MG	YA	3358	1/1	0.76	0.85	-	90,90,90,90	0
56	MG	YA	3442	1/1	0.70	0.56	-	90,90,90,90	0
56	MG	YB	203	1/1	0.57	0.25	-	72,72,72,72	0
56	MG	YA	3229	1/1	0.81	0.30	-	83,83,83,83	0
56	MG	YA	3566	1/1	0.76	0.42	-	73,73,73,73	0
56	MG	RA	4016	1/1	0.72	0.45	-	87,87,87,87	0
56	MG	XA	1790	1/1	0.62	0.84	-	87,87,87,87	0
56	MG	RA	3519	1/1	0.70	0.94	-	86,86,86,86	0
56	MG	YA	3520	1/1	0.74	0.22	-	100,100,100,100	0
56	MG	YA	3654	1/1	0.48	0.38	-	91,91,91,91	0
56	MG	XA	1761	1/1	0.95	0.66	-	80,80,80,80	0
56	MG	QA	1875	1/1	0.74	0.32	-	78,78,78,78	0
56	MG	RA	3579	1/1	0.65	0.62	-	63,63,63,63	0
56	MG	YA	3113	1/1	0.43	0.63	-	79,79,79,79	0
56	MG	RA	3569	1/1	0.95	0.45	-	62,62,62,62	0
56	MG	RA	3264	1/1	0.89	0.37	-	84,84,84,84	0
56	MG	QA	1605	1/1	0.81	0.17	-	90,90,90,90	0
56	MG	RP	202	1/1	-0.23	0.48	-	98,98,98,98	0
56	MG	QG	203	1/1	-0.15	1.46	-	97,97,97,97	0
56	MG	RA	3961	1/1	0.62	0.49	-	87,87,87,87	0
56	MG	RA	3081	1/1	0.43	0.52	-	92,92,92,92	0
56	MG	YA	3553	1/1	0.77	0.71	-	73,73,73,73	0
56	MG	RA	3414	1/1	0.94	0.42	-	62,62,62,62	0
56	MG	RB	213	1/1	0.83	0.81	-	71,71,71,71	0
56	MG	QA	1707	1/1	0.88	0.51	-	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3719	1/1	0.88	0.30	-	79,79,79,79	0
56	MG	YA	3696	1/1	0.47	0.82	-	91,91,91,91	0
56	MG	QA	1730	1/1	0.55	0.32	-	73,73,73,73	0
56	MG	QE	202	1/1	0.58	0.69	-	88,88,88,88	0
56	MG	XA	1679	1/1	0.91	0.67	-	102,102,102,102	0
56	MG	QA	1834	1/1	-0.18	0.92	-	97,97,97,97	0
56	MG	YA	3562	1/1	0.37	0.53	-	82,82,82,82	0
56	MG	YA	3262	1/1	0.79	0.56	-	88,88,88,88	0
56	MG	RA	3880	1/1	0.98	0.62	-	62,62,62,62	0
56	MG	QA	1824	1/1	0.78	0.58	-	69,69,69,69	0
56	MG	YA	3288	1/1	0.90	0.65	-	62,62,62,62	0
56	MG	RA	3725	1/1	0.68	0.45	-	86,86,86,86	0
56	MG	RA	3849	1/1	0.54	0.86	-	85,85,85,85	0
56	MG	RA	3183	1/1	0.61	0.50	-	97,97,97,97	0
56	MG	RA	3764	1/1	0.30	0.47	-	77,77,77,77	0
56	MG	RA	3488	1/1	0.91	0.19	-	67,67,67,67	0
56	MG	QA	1604	1/1	0.46	0.66	-	96,96,96,96	0
56	MG	RA	3031	1/1	0.65	0.49	-	96,96,96,96	0
56	MG	QA	1813	1/1	0.83	0.46	-	90,90,90,90	0
56	MG	YA	3519	1/1	0.73	0.36	-	72,72,72,72	0
56	MG	XA	1622	1/1	0.71	0.59	-	78,78,78,78	0
56	MG	RT	203	1/1	-0.29	2.40	-	100,100,100,100	0
56	MG	RA	3362	1/1	0.55	0.60	-	91,91,91,91	0
56	MG	RA	3206	1/1	0.84	0.31	-	86,86,86,86	0
56	MG	XA	1756	1/1	0.73	1.16	-	81,81,81,81	0
56	MG	RA	3172	1/1	0.04	0.71	-	105,105,105,105	0
56	MG	XA	1672	1/1	-0.05	0.99	-	95,95,95,95	0
56	MG	QA	1632	1/1	0.67	0.50	-	91,91,91,91	0
56	MG	RA	3587	1/1	0.68	0.48	-	78,78,78,78	0
56	MG	RA	3934	1/1	0.93	0.54	-	81,81,81,81	0
56	MG	QA	1764	1/1	0.33	1.28	-	83,83,83,83	0
56	MG	YA	3717	1/1	0.62	0.72	-	100,100,100,100	0
56	MG	RA	3441	1/1	0.54	0.77	-	67,67,67,67	0
56	MG	RA	3011	1/1	0.39	0.69	-	93,93,93,93	0
56	MG	RA	3531	1/1	-0.06	0.58	-	90,90,90,90	0
56	MG	RA	3984	1/1	0.62	0.57	-	87,87,87,87	0
56	MG	QE	201	1/1	0.47	0.33	-	95,95,95,95	0
56	MG	QV	102	1/1	0.90	0.22	-	94,94,94,94	0
56	MG	RA	3753	1/1	0.50	0.70	-	92,92,92,92	0
