



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2016 – 12:16 AM EDT

PDB ID : 4ZER
Title : Crystal structure of the Onc112 antimicrobial peptide bound to the *Thermus thermophilus* 70S ribosome
Authors : Seefeldt, A.C.; Nguyen, F.; Antunes, S.; Perebaskine, N.; Graf, M.; Arenz, S.; Inampudi, K.K.; Douat, C.; Guichard, G.; Wilson, D.N.; Innis, C.A.
Deposited on : 2015-04-20
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

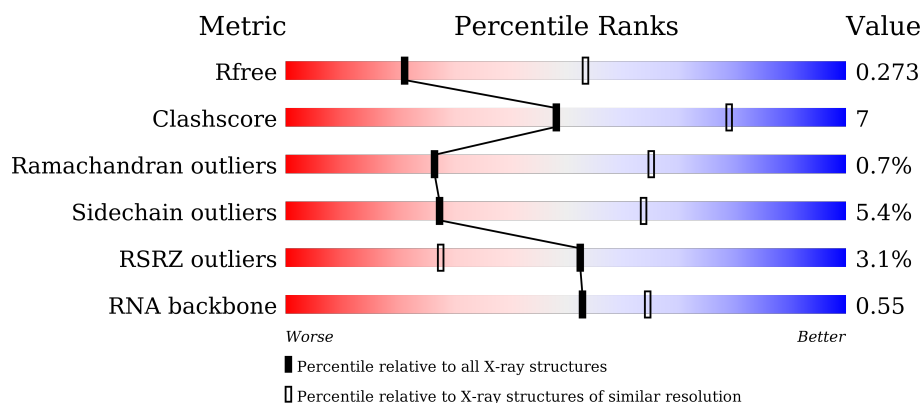
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









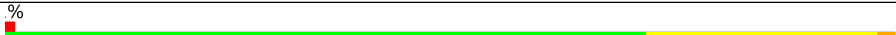
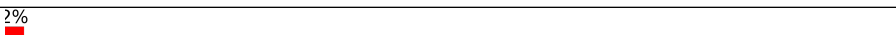
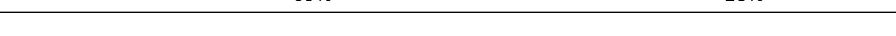
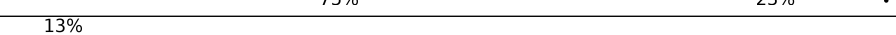
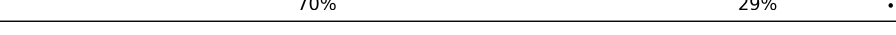
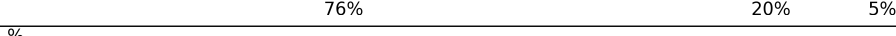













Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1A	2915	<div> <div>3%</div> <div>62% 29% 6% .</div> </div>
1	2A	2915	<div> <div>4%</div> <div>61% 31% 7% .</div> </div>
2	1B	120	<div> <div>61% 34% . .</div> </div>
2	2B	120	<div> <div>70% 27% .</div> </div>


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1D	275	 82% 16% .
3	2D	275	 81% 16% .
4	1E	204	 78% 18% .
4	2E	204	 77% 20% .
5	1F	203	 72% 25% .
5	2F	203	 74% 24% .
6	1G	181	 72% 26% .
6	2G	181	 69% 28% .
7	1H	174	 75% 23% .
7	2H	174	 70% 29% ..
8	1I	147	 76% 20% 5% .
8	2I	147	 76% 21% ..
9	1N	140	 82% 18% .
9	2N	140	 80% 18% .
10	1O	122	 81% 18% .
10	2O	122	 75% 25% .
11	1P	149	 77% 21% .
11	2P	149	 81% 19% .
12	1Q	141	 77% 21% .
12	2Q	141	 74% 23% .
13	1R	118	 75% 21% .
13	2R	118	 72% 24% .
14	1S	110	 75% 23% ..
14	2S	110	 75% 24% .
15	1T	131	 74% 24% .





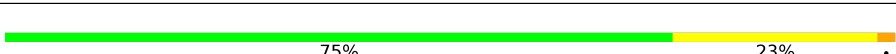
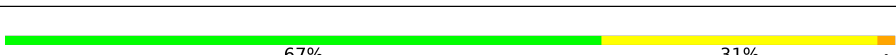
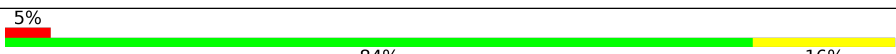
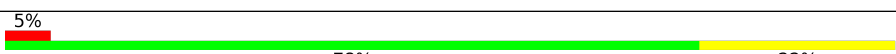
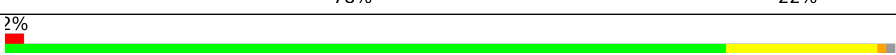

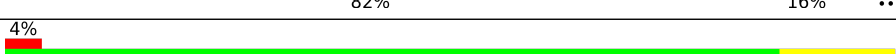
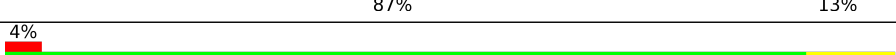
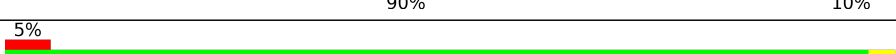
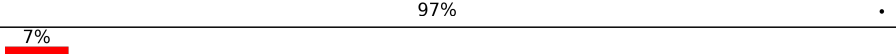
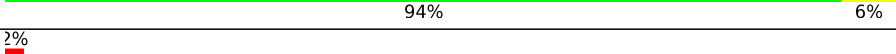
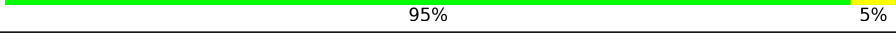
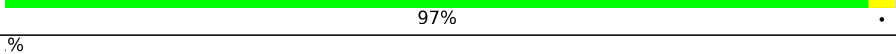
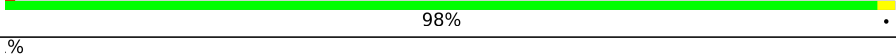
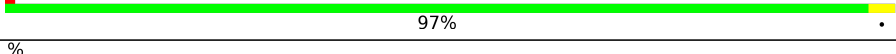
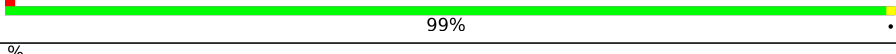
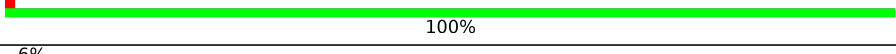
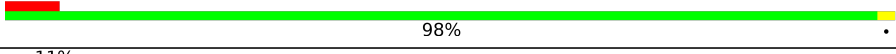
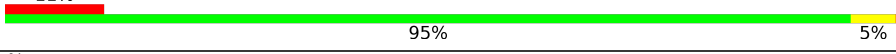
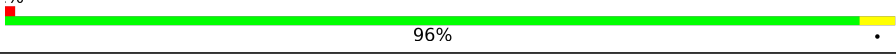
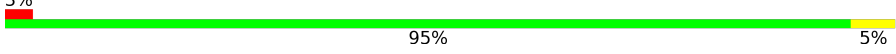
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	131	 77% 23%
16	1U	116	 81% 18% .
16	2U	116	 81% 18% .
17	1V	101	 70% 28% .
17	2V	101	 72% 24% .
18	1W	112	 85% 14% .
18	2W	112	 76% 22% .
19	1X	95	 75% 25%
19	2X	95	 78% 21% .
20	1Y	107	 64% 35% .
20	2Y	107	 73% 26% .
21	1Z	203	 76% 22% .
21	2Z	203	 76% 20% . .
22	10	77	 83% 14% .
22	20	77	 81% 19%
23	11	97	 84% 16%
23	21	97	 71% 29%
24	12	70	 83% 17%
24	22	70	 84% 16%
25	13	59	 71% 22% 7%
25	23	59	 80% 17% .
26	14	69	 59% 35% . .
26	24	69	 61% 35% .
27	15	59	 86% 12% .
27	25	59	 86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	16	53	
28	26	53	
29	17	48	
29	27	48	
30	18	64	
30	28	64	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	231	
33	2b	231	
34	1c	206	
34	2c	206	
35	1d	208	
35	2d	208	
36	1e	148	
36	2e	148	
37	1f	100	
37	2f	100	
38	1g	155	
38	2g	155	
39	1h	137	
39	2h	137	
40	1i	127	


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	2i	127	<div> <div>23%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
41	1j	97	<div> <div>16%</div> <div>94%</div> <div>6%</div> <div>.</div> </div>
41	2j	97	<div> <div>23%</div> <div>96%</div> <div>.</div> <div>.</div> </div>
42	1k	114	<div> <div>97%</div> <div>.</div> </div>
42	2k	114	<div> <div>2%</div> <div>97%</div> <div>.</div> </div>
43	1l	122	<div> <div>2%</div> <div>97%</div> <div>.</div> </div>
43	2l	122	<div> <div>2%</div> <div>97%</div> <div>.</div> </div>
44	1m	116	<div> <div>5%</div> <div>94%</div> <div>6%</div> <div>.</div> </div>
44	2m	116	<div> <div>12%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
45	1n	60	<div> <div>5%</div> <div>95%</div> <div>5%</div> <div>.</div> </div>
45	2n	60	<div> <div>23%</div> <div>98%</div> <div>.</div> </div>
46	1o	88	<div> <div>%</div> <div>97%</div> <div>.</div> </div>
46	2o	88	<div> <div>%</div> <div>93%</div> <div>7%</div> <div>.</div> </div>
47	1p	82	<div> <div>9%</div> <div>93%</div> <div>7%</div> <div>.</div> </div>
47	2p	82	<div> <div>2%</div> <div>93%</div> <div>7%</div> <div>.</div> </div>
48	1q	99	<div> <div>98%</div> <div>.</div> </div>
48	2q	99	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
49	1r	68	<div> <div>99%</div> <div>.</div> </div>
49	2r	68	<div> <div>%</div> <div>99%</div> <div>.</div> </div>
50	1s	83	<div> <div>13%</div> <div>95%</div> <div>5%</div> <div>.</div> </div>
50	2s	83	<div> <div>24%</div> <div>94%</div> <div>6%</div> <div>.</div> </div>
51	1t	98	<div> <div>3%</div> <div>94%</div> <div>.</div> <div>.</div> <div>.</div> </div>
51	2t	98	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>
52	1u	23	<div> <div>9%</div> <div>100%</div> </div>
52	2u	23	<div> <div>48%</div> <div>96%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1x	76	
53	2x	76	
54	1y	19	
54	2y	19	
55	A	27	
55	B	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	15	101	-	-	-	X
56	MG	1A	3001	-	-	-	X
56	MG	1A	3006	-	-	-	X
56	MG	1A	3013	-	-	-	X
56	MG	1A	3019	-	-	-	X
56	MG	1A	3021	-	-	-	X
56	MG	1A	3022	-	-	-	X
56	MG	1A	3024	-	-	-	X
56	MG	1A	3026	-	-	-	X
56	MG	1A	3027	-	-	-	X
56	MG	1A	3038	-	-	-	X
56	MG	1A	3039	-	-	-	X
56	MG	1A	3041	-	-	-	X
56	MG	1A	3047	-	-	-	X
56	MG	1A	3059	-	-	-	X
56	MG	1A	3069	-	-	-	X
56	MG	1A	3071	-	-	-	X
56	MG	1A	3072	-	-	-	X
56	MG	1A	3076	-	-	-	X
56	MG	1A	3085	-	-	-	X
56	MG	1A	3100	-	-	-	X
56	MG	1A	3104	-	-	-	X
56	MG	1A	3107	-	-	-	X
56	MG	1A	3109	-	-	-	X
56	MG	1A	3112	-	-	-	X
56	MG	1A	3118	-	-	-	X
56	MG	1A	3121	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3129	-	-	-	X
56	MG	1A	3130	-	-	-	X
56	MG	1A	3134	-	-	-	X
56	MG	1A	3136	-	-	-	X
56	MG	1A	3137	-	-	-	X
56	MG	1A	3146	-	-	-	X
56	MG	1A	3149	-	-	-	X
56	MG	1A	3150	-	-	-	X
56	MG	1A	3152	-	-	-	X
56	MG	1A	3155	-	-	-	X
56	MG	1A	3164	-	-	-	X
56	MG	1A	3169	-	-	-	X
56	MG	1A	3187	-	-	-	X
56	MG	1A	3189	-	-	-	X
56	MG	1A	3190	-	-	-	X
56	MG	1A	3201	-	-	-	X
56	MG	1A	3211	-	-	-	X
56	MG	1A	3212	-	-	-	X
56	MG	1A	3214	-	-	-	X
56	MG	1A	3218	-	-	-	X
56	MG	1A	3221	-	-	-	X
56	MG	1A	3225	-	-	-	X
56	MG	1A	3228	-	-	-	X
56	MG	1A	3237	-	-	-	X
56	MG	1A	3242	-	-	-	X
56	MG	1A	3255	-	-	-	X
56	MG	1A	3256	-	-	-	X
56	MG	1A	3266	-	-	-	X
56	MG	1A	3271	-	-	-	X
56	MG	1A	3273	-	-	-	X
56	MG	1A	3291	-	-	-	X
56	MG	1A	3297	-	-	-	X
56	MG	1A	3360	-	-	-	X
56	MG	1A	3371	-	-	-	X
56	MG	1A	3386	-	-	-	X
56	MG	1A	3416	-	-	-	X
56	MG	1A	3426	-	-	-	X
56	MG	1A	3432	-	-	-	X
56	MG	1A	3437	-	-	-	X
56	MG	1A	3466	-	-	-	X
56	MG	1A	3482	-	-	-	X
56	MG	1A	3522	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3527	-	-	-	X
56	MG	1A	3535	-	-	-	X
56	MG	1A	3552	-	-	-	X
56	MG	1A	3556	-	-	-	X
56	MG	1A	3558	-	-	-	X
56	MG	1A	3563	-	-	-	X
56	MG	1A	3578	-	-	-	X
56	MG	1A	3579	-	-	-	X
56	MG	1A	3586	-	-	-	X
56	MG	1A	3601	-	-	-	X
56	MG	1A	3618	-	-	-	X
56	MG	1A	3619	-	-	-	X
56	MG	1A	3630	-	-	-	X
56	MG	1A	3644	-	-	-	X
56	MG	1A	3645	-	-	-	X
56	MG	1A	3657	-	-	-	X
56	MG	1A	3659	-	-	-	X
56	MG	1A	3667	-	-	-	X
56	MG	1A	3673	-	-	-	X
56	MG	1A	3703	-	-	-	X
56	MG	1A	3712	-	-	-	X
56	MG	1A	3729	-	-	-	X
56	MG	1A	3737	-	-	-	X
56	MG	1A	3767	-	-	-	X
56	MG	1A	3776	-	-	-	X
56	MG	1A	3782	-	-	-	X
56	MG	1A	3810	-	-	-	X
56	MG	1A	3857	-	-	-	X
56	MG	1A	3885	-	-	-	X
56	MG	1A	3886	-	-	-	X
56	MG	1A	3891	-	-	-	X
56	MG	1A	3892	-	-	-	X
56	MG	1A	3893	-	-	-	X
56	MG	1A	3898	-	-	-	X
56	MG	1A	3919	-	-	-	X
56	MG	1A	3922	-	-	-	X
56	MG	1A	3923	-	-	-	X
56	MG	1A	3925	-	-	-	X
56	MG	1A	3926	-	-	-	X
56	MG	1A	3928	-	-	-	X
56	MG	1A	3929	-	-	-	X
56	MG	1A	3930	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3931	-	-	-	X
56	MG	1A	3935	-	-	-	X
56	MG	1A	3936	-	-	-	X
56	MG	1A	3937	-	-	-	X
56	MG	1A	3938	-	-	-	X
56	MG	1A	3939	-	-	-	X
56	MG	1A	3945	-	-	-	X
56	MG	1A	3946	-	-	-	X
56	MG	1A	3948	-	-	-	X
56	MG	1B	205	-	-	-	X
56	MG	1B	208	-	-	-	X
56	MG	1D	302	-	-	-	X
56	MG	1D	303	-	-	-	X
56	MG	1D	304	-	-	-	X
56	MG	1D	306	-	-	-	X
56	MG	1D	312	-	-	-	X
56	MG	1D	313	-	-	-	X
56	MG	1D	316	-	-	-	X
56	MG	1D	317	-	-	-	X
56	MG	1D	321	-	-	-	X
56	MG	1E	302	-	-	-	X
56	MG	1E	303	-	-	-	X
56	MG	1F	302	-	-	-	X
56	MG	1F	303	-	-	-	X
56	MG	1F	304	-	-	-	X
56	MG	1F	305	-	-	-	X
56	MG	1F	306	-	-	-	X
56	MG	1N	201	-	-	-	X
56	MG	1R	201	-	-	-	X
56	MG	1R	203	-	-	-	X
56	MG	1U	204	-	-	-	X
56	MG	1V	201	-	-	-	X
56	MG	1a	1606	-	-	-	X
56	MG	1a	1615	-	-	-	X
56	MG	1a	1617	-	-	-	X
56	MG	1a	1619	-	-	-	X
56	MG	1a	1625	-	-	-	X
56	MG	1a	1633	-	-	-	X
56	MG	1a	1637	-	-	-	X
56	MG	1a	1639	-	-	-	X
56	MG	1a	1644	-	-	-	X
56	MG	1a	1648	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	1652	-	-	-	X
56	MG	1a	1653	-	-	-	X
56	MG	1a	1655	-	-	-	X
56	MG	1a	1661	-	-	-	X
56	MG	1a	1667	-	-	-	X
56	MG	1a	1668	-	-	-	X
56	MG	1a	1695	-	-	-	X
56	MG	1a	1698	-	-	-	X
56	MG	1a	1710	-	-	-	X
56	MG	1a	1722	-	-	-	X
56	MG	1a	1728	-	-	-	X
56	MG	1a	1732	-	-	-	X
56	MG	1a	1754	-	-	-	X
56	MG	1a	1756	-	-	-	X
56	MG	1a	1766	-	-	-	X
56	MG	1a	1831	-	-	-	X
56	MG	1a	1840	-	-	-	X
56	MG	1a	1842	-	-	-	X
56	MG	1a	1856	-	-	-	X
56	MG	1a	1862	-	-	-	X
56	MG	1e	203	-	-	-	X
56	MG	1o	101	-	-	-	X
56	MG	23	101	-	-	-	X
56	MG	2A	3002	-	-	-	X
56	MG	2A	3010	-	-	-	X
56	MG	2A	3011	-	-	-	X
56	MG	2A	3014	-	-	-	X
56	MG	2A	3017	-	-	-	X
56	MG	2A	3026	-	-	-	X
56	MG	2A	3028	-	-	-	X
56	MG	2A	3046	-	-	-	X
56	MG	2A	3054	-	-	-	X
56	MG	2A	3055	-	-	-	X
56	MG	2A	3057	-	-	-	X
56	MG	2A	3061	-	-	-	X
56	MG	2A	3066	-	-	-	X
56	MG	2A	3071	-	-	-	X
56	MG	2A	3084	-	-	-	X
56	MG	2A	3086	-	-	-	X
56	MG	2A	3087	-	-	-	X
56	MG	2A	3093	-	-	-	X
56	MG	2A	3094	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3096	-	-	-	X
56	MG	2A	3099	-	-	-	X
56	MG	2A	3104	-	-	-	X
56	MG	2A	3106	-	-	-	X
56	MG	2A	3107	-	-	-	X
56	MG	2A	3114	-	-	-	X
56	MG	2A	3124	-	-	-	X
56	MG	2A	3129	-	-	-	X
56	MG	2A	3137	-	-	-	X
56	MG	2A	3140	-	-	-	X
56	MG	2A	3142	-	-	-	X
56	MG	2A	3152	-	-	-	X
56	MG	2A	3168	-	-	-	X
56	MG	2A	3171	-	-	-	X
56	MG	2A	3181	-	-	-	X
56	MG	2A	3183	-	-	-	X
56	MG	2A	3192	-	-	-	X
56	MG	2A	3198	-	-	-	X
56	MG	2A	3220	-	-	-	X
56	MG	2A	3224	-	-	-	X
56	MG	2A	3242	-	-	-	X
56	MG	2A	3243	-	-	-	X
56	MG	2A	3254	-	-	-	X
56	MG	2A	3258	-	-	-	X
56	MG	2A	3264	-	-	-	X
56	MG	2A	3270	-	-	-	X
56	MG	2A	3272	-	-	-	X
56	MG	2A	3273	-	-	-	X
56	MG	2A	3286	-	-	-	X
56	MG	2A	3296	-	-	-	X
56	MG	2A	3300	-	-	-	X
56	MG	2A	3338	-	-	-	X
56	MG	2A	3344	-	-	-	X
56	MG	2A	3384	-	-	-	X
56	MG	2A	3392	-	-	-	X
56	MG	2A	3398	-	-	-	X
56	MG	2A	3417	-	-	-	X
56	MG	2A	3418	-	-	-	X
56	MG	2A	3466	-	-	-	X
56	MG	2A	3475	-	-	-	X
56	MG	2A	3493	-	-	-	X
56	MG	2A	3534	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3539	-	-	-	X
56	MG	2A	3563	-	-	-	X
56	MG	2A	3572	-	-	-	X
56	MG	2A	3601	-	-	-	X
56	MG	2A	3602	-	-	-	X
56	MG	2A	3642	-	-	-	X
56	MG	2A	3644	-	-	-	X
56	MG	2A	3652	-	-	-	X
56	MG	2A	3653	-	-	-	X
56	MG	2A	3654	-	-	-	X
56	MG	2A	3657	-	-	-	X
56	MG	2A	3662	-	-	-	X
56	MG	2A	3663	-	-	-	X
56	MG	2A	3670	-	-	-	X
56	MG	2A	3672	-	-	-	X
56	MG	2A	3674	-	-	-	X
56	MG	2A	3678	-	-	-	X
56	MG	2A	3679	-	-	-	X
56	MG	2D	305	-	-	-	X
56	MG	2D	306	-	-	-	X
56	MG	2D	307	-	-	-	X
56	MG	2E	301	-	-	-	X
56	MG	2F	303	-	-	-	X
56	MG	2Q	201	-	-	-	X
56	MG	2U	202	-	-	-	X
56	MG	2V	202	-	-	-	X
56	MG	2a	1610	-	-	-	X
56	MG	2a	1621	-	-	-	X
56	MG	2a	1624	-	-	-	X
56	MG	2a	1625	-	-	-	X
56	MG	2a	1626	-	-	-	X
56	MG	2a	1628	-	-	-	X
56	MG	2a	1630	-	-	-	X
56	MG	2a	1633	-	-	-	X
56	MG	2a	1634	-	-	-	X
56	MG	2a	1640	-	-	-	X
56	MG	2a	1651	-	-	-	X
56	MG	2a	1653	-	-	-	X
56	MG	2a	1678	-	-	-	X
56	MG	2a	1702	-	-	-	X
56	MG	2a	1712	-	-	-	X
56	MG	2a	1729	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2a	1754	-	-	-	X
56	MG	2a	1756	-	-	-	X
56	MG	2a	1772	-	-	-	X
56	MG	2n	101	-	-	-	X
56	MG	2t	3001	-	-	-	X
56	MG	2x	108	-	-	-	X
57	UNX	2A	3667	-	-	-	X
58	MPD	1A	3907	-	-	-	X
59	ARG	1B	229	-	-	-	X

2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 293672 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2824	Total	C	N	O	P	0	0	0
			60842	27081	11388	19550	2823			
1	2A	2869	Total	C	N	O	P	0	0	0
			61801	27510	11560	19864	2867			

- Molecule 2 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	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	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	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	2O	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	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	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	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	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	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	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	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	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	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	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	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	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	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	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	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	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	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	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	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16s ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	2e	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	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	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	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	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	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	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	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	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	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	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	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called tRNA met.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
53	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
53	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 54 is a protein called Onc112.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	1y	12	Total	C	N	O	0	0	0
			101	67	19	15			
54	2y	12	Total	C	N	O	0	0	0
			101	67	19	15			

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	A	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			
55	B	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	7	Total	Mg	0	0
			7	7		
56	17	2	Total	Mg	0	0
			2	2		
56	1T	2	Total	Mg	0	0
			2	2		
56	1N	3	Total	Mg	0	0
			3	3		
56	20	1	Total	Mg	0	0
			1	1		
56	18	1	Total	Mg	0	0
			1	1		
56	1o	2	Total	Mg	0	0
			2	2		
56	2W	1	Total	Mg	0	0
			1	1		
56	1Y	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2I	1	Total 1	Mg 1	0	0
56	13	3	Total 3	Mg 3	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1P	2	Total 2	Mg 2	0	0
56	2B	17	Total 17	Mg 17	0	0
56	2a	183	Total 183	Mg 183	0	0
56	1E	6	Total 6	Mg 6	0	0
56	1b	1	Total 1	Mg 1	0	0
56	2I	1	Total 1	Mg 1	0	0
56	2F	3	Total 3	Mg 3	0	0
56	28	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1W	3	Total 3	Mg 3	0	0
56	1A	946	Total 946	Mg 946	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	2P	1	Total 1	Mg 1	0	0
56	1X	1	Total 1	Mg 1	0	0
56	2p	1	Total 1	Mg 1	0	0
56	2T	4	Total 4	Mg 4	0	0
56	1D	21	Total 21	Mg 21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2N	1	Total 1	Mg 1	0	0
56	1e	4	Total 4	Mg 4	0	0
56	2G	2	Total 2	Mg 2	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	3	Total 3	Mg 3	0	0
56	2X	1	Total 1	Mg 1	0	0
56	1a	261	Total 261	Mg 261	0	0
56	2Q	2	Total 2	Mg 2	0	0
56	15	3	Total 3	Mg 3	0	0
56	1x	12	Total 12	Mg 12	0	0
56	2j	1	Total 1	Mg 1	0	0
56	1R	4	Total 4	Mg 4	0	0
56	2U	2	Total 2	Mg 2	0	0
56	1G	4	Total 4	Mg 4	0	0
56	2O	2	Total 2	Mg 2	0	0
56	11	3	Total 3	Mg 3	0	0
56	1d	4	Total 4	Mg 4	0	0
56	2n	1	Total 1	Mg 1	0	0
56	1H	2	Total 2	Mg 2	0	0
56	21	1	Total 1	Mg 1	0	0
56	1i	1	Total 1	Mg 1	0	0

Continued on next page...

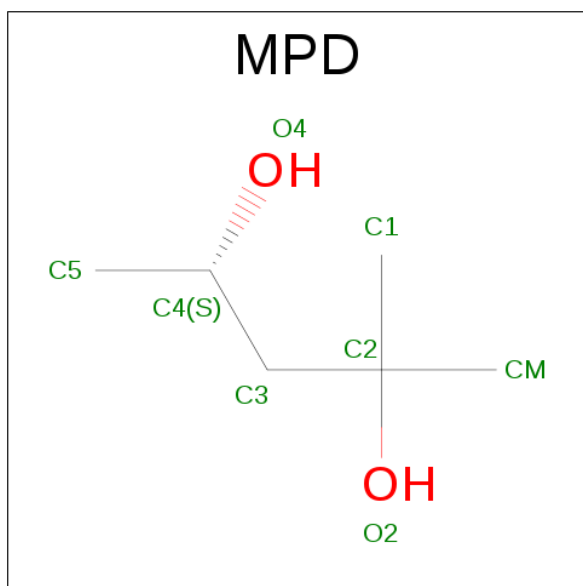
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2Y	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	2x	10	Total 10	Mg 10	0	0
56	2R	1	Total 1	Mg 1	0	0
56	1Z	1	Total 1	Mg 1	0	0
56	2D	8	Total 8	Mg 8	0	0
56	2q	1	Total 1	Mg 1	0	0
56	2k	1	Total 1	Mg 1	0	0
56	1U	5	Total 5	Mg 5	0	0
56	1O	1	Total 1	Mg 1	0	0
56	1r	1	Total 1	Mg 1	0	0
56	19	2	Total 2	Mg 2	0	0
56	1l	1	Total 1	Mg 1	0	0
56	2V	3	Total 3	Mg 3	0	0
56	1F	9	Total 9	Mg 9	0	0
56	10	7	Total 7	Mg 7	0	0
56	1g	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	1Q	4	Total 4	Mg 4	0	0
56	2A	679	Total 679	Mg 679	0	0
56	1B	29	Total 29	Mg 29	0	0

- Molecule 57 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

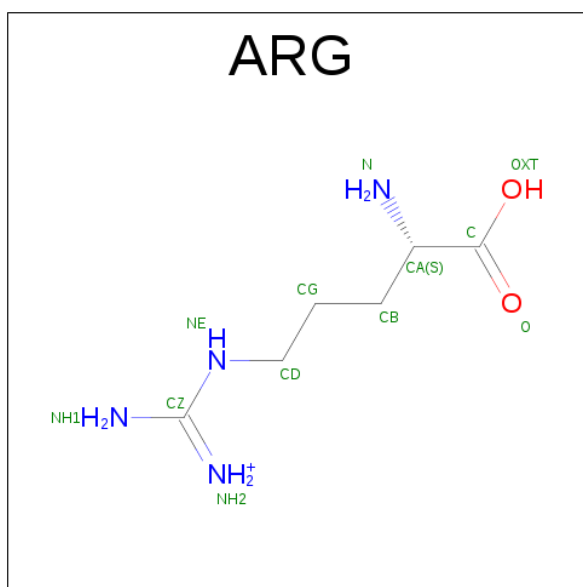
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1	Total	X	0	0
			1	1		
57	2A	1	Total	X	0	0
			1	1		

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1A	1	Total	C	O	0	0
			8	6	2		
58	1a	1	Total	C	O	0	0
			8	6	2		

- Molecule 59 is ARGinine (three-letter code: ARG) (formula: C₆H₁₅N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

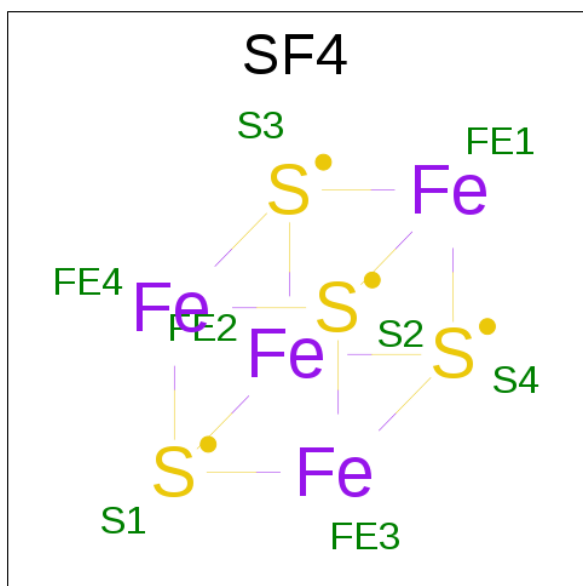
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	29	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	2n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	16	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2A	1	Total	K	0	0
			1	1		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1A	1632	Total	O	0	0
			1632	1632		
63	1B	50	Total	O	0	0
			50	50		
63	1D	20	Total	O	0	0
			20	20		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1E	17	Total	O	0	0
			17	17		
63	1F	14	Total	O	0	0
			14	14		
63	1G	5	Total	O	0	0
			5	5		
63	1H	4	Total	O	0	0
			4	4		
63	1N	7	Total	O	0	0
			7	7		
63	1O	2	Total	O	0	0
			2	2		
63	1P	18	Total	O	0	0
			18	18		
63	1Q	5	Total	O	0	0
			5	5		
63	1R	7	Total	O	0	0
			7	7		
63	1T	4	Total	O	0	0
			4	4		
63	1U	3	Total	O	0	0
			3	3		
63	1V	3	Total	O	0	0
			3	3		
63	1X	6	Total	O	0	0
			6	6		
63	1Y	2	Total	O	0	0
			2	2		
63	10	4	Total	O	0	0
			4	4		
63	11	3	Total	O	0	0
			3	3		
63	13	6	Total	O	0	0
			6	6		
63	15	2	Total	O	0	0
			2	2		
63	16	3	Total	O	0	0
			3	3		
63	18	7	Total	O	0	0
			7	7		
63	19	3	Total	O	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1a	369	Total 369	O 369	0	0
63	1c	1	Total 1	O 1	0	0
63	1d	6	Total 6	O 6	0	0
63	1e	3	Total 3	O 3	0	0
63	1f	1	Total 1	O 1	0	0
63	1h	1	Total 1	O 1	0	0
63	1l	3	Total 3	O 3	0	0
63	1m	1	Total 1	O 1	0	0
63	1n	1	Total 1	O 1	0	0
63	1o	2	Total 2	O 2	0	0
63	1p	1	Total 1	O 1	0	0
63	1t	1	Total 1	O 1	0	0
63	1x	2	Total 2	O 2	0	0
63	2A	1221	Total 1221	O 1221	0	0
63	2B	33	Total 33	O 33	0	0
63	2D	13	Total 13	O 13	0	0
63	2E	12	Total 12	O 12	0	0
63	2F	4	Total 4	O 4	0	0
63	2N	2	Total 2	O 2	0	0
63	2O	4	Total 4	O 4	0	0
63	2P	7	Total 7	O 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2Q	5	Total 5	O 5	0	0
63	2R	2	Total 2	O 2	0	0
63	2T	2	Total 2	O 2	0	0
63	2U	3	Total 3	O 3	0	0
63	2X	4	Total 4	O 4	0	0
63	2Y	1	Total 1	O 1	0	0
63	20	2	Total 2	O 2	0	0
63	21	2	Total 2	O 2	0	0
63	23	2	Total 2	O 2	0	0
63	25	1	Total 1	O 1	0	0
63	26	2	Total 2	O 2	0	0
63	28	5	Total 5	O 5	0	0
63	2a	305	Total 305	O 305	0	0
63	2d	3	Total 3	O 3	0	0
63	2e	1	Total 1	O 1	0	0
63	2j	2	Total 2	O 2	0	0
63	2l	1	Total 1	O 1	0	0
63	2n	1	Total 1	O 1	0	0
63	2p	1	Total 1	O 1	0	0
63	2r	1	Total 1	O 1	0	0
63	2t	1	Total 1	O 1	0	0

Continued on next page...