56	MG	RA	3826	1/1	0.72	0.30	-	95,95,95,95	0
56	MG	YR	201	1/1	0.78	0.46	-	82,82,82,82	0
56	MG	QA	1819	1/1	0.06	0.82	-	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3422	1/1	0.65	0.55	-	73,73,73,73	0
56	MG	RA	3267	1/1	0.77	0.71	-	85,85,85,85	0
56	MG	XV	103	1/1	0.58	0.59	-	84,84,84,84	0
56	MG	RA	3004	1/1	0.85	0.17	-	63,63,63,63	0
56	MG	RA	3944	1/1	0.57	0.60	-	97,97,97,97	0
56	MG	RA	3192	1/1	0.31	0.37	-	83,83,83,83	0
56	MG	YA	3697	1/1	0.61	0.41	-	78,78,78,78	0
56	MG	YA	3631	1/1	0.67	0.44	-	76,76,76,76	0
56	MG	RA	3883	1/1	0.53	0.88	-	88,88,88,88	0
56	MG	RD	311	1/1	0.56	0.84	-	101,101,101,101	0
56	MG	RA	3960	1/1	0.18	0.72	-	92,92,92,92	0
56	MG	YA	3662	1/1	0.80	0.51	-	68,68,68,68	0
56	MG	YT	203	1/1	0.73	0.55	-	91,91,91,91	0
56	MG	RA	3565	1/1	0.49	0.56	-	103,103,103,103	0
56	MG	XA	1729	1/1	0.22	0.74	-	83,83,83,83	0
56	MG	RA	3942	1/1	0.68	0.43	-	95,95,95,95	0
56	MG	RA	3937	1/1	0.77	0.81	-	80,80,80,80	0
56	MG	YA	3463	1/1	0.15	0.92	-	86,86,86,86	0
56	MG	RA	3198	1/1	0.14	3.01	-	98,98,98,98	0
56	MG	QA	1675	1/1	0.81	0.49	-	91,91,91,91	0
56	MG	RA	3794	1/1	0.80	0.36	-	72,72,72,72	0
56	MG	QA	1732	1/1	0.72	0.57	-	72,72,72,72	0
56	MG	XA	1681	1/1	0.79	0.17	-	100,100,100,100	0
56	MG	RA	3347	1/1	0.94	0.74	-	62,62,62,62	0
56	MG	QA	1755	1/1	0.49	0.89	-	81,81,81,81	0
56	MG	YA	3422	1/1	0.82	0.32	-	90,90,90,90	0
56	MG	RA	3833	1/1	0.24	0.53	-	92,92,92,92	0
56	MG	RA	3864	1/1	0.51	0.82	-	93,93,93,93	0
56	MG	RA	3309	1/1	0.18	0.90	-	93,93,93,93	0
56	MG	YA	3432	1/1	0.80	0.36	-	76,76,76,76	0
56	MG	XA	1603	1/1	0.81	0.33	-	83,83,83,83	0
56	MG	XA	1608	1/1	0.62	0.71	-	76,76,76,76	0
56	MG	RA	3182	1/1	0.72	0.99	-	97,97,97,97	0
56	MG	QG	202	1/1	0.59	0.71	-	87,87,87,87	0
56	MG	XA	1787	1/1	0.59	0.65	-	78,78,78,78	0
56	MG	RA	3855	1/1	0.96	0.33	-	71,71,71,71	0
56	MG	RA	3033	1/1	-0.07	0.48	-	100,100,100,100	0
56	MG	YA	3527	1/1	0.67	0.38	-	74,74,74,74	0
56	MG	QA	1752	1/1	0.81	0.37	-	94,94,94,94	0
56	MG	XA	1757	1/1	0.95	0.61	-	76,76,76,76	0
56	MG	QA	1758	1/1	0.74	0.35	-	93,93,93,93	0
56	MG	RA	3846	1/1	0.65	0.53	-	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3309	1/1	0.07	1.03	-	90,90,90,90	0
56	MG	RA	3038	1/1	0.90	0.15	-	86,86,86,86	0
56	MG	RA	3169	1/1	0.64	0.23	-	90,90,90,90	0
56	MG	RA	3830	1/1	0.75	1.56	-	78,78,78,78	0
56	MG	YQ	202	1/1	0.20	0.69	-	89,89,89,89	0
56	MG	YA	3663	1/1	0.33	1.33	-	98,98,98,98	0
56	MG	XA	1634	1/1	0.98	0.48	-	69,69,69,69	0
56	MG	RA	3743	1/1	0.63	0.78	-	89,89,89,89	0
56	MG	RA	3100	1/1	0.57	0.53	-	102,102,102,102	0
56	MG	XA	1711	1/1	0.42	0.69	-	94,94,94,94	0
56	MG	YB	219	1/1	0.88	0.47	-	63,63,63,63	0
56	MG	YA	3099	1/1	0.48	0.38	-	82,82,82,82	0
56	MG	XA	1668	1/1	0.92	0.52	-	92,92,92,92	0
56	MG	QA	1701	1/1	0.61	0.50	-	77,77,77,77	0
56	MG	RA	3126	1/1	0.65	0.91	-	89,89,89,89	0
56	MG	RA	3281	1/1	0.76	0.24	-	90,90,90,90	0
56	MG	QA	1754	1/1	0.90	0.27	-	85,85,85,85	0
56	MG	RA	3612	1/1	0.63	0.20	-	80,80,80,80	0