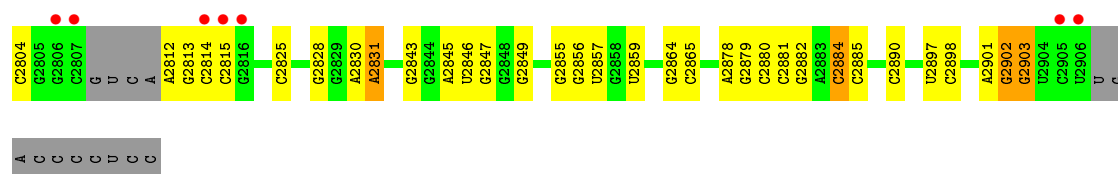
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2x	2	Total	O	0	0
			2	2		
63	A	1	Total	O	0	0
			1	1		

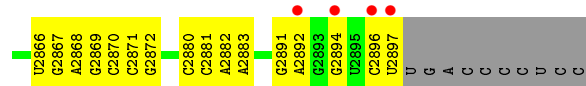
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

- [illegible]

C2692	U2559	A2437	C2338	A2237	U2097	U1977	G1854	C1731	C1594	G1495	G1401	G1290	A1774
U2699	C2560	G2441	C2238	G2240	U2101	U1985	G1857	U1735	C1595	A1496	G1404	G1291	A1775
U2700	C2562	A2442	G2240	G2240	U2102	U1986	G1858	A1736	C1596	A1405	G1405	G1292	U1776
C2702	U2563	A2446	U2244	U2245	U2103	G1989	G1859	A1737	C1597	A1406	G1406	A1299	C1180
C2703	C2565	A2447	U2246	U2246	U2114	C1990	G1870	G1743	A1613	G1409	G1409	G1302	G1181
U2710	U2567	A2450	G2250	G2250	G2115	A1991	G1871	A1747	A1616	G1410	G1410	C1303	G1182
C2711	C2568	A2451	G2251	G2251	C2119	A1992	G1872	A1748	U1625	C1514	G1414	G1304	C1185
C2712	C2569	C2452	C2252	C2252	U2120	A1993	G1873	G1749	U1626	G1517	G1415	G1305	U1186
U2714	C2570	C2453	A2253	A2253	U2121	A1994	G1874	G1750	A1626	G1518	G1416	G1310	U1187
U2715	C2573	C2454	G2254	G2254	U2122	G2014	A1878	G1751	A1627	G1519	G1417	A1311	A1188
C2716	C2576	C2455	U2255	U2255	U2123	U2015	A1879	G1752	C1631	C1521	U1418	G1312	G1195
C2717	C2577	C2456	U2256	U2256	U2124	C2018	G1889	U1753	A1632	G1522	U1419	U1313	G1199
U2721	A2576	C2457	U2257	U2257	C2125	G2019	A1990	U1765	G1639	G1525	A1425	A1314	C1199
U2724	C2578	C2458	G2258	G2258	U2126	C2020	G1991	G1766	G1640	G1529	A1426	A1315	G1200
A2725	C2579	A2459	A2259	A2259	C2127	A2023	G1992	A1767	C1653	G1532	G1432	C1316	A1201
A2726	C2580	C2460	G2263	G2263	G2128	G2024	G1993	U1768	A1654	G1533	A1433	G1317	A1202
C2727	C2586	U2474	U2370	U2370	C2130	A1996	G1994	U1769	A1655	G1534	A1434	A1318	G1206
A2734	C2587	C2475	A2280	A2280	U2131	G2031	C1897	G1771	A1656	G1539	G1435	A1321	C1211
C2739	C2594	C2476	A2281	A2281	C2132	G2034	A1898	G1785	A1662	A1540	G1436	A1324	C1212
G2740	U2597	A2480	A2285	A2285	C2133	A2035	G1900	A1788	A1668	A1542	U1437	G1331	G1217
G2745	C2598	A2481	A2286	A2286	G2134	A2036	C1901	U1788	G1668	A1543	U1438	C1335	G1218
A2746	A2602	C2488	G2289	G2289	A2136	U2044	G1905	G1794	G1682	C1551	A1441	C1336	A1219
A2747	C2603	C2489	A2290	A2290	C2137	G2045	C1906	G1795	C1683	C1552	U1442	U1338	U1220
C2748	C2614	G2495	G2291	G2291	U2139	U2046	G1907	G1812	A1686	A1553	U1443	C1339	G1221
C2760	A2615	C2496	C2295	C2295	U2140	G2049	A1911	A1804	U1687	C1554	U1444	C1342	A1222
A2761	U2616	A2500	C2296	C2296	A2141	U2050	G1912	C1805	C1687	C1555	U1445	G1343	C1223
C2762	C2620	C2503	C2297	C2297	G2142	G2051	A1922	U1805	A1688	C1556	U1446	U1344	C1224
C2768	U2621	U2503	A2298	A2298	U2143	A2052	G1922	A1811	A1689	A1557	U1447	U1345	C1225
C2769	C2622	C2495	G2299	G2299	U2144	G2053	G1925	G1812	G1690	A1558	G1459	A1347	G1231
A2771	U2623	C2510	C2300	C2300	G2146	A2055	G1928	C1813	C1691	C1559	G1460	A1348	G1232
C2778	C2624	C2511	G2301	G2301	G2147	C2058	G1929	A1814	C1695	U1560	G1462	U1233	U1233
G2779	C2629	U2512	C2302	C2302	A2148	G2059	A1934	A1817	A1699	C1561	G1463	G1357	A1234
C2780	C2639	C2513	U2303	U2303	C2149	G2060	A1935	G1830	A1700	U1562	G1464	U1358	A1239
C2784	C2640	U2515	C2305	C2305	U2150	C2061	C1936	C1821	A1701	G1563	U1465	U1359	C1245
C2785	A2641	G2516	C2306	C2306	C2151	C2062	U1937	A1822	A1701	G1564	U1466	C1360	C1246
C2786	C2642	U2517	C2307	C2307	U2152	U2063	A1940	G1823	C1704	U1566	G1467	C1361	C1247
C2787	G2643	U2518	U2308	U2308	U2153	C2064	A1941	U1829	C1705	G1567	G1471	A1363	G1248
A2791	C2644	C2524	G2316	G2316	U2154	C2065	C1942	U1830	C1705	A1575	G1472	A1367	A1255
U2792	C2658	G2525	A2317	A2317	A2155	C2077	G1951	G1831	G1710	C1579	A1473	A1367	U1256
C2793	U2659	U2526	C2317	C2317	A2156	G2078	G1952	G1832	A1711	G	G1474	G1378	C1263
A2794	C2660	C2417	U2324	U2324	C2158	A2081	G1953	A1834	A1712	U	G1475	U1386	A1263
C2798	U2661	G2422	G2327	G2327	C2160	A2082	U1954	C1835	A1715	A	G1481	U1387	G1277
U2799	U2662	C2328	C2328	C2328	C2161	G2083	G1955	U1836	A1716	C	G1482	U1387	G1277
C2799	A2666	G2426	U2330	U2330	A2084	A2084	G1956	U1836	G1721	G1584	C1483	C1391	G1281
C2800	C2667	C2331	G2231	G2231	C2164	U2090	G1957	A1841	G1721	G1585	A1491	C1391	G1281
A2801	A2674	A2332	G2232	G2232	C2165	G2091	A1958	G1842	G1725	G1586	A1492	U1398	G1282
C2802	C2676	G2333	G2233	G2233	U2166	U2091	A1959	A1846	G1725	U1587	C1492	A1399	G1285
A2803	C2686	A2434	G2236	G2236	C2168	U2096	A1961	G1847	C1730	G1588	G1494	A1400	U1286

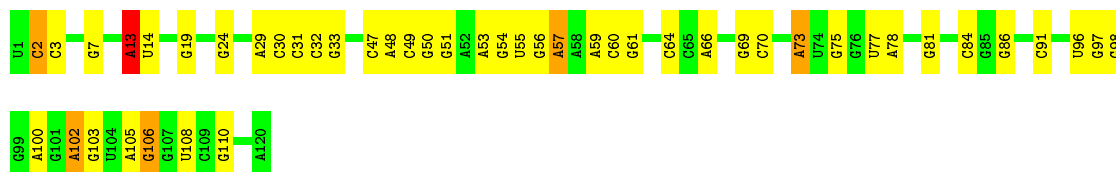


C2745	C2635	G2559	A2430	G2334	U2232	G2148	U2075	C1962	A1812	A1664	G1525	C1428	U1211
U2746	U2636	G2559	A2435	A2335	U2233	G2149	U2076	C1963	A1816	G1667	G1529	G1429	C1297
A2747	G2637	U2537	A2439	A2336	G2234	G2150	U2079	G1964	A1819	A1668	G1529	U1430	C1218
U2756	G2638	C2538	A2443	G2340	G2238	G2151	G2080	U1967	A1820	A1669	U1300	U1431	A1220
A2757	G2640	C2540	C2441	G2343	G2239	G2152	A2082	C1967	A1823	G1675	G1533	C1432	G1221A
A2758	G2641	C2541	C2442	U2344	G2240	G2153	G2086	A1970	G1824	C1674	U1312	C1222	C1221A
		A2542	C2443	G2347	U2245	G2154	G2087	A1971	A1825	C1675	A	G1441	G1223
A2764	U2647	C2543	G2444	U2348	G2246	G2155	U2086	A1972	G1826	C1676	C1536	G1442	
A2765	U2648	G2544	G2445	U2349	G2247	G2156	G2087	A1973	G1827	U1688	A1542	U1316	A1226
	U2649		G2446	G2350	G2251	G2157	G2093	C1974	G1828	U1688	C1543	G1443	A1227
C2769		U2547	G2447	G2351	G2252	G2158	G2160	A1700	A1829	A1700	C1547	G1444	G1227
	A2654	G2548	A2448	G2352	A2268	G2159	G2161	A1701	G1830	A1701	C1547	G1445	G1228
A2776	G2659	G2549	A2451	A2352	A2269	G2162	G2101		G1835			G1446	G1229
C2777	A2660	G2550		A2353	A2270	G2163	G2102	U1991	G1836	U1709	A1558	A1449	G1230
A2778	G2661	C2551	U2457	A2360	A2271	G2164	G2103	G1992	A1837	C1710	G1559	G1450	G1231
	A2662	G2552		A2361	A2272	G2165	G2104	U1993	G1839	C1711		C1450A	
A2781	G2663	G2553	U2462	A2362	C2275	G2166	G2105	C1996	G1842		A1566	G1459	G1235
G2782		U2554		G2365	G2276	G2167	G2106	G1997	G1843	G1721	A1569	A1460	G1236
	U2682	C2556	C2466	G2366	G2277	G2168	G2107	C1998	A1847	A1722	C1569	A1461	A1237
C2788	G2683	C2557	G2467	G2367	G2278	G2169	G2108	C1999	A1848	U1739	U1578	G1466	G1238
C2789		A2561	G2468	G2368	G2279	G2170	G2109		A1849	G1740	A1579	C1467	G1239
A	U2687		A2469	G2369	G2280	G2171	G2110		A1850	A1741	A1580	G1468	U1240
C2792	U2688	A2562	G2472	G2370	A2281	G2172	G2111	G2004	G1861	G1746		G1470	A1241
G2793	U2689	A2563	G2473	G2371	A2282	G2173	U2113	A2005	A1877			A1471	G1244
C2794	G2690	A2564	G2474	G2372	A2283	G2174	A2114	G2010	A1878	C1754	A1586	A1571	A1247
G	C2691	C2565	C2475	G2373	G2284	G2175	G2115	G2011	G1879	A1755		G1474	G1250
U		G2566	G2476	U2377	U2285	G2176	G2116	U2012	A1889	G1756	G1593	G1364	
C	G2695	C2567	C2477	A2378	G2286	G2177	G2117	G2013			G1594	A1365	
A	U2696	A2572	G2478	G2379	G2287	G2178	G2118	A2014	G1899	C1761		G1482	A1253
A2801A	G2697	C2573	A2478	G2380	U2288	G2179	G2119		A1900	A1762	C1598	G1491	A1254
C2802	U2698	G2574	G2479	G2381	A2289	G2180	G2120	U2022	A1877	G1763		G1492	G1255
C2803	G2699	C2575	G2480	G2382	G2290	G2181	G2121	G2023	A1878	G1764	U1602	C1493	G1256
G2804		G2576	G2485	G2383	G2291	G2182	G2122		A1879		A1603	A1494	U1263
C2805	U2702	A2577	A2488	G2384	G2303	G2183	G2123	A2031	A1919	A1773	C1607	A1495	G1264
G2807	C2703		G2489	U2390	A2304	G2184	G2124	G3082	A1927	A1780	A1608	A1496	A1265
U2808	C2704	G2582	G2490	G2399	G2305	G2185	G2125	A2033	A1928	C1781	A1609	U1497	G1266
A2809	A2705	U2585	U2491	G2400	G2306	G2186	A2126	A2033	A1929	C1782	A1610	C1498	U1267
			G2492	G2401	G2307	G2187	G2127	C2040	G1930	A1783		C1499	U1268
C2816	C2710		G2493	G2402	A2308	G2188	G2128	C2043	G1931	A1786	A1614	G1500	A1268
G2817	A2711	A2602	U2494	G2403	A2309	G2189	G2129		U1932				A1269
U2712	U2712	G2602	G2495	G2404	A2310	G2190	G2130	C2055	A1933	A1791	C1622	U1503	G1270
A2712A		C2606	G2496	U2406	A2311	G2191	U2131	G2056	A1934	U1794	C1404	C1504	A1272
A2820	A2713	G2607	G2497	G2407	U2312	G2192	G2132	G2059	A1935	C1795	C1404	C1505	U1273
G2822	G2714	G2608	A2411	G2410	C2313	G2193	G2133	A2060	A1936	C1796	U1406	C1506	
			G2412	A2412	G2314	G2194	G2134	G2061	A1937	U1797	A1412	A1507	A1278
G2823		G2502	G2414	G2413	C2315	G2195	A2135	A2062	A1938	C1797	A1413	C1508	G1279
	G2718	U2611	G2503	G2415	G2316	G2196	G2136	G2067		U1798	A1641	A1509A	U1282
G2719	G2719	C2612	U2504	G2416	G2317	G2197	G2137	G2068	G1945	C1799	G1416	G1283	G1283
		U2613	G2505	G2417	G2318	A2198	G2138	G2069	G1946	U1799	C1417	A1513	A1284
C2723	C2723	A2614	U2506	G2418	G2319		C2139	G2070	U1947	C1640	C1417	U1514	G1285
		A2615	A2422	G2420	A2320	U2203	G2140	A2071	A1802	A1641	U1420	G1515	A1286
G2839	U2726	C2617	U2511	G2421	G2321	C2205	G2141	G2072	A1803	A1641	G1421	G1516	A1287
G2845	G2727		G2512	U2423	A2322	G2206	G2142	C2073	A1810	C1800	G1422	U1517	U1292
G2846	U2728	C2620	G2513	G2424	G2323	G2207	G2143	G2074	A1811	G1801	G1423	U1518	C1293
U2847			G2514	A2425	G2324	A2208	G2144	A2072					
U2848		A2629	A2518	G2426	G2325	G2224	U2145	A2073					
U2849	A2732	G2630	U2519	G2427	G2326	G2225	C2146	C2074					
A2850	A2733		G2520	A2428	A2327	G2226	G2147	U2074					



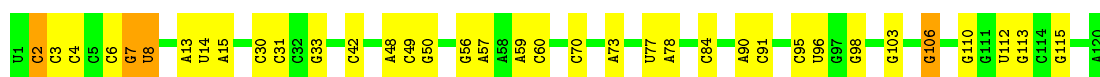
- Molecule 2: 5s ribosomal RNA

Chain 1B: 61% 34%



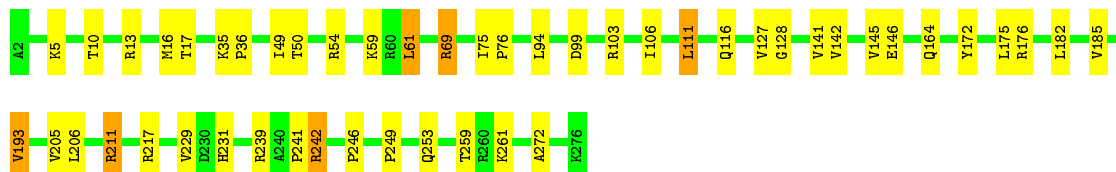
- Molecule 2: 5s ribosomal RNA

Chain 2B: 70% 27%



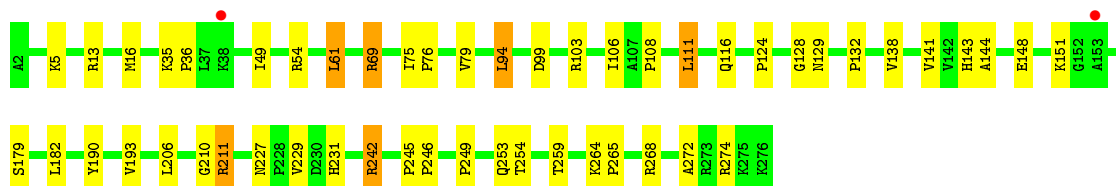
- Molecule 3: 50S ribosomal protein L2

Chain 1D: 82% 16%



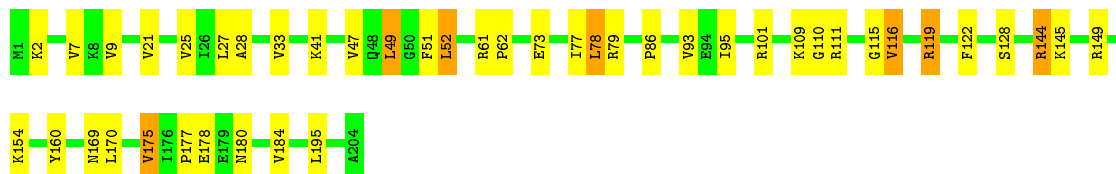
- Molecule 3: 50S ribosomal protein L2

Chain 2D: 81% 16%

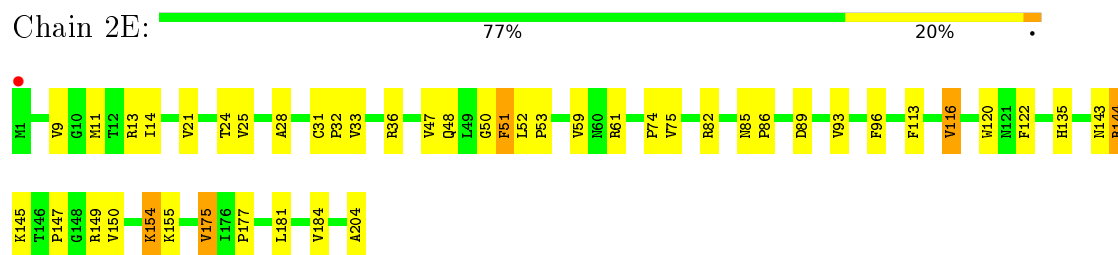


- Molecule 4: 50S ribosomal protein L3

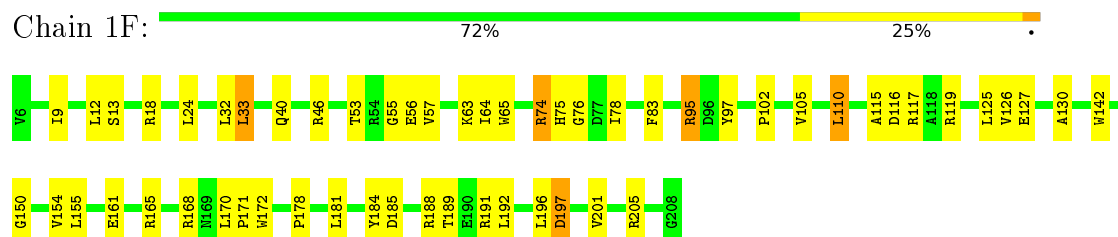
Chain 1E: 78% 18%



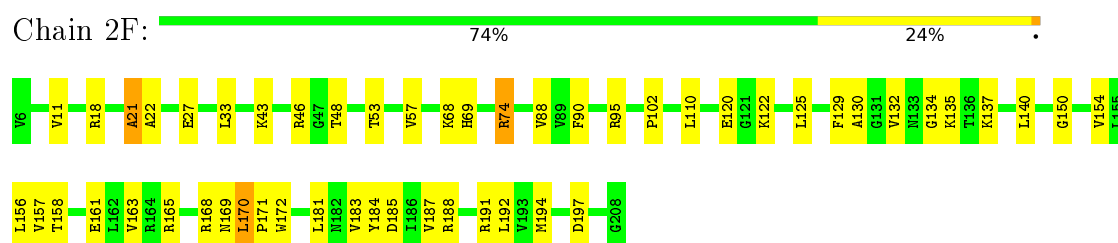
- Molecule 4: 50S ribosomal protein L3



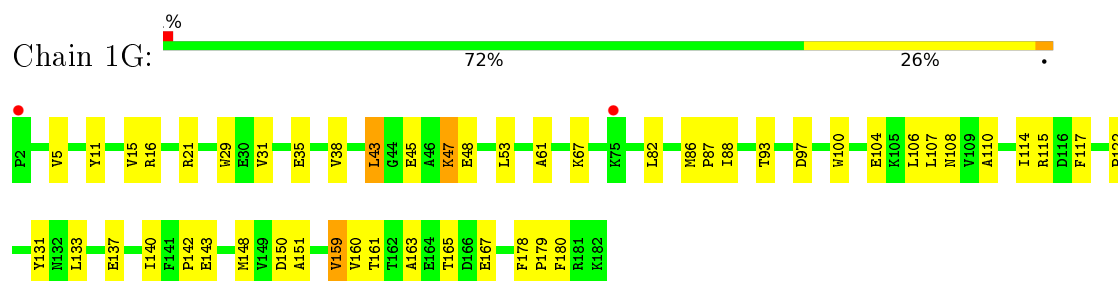
- Molecule 5: 50S ribosomal protein L4



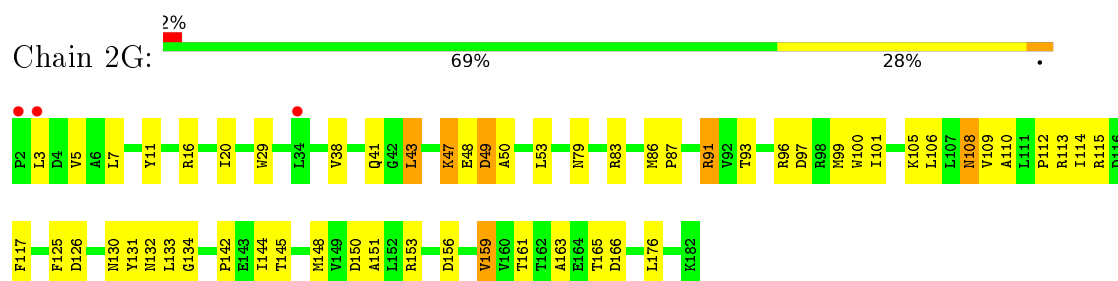
- Molecule 5: 50S ribosomal protein L4



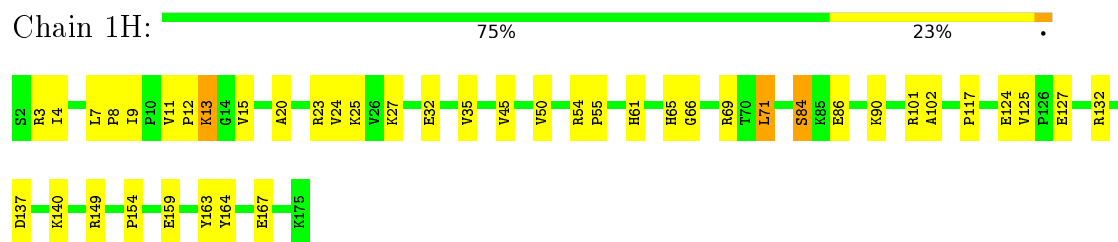
- Molecule 6: 50S ribosomal protein L5



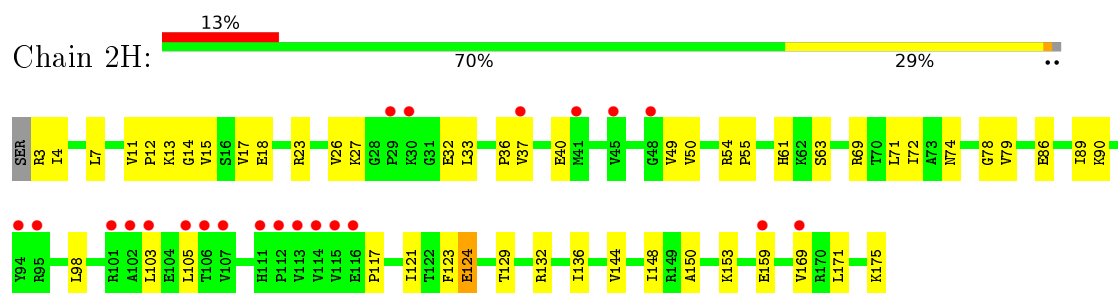
- Molecule 6: 50S ribosomal protein L5



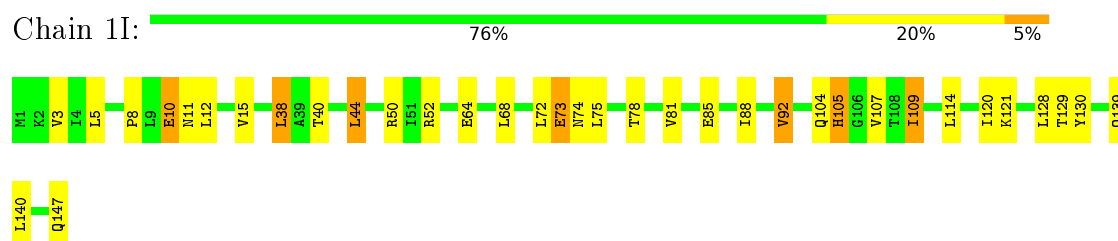
- Molecule 7: 50S ribosomal protein L6



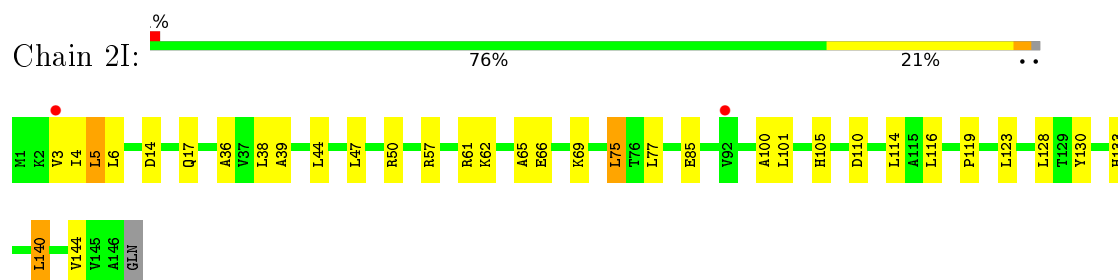
- Molecule 7: 50S ribosomal protein L6



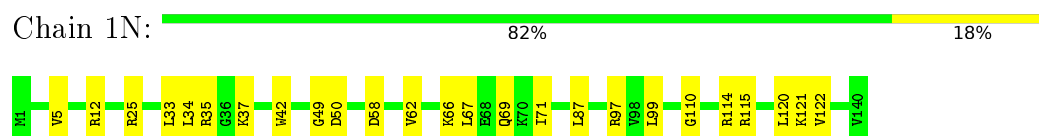
- Molecule 8: 50S ribosomal protein L9



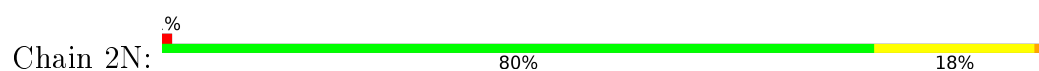
- Molecule 8: 50S ribosomal protein L9

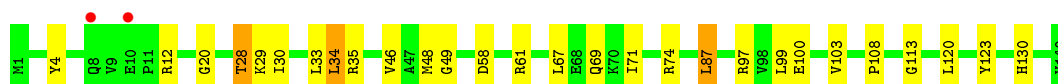


- Molecule 9: 50S ribosomal protein L13

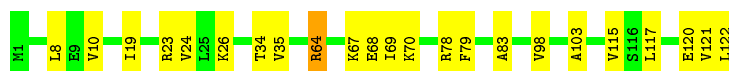
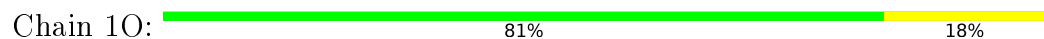


- Molecule 9: 50S ribosomal protein L13

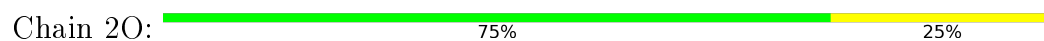




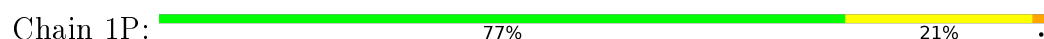
- Molecule 10: 50S ribosomal protein L14



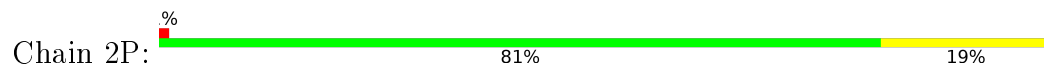
- Molecule 10: 50S ribosomal protein L14



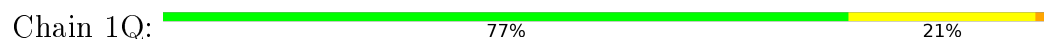
- Molecule 11: 50S ribosomal protein L15



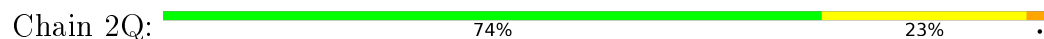
- Molecule 11: 50S ribosomal protein L15




- Molecule 12: 50S ribosomal protein L16

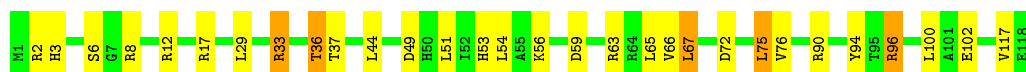


- Molecule 12: 50S ribosomal protein L16



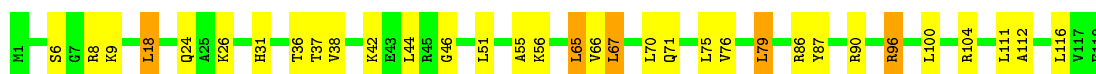
- Molecule 13: 50S ribosomal protein L17

Chain 1R:  75% 21% .



- Molecule 13: 50S ribosomal protein L17

Chain 2R:  72% 24% .




- Molecule 14: 50S ribosomal protein L18

Chain 1S:  75% 23% ..




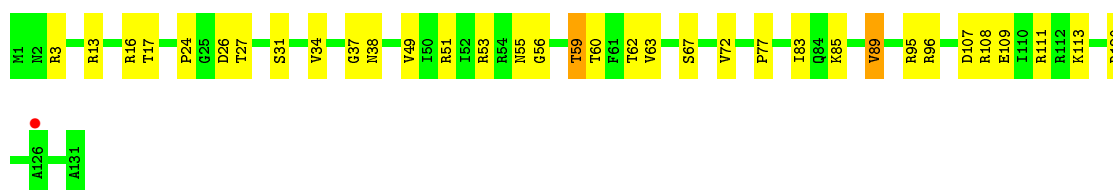
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  5% 75% 24% .




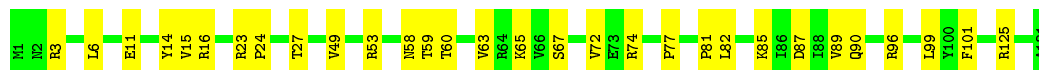
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  % 74% 24% .




- Molecule 15: 50S ribosomal protein L19

Chain 2T:  77% 23% .

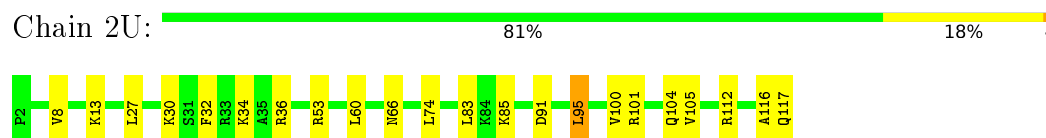


- Molecule 16: 50S ribosomal protein L20

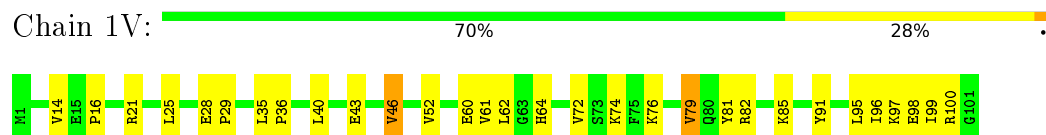
Chain 1U:  81% 18% .



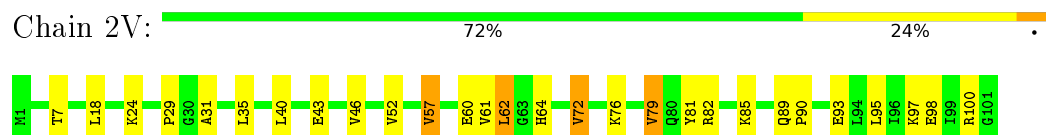
- Molecule 16: 50S ribosomal protein L20



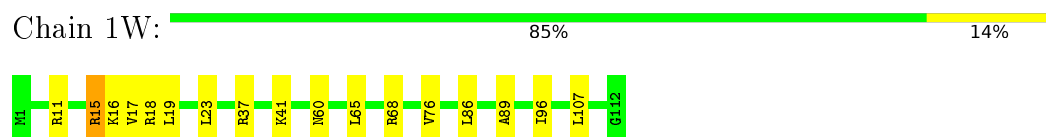
- Molecule 17: 50S ribosomal protein L21



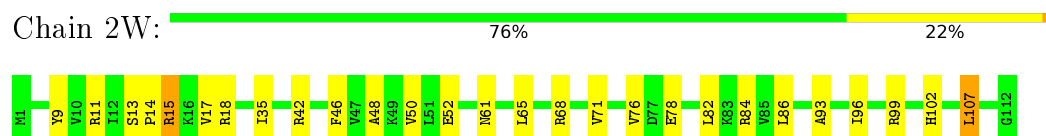
- Molecule 17: 50S ribosomal protein L21



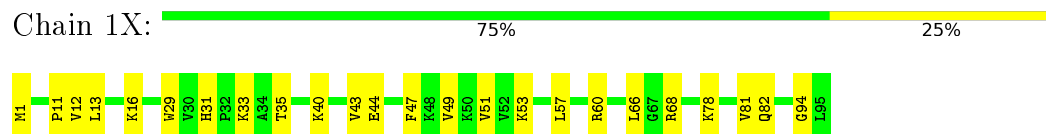
- Molecule 18: 50S ribosomal protein L22



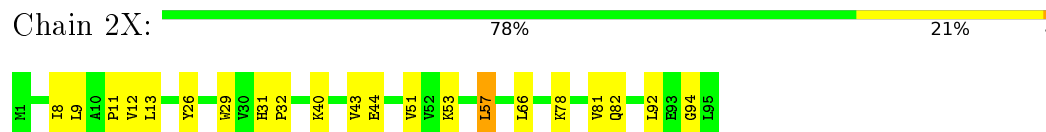
- Molecule 18: 50S ribosomal protein L22



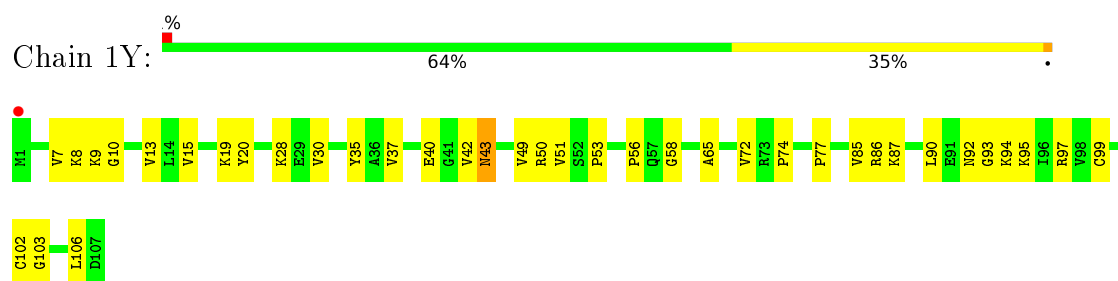
- Molecule 19: 50S ribosomal protein L23



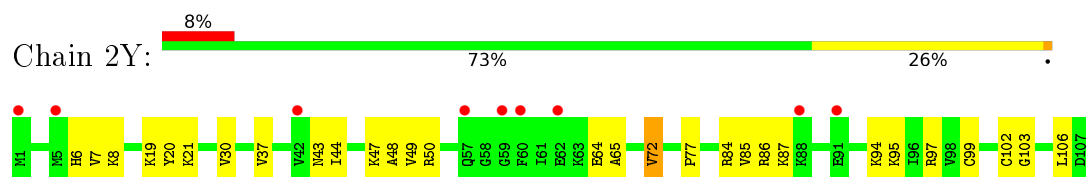
- Molecule 19: 50S ribosomal protein L23



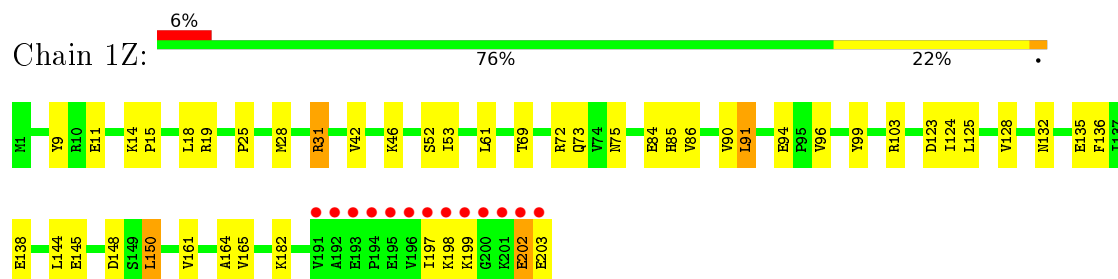
- Molecule 20: 50S ribosomal protein L24



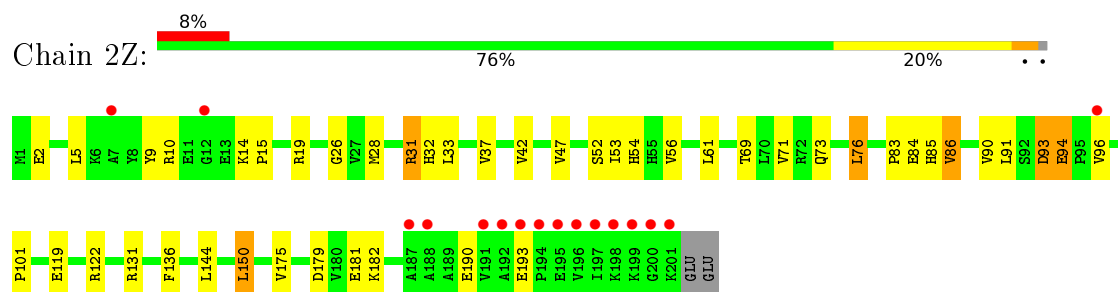
- Molecule 20: 50S ribosomal protein L24



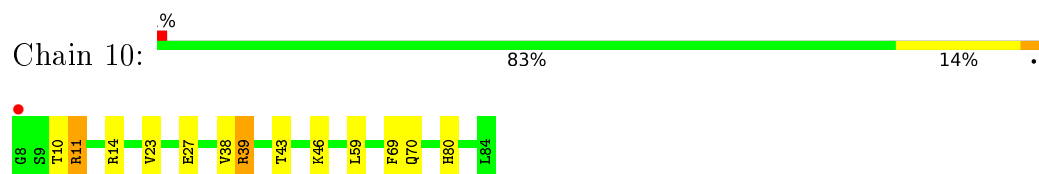
- Molecule 21: 50S ribosomal protein L25



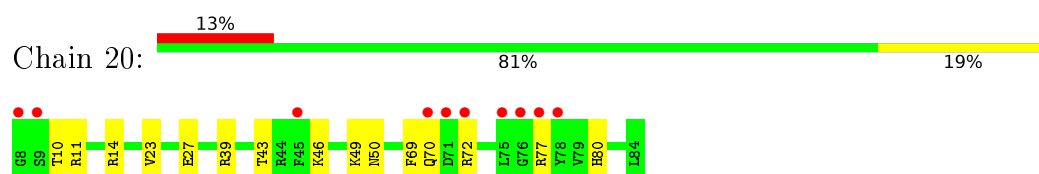
- Molecule 21: 50S ribosomal protein L25



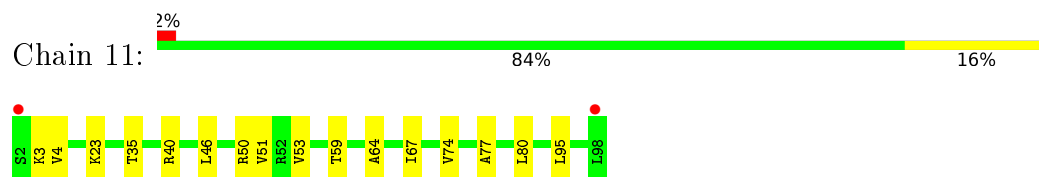
- Molecule 22: 50S ribosomal protein L27



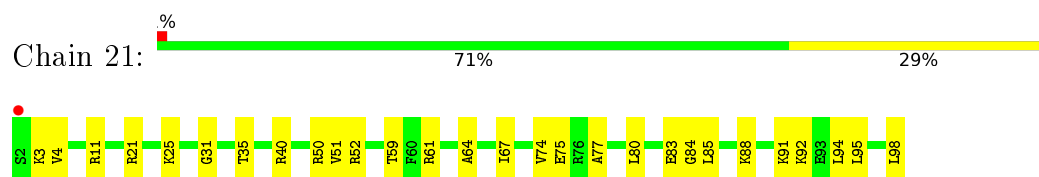
- Molecule 22: 50S ribosomal protein L27



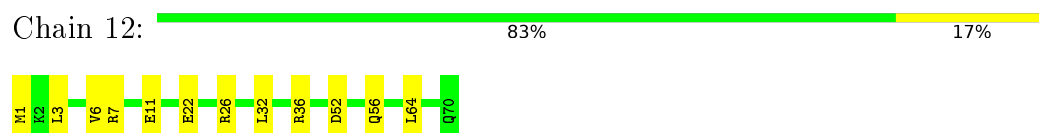
- Molecule 23: 50S ribosomal protein L28



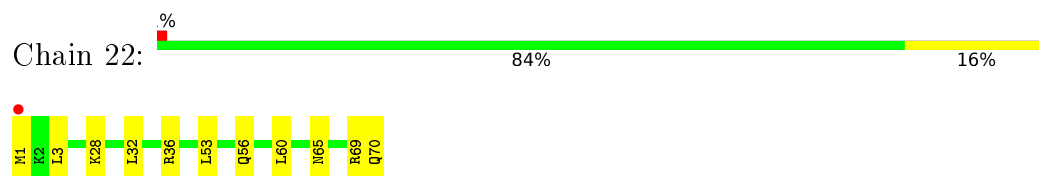
- Molecule 23: 50S ribosomal protein L28



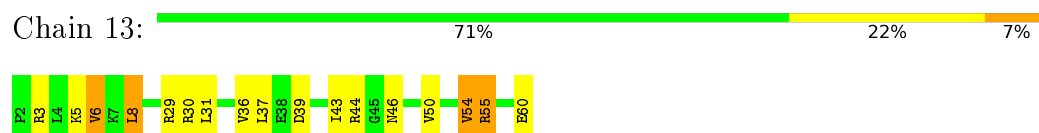
- Molecule 24: 50S ribosomal protein L29