56	MG	YA	3141	1/1	0.68	0.44	-	79,79,79,79	0
56	MG	YA	3721	1/1	0.55	0.69	-	74,74,74,74	0
56	MG	RA	3865	1/1	0.90	0.33	-	93,93,93,93	0
56	MG	RA	3879	1/1	0.11	0.96	-	93,93,93,93	0
56	MG	RA	3559	1/1	0.34	0.73	-	84,84,84,84	0
56	MG	QA	1861	1/1	0.86	0.38	-	72,72,72,72	0
56	MG	RA	3499	1/1	0.22	1.30	-	80,80,80,80	0
56	MG	RA	3152	1/1	0.81	0.26	-	93,93,93,93	0
56	MG	YA	3371	1/1	0.84	1.01	-	68,68,68,68	0
56	MG	RA	3280	1/1	0.56	0.84	-	95,95,95,95	0
56	MG	RA	3728	1/1	0.14	0.76	-	99,99,99,99	0
56	MG	RA	3380	1/1	0.91	0.68	-	64,64,64,64	0
56	MG	RA	3151	1/1	0.81	0.52	-	84,84,84,84	0
56	MG	XA	1717	1/1	0.84	0.38	-	82,82,82,82	0
56	MG	XA	1784	1/1	0.93	0.34	-	80,80,80,80	0
56	MG	RA	3890	1/1	0.77	0.99	-	77,77,77,77	0
56	MG	YA	3259	1/1	0.75	0.78	-	98,98,98,98	0
56	MG	YA	3147	1/1	-0.08	1.01	-	86,86,86,86	0
56	MG	YA	3073	1/1	0.83	0.31	-	86,86,86,86	0
56	MG	YA	3716	1/1	0.32	0.89	-	87,87,87,87	0
56	MG	YA	3125	1/1	0.42	0.34	-	81,81,81,81	0
56	MG	YB	208	1/1	0.72	0.47	-	93,93,93,93	0
56	MG	YA	3641	1/1	0.83	0.94	-	83,83,83,83	0
56	MG	RA	3061	1/1	0.57	0.25	-	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3069	1/1	0.77	0.58	-	98,98,98,98	0
56	MG	YA	3390	1/1	0.47	0.33	-	88,88,88,88	0
56	MG	YA	3220	1/1	0.74	0.56	-	105,105,105,105	0
56	MG	XA	1643	1/1	0.94	0.31	-	81,81,81,81	0
56	MG	YA	3261	1/1	0.75	0.59	-	85,85,85,85	0
56	MG	RA	3780	1/1	0.66	0.48	-	89,89,89,89	0
56	MG	QA	1694	1/1	0.18	0.77	-	91,91,91,91	0
56	MG	YA	3168	1/1	0.29	0.90	-	100,100,100,100	0
56	MG	RA	3411	1/1	0.73	0.52	-	93,93,93,93	0
56	MG	YA	3226	1/1	0.59	0.56	-	87,87,87,87	0
56	MG	YA	3330	1/1	0.91	1.11	-	62,62,62,62	0
56	MG	QA	1804	1/1	0.86	0.40	-	85,85,85,85	0
56	MG	RA	3558	1/1	0.74	0.36	-	76,76,76,76	0
56	MG	QA	1801	1/1	0.59	0.33	-	76,76,76,76	0
56	MG	XA	1620	1/1	0.17	0.17	-	93,93,93,93	0
56	MG	YA	3208	1/1	-0.55	1.38	-	102,102,102,102	0
56	MG	RA	3716	1/1	0.03	0.37	-	91,91,91,91	0
56	MG	YA	3564	1/1	0.96	0.29	-	63,63,63,63	0
56	MG	RA	3766	1/1	0.93	1.11	-	71,71,71,71	0
56	MG	RA	3691	1/1	0.69	1.05	-	93,93,93,93	0
56	MG	RA	3253	1/1	0.57	0.52	-	81,81,81,81	0
56	MG	RA	3642	1/1	0.49	0.55	-	92,92,92,92	0
56	MG	RA	3057	1/1	0.36	0.58	-	96,96,96,96	0
56	MG	RA	3469	1/1	0.95	0.39	-	68,68,68,68	0
56	MG	QA	1687	1/1	0.72	0.62	-	94,94,94,94	0
56	MG	RA	3351	1/1	0.93	0.19	-	89,89,89,89	0
56	MG	QA	1811	1/1	0.77	0.23	-	78,78,78,78	0
56	MG	YA	3693	1/1	0.75	0.64	-	70,70,70,70	0
56	MG	RA	3288	1/1	0.56	0.53	-	96,96,96,96	0
56	MG	RA	3242	1/1	0.47	0.43	-	99,99,99,99	0
56	MG	YA	3143	1/1	0.54	0.45	-	106,106,106,106	0
56	MG	RA	3907	1/1	0.96	0.45	-	70,70,70,70	0
56	MG	QA	1792	1/1	0.88	0.82	-	84,84,84,84	0
56	MG	RA	3651	1/1	0.79	0.40	-	80,80,80,80	0
56	MG	QA	1670	1/1	0.67	0.42	-	84,84,84,84	0
56	MG	YA	3622	1/1	0.88	0.37	-	66,66,66,66	0
56	MG	YB	204	1/1	0.77	0.52	-	95,95,95,95	0
56	MG	YA	3031	1/1	0.71	0.32	-	63,63,63,63	0
56	MG	RA	3695	1/1	0.59	0.83	-	107,107,107,107	0
56	MG	RA	3791	1/1	0.37	0.47	-	84,84,84,84	0
56	MG	YB	211	1/1	0.51	0.30	-	80,80,80,80	0
56	MG	YA	3067	1/1	0.77	0.32	-	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3411	1/1	0.37	0.64	-	90,90,90,90	0
56	MG	RA	3804	1/1	0.17	0.52	-	92,92,92,92	0
56	MG	XA	1767	1/1	0.63	0.81	-	78,78,78,78	0
56	MG	RA	3998	1/1	0.89	0.46	-	84,84,84,84	0
56	MG	YA	3144	1/1	0.90	0.10	-	82,82,82,82	0
56	MG	YA	3530	1/1	-0.14	0.59	-	102,102,102,102	0
56	MG	RA	3498	1/1	-0.14	0.57	-	83,83,83,83	0
56	MG	YA	3451	1/1	0.63	0.64	-	94,94,94,94	0
56	MG	XA	1692	1/1	0.82	0.55	-	69,69,69,69	0
56	MG	YA	3061	1/1	0.65	0.48	-	65,65,65,65	0
56	MG	YA	3079	1/1	0.51	0.67	-	97,97,97,97	0
56	MG	YA	3596	1/1	0.63	0.57	-	66,66,66,66	0
56	MG	RQ	202	1/1	0.78	0.69	-	73,73,73,73	0
56	MG	QA	1713	1/1	0.04	0.73	-	95,95,95,95	0
56	MG	RA	3105	1/1	0.37	1.08	-	92,92,92,92	0
56	MG	YA	3481	1/1	0.65	0.60	-	79,79,79,79	0
56	MG	RA	3951	1/1	0.31	0.77	-	85,85,85,85	0
56	MG	RA	3354	1/1	0.73	0.67	-	70,70,70,70	0
56	MG	YA	3672	1/1	0.56	0.67	-	76,76,76,76	0
56	MG	RA	3661	1/1	0.77	0.34	-	73,73,73,73	0
56	MG	RA	3866	1/1	0.64	0.38	-	76,76,76,76	0
56	MG	YA	3160	1/1	0.78	0.30	-	88,88,88,88	0
56	MG	XA	1748	1/1	0.55	0.73	-	79,79,79,79	0
56	MG	YA	3708	1/1	0.74	1.08	-	66,66,66,66	0
56	MG	RA	3159	1/1	0.49	0.67	-	94,94,94,94	0
56	MG	XA	1675	1/1	0.56	0.43	-	90,90,90,90	0
56	MG	RA	3542	1/1	0.77	0.72	-	79,79,79,79	0
56	MG	XA	1601	1/1	0.11	0.89	-	93,93,93,93	0
56	MG	RA	3340	1/1	0.61	0.56	-	82,82,82,82	0
56	MG	RA	3298	1/1	0.65	0.16	-	79,79,79,79	0
56	MG	RA	3863	1/1	0.86	0.29	-	86,86,86,86	0
56	MG	YA	3035	1/1	-0.27	1.00	-	93,93,93,93	0
56	MG	YA	3551	1/1	0.31	0.50	-	73,73,73,73	0
56	MG	RA	3608	1/1	0.62	0.62	-	83,83,83,83	0
56	MG	QA	1646	1/1	0.46	0.74	-	71,71,71,71	0
56	MG	YA	3599	1/1	-0.13	0.96	-	83,83,83,83	0
56	MG	XA	1689	1/1	0.94	0.44	-	75,75,75,75	0
56	MG	RA	3344	1/1	0.97	0.25	-	67,67,67,67	0
56	MG	RA	3457	1/1	0.70	0.17	-	89,89,89,89	0
56	MG	RA	3980	1/1	0.90	0.36	-	77,77,77,77	0
56	MG	XA	1665	1/1	0.72	0.28	-	72,72,72,72	0
56	MG	YA	3278	1/1	0.60	0.96	-	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3091	1/1	0.70	1.15	-	102,102,102,102	0
56	MG	RA	3975	1/1	0.46	0.34	-	98,98,98,98	0
56	MG	YA	3224	1/1	0.93	0.35	-	71,71,71,71	0
56	MG	RA	3950	1/1	0.71	1.05	-	86,86,86,86	0
56	MG	RA	3672	1/1	0.61	0.47	-	89,89,89,89	0
56	MG	RA	3334	1/1	0.88	0.43	-	82,82,82,82	0
56	MG	QA	1815	1/1	0.84	0.32	-	87,87,87,87	0
56	MG	RA	3783	1/1	-0.35	0.71	-	96,96,96,96	0
56	MG	RA	3730	1/1	0.76	0.70	-	89,89,89,89	0
56	MG	RA	3079	1/1	0.24	0.80	-	111,111,111,111	0
56	MG	YA	3719	1/1	0.33	0.25	-	89,89,89,89	0
56	MG	YA	3001	1/1	0.39	0.75	-	96,96,96,96	0
56	MG	RA	3416	1/1	0.93	0.36	-	75,75,75,75	0
56	MG	YA	3197	1/1	0.73	0.45	-	93,93,93,93	0
56	MG	QA	1648	1/1	0.86	0.17	-	87,87,87,87	0
56	MG	QA	1855	1/1	-0.48	0.73	-	106,106,106,106	0
56	MG	QV	104	1/1	0.69	0.60	-	79,79,79,79	0
56	MG	YA	3200	1/1	0.66	0.47	-	77,77,77,77	0
56	MG	RA	3673	1/1	0.65	0.38	-	86,86,86,86	0