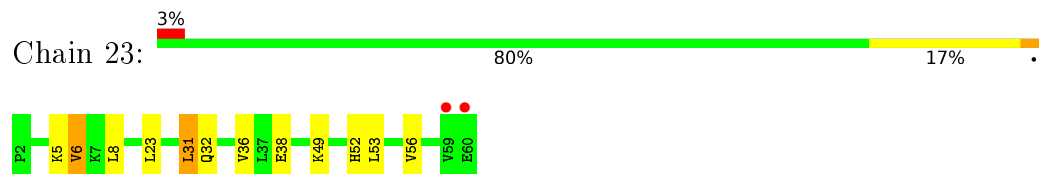
- Molecule 24: 50S ribosomal protein L29



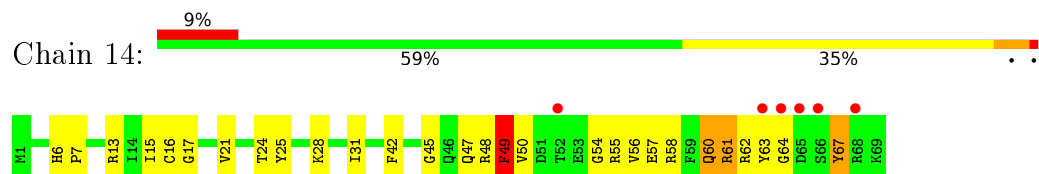
- Molecule 25: 50S ribosomal protein L30



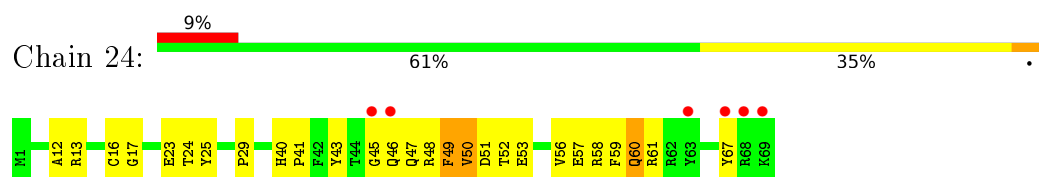
- Molecule 25: 50S ribosomal protein L30



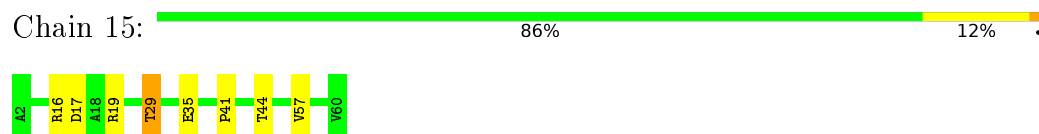
- Molecule 26: 50S ribosomal protein L31



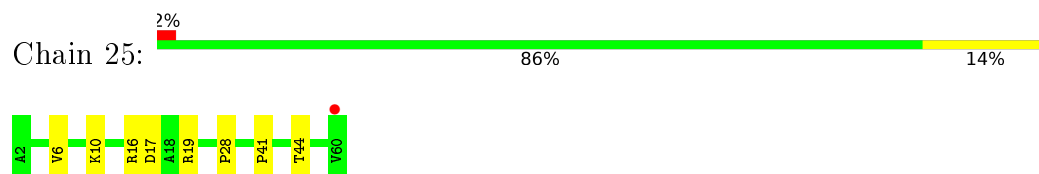
- Molecule 26: 50S ribosomal protein L31



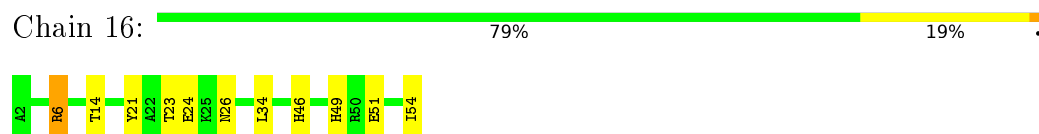
- Molecule 27: 50S ribosomal protein L32



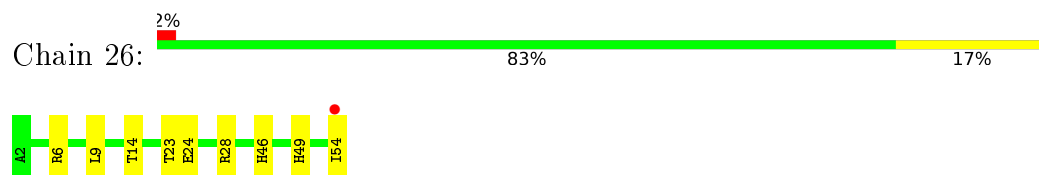
- Molecule 27: 50S ribosomal protein L32



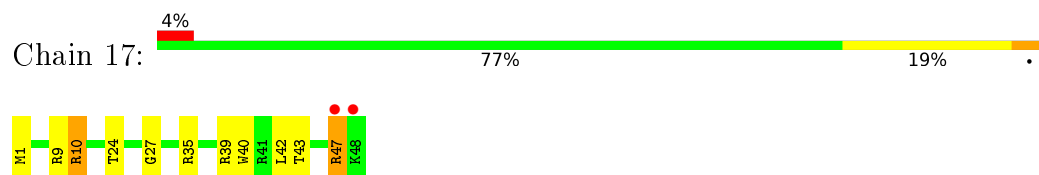
- Molecule 28: 50S ribosomal protein L33



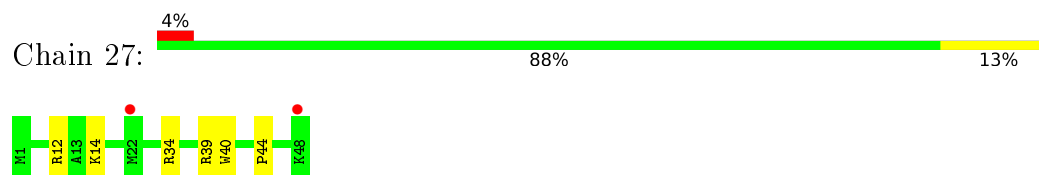
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35

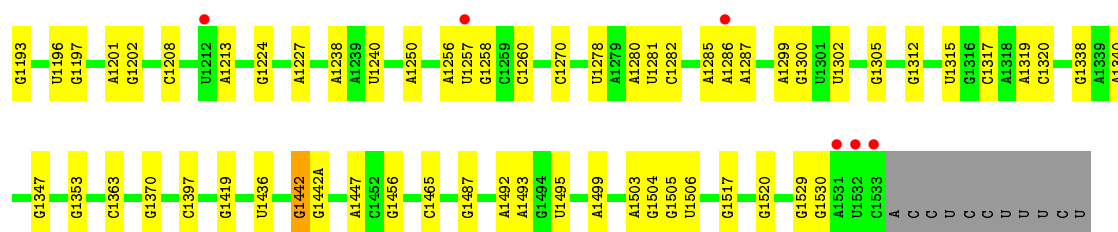
- Molecule 30: 50S ribosomal protein L35

- Molecule 31: 50S ribosomal protein L36

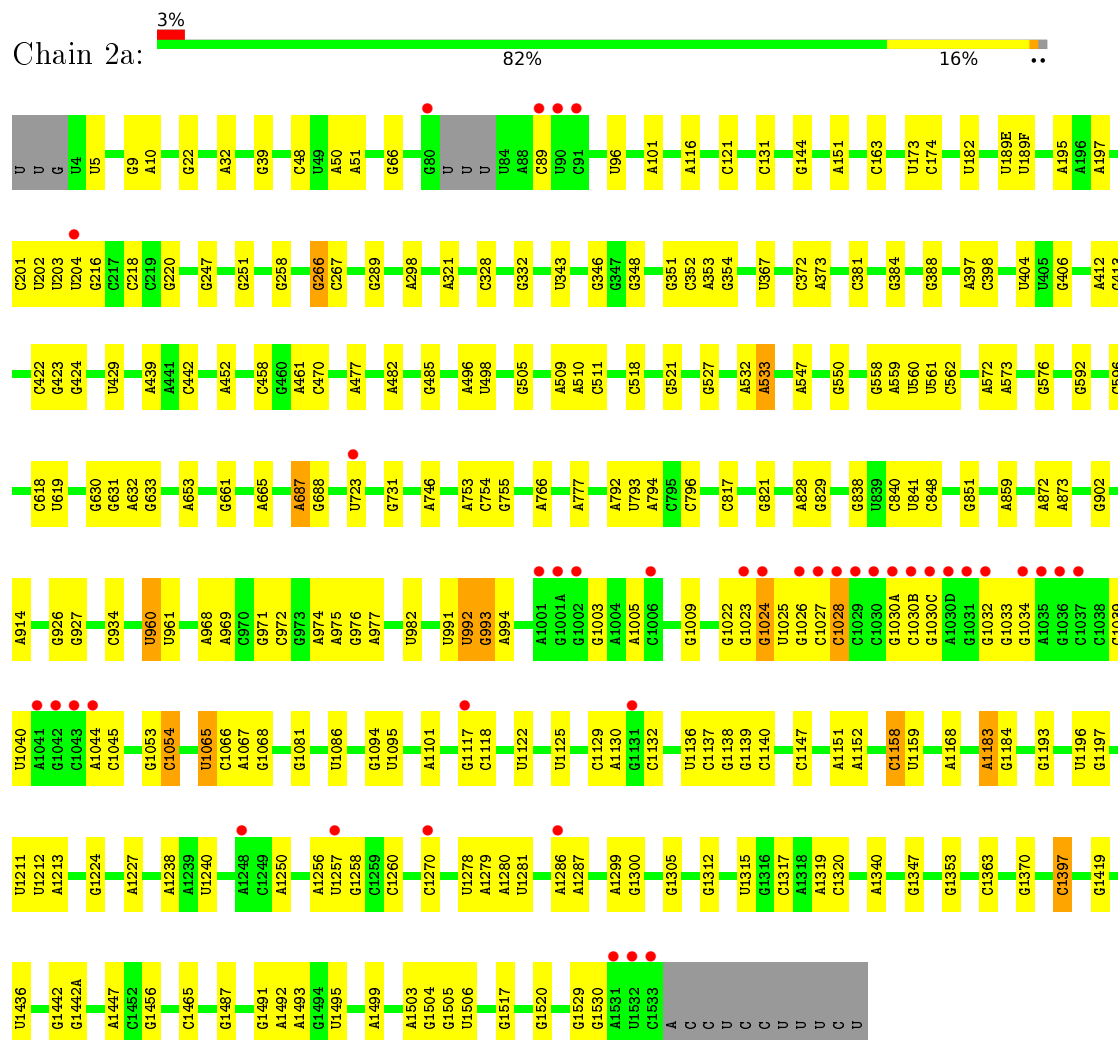
- Molecule 31: 50S ribosomal protein L36

- Molecule 32: 16s ribosomal RNA

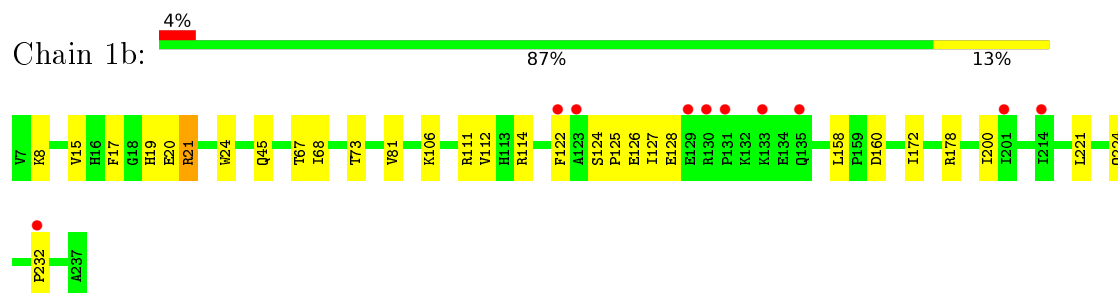
G1030C	G1030D	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	U1040	G1043	A1044	C1045	G1053	C1054	U1065	C1066	A1067	G1068	G1081	U1086	G1094	A1101	C1118	U1122	U1125	A1130	G1131	C1132	G1133	G1134	U1135	U1136	C1137	G1138	G1139	A1151	A1152	U1159	A1168	A1183	G1184
--------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------



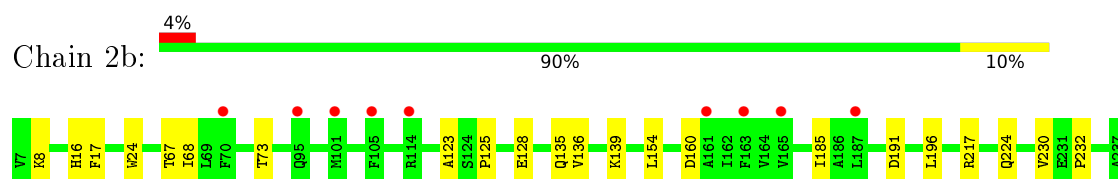
• Molecule 32: 16s ribosomal RNA



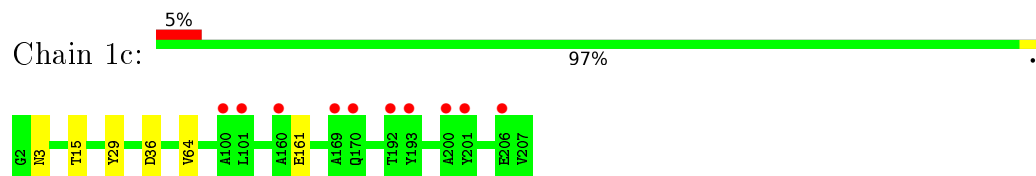
• Molecule 33: 30S ribosomal protein S2



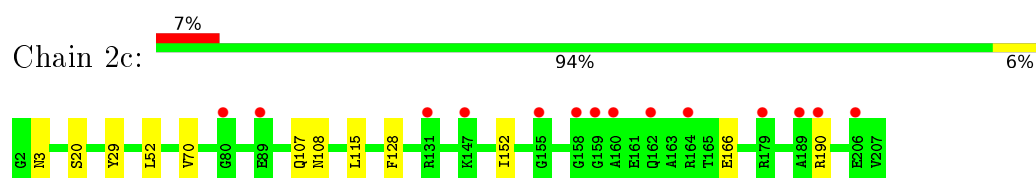
• Molecule 33: 30S ribosomal protein S2



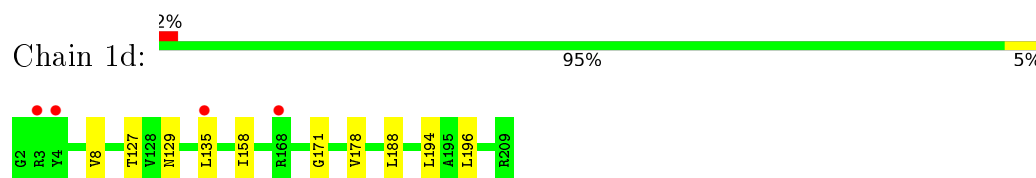
- Molecule 34: 30S ribosomal protein S3



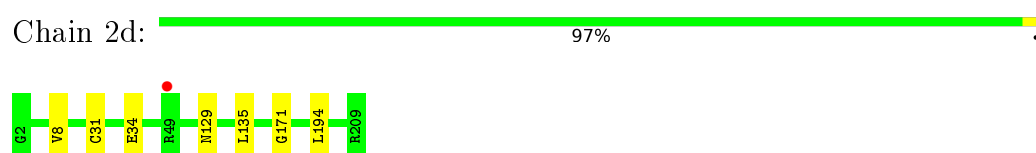
- Molecule 34: 30S ribosomal protein S3



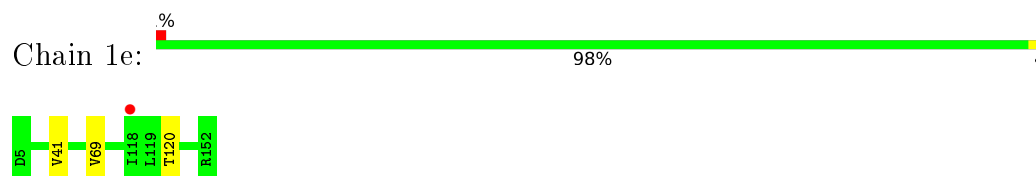
- Molecule 35: 30S ribosomal protein S4



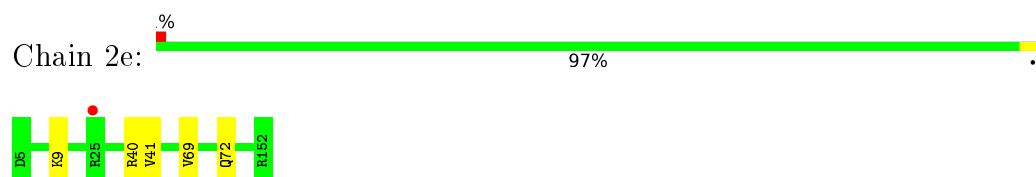
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



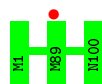
- Molecule 36: 30S ribosomal protein S5



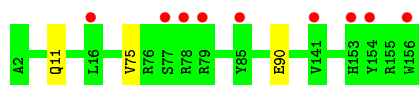
- Molecule 37: 30S ribosomal protein S6



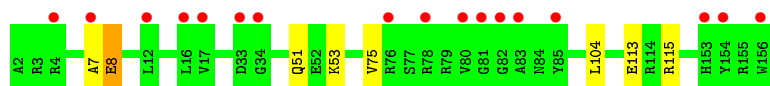
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



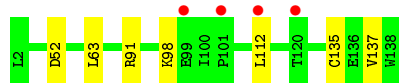
- Molecule 38: 30S ribosomal protein S7



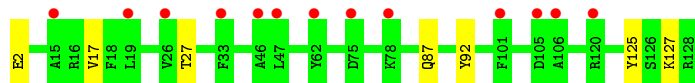
- Molecule 39: 30S ribosomal protein S8



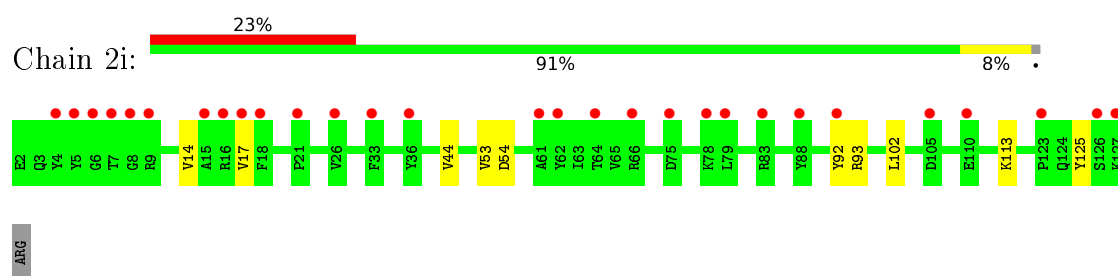
- Molecule 39: 30S ribosomal protein S8



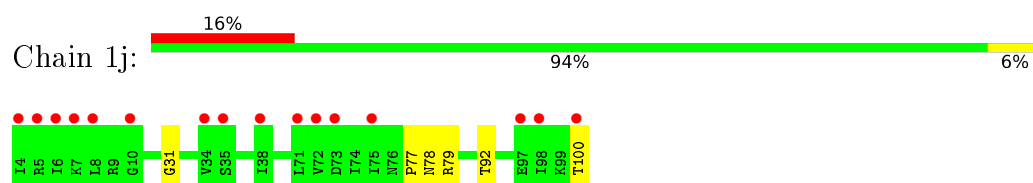
- Molecule 40: 30S ribosomal protein S9



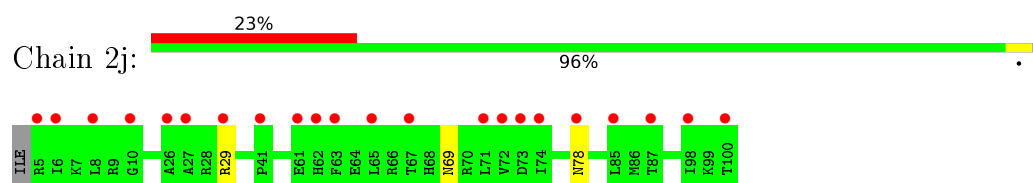
- Molecule 40: 30S ribosomal protein S9



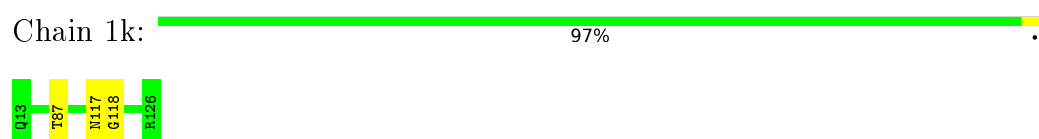
- Molecule 41: 30S ribosomal protein S10



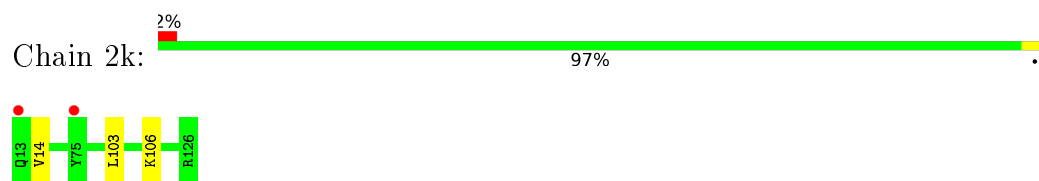
- Molecule 41: 30S ribosomal protein S10



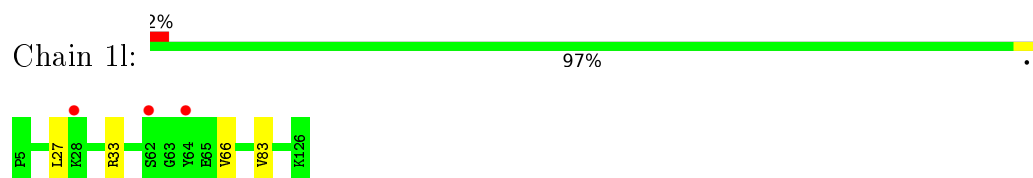
- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11

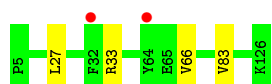


- Molecule 43: 30S ribosomal protein S12

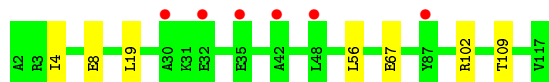


- Molecule 43: 30S ribosomal protein S12

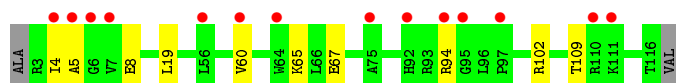




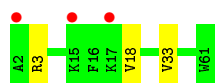
- Molecule 44: 30S ribosomal protein S13



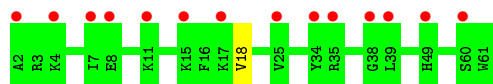
- Molecule 44: 30S ribosomal protein S13



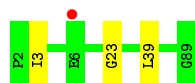
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

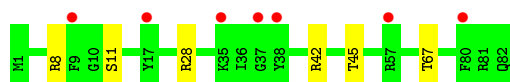


- Molecule 46: 30S ribosomal protein S15

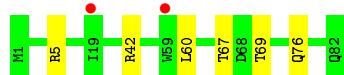


- Molecule 47: 30S ribosomal protein S16





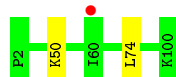
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



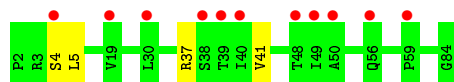
- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

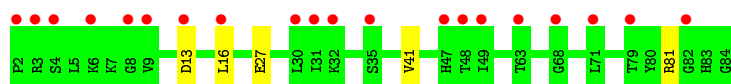


- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

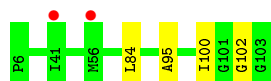




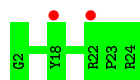
- Molecule 51: 30S ribosomal protein S20



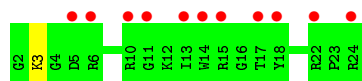
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



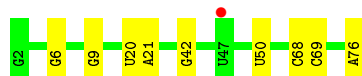
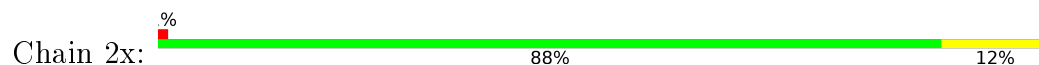
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: tRNA met

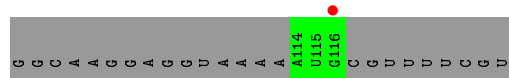


- Molecule 53: tRNA met



- Molecule 54: Onc112





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.30Å 452.29Å 625.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.10 49.72 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.72-3.10) 99.1 (49.72-3.10)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.231 , 0.271 0.234 , 0.273	Depositor DCC
R_{free} test set	52535 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 15.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 1050694 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	293672	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, ZN, 4SU, OMG, 5MC, MA6, G7M, MG, SF4, 0TD, MPD, UNX, 2MA, 2MG, OMU, UR3, 4OC, M2G, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1A	0.45	0/67879	0.88	48/105953 (0.0%)
1	2A	0.35	0/68951	0.85	38/107627 (0.0%)
2	1B	0.42	0/2876	1.00	8/4486 (0.2%)
2	2B	0.34	0/2878	0.84	0/4490
3	1D	0.31	0/2181	0.51	0/2940
3	2D	0.28	0/2186	0.50	0/2944
4	1E	0.32	0/1592	0.52	0/2149
4	2E	0.27	0/1592	0.52	0/2149
5	1F	0.31	0/1619	0.50	0/2193
5	2F	0.28	0/1615	0.49	0/2188
6	1G	0.26	0/1451	0.51	0/1961
6	2G	0.27	0/1449	0.49	0/1957
7	1H	0.29	0/1356	0.49	0/1834
7	2H	0.26	0/1350	0.49	0/1826
8	1I	0.27	0/1109	0.53	0/1512
8	2I	0.26	0/1091	0.50	0/1490
9	1N	0.29	0/1148	0.48	0/1547
9	2N	0.25	0/1144	0.46	0/1543
10	1O	0.35	0/943	0.51	0/1269
10	2O	0.31	0/943	0.49	0/1269
11	1P	0.32	0/1152	0.51	0/1533
11	2P	0.26	0/1152	0.48	0/1533
12	1Q	0.32	0/1143	0.48	0/1527
12	2Q	0.27	0/1143	0.44	0/1527
13	1R	0.30	0/982	0.52	0/1312
13	2R	0.26	0/982	0.46	0/1312
14	1S	0.27	0/887	0.52	0/1180
14	2S	0.26	0/880	0.48	0/1172
15	1T	0.32	0/1105	0.52	0/1477
15	2T	0.27	0/1097	0.48	0/1468
16	1U	0.34	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.28	0/977	0.45	0/1301
17	1V	0.32	0/786	0.49	0/1053
17	2V	0.28	0/782	0.50	0/1049
18	1W	0.34	0/897	0.49	0/1205
18	2W	0.27	0/897	0.45	0/1205
19	1X	0.34	0/764	0.52	0/1025
19	2X	0.28	0/764	0.51	0/1025
20	1Y	0.32	0/823	0.51	0/1099
20	2Y	0.27	0/823	0.50	0/1100
21	1Z	0.27	0/1620	0.47	0/2200
21	2Z	0.26	0/1590	0.47	0/2162
22	10	0.31	0/616	0.49	0/821
22	20	0.27	0/616	0.48	0/821
23	11	0.30	0/761	0.49	0/1013
23	21	0.28	0/766	0.46	0/1018
24	12	0.29	0/590	0.48	0/781
24	22	0.27	0/594	0.43	0/785
25	13	0.29	0/474	0.46	0/635
25	23	0.24	0/469	0.43	0/630
26	14	0.29	0/559	0.57	0/754
26	24	0.34	0/549	0.57	0/741
27	15	0.32	0/473	0.49	0/639
27	25	0.27	0/469	0.48	0/635
28	16	0.30	0/460	0.45	0/613
28	26	0.26	0/456	0.44	0/608
29	17	0.34	0/426	0.53	0/561
29	27	0.27	0/426	0.48	0/561
30	18	0.32	0/525	0.48	0/691
30	28	0.28	0/525	0.47	0/691
31	19	0.32	0/310	0.51	0/407
31	29	0.28	0/310	0.48	0/407
32	1a	0.35	0/35795	0.85	32/55864 (0.1%)
32	2a	0.34	0/35890	0.86	40/56012 (0.1%)
33	1b	0.27	0/1876	0.52	0/2533
33	2b	0.29	0/1860	0.49	0/2518
34	1c	0.26	0/1582	0.44	0/2137
34	2c	0.28	0/1566	0.45	0/2119
35	1d	0.27	0/1695	0.48	0/2274
35	2d	0.26	0/1698	0.47	0/2277
36	1e	0.26	0/1149	0.49	0/1548
36	2e	0.26	0/1149	0.49	0/1548
37	1f	0.26	0/827	0.44	0/1120
37	2f	0.27	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.24	0/1254	0.44	0/1683
38	2g	0.25	0/1248	0.44	0/1676
39	1h	0.24	0/1118	0.48	0/1506
39	2h	0.25	0/1108	0.47	0/1494
40	1i	0.27	0/1005	0.48	0/1351
40	2i	0.30	0/985	0.50	0/1329
41	1j	0.28	0/732	0.51	0/993
41	2j	0.29	0/723	0.51	0/984
42	1k	0.27	0/849	0.47	0/1150
42	2k	0.27	0/848	0.49	0/1149
43	1l	0.27	0/937	0.48	0/1260
43	2l	0.27	0/937	0.55	0/1260
44	1m	0.25	0/924	0.49	0/1242
44	2m	0.27	0/905	0.49	0/1217
45	1n	0.25	0/501	0.45	0/664
45	2n	0.28	0/501	0.41	0/664
46	1o	0.26	0/739	0.46	0/985
46	2o	0.26	0/739	0.45	0/985
47	1p	0.26	0/697	0.47	0/939
47	2p	0.26	0/693	0.49	0/935
48	1q	0.27	0/836	0.50	0/1117
48	2q	0.26	0/836	0.47	0/1117
49	1r	0.27	0/560	0.47	0/746
49	2r	0.26	0/560	0.45	0/746
50	1s	0.26	0/663	0.49	0/895
50	2s	0.27	0/660	0.54	0/893
51	1t	0.26	0/734	0.48	0/969
51	2t	0.25	0/736	0.44	0/976
52	1u	0.24	0/203	0.46	0/266
52	2u	0.27	0/203	0.47	0/266
53	1x	0.41	0/1725	0.95	0/2689
53	2x	0.40	0/1725	0.93	1/2689 (0.0%)
54	1y	0.33	0/106	0.63	0/146
54	2y	0.27	0/106	0.55	0/146
55	A	0.58	0/72	1.13	0/110
55	B	0.53	0/72	1.09	0/110
All	All	0.35	0/311106	0.78	167/465325 (0.0%)

There are no bond length outliers.

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1100	A	OP1-P-OP2	16.92	144.98	119.60
1	1A	1100	A	O5'-P-OP1	-14.97	92.23	105.70
1	1A	1099	C	OP1-P-O3'	-14.88	72.47	105.20
1	1A	1099	C	OP2-P-O3'	-13.42	75.67	105.20
1	1A	720	C	C2-N3-C4	-9.29	115.26	119.90

There are no chirality outliers.

There are no planarity outliers.

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	1A	60842	0	30688	557	0
1	2A	61801	0	31173	640	0
2	1B	2572	0	1305	31	0
2	2B	2573	0	1306	28	0
3	1D	2131	0	2207	37	0
3	2D	2136	0	2218	44	0
4	1E	1559	0	1618	27	0
4	2E	1559	0	1618	34	0
5	1F	1584	0	1625	36	0
5	2F	1580	0	1619	32	0
6	1G	1426	0	1445	28	0
6	2G	1424	0	1441	36	0
7	1H	1330	0	1407	31	0
7	2H	1324	0	1402	31	0
8	1I	1094	0	1127	22	0
8	2I	1076	0	1094	21	0
9	1N	1121	0	1194	11	0
9	2N	1117	0	1184	20	0
10	1O	933	0	996	18	0
10	2O	933	0	996	23	0
11	1P	1135	0	1212	21	0
11	2P	1135	0	1212	17	0
12	1Q	1122	0	1179	22	0
12	2Q	1122	0	1179	25	0
13	1R	968	0	1033	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	2R	968	0	1033	20	0
14	1S	877	0	938	22	0
14	2S	870	0	923	23	0
15	1T	1091	0	1151	19	0
15	2T	1083	0	1136	19	0
16	1U	959	0	1019	13	0
16	2U	959	0	1019	12	0
17	1V	775	0	841	13	0
17	2V	771	0	829	13	0
18	1W	886	0	940	8	0
18	2W	886	0	940	19	0
19	1X	750	0	814	18	0
19	2X	750	0	814	12	0
20	1Y	810	0	892	24	0
20	2Y	810	0	887	20	0
21	1Z	1587	0	1598	30	0
21	2Z	1557	0	1564	29	0
22	10	608	0	622	9	0
22	20	608	0	622	10	0
23	11	754	0	823	9	0
23	21	759	0	837	17	0
24	12	588	0	643	9	0
24	22	592	0	654	6	0
25	13	469	0	518	12	0
25	23	464	0	514	7	0
26	14	546	0	522	20	0
26	24	536	0	514	18	0
27	15	459	0	476	6	0
27	25	455	0	465	6	0
28	16	453	0	473	8	0
28	26	449	0	469	6	0
29	17	418	0	467	10	0
29	27	418	0	467	6	0
30	18	517	0	582	10	0
30	28	517	0	582	14	0
31	19	307	0	335	4	0
31	29	307	0	335	6	0
32	1a	32246	0	16294	0	0
32	2a	32331	0	16338	0	0
33	1b	1842	0	1862	0	0
33	2b	1825	0	1828	0	0
34	1c	1558	0	1557	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	2c	1542	0	1517	0	0
35	1d	1665	0	1687	0	0
35	2d	1668	0	1703	0	0
36	1e	1133	0	1191	0	0
36	2e	1133	0	1191	0	0
37	1f	814	0	808	0	0
37	2f	816	0	808	0	0
38	1g	1235	0	1249	0	0
38	2g	1229	0	1238	0	0
39	1h	1098	0	1143	0	0
39	2h	1088	0	1126	0	0
40	1i	986	0	990	0	0
40	2i	966	0	953	0	0
41	1j	719	0	672	0	0
41	2j	710	0	661	0	0
42	1k	834	0	838	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	914	0	954	0	0
44	2m	895	0	920	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	648	0	658	0	0
50	2s	645	0	635	0	0
51	1t	732	0	809	0	0
51	2t	733	0	795	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1x	1625	0	829	0	0
53	2x	1625	0	829	0	0
54	1y	101	0	109	0	0
54	2y	101	0	109	0	0
55	A	65	0	33	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B	65	0	33	0	0
56	10	7	0	0	0	0
56	11	3	0	0	0	0
56	13	3	0	0	0	0
56	15	3	0	0	0	0
56	17	2	0	0	0	0
56	18	1	0	0	0	0
56	19	2	0	0	0	0
56	1A	946	0	0	0	0
56	1B	29	0	0	0	0
56	1D	21	0	0	0	0
56	1E	6	0	0	0	0
56	1F	9	0	0	0	0
56	1G	4	0	0	0	0
56	1H	2	0	0	0	0
56	1N	3	0	0	0	0
56	1O	1	0	0	0	0
56	1P	2	0	0	0	0
56	1Q	4	0	0	0	0
56	1R	4	0	0	0	0
56	1T	2	0	0	0	0
56	1U	5	0	0	0	0
56	1V	3	0	0	0	0
56	1W	3	0	0	0	0
56	1X	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	1	0	0	0	0
56	1a	261	0	0	0	0
56	1b	1	0	0	0	0
56	1d	4	0	0	0	0
56	1e	4	0	0	0	0
56	1f	1	0	0	0	0
56	1g	1	0	0	0	0
56	1i	1	0	0	0	0
56	1l	1	0	0	0	0
56	1n	1	0	0	0	0
56	1o	2	0	0	0	0
56	1r	1	0	0	0	0
56	1t	1	0	0	0	0
56	1x	12	0	0	0	0
56	20	1	0	0	0	0
56	21	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	23	1	0	0	0	0
56	28	2	0	0	0	0
56	2A	679	0	0	0	0
56	2B	17	0	0	0	0
56	2D	8	0	0	0	0
56	2E	7	0	0	0	0
56	2F	3	0	0	0	0
56	2G	2	0	0	0	0
56	2I	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	2	0	0	0	0
56	2R	1	0	0	0	0
56	2T	4	0	0	0	0
56	2U	2	0	0	0	0
56	2V	3	0	0	0	0
56	2W	1	0	0	0	0
56	2X	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2a	183	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	1	0	0	0	0
56	2n	1	0	0	0	0
56	2p	1	0	0	0	0
56	2q	1	0	0	0	0
56	2t	1	0	0	0	0
56	2x	10	0	0	0	0
57	1A	1	0	0	0	0
57	2A	1	0	0	0	0
58	1A	8	0	14	1	0
58	1a	8	0	14	0	0
59	1B	12	0	12	1	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	2A	1	0	0	0	0
63	10	4	0	0	0	0
63	11	3	0	0	0	0
63	13	6	0	0	1	0
63	15	2	0	0	0	0
63	16	3	0	0	0	0
63	18	7	0	0	0	0
63	19	3	0	0	1	0
63	1A	1632	0	0	8	0
63	1B	50	0	0	0	0
63	1D	20	0	0	0	0
63	1E	17	0	0	0	0
63	1F	14	0	0	1	0
63	1G	5	0	0	0	0
63	1H	4	0	0	0	0
63	1N	7	0	0	0	0
63	1O	2	0	0	0	0
63	1P	18	0	0	0	0
63	1Q	5	0	0	0	0
63	1R	7	0	0	1	0
63	1T	4	0	0	0	0
63	1U	3	0	0	0	0
63	1V	3	0	0	0	0
63	1X	6	0	0	0	0
63	1Y	2	0	0	0	0
63	1a	369	0	0	0	0
63	1c	1	0	0	0	0
63	1d	6	0	0	0	0
63	1e	3	0	0	0	0
63	1f	1	0	0	0	0
63	1h	1	0	0	0	0
63	1l	3	0	0	0	0
63	1m	1	0	0	0	0
63	1n	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	1o	2	0	0	0	0
63	1p	1	0	0	0	0
63	1t	1	0	0	0	0
63	1x	2	0	0	0	0
63	20	2	0	0	0	0
63	21	2	0	0	0	0
63	23	2	0	0	0	0
63	25	1	0	0	0	0
63	26	2	0	0	0	0
63	28	5	0	0	0	0
63	2A	1221	0	0	6	0
63	2B	33	0	0	1	0
63	2D	13	0	0	0	0
63	2E	12	0	0	1	0
63	2F	4	0	0	0	0
63	2N	2	0	0	0	0
63	2O	4	0	0	0	0
63	2P	7	0	0	0	0
63	2Q	5	0	0	0	0
63	2R	2	0	0	0	0
63	2T	2	0	0	0	0
63	2U	3	0	0	0	0
63	2X	4	0	0	0	0
63	2Y	1	0	0	0	0
63	2a	305	0	0	0	0
63	2d	3	0	0	0	0
63	2e	1	0	0	0	0
63	2j	2	0	0	0	0
63	2l	1	0	0	0	0
63	2n	1	0	0	0	0
63	2p	1	0	0	0	0
63	2r	1	0	0	0	0
63	2t	1	0	0	0	0
63	2x	2	0	0	0	0
63	A	1	0	0	0	0
All	All	293672	0	194336	2003	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 2003 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2564:OMU:C4	1:1A:2564:OMU:C5	1.78	1.59
1:2A:2552:OMU:C4	1:2A:2552:OMU:C5	1.78	1.58
1:1A:1405:A:N6	1:1A:1418:U:H3	1.34	1.23
1:1A:2159:C:N4	1:1A:2176:G:H1	1.52	1.07
2:2B:6:C:H42	2:2B:115:G:H1	1.01	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/275 (99%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/275 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	34	72
4	2E	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	34	72
5	1F	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	34	72
5	2F	201/203 (99%)	195 (97%)	4 (2%)	2 (1%)	19	58
6	1G	179/181 (99%)	167 (93%)	10 (6%)	2 (1%)	17	55
6	2G	179/181 (99%)	163 (91%)	13 (7%)	3 (2%)	11	43
7	1H	172/174 (99%)	162 (94%)	10 (6%)	0	100	100
7	2H	171/174 (98%)	162 (95%)	9 (5%)	0	100	100
8	1I	145/147 (99%)	132 (91%)	9 (6%)	4 (3%)	6	30
8	2I	144/147 (98%)	134 (93%)	9 (6%)	1 (1%)	26	65
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	26	65
11	2P	147/149 (99%)	139 (95%)	7 (5%)	1 (1%)	26	65
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	21	61
14	2S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
15	1T	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
15	2T	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
16	1U	114/116 (98%)	114 (100%)	0	0	100	100
16	2U	114/116 (98%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	19	58
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	19	58
18	1W	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/95 (98%)	91 (98%)	1 (1%)	1 (1%)	17	55
19	2X	93/95 (98%)	90 (97%)	2 (2%)	1 (1%)	17	55
20	1Y	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
21	1Z	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
21	2Z	199/203 (98%)	183 (92%)	16 (8%)	0	100	100
22	10	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
22	20	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
23	11	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
23	21	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
24	12	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
24	22	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
25	13	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
25	23	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
26	14	67/69 (97%)	52 (78%)	12 (18%)	3 (4%)	3	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/69 (97%)	51 (76%)	12 (18%)	4 (6%)	2	11
27	15	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
27	25	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
28	16	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
28	26	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
29	17	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
29	27	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
30	18	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
30	28	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/231 (99%)	199 (87%)	21 (9%)	9 (4%)	4	22
33	2b	229/231 (99%)	200 (87%)	23 (10%)	6 (3%)	7	32
34	1c	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
34	2c	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	19	58
35	1d	206/208 (99%)	193 (94%)	11 (5%)	2 (1%)	19	58
35	2d	206/208 (99%)	196 (95%)	8 (4%)	2 (1%)	19	58
36	1e	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
36	2e	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
38	2g	153/155 (99%)	143 (94%)	8 (5%)	2 (1%)	15	50
39	1h	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	24	63
40	2i	124/127 (98%)	111 (90%)	11 (9%)	2 (2%)	12	44
41	1j	95/97 (98%)	82 (86%)	9 (10%)	4 (4%)	3	19
41	2j	94/97 (97%)	84 (89%)	9 (10%)	1 (1%)	17	55
42	1k	112/114 (98%)	105 (94%)	6 (5%)	1 (1%)	21	61
42	2k	112/114 (98%)	107 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/122 (98%)	110 (92%)	9 (8%)	0	100	100
44	1m	114/116 (98%)	106 (93%)	7 (6%)	1 (1%)	21	61
44	2m	112/116 (97%)	105 (94%)	5 (4%)	2 (2%)	11	42
45	1n	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/88 (98%)	84 (98%)	1 (1%)	1 (1%)	16	52
46	2o	86/88 (98%)	81 (94%)	3 (4%)	2 (2%)	8	35
47	1p	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
47	2p	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	19	58
48	2q	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
49	1r	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
50	2s	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
51	1t	94/98 (96%)	90 (96%)	1 (1%)	3 (3%)	5	26
51	2t	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	27
52	1u	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	3	17
54	1y	10/19 (53%)	9 (90%)	1 (10%)	0	100	100
54	2y	10/19 (53%)	9 (90%)	1 (10%)	0	100	100
All	All	11460/11686 (98%)	10814 (94%)	571 (5%)	75 (1%)	26	65