56	MG	RA	3035	1/1	0.58	0.35	-	95,95,95,95	0
56	MG	XA	1638	1/1	0.25	0.82	-	98,98,98,98	0
56	MG	YA	3586	1/1	0.63	1.11	-	76,76,76,76	0
56	MG	RA	3255	1/1	0.77	0.57	-	97,97,97,97	0
56	MG	XA	1653	1/1	0.63	0.58	-	89,89,89,89	0
56	MG	YA	3365	1/1	0.57	0.38	-	86,86,86,86	0
56	MG	QA	1664	1/1	-0.25	1.44	-	91,91,91,91	0
56	MG	QA	1793	1/1	0.28	0.79	-	93,93,93,93	0
56	MG	RA	3921	1/1	0.93	0.88	-	63,63,63,63	0
56	MG	RA	3996	1/1	0.48	0.59	-	89,89,89,89	0
56	MG	RA	3143	1/1	0.83	0.28	-	77,77,77,77	0
56	MG	YA	3608	1/1	0.90	0.30	-	66,66,66,66	0
56	MG	YA	3121	1/1	0.94	0.09	-	77,77,77,77	0
56	MG	RA	3615	1/1	0.75	0.51	-	62,62,62,62	0
56	MG	RA	3054	1/1	-0.05	0.86	-	94,94,94,94	0
56	MG	QA	1805	1/1	0.66	0.94	-	76,76,76,76	0
56	MG	RA	3191	1/1	0.77	0.28	-	90,90,90,90	0
56	MG	RA	3824	1/1	0.24	0.61	-	92,92,92,92	0
56	MG	RA	3604	1/1	0.40	0.77	-	107,107,107,107	0
56	MG	QD	304	1/1	0.67	0.52	-	97,97,97,97	0
56	MG	XA	1605	1/1	0.21	1.09	-	96,96,96,96	0
56	MG	XA	1740	1/1	0.75	0.59	-	70,70,70,70	0
56	MG	R7	101	1/1	0.26	0.54	-	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	R9	101	1/1	0.12	0.47	-	100,100,100,100	0
56	MG	XA	1709	1/1	0.84	0.26	-	88,88,88,88	0
56	MG	RA	3584	1/1	0.63	0.57	-	76,76,76,76	0
56	MG	RA	3439	1/1	0.52	0.24	-	84,84,84,84	0
56	MG	RA	3237	1/1	0.49	0.96	-	96,96,96,96	0
56	MG	RA	3026	1/1	0.93	1.22	-	100,100,100,100	0
56	MG	YA	3242	1/1	0.55	0.85	-	107,107,107,107	0
56	MG	RA	3318	1/1	0.93	0.73	-	71,71,71,71	0
56	MG	RA	3920	1/1	0.69	0.46	-	80,80,80,80	0
56	MG	QA	1657	1/1	0.76	0.42	-	101,101,101,101	0
56	MG	XA	1733	1/1	0.77	0.98	-	69,69,69,69	0
56	MG	YA	3155	1/1	0.90	0.65	-	85,85,85,85	0
56	MG	YA	3738	1/1	0.80	0.93	-	99,99,99,99	0
56	MG	YA	3571	1/1	0.94	0.69	-	64,64,64,64	0
56	MG	YA	3225	1/1	0.47	0.96	-	96,96,96,96	0
56	MG	RA	3134	1/1	0.16	0.99	-	96,96,96,96	0
56	MG	QA	1830	1/1	0.95	0.37	-	69,69,69,69	0
56	MG	RA	3580	1/1	0.92	0.41	-	64,64,64,64	0
56	MG	XA	1610	1/1	0.53	1.06	-	88,88,88,88	0
56	MG	RA	3250	1/1	0.24	0.93	-	84,84,84,84	0
56	MG	YA	3575	1/1	0.93	0.75	-	67,67,67,67	0
56	MG	RA	3087	1/1	0.76	1.00	-	113,113,113,113	0
56	MG	YA	3591	1/1	0.92	0.79	-	62,62,62,62	0
56	MG	YA	3431	1/1	0.78	0.97	-	84,84,84,84	0
56	MG	RA	3114	1/1	0.71	0.52	-	95,95,95,95	0
56	MG	XA	1766	1/1	0.55	1.07	-	88,88,88,88	0
56	MG	XA	1648	1/1	0.49	0.29	-	89,89,89,89	0
56	MG	RA	3358	1/1	0.70	0.26	-	81,81,81,81	0
56	MG	RA	3207	1/1	0.72	0.62	-	96,96,96,96	0
56	MG	RA	3816	1/1	0.75	0.29	-	79,79,79,79	0
56	MG	RA	3761	1/1	0.83	0.26	-	70,70,70,70	0
56	MG	YE	306	1/1	0.65	0.81	-	62,62,62,62	0
56	MG	YA	3302	1/1	0.71	0.27	-	89,89,89,89	0
56	MG	YA	3583	1/1	0.80	0.52	-	74,74,74,74	0
56	MG	RA	3150	1/1	0.33	0.27	-	84,84,84,84	0
56	MG	QA	1659	1/1	0.83	0.97	-	92,92,92,92	0
56	MG	RA	3534	1/1	0.85	0.38	-	75,75,75,75	0
56	MG	QA	1803	1/1	0.58	0.37	-	81,81,81,81	0
56	MG	YA	3484	1/1	-0.11	0.63	-	99,99,99,99	0
56	MG	RA	3857	1/1	0.86	0.69	-	76,76,76,76	0