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
8	1I	105	HIS
26	14	49	PHE
35	1d	171	GLY
40	1i	127	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/217 (99%)	202 (94%)	12 (6%)	26	62
3	2D	215/217 (99%)	204 (95%)	11 (5%)	29	66
4	1E	164/165 (99%)	152 (93%)	12 (7%)	17	52
4	2E	164/165 (99%)	156 (95%)	8 (5%)	31	68
5	1F	160/161 (99%)	149 (93%)	11 (7%)	19	55
5	2F	159/161 (99%)	147 (92%)	12 (8%)	17	51
6	1G	144/155 (93%)	133 (92%)	11 (8%)	16	51
6	2G	142/155 (92%)	133 (94%)	9 (6%)	22	58
7	1H	144/145 (99%)	139 (96%)	5 (4%)	43	78
7	2H	143/145 (99%)	138 (96%)	5 (4%)	43	78
8	1I	111/123 (90%)	100 (90%)	11 (10%)	10	34
8	2I	108/123 (88%)	101 (94%)	7 (6%)	21	57
9	1N	119/119 (100%)	110 (92%)	9 (8%)	16	51
9	2N	118/119 (99%)	112 (95%)	6 (5%)	29	66
10	1O	100/100 (100%)	96 (96%)	4 (4%)	38	75
10	2O	100/100 (100%)	96 (96%)	4 (4%)	38	75
11	1P	115/116 (99%)	106 (92%)	9 (8%)	16	49
11	2P	115/116 (99%)	111 (96%)	4 (4%)	43	78
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	22	58
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	22	58
13	1R	101/101 (100%)	91 (90%)	10 (10%)	10	34
13	2R	101/101 (100%)	88 (87%)	13 (13%)	5	21
14	1S	87/87 (100%)	84 (97%)	3 (3%)	44	79
14	2S	85/87 (98%)	81 (95%)	4 (5%)	32	70
15	1T	115/115 (100%)	109 (95%)	6 (5%)	29	65
15	2T	113/115 (98%)	110 (97%)	3 (3%)	52	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/93 (100%)	87 (94%)	6 (6%)	21	57
16	2U	93/93 (100%)	87 (94%)	6 (6%)	21	57
17	1V	81/82 (99%)	73 (90%)	8 (10%)	10	34
17	2V	80/82 (98%)	72 (90%)	8 (10%)	9	34
18	1W	90/91 (99%)	83 (92%)	7 (8%)	16	49
18	2W	90/91 (99%)	86 (96%)	4 (4%)	35	71
19	1X	77/77 (100%)	76 (99%)	1 (1%)	76	91
19	2X	77/77 (100%)	74 (96%)	3 (4%)	39	75
20	1Y	86/88 (98%)	82 (95%)	4 (5%)	32	70
20	2Y	86/88 (98%)	83 (96%)	3 (4%)	43	78
21	1Z	169/176 (96%)	156 (92%)	13 (8%)	16	50
21	2Z	165/176 (94%)	155 (94%)	10 (6%)	23	59
22	10	61/62 (98%)	58 (95%)	3 (5%)	31	68
22	20	61/62 (98%)	59 (97%)	2 (3%)	45	79
23	11	79/82 (96%)	77 (98%)	2 (2%)	55	84
23	21	81/82 (99%)	77 (95%)	4 (5%)	31	68
24	12	65/66 (98%)	64 (98%)	1 (2%)	72	90
24	22	66/66 (100%)	64 (97%)	2 (3%)	48	81
25	13	51/51 (100%)	47 (92%)	4 (8%)	16	49
25	23	50/51 (98%)	47 (94%)	3 (6%)	24	60
26	14	58/62 (94%)	53 (91%)	5 (9%)	13	45
26	24	54/62 (87%)	51 (94%)	3 (6%)	26	62
27	15	51/51 (100%)	49 (96%)	2 (4%)	39	75
27	25	50/51 (98%)	49 (98%)	1 (2%)	63	86
28	16	51/51 (100%)	48 (94%)	3 (6%)	24	60
28	26	50/51 (98%)	47 (94%)	3 (6%)	24	60
29	17	41/41 (100%)	37 (90%)	4 (10%)	10	36
29	27	41/41 (100%)	41 (100%)	0	100	100
30	18	54/54 (100%)	50 (93%)	4 (7%)	17	51
30	28	54/54 (100%)	51 (94%)	3 (6%)	26	62
31	19	34/34 (100%)	34 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	191/199 (96%)	169 (88%)	22 (12%)	7	27
33	2b	187/199 (94%)	171 (91%)	16 (9%)	13	45
34	1c	144/160 (90%)	138 (96%)	6 (4%)	36	73
34	2c	140/160 (88%)	130 (93%)	10 (7%)	18	54
35	1d	171/180 (95%)	163 (95%)	8 (5%)	32	70
35	2d	172/180 (96%)	167 (97%)	5 (3%)	50	81
36	1e	114/114 (100%)	111 (97%)	3 (3%)	54	83
36	2e	114/114 (100%)	109 (96%)	5 (4%)	35	71
37	1f	85/90 (94%)	84 (99%)	1 (1%)	78	92
37	2f	85/90 (94%)	85 (100%)	0	100	100
38	1g	120/126 (95%)	117 (98%)	3 (2%)	55	84
38	2g	119/126 (94%)	112 (94%)	7 (6%)	24	60
39	1h	116/118 (98%)	111 (96%)	5 (4%)	35	72
39	2h	114/118 (97%)	107 (94%)	7 (6%)	23	59
40	1i	91/98 (93%)	85 (93%)	6 (7%)	21	56
40	2i	88/98 (90%)	80 (91%)	8 (9%)	12	40
41	1j	68/87 (78%)	66 (97%)	2 (3%)	50	81
41	2j	68/87 (78%)	66 (97%)	2 (3%)	50	81
42	1k	83/86 (96%)	81 (98%)	2 (2%)	57	84
42	2k	83/86 (96%)	80 (96%)	3 (4%)	42	77
43	1l	96/102 (94%)	92 (96%)	4 (4%)	36	73
43	2l	96/102 (94%)	92 (96%)	4 (4%)	36	73
44	1m	90/94 (96%)	84 (93%)	6 (7%)	20	56
44	2m	87/94 (93%)	79 (91%)	8 (9%)	11	40
45	1n	49/49 (100%)	46 (94%)	3 (6%)	23	59
45	2n	49/49 (100%)	48 (98%)	1 (2%)	63	86
46	1o	78/79 (99%)	76 (97%)	2 (3%)	54	83
46	2o	78/79 (99%)	74 (95%)	4 (5%)	29	66
47	1p	69/71 (97%)	63 (91%)	6 (9%)	13	44
47	2p	68/71 (96%)	62 (91%)	6 (9%)	12	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/94 (100%)	93 (99%)	1 (1%)	80	93
48	2q	94/94 (100%)	92 (98%)	2 (2%)	61	86
49	1r	59/59 (100%)	58 (98%)	1 (2%)	68	89
49	2r	59/59 (100%)	58 (98%)	1 (2%)	68	89
50	1s	68/72 (94%)	64 (94%)	4 (6%)	24	60
50	2s	67/72 (93%)	62 (92%)	5 (8%)	17	51
51	1t	71/76 (93%)	69 (97%)	2 (3%)	51	82
51	2t	70/76 (92%)	69 (99%)	1 (1%)	74	90
52	1u	18/18 (100%)	18 (100%)	0	100	100
52	2u	18/18 (100%)	18 (100%)	0	100	100
54	1y	12/19 (63%)	12 (100%)	0	100	100
54	2y	12/19 (63%)	12 (100%)	0	100	100
All	All	9387/9734 (96%)	8880 (95%)	507 (5%)	27	64

5 of 507 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	1i	92	TYR
5	2F	18	ARG
40	2i	113	LYS
43	1l	33	ARG
49	1r	76	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
48	1q	26	GLN
12	2Q	123	HIS
46	2o	62	GLN
50	1s	47	HIS
5	2F	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2814/2915 (96%)	427 (15%)	31 (1%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2859/2915 (98%)	486 (16%)	28 (0%)
2	1B	119/120 (99%)	10 (8%)	0
2	2B	119/120 (99%)	12 (10%)	0
32	1a	1494/1521 (98%)	255 (17%)	0
32	2a	1498/1521 (98%)	249 (16%)	0
53	1x	75/76 (98%)	7 (9%)	0
53	2x	75/76 (98%)	8 (10%)	0
55	A	2/27 (7%)	0	0
55	B	2/27 (7%)	0	0
All	All	9057/9318 (97%)	1454 (16%)	59 (0%)

5 of 1454 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	54	G

5 of 59 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2434	A
1	2A	266	G
1	2A	2171	A
1	1A	2442	A
1	1A	2701	U

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

56 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
1	PSU	1A	1933	1	15,21,22	1.95	3 (20%)	16,30,33	2.77	3 (18%)
1	5MU	1A	1937	1	13,22,23	1.49	1 (7%)	16,32,35	3.54	2 (12%)
1	PSU	1A	1939	1,56	15,21,22	1.85	3 (20%)	16,30,33	2.84	2 (12%)
1	OMC	1A	1942	1,56	15,22,23	2.32	6 (40%)	20,31,34	1.20	2 (10%)
1	5MU	1A	1961	1	13,22,23	1.42	2 (15%)	16,32,35	3.56	2 (12%)
1	5MC	1A	1964	1	14,22,23	0.77	0	17,32,35	0.93	1 (5%)
1	5MC	1A	1984	1	14,22,23	0.86	1 (7%)	17,32,35	0.86	1 (5%)
1	OMG	1A	2263	1,56,53	18,26,27	2.52	6 (33%)	21,38,41	2.85	5 (23%)
1	2MA	1A	2515	1,56	17,25,26	2.59	6 (35%)	18,37,40	4.51	4 (22%)
1	OMU	1A	2564	1	14,22,23	7.77	8 (57%)	19,31,34	1.49	3 (15%)
1	PSU	1A	2617	1	15,21,22	2.22	4 (26%)	16,30,33	2.96	6 (37%)
32	2MG	1a	1207	32,56	18,26,27	2.77	6 (33%)	21,38,41	3.19	9 (42%)
32	5MC	1a	1400	32	14,22,23	0.76	0	17,32,35	0.85	1 (5%)
32	4OC	1a	1402	32	15,23,24	2.27	6 (40%)	21,32,35	1.68	3 (14%)
32	5MC	1a	1404	32	14,22,23	0.89	0	17,32,35	0.84	1 (5%)
32	5MC	1a	1407	32	14,22,23	0.89	0	17,32,35	0.92	1 (5%)
32	UR3	1a	1498	32	13,22,23	1.90	3 (23%)	18,32,35	0.69	0
32	MA6	1a	1518	32	18,26,27	0.92	2 (11%)	15,38,41	3.81	3 (20%)
32	MA6	1a	1519	32	18,26,27	0.95	2 (11%)	15,38,41	3.73	3 (20%)
32	PSU	1a	516	32	15,21,22	2.27	5 (33%)	16,30,33	3.09	5 (31%)
32	G7M	1a	527	32,56	18,26,27	3.74	7 (38%)	21,39,42	1.85	3 (14%)
32	M2G	1a	966	32	18,27,28	3.03	6 (33%)	22,40,43	1.69	4 (18%)
32	5MC	1a	967	32	14,22,23	0.75	0	17,32,35	0.83	1 (5%)
43	0TD	1l	92	43	4,9,10	2.11	2 (50%)	4,11,13	3.05	2 (50%)
53	5MC	1x	32	53	14,22,23	0.89	0	17,32,35	0.85	1 (5%)
53	5MU	1x	54	53	13,22,23	1.51	1 (7%)	16,32,35	3.84	2 (12%)
53	PSU	1x	55	53	15,21,22	1.99	3 (20%)	16,30,33	2.89	5 (31%)
53	4SU	1x	8	53	12,21,22	1.27	2 (16%)	15,30,33	1.95	1 (6%)
1	PSU	2A	1911	1	15,21,22	1.87	3 (20%)	16,30,33	2.87	5 (31%)
1	5MU	2A	1915	1	13,22,23	1.52	2 (15%)	16,32,35	3.66	2 (12%)
1	PSU	2A	1917	1	15,21,22	1.92	4 (26%)	16,30,33	2.97	5 (31%)
1	OMC	2A	1920	1	15,22,23	2.41	6 (40%)	20,31,34	1.34	1 (5%)
1	5MU	2A	1939	1	13,22,23	1.37	1 (7%)	16,32,35	3.67	2 (12%)
1	5MC	2A	1942	1	14,22,23	0.81	0	17,32,35	0.84	1 (5%)
1	5MC	2A	1962	1,56	14,22,23	0.85	0	17,32,35	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	2A	2251	1,56,53	18,26,27	2.47	6 (33%)	21,38,41	2.83	4 (19%)
1	2MA	2A	2503	1,56	17,25,26	2.62	6 (35%)	18,37,40	4.82	4 (22%)
1	OMU	2A	2552	1,56	14,22,23	7.88	8 (57%)	19,31,34	1.49	2 (10%)
1	PSU	2A	2605	1	15,21,22	2.27	4 (26%)	16,30,33	2.96	5 (31%)
32	2MG	2a	1207	32	18,26,27	2.71	6 (33%)	21,38,41	3.02	8 (38%)
32	5MC	2a	1400	32	14,22,23	0.81	0	17,32,35	0.88	1 (5%)
32	4OC	2a	1402	32	15,23,24	2.30	6 (40%)	21,32,35	1.64	3 (14%)
32	5MC	2a	1404	32	14,22,23	0.91	0	17,32,35	0.86	1 (5%)
32	5MC	2a	1407	32	14,22,23	0.81	0	17,32,35	0.93	1 (5%)
32	UR3	2a	1498	32	13,22,23	1.96	3 (23%)	18,32,35	0.69	0
32	MA6	2a	1518	32	18,26,27	0.90	2 (11%)	15,38,41	3.95	3 (20%)
32	MA6	2a	1519	32	18,26,27	0.95	2 (11%)	15,38,41	3.77	3 (20%)
32	PSU	2a	516	32	15,21,22	2.41	5 (33%)	16,30,33	2.95	5 (31%)
32	G7M	2a	527	32,56	18,26,27	3.74	7 (38%)	21,39,42	2.11	5 (23%)
32	M2G	2a	966	32	18,27,28	3.09	6 (33%)	22,40,43	1.69	5 (22%)
32	5MC	2a	967	32	14,22,23	0.82	0	17,32,35	0.89	1 (5%)
43	0TD	2l	92	43	4,9,10	1.90	2 (50%)	4,11,13	2.70	2 (50%)
53	5MC	2x	32	53	14,22,23	0.80	0	17,32,35	0.92	1 (5%)
53	5MU	2x	54	53	13,22,23	1.45	1 (7%)	16,32,35	3.69	2 (12%)
53	PSU	2x	55	53	15,21,22	2.19	5 (33%)	16,30,33	2.86	5 (31%)
53	4SU	2x	8	56,53	12,21,22	1.61	3 (25%)	15,30,33	2.23	1 (6%)

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
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
1	OMC	1A	1942	1,56	-	0/5/27/28	0/2/2/2
1	5MU	1A	1961	1	-	0/3/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/3/25/26	0/2/2/2
1	5MC	1A	1984	1	-	0/3/25/26	0/2/2/2
1	OMG	1A	2263	1,56,53	-	0/5/27/28	0/3/3/3
1	2MA	1A	2515	1,56	-	0/3/25/26	0/3/3/3
1	OMU	1A	2564	1	-	0/5/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32,56	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	0/3/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	1l	92	43	-	0/2/12/14	0/0/0/0
53	5MC	1x	32	53	-	0/3/25/26	0/2/2/2
53	5MU	1x	54	53	-	0/3/25/26	0/2/2/2
53	PSU	1x	55	53	-	0/7/25/26	0/2/2/2
53	4SU	1x	8	53	-	0/3/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/3/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/5/27/28	0/2/2/2
1	5MU	2A	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/3/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/3/25/26	0/2/2/2
1	OMG	2A	2251	1,56,53	-	0/5/27/28	0/3/3/3
1	2MA	2A	2503	1,56	-	0/3/25/26	0/3/3/3
1	OMU	2A	2552	1,56	-	0/5/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,56	-	0/3/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	2l	92	43	-	0/2/12/14	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	5MC	2x	32	53	-	0/3/25/26	0/2/2/2
53	5MU	2x	54	53	-	0/3/25/26	0/2/2/2
53	PSU	2x	55	53	-	0/7/25/26	0/2/2/2
53	4SU	2x	8	56,53	-	0/3/25/26	0/2/2/2

The worst 5 of 173 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	OMU	C6-C5	-12.22	1.11	1.38
1	2A	2552	OMU	C6-C5	-12.18	1.11	1.38
1	1A	2564	OMU	C4-N3	-11.64	1.12	1.33
1	2A	2552	OMU	C4-N3	-11.35	1.12	1.33
1	1A	2564	OMU	C3'-C2'	-8.86	1.33	1.53

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1x	54	5MU	C5-C4-N3	-10.96	116.15	125.35
32	2a	1518	MA6	N3-C2-N1	-10.93	120.29	128.87
32	2a	1519	MA6	N3-C2-N1	-10.87	120.34	128.87
32	1a	1519	MA6	N3-C2-N1	-10.81	120.38	128.87
1	2A	1939	5MU	C5-C4-N3	-10.72	116.35	125.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1942	OMC	1	0
1	1A	1961	5MU	1	0
1	1A	2263	OMG	1	0
1	1A	2515	2MA	1	0
1	1A	2564	OMU	2	0
1	2A	1962	5MC	1	0
1	2A	2251	OMG	1	0
1	2A	2503	2MA	1	0
1	2A	2552	OMU	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2322 ligands modelled in this entry, 2 are unknown and 2315 are monoatomic - leaving 5 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	MPD	1A	3907	-	6,7,7	0.35	0	6,10,10	0.20	0
59	ARG	1B	229	-	5,11,11	0.25	0	3,13,13	0.12	0
58	MPD	1a	1860	-	6,7,7	0.34	0	6,10,10	0.27	0
61	SF4	1d	501	35	0,12,12	0.00	-	0,24,24	0.00	-
61	SF4	2d	501	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	MPD	1A	3907	-	-	0/5/5/5	0/0/0/0
59	ARG	1B	229	-	-	0/5/11/11	0/0/0/0
58	MPD	1a	1860	-	-	0/5/5/5	0/0/0/0
61	SF4	1d	501	35	-	0/0/48/48	0/6/5/5
61	SF4	2d	501	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1A	3907	MPD	1	0
59	1B	229	ARG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1A	1151:U	O3'	1152:G	P	3.02

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	1A	2813/2915 (96%)	-0.13	74 (2%) 59 35	23, 42, 82, 95	0
1	2A	2858/2915 (98%)	-0.13	103 (3%) 46 23	40, 59, 86, 96	0
2	1B	120/120 (100%)	-0.52	0 100 100	38, 57, 63, 76	0
2	2B	120/120 (100%)	-0.20	0 100 100	62, 75, 81, 82	0
3	1D	275/275 (100%)	-0.29	0 100 100	30, 44, 54, 67	0
3	2D	275/275 (100%)	-0.20	2 (0%) 89 78	43, 55, 62, 69	0
4	1E	204/204 (100%)	-0.27	0 100 100	28, 47, 60, 69	0
4	2E	204/204 (100%)	-0.15	1 (0%) 91 83	43, 59, 67, 75	0
5	1F	203/203 (100%)	-0.30	0 100 100	26, 49, 66, 73	0
5	2F	203/203 (100%)	-0.20	0 100 100	44, 65, 72, 79	0
6	1G	181/181 (100%)	-0.40	2 (1%) 82 66	55, 64, 72, 80	0
6	2G	181/181 (100%)	0.23	3 (1%) 73 52	71, 75, 79, 85	0
7	1H	174/174 (100%)	-0.29	0 100 100	43, 54, 62, 65	0
7	2H	173/174 (99%)	0.62	22 (12%) 5 2	66, 75, 79, 85	0
8	1I	147/147 (100%)	-0.23	0 100 100	51, 67, 74, 76	0
8	2I	146/147 (99%)	0.14	2 (1%) 78 60	59, 75, 79, 82	0
9	1N	140/140 (100%)	-0.20	0 100 100	35, 45, 61, 67	0
9	2N	140/140 (100%)	0.01	2 (1%) 78 60	52, 63, 71, 78	0
10	1O	122/122 (100%)	-0.15	0 100 100	38, 47, 58, 62	0
10	2O	122/122 (100%)	-0.28	0 100 100	50, 57, 65, 69	0
11	1P	149/149 (100%)	-0.24	0 100 100	28, 50, 61, 73	0
11	2P	149/149 (100%)	0.05	2 (1%) 79 62	46, 67, 75, 78	0
12	1Q	141/141 (100%)	-0.22	0 100 100	36, 49, 56, 63	0
12	2Q	141/141 (100%)	-0.31	0 100 100	51, 64, 69, 75	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.21	0 100 100	35, 42, 53, 65	0
13	2R	118/118 (100%)	-0.13	0 100 100	48, 56, 62, 69	0
14	1S	110/110 (100%)	-0.13	0 100 100	45, 53, 60, 64	0
14	2S	110/110 (100%)	0.44	5 (4%) 37 17	65, 71, 74, 76	0
15	1T	131/131 (100%)	-0.28	1 (0%) 87 75	42, 51, 67, 74	0
15	2T	131/131 (100%)	-0.21	0 100 100	55, 60, 70, 75	0
16	1U	116/116 (100%)	-0.29	0 100 100	30, 40, 52, 58	0
16	2U	116/116 (100%)	-0.17	0 100 100	50, 60, 69, 74	0
17	1V	101/101 (100%)	-0.24	0 100 100	27, 49, 59, 64	0
17	2V	101/101 (100%)	-0.05	0 100 100	48, 67, 73, 76	0
18	1W	112/112 (100%)	-0.31	0 100 100	31, 38, 54, 71	0
18	2W	112/112 (100%)	-0.08	0 100 100	46, 54, 64, 71	0
19	1X	95/95 (100%)	-0.12	0 100 100	34, 44, 60, 67	0
19	2X	95/95 (100%)	-0.02	0 100 100	53, 61, 68, 69	0
20	1Y	107/107 (100%)	-0.17	1 (0%) 85 72	46, 53, 65, 68	0
20	2Y	107/107 (100%)	0.70	9 (8%) 14 4	62, 68, 73, 83	0
21	1Z	203/203 (100%)	0.03	13 (6%) 23 9	50, 61, 72, 81	0
21	2Z	201/203 (99%)	0.43	16 (7%) 15 5	66, 73, 79, 82	0
22	10	77/77 (100%)	-0.22	1 (1%) 79 62	37, 45, 53, 57	0
22	20	77/77 (100%)	0.75	10 (12%) 5 2	57, 63, 68, 70	0
23	11	97/97 (100%)	0.03	2 (2%) 67 44	32, 48, 65, 71	0
23	21	97/97 (100%)	0.28	1 (1%) 84 69	47, 59, 70, 74	0
24	12	70/70 (100%)	-0.19	0 100 100	44, 52, 58, 71	0
24	22	70/70 (100%)	0.10	1 (1%) 78 60	61, 67, 72, 74	0
25	13	59/59 (100%)	-0.16	0 100 100	36, 45, 62, 70	0
25	23	59/59 (100%)	0.64	2 (3%) 49 24	57, 62, 69, 72	0
26	14	69/69 (100%)	0.29	6 (8%) 13 4	62, 73, 82, 84	0
26	24	69/69 (100%)	0.72	6 (8%) 13 4	75, 80, 84, 85	0
27	15	59/59 (100%)	-0.24	0 100 100	28, 45, 57, 63	0
27	25	59/59 (100%)	-0.26	1 (1%) 73 52	46, 57, 68, 73	0
28	16	53/53 (100%)	-0.22	0 100 100	45, 50, 58, 60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/53 (100%)	0.34	1 (1%) 70 48	59, 63, 67, 72	0
29	17	48/48 (100%)	-0.01	2 (4%) 40 19	30, 33, 52, 56	0
29	27	48/48 (100%)	0.14	2 (4%) 40 19	43, 48, 61, 69	0
30	18	64/64 (100%)	-0.10	0 100 100	35, 41, 46, 48	0
30	28	64/64 (100%)	0.13	0 100 100	52, 57, 62, 64	0
31	19	37/37 (100%)	0.30	2 (5%) 29 12	40, 48, 58, 62	0
31	29	37/37 (100%)	0.59	2 (5%) 29 12	62, 66, 70, 71	0
32	1a	1488/1521 (97%)	-0.12	34 (2%) 64 40	45, 72, 87, 97	0
32	2a	1492/1521 (98%)	-0.11	40 (2%) 58 34	52, 73, 88, 95	0
33	1b	231/231 (100%)	0.09	10 (4%) 39 18	69, 75, 81, 84	0
33	2b	231/231 (100%)	0.27	9 (3%) 43 21	72, 77, 82, 84	0
34	1c	206/206 (100%)	0.38	10 (4%) 33 14	70, 76, 79, 81	0
34	2c	206/206 (100%)	0.32	14 (6%) 20 7	73, 78, 81, 84	0
35	1d	208/208 (100%)	0.12	4 (1%) 70 48	65, 74, 78, 81	0
35	2d	208/208 (100%)	0.02	1 (0%) 91 83	64, 70, 75, 78	0
36	1e	148/148 (100%)	-0.03	1 (0%) 89 78	61, 68, 73, 82	0
36	2e	148/148 (100%)	0.00	1 (0%) 89 78	65, 71, 76, 83	0
37	1f	100/100 (100%)	-0.17	1 (1%) 84 69	63, 70, 73, 76	0
37	2f	100/100 (100%)	-0.26	1 (1%) 84 69	67, 71, 75, 77	0
38	1g	155/155 (100%)	0.22	9 (5%) 26 11	67, 73, 80, 85	0
38	2g	155/155 (100%)	0.57	17 (10%) 7 2	74, 77, 80, 86	0
39	1h	137/137 (100%)	-0.02	1 (0%) 89 78	64, 68, 72, 76	0
39	2h	137/137 (100%)	0.19	4 (2%) 55 31	67, 71, 74, 75	0
40	1i	127/127 (100%)	0.76	13 (10%) 9 3	69, 78, 81, 83	0
40	2i	126/127 (99%)	1.27	29 (23%) 1 0	72, 80, 83, 85	0
41	1j	97/97 (100%)	1.13	16 (16%) 2 1	71, 78, 80, 83	0
41	2j	96/97 (98%)	1.12	22 (22%) 1 0	74, 80, 83, 85	0
42	1k	114/114 (100%)	-0.24	0 100 100	56, 68, 72, 74	0
42	2k	114/114 (100%)	-0.04	2 (1%) 71 50	63, 72, 75, 79	0
43	1l	121/122 (99%)	0.22	3 (2%) 61 37	58, 66, 70, 74	0
43	2l	121/122 (99%)	0.06	2 (1%) 73 52	60, 65, 70, 74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/116 (100%)	0.32	6 (5%) 31 13	64, 74, 78, 80	0
44	2m	114/116 (98%)	0.66	14 (12%) 5 2	73, 79, 82, 82	0
45	1n	60/60 (100%)	0.37	3 (5%) 32 13	71, 74, 77, 79	0
45	2n	60/60 (100%)	1.04	14 (23%) 1 0	74, 78, 81, 82	0
46	1o	88/88 (100%)	-0.05	1 (1%) 82 66	57, 66, 73, 76	0
46	2o	88/88 (100%)	0.09	1 (1%) 82 66	63, 69, 74, 76	0
47	1p	82/82 (100%)	0.70	7 (8%) 13 4	67, 73, 77, 79	0
47	2p	82/82 (100%)	0.25	2 (2%) 62 39	63, 69, 74, 76	0
48	1q	99/99 (100%)	0.08	0 100 100	62, 66, 72, 73	0
48	2q	99/99 (100%)	0.22	1 (1%) 84 69	63, 69, 73, 75	0
49	1r	68/68 (100%)	0.20	0 100 100	64, 69, 75, 77	0
49	2r	68/68 (100%)	0.34	1 (1%) 76 58	68, 71, 76, 77	0
50	1s	83/83 (100%)	0.88	11 (13%) 4 2	70, 76, 79, 81	0
50	2s	83/83 (100%)	1.39	20 (24%) 1 0	71, 80, 82, 83	0
51	1t	96/98 (97%)	0.38	3 (3%) 52 28	65, 70, 75, 78	0
51	2t	98/98 (100%)	0.27	2 (2%) 68 46	62, 68, 75, 75	0
52	1u	23/23 (100%)	0.87	2 (8%) 13 4	70, 73, 76, 77	0
52	2u	23/23 (100%)	1.65	11 (47%) 0 0	76, 77, 79, 80	0
53	1x	72/76 (94%)	-0.20	0 100 100	41, 66, 76, 80	0
53	2x	72/76 (94%)	0.09	1 (1%) 78 60	56, 73, 81, 90	0
54	1y	12/19 (63%)	0.40	0 100 100	37, 48, 57, 59	0
54	2y	12/19 (63%)	1.03	3 (25%) 1 0	52, 59, 62, 69	0
55	A	3/27 (11%)	2.11	1 (33%) 0 0	70, 70, 71, 74	0
55	B	3/27 (11%)	0.58	1 (33%) 0 0	64, 64, 65, 69	0
All	All	20701/21004 (98%)	-0.00	646 (3%) 52 28	23, 65, 82, 97	0