56	MG	RB	216	1/1	0.81	0.55	-	88,88,88,88	0
56	MG	YA	3706	1/1	0.74	0.88	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	QA	1641	1/1	0.94	0.31	-	95,95,95,95	0
56	MG	QA	1651	1/1	0.70	0.47	-	90,90,90,90	0
56	MG	XA	1726	1/1	0.46	0.53	-	96,96,96,96	0
56	MG	RA	3474	1/1	0.95	0.38	-	70,70,70,70	0
56	MG	XA	1615	1/1	0.90	0.19	-	89,89,89,89	0
56	MG	XV	102	1/1	0.48	0.13	-	84,84,84,84	0
56	MG	YA	3127	1/1	0.93	0.36	-	70,70,70,70	0
56	MG	YA	3294	1/1	0.96	0.69	-	62,62,62,62	0
56	MG	RA	3982	1/1	0.91	0.14	-	79,79,79,79	0
56	MG	RA	3667	1/1	0.87	0.63	-	88,88,88,88	0
56	MG	QA	1879	1/1	-0.07	1.40	-	105,105,105,105	0
56	MG	RA	3212	1/1	0.88	0.60	-	80,80,80,80	0
56	MG	RA	3450	1/1	0.54	0.28	-	79,79,79,79	0
56	MG	XA	1647	1/1	0.96	0.88	-	70,70,70,70	0
56	MG	QA	1689	1/1	0.91	0.49	-	81,81,81,81	0
56	MG	RA	3675	1/1	0.68	0.60	-	84,84,84,84	0
56	MG	RA	3010	1/1	0.91	0.50	-	79,79,79,79	0
56	MG	YA	3513	1/1	0.60	0.85	-	81,81,81,81	0
56	MG	YA	3289	1/1	-0.12	1.36	-	92,92,92,92	0
56	MG	YA	3086	1/1	-0.10	0.76	-	92,92,92,92	0
56	MG	RA	3037	1/1	0.68	0.48	-	100,100,100,100	0
56	MG	YA	3118	1/1	0.80	0.44	-	74,74,74,74	0
56	MG	YA	3609	1/1	0.88	0.59	-	75,75,75,75	0
56	MG	RA	3640	1/1	0.56	0.49	-	84,84,84,84	0
56	MG	YA	3572	1/1	0.88	0.43	-	72,72,72,72	0
56	MG	RA	3567	1/1	0.55	0.44	-	90,90,90,90	0
56	MG	RA	3376	1/1	0.68	0.78	-	78,78,78,78	0
56	MG	RB	222	1/1	0.62	0.48	-	79,79,79,79	0
56	MG	RA	3894	1/1	0.82	0.78	-	69,69,69,69	0
56	MG	RA	4011	1/1	-0.10	0.38	-	102,102,102,102	0
56	MG	RA	3648	1/1	0.24	0.29	-	97,97,97,97	0
56	MG	RA	3001	1/1	0.61	0.47	-	91,91,91,91	0
56	MG	YO	201	1/1	0.45	0.64	-	86,86,86,86	0
56	MG	RA	3056	1/1	0.83	0.84	-	87,87,87,87	0
56	MG	RA	3195	1/1	0.95	0.61	-	97,97,97,97	0
56	MG	RA	3147	1/1	0.99	0.17	-	84,84,84,84	0
56	MG	RA	3706	1/1	0.91	0.47	-	78,78,78,78	0
56	MG	RA	3610	1/1	0.81	0.49	-	91,91,91,91	0
56	MG	XA	1671	1/1	0.92	0.25	-	84,84,84,84	0
56	MG	YA	3234	1/1	0.93	0.35	-	92,92,92,92	0
56	MG	RA	3500	1/1	0.78	0.63	-	94,94,94,94	0
56	MG	YA	3279	1/1	0.93	0.81	-	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3364	1/1	0.65	0.23	-	81,81,81,81	0
56	MG	RA	3646	1/1	0.74	0.35	-	92,92,92,92	0
56	MG	QA	1703	1/1	0.56	0.41	-	63,63,63,63	0
56	MG	RA	3135	1/1	0.93	0.37	-	91,91,91,91	0
56	MG	YA	3522	1/1	0.79	0.60	-	75,75,75,75	0
56	MG	RA	3593	1/1	0.86	1.02	-	84,84,84,84	0
56	MG	RA	3721	1/1	0.66	0.86	-	67,67,67,67	0
56	MG	RA	3240	1/1	0.82	0.52	-	106,106,106,106	0
56	MG	YA	3040	1/1	0.56	0.48	-	88,88,88,88	0
56	MG	XA	1779	1/1	0.71	0.43	-	92,92,92,92	0
56	MG	YA	3173	1/1	0.25	0.58	-	99,99,99,99	0
56	MG	RA	3076	1/1	0.25	1.20	-	96,96,96,96	0
56	MG	RA	3735	1/1	0.53	0.59	-	77,77,77,77	0
56	MG	YA	3338	1/1	0.61	1.04	-	85,85,85,85	0
56	MG	QA	1624	1/1	0.79	0.51	-	74,74,74,74	0
56	MG	YA	3389	1/1	0.68	0.62	-	71,71,71,71	0
56	MG	YA	3486	1/1	-0.02	1.11	-	105,105,105,105	0
56	MG	RA	3801	1/1	0.75	0.32	-	92,92,92,92	0
56	MG	YA	3124	1/1	0.94	0.17	-	93,93,93,93	0