The worst 5 of 646 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	1Z	192	ALA	8.1
21	1Z	198	LYS	8.0
21	1Z	193	GLU	8.0
21	1Z	200	GLY	7.9
32	2a	1030(B)	C	7.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
32	5MC	2a	1404	21/22	0.96	0.16	-	59,60,62,62	0
1	PSU	2A	1911	20/21	0.96	0.09	-	67,68,69,69	0
53	5MC	2x	32	21/22	0.94	0.16	-	70,71,72,73	0
53	5MU	1x	54	21/22	0.96	0.16	-	67,69,72,75	0
53	4SU	2x	8	20/21	0.92	0.15	-	72,75,76,77	0
32	PSU	2a	516	20/21	0.88	0.17	-	73,74,78,78	0
1	PSU	1A	1939	20/21	0.92	0.15	-	62,65,68,69	0
1	5MU	1A	1961	21/22	0.97	0.21	-	37,39,40,40	0
32	5MC	1a	1400	21/22	0.94	0.18	-	62,64,65,65	0
1	2MA	2A	2503	23/24	0.93	0.26	-	41,43,46,48	0
1	PSU	1A	2617	20/21	0.96	0.22	-	36,37,38,39	0
1	PSU	1A	1933	20/21	0.96	0.14	-	58,61,63,64	0
32	2MG	2a	1207	24/25	0.93	0.20	-	75,77,78,79	0
32	5MC	2a	1400	21/22	0.95	0.21	-	67,69,71,71	0
32	5MC	1a	967	21/22	0.95	0.17	-	67,68,69,70	0
53	5MC	1x	32	21/22	0.92	0.20	-	65,66,69,69	0
1	OMG	1A	2263	24/25	0.98	0.18	-	31,33,36,36	0
32	5MC	1a	1407	21/22	0.95	0.18	-	52,56,59,60	0
53	PSU	1x	55	20/21	0.93	0.16	-	66,67,69,69	0
32	2MG	1a	1207	24/25	0.92	0.13	-	72,75,78,79	0
32	UR3	2a	1498	21/22	0.96	0.16	-	60,61,63,64	0
1	5MU	2A	1939	21/22	0.96	0.18	-	46,49,50,50	0
32	G7M	1a	527	24/25	0.96	0.16	-	66,67,68,68	0
53	4SU	1x	8	20/21	0.93	0.14	-	66,68,68,69	0
1	5MU	2A	1915	21/22	0.92	0.17	-	78,80,84,87	0
32	MA6	1a	1519	24/25	0.96	0.22	-	51,55,55,56	0
32	MA6	1a	1518	24/25	0.96	0.21	-	53,54,56,57	0
32	PSU	1a	516	20/21	0.86	0.17	-	69,72,73,73	0
32	M2G	1a	966	25/26	0.94	0.20	-	66,67,69,70	0
32	MA6	2a	1519	24/25	0.96	0.19	-	58,59,60,60	0
43	0TD	1l	92	10/11	0.90	0.26	-	66,66,67,69	0
1	5MC	1A	1964	21/22	0.97	0.12	-	40,43,44,45	0
1	OMC	2A	1920	21/22	0.96	0.17	-	62,64,66,66	0
32	5MC	2a	967	21/22	0.95	0.16	-	70,71,74,77	0
1	5MC	2A	1942	21/22	0.97	0.14	-	55,56,57,57	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	5MC	1a	1404	21/22	0.96	0.17	-	57,59,61,61	0
1	2MA	1A	2515	23/24	0.97	0.21	-	24,26,28,30	0
32	4OC	1a	1402	22/23	0.96	0.22	-	60,61,62,62	0
1	OMG	2A	2251	24/25	0.97	0.20	-	45,46,50,51	0
1	PSU	2A	2605	20/21	0.96	0.19	-	42,45,45,45	0
32	G7M	2a	527	24/25	0.92	0.20	-	69,70,71,72	0
32	4OC	2a	1402	22/23	0.93	0.20	-	64,66,67,69	0
1	OMU	2A	2552	21/22	0.97	0.15	-	45,46,48,48	0
43	0TD	2l	92	10/11	0.92	0.18	-	65,65,66,67	0
1	5MC	2A	1962	21/22	0.98	0.15	-	53,54,57,58	0
1	5MC	1A	1984	21/22	0.96	0.15	-	42,43,46,49	0
53	PSU	2x	55	20/21	0.85	0.18	-	74,74,76,76	0
32	MA6	2a	1518	24/25	0.96	0.18	-	60,61,62,62	0
32	M2G	2a	966	25/26	0.94	0.21	-	68,70,72,73	0
1	OMU	1A	2564	21/22	0.94	0.20	-	35,37,38,39	0
1	5MU	1A	1937	21/22	0.91	0.21	-	69,72,80,81	0
32	5MC	2a	1407	21/22	0.94	0.19	-	58,63,64,65	0
1	PSU	2A	1917	20/21	0.95	0.10	-	67,70,73,74	0
53	5MU	2x	54	21/22	0.93	0.17	-	73,74,76,77	0
1	OMC	1A	1942	21/22	0.96	0.20	-	54,57,58,59	0
32	UR3	1a	1498	21/22	0.97	0.16	-	56,57,60,61	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	1A	3225	1/1	0.96	1.06	60.01	38,38,38,38	0
56	MG	1A	3104	1/1	0.92	1.00	50.36	32,32,32,32	0
56	MG	1A	3024	1/1	0.91	0.61	44.85	34,34,34,34	0
56	MG	1A	3026	1/1	0.92	0.76	41.24	32,32,32,32	0
56	MG	1A	3211	1/1	0.87	0.82	41.09	30,30,30,30	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	1A	3150	1/1	0.89	0.88	41.01	32,32,32,32	0
56	MG	1A	3218	1/1	0.93	0.54	39.05	35,35,35,35	0
56	MG	1A	3930	1/1	0.86	0.88	38.80	32,32,32,32	0
56	MG	1A	3256	1/1	0.93	1.30	36.94	48,48,48,48	0
56	MG	1A	3556	1/1	0.89	0.69	36.51	39,39,39,39	0
56	MG	1U	204	1/1	0.91	0.76	35.88	35,35,35,35	0
56	MG	2A	3061	1/1	0.90	0.90	35.71	61,61,61,61	0
56	MG	1F	304	1/1	0.90	0.68	34.61	32,32,32,32	0
56	MG	1D	302	1/1	0.97	0.70	31.74	34,34,34,34	0
56	MG	2a	1624	1/1	0.93	0.47	31.64	64,64,64,64	0
56	MG	1A	3893	1/1	0.89	1.39	30.71	39,39,39,39	0
56	MG	1A	3922	1/1	0.78	0.85	30.16	31,31,31,31	0
56	MG	1A	3221	1/1	0.97	0.76	29.62	29,29,29,29	0
56	MG	2A	3017	1/1	0.95	0.82	29.26	48,48,48,48	0
56	MG	1a	1732	1/1	0.62	0.72	29.05	74,74,74,74	0
56	MG	2a	1640	1/1	0.89	0.51	28.25	71,71,71,71	0
56	MG	1A	3935	1/1	0.91	0.80	27.55	38,38,38,38	0
56	MG	1A	3076	1/1	0.89	0.87	27.35	37,37,37,37	0
56	MG	1D	321	1/1	0.97	0.59	26.90	46,46,46,46	0
56	MG	1A	3703	1/1	0.92	0.59	26.07	43,43,43,43	0
56	MG	2A	3152	1/1	0.96	0.48	25.99	51,51,51,51	0
56	MG	2A	3654	1/1	0.93	0.86	25.94	50,50,50,50	0
56	MG	1A	3212	1/1	0.84	0.69	25.32	30,30,30,30	0
56	MG	1a	1637	1/1	0.96	0.38	25.10	52,52,52,52	0
56	MG	1A	3069	1/1	0.95	0.74	24.64	30,30,30,30	0
56	MG	2A	3087	1/1	0.83	0.44	24.39	51,51,51,51	0
56	MG	1A	3130	1/1	0.92	0.71	24.30	31,31,31,31	0
56	MG	2A	3183	1/1	0.54	0.51	24.24	54,54,54,54	0
56	MG	2A	3663	1/1	0.83	0.52	24.14	55,55,55,55	0
56	MG	1D	317	1/1	0.91	0.66	23.38	35,35,35,35	0
56	MG	2A	3653	1/1	0.93	0.72	23.37	52,52,52,52	0
56	MG	1A	3273	1/1	0.92	0.42	23.27	41,41,41,41	0
56	MG	1E	302	1/1	0.95	0.68	23.10	30,30,30,30	0
56	MG	1A	3155	1/1	0.93	0.40	22.88	32,32,32,32	0
56	MG	1a	1653	1/1	0.70	0.43	22.36	56,56,56,56	0
56	MG	1A	3767	1/1	0.91	0.54	22.09	43,43,43,43	0
56	MG	1A	3019	1/1	0.96	0.76	21.35	27,27,27,27	0
56	MG	2A	3674	1/1	0.86	0.85	21.29	50,50,50,50	0
56	MG	1F	303	1/1	0.91	0.69	21.20	38,38,38,38	0
56	MG	2A	3124	1/1	0.84	0.57	21.18	63,63,63,63	0
56	MG	1A	3100	1/1	0.83	0.56	20.84	28,28,28,28	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	1A	3027	1/1	0.94	0.69	20.66	39,39,39,39	0
56	MG	1A	3152	1/1	0.96	0.74	19.96	36,36,36,36	0
56	MG	1A	3928	1/1	0.93	0.89	19.56	35,35,35,35	0
56	MG	1A	3945	1/1	0.84	0.57	19.37	38,38,38,38	0
56	MG	1A	3071	1/1	0.93	0.55	19.03	32,32,32,32	0
56	MG	1A	3129	1/1	0.93	0.64	18.87	30,30,30,30	0
56	MG	2a	1772	1/1	0.94	0.33	18.46	62,62,62,62	0
56	MG	1V	201	1/1	0.94	0.38	18.39	45,45,45,45	0
56	MG	15	101	1/1	0.90	0.58	18.37	32,32,32,32	0
56	MG	2A	3192	1/1	0.94	0.49	18.33	50,50,50,50	0
56	MG	2a	1630	1/1	0.71	1.06	18.31	76,76,76,76	0
56	MG	1A	3149	1/1	0.78	0.63	18.26	35,35,35,35	0
56	MG	1R	201	1/1	0.86	0.42	18.17	35,35,35,35	0
56	MG	1A	3112	1/1	0.94	0.45	18.10	37,37,37,37	0
56	MG	1a	1661	1/1	0.94	0.48	18.09	66,66,66,66	0
56	MG	1A	3579	1/1	0.86	0.49	17.19	37,37,37,37	0
56	MG	2a	1610	1/1	0.90	0.48	17.04	72,72,72,72	0
56	MG	2a	1625	1/1	0.84	0.58	16.73	72,72,72,72	0
56	MG	1A	3936	1/1	0.88	0.52	16.03	32,32,32,32	0
56	MG	1A	3164	1/1	0.96	0.63	15.65	29,29,29,29	0
56	MG	1A	3563	1/1	0.91	0.34	15.53	23,23,23,23	0
56	MG	1F	305	1/1	0.94	0.44	15.26	28,28,28,28	0
56	MG	2A	3534	1/1	0.96	0.45	15.24	50,50,50,50	0
56	MG	1a	1862	1/1	0.84	0.58	15.18	70,70,70,70	0
56	MG	2a	1678	1/1	0.86	0.51	14.88	64,64,64,64	0
56	MG	2A	3662	1/1	0.84	0.82	14.65	63,63,63,63	0
56	MG	1A	3047	1/1	0.96	0.68	14.54	44,44,44,44	0
56	MG	1a	1766	1/1	0.85	0.26	14.47	72,72,72,72	0
56	MG	1a	1655	1/1	0.96	0.35	14.25	51,51,51,51	0
56	MG	1A	3659	1/1	0.93	0.35	14.11	38,38,38,38	0
56	MG	1a	1652	1/1	0.74	0.30	13.96	55,55,55,55	0
56	MG	1A	3558	1/1	0.95	0.60	13.85	31,31,31,31	0
56	MG	1E	303	1/1	0.88	0.72	13.58	33,33,33,33	0
56	MG	1A	3255	1/1	0.89	0.59	13.10	30,30,30,30	0
56	MG	1A	3134	1/1	0.93	0.31	13.10	38,38,38,38	0
56	MG	1A	3228	1/1	0.86	0.57	12.75	40,40,40,40	0
56	MG	1B	205	1/1	0.79	0.22	12.66	57,57,57,57	0
56	MG	2A	3014	1/1	0.89	0.37	12.44	76,76,76,76	0
56	MG	1A	3189	1/1	0.87	0.84	12.42	43,43,43,43	0
56	MG	1A	3107	1/1	0.85	0.33	12.25	32,32,32,32	0
56	MG	1A	3038	1/1	0.82	0.40	12.22	39,39,39,39	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	2A	3220	1/1	0.56	0.44	12.20	51,51,51,51	0
56	MG	1A	3892	1/1	0.93	0.33	12.10	31,31,31,31	0
59	ARG	1B	229	12/12	0.93	0.31	12.03	41,46,51,52	0
56	MG	1A	3929	1/1	0.91	0.56	11.97	31,31,31,31	0
56	MG	1A	3137	1/1	0.98	0.48	11.92	32,32,32,32	0
56	MG	1A	3630	1/1	0.87	0.33	11.84	37,37,37,37	0
56	MG	1a	1754	1/1	0.87	0.50	11.71	68,68,68,68	0
56	MG	2A	3055	1/1	0.65	0.26	11.60	62,62,62,62	0
56	MG	1F	302	1/1	0.96	0.49	11.45	31,31,31,31	0
56	MG	2A	3181	1/1	0.94	0.38	11.38	57,57,57,57	0
56	MG	1A	3021	1/1	0.94	0.48	11.20	36,36,36,36	0
56	MG	1A	3919	1/1	0.92	0.45	11.13	41,41,41,41	0
56	MG	2A	3198	1/1	0.92	0.41	11.11	59,59,59,59	0
56	MG	2A	3054	1/1	0.94	0.73	10.91	66,66,66,66	0
56	MG	2A	3002	1/1	0.96	0.23	10.68	59,59,59,59	0
56	MG	1A	3118	1/1	0.96	0.41	10.62	39,39,39,39	0
56	MG	1A	3657	1/1	0.93	0.35	10.59	41,41,41,41	0
56	MG	1F	306	1/1	0.95	0.44	10.57	31,31,31,31	0
56	MG	2U	202	1/1	0.78	0.62	10.52	59,59,59,59	0
56	MG	1A	3937	1/1	0.96	0.49	10.06	32,32,32,32	0
56	MG	2A	3137	1/1	0.96	0.31	9.99	49,49,49,49	0
56	MG	1a	1619	1/1	0.84	0.48	9.83	74,74,74,74	0
56	MG	1N	201	1/1	0.94	0.72	9.80	41,41,41,41	0
56	MG	1A	3886	1/1	0.88	0.38	9.78	38,38,38,38	0
56	MG	2A	3243	1/1	0.78	0.28	9.70	50,50,50,50	0
56	MG	1A	3891	1/1	0.94	0.44	9.62	38,38,38,38	0
56	MG	2A	3104	1/1	0.95	0.38	9.62	48,48,48,48	0
56	MG	1A	3136	1/1	0.92	0.32	9.61	33,33,33,33	0
56	MG	1A	3169	1/1	0.96	0.48	9.60	37,37,37,37	0
56	MG	1a	1615	1/1	0.89	0.31	9.55	71,71,71,71	0
56	MG	2a	1634	1/1	0.88	0.26	9.40	69,69,69,69	0
56	MG	1A	3416	1/1	0.95	0.28	9.29	44,44,44,44	0
56	MG	1A	3482	1/1	0.84	0.36	9.24	28,28,28,28	0
56	MG	1D	306	1/1	0.84	0.30	9.06	35,35,35,35	0
56	MG	1A	3466	1/1	0.94	0.31	8.95	29,29,29,29	0
56	MG	1A	3586	1/1	0.91	0.39	8.90	36,36,36,36	0
56	MG	1A	3146	1/1	0.66	0.31	8.86	52,52,52,52	0
56	MG	1A	3946	1/1	0.94	0.36	8.81	29,29,29,29	0
56	MG	1o	101	1/1	0.65	0.44	8.78	66,66,66,66	0
56	MG	1A	3121	1/1	0.93	0.25	8.50	68,68,68,68	0
56	MG	2A	3096	1/1	0.97	0.22	8.32	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	2A	3652	1/1	0.91	0.37	8.29	41,41,41,41	0
56	MG	2a	1653	1/1	0.89	0.38	8.28	67,67,67,67	0
56	MG	1A	3085	1/1	0.89	0.49	8.10	42,42,42,42	0
56	MG	1a	1710	1/1	0.98	0.32	8.01	58,58,58,58	0
56	MG	1A	3948	1/1	0.90	0.41	7.96	44,44,44,44	0
56	MG	2A	3344	1/1	0.98	0.33	7.90	61,61,61,61	0
56	MG	1a	1639	1/1	0.70	0.37	7.88	61,61,61,61	0
56	MG	2A	3670	1/1	0.94	0.46	7.61	50,50,50,50	0
56	MG	2A	3057	1/1	0.81	0.76	7.59	53,53,53,53	0
56	MG	2A	3114	1/1	0.79	0.37	7.39	50,50,50,50	0
56	MG	2x	108	1/1	0.75	0.64	7.21	57,57,57,57	0
56	MG	2A	3028	1/1	0.87	0.31	7.14	51,51,51,51	0
56	MG	2A	3086	1/1	0.78	0.28	7.08	58,58,58,58	0
56	MG	2A	3084	1/1	0.86	0.36	7.08	42,42,42,42	0
56	MG	1A	3022	1/1	0.88	0.28	7.04	43,43,43,43	0
56	MG	2a	1626	1/1	0.90	0.28	7.04	61,61,61,61	0
56	MG	2A	3046	1/1	0.83	0.26	6.74	61,61,61,61	0
56	MG	1A	3618	1/1	0.95	0.34	6.70	30,30,30,30	0
56	MG	1A	3938	1/1	0.96	0.55	6.65	33,33,33,33	0
56	MG	1A	3645	1/1	0.73	0.61	6.61	37,37,37,37	0
56	MG	1A	3729	1/1	0.92	0.34	6.53	32,32,32,32	0
56	MG	1A	3857	1/1	0.97	0.26	6.51	44,44,44,44	0
56	MG	2A	3338	1/1	0.94	0.30	6.42	40,40,40,40	0
56	MG	2a	1754	1/1	0.62	0.23	6.32	69,69,69,69	0
56	MG	2A	3273	1/1	0.93	0.28	6.24	61,61,61,61	0
56	MG	2a	1621	1/1	0.70	0.22	6.20	60,60,60,60	0
56	MG	2a	1729	1/1	0.95	0.21	6.18	64,64,64,64	0
56	MG	2a	1651	1/1	0.96	0.58	6.06	62,62,62,62	0
56	MG	1A	3667	1/1	0.93	0.23	6.05	37,37,37,37	0
56	MG	2t	3001	1/1	0.78	0.52	6.03	66,66,66,66	0
56	MG	1A	3925	1/1	0.94	0.42	5.96	42,42,42,42	0
56	MG	2A	3066	1/1	0.98	0.47	5.95	59,59,59,59	0
56	MG	1A	3297	1/1	0.98	0.27	5.94	37,37,37,37	0
56	MG	1A	3619	1/1	0.75	0.25	5.92	32,32,32,32	0
56	MG	2A	3224	1/1	0.89	0.32	5.84	46,46,46,46	0
56	MG	2D	305	1/1	0.90	0.32	5.81	46,46,46,46	0
56	MG	1D	303	1/1	0.91	0.42	5.81	41,41,41,41	0
56	MG	2A	3300	1/1	0.97	0.28	5.75	42,42,42,42	0
56	MG	1A	3644	1/1	0.86	0.34	5.73	38,38,38,38	0
56	MG	2A	3384	1/1	0.85	0.30	5.67	48,48,48,48	0
56	MG	1A	3190	1/1	0.94	0.28	5.64	44,44,44,44	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	1a	1648	1/1	0.95	0.39	5.64	57,57,57,57	0
56	MG	1D	312	1/1	0.93	0.69	5.61	48,48,48,48	0
56	MG	1A	3885	1/1	0.96	0.31	5.57	30,30,30,30	0
56	MG	1A	3939	1/1	0.95	0.43	5.51	32,32,32,32	0
56	MG	2A	3657	1/1	0.94	0.32	5.42	49,49,49,49	0
56	MG	1A	3926	1/1	0.90	0.56	5.39	45,45,45,45	0
56	MG	2A	3010	1/1	0.94	0.28	5.35	43,43,43,43	0
56	MG	1A	3237	1/1	0.99	0.30	5.35	38,38,38,38	0
56	MG	2A	3071	1/1	0.86	0.18	5.27	65,65,65,65	0
56	MG	2a	1633	1/1	0.76	0.28	5.23	54,54,54,54	0
56	MG	2A	3258	1/1	0.90	0.28	5.19	58,58,58,58	0
56	MG	1A	3527	1/1	0.89	0.23	5.18	49,49,49,49	0
56	MG	1A	3291	1/1	0.86	0.30	5.13	26,26,26,26	0
56	MG	1A	3059	1/1	0.85	0.23	5.01	60,60,60,60	0
56	MG	1A	3712	1/1	0.80	0.26	5.00	48,48,48,48	0
56	MG	2D	306	1/1	0.94	0.40	4.97	54,54,54,54	0
56	MG	2A	3094	1/1	0.98	0.28	4.90	55,55,55,55	0
56	MG	1A	3271	1/1	0.96	0.32	4.88	42,42,42,42	0
56	MG	2a	1712	1/1	0.83	0.24	4.80	66,66,66,66	0
56	MG	1D	304	1/1	0.82	0.76	4.75	49,49,49,49	0
56	MG	1A	3737	1/1	0.93	0.24	4.75	31,31,31,31	0
56	MG	2A	3563	1/1	0.78	0.34	4.74	45,45,45,45	0
56	MG	1A	3898	1/1	0.89	0.29	4.73	43,43,43,43	0
56	MG	1A	3931	1/1	0.94	0.41	4.67	42,42,42,42	0
56	MG	1a	1667	1/1	0.78	0.46	4.64	83,83,83,83	0
56	MG	2A	3272	1/1	0.79	0.22	4.62	54,54,54,54	0
56	MG	1a	1856	1/1	0.89	0.27	4.62	62,62,62,62	0
56	MG	2A	3296	1/1	0.85	0.30	4.52	42,42,42,42	0
56	MG	2A	3642	1/1	0.96	0.47	4.48	51,51,51,51	0
56	MG	1A	3041	1/1	0.92	0.19	4.47	46,46,46,46	0
56	MG	1A	3522	1/1	0.86	0.24	4.44	39,39,39,39	0
56	MG	1A	3072	1/1	0.85	0.21	4.42	43,43,43,43	0
56	MG	1A	3187	1/1	0.95	0.28	4.40	41,41,41,41	0
56	MG	2a	1628	1/1	0.79	0.30	4.39	58,58,58,58	0
56	MG	1R	203	1/1	0.85	0.31	4.34	39,39,39,39	0
56	MG	23	101	1/1	0.84	0.68	4.29	58,58,58,58	0
56	MG	1a	1606	1/1	0.89	0.27	4.26	62,62,62,62	0
56	MG	2A	3142	1/1	0.89	0.26	4.23	61,61,61,61	0
56	MG	1A	3810	1/1	0.97	0.31	4.18	28,28,28,28	0
56	MG	1A	3371	1/1	0.73	0.24	4.17	30,30,30,30	0
56	MG	2A	3171	1/1	0.88	0.19	4.08	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	2A	3011	1/1	0.92	0.20	4.08	59,59,59,59	0
56	MG	1A	3601	1/1	0.83	0.23	4.08	31,31,31,31	0
56	MG	2D	307	1/1	0.90	0.37	4.06	46,46,46,46	0
56	MG	1a	1698	1/1	0.65	0.26	4.06	72,72,72,72	0
56	MG	1A	3552	1/1	0.90	0.26	4.03	32,32,32,32	0
56	MG	2A	3644	1/1	0.87	0.23	4.00	56,56,56,56	0
56	MG	2A	3602	1/1	0.90	0.26	3.96	47,47,47,47	0
56	MG	1D	316	1/1	0.94	0.33	3.96	34,34,34,34	0
56	MG	2A	3129	1/1	0.93	0.23	3.96	49,49,49,49	0
56	MG	1A	3426	1/1	0.83	0.24	3.94	32,32,32,32	0
56	MG	1A	3266	1/1	0.98	0.24	3.93	31,31,31,31	0
56	MG	1A	3001	1/1	0.96	0.23	3.92	42,42,42,42	0
56	MG	2A	3466	1/1	0.83	0.20	3.89	57,57,57,57	0
56	MG	1A	3039	1/1	0.97	0.24	3.89	53,53,53,53	0
56	MG	1A	3013	1/1	0.97	0.24	3.86	29,29,29,29	0
56	MG	1A	3109	1/1	0.97	0.41	3.80	40,40,40,40	0
56	MG	1a	1633	1/1	0.95	0.28	3.76	51,51,51,51	0
56	MG	1A	3776	1/1	0.85	0.22	3.69	40,40,40,40	0
56	MG	2F	303	1/1	0.93	0.36	3.59	50,50,50,50	0
56	MG	1A	3535	1/1	0.71	0.23	3.52	34,34,34,34	0
56	MG	1a	1842	1/1	0.91	0.23	3.51	62,62,62,62	0
56	MG	2V	202	1/1	0.93	0.46	3.49	53,53,53,53	0
56	MG	1A	3006	1/1	0.87	0.25	3.48	34,34,34,34	0
56	MG	1B	208	1/1	0.92	0.22	3.39	54,54,54,54	0
56	MG	2A	3418	1/1	0.84	0.24	3.39	65,65,65,65	0
56	MG	1D	313	1/1	0.91	0.30	3.39	41,41,41,41	0
56	MG	1A	3214	1/1	0.94	0.31	3.36	30,30,30,30	0
56	MG	1a	1722	1/1	0.84	0.23	3.35	67,67,67,67	0
56	MG	1a	1728	1/1	0.79	0.45	3.34	75,75,75,75	0
58	MPD	1A	3907	8/8	0.93	0.22	3.26	51,53,55,56	0
56	MG	1a	1644	1/1	0.91	0.24	3.25	62,62,62,62	0
56	MG	2A	3264	1/1	0.82	0.23	3.25	49,49,49,49	0
56	MG	2E	301	1/1	0.94	0.35	3.14	45,45,45,45	0
57	UNX	2A	3667	1/1	0.97	0.38	3.10	45,45,45,45	0
56	MG	2A	3140	1/1	0.93	0.34	3.09	65,65,65,65	0
56	MG	2A	3539	1/1	0.86	0.22	3.07	57,57,57,57	0
56	MG	2A	3398	1/1	0.81	0.24	3.04	64,64,64,64	0
56	MG	1A	3432	1/1	0.86	0.23	3.02	34,34,34,34	0
56	MG	1A	3437	1/1	0.80	0.25	3.01	26,26,26,26	0
56	MG	1a	1831	1/1	0.76	0.22	2.97	69,69,69,69	0
56	MG	1A	3360	1/1	0.92	0.22	2.94	44,44,44,44	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	1A	3386	1/1	0.81	0.21	2.91	32,32,32,32	0
56	MG	2n	101	1/1	0.97	0.36	2.90	77,77,77,77	0
56	MG	1a	1617	1/1	0.97	0.26	2.90	69,69,69,69	0
56	MG	1a	1625	1/1	0.81	0.20	2.89	71,71,71,71	0
56	MG	2A	3493	1/1	0.88	0.20	2.83	61,61,61,61	0
56	MG	2A	3572	1/1	0.95	0.25	2.83	61,61,61,61	0
56	MG	2A	3392	1/1	0.93	0.18	2.79	52,52,52,52	0
56	MG	2a	1702	1/1	0.92	0.16	2.76	62,62,62,62	0
56	MG	2A	3242	1/1	0.92	0.23	2.74	55,55,55,55	0
56	MG	2A	3168	1/1	0.88	0.22	2.74	52,52,52,52	0
56	MG	2A	3417	1/1	0.89	0.18	2.72	62,62,62,62	0
56	MG	2A	3099	1/1	0.81	0.30	2.69	57,57,57,57	0
56	MG	1A	3673	1/1	0.97	0.25	2.67	44,44,44,44	0
56	MG	1a	1840	1/1	0.91	0.20	2.63	67,67,67,67	0
56	MG	1A	3201	1/1	0.92	0.22	2.63	25,25,25,25	0
56	MG	1a	1695	1/1	0.93	0.22	2.57	67,67,67,67	0
56	MG	2A	3672	1/1	0.76	0.34	2.57	64,64,64,64	0
56	MG	2a	1756	1/1	0.93	0.27	2.54	73,73,73,73	0
56	MG	1A	3578	1/1	0.95	0.21	2.51	36,36,36,36	0
56	MG	2A	3107	1/1	0.86	0.17	2.49	66,66,66,66	0
56	MG	2A	3026	1/1	0.91	0.18	2.49	41,41,41,41	0
56	MG	1a	1756	1/1	0.87	0.18	2.49	58,58,58,58	0
56	MG	2A	3254	1/1	0.85	0.36	2.47	42,42,42,42	0
56	MG	2Q	201	1/1	0.96	0.26	2.47	59,59,59,59	0
56	MG	1A	3242	1/1	0.97	0.24	2.47	29,29,29,29	0
56	MG	2A	3679	1/1	0.87	0.37	2.44	53,53,53,53	0
56	MG	1A	3923	1/1	0.99	0.24	2.39	36,36,36,36	0
56	MG	1A	3782	1/1	0.92	0.19	2.31	44,44,44,44	0
56	MG	2A	3093	1/1	0.95	0.21	2.29	61,61,61,61	0
56	MG	2A	3678	1/1	0.96	0.19	2.12	53,53,53,53	0
56	MG	2A	3601	1/1	0.90	0.23	2.11	54,54,54,54	0
56	MG	2A	3286	1/1	0.96	0.18	2.09	51,51,51,51	0
56	MG	2A	3106	1/1	0.94	0.23	2.07	49,49,49,49	0
56	MG	2A	3270	1/1	0.95	0.19	2.02	50,50,50,50	0
56	MG	2A	3475	1/1	0.21	0.27	2.01	48,48,48,48	0
56	MG	1e	203	1/1	0.93	0.35	2.01	63,63,63,63	0
56	MG	1a	1620	1/1	0.90	0.24	2.00	60,60,60,60	0
56	MG	2A	3436	1/1	0.93	0.18	1.99	41,41,41,41	0
56	MG	2A	3256	1/1	0.97	0.15	1.94	56,56,56,56	0
56	MG	2A	3556	1/1	0.95	0.23	1.92	47,47,47,47	0
56	MG	1A	3005	1/1	0.82	0.18	1.88	40,40,40,40	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	1A	3354	1/1	0.95	0.21	1.84	31,31,31,31	0
56	MG	1A	3496	1/1	0.81	0.18	1.81	40,40,40,40	0
56	MG	2A	3508	1/1	0.95	0.21	1.77	50,50,50,50	0
56	MG	2a	1684	1/1	0.68	0.16	1.70	66,66,66,66	0
56	MG	2A	3520	1/1	0.81	0.23	1.67	46,46,46,46	0
56	MG	1A	3612	1/1	0.89	0.19	1.67	65,65,65,65	0
56	MG	1B	221	1/1	0.98	0.22	1.62	51,51,51,51	0
56	MG	1a	1621	1/1	0.94	0.22	1.59	71,71,71,71	0
56	MG	10	103	1/1	0.95	0.21	1.57	42,42,42,42	0
56	MG	1A	3473	1/1	0.93	0.20	1.56	39,39,39,39	0
56	MG	2A	3276	1/1	0.89	0.19	1.51	47,47,47,47	0
56	MG	1A	3023	1/1	0.94	0.21	1.50	35,35,35,35	0
58	MPD	1a	1860	8/8	0.77	0.31	1.50	65,70,76,77	0
56	MG	1a	1668	1/1	0.78	0.41	1.47	70,70,70,70	0
56	MG	1a	1765	1/1	0.88	0.17	1.47	80,80,80,80	0
56	MG	1A	3321	1/1	0.92	0.20	1.47	26,26,26,26	0
56	MG	2A	3160	1/1	0.78	0.22	1.40	63,63,63,63	0
56	MG	1A	3699	1/1	0.87	0.20	1.37	32,32,32,32	0
56	MG	1A	3330	1/1	0.97	0.21	1.33	33,33,33,33	0
56	MG	1b	3001	1/1	0.92	0.19	1.32	73,73,73,73	0
56	MG	2A	3531	1/1	0.92	0.36	1.31	65,65,65,65	0
56	MG	1E	305	1/1	0.92	0.25	1.30	31,31,31,31	0
56	MG	1A	3573	1/1	0.91	0.21	1.29	35,35,35,35	0
56	MG	1a	1676	1/1	0.92	0.23	1.29	54,54,54,54	0
56	MG	1D	315	1/1	0.95	0.18	1.29	49,49,49,49	0
56	MG	1A	3876	1/1	0.83	0.22	1.28	32,32,32,32	0
56	MG	1A	3413	1/1	0.93	0.24	1.23	24,24,24,24	0
56	MG	1A	3269	1/1	0.85	0.32	1.20	41,41,41,41	0
56	MG	2A	3651	1/1	0.91	0.16	1.13	65,65,65,65	0
56	MG	2A	3037	1/1	0.86	0.15	1.12	66,66,66,66	0
56	MG	1A	3193	1/1	0.98	0.20	1.10	33,33,33,33	0
56	MG	2a	1761	1/1	0.79	0.28	1.04	63,63,63,63	0
56	MG	1A	3381	1/1	0.88	0.23	1.03	38,38,38,38	0
56	MG	2F	301	1/1	0.93	0.28	1.00	45,45,45,45	0
56	MG	2A	3362	1/1	0.76	0.20	1.00	46,46,46,46	0
56	MG	1A	3675	1/1	0.79	0.22	0.98	36,36,36,36	0
57	UNX	1A	3906	1/1	0.94	0.27	0.97	38,38,38,38	0
56	MG	1a	1666	1/1	0.95	0.27	0.97	65,65,65,65	0
56	MG	1A	3300	1/1	0.89	0.20	0.96	45,45,45,45	0
56	MG	1A	3295	1/1	0.94	0.15	0.94	50,50,50,50	0
56	MG	1a	1859	1/1	0.90	0.21	0.89	62,62,62,62	0
56	MG	1n	101	1/1	0.93	0.32	0.84	71,71,71,71	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	2a	1641	1/1	0.77	0.36	0.82	76,76,76,76	0
56	MG	2A	3578	1/1	0.97	0.23	0.78	51,51,51,51	0
56	MG	2A	3409	1/1	0.89	0.18	0.78	56,56,56,56	0
56	MG	1A	3654	1/1	0.96	0.14	0.75	49,49,49,49	0
56	MG	2A	3025	1/1	0.87	0.20	0.70	56,56,56,56	0
56	MG	2A	3315	1/1	0.78	0.18	0.70	48,48,48,48	0
56	MG	2a	1689	1/1	0.90	0.14	0.65	75,75,75,75	0
56	MG	1A	3690	1/1	0.91	0.23	0.65	42,42,42,42	0
56	MG	2A	3036	1/1	0.96	0.15	0.63	65,65,65,65	0
56	MG	2A	3380	1/1	0.95	0.18	0.60	59,59,59,59	0
56	MG	17	102	1/1	0.95	0.22	0.59	35,35,35,35	0
56	MG	1A	3838	1/1	0.98	0.29	0.54	45,45,45,45	0
56	MG	1B	224	1/1	0.82	0.16	0.53	54,54,54,54	0
56	MG	1D	310	1/1	0.93	0.20	0.52	36,36,36,36	0
56	MG	1A	3492	1/1	0.94	0.17	0.51	45,45,45,45	0
56	MG	2a	1782	1/1	0.97	0.15	0.48	63,63,63,63	0
56	MG	2A	3570	1/1	0.66	0.23	0.39	43,43,43,43	0
56	MG	1a	1630	1/1	0.95	0.17	0.38	64,64,64,64	0
56	MG	1A	3688	1/1	0.93	0.17	0.34	40,40,40,40	0
56	MG	1Q	201	1/1	0.89	0.21	0.31	41,41,41,41	0
56	MG	1A	3451	1/1	0.92	0.13	0.29	38,38,38,38	0
56	MG	1a	1767	1/1	0.90	0.13	0.29	72,72,72,72	0
56	MG	2a	1763	1/1	0.70	0.22	0.26	82,82,82,82	0
56	MG	1a	1623	1/1	0.91	0.23	0.26	65,65,65,65	0
56	MG	1a	1649	1/1	0.94	0.18	0.23	70,70,70,70	0
56	MG	1A	3206	1/1	0.94	0.19	0.16	35,35,35,35	0
56	MG	2A	3557	1/1	0.83	0.18	0.15	51,51,51,51	0
56	MG	2A	3321	1/1	0.90	0.20	0.14	48,48,48,48	0
56	MG	2A	3293	1/1	0.88	0.14	0.12	63,63,63,63	0
60	ZN	24	501	1/1	0.85	0.23	0.07	94,94,94,94	0
56	MG	1A	3067	1/1	0.98	0.21	0.04	35,35,35,35	0
56	MG	1A	3299	1/1	0.87	0.17	0.01	47,47,47,47	0
56	MG	1A	3484	1/1	0.83	0.17	0.01	43,43,43,43	0
56	MG	2f	3001	1/1	0.98	0.21	-0.05	67,67,67,67	0
56	MG	2A	3297	1/1	0.94	0.19	-0.06	43,43,43,43	0
56	MG	10	101	1/1	0.95	0.17	-0.08	48,48,48,48	0
56	MG	2D	308	1/1	0.86	0.19	-0.11	47,47,47,47	0
56	MG	2a	1681	1/1	0.86	0.14	-0.13	69,69,69,69	0
56	MG	2a	1780	1/1	0.93	0.16	-0.13	70,70,70,70	0
56	MG	2A	3050	1/1	0.86	0.14	-0.13	56,56,56,56	0
56	MG	1A	3643	1/1	0.95	0.18	-0.14	37,37,37,37	0
56	MG	1a	1845	1/1	0.95	0.15	-0.14	61,61,61,61	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	1A	3920	1/1	0.91	0.21	-0.19	47,47,47,47	0
56	MG	1A	3887	1/1	0.94	0.21	-0.21	36,36,36,36	0
56	MG	1A	3889	1/1	0.93	0.18	-0.23	35,35,35,35	0
56	MG	1a	1634	1/1	0.90	0.15	-0.24	63,63,63,63	0
56	MG	1A	3870	1/1	0.62	0.16	-0.25	35,35,35,35	0
56	MG	2A	3083	1/1	0.77	0.15	-0.26	76,76,76,76	0
56	MG	2A	3029	1/1	0.91	0.17	-0.26	50,50,50,50	0
56	MG	2A	3352	1/1	0.82	0.20	-0.27	49,49,49,49	0
56	MG	2A	3499	1/1	0.84	0.21	-0.28	41,41,41,41	0
56	MG	1a	1618	1/1	0.92	0.17	-0.28	73,73,73,73	0
56	MG	1a	1687	1/1	0.86	0.21	-0.29	71,71,71,71	0
56	MG	2a	1783	1/1	0.94	0.15	-0.31	67,67,67,67	0
60	ZN	14	501	1/1	0.90	0.14	-0.33	89,89,89,89	0
56	MG	2E	304	1/1	0.95	0.19	-0.33	47,47,47,47	0
56	MG	2A	3341	1/1	0.96	0.17	-0.33	55,55,55,55	0
56	MG	1d	505	1/1	0.34	0.16	-0.33	77,77,77,77	0
56	MG	2A	3357	1/1	0.85	0.16	-0.33	51,51,51,51	0
56	MG	1x	104	1/1	0.80	0.14	-0.35	69,69,69,69	0
56	MG	2A	3358	1/1	0.86	0.18	-0.39	43,43,43,43	0
56	MG	1A	3915	1/1	0.85	0.18	-0.41	29,29,29,29	0
56	MG	1a	1656	1/1	0.96	0.14	-0.42	73,73,73,73	0
56	MG	2a	1655	1/1	0.94	0.15	-0.44	68,68,68,68	0
56	MG	2B	3012	1/1	0.72	0.10	-0.46	64,64,64,64	0
56	MG	2A	3681	1/1	0.94	0.16	-0.48	54,54,54,54	0
56	MG	2A	3080	1/1	0.87	0.13	-0.49	61,61,61,61	0
56	MG	1A	3439	1/1	0.85	0.19	-0.49	31,31,31,31	0
56	MG	1A	3741	1/1	0.87	0.17	-0.50	31,31,31,31	0
56	MG	1a	1718	1/1	0.92	0.14	-0.50	73,73,73,73	0
56	MG	2A	3400	1/1	0.89	0.19	-0.53	54,54,54,54	0
56	MG	1A	3428	1/1	0.86	0.20	-0.53	24,24,24,24	0
56	MG	1D	308	1/1	0.96	0.20	-0.53	42,42,42,42	0
56	MG	1a	1705	1/1	0.91	0.18	-0.54	51,51,51,51	0
56	MG	1A	3431	1/1	0.89	0.18	-0.61	29,29,29,29	0
56	MG	1A	3320	1/1	0.74	0.19	-0.62	26,26,26,26	0
56	MG	2A	3464	1/1	0.93	0.13	-0.63	65,65,65,65	0
56	MG	1A	3542	1/1	0.96	0.15	-0.66	49,49,49,49	0
56	MG	1A	3701	1/1	0.95	0.17	-0.66	47,47,47,47	0
56	MG	2A	3365	1/1	0.96	0.15	-0.67	48,48,48,48	0
60	ZN	25	101	1/1	0.99	0.09	-0.69	65,65,65,65	0
56	MG	1A	3341	1/1	0.90	0.16	-0.73	35,35,35,35	0
56	MG	28	101	1/1	0.94	0.15	-0.74	62,62,62,62	0
56	MG	2A	3379	1/1	0.60	0.14	-0.74	55,55,55,55	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	2a	1744	1/1	0.82	0.15	-0.75	62,62,62,62	0
56	MG	2A	3282	1/1	0.96	0.14	-0.75	49,49,49,49	0
56	MG	1X	101	1/1	0.94	0.12	-0.77	39,39,39,39	0
56	MG	1A	3916	1/1	0.98	0.16	-0.78	42,42,42,42	0
56	MG	2B	3009	1/1	0.93	0.10	-0.79	66,66,66,66	0
56	MG	2A	3504	1/1	0.88	0.14	-0.80	64,64,64,64	0
56	MG	2a	1767	1/1	0.97	0.15	-0.80	63,63,63,63	0
56	MG	2A	3673	1/1	0.96	0.17	-0.82	51,51,51,51	0
56	MG	2A	3639	1/1	0.94	0.16	-0.82	57,57,57,57	0
56	MG	2A	3478	1/1	0.79	0.15	-0.87	50,50,50,50	0
56	MG	2A	3559	1/1	0.66	0.19	-0.88	47,47,47,47	0
56	MG	2a	1616	1/1	0.88	0.15	-0.90	57,57,57,57	0
56	MG	1r	3001	1/1	0.78	0.19	-0.95	70,70,70,70	0
56	MG	1a	1646	1/1	0.83	0.13	-0.96	72,72,72,72	0
56	MG	2V	201	1/1	0.98	0.12	-0.96	64,64,64,64	0
56	MG	2A	3551	1/1	0.92	0.16	-0.98	48,48,48,48	0
56	MG	2A	3391	1/1	0.82	0.17	-0.98	48,48,48,48	0
56	MG	1a	1711	1/1	0.78	0.15	-0.99	77,77,77,77	0
56	MG	1a	1805	1/1	0.82	0.12	-1.02	70,70,70,70	0
56	MG	1A	3477	1/1	0.93	0.13	-1.02	49,49,49,49	0
56	MG	2A	3442	1/1	0.86	0.13	-1.05	64,64,64,64	0
56	MG	2a	1619	1/1	0.84	0.14	-1.05	65,65,65,65	0
60	ZN	19	102	1/1	0.99	0.11	-1.06	52,52,52,52	0
56	MG	1A	3286	1/1	0.80	0.15	-1.09	27,27,27,27	0
60	ZN	16	101	1/1	0.98	0.12	-1.11	49,49,49,49	0
56	MG	1A	3298	1/1	0.97	0.16	-1.11	28,28,28,28	0
61	SF4	1d	501	8/8	0.96	0.15	-1.13	72,75,79,82	0
56	MG	1A	3346	1/1	0.93	0.14	-1.13	43,43,43,43	0
56	MG	1A	3007	1/1	0.98	0.12	-1.14	50,50,50,50	0
56	MG	2A	3427	1/1	0.89	0.08	-1.18	63,63,63,63	0
56	MG	1A	3811	1/1	0.90	0.20	-1.18	30,30,30,30	0
56	MG	28	102	1/1	0.92	0.20	-1.20	49,49,49,49	0
56	MG	1A	3444	1/1	0.94	0.19	-1.20	31,31,31,31	0
56	MG	1A	3848	1/1	0.84	0.12	-1.21	54,54,54,54	0
61	SF4	2d	501	8/8	0.98	0.14	-1.22	70,73,77,79	0
56	MG	2a	1614	1/1	0.84	0.13	-1.27	65,65,65,65	0
56	MG	2a	1736	1/1	0.97	0.10	-1.30	66,66,66,66	0
56	MG	2A	3416	1/1	0.97	0.10	-1.31	62,62,62,62	0
56	MG	1A	3210	1/1	0.97	0.13	-1.32	33,33,33,33	0
56	MG	1A	3314	1/1	0.93	0.16	-1.34	32,32,32,32	0
56	MG	1A	3812	1/1	0.95	0.17	-1.35	37,37,37,37	0
60	ZN	29	501	1/1	0.93	0.07	-1.36	67,67,67,67	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	1G	3004	1/1	0.90	0.11	-1.37	59,59,59,59	0
60	ZN	2n	102	1/1	0.95	0.06	-1.37	84,84,84,84	0
56	MG	1A	3918	1/1	0.97	0.15	-1.37	27,27,27,27	0
56	MG	2a	1611	1/1	0.96	0.13	-1.37	59,59,59,59	0
56	MG	2A	3503	1/1	0.77	0.12	-1.39	62,62,62,62	0
56	MG	1A	3343	1/1	0.92	0.17	-1.39	25,25,25,25	0
56	MG	2a	1768	1/1	0.79	0.14	-1.42	69,69,69,69	0
56	MG	1A	3710	1/1	0.89	0.16	-1.42	30,30,30,30	0
56	MG	2A	3019	1/1	0.96	0.12	-1.45	51,51,51,51	0
56	MG	1A	3345	1/1	0.74	0.14	-1.46	45,45,45,45	0
56	MG	2G	202	1/1	0.89	0.10	-1.46	74,74,74,74	0
56	MG	2A	3369	1/1	0.96	0.15	-1.47	45,45,45,45	0
56	MG	1A	3802	1/1	0.94	0.12	-1.49	54,54,54,54	0
60	ZN	15	102	1/1	0.98	0.10	-1.51	54,54,54,54	0
56	MG	1a	1838	1/1	0.87	0.08	-1.53	69,69,69,69	0
56	MG	1A	3313	1/1	0.85	0.17	-1.53	35,35,35,35	0
56	MG	1a	1861	1/1	0.96	0.11	-1.54	72,72,72,72	0
56	MG	2A	3425	1/1	0.93	0.16	-1.54	48,48,48,48	0
56	MG	2A	3376	1/1	0.92	0.14	-1.55	50,50,50,50	0
56	MG	1D	301	1/1	0.97	0.17	-1.55	35,35,35,35	0
56	MG	1A	3781	1/1	0.77	0.09	-1.56	66,66,66,66	0
56	MG	18	101	1/1	0.94	0.12	-1.59	49,49,49,49	0
56	MG	1A	3378	1/1	0.95	0.14	-1.60	40,40,40,40	0
56	MG	1A	3393	1/1	0.88	0.16	-1.60	31,31,31,31	0
56	MG	2a	1770	1/1	0.80	0.13	-1.61	68,68,68,68	0
56	MG	2A	3671	1/1	0.89	0.18	-1.61	44,44,44,44	0
56	MG	1A	3479	1/1	0.91	0.15	-1.61	33,33,33,33	0
56	MG	1B	217	1/1	0.83	0.11	-1.65	59,59,59,59	0
56	MG	1A	3280	1/1	0.97	0.14	-1.65	35,35,35,35	0
56	MG	2A	3012	1/1	0.98	0.17	-1.66	45,45,45,45	0
56	MG	1a	1772	1/1	0.97	0.13	-1.67	68,68,68,68	0
56	MG	1D	305	1/1	0.98	0.15	-1.68	34,34,34,34	0
60	ZN	26	101	1/1	0.98	0.06	-1.70	67,67,67,67	0
56	MG	2A	3530	1/1	0.82	0.13	-1.70	56,56,56,56	0
56	MG	1A	3472	1/1	0.95	0.17	-1.71	42,42,42,42	0
56	MG	1a	1801	1/1	0.67	0.13	-1.71	85,85,85,85	0
60	ZN	2Y	202	1/1	0.97	0.04	-1.73	77,77,77,77	0
56	MG	2A	3515	1/1	0.97	0.10	-1.74	62,62,62,62	0
56	MG	1A	3858	1/1	0.97	0.16	-1.81	38,38,38,38	0
60	ZN	1n	102	1/1	0.93	0.09	-1.83	76,76,76,76	0
56	MG	1A	3122	1/1	0.88	0.09	-1.86	37,37,37,37	0
56	MG	1a	1815	1/1	0.84	0.13	-1.87	57,57,57,57	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	2A	3354	1/1	0.96	0.12	-1.87	59,59,59,59	0
56	MG	2a	1771	1/1	0.86	0.15	-1.89	79,79,79,79	0
56	MG	1a	1857	1/1	0.91	0.09	-1.89	64,64,64,64	0
56	MG	2A	3257	1/1	0.93	0.11	-1.92	46,46,46,46	0
56	MG	2A	3245	1/1	0.97	0.12	-1.93	56,56,56,56	0
56	MG	1A	3565	1/1	0.96	0.14	-1.94	31,31,31,31	0
56	MG	1A	3315	1/1	0.95	0.11	-1.94	48,48,48,48	0
56	MG	1G	3001	1/1	0.85	0.12	-1.95	69,69,69,69	0
56	MG	1A	3456	1/1	0.88	0.14	-2.00	36,36,36,36	0
56	MG	2A	3596	1/1	0.91	0.12	-2.03	56,56,56,56	0
56	MG	1a	1802	1/1	0.70	0.12	-2.03	71,71,71,71	0
56	MG	2a	1760	1/1	0.76	0.11	-2.03	65,65,65,65	0
56	MG	1a	1602	1/1	0.90	0.08	-2.04	82,82,82,82	0
56	MG	2A	3422	1/1	0.93	0.12	-2.04	54,54,54,54	0
56	MG	2A	3549	1/1	0.96	0.15	-2.04	53,53,53,53	0
56	MG	1B	204	1/1	0.95	0.09	-2.06	56,56,56,56	0
56	MG	1A	3934	1/1	0.95	0.09	-2.07	44,44,44,44	0
56	MG	1A	3680	1/1	0.97	0.14	-2.10	30,30,30,30	0
56	MG	2a	1765	1/1	0.99	0.12	-2.17	66,66,66,66	0
56	MG	1A	3370	1/1	0.94	0.18	-2.19	35,35,35,35	0
56	MG	2I	3001	1/1	0.81	0.18	-2.20	74,74,74,74	0
56	MG	2A	3082	1/1	0.94	0.14	-2.24	47,47,47,47	0
56	MG	1A	3629	1/1	0.90	0.09	-2.26	64,64,64,64	0
56	MG	2A	3203	1/1	0.93	0.08	-2.33	71,71,71,71	0
56	MG	1A	3293	1/1	0.97	0.11	-2.36	35,35,35,35	0
56	MG	2A	3655	1/1	0.89	0.12	-2.38	46,46,46,46	0
60	ZN	1Y	501	1/1	0.97	0.07	-2.38	63,63,63,63	0
56	MG	1A	3355	1/1	0.85	0.15	-2.43	31,31,31,31	0
56	MG	1A	3786	1/1	0.80	0.16	-2.43	38,38,38,38	0
56	MG	1A	3817	1/1	0.74	0.14	-2.43	32,32,32,32	0
56	MG	2x	101	1/1	0.91	0.08	-2.43	70,70,70,70	0
56	MG	2A	3533	1/1	0.93	0.08	-2.45	60,60,60,60	0
56	MG	2A	3635	1/1	0.96	0.14	-2.46	48,48,48,48	0
56	MG	11	101	1/1	0.98	0.11	-2.47	34,34,34,34	0
56	MG	2A	3295	1/1	0.97	0.12	-2.54	52,52,52,52	0
56	MG	2a	1750	1/1	0.82	0.08	-2.57	76,76,76,76	0
56	MG	1A	3698	1/1	0.96	0.10	-2.57	30,30,30,30	0
56	MG	2A	3617	1/1	0.83	0.14	-2.58	49,49,49,49	0
56	MG	2A	3495	1/1	0.73	0.09	-2.58	65,65,65,65	0
56	MG	1A	3425	1/1	0.98	0.10	-2.60	44,44,44,44	0
56	MG	1A	3467	1/1	0.88	0.14	-2.62	48,48,48,48	0
56	MG	1A	3540	1/1	0.94	0.12	-2.66	42,42,42,42	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	2A	3307	1/1	0.93	0.10	-2.67	48,48,48,48	0
56	MG	2x	104	1/1	0.88	0.10	-2.68	72,72,72,72	0
56	MG	1A	3367	1/1	0.96	0.14	-2.68	33,33,33,33	0
56	MG	1A	3465	1/1	0.88	0.10	-2.69	50,50,50,50	0
56	MG	1a	1702	1/1	0.92	0.12	-2.73	51,51,51,51	0
56	MG	1a	1821	1/1	0.91	0.10	-2.75	76,76,76,76	0
56	MG	1A	3376	1/1	0.86	0.16	-2.75	29,29,29,29	0
56	MG	1A	3840	1/1	0.96	0.07	-2.75	39,39,39,39	0
56	MG	1A	3572	1/1	0.92	0.15	-2.75	35,35,35,35	0
56	MG	1A	3356	1/1	0.94	0.15	-2.75	26,26,26,26	0
56	MG	1A	3030	1/1	0.93	0.11	-2.76	28,28,28,28	0
56	MG	2A	3304	1/1	0.92	0.10	-2.77	53,53,53,53	0
56	MG	1A	3649	1/1	0.94	0.15	-2.78	36,36,36,36	0
56	MG	1A	3457	1/1	0.72	0.15	-2.84	28,28,28,28	0
56	MG	1a	1829	1/1	0.93	0.11	-2.90	55,55,55,55	0
56	MG	2A	3310	1/1	0.94	0.15	-2.90	48,48,48,48	0
56	MG	1A	3436	1/1	0.89	0.15	-2.91	33,33,33,33	0
56	MG	2a	1739	1/1	0.96	0.09	-2.94	57,57,57,57	0
56	MG	1x	101	1/1	0.96	0.07	-2.95	69,69,69,69	0
56	MG	1A	3430	1/1	0.90	0.12	-2.97	32,32,32,32	0
56	MG	1A	3461	1/1	0.93	0.12	-2.98	30,30,30,30	0
56	MG	1A	3515	1/1	0.95	0.10	-2.99	46,46,46,46	0
56	MG	1V	202	1/1	0.98	0.11	-3.04	46,46,46,46	0
56	MG	2a	1699	1/1	0.77	0.13	-3.07	59,59,59,59	0
56	MG	1P	201	1/1	0.96	0.09	-3.08	34,34,34,34	0
56	MG	2A	3267	1/1	0.97	0.12	-3.11	49,49,49,49	0
56	MG	2A	3373	1/1	0.91	0.15	-3.12	45,45,45,45	0
56	MG	1a	1643	1/1	0.89	0.14	-3.13	65,65,65,65	0
56	MG	2A	3605	1/1	0.92	0.14	-3.15	49,49,49,49	0
56	MG	1A	3554	1/1	0.97	0.09	-3.19	45,45,45,45	0
56	MG	2A	3455	1/1	0.89	0.13	-3.31	53,53,53,53	0
56	MG	1A	3779	1/1	0.63	0.13	-3.32	46,46,46,46	0
56	MG	1a	1610	1/1	0.97	0.10	-3.33	71,71,71,71	0
56	MG	2U	201	1/1	0.89	0.12	-3.36	52,52,52,52	0
56	MG	2A	3638	1/1	0.92	0.09	-3.36	58,58,58,58	0
56	MG	1a	1835	1/1	0.96	0.05	-3.36	64,64,64,64	0
56	MG	2a	1692	1/1	0.86	0.07	-3.39	62,62,62,62	0
56	MG	1A	3787	1/1	0.85	0.12	-3.40	31,31,31,31	0
56	MG	1A	3264	1/1	0.99	0.17	-3.40	34,34,34,34	0
56	MG	2A	3669	1/1	0.95	0.14	-3.45	47,47,47,47	0
56	MG	1A	3351	1/1	0.96	0.15	-3.45	29,29,29,29	0
56	MG	1A	3814	1/1	0.91	0.08	-3.50	42,42,42,42	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	2A	3561	1/1	0.89	0.08	-3.51	58,58,58,58	0
56	MG	1I	102	1/1	0.99	0.05	-3.53	41,41,41,41	0
56	MG	2A	3588	1/1	0.99	0.12	-3.54	47,47,47,47	0
56	MG	1A	3913	1/1	0.96	0.11	-3.61	32,32,32,32	0
56	MG	2A	3546	1/1	0.94	0.05	-3.63	56,56,56,56	0
56	MG	2A	3347	1/1	0.92	0.17	-3.63	42,42,42,42	0
56	MG	2B	3015	1/1	0.86	0.09	-3.70	76,76,76,76	0
56	MG	2A	3453	1/1	0.78	0.10	-3.75	47,47,47,47	0
56	MG	1A	3446	1/1	0.97	0.08	-3.79	46,46,46,46	0
56	MG	1A	3358	1/1	0.88	0.15	-3.80	30,30,30,30	0
56	MG	2A	3615	1/1	0.94	0.07	-3.84	63,63,63,63	0
56	MG	1A	3695	1/1	0.93	0.08	-3.90	38,38,38,38	0
56	MG	2A	3550	1/1	0.88	0.10	-3.95	43,43,43,43	0
56	MG	1A	3732	1/1	0.91	0.10	-3.98	46,46,46,46	0
56	MG	1A	3494	1/1	0.95	0.10	-4.01	42,42,42,42	0
56	MG	1A	3596	1/1	0.96	0.14	-4.06	41,41,41,41	0
56	MG	1A	3664	1/1	0.94	0.13	-4.17	44,44,44,44	0
56	MG	1A	3323	1/1	0.94	0.06	-4.39	42,42,42,42	0
56	MG	1A	3489	1/1	0.92	0.12	-4.48	32,32,32,32	0
56	MG	2a	1762	1/1	0.92	0.07	-4.48	79,79,79,79	0
56	MG	1A	3374	1/1	0.93	0.09	-4.49	31,31,31,31	0
56	MG	2A	3633	1/1	0.97	0.06	-4.54	48,48,48,48	0
56	MG	1A	3493	1/1	0.96	0.08	-4.56	29,29,29,29	0
56	MG	2a	1749	1/1	0.95	0.12	-4.64	59,59,59,59	0
56	MG	1A	3397	1/1	0.99	0.06	-4.65	34,34,34,34	0
56	MG	1A	3462	1/1	0.99	0.14	-4.78	30,30,30,30	0
56	MG	2A	3268	1/1	0.98	0.10	-4.86	45,45,45,45	0
56	MG	1A	3662	1/1	0.91	0.09	-4.91	39,39,39,39	0
56	MG	2A	3330	1/1	0.98	0.12	-5.11	48,48,48,48	0
56	MG	1A	3471	1/1	0.97	0.12	-5.11	33,33,33,33	0
56	MG	2A	3540	1/1	0.90	0.12	-5.17	47,47,47,47	0
56	MG	2a	1730	1/1	0.81	0.10	-5.18	66,66,66,66	0
56	MG	2A	3610	1/1	0.95	0.06	-5.32	62,62,62,62	0
56	MG	1A	3364	1/1	0.94	0.10	-5.37	39,39,39,39	0
56	MG	2A	3298	1/1	0.83	0.13	-5.39	46,46,46,46	0
56	MG	1a	1844	1/1	0.93	0.07	-5.41	68,68,68,68	0
56	MG	1D	314	1/1	0.99	0.10	-5.46	33,33,33,33	0
56	MG	1A	3028	1/1	0.97	0.15	-5.49	39,39,39,39	0
56	MG	2A	3290	1/1	0.95	0.04	-5.52	55,55,55,55	0
56	MG	2A	3444	1/1	0.98	0.07	-5.69	46,46,46,46	0
56	MG	2A	3606	1/1	0.69	0.11	-5.75	47,47,47,47	0
56	MG	1A	3405	1/1	0.96	0.15	-5.79	26,26,26,26	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	2A	3313	1/1	0.94	0.09	-5.85	44,44,44,44	0
56	MG	1A	3349	1/1	0.96	0.12	-5.85	26,26,26,26	0
56	MG	2A	3325	1/1	0.98	0.06	-6.00	50,50,50,50	0
56	MG	2A	3018	1/1	0.99	0.10	-6.07	48,48,48,48	0
56	MG	2A	3524	1/1	0.92	0.09	-6.31	42,42,42,42	0
56	MG	2A	3363	1/1	0.90	0.12	-6.32	44,44,44,44	0
56	MG	1A	3336	1/1	0.98	0.10	-6.35	41,41,41,41	0
56	MG	1A	3837	1/1	0.86	0.10	-6.39	46,46,46,46	0
56	MG	1A	3869	1/1	0.95	0.06	-6.53	46,46,46,46	0
56	MG	1a	1726	1/1	0.79	0.09	-6.55	60,60,60,60	0
56	MG	1A	3634	1/1	0.97	0.06	-6.73	34,34,34,34	0
56	MG	2a	1748	1/1	0.97	0.04	-6.77	60,60,60,60	0
56	MG	1A	3288	1/1	0.97	0.15	-6.79	25,25,25,25	0
56	MG	1A	3388	1/1	0.92	0.09	-6.80	42,42,42,42	0
56	MG	2A	3560	1/1	0.97	0.06	-6.81	54,54,54,54	0
56	MG	1A	3307	1/1	0.96	0.11	-6.87	34,34,34,34	0
56	MG	1A	3862	1/1	0.97	0.13	-6.92	31,31,31,31	0
56	MG	1A	3197	1/1	0.99	0.11	-6.95	29,29,29,29	0
56	MG	1a	1614	1/1	0.87	0.11	-6.97	51,51,51,51	0
56	MG	1A	3157	1/1	0.92	0.11	-6.99	33,33,33,33	0
56	MG	1A	3771	1/1	0.98	0.10	-7.05	33,33,33,33	0
56	MG	1A	3642	1/1	0.97	0.09	-7.45	32,32,32,32	0
56	MG	1A	3443	1/1	0.94	0.11	-7.75	35,35,35,35	0
56	MG	1A	3592	1/1	0.93	0.07	-7.77	43,43,43,43	0
56	MG	1A	3784	1/1	0.99	0.05	-8.14	39,39,39,39	0
56	MG	1A	3734	1/1	0.95	0.08	-8.30	49,49,49,49	0
56	MG	2A	3593	1/1	0.96	0.06	-8.37	48,48,48,48	0
56	MG	2A	3359	1/1	0.92	0.09	-8.61	47,47,47,47	0
56	MG	1A	3773	1/1	0.92	0.09	-8.94	44,44,44,44	0
56	MG	1A	3348	1/1	0.97	0.10	-8.96	32,32,32,32	0
56	MG	1A	3106	1/1	0.96	0.12	-9.21	39,39,39,39	0
56	MG	1A	3803	1/1	0.98	0.06	-9.69	53,53,53,53	0
56	MG	1A	3599	1/1	0.95	0.07	-10.02	35,35,35,35	0
56	MG	2A	3535	1/1	0.97	0.05	-10.07	52,52,52,52	0
56	MG	1A	3758	1/1	0.97	0.05	-10.16	31,31,31,31	0
56	MG	1A	3743	1/1	0.94	0.11	-10.20	41,41,41,41	0
56	MG	1A	3125	1/1	0.97	0.09	-10.44	29,29,29,29	0
56	MG	1A	3799	1/1	0.97	0.05	-10.74	32,32,32,32	0
56	MG	2A	3468	1/1	0.88	0.07	-10.76	69,69,69,69	0
56	MG	1A	3383	1/1	0.85	0.10	-11.19	33,33,33,33	0
56	MG	2A	3590	1/1	0.97	0.09	-11.39	47,47,47,47	0
56	MG	2A	3589	1/1	0.97	0.09	-11.47	47,47,47,47	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	1A	3419	1/1	0.99	0.09	-12.69	42,42,42,42	0
56	MG	1A	3702	1/1	0.87	0.14	-12.73	37,37,37,37	0
56	MG	1A	3543	1/1	0.98	0.04	-19.56	36,36,36,36	0
56	MG	1A	3711	1/1	0.86	0.16	-	45,45,45,45	0
56	MG	1o	102	1/1	0.91	0.22	-	49,49,49,49	0
56	MG	1A	3794	1/1	0.91	0.06	-	44,44,44,44	0
56	MG	2A	3212	1/1	0.90	0.34	-	53,53,53,53	0
56	MG	2A	3210	1/1	0.94	0.26	-	42,42,42,42	0
56	MG	2A	3134	1/1	0.91	0.12	-	68,68,68,68	0
56	MG	2A	3127	1/1	0.68	0.33	-	61,61,61,61	0
56	MG	1A	3031	1/1	0.97	0.26	-	32,32,32,32	0
56	MG	1A	3637	1/1	0.94	0.26	-	33,33,33,33	0
56	MG	2A	3575	1/1	0.90	0.14	-	65,65,65,65	0
56	MG	2A	3432	1/1	0.92	0.16	-	49,49,49,49	0
56	MG	1A	3403	1/1	0.96	0.15	-	35,35,35,35	0
56	MG	2A	3483	1/1	0.96	0.29	-	51,51,51,51	0
56	MG	1A	3139	1/1	0.94	0.17	-	33,33,33,33	0
56	MG	2A	3180	1/1	0.78	0.10	-	65,65,65,65	0
56	MG	2A	3477	1/1	0.93	0.22	-	50,50,50,50	0
56	MG	2A	3647	1/1	0.98	0.15	-	60,60,60,60	0
56	MG	2a	1671	1/1	0.88	0.39	-	71,71,71,71	0
56	MG	2A	3285	1/1	0.94	0.23	-	49,49,49,49	0
56	MG	1A	3177	1/1	0.89	0.47	-	35,35,35,35	0
56	MG	1A	3899	1/1	0.95	0.18	-	41,41,41,41	0
56	MG	2A	3457	1/1	0.86	0.25	-	63,63,63,63	0
56	MG	1A	3597	1/1	0.79	0.20	-	34,34,34,34	0
56	MG	1A	3120	1/1	0.94	0.06	-	55,55,55,55	0
56	MG	2A	3421	1/1	0.95	0.26	-	61,61,61,61	0
56	MG	2A	3522	1/1	0.75	0.20	-	50,50,50,50	0
56	MG	1a	1693	1/1	0.92	0.17	-	75,75,75,75	0
56	MG	1A	3708	1/1	0.87	0.12	-	35,35,35,35	0
56	MG	1B	201	1/1	0.95	0.25	-	53,53,53,53	0
56	MG	1a	1735	1/1	0.92	0.06	-	62,62,62,62	0
56	MG	1A	3826	1/1	0.93	0.09	-	47,47,47,47	0
56	MG	1A	3569	1/1	0.85	0.24	-	30,30,30,30	0
56	MG	1a	1683	1/1	0.93	0.21	-	67,67,67,67	0
56	MG	2A	3182	1/1	0.80	0.39	-	57,57,57,57	0
56	MG	1A	3686	1/1	0.99	0.07	-	49,49,49,49	0
56	MG	1A	3719	1/1	0.79	0.10	-	42,42,42,42	0
56	MG	2A	3470	1/1	0.83	0.22	-	57,57,57,57	0
56	MG	1A	3731	1/1	0.98	0.12	-	32,32,32,32	0
56	MG	2A	3528	1/1	0.93	0.58	-	51,51,51,51	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	2a	1632	1/1	0.65	0.38	-	60,60,60,60	0
56	MG	10	106	1/1	0.94	0.08	-	46,46,46,46	0
56	MG	2A	3625	1/1	0.90	0.10	-	65,65,65,65	0
56	MG	1A	3613	1/1	0.68	0.21	-	68,68,68,68	0
56	MG	2A	3519	1/1	0.83	0.25	-	44,44,44,44	0
56	MG	1a	1605	1/1	0.86	0.41	-	67,67,67,67	0
56	MG	2A	3368	1/1	0.85	0.27	-	55,55,55,55	0
56	MG	2A	3441	1/1	0.85	0.14	-	65,65,65,65	0
56	MG	1A	3628	1/1	0.96	0.13	-	43,43,43,43	0
56	MG	1A	3834	1/1	0.94	0.08	-	47,47,47,47	0
56	MG	1A	3359	1/1	0.92	0.09	-	34,34,34,34	0
56	MG	2A	3554	1/1	0.94	0.09	-	63,63,63,63	0
56	MG	1A	3796	1/1	0.94	0.42	-	37,37,37,37	0
56	MG	1A	3587	1/1	0.93	0.24	-	45,45,45,45	0
56	MG	2A	3100	1/1	0.79	0.28	-	60,60,60,60	0
56	MG	2T	3002	1/1	0.96	0.29	-	58,58,58,58	0
56	MG	1A	3116	1/1	0.75	0.67	-	40,40,40,40	0
56	MG	2A	3091	1/1	0.87	0.21	-	54,54,54,54	0
56	MG	1A	3668	1/1	0.96	0.19	-	51,51,51,51	0
56	MG	1A	3670	1/1	0.95	0.27	-	46,46,46,46	0
56	MG	1A	3366	1/1	0.95	0.29	-	44,44,44,44	0
56	MG	2A	3505	1/1	0.96	0.10	-	59,59,59,59	0
56	MG	1A	3604	1/1	0.85	0.07	-	54,54,54,54	0
56	MG	2A	3032	1/1	0.80	0.19	-	63,63,63,63	0
56	MG	1A	3589	1/1	0.95	0.09	-	46,46,46,46	0
56	MG	1A	3380	1/1	0.80	0.12	-	44,44,44,44	0
56	MG	1A	3338	1/1	0.99	0.20	-	31,31,31,31	0
56	MG	1A	3049	1/1	0.93	0.24	-	28,28,28,28	0
56	MG	2A	3006	1/1	0.76	0.45	-	52,52,52,52	0
56	MG	2A	3521	1/1	0.81	0.18	-	49,49,49,49	0
56	MG	1A	3881	1/1	0.83	0.28	-	53,53,53,53	0
56	MG	2A	3494	1/1	0.89	0.20	-	60,60,60,60	0
56	MG	2A	3058	1/1	0.97	0.16	-	31,31,31,31	0
56	MG	2a	1676	1/1	0.94	0.10	-	68,68,68,68	0
56	MG	1A	3126	1/1	0.86	0.37	-	32,32,32,32	0
56	MG	2A	3614	1/1	0.75	0.13	-	64,64,64,64	0
56	MG	2a	1764	1/1	0.72	0.16	-	66,66,66,66	0
56	MG	2A	3228	1/1	0.91	0.38	-	46,46,46,46	0
56	MG	1A	3798	1/1	0.95	0.11	-	37,37,37,37	0
56	MG	2a	1711	1/1	0.91	0.62	-	77,77,77,77	0
56	MG	2T	3004	1/1	0.94	0.17	-	50,50,50,50	0
56	MG	1A	3677	1/1	0.98	0.08	-	40,40,40,40	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	1A	3441	1/1	0.90	0.09	-	40,40,40,40	0
56	MG	2A	3552	1/1	0.98	0.07	-	47,47,47,47	0
56	MG	2a	1656	1/1	0.77	0.26	-	68,68,68,68	0
56	MG	1A	3002	1/1	0.87	0.37	-	44,44,44,44	0
56	MG	1a	1739	1/1	0.91	0.55	-	65,65,65,65	0
56	MG	2A	3271	1/1	0.98	0.08	-	60,60,60,60	0
56	MG	1A	3879	1/1	0.94	0.07	-	66,66,66,66	0
56	MG	2A	3275	1/1	0.96	0.22	-	55,55,55,55	0
56	MG	2A	3374	1/1	0.91	0.18	-	74,74,74,74	0
56	MG	1A	3724	1/1	0.98	0.36	-	44,44,44,44	0
56	MG	2A	3645	1/1	0.98	0.09	-	50,50,50,50	0
56	MG	2a	1698	1/1	0.87	0.14	-	77,77,77,77	0
56	MG	1A	3855	1/1	0.88	0.54	-	42,42,42,42	0
56	MG	2A	3595	1/1	0.84	0.10	-	66,66,66,66	0
56	MG	1A	3598	1/1	0.75	0.37	-	55,55,55,55	0
56	MG	1l	201	1/1	0.91	0.19	-	63,63,63,63	0
56	MG	1A	3093	1/1	0.85	0.27	-	50,50,50,50	0
56	MG	1A	3188	1/1	0.88	0.31	-	42,42,42,42	0
56	MG	1a	1786	1/1	0.40	0.40	-	65,65,65,65	0
56	MG	1A	3181	1/1	0.81	0.29	-	45,45,45,45	0
56	MG	1A	3531	1/1	0.89	0.13	-	52,52,52,52	0
56	MG	2A	3191	1/1	0.70	0.44	-	50,50,50,50	0
56	MG	2A	3189	1/1	0.94	0.15	-	49,49,49,49	0
56	MG	1E	301	1/1	0.97	0.14	-	34,34,34,34	0
56	MG	1A	3747	1/1	0.97	0.10	-	40,40,40,40	0
56	MG	1a	1716	1/1	0.98	0.08	-	49,49,49,49	0
56	MG	1A	3098	1/1	0.82	0.23	-	51,51,51,51	0
56	MG	2A	3205	1/1	0.91	0.28	-	51,51,51,51	0
56	MG	2A	3158	1/1	0.74	0.08	-	78,78,78,78	0
56	MG	1A	3474	1/1	0.92	0.15	-	56,56,56,56	0
56	MG	2A	3049	1/1	0.91	0.15	-	62,62,62,62	0
56	MG	1A	3829	1/1	0.92	0.07	-	40,40,40,40	0
56	MG	1a	1777	1/1	0.91	0.15	-	74,74,74,74	0
56	MG	1A	3423	1/1	0.87	0.09	-	57,57,57,57	0
56	MG	2A	3117	1/1	0.83	0.15	-	55,55,55,55	0
56	MG	1a	1783	1/1	0.89	0.42	-	63,63,63,63	0
56	MG	1A	3302	1/1	0.99	0.10	-	36,36,36,36	0
56	MG	1Q	202	1/1	0.89	0.17	-	35,35,35,35	0
56	MG	1A	3339	1/1	0.95	0.10	-	43,43,43,43	0
56	MG	2A	3035	1/1	0.90	0.21	-	70,70,70,70	0
56	MG	1H	8002	1/1	0.93	0.23	-	44,44,44,44	0
56	MG	1A	3873	1/1	0.82	0.26	-	55,55,55,55	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	2A	3435	1/1	0.93	0.10	-	54,54,54,54	0
56	MG	2A	3471	1/1	0.90	0.22	-	48,48,48,48	0
56	MG	1A	3842	1/1	0.93	0.30	-	47,47,47,47	0
56	MG	1A	3390	1/1	0.96	0.15	-	35,35,35,35	0
56	MG	2a	1609	1/1	0.83	0.25	-	67,67,67,67	0
56	MG	2A	3437	1/1	0.25	0.52	-	62,62,62,62	0
56	MG	1a	1686	1/1	0.97	0.13	-	67,67,67,67	0
56	MG	1A	3632	1/1	0.85	0.32	-	34,34,34,34	0
56	MG	1A	3513	1/1	0.85	0.13	-	49,49,49,49	0
56	MG	1a	1741	1/1	0.98	0.07	-	63,63,63,63	0
56	MG	1W	3001	1/1	0.97	0.20	-	38,38,38,38	0
56	MG	1A	3921	1/1	0.94	0.09	-	55,55,55,55	0
56	MG	1A	3238	1/1	0.93	0.08	-	65,65,65,65	0
56	MG	1A	3753	1/1	0.93	0.18	-	51,51,51,51	0
56	MG	1A	3265	1/1	0.93	0.33	-	32,32,32,32	0
56	MG	2a	1669	1/1	0.64	0.23	-	63,63,63,63	0
56	MG	1A	3429	1/1	0.76	0.18	-	34,34,34,34	0
56	MG	1A	3504	1/1	0.93	0.17	-	44,44,44,44	0
56	MG	1A	3497	1/1	0.93	0.22	-	45,45,45,45	0
56	MG	2A	3199	1/1	0.94	0.23	-	56,56,56,56	0
56	MG	2A	3411	1/1	0.82	0.39	-	58,58,58,58	0
56	MG	1A	3282	1/1	0.88	0.08	-	67,67,67,67	0
56	MG	1A	3833	1/1	0.94	0.20	-	59,59,59,59	0
56	MG	1A	3533	1/1	0.92	0.34	-	51,51,51,51	0
56	MG	1A	3227	1/1	0.92	0.21	-	39,39,39,39	0
56	MG	2A	3564	1/1	0.84	0.09	-	68,68,68,68	0
56	MG	1A	3284	1/1	0.99	0.12	-	39,39,39,39	0
56	MG	1A	3127	1/1	0.89	0.55	-	28,28,28,28	0
56	MG	2a	1723	1/1	0.86	0.13	-	62,62,62,62	0
56	MG	1a	1730	1/1	0.94	0.07	-	55,55,55,55	0
56	MG	2A	3070	1/1	0.78	0.65	-	49,49,49,49	0
56	MG	1A	3045	1/1	0.91	0.33	-	40,40,40,40	0
56	MG	2A	3248	1/1	0.82	0.21	-	51,51,51,51	0
56	MG	1N	202	1/1	0.93	0.45	-	46,46,46,46	0
56	MG	1A	3400	1/1	0.89	0.07	-	61,61,61,61	0
56	MG	1A	3151	1/1	0.98	0.42	-	31,31,31,31	0
56	MG	2A	3193	1/1	0.97	0.28	-	66,66,66,66	0
56	MG	1a	1616	1/1	0.89	0.14	-	73,73,73,73	0
56	MG	2A	3289	1/1	0.84	0.27	-	55,55,55,55	0
56	MG	1a	1700	1/1	0.97	0.09	-	50,50,50,50	0
56	MG	2a	1608	1/1	0.62	1.47	-	69,69,69,69	0
56	MG	2a	1735	1/1	0.92	0.16	-	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	1a	1689	1/1	0.81	0.43	-	69,69,69,69	0
56	MG	1a	1761	1/1	0.44	0.37	-	68,68,68,68	0
56	MG	2a	1601	1/1	0.90	0.43	-	58,58,58,58	0
56	MG	2a	1666	1/1	0.86	0.29	-	84,84,84,84	0
56	MG	1A	3900	1/1	0.85	0.26	-	33,33,33,33	0
56	MG	1A	3835	1/1	0.91	0.08	-	59,59,59,59	0
56	MG	1a	1713	1/1	0.82	0.37	-	72,72,72,72	0
56	MG	2A	3153	1/1	0.91	0.42	-	51,51,51,51	0
56	MG	1A	3828	1/1	0.97	0.21	-	43,43,43,43	0
56	MG	1A	3736	1/1	0.90	0.11	-	37,37,37,37	0
56	MG	2A	3241	1/1	0.94	0.32	-	45,45,45,45	0
56	MG	1a	1750	1/1	0.83	0.40	-	63,63,63,63	0
56	MG	2A	3329	1/1	0.97	0.07	-	50,50,50,50	0
56	MG	1A	3062	1/1	0.96	0.30	-	41,41,41,41	0
56	MG	2A	3569	1/1	0.97	0.26	-	66,66,66,66	0
56	MG	1A	3875	1/1	0.97	0.14	-	28,28,28,28	0