56	MG	RA	3161	1/1	0.91	0.28	-	83,83,83,83	0
56	MG	RA	3760	1/1	0.36	0.80	-	98,98,98,98	0
56	MG	RA	3480	1/1	0.91	0.50	-	62,62,62,62	0
56	MG	YA	3120	1/1	0.72	0.61	-	86,86,86,86	0
56	MG	YA	3331	1/1	0.88	0.73	-	62,62,62,62	0
56	MG	RA	3995	1/1	0.24	0.46	-	91,91,91,91	0
56	MG	RA	3373	1/1	0.44	0.77	-	82,82,82,82	0
56	MG	RA	3492	1/1	0.46	0.56	-	78,78,78,78	0
56	MG	RA	3729	1/1	0.44	0.69	-	82,82,82,82	0
56	MG	QA	1612	1/1	0.44	0.56	-	89,89,89,89	0
56	MG	R7	102	1/1	0.47	0.66	-	75,75,75,75	0
56	MG	RA	3293	1/1	0.85	0.26	-	87,87,87,87	0
56	MG	RA	3314	1/1	0.71	0.55	-	77,77,77,77	0
56	MG	RA	3772	1/1	0.52	0.56	-	69,69,69,69	0
56	MG	RA	3274	1/1	0.79	0.37	-	88,88,88,88	0
56	MG	YA	3636	1/1	0.79	0.93	-	72,72,72,72	0
56	MG	RA	3018	1/1	0.84	0.48	-	95,95,95,95	0
56	MG	RA	3590	1/1	0.38	0.73	-	100,100,100,100	0
56	MG	RO	201	1/1	0.89	0.26	-	72,72,72,72	0
56	MG	XA	1640	1/1	0.74	0.47	-	92,92,92,92	0
56	MG	RA	3822	1/1	0.95	0.55	-	73,73,73,73	0
56	MG	XA	1662	1/1	-0.18	0.37	-	97,97,97,97	0
56	MG	YA	3692	1/1	0.57	0.53	-	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	XA	1715	1/1	0.23	0.96	-	94,94,94,94	0
56	MG	QA	1639	1/1	0.78	0.18	-	93,93,93,93	0
56	MG	RA	3628	1/1	0.04	1.22	-	89,89,89,89	0
56	MG	RA	3003	1/1	0.49	0.56	-	91,91,91,91	0
56	MG	XJ	201	1/1	0.40	0.38	-	97,97,97,97	0
56	MG	YA	3491	1/1	0.88	0.54	-	91,91,91,91	0
56	MG	RA	3511	1/1	0.87	0.16	-	71,71,71,71	0
56	MG	YA	3712	1/1	0.56	0.77	-	80,80,80,80	0
56	MG	QA	1768	1/1	0.24	0.54	-	89,89,89,89	0
56	MG	RA	3596	1/1	0.67	0.38	-	98,98,98,98	0
56	MG	YA	3169	1/1	0.80	0.40	-	85,85,85,85	0
56	MG	RA	3467	1/1	0.02	0.66	-	89,89,89,89	0
56	MG	QA	1827	1/1	0.81	0.40	-	74,74,74,74	0
56	MG	RA	4053	1/1	0.26	1.73	-	103,103,103,103	0
56	MG	RA	3218	1/1	0.07	0.46	-	88,88,88,88	0
56	MG	RA	3817	1/1	0.57	0.80	-	92,92,92,92	0
56	MG	XA	1663	1/1	0.73	0.23	-	83,83,83,83	0
56	MG	YA	3504	1/1	0.12	0.54	-	93,93,93,93	0
56	MG	RA	3837	1/1	0.53	0.63	-	90,90,90,90	0
56	MG	RA	3104	1/1	0.94	0.32	-	77,77,77,77	0
56	MG	QQ	201	1/1	0.79	0.24	-	91,91,91,91	0
56	MG	YA	3620	1/1	0.53	0.34	-	75,75,75,75	0
56	MG	RA	3389	1/1	0.90	0.82	-	69,69,69,69	0
56	MG	YA	3396	1/1	0.42	0.89	-	67,67,67,67	0
56	MG	RA	3655	1/1	0.52	0.27	-	94,94,94,94	0
56	MG	RA	3085	1/1	0.31	0.86	-	91,91,91,91	0
56	MG	XA	1685	1/1	0.40	0.77	-	62,62,62,62	0
56	MG	RT	201	1/1	0.82	1.45	-	78,78,78,78	0
56	MG	QA	1721	1/1	0.92	0.69	-	62,62,62,62	0
56	MG	RA	3870	1/1	0.92	1.64	-	86,86,86,86	0
56	MG	RA	3790	1/1	0.62	0.58	-	102,102,102,102	0
56	MG	YA	3054	1/1	0.82	0.45	-	102,102,102,102	0
56	MG	YA	3615	1/1	0.91	0.26	-	65,65,65,65	0
56	MG	YA	3135	1/1	0.82	0.40	-	63,63,63,63	0
56	MG	RA	3949	1/1	0.71	0.77	-	95,95,95,95	0
56	MG	RA	3225	1/1	0.14	0.97	-	111,111,111,111	0
56	MG	RA	3699	1/1	0.76	0.50	-	107,107,107,107	0
56	MG	QA	1822	1/1	0.88	0.33	-	97,97,97,97	0
56	MG	QH	202	1/1	0.52	0.47	-	91,91,91,91	0
56	MG	RA	3051	1/1	0.81	0.75	-	97,97,97,97	0
56	MG	YA	3683	1/1	0.74	0.27	-	82,82,82,82	0
56	MG	YA	3646	1/1	0.83	0.43	-	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	YA	3277	1/1	0.92	0.52	-	62,62,62,62	0
56	MG	YA	3450	1/1	0.48	0.94	-	79,79,79,79	0
56	MG	Y7	101	1/1	0.90	0.93	-	99,99,99,99	0
56	MG	YA	3032	1/1	0.35	0.72	-	93,93,93,93	0
56	MG	RA	3602	1/1	0.74	1.58	-	97,97,97,97	0
56	MG	RA	3891	1/1	0.87	0.92	-	69,69,69,69	0
56	MG	QA	1799	1/1	0.23	0.66	-	99,99,99,99	0
56	MG	RA	3405	1/1	0.74	0.19	-	85,85,85,85	0
56	MG	RA	3451	1/1	0.71	1.35	-	74,74,74,74	0
56	MG	YA	3435	1/1	0.11	1.10	-	87,87,87,87	0
56	MG	YA	3443	1/1	0.87	0.27	-	83,83,83,83	0
56	MG	YA	3175	1/1	-0.01	1.24	-	101,101,101,101	0
56	MG	RA	3224	1/1	0.44	0.73	-	93,93,93,93	0
56	MG	RA	3166	1/1	0.60	0.82	-	83,83,83,83	0
56	MG	YA	3202	1/1	0.52	0.42	-	82,82,82,82	0
56	MG	QA	1653	1/1	0.76	0.55	-	84,84,84,84	0
56	MG	RA	3046	1/1	0.94	0.80	-	99,99,99,99	0
56	MG	RA	3958	1/1	0.45	0.48	-	80,80,80,80	0
56	MG	RE	301	1/1	0.91	0.57	-	107,107,107,107	0
56	MG	RA	3945	1/1	0.83	0.21	-	63,63,63,63	0
56	MG	YA	3084	1/1	0.03	1.21	-	101,101,101,101	0
56	MG	QA	1825	1/1	0.62	0.59	-	86,86,86,86	0
56	MG	YA	3595	1/1	0.77	0.48	-	83,83,83,83	0
56	MG	YA	3561	1/1	0.27	1.18	-	89,89,89,89	0
56	MG	YA	3558	1/1	0.54	0.70	-	87,87,87,87	0
56	MG	YA	3466	1/1	0.72	0.56	-	79,79,79,79	0
56	MG	RA	3353	1/1	0.72	0.65	-	84,84,84,84	0
56	MG	XA	1768	1/1	0.96	0.89	-	62,62,62,62	0
56	MG	YA	3671	1/1	0.97	0.53	-	62,62,62,62	0
56	MG	RA	3489	1/1	0.65	0.38	-	67,67,67,67	0
56	MG	XA	1724	1/1	0.81	0.36	-	75,75,75,75	0
56	MG	YA	3056	1/1	0.77	0.46	-	86,86,86,86	0
56	MG	RA	3283	1/1	0.88	0.57	-	88,88,88,88	0
56	MG	YA	3232	1/1	0.87	0.25	-	84,84,84,84	0
56	MG	YA	3402	1/1	0.83	0.27	-	86,86,86,86	0
56	MG	YA	3280	1/1	0.90	0.33	-	64,64,64,64	0
56	MG	RG	203	1/1	0.27	0.81	-	83,83,83,83	0
56	MG	YA	3385	1/1	0.79	0.49	-	69,69,69,69	0
56	MG	RA	3872	1/1	0.12	0.60	-	83,83,83,83	0
56	MG	RA	3440	1/1	-0.17	1.18	-	89,89,89,89	0
56	MG	RA	3164	1/1	0.33	0.79	-	100,100,100,100	0
56	MG	RA	3643	1/1	0.78	0.48	-	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	RA	3527	1/1	0.44	1.07	-	73,73,73,73	0
56	MG	YA	3425	1/1	0.16	0.55	-	88,88,88,88	0
56	MG	RA	3454	1/1	0.76	0.41	-	87,87,87,87	0
56	MG	QA	1788	1/1	0.93	0.58	-	93,93,93,93	0
56	MG	QA	1629	1/1	0.84	0.89	-	83,83,83,83	0
56	MG	RB	220	1/1	0.90	0.71	-	75,75,75,75	0
56	MG	RF	307	1/1	0.82	0.66	-	74,74,74,74	0
56	MG	RF	302	1/1	0.39	0.76	-	80,80,80,80	0
56	MG	RA	3295	1/1	0.47	0.44	-	92,92,92,92	0
56	MG	RA	3301	1/1	0.45	1.69	-	93,93,93,93	0
56	MG	RA	3931	1/1	0.70	0.47	-	78,78,78,78	0
56	MG	YA	3275	1/1	0.85	0.51	-	89,89,89,89	0
56	MG	YA	3204	1/1	0.67	0.38	-	89,89,89,89	0
56	MG	QA	1734	1/1	0.49	0.77	-	84,84,84,84	0
56	MG	XA	1604	1/1	0.71	1.05	-	98,98,98,98	0
56	MG	RA	3845	1/1	0.57	0.73	-	97,97,97,97	0
56	MG	QA	1649	1/1	0.93	0.27	-	73,73,73,73	0
56	MG	RA	3181	1/1	0.16	0.82	-	86,86,86,86	0
56	MG	YA	3044	1/1	0.87	0.30	-	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.