56	MG	2A	3488	1/1	0.90	0.14	-	74,74,74,74	0
56	MG	1a	1708	1/1	0.83	0.29	-	64,64,64,64	0
56	MG	1a	1665	1/1	0.73	0.50	-	55,55,55,55	0
56	MG	1A	3614	1/1	0.89	0.27	-	42,42,42,42	0
56	MG	2a	1612	1/1	0.94	0.25	-	66,66,66,66	0
56	MG	2A	3115	1/1	0.92	0.22	-	46,46,46,46	0
56	MG	2A	3141	1/1	0.97	0.30	-	57,57,57,57	0
56	MG	2A	3351	1/1	0.77	0.18	-	53,53,53,53	0
56	MG	1A	3666	1/1	0.97	0.12	-	37,37,37,37	0
56	MG	2A	3148	1/1	0.70	0.42	-	66,66,66,66	0
56	MG	2A	3274	1/1	0.94	0.13	-	54,54,54,54	0
56	MG	2A	3326	1/1	0.97	0.07	-	55,55,55,55	0
56	MG	1A	3196	1/1	0.96	0.19	-	41,41,41,41	0
56	MG	1A	3140	1/1	0.99	0.11	-	31,31,31,31	0
56	MG	1g	3001	1/1	0.84	0.18	-	62,62,62,62	0
56	MG	1A	3669	1/1	0.95	0.12	-	64,64,64,64	0
56	MG	2A	3229	1/1	0.88	0.44	-	45,45,45,45	0
56	MG	1A	3585	1/1	0.91	0.28	-	39,39,39,39	0
56	MG	1A	3229	1/1	0.77	0.49	-	32,32,32,32	0
56	MG	2A	3005	1/1	0.69	0.51	-	53,53,53,53	0
56	MG	1A	3816	1/1	0.88	0.49	-	42,42,42,42	0
56	MG	1a	1743	1/1	0.94	0.25	-	73,73,73,73	0
56	MG	2A	3408	1/1	0.94	0.06	-	66,66,66,66	0
56	MG	1a	1836	1/1	0.82	0.10	-	61,61,61,61	0
56	MG	1A	3545	1/1	0.65	0.45	-	54,54,54,54	0
56	MG	2A	3480	1/1	0.94	0.20	-	49,49,49,49	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	1a	1662	1/1	0.94	0.25	-	70,70,70,70	0
56	MG	2A	3517	1/1	0.93	0.13	-	60,60,60,60	0
56	MG	1A	3328	1/1	0.94	0.17	-	49,49,49,49	0
56	MG	1E	306	1/1	0.96	0.10	-	47,47,47,47	0
56	MG	2a	1683	1/1	0.78	0.57	-	71,71,71,71	0
56	MG	1A	3319	1/1	0.87	0.09	-	43,43,43,43	0
56	MG	1a	1729	1/1	0.95	0.14	-	52,52,52,52	0
56	MG	1a	1811	1/1	0.93	0.07	-	73,73,73,73	0
56	MG	1A	3933	1/1	0.98	0.38	-	49,49,49,49	0
56	MG	1A	3096	1/1	0.81	0.71	-	33,33,33,33	0
56	MG	1A	3576	1/1	0.88	0.22	-	43,43,43,43	0
56	MG	2A	3668	1/1	0.89	0.10	-	62,62,62,62	0
56	MG	1a	1658	1/1	0.95	0.33	-	67,67,67,67	0
56	MG	1A	3785	1/1	0.98	0.05	-	36,36,36,36	0
56	MG	2A	3386	1/1	0.93	0.29	-	48,48,48,48	0
56	MG	1A	3123	1/1	0.52	0.45	-	41,41,41,41	0
56	MG	2B	3016	1/1	0.97	0.10	-	71,71,71,71	0
56	MG	1A	3389	1/1	0.94	0.10	-	44,44,44,44	0
56	MG	2A	3571	1/1	0.89	0.16	-	57,57,57,57	0
56	MG	2a	1743	1/1	0.91	0.20	-	60,60,60,60	0
56	MG	1e	202	1/1	0.79	0.17	-	64,64,64,64	0
56	MG	1D	307	1/1	0.84	0.24	-	45,45,45,45	0
56	MG	1R	202	1/1	0.98	0.07	-	38,38,38,38	0
56	MG	1A	3363	1/1	0.92	0.08	-	54,54,54,54	0
56	MG	1A	3491	1/1	0.85	0.16	-	35,35,35,35	0
56	MG	1B	227	1/1	0.86	0.09	-	51,51,51,51	0
56	MG	1a	1674	1/1	0.81	0.36	-	74,74,74,74	0
56	MG	2A	3222	1/1	0.82	0.26	-	57,57,57,57	0
56	MG	1P	202	1/1	0.95	0.10	-	55,55,55,55	0
56	MG	2a	1696	1/1	0.68	0.55	-	63,63,63,63	0
56	MG	1A	3414	1/1	0.97	0.07	-	63,63,63,63	0
56	MG	1B	211	1/1	0.96	0.14	-	41,41,41,41	0
56	MG	2A	3105	1/1	0.92	0.13	-	42,42,42,42	0
56	MG	2A	3247	1/1	0.84	0.12	-	52,52,52,52	0
56	MG	1A	3713	1/1	0.77	0.56	-	59,59,59,59	0
56	MG	2a	1690	1/1	0.90	0.28	-	65,65,65,65	0
56	MG	2A	3452	1/1	0.94	0.18	-	66,66,66,66	0
56	MG	1A	3160	1/1	0.90	0.20	-	40,40,40,40	0
56	MG	1a	1858	1/1	0.70	0.24	-	62,62,62,62	0
56	MG	1A	3303	1/1	0.87	0.16	-	32,32,32,32	0
56	MG	2A	3176	1/1	0.78	0.41	-	52,52,52,52	0
56	MG	1a	1642	1/1	0.96	0.41	-	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	1A	3372	1/1	0.90	0.12	-	28,28,28,28	0
56	MG	2a	1773	1/1	0.94	0.07	-	63,63,63,63	0
56	MG	1G	3003	1/1	0.93	0.31	-	60,60,60,60	0
56	MG	1a	1607	1/1	0.91	0.26	-	60,60,60,60	0
56	MG	1A	3813	1/1	0.87	0.12	-	35,35,35,35	0
56	MG	2A	3232	1/1	0.93	0.40	-	50,50,50,50	0
56	MG	1A	3404	1/1	0.99	0.09	-	32,32,32,32	0
56	MG	1a	1841	1/1	0.94	0.27	-	67,67,67,67	0
56	MG	2A	3167	1/1	0.83	0.17	-	66,66,66,66	0
56	MG	1A	3520	1/1	0.94	0.21	-	40,40,40,40	0
56	MG	1A	3249	1/1	0.92	0.18	-	48,48,48,48	0
56	MG	1a	1784	1/1	0.93	0.14	-	60,60,60,60	0
56	MG	1A	3035	1/1	0.90	0.16	-	33,33,33,33	0
56	MG	2A	3251	1/1	0.96	0.26	-	53,53,53,53	0
56	MG	1A	3752	1/1	0.68	0.10	-	50,50,50,50	0
56	MG	1T	202	1/1	0.94	0.18	-	51,51,51,51	0
56	MG	1a	1645	1/1	0.94	0.66	-	59,59,59,59	0
56	MG	2A	3600	1/1	0.80	0.43	-	80,80,80,80	0
56	MG	1A	3570	1/1	0.85	0.19	-	42,42,42,42	0
56	MG	2B	3014	1/1	0.94	0.05	-	64,64,64,64	0
56	MG	1A	3648	1/1	0.96	0.12	-	37,37,37,37	0
56	MG	2A	3154	1/1	0.93	0.38	-	48,48,48,48	0
56	MG	2A	3157	1/1	0.84	0.18	-	47,47,47,47	0
56	MG	2a	1719	1/1	0.81	0.17	-	63,63,63,63	0
56	MG	2a	1707	1/1	0.96	0.17	-	68,68,68,68	0
56	MG	1a	1681	1/1	0.94	0.21	-	56,56,56,56	0
56	MG	1a	1719	1/1	0.98	0.14	-	71,71,71,71	0
56	MG	1a	1660	1/1	0.95	0.25	-	68,68,68,68	0
56	MG	1a	1697	1/1	0.91	0.10	-	55,55,55,55	0
56	MG	1d	503	1/1	0.79	0.24	-	70,70,70,70	0
56	MG	1A	3485	1/1	0.92	0.09	-	47,47,47,47	0
56	MG	1a	1851	1/1	0.86	0.21	-	78,78,78,78	0
56	MG	1a	1764	1/1	0.55	0.13	-	70,70,70,70	0
56	MG	2A	3448	1/1	0.77	0.15	-	47,47,47,47	0
56	MG	2A	3235	1/1	0.96	0.42	-	49,49,49,49	0
56	MG	2a	1659	1/1	0.92	0.39	-	77,77,77,77	0
56	MG	1A	3044	1/1	0.98	0.06	-	26,26,26,26	0
56	MG	1A	3060	1/1	0.90	0.18	-	33,33,33,33	0
56	MG	2A	3511	1/1	0.77	0.09	-	64,64,64,64	0
56	MG	2A	3439	1/1	0.86	0.45	-	70,70,70,70	0
56	MG	1A	3166	1/1	0.93	0.79	-	36,36,36,36	0
56	MG	1B	215	1/1	0.39	0.64	-	71,71,71,71	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	2A	3162	1/1	0.93	0.53	-	57,57,57,57	0
56	MG	2A	3185	1/1	0.79	0.30	-	56,56,56,56	0
56	MG	1A	3908	1/1	0.92	0.19	-	41,41,41,41	0
56	MG	1A	3615	1/1	0.96	0.12	-	59,59,59,59	0
56	MG	1A	3581	1/1	0.92	0.35	-	29,29,29,29	0
56	MG	2A	3396	1/1	0.89	0.23	-	58,58,58,58	0
56	MG	1A	3460	1/1	0.92	0.17	-	44,44,44,44	0
56	MG	2a	1714	1/1	0.81	0.34	-	62,62,62,62	0
56	MG	1F	307	1/1	0.94	0.19	-	36,36,36,36	0
56	MG	1A	3086	1/1	0.90	0.24	-	52,52,52,52	0
56	MG	1a	1638	1/1	0.98	0.12	-	68,68,68,68	0
56	MG	1A	3215	1/1	0.88	0.22	-	48,48,48,48	0
56	MG	1A	3568	1/1	0.98	0.14	-	44,44,44,44	0
56	MG	1a	1671	1/1	0.91	0.14	-	57,57,57,57	0
56	MG	2a	1673	1/1	0.80	0.25	-	65,65,65,65	0
56	MG	2a	1642	1/1	0.96	0.33	-	75,75,75,75	0
56	MG	1A	3412	1/1	0.89	0.23	-	28,28,28,28	0
56	MG	2A	3643	1/1	0.98	0.09	-	54,54,54,54	0
56	MG	1a	1677	1/1	0.98	0.13	-	49,49,49,49	0
56	MG	2A	3038	1/1	0.81	0.73	-	49,49,49,49	0
56	MG	2a	1708	1/1	0.94	0.14	-	56,56,56,56	0
56	MG	2a	1705	1/1	0.95	0.08	-	62,62,62,62	0
56	MG	2A	3406	1/1	0.97	0.09	-	56,56,56,56	0
56	MG	1a	1701	1/1	0.94	0.08	-	53,53,53,53	0
56	MG	2A	3022	1/1	0.87	0.24	-	59,59,59,59	0
56	MG	1A	3170	1/1	0.89	0.21	-	42,42,42,42	0
56	MG	1A	3165	1/1	0.86	0.28	-	36,36,36,36	0
56	MG	1a	1849	1/1	0.90	0.21	-	62,62,62,62	0
56	MG	1A	3718	1/1	0.87	0.07	-	72,72,72,72	0
56	MG	2A	3043	1/1	0.91	0.35	-	61,61,61,61	0
56	MG	1a	1624	1/1	0.63	0.47	-	51,51,51,51	0
56	MG	1A	3746	1/1	0.91	0.19	-	40,40,40,40	0
56	MG	2A	3322	1/1	0.74	0.11	-	71,71,71,71	0
56	MG	2A	3184	1/1	0.64	0.33	-	59,59,59,59	0
56	MG	1B	230	1/1	0.94	0.09	-	55,55,55,55	0
56	MG	1A	3220	1/1	0.88	0.31	-	28,28,28,28	0
56	MG	1A	3305	1/1	0.98	0.28	-	47,47,47,47	0
56	MG	15	103	1/1	0.93	0.10	-	39,39,39,39	0
56	MG	1A	3411	1/1	0.96	0.09	-	62,62,62,62	0
56	MG	2D	301	1/1	0.96	0.24	-	49,49,49,49	0
56	MG	2A	3336	1/1	0.86	0.14	-	78,78,78,78	0
56	MG	2A	3387	1/1	0.90	0.08	-	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	2a	1687	1/1	0.95	0.16	-	62,62,62,62	0
56	MG	1A	3281	1/1	0.97	0.10	-	35,35,35,35	0
56	MG	1A	3553	1/1	0.87	0.17	-	58,58,58,58	0
56	MG	1a	1703	1/1	0.95	0.07	-	72,72,72,72	0
56	MG	2A	3548	1/1	0.88	0.16	-	46,46,46,46	0
56	MG	1A	3391	1/1	0.84	0.10	-	50,50,50,50	0
56	MG	1B	207	1/1	0.94	0.22	-	45,45,45,45	0
56	MG	2a	1620	1/1	0.90	0.60	-	56,56,56,56	0
56	MG	2a	1757	1/1	0.97	0.10	-	69,69,69,69	0
56	MG	2a	1724	1/1	0.43	0.13	-	74,74,74,74	0
56	MG	1a	1804	1/1	0.81	0.53	-	67,67,67,67	0
56	MG	1A	3101	1/1	0.90	0.65	-	32,32,32,32	0
56	MG	1A	3836	1/1	0.95	0.12	-	42,42,42,42	0
56	MG	2N	8001	1/1	0.99	0.09	-	55,55,55,55	0
56	MG	2a	1727	1/1	0.70	0.12	-	64,64,64,64	0
56	MG	2A	3081	1/1	0.69	1.07	-	62,62,62,62	0
56	MG	1a	1723	1/1	0.60	0.11	-	69,69,69,69	0
56	MG	2A	3303	1/1	0.82	0.17	-	44,44,44,44	0
56	MG	1Z	8001	1/1	0.70	0.38	-	60,60,60,60	0
56	MG	1A	3481	1/1	0.97	0.19	-	54,54,54,54	0
56	MG	1a	1819	1/1	0.89	0.23	-	69,69,69,69	0
56	MG	2a	1722	1/1	0.91	0.08	-	66,66,66,66	0
56	MG	1a	1609	1/1	0.76	0.25	-	68,68,68,68	0
56	MG	1A	3163	1/1	0.92	0.16	-	33,33,33,33	0
56	MG	2A	3120	1/1	0.88	0.14	-	60,60,60,60	0
56	MG	1A	3577	1/1	0.98	0.18	-	28,28,28,28	0
56	MG	2A	3151	1/1	0.89	0.20	-	41,41,41,41	0
56	MG	2a	1606	1/1	0.56	0.64	-	59,59,59,59	0
56	MG	1A	3536	1/1	0.97	0.14	-	35,35,35,35	0
56	MG	2A	3356	1/1	0.89	0.27	-	55,55,55,55	0
56	MG	1A	3795	1/1	0.73	0.46	-	39,39,39,39	0
56	MG	2A	3122	1/1	0.97	0.32	-	44,44,44,44	0
56	MG	1F	309	1/1	0.88	0.34	-	43,43,43,43	0
56	MG	1B	214	1/1	0.98	0.13	-	44,44,44,44	0
56	MG	1A	3490	1/1	0.88	0.28	-	44,44,44,44	0
56	MG	1A	3329	1/1	0.98	0.07	-	49,49,49,49	0
56	MG	2A	3545	1/1	0.95	0.10	-	57,57,57,57	0
56	MG	1A	3911	1/1	0.93	0.23	-	28,28,28,28	0
56	MG	1A	3224	1/1	0.79	0.28	-	46,46,46,46	0
56	MG	1A	3317	1/1	0.84	0.17	-	45,45,45,45	0
56	MG	1A	3259	1/1	0.88	0.09	-	71,71,71,71	0
56	MG	1e	201	1/1	0.75	0.55	-	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	1D	318	1/1	0.89	0.59	-	51,51,51,51	0
56	MG	2A	3389	1/1	0.94	0.27	-	49,49,49,49	0
56	MG	2A	3041	1/1	0.87	0.22	-	63,63,63,63	0
56	MG	1d	502	1/1	0.76	0.27	-	68,68,68,68	0
56	MG	1A	3361	1/1	0.96	0.24	-	47,47,47,47	0
56	MG	2A	3424	1/1	0.89	0.12	-	63,63,63,63	0
56	MG	1V	203	1/1	0.91	0.29	-	62,62,62,62	0
56	MG	1A	3034	1/1	0.93	0.34	-	45,45,45,45	0
56	MG	2T	3001	1/1	0.83	0.31	-	54,54,54,54	0
56	MG	1R	204	1/1	0.92	0.20	-	39,39,39,39	0
56	MG	2A	3490	1/1	0.98	0.17	-	42,42,42,42	0
56	MG	2A	3126	1/1	0.85	0.34	-	57,57,57,57	0
56	MG	2A	3491	1/1	0.91	0.63	-	58,58,58,58	0
56	MG	1a	1635	1/1	0.89	0.41	-	75,75,75,75	0
56	MG	1A	3254	1/1	0.96	0.15	-	52,52,52,52	0
56	MG	1A	3584	1/1	0.95	0.27	-	61,61,61,61	0
56	MG	1A	3626	1/1	0.97	0.06	-	51,51,51,51	0
56	MG	2A	3340	1/1	0.96	0.09	-	50,50,50,50	0
56	MG	2A	3324	1/1	0.95	0.12	-	51,51,51,51	0
56	MG	1A	3362	1/1	0.94	0.16	-	41,41,41,41	0
56	MG	2a	1657	1/1	0.93	0.19	-	69,69,69,69	0
56	MG	1A	3408	1/1	0.94	0.26	-	42,42,42,42	0
56	MG	2A	3661	1/1	0.71	0.64	-	62,62,62,62	0
56	MG	2A	3259	1/1	0.95	0.17	-	59,59,59,59	0
56	MG	2a	1716	1/1	0.93	0.17	-	72,72,72,72	0
56	MG	1A	3901	1/1	0.97	0.25	-	51,51,51,51	0
56	MG	1F	301	1/1	0.95	0.10	-	44,44,44,44	0
56	MG	2A	3523	1/1	0.93	0.07	-	57,57,57,57	0
56	MG	1A	3051	1/1	0.88	0.72	-	32,32,32,32	0
56	MG	2A	3446	1/1	0.92	0.10	-	60,60,60,60	0
56	MG	2a	1704	1/1	0.90	0.12	-	70,70,70,70	0
56	MG	2A	3632	1/1	0.97	0.05	-	55,55,55,55	0
56	MG	2A	3308	1/1	0.85	0.17	-	51,51,51,51	0
56	MG	1F	308	1/1	0.89	0.60	-	56,56,56,56	0
56	MG	2B	3017	1/1	0.86	0.08	-	66,66,66,66	0
56	MG	1A	3334	1/1	0.98	0.22	-	33,33,33,33	0
56	MG	2a	1695	1/1	0.95	0.19	-	58,58,58,58	0
56	MG	2A	3145	1/1	0.94	0.42	-	53,53,53,53	0
56	MG	1A	3235	1/1	0.98	0.21	-	32,32,32,32	0
56	MG	2a	1638	1/1	0.94	0.22	-	71,71,71,71	0
56	MG	1A	3623	1/1	0.77	0.36	-	53,53,53,53	0
56	MG	2A	3501	1/1	0.85	0.12	-	60,60,60,60	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	2A	3631	1/1	0.92	0.08	-	57,57,57,57	0
56	MG	1A	3884	1/1	0.96	0.12	-	44,44,44,44	0
56	MG	1A	3697	1/1	0.96	0.36	-	37,37,37,37	0
56	MG	2a	1701	1/1	0.80	0.23	-	61,61,61,61	0
56	MG	2A	3388	1/1	0.97	0.15	-	48,48,48,48	0
56	MG	1A	3017	1/1	0.98	0.28	-	25,25,25,25	0
56	MG	1A	3119	1/1	0.93	0.33	-	30,30,30,30	0
56	MG	2A	3553	1/1	0.86	0.13	-	63,63,63,63	0
56	MG	2A	3342	1/1	0.95	0.23	-	61,61,61,61	0
56	MG	2A	3016	1/1	0.99	0.14	-	50,50,50,50	0
56	MG	1A	3433	1/1	0.92	0.16	-	48,48,48,48	0
56	MG	2q	201	1/1	0.97	0.28	-	62,62,62,62	0
56	MG	1a	1745	1/1	0.95	0.07	-	54,54,54,54	0
56	MG	1a	1823	1/1	0.62	0.84	-	54,54,54,54	0
56	MG	1A	3807	1/1	0.86	0.14	-	60,60,60,60	0
56	MG	1a	1774	1/1	0.98	0.15	-	70,70,70,70	0
56	MG	2a	1636	1/1	0.81	0.09	-	81,81,81,81	0
56	MG	1A	3624	1/1	0.87	0.15	-	62,62,62,62	0
56	MG	2A	3664	1/1	0.90	0.30	-	55,55,55,55	0
56	MG	1t	3001	1/1	0.90	0.23	-	69,69,69,69	0
56	MG	1x	103	1/1	0.91	0.21	-	63,63,63,63	0
56	MG	2p	101	1/1	0.84	0.43	-	58,58,58,58	0
56	MG	2A	3484	1/1	0.96	0.10	-	53,53,53,53	0
56	MG	1A	3081	1/1	0.96	0.74	-	39,39,39,39	0
56	MG	1A	3088	1/1	0.82	0.68	-	32,32,32,32	0
56	MG	1A	3082	1/1	0.99	0.10	-	59,59,59,59	0
56	MG	2A	3216	1/1	0.95	0.14	-	52,52,52,52	0
56	MG	1A	3865	1/1	0.95	0.06	-	44,44,44,44	0
56	MG	2a	1675	1/1	0.82	0.76	-	69,69,69,69	0
56	MG	1a	1787	1/1	0.73	0.13	-	65,65,65,65	0
56	MG	2A	3509	1/1	0.94	0.12	-	59,59,59,59	0
56	MG	1A	3308	1/1	0.96	0.15	-	58,58,58,58	0
56	MG	2A	3648	1/1	0.92	0.13	-	64,64,64,64	0
56	MG	1A	3566	1/1	0.85	0.26	-	41,41,41,41	0
56	MG	2A	3360	1/1	0.91	0.13	-	62,62,62,62	0
56	MG	2a	1747	1/1	0.83	0.14	-	66,66,66,66	0
56	MG	1A	3487	1/1	0.90	0.34	-	51,51,51,51	0
56	MG	1A	3943	1/1	0.95	0.22	-	47,47,47,47	0
56	MG	1a	1659	1/1	0.78	0.38	-	64,64,64,64	0
56	MG	2A	3103	1/1	0.98	0.11	-	63,63,63,63	0
56	MG	1a	1799	1/1	0.73	0.24	-	66,66,66,66	0
56	MG	1a	1757	1/1	0.95	0.15	-	55,55,55,55	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	2A	3618	1/1	0.98	0.04	-	42,42,42,42	0
56	MG	1x	110	1/1	0.83	0.11	-	58,58,58,58	0
56	MG	2A	3461	1/1	0.96	0.07	-	53,53,53,53	0
56	MG	1a	1791	1/1	0.90	0.24	-	74,74,74,74	0
56	MG	1U	201	1/1	0.92	0.28	-	37,37,37,37	0
56	MG	2a	1602	1/1	0.78	0.55	-	64,64,64,64	0
56	MG	1A	3036	1/1	0.86	0.07	-	58,58,58,58	0
56	MG	2A	3370	1/1	0.94	0.27	-	62,62,62,62	0
56	MG	2A	3206	1/1	0.79	0.32	-	57,57,57,57	0
56	MG	1A	3510	1/1	0.93	0.10	-	52,52,52,52	0
56	MG	2A	3261	1/1	0.90	0.13	-	52,52,52,52	0
56	MG	2A	3214	1/1	0.94	0.47	-	49,49,49,49	0
56	MG	1a	1769	1/1	0.96	0.17	-	68,68,68,68	0
56	MG	1A	3530	1/1	0.98	0.11	-	43,43,43,43	0
56	MG	1A	3877	1/1	0.92	0.10	-	35,35,35,35	0
56	MG	2a	1622	1/1	0.79	0.59	-	56,56,56,56	0
56	MG	2a	1627	1/1	0.98	0.14	-	58,58,58,58	0
56	MG	1a	1672	1/1	0.85	0.54	-	61,61,61,61	0
56	MG	1a	1825	1/1	0.93	0.07	-	66,66,66,66	0
56	MG	1A	3468	1/1	0.96	0.06	-	47,47,47,47	0
56	MG	1A	3809	1/1	0.91	0.09	-	40,40,40,40	0
56	MG	2A	3277	1/1	0.99	0.15	-	67,67,67,67	0
56	MG	1T	201	1/1	0.84	0.23	-	52,52,52,52	0
56	MG	2A	3052	1/1	0.89	0.18	-	62,62,62,62	0
56	MG	1A	3014	1/1	0.96	0.09	-	41,41,41,41	0
56	MG	1A	3600	1/1	0.80	0.26	-	38,38,38,38	0
56	MG	1A	3276	1/1	0.98	0.12	-	49,49,49,49	0
56	MG	1a	1632	1/1	0.85	0.15	-	63,63,63,63	0
56	MG	2A	3118	1/1	0.88	0.36	-	47,47,47,47	0
56	MG	2A	3532	1/1	0.63	0.16	-	50,50,50,50	0
56	MG	1a	1736	1/1	0.81	0.32	-	73,73,73,73	0
56	MG	2A	3079	1/1	0.94	0.23	-	51,51,51,51	0
56	MG	1A	3310	1/1	0.94	0.11	-	30,30,30,30	0
56	MG	1A	3638	1/1	0.97	0.08	-	44,44,44,44	0
56	MG	1A	3818	1/1	0.86	0.34	-	29,29,29,29	0
56	MG	2A	3410	1/1	0.61	0.41	-	63,63,63,63	0
56	MG	1x	106	1/1	0.93	0.21	-	62,62,62,62	0
56	MG	1A	3409	1/1	0.99	0.06	-	38,38,38,38	0
56	MG	2A	3187	1/1	0.70	0.70	-	57,57,57,57	0
56	MG	2a	1742	1/1	0.92	0.16	-	70,70,70,70	0
56	MG	1A	3792	1/1	0.87	0.18	-	34,34,34,34	0
56	MG	2A	3213	1/1	0.88	0.41	-	53,53,53,53	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	2A	3390	1/1	0.91	0.24	-	49,49,49,49	0
56	MG	2E	302	1/1	0.93	0.19	-	52,52,52,52	0
56	MG	1A	3042	1/1	0.97	0.45	-	21,21,21,21	0
56	MG	1B	220	1/1	0.95	0.10	-	44,44,44,44	0
56	MG	2A	3020	1/1	0.90	0.64	-	49,49,49,49	0
56	MG	1A	3944	1/1	0.83	0.14	-	31,31,31,31	0
56	MG	2A	3169	1/1	0.79	0.13	-	50,50,50,50	0
56	MG	1A	3368	1/1	0.92	0.19	-	58,58,58,58	0
56	MG	2a	1618	1/1	0.69	0.15	-	80,80,80,80	0
56	MG	2A	3089	1/1	0.79	0.45	-	69,69,69,69	0
56	MG	1x	112	1/1	0.94	0.37	-	65,65,65,65	0
56	MG	2A	3649	1/1	0.84	0.37	-	57,57,57,57	0
56	MG	2a	1664	1/1	0.86	0.69	-	65,65,65,65	0
56	MG	1A	3095	1/1	0.90	0.67	-	44,44,44,44	0
56	MG	1A	3789	1/1	0.97	0.06	-	41,41,41,41	0
56	MG	2a	1751	1/1	0.69	0.19	-	77,77,77,77	0
56	MG	2a	1670	1/1	0.83	0.27	-	58,58,58,58	0
56	MG	1A	3541	1/1	0.94	0.24	-	35,35,35,35	0
56	MG	2B	3002	1/1	0.93	0.22	-	72,72,72,72	0
56	MG	1A	3739	1/1	0.91	0.24	-	28,28,28,28	0
56	MG	1A	3860	1/1	0.96	0.21	-	35,35,35,35	0
56	MG	2A	3587	1/1	0.95	0.06	-	70,70,70,70	0
56	MG	2a	1663	1/1	0.76	0.30	-	65,65,65,65	0
56	MG	2A	3608	1/1	0.82	0.21	-	62,62,62,62	0
56	MG	2A	3098	1/1	0.88	0.26	-	59,59,59,59	0
56	MG	1i	3001	1/1	0.72	0.21	-	68,68,68,68	0
56	MG	1A	3083	1/1	0.91	0.27	-	34,34,34,34	0
56	MG	2A	3429	1/1	0.97	0.22	-	58,58,58,58	0
56	MG	1A	3420	1/1	0.94	0.11	-	43,43,43,43	0
56	MG	2A	3204	1/1	0.71	0.18	-	56,56,56,56	0
56	MG	1a	1612	1/1	0.88	0.28	-	56,56,56,56	0
56	MG	2A	3364	1/1	0.94	0.13	-	58,58,58,58	0
56	MG	1A	3924	1/1	0.94	0.21	-	51,51,51,51	0
56	MG	1A	3791	1/1	0.52	0.12	-	60,60,60,60	0
56	MG	1a	1792	1/1	0.79	0.21	-	68,68,68,68	0
56	MG	1B	213	1/1	0.85	0.09	-	49,49,49,49	0
56	MG	2a	1639	1/1	0.92	0.50	-	68,68,68,68	0
56	MG	2A	3013	1/1	0.98	0.17	-	57,57,57,57	0
56	MG	1G	3002	1/1	0.96	0.08	-	57,57,57,57	0
56	MG	2A	3529	1/1	0.96	0.18	-	59,59,59,59	0
56	MG	2A	3178	1/1	0.75	0.39	-	49,49,49,49	0
56	MG	1A	3721	1/1	0.91	0.14	-	53,53,53,53	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	1A	3797	1/1	0.94	0.22	-	45,45,45,45	0
56	MG	2A	3331	1/1	0.82	0.23	-	57,57,57,57	0
56	MG	2A	3073	1/1	0.94	0.35	-	50,50,50,50	0
56	MG	2O	201	1/1	0.94	0.13	-	54,54,54,54	0
56	MG	2A	3309	1/1	0.94	0.33	-	61,61,61,61	0
56	MG	1a	1822	1/1	0.92	0.07	-	60,60,60,60	0
56	MG	2A	3393	1/1	0.97	0.37	-	54,54,54,54	0
56	MG	1A	3253	1/1	0.88	0.28	-	40,40,40,40	0
56	MG	1A	3562	1/1	0.90	0.07	-	45,45,45,45	0
56	MG	1A	3248	1/1	0.99	0.15	-	37,37,37,37	0
56	MG	1A	3239	1/1	0.97	0.09	-	41,41,41,41	0
56	MG	1a	1680	1/1	0.88	0.60	-	45,45,45,45	0
56	MG	2A	3218	1/1	0.91	0.59	-	55,55,55,55	0
56	MG	2A	3486	1/1	0.96	0.13	-	54,54,54,54	0
56	MG	2a	1746	1/1	0.94	0.09	-	71,71,71,71	0
56	MG	1A	3110	1/1	0.97	0.12	-	35,35,35,35	0
56	MG	1A	3806	1/1	0.90	0.14	-	60,60,60,60	0
56	MG	1A	3186	1/1	0.87	0.23	-	34,34,34,34	0
56	MG	2A	3627	1/1	0.97	0.10	-	46,46,46,46	0
56	MG	2a	1703	1/1	0.80	0.37	-	77,77,77,77	0
56	MG	1a	1740	1/1	0.92	0.17	-	70,70,70,70	0
56	MG	1A	3748	1/1	0.97	0.06	-	49,49,49,49	0
56	MG	1a	1685	1/1	0.87	0.52	-	67,67,67,67	0
56	MG	1A	3551	1/1	0.85	0.44	-	54,54,54,54	0
56	MG	1A	3184	1/1	0.95	0.13	-	37,37,37,37	0
56	MG	1A	3275	1/1	0.58	0.18	-	70,70,70,70	0
56	MG	1A	3727	1/1	0.92	0.23	-	67,67,67,67	0
56	MG	1A	3094	1/1	0.92	0.26	-	36,36,36,36	0
56	MG	1A	3676	1/1	0.88	0.34	-	34,34,34,34	0
56	MG	1A	3066	1/1	0.98	0.27	-	13,13,13,13	0
56	MG	1a	1852	1/1	0.95	0.22	-	63,63,63,63	0
56	MG	2A	3433	1/1	0.98	0.09	-	52,52,52,52	0
56	MG	1A	3434	1/1	0.93	0.14	-	38,38,38,38	0
56	MG	1A	3574	1/1	0.91	0.14	-	32,32,32,32	0
56	MG	1A	3289	1/1	0.95	0.18	-	32,32,32,32	0
56	MG	2A	3201	1/1	0.61	0.30	-	53,53,53,53	0
56	MG	2a	1635	1/1	0.92	0.44	-	73,73,73,73	0
56	MG	1A	3617	1/1	0.98	0.05	-	60,60,60,60	0
56	MG	1A	3294	1/1	0.91	0.14	-	42,42,42,42	0
56	MG	1A	3609	1/1	0.95	0.12	-	43,43,43,43	0
56	MG	1A	3198	1/1	0.85	0.14	-	60,60,60,60	0
56	MG	1a	1706	1/1	0.61	0.61	-	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	1A	3808	1/1	0.92	0.17	-	55,55,55,55	0
56	MG	1a	1742	1/1	0.89	0.13	-	71,71,71,71	0
56	MG	1A	3896	1/1	0.96	0.17	-	31,31,31,31	0
56	MG	1A	3040	1/1	0.93	0.20	-	49,49,49,49	0
56	MG	1A	3506	1/1	0.84	0.10	-	44,44,44,44	0
56	MG	1A	3788	1/1	0.98	0.08	-	55,55,55,55	0
56	MG	2a	1718	1/1	0.95	0.21	-	62,62,62,62	0
56	MG	1A	3480	1/1	0.94	0.08	-	35,35,35,35	0
56	MG	2R	8001	1/1	0.96	0.17	-	50,50,50,50	0
56	MG	2A	3544	1/1	0.85	0.10	-	61,61,61,61	0
56	MG	1A	3445	1/1	0.95	0.15	-	42,42,42,42	0
56	MG	13	102	1/1	0.95	0.46	-	53,53,53,53	0
56	MG	1A	3684	1/1	0.92	0.17	-	50,50,50,50	0
56	MG	1B	218	1/1	0.90	0.08	-	39,39,39,39	0
56	MG	2A	3426	1/1	0.92	0.35	-	60,60,60,60	0
56	MG	1A	3872	1/1	0.78	0.21	-	58,58,58,58	0
56	MG	2a	1674	1/1	0.88	0.37	-	64,64,64,64	0
56	MG	2A	3007	1/1	0.90	0.20	-	51,51,51,51	0
56	MG	1A	3352	1/1	0.94	0.08	-	40,40,40,40	0
56	MG	2A	3566	1/1	0.88	0.15	-	62,62,62,62	0
56	MG	1A	3377	1/1	0.84	0.13	-	34,34,34,34	0
56	MG	1A	3606	1/1	0.82	0.50	-	40,40,40,40	0
56	MG	1a	1759	1/1	0.84	0.32	-	69,69,69,69	0
56	MG	2A	3314	1/1	0.90	0.05	-	65,65,65,65	0
56	MG	1A	3519	1/1	0.96	0.05	-	56,56,56,56	0
56	MG	1A	3650	1/1	0.94	0.07	-	40,40,40,40	0
56	MG	1A	3279	1/1	0.64	0.12	-	49,49,49,49	0
56	MG	2a	1774	1/1	0.75	0.36	-	68,68,68,68	0
56	MG	2E	307	1/1	0.71	0.19	-	52,52,52,52	0
56	MG	2A	3537	1/1	0.91	0.09	-	60,60,60,60	0
56	MG	1A	3092	1/1	0.87	0.32	-	33,33,33,33	0
56	MG	1A	3517	1/1	0.87	0.19	-	33,33,33,33	0
56	MG	1A	3652	1/1	0.95	0.25	-	40,40,40,40	0
56	MG	1A	3610	1/1	0.97	0.11	-	45,45,45,45	0
56	MG	2A	3116	1/1	0.75	0.18	-	73,73,73,73	0
56	MG	2A	3485	1/1	0.97	0.07	-	53,53,53,53	0
56	MG	1a	1690	1/1	0.86	0.18	-	55,55,55,55	0
56	MG	2A	3640	1/1	0.98	0.43	-	59,59,59,59	0
56	MG	2A	3287	1/1	0.96	0.13	-	60,60,60,60	0
56	MG	19	101	1/1	0.86	0.28	-	48,48,48,48	0
56	MG	2A	3072	1/1	0.85	0.48	-	54,54,54,54	0
56	MG	1A	3337	1/1	0.97	0.20	-	36,36,36,36	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	2A	3514	1/1	0.82	0.08	-	63,63,63,63	0
56	MG	1A	3755	1/1	0.81	0.10	-	45,45,45,45	0
56	MG	1x	102	1/1	0.96	0.15	-	64,64,64,64	0
56	MG	1A	3073	1/1	0.97	0.34	-	32,32,32,32	0
56	MG	1B	225	1/1	0.90	0.31	-	55,55,55,55	0
56	MG	2A	3516	1/1	0.97	0.30	-	57,57,57,57	0
56	MG	1A	3306	1/1	0.96	0.20	-	40,40,40,40	0
56	MG	1a	1809	1/1	0.85	0.20	-	62,62,62,62	0
56	MG	2A	3404	1/1	0.72	0.36	-	55,55,55,55	0
56	MG	1A	3075	1/1	0.90	0.22	-	37,37,37,37	0
56	MG	1a	1603	1/1	0.94	0.35	-	64,64,64,64	0
56	MG	2A	3090	1/1	0.92	0.08	-	58,58,58,58	0
56	MG	2A	3163	1/1	0.95	0.35	-	48,48,48,48	0
56	MG	1A	3205	1/1	0.93	0.19	-	30,30,30,30	0
56	MG	2a	1665	1/1	0.95	0.17	-	81,81,81,81	0
56	MG	2A	3292	1/1	0.73	0.30	-	60,60,60,60	0
56	MG	1A	3805	1/1	0.97	0.04	-	31,31,31,31	0
56	MG	1A	3567	1/1	0.94	0.15	-	52,52,52,52	0
56	MG	1A	3296	1/1	0.83	0.10	-	45,45,45,45	0
56	MG	2E	305	1/1	0.87	0.34	-	45,45,45,45	0
56	MG	1A	3511	1/1	0.97	0.21	-	47,47,47,47	0
56	MG	1a	1775	1/1	0.95	0.23	-	66,66,66,66	0
56	MG	1A	3070	1/1	0.92	0.29	-	31,31,31,31	0
56	MG	1A	3032	1/1	0.93	0.50	-	35,35,35,35	0
56	MG	2a	1694	1/1	0.97	0.07	-	63,63,63,63	0
56	MG	1A	3312	1/1	0.97	0.21	-	27,27,27,27	0
56	MG	2A	3033	1/1	0.93	0.11	-	58,58,58,58	0
56	MG	2a	1623	1/1	0.91	0.49	-	49,49,49,49	0
56	MG	1Q	203	1/1	0.94	0.30	-	47,47,47,47	0
56	MG	1e	204	1/1	0.93	0.07	-	63,63,63,63	0
56	MG	1A	3801	1/1	0.96	0.06	-	51,51,51,51	0
56	MG	1E	304	1/1	0.92	0.15	-	50,50,50,50	0
56	MG	1A	3080	1/1	0.85	1.21	-	33,33,33,33	0
56	MG	1A	3142	1/1	0.83	0.19	-	34,34,34,34	0
56	MG	2A	3064	1/1	0.96	0.27	-	46,46,46,46	0
56	MG	2A	3428	1/1	0.94	0.09	-	57,57,57,57	0
56	MG	1A	3385	1/1	0.95	0.14	-	53,53,53,53	0
56	MG	1A	3108	1/1	0.88	0.61	-	40,40,40,40	0
56	MG	2A	3069	1/1	0.86	0.30	-	41,41,41,41	0
56	MG	1A	3478	1/1	0.88	0.11	-	41,41,41,41	0
56	MG	1A	3726	1/1	0.95	0.08	-	51,51,51,51	0
56	MG	1a	1738	1/1	0.96	0.10	-	57,57,57,57	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	1A	3607	1/1	0.76	0.24	-	45,45,45,45	0
56	MG	1A	3207	1/1	0.87	0.77	-	35,35,35,35	0
56	MG	2B	3011	1/1	0.75	0.17	-	78,78,78,78	0
56	MG	1A	3523	1/1	0.94	0.16	-	57,57,57,57	0
56	MG	2A	3263	1/1	0.89	0.23	-	52,52,52,52	0
56	MG	2G	201	1/1	0.88	0.16	-	72,72,72,72	0
56	MG	1A	3099	1/1	0.95	1.09	-	34,34,34,34	0
62	K	2A	3665	1/1	0.85	0.48	-	60,60,60,60	0
56	MG	2A	3291	1/1	0.85	0.12	-	52,52,52,52	0
56	MG	2A	3159	1/1	0.85	0.33	-	53,53,53,53	0
56	MG	2A	3628	1/1	0.84	0.23	-	58,58,58,58	0
56	MG	2A	3592	1/1	0.92	0.11	-	47,47,47,47	0
56	MG	1A	3763	1/1	0.89	0.18	-	33,33,33,33	0
56	MG	1A	3689	1/1	0.93	0.14	-	37,37,37,37	0
56	MG	1A	3516	1/1	0.98	0.08	-	38,38,38,38	0
56	MG	1a	1691	1/1	0.89	0.08	-	67,67,67,67	0
56	MG	2A	3173	1/1	0.84	0.15	-	56,56,56,56	0
56	MG	1A	3243	1/1	0.90	0.24	-	55,55,55,55	0
56	MG	2a	1672	1/1	0.91	0.45	-	52,52,52,52	0
56	MG	2A	3302	1/1	0.88	0.20	-	51,51,51,51	0
56	MG	2B	3004	1/1	0.81	0.29	-	64,64,64,64	0
56	MG	2A	3481	1/1	0.96	0.13	-	59,59,59,59	0
56	MG	2A	3164	1/1	0.91	0.25	-	46,46,46,46	0
56	MG	2a	1738	1/1	0.69	0.10	-	58,58,58,58	0
56	MG	1a	1832	1/1	0.93	0.04	-	73,73,73,73	0
56	MG	1A	3091	1/1	0.98	0.38	-	23,23,23,23	0
56	MG	1A	3245	1/1	0.90	0.28	-	44,44,44,44	0
56	MG	1a	1782	1/1	0.93	0.38	-	58,58,58,58	0
56	MG	2A	3412	1/1	0.94	0.06	-	47,47,47,47	0
56	MG	2A	3244	1/1	0.93	0.06	-	58,58,58,58	0
56	MG	1B	228	1/1	0.87	0.20	-	67,67,67,67	0
56	MG	1A	3135	1/1	0.99	0.18	-	33,33,33,33	0
56	MG	1a	1785	1/1	0.88	0.26	-	71,71,71,71	0
56	MG	1A	3717	1/1	0.70	0.20	-	57,57,57,57	0
56	MG	2k	201	1/1	0.84	0.22	-	64,64,64,64	0
56	MG	2A	3489	1/1	0.92	0.33	-	55,55,55,55	0
56	MG	2A	3579	1/1	0.93	0.34	-	50,50,50,50	0
56	MG	1A	3822	1/1	0.85	0.26	-	37,37,37,37	0
56	MG	1a	1640	1/1	0.67	0.33	-	71,71,71,71	0
56	MG	2A	3450	1/1	0.86	0.07	-	50,50,50,50	0
56	MG	1a	1763	1/1	0.88	0.15	-	82,82,82,82	0
56	MG	2A	3249	1/1	0.91	0.14	-	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	1A	3772	1/1	0.93	0.10	-	45,45,45,45	0
56	MG	1A	3605	1/1	0.90	0.12	-	47,47,47,47	0
56	MG	2A	3353	1/1	0.86	0.40	-	53,53,53,53	0
56	MG	1A	3733	1/1	0.96	0.18	-	29,29,29,29	0
56	MG	1A	3202	1/1	0.94	0.20	-	29,29,29,29	0
56	MG	1A	3627	1/1	0.95	0.07	-	40,40,40,40	0
56	MG	1A	3608	1/1	0.85	0.11	-	36,36,36,36	0
56	MG	2A	3097	1/1	0.63	0.38	-	62,62,62,62	0
56	MG	1A	3046	1/1	0.97	0.25	-	37,37,37,37	0
56	MG	2A	3003	1/1	0.96	0.12	-	54,54,54,54	0
56	MG	2a	1658	1/1	0.65	0.66	-	58,58,58,58	0
56	MG	1A	3406	1/1	0.98	0.07	-	34,34,34,34	0
56	MG	2A	3395	1/1	0.95	0.16	-	58,58,58,58	0
56	MG	2a	1686	1/1	0.96	0.07	-	69,69,69,69	0
56	MG	1A	3395	1/1	0.95	0.07	-	43,43,43,43	0
56	MG	1A	3905	1/1	0.75	0.21	-	54,54,54,54	0
56	MG	1A	3325	1/1	0.94	0.18	-	42,42,42,42	0
56	MG	1A	3693	1/1	0.79	0.15	-	34,34,34,34	0
56	MG	1a	1733	1/1	0.87	0.13	-	65,65,65,65	0
56	MG	10	105	1/1	0.88	0.09	-	49,49,49,49	0
56	MG	1A	3764	1/1	0.64	0.47	-	47,47,47,47	0
56	MG	2A	3650	1/1	0.36	0.20	-	70,70,70,70	0
56	MG	1A	3651	1/1	0.84	0.17	-	74,74,74,74	0
56	MG	1a	1747	1/1	0.89	0.17	-	56,56,56,56	0
56	MG	1A	3192	1/1	0.99	0.15	-	32,32,32,32	0
56	MG	1a	1800	1/1	0.80	0.08	-	66,66,66,66	0
56	MG	1A	3505	1/1	0.99	0.07	-	50,50,50,50	0
56	MG	1A	3804	1/1	0.98	0.04	-	37,37,37,37	0
56	MG	1A	3147	1/1	0.90	0.54	-	36,36,36,36	0
56	MG	1x	107	1/1	0.96	0.14	-	56,56,56,56	0
56	MG	2A	3150	1/1	0.91	0.40	-	46,46,46,46	0
56	MG	1x	111	1/1	0.61	0.19	-	72,72,72,72	0
56	MG	1A	3754	1/1	0.97	0.13	-	41,41,41,41	0
56	MG	2a	1677	1/1	0.88	0.47	-	76,76,76,76	0
56	MG	2a	1715	1/1	0.80	0.15	-	75,75,75,75	0
56	MG	2a	1648	1/1	0.91	0.15	-	70,70,70,70	0
56	MG	2A	3179	1/1	0.91	0.61	-	52,52,52,52	0
56	MG	1A	3087	1/1	0.99	0.29	-	38,38,38,38	0
56	MG	1A	3864	1/1	0.95	0.28	-	42,42,42,42	0
56	MG	2x	106	1/1	0.95	0.10	-	63,63,63,63	0
56	MG	2a	1721	1/1	0.89	0.22	-	71,71,71,71	0
56	MG	2e	201	1/1	0.92	0.28	-	57,57,57,57	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	1A	3735	1/1	0.92	0.13	-	55,55,55,55	0
56	MG	1A	3270	1/1	0.89	0.18	-	49,49,49,49	0
56	MG	2A	3568	1/1	0.61	0.77	-	56,56,56,56	0
56	MG	2A	3209	1/1	0.91	0.59	-	61,61,61,61	0
56	MG	2A	3266	1/1	0.83	0.15	-	50,50,50,50	0
56	MG	1A	3357	1/1	0.82	0.19	-	29,29,29,29	0
56	MG	1A	3742	1/1	0.94	0.22	-	33,33,33,33	0
56	MG	1A	3415	1/1	0.96	0.05	-	55,55,55,55	0
56	MG	1A	3725	1/1	0.91	0.11	-	46,46,46,46	0
56	MG	1A	3538	1/1	0.86	0.31	-	56,56,56,56	0
56	MG	1f	8001	1/1	0.78	0.14	-	63,63,63,63	0
56	MG	2A	3367	1/1	0.98	0.14	-	59,59,59,59	0
56	MG	2A	3196	1/1	0.71	0.35	-	52,52,52,52	0
56	MG	1A	3216	1/1	0.94	0.77	-	34,34,34,34	0
56	MG	2A	3656	1/1	0.94	0.40	-	50,50,50,50	0
56	MG	1a	1797	1/1	0.91	0.22	-	76,76,76,76	0
56	MG	1A	3054	1/1	0.95	0.17	-	30,30,30,30	0
56	MG	1A	3020	1/1	0.96	0.20	-	36,36,36,36	0
56	MG	1A	3745	1/1	0.87	0.23	-	49,49,49,49	0
56	MG	1A	3593	1/1	0.81	0.43	-	52,52,52,52	0
56	MG	2A	3332	1/1	0.94	0.26	-	43,43,43,43	0
56	MG	1A	3868	1/1	0.86	0.32	-	56,56,56,56	0
56	MG	1A	3148	1/1	0.95	0.25	-	32,32,32,32	0
56	MG	1A	3591	1/1	0.85	0.23	-	54,54,54,54	0
56	MG	2A	3402	1/1	0.87	0.06	-	52,52,52,52	0
56	MG	2A	3616	1/1	0.94	0.18	-	73,73,73,73	0
56	MG	1A	3292	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	2A	3130	1/1	0.95	0.16	-	62,62,62,62	0
56	MG	2a	1607	1/1	0.98	0.07	-	70,70,70,70	0
56	MG	1A	3004	1/1	0.88	0.19	-	37,37,37,37	0
56	MG	2A	3407	1/1	0.89	0.05	-	59,59,59,59	0
56	MG	1A	3672	1/1	0.94	0.08	-	45,45,45,45	0
56	MG	1A	3387	1/1	0.94	0.11	-	34,34,34,34	0
56	MG	1A	3326	1/1	0.91	0.18	-	48,48,48,48	0
56	MG	1a	1628	1/1	0.85	0.32	-	63,63,63,63	0
56	MG	2A	3372	1/1	0.94	0.10	-	58,58,58,58	0
56	MG	1a	1752	1/1	0.98	0.18	-	67,67,67,67	0
56	MG	1a	1714	1/1	0.94	0.08	-	53,53,53,53	0
56	MG	1A	3159	1/1	0.92	0.69	-	38,38,38,38	0
56	MG	1A	3056	1/1	0.89	0.17	-	55,55,55,55	0
56	MG	1a	1608	1/1	0.90	0.10	-	78,78,78,78	0
56	MG	1A	3841	1/1	0.95	0.14	-	45,45,45,45	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	2A	3438	1/1	0.95	0.06	-	56,56,56,56	0
56	MG	2A	3621	1/1	0.86	0.08	-	76,76,76,76	0
56	MG	2a	1717	1/1	0.82	0.27	-	67,67,67,67	0
56	MG	1a	1731	1/1	0.93	0.20	-	63,63,63,63	0
56	MG	1a	1803	1/1	0.84	0.48	-	63,63,63,63	0
56	MG	1A	3173	1/1	0.95	0.14	-	40,40,40,40	0
56	MG	1A	3335	1/1	0.94	0.13	-	44,44,44,44	0
56	MG	2A	3479	1/1	0.92	0.24	-	49,49,49,49	0
56	MG	1A	3549	1/1	0.95	0.28	-	32,32,32,32	0
56	MG	1B	222	1/1	0.95	0.08	-	49,49,49,49	0
56	MG	2V	203	1/1	0.72	0.28	-	61,61,61,61	0
56	MG	2A	3221	1/1	0.98	0.28	-	51,51,51,51	0
56	MG	2A	3135	1/1	0.93	0.54	-	43,43,43,43	0
56	MG	1A	3640	1/1	0.94	0.42	-	43,43,43,43	0
56	MG	1a	1751	1/1	0.96	0.15	-	69,69,69,69	0
56	MG	2a	1685	1/1	0.84	0.07	-	68,68,68,68	0
56	MG	1A	3171	1/1	0.83	0.85	-	42,42,42,42	0
56	MG	1A	3580	1/1	0.92	0.19	-	48,48,48,48	0
56	MG	1A	3138	1/1	0.89	0.15	-	50,50,50,50	0
56	MG	2A	3265	1/1	0.95	0.07	-	60,60,60,60	0
56	MG	2a	1646	1/1	0.90	0.51	-	66,66,66,66	0
56	MG	2A	3328	1/1	0.74	0.47	-	71,71,71,71	0
56	MG	2A	3414	1/1	0.93	0.14	-	53,53,53,53	0
56	MG	2a	1775	1/1	0.94	0.07	-	65,65,65,65	0
56	MG	2A	3175	1/1	0.85	0.26	-	58,58,58,58	0
56	MG	1a	1796	1/1	0.97	0.22	-	68,68,68,68	0
56	MG	2A	3449	1/1	0.95	0.12	-	42,42,42,42	0
56	MG	2A	3172	1/1	0.87	0.13	-	68,68,68,68	0
56	MG	1H	8001	1/1	0.77	0.26	-	61,61,61,61	0
56	MG	2a	1700	1/1	0.97	0.08	-	65,65,65,65	0
56	MG	2A	3659	1/1	0.91	0.11	-	60,60,60,60	0
56	MG	2A	3121	1/1	0.88	0.15	-	68,68,68,68	0
56	MG	1A	3800	1/1	0.95	0.07	-	51,51,51,51	0
56	MG	2A	3496	1/1	0.78	0.14	-	45,45,45,45	0
56	MG	2A	3527	1/1	0.95	0.17	-	60,60,60,60	0
56	MG	2A	3658	1/1	0.84	0.22	-	49,49,49,49	0
56	MG	1a	1795	1/1	0.76	0.21	-	76,76,76,76	0
56	MG	2A	3021	1/1	0.75	0.19	-	67,67,67,67	0
56	MG	2A	3403	1/1	0.98	0.43	-	60,60,60,60	0
56	MG	1a	1678	1/1	0.83	0.29	-	74,74,74,74	0
56	MG	2x	107	1/1	0.84	0.18	-	69,69,69,69	0
56	MG	2A	3008	1/1	0.91	0.18	-	45,45,45,45	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	1A	3333	1/1	0.95	0.16	-	45,45,45,45	0
56	MG	2A	3603	1/1	0.83	0.16	-	46,46,46,46	0
56	MG	11	103	1/1	0.91	0.25	-	41,41,41,41	0
56	MG	2A	3525	1/1	0.94	0.13	-	55,55,55,55	0
56	MG	2a	1617	1/1	0.92	0.17	-	51,51,51,51	0
56	MG	2A	3498	1/1	0.96	0.09	-	42,42,42,42	0
56	MG	2A	3487	1/1	0.95	0.06	-	56,56,56,56	0
56	MG	1A	3839	1/1	0.99	0.18	-	41,41,41,41	0
56	MG	1A	3448	1/1	0.96	0.21	-	30,30,30,30	0
56	MG	1A	3222	1/1	0.91	0.16	-	62,62,62,62	0
56	MG	2A	3031	1/1	0.94	0.27	-	56,56,56,56	0
56	MG	13	101	1/1	0.97	0.11	-	38,38,38,38	0
56	MG	1A	3914	1/1	0.81	0.40	-	57,57,57,57	0
56	MG	1A	3226	1/1	0.79	0.76	-	36,36,36,36	0
56	MG	2A	3207	1/1	0.86	0.27	-	68,68,68,68	0
56	MG	1A	3132	1/1	0.99	0.24	-	39,39,39,39	0
56	MG	1A	3550	1/1	0.86	0.15	-	51,51,51,51	0
56	MG	1A	3679	1/1	0.93	0.15	-	32,32,32,32	0
56	MG	2A	3312	1/1	0.69	0.13	-	69,69,69,69	0
56	MG	1A	3057	1/1	0.96	0.33	-	32,32,32,32	0
56	MG	2A	3630	1/1	0.94	0.24	-	50,50,50,50	0
56	MG	1A	3534	1/1	0.94	0.14	-	36,36,36,36	0
56	MG	1a	1663	1/1	0.93	0.15	-	74,74,74,74	0
56	MG	1a	1816	1/1	0.78	0.19	-	57,57,57,57	0
56	MG	1A	3646	1/1	0.88	0.12	-	37,37,37,37	0
56	MG	2A	3474	1/1	0.96	0.14	-	47,47,47,47	0
56	MG	1A	3103	1/1	0.99	0.15	-	48,48,48,48	0
56	MG	1A	3823	1/1	0.88	0.14	-	59,59,59,59	0
56	MG	1a	1704	1/1	0.93	0.06	-	63,63,63,63	0
56	MG	1A	3514	1/1	0.99	0.06	-	42,42,42,42	0
56	MG	1A	3090	1/1	0.95	0.56	-	29,29,29,29	0
56	MG	2A	3318	1/1	0.67	0.18	-	50,50,50,50	0
56	MG	2A	3067	1/1	0.85	0.67	-	42,42,42,42	0
56	MG	1A	3128	1/1	0.90	0.32	-	43,43,43,43	0
56	MG	1B	216	1/1	0.79	0.26	-	49,49,49,49	0
56	MG	2A	3580	1/1	0.97	0.35	-	52,52,52,52	0
56	MG	1A	3309	1/1	0.83	0.11	-	36,36,36,36	0
56	MG	1a	1847	1/1	0.94	0.06	-	72,72,72,72	0
56	MG	1a	1793	1/1	0.86	0.24	-	71,71,71,71	0
56	MG	2A	3497	1/1	0.92	0.18	-	51,51,51,51	0
56	MG	2a	1603	1/1	0.83	0.63	-	60,60,60,60	0
56	MG	1A	3048	1/1	0.94	0.59	-	40,40,40,40	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	1A	3663	1/1	0.84	0.09	-	48,48,48,48	0
56	MG	2A	3109	1/1	0.90	0.17	-	54,54,54,54	0
56	MG	2A	3092	1/1	0.94	0.64	-	61,61,61,61	0
56	MG	2A	3215	1/1	0.99	0.09	-	47,47,47,47	0
56	MG	2A	3161	1/1	0.87	0.31	-	47,47,47,47	0
56	MG	1A	3469	1/1	0.89	0.28	-	39,39,39,39	0
56	MG	1A	3421	1/1	0.89	0.07	-	55,55,55,55	0
56	MG	2A	3139	1/1	0.78	0.92	-	57,57,57,57	0
56	MG	2A	3236	1/1	0.96	0.20	-	50,50,50,50	0
56	MG	2a	1776	1/1	0.75	0.32	-	65,65,65,65	0
56	MG	1A	3582	1/1	0.92	0.39	-	39,39,39,39	0
56	MG	1A	3769	1/1	0.87	0.17	-	67,67,67,67	0
56	MG	2A	3323	1/1	0.94	0.18	-	50,50,50,50	0
56	MG	2A	3465	1/1	0.95	0.15	-	57,57,57,57	0
56	MG	1A	3252	1/1	0.87	0.53	-	41,41,41,41	0
56	MG	1a	1675	1/1	0.83	0.25	-	46,46,46,46	0
56	MG	2B	3003	1/1	0.83	0.28	-	68,68,68,68	0
56	MG	2A	3063	1/1	0.73	0.17	-	53,53,53,53	0
56	MG	1a	1737	1/1	0.84	0.11	-	74,74,74,74	0
56	MG	2A	3279	1/1	0.86	0.23	-	60,60,60,60	0
56	MG	2A	3622	1/1	0.98	0.12	-	67,67,67,67	0
56	MG	2A	3598	1/1	0.91	0.11	-	54,54,54,54	0
56	MG	1A	3450	1/1	0.95	0.09	-	35,35,35,35	0
56	MG	2A	3611	1/1	0.96	0.07	-	57,57,57,57	0
56	MG	2A	3394	1/1	0.92	0.21	-	62,62,62,62	0
56	MG	2A	3147	1/1	0.87	0.14	-	54,54,54,54	0
56	MG	1A	3756	1/1	0.95	0.10	-	39,39,39,39	0
56	MG	1A	3759	1/1	0.82	0.58	-	53,53,53,53	0
56	MG	1A	3084	1/1	0.75	0.41	-	49,49,49,49	0
56	MG	1A	3707	1/1	0.91	0.18	-	52,52,52,52	0
56	MG	1A	3458	1/1	0.95	0.11	-	69,69,69,69	0
56	MG	1A	3602	1/1	0.78	0.13	-	48,48,48,48	0
56	MG	1A	3182	1/1	0.89	0.20	-	60,60,60,60	0
56	MG	1A	3179	1/1	0.97	0.12	-	57,57,57,57	0
56	MG	1A	3525	1/1	0.86	0.23	-	31,31,31,31	0
56	MG	2A	3027	1/1	0.93	0.40	-	42,42,42,42	0
56	MG	1a	1631	1/1	0.92	1.45	-	72,72,72,72	0
56	MG	1A	3331	1/1	0.97	0.05	-	40,40,40,40	0
56	MG	2A	3385	1/1	0.96	0.28	-	53,53,53,53	0
56	MG	1A	3204	1/1	0.91	0.13	-	45,45,45,45	0
56	MG	1A	3316	1/1	0.86	0.31	-	45,45,45,45	0
56	MG	1A	3852	1/1	0.98	0.03	-	47,47,47,47	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	1a	1636	1/1	0.91	1.05	-	60,60,60,60	0
56	MG	1a	1778	1/1	0.88	0.20	-	63,63,63,63	0
56	MG	1a	1734	1/1	0.92	0.12	-	54,54,54,54	0
56	MG	2a	1688	1/1	0.91	0.06	-	58,58,58,58	0
56	MG	2A	3675	1/1	0.98	0.17	-	59,59,59,59	0
56	MG	2A	3074	1/1	0.87	0.31	-	48,48,48,48	0
56	MG	2A	3306	1/1	0.94	0.28	-	59,59,59,59	0
56	MG	1A	3681	1/1	0.87	0.09	-	47,47,47,47	0
56	MG	2A	3585	1/1	0.97	0.18	-	59,59,59,59	0
56	MG	2A	3399	1/1	0.72	0.55	-	53,53,53,53	0
56	MG	1A	3620	1/1	0.90	0.07	-	48,48,48,48	0
56	MG	1a	1746	1/1	0.86	0.17	-	69,69,69,69	0
56	MG	1A	3037	1/1	0.91	0.34	-	38,38,38,38	0
56	MG	1A	3274	1/1	0.91	0.42	-	41,41,41,41	0
56	MG	1A	3424	1/1	0.94	0.19	-	51,51,51,51	0
56	MG	2A	3502	1/1	0.96	0.09	-	70,70,70,70	0
56	MG	1a	1684	1/1	0.81	0.60	-	56,56,56,56	0
56	MG	2A	3024	1/1	0.90	0.23	-	45,45,45,45	0
56	MG	2A	3131	1/1	0.94	0.33	-	63,63,63,63	0
56	MG	2a	1741	1/1	0.92	0.18	-	68,68,68,68	0
56	MG	2A	3177	1/1	0.74	0.39	-	54,54,54,54	0
56	MG	2A	3039	1/1	0.88	0.24	-	56,56,56,56	0
56	MG	1A	3257	1/1	0.83	0.20	-	55,55,55,55	0
56	MG	2D	302	1/1	0.57	1.22	-	48,48,48,48	0
56	MG	1A	3783	1/1	0.98	0.05	-	51,51,51,51	0
56	MG	2A	3051	1/1	0.82	0.75	-	49,49,49,49	0
56	MG	1A	3499	1/1	0.89	0.33	-	43,43,43,43	0
56	MG	1A	3311	1/1	0.94	0.12	-	28,28,28,28	0
56	MG	2a	1652	1/1	0.82	0.52	-	58,58,58,58	0
56	MG	2a	1710	1/1	0.97	0.04	-	73,73,73,73	0
56	MG	2A	3225	1/1	0.95	0.17	-	57,57,57,57	0
56	MG	2W	201	1/1	0.86	0.30	-	62,62,62,62	0
56	MG	2A	3482	1/1	0.85	0.10	-	74,74,74,74	0
56	MG	1A	3463	1/1	0.88	0.14	-	31,31,31,31	0
56	MG	1A	3261	1/1	0.90	0.25	-	52,52,52,52	0
56	MG	2a	1645	1/1	0.89	0.20	-	68,68,68,68	0
56	MG	2A	3577	1/1	0.94	0.09	-	48,48,48,48	0
56	MG	1B	209	1/1	0.83	0.38	-	61,61,61,61	0
56	MG	10	102	1/1	0.90	0.19	-	43,43,43,43	0
56	MG	2A	3226	1/1	0.92	0.33	-	56,56,56,56	0
56	MG	2a	1644	1/1	0.93	0.67	-	69,69,69,69	0
56	MG	1A	3537	1/1	0.95	0.14	-	32,32,32,32	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	17	101	1/1	0.94	0.09	-	36,36,36,36	0
56	MG	1A	3854	1/1	0.91	0.57	-	59,59,59,59	0
56	MG	2A	3447	1/1	0.85	0.34	-	42,42,42,42	0
56	MG	1A	3111	1/1	0.93	0.47	-	30,30,30,30	0
56	MG	2A	3660	1/1	0.97	0.55	-	47,47,47,47	0
56	MG	1A	3078	1/1	0.84	0.29	-	45,45,45,45	0
56	MG	1A	3502	1/1	0.98	0.12	-	43,43,43,43	0
56	MG	2A	3542	1/1	0.92	0.05	-	56,56,56,56	0
56	MG	1A	3894	1/1	0.94	0.08	-	53,53,53,53	0
56	MG	2A	3034	1/1	0.97	0.20	-	49,49,49,49	0
56	MG	2A	3077	1/1	0.74	0.76	-	56,56,56,56	0
56	MG	1a	1622	1/1	0.89	0.22	-	65,65,65,65	0
56	MG	1A	3161	1/1	0.95	0.12	-	35,35,35,35	0
56	MG	2A	3239	1/1	0.95	0.17	-	63,63,63,63	0
56	MG	2A	3574	1/1	0.91	0.12	-	60,60,60,60	0
56	MG	2A	3280	1/1	0.91	0.20	-	42,42,42,42	0
56	MG	2B	3001	1/1	0.95	0.17	-	71,71,71,71	0
56	MG	1A	3512	1/1	0.94	0.09	-	54,54,54,54	0
56	MG	2A	3317	1/1	0.74	0.13	-	54,54,54,54	0
56	MG	2A	3234	1/1	0.91	0.20	-	55,55,55,55	0
56	MG	1a	1794	1/1	0.88	0.44	-	69,69,69,69	0
56	MG	1a	1789	1/1	0.91	0.24	-	74,74,74,74	0
56	MG	2A	3255	1/1	0.93	0.10	-	69,69,69,69	0
56	MG	1A	3639	1/1	0.62	0.28	-	45,45,45,45	0
56	MG	2A	3613	1/1	0.94	0.05	-	56,56,56,56	0
56	MG	1A	3539	1/1	0.94	0.20	-	53,53,53,53	0
56	MG	1A	3844	1/1	0.95	0.20	-	32,32,32,32	0
56	MG	1A	3074	1/1	0.95	0.20	-	32,32,32,32	0
56	MG	19	103	1/1	0.89	0.15	-	51,51,51,51	0
56	MG	1A	3068	1/1	0.97	0.20	-	40,40,40,40	0
56	MG	1A	3342	1/1	0.91	0.26	-	33,33,33,33	0
56	MG	1A	3524	1/1	0.80	0.13	-	55,55,55,55	0
56	MG	1A	3861	1/1	0.87	0.08	-	50,50,50,50	0
56	MG	1A	3845	1/1	0.95	0.21	-	32,32,32,32	0
56	MG	1A	3509	1/1	0.98	0.14	-	39,39,39,39	0
56	MG	1A	3656	1/1	0.85	0.14	-	41,41,41,41	0
56	MG	1a	1826	1/1	0.98	0.24	-	68,68,68,68	0
56	MG	2A	3197	1/1	0.96	0.29	-	50,50,50,50	0
56	MG	1A	3209	1/1	0.84	0.54	-	40,40,40,40	0
56	MG	1A	3821	1/1	0.82	0.72	-	37,37,37,37	0
56	MG	2A	3101	1/1	0.93	0.42	-	47,47,47,47	0
56	MG	1a	1830	1/1	0.96	0.30	-	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	2A	3463	1/1	0.87	0.32	-	52,52,52,52	0
56	MG	2E	306	1/1	0.94	0.07	-	46,46,46,46	0
56	MG	2A	3238	1/1	0.86	0.30	-	55,55,55,55	0
56	MG	1A	3740	1/1	0.92	0.13	-	47,47,47,47	0
56	MG	1A	3318	1/1	0.89	0.12	-	25,25,25,25	0
56	MG	2a	1662	1/1	0.81	1.11	-	77,77,77,77	0
56	MG	1a	1604	1/1	0.68	0.36	-	72,72,72,72	0
56	MG	1D	309	1/1	0.56	0.95	-	42,42,42,42	0
56	MG	2T	3003	1/1	0.93	0.32	-	56,56,56,56	0
56	MG	2A	3636	1/1	0.90	0.15	-	52,52,52,52	0
56	MG	1a	1664	1/1	0.90	0.33	-	71,71,71,71	0
56	MG	1A	3830	1/1	0.96	0.11	-	33,33,33,33	0
56	MG	2A	3345	1/1	0.93	0.14	-	64,64,64,64	0
56	MG	1a	1707	1/1	0.95	0.07	-	47,47,47,47	0
56	MG	2A	3260	1/1	0.98	0.13	-	63,63,63,63	0
56	MG	2A	3056	1/1	0.90	0.32	-	41,41,41,41	0
56	MG	1a	1692	1/1	0.92	0.14	-	70,70,70,70	0
56	MG	1x	109	1/1	0.91	0.18	-	63,63,63,63	0
56	MG	1a	1846	1/1	0.89	0.10	-	48,48,48,48	0
56	MG	1A	3832	1/1	0.71	0.17	-	45,45,45,45	0
56	MG	2A	3262	1/1	0.96	0.23	-	49,49,49,49	0
56	MG	1A	3947	1/1	0.85	0.22	-	56,56,56,56	0
56	MG	2A	3526	1/1	0.82	0.17	-	60,60,60,60	0
56	MG	1A	3263	1/1	0.95	0.27	-	36,36,36,36	0
56	MG	1a	1753	1/1	0.96	0.17	-	50,50,50,50	0
56	MG	2A	3149	1/1	0.80	0.35	-	44,44,44,44	0
56	MG	1A	3016	1/1	0.96	0.70	-	30,30,30,30	0
56	MG	2A	3194	1/1	0.95	0.14	-	54,54,54,54	0
56	MG	1A	3394	1/1	0.98	0.10	-	33,33,33,33	0
56	MG	1A	3442	1/1	0.94	0.06	-	61,61,61,61	0
56	MG	10	107	1/1	0.89	0.10	-	54,54,54,54	0
56	MG	1A	3453	1/1	0.94	0.15	-	46,46,46,46	0
56	MG	1a	1721	1/1	0.96	0.09	-	55,55,55,55	0
56	MG	1a	1776	1/1	0.95	0.08	-	80,80,80,80	0
56	MG	1A	3658	1/1	0.49	0.38	-	50,50,50,50	0
56	MG	1A	3234	1/1	0.84	0.34	-	41,41,41,41	0
56	MG	2A	3015	1/1	0.95	0.19	-	51,51,51,51	0
56	MG	1a	1780	1/1	0.91	0.13	-	71,71,71,71	0
56	MG	1a	1770	1/1	0.87	0.54	-	65,65,65,65	0
56	MG	2A	3132	1/1	0.90	0.28	-	49,49,49,49	0
56	MG	1A	3611	1/1	0.93	0.14	-	50,50,50,50	0
56	MG	1A	3213	1/1	0.96	0.89	-	37,37,37,37	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	2A	3299	1/1	0.62	0.90	-	66,66,66,66	0
56	MG	2a	1737	1/1	0.89	0.07	-	74,74,74,74	0
56	MG	1A	3301	1/1	0.91	0.12	-	40,40,40,40	0
56	MG	2A	3510	1/1	0.89	0.16	-	67,67,67,67	0
56	MG	1A	3851	1/1	0.88	0.10	-	63,63,63,63	0
56	MG	1a	1808	1/1	0.86	0.26	-	66,66,66,66	0
56	MG	1A	3251	1/1	0.97	0.16	-	47,47,47,47	0
56	MG	2D	303	1/1	0.90	0.20	-	58,58,58,58	0
56	MG	1A	3571	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	1A	3350	1/1	0.86	0.20	-	32,32,32,32	0
56	MG	1A	3819	1/1	0.96	0.24	-	53,53,53,53	0
56	MG	2Y	201	1/1	0.96	0.10	-	60,60,60,60	0
56	MG	1x	108	1/1	0.90	0.11	-	65,65,65,65	0
56	MG	1A	3692	1/1	0.81	0.12	-	58,58,58,58	0
56	MG	1a	1727	1/1	0.94	0.11	-	51,51,51,51	0
56	MG	1A	3575	1/1	0.96	0.09	-	55,55,55,55	0
56	MG	2A	3637	1/1	0.97	0.10	-	60,60,60,60	0
56	MG	1A	3488	1/1	0.86	0.12	-	46,46,46,46	0
56	MG	2x	105	1/1	0.84	0.21	-	75,75,75,75	0
56	MG	1a	1679	1/1	0.98	0.10	-	81,81,81,81	0
56	MG	1A	3942	1/1	0.91	0.43	-	55,55,55,55	0
56	MG	1A	3636	1/1	0.90	0.15	-	42,42,42,42	0
56	MG	2A	3188	1/1	0.90	0.54	-	55,55,55,55	0
56	MG	2a	1661	1/1	0.66	0.27	-	65,65,65,65	0
56	MG	2A	3512	1/1	0.96	0.21	-	45,45,45,45	0
56	MG	1A	3475	1/1	0.94	0.07	-	32,32,32,32	0
56	MG	1A	3410	1/1	0.96	0.09	-	50,50,50,50	0
56	MG	2A	3440	1/1	0.94	0.06	-	55,55,55,55	0
56	MG	1a	1641	1/1	0.83	0.36	-	75,75,75,75	0
56	MG	1A	3910	1/1	0.91	0.33	-	39,39,39,39	0
56	MG	2A	3469	1/1	0.98	0.17	-	51,51,51,51	0
56	MG	1A	3375	1/1	0.80	0.14	-	56,56,56,56	0
56	MG	1A	3454	1/1	0.98	0.10	-	36,36,36,36	0
56	MG	1A	3917	1/1	0.90	0.24	-	40,40,40,40	0
56	MG	1A	3532	1/1	0.96	0.14	-	40,40,40,40	0
56	MG	1A	3399	1/1	0.89	0.13	-	49,49,49,49	0
56	MG	2A	3059	1/1	0.95	0.32	-	46,46,46,46	0
56	MG	1A	3897	1/1	0.92	0.49	-	34,34,34,34	0
56	MG	2A	3138	1/1	0.95	0.23	-	42,42,42,42	0
56	MG	1A	3285	1/1	0.70	0.19	-	37,37,37,37	0
56	MG	1A	3723	1/1	0.96	0.09	-	51,51,51,51	0
56	MG	1A	3174	1/1	0.90	0.22	-	56,56,56,56	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	2A	3269	1/1	0.84	0.28	-	43,43,43,43	0
56	MG	2A	3045	1/1	0.93	0.18	-	56,56,56,56	0
56	MG	2A	3113	1/1	0.88	0.09	-	59,59,59,59	0
56	MG	1a	1812	1/1	0.94	0.24	-	67,67,67,67	0
56	MG	1a	1709	1/1	0.94	0.20	-	56,56,56,56	0
56	MG	2A	3619	1/1	0.96	0.06	-	55,55,55,55	0
56	MG	1A	3115	1/1	0.96	0.28	-	41,41,41,41	0
56	MG	1a	1748	1/1	0.93	0.10	-	74,74,74,74	0
56	MG	1A	3172	1/1	0.96	0.25	-	37,37,37,37	0
56	MG	1a	1818	1/1	0.89	0.23	-	73,73,73,73	0
56	MG	2A	3420	1/1	0.92	0.10	-	64,64,64,64	0
56	MG	2A	3133	1/1	0.87	0.28	-	52,52,52,52	0
56	MG	2j	8001	1/1	0.59	0.17	-	79,79,79,79	0
56	MG	1A	3683	1/1	0.90	0.09	-	46,46,46,46	0
56	MG	1a	1611	1/1	0.79	0.51	-	49,49,49,49	0
56	MG	1U	203	1/1	0.92	0.48	-	36,36,36,36	0
56	MG	1A	3422	1/1	0.89	0.06	-	40,40,40,40	0
56	MG	2A	3586	1/1	0.96	0.07	-	68,68,68,68	0
56	MG	1B	210	1/1	0.89	0.08	-	57,57,57,57	0
56	MG	1A	3940	1/1	0.84	0.08	-	42,42,42,42	0
56	MG	1A	3033	1/1	0.86	0.20	-	45,45,45,45	0
56	MG	1a	1798	1/1	0.93	0.15	-	71,71,71,71	0
56	MG	1A	3704	1/1	0.93	0.35	-	36,36,36,36	0
56	MG	2A	3237	1/1	0.80	0.54	-	58,58,58,58	0
56	MG	1A	3219	1/1	0.93	0.17	-	34,34,34,34	0
56	MG	2A	3110	1/1	0.67	0.55	-	53,53,53,53	0
56	MG	1A	3203	1/1	0.90	0.12	-	65,65,65,65	0
56	MG	1A	3714	1/1	0.88	0.43	-	52,52,52,52	0
56	MG	2A	3284	1/1	0.99	0.14	-	44,44,44,44	0
56	MG	2a	1728	1/1	0.95	0.10	-	70,70,70,70	0
56	MG	1A	3452	1/1	0.97	0.06	-	40,40,40,40	0
56	MG	1A	3162	1/1	0.98	0.14	-	36,36,36,36	0
56	MG	2A	3186	1/1	0.93	0.24	-	59,59,59,59	0
56	MG	2A	3253	1/1	0.86	0.09	-	53,53,53,53	0
56	MG	1A	3691	1/1	0.93	0.11	-	48,48,48,48	0
56	MG	1A	3621	1/1	0.98	0.11	-	53,53,53,53	0
56	MG	1A	3058	1/1	0.94	0.12	-	52,52,52,52	0
56	MG	1A	3903	1/1	0.95	0.15	-	53,53,53,53	0
56	MG	1A	3195	1/1	0.90	0.47	-	41,41,41,41	0
56	MG	1A	3332	1/1	0.97	0.10	-	48,48,48,48	0
56	MG	2a	1691	1/1	0.94	0.10	-	60,60,60,60	0
56	MG	2A	3459	1/1	0.86	0.15	-	56,56,56,56	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	2A	3349	1/1	0.52	0.20	-	55,55,55,55	0
56	MG	1A	3141	1/1	0.93	0.14	-	43,43,43,43	0
56	MG	1a	1773	1/1	0.56	0.62	-	82,82,82,82	0
56	MG	1A	3682	1/1	0.96	0.12	-	41,41,41,41	0
56	MG	2A	3047	1/1	0.82	0.25	-	56,56,56,56	0
56	MG	2P	3401	1/1	0.98	0.16	-	55,55,55,55	0
56	MG	1A	3233	1/1	0.96	0.36	-	50,50,50,50	0
56	MG	1A	3168	1/1	0.91	0.27	-	39,39,39,39	0
56	MG	2A	3246	1/1	0.95	0.27	-	54,54,54,54	0
56	MG	1a	1657	1/1	0.65	0.16	-	71,71,71,71	0
56	MG	1W	3003	1/1	0.95	0.75	-	33,33,33,33	0
56	MG	2x	103	1/1	0.69	0.34	-	73,73,73,73	0
56	MG	15	104	1/1	0.76	0.35	-	63,63,63,63	0
56	MG	1A	3144	1/1	0.97	0.33	-	36,36,36,36	0
56	MG	1A	3369	1/1	0.95	0.07	-	43,43,43,43	0
56	MG	1a	1779	1/1	0.83	0.10	-	66,66,66,66	0
56	MG	1A	3720	1/1	0.98	0.08	-	34,34,34,34	0
56	MG	2A	3252	1/1	0.92	0.15	-	41,41,41,41	0
56	MG	2A	3144	1/1	0.97	0.11	-	49,49,49,49	0
56	MG	1A	3774	1/1	0.98	0.04	-	45,45,45,45	0
56	MG	1A	3260	1/1	0.85	0.19	-	42,42,42,42	0
56	MG	1A	3230	1/1	0.93	0.42	-	36,36,36,36	0
56	MG	1A	3824	1/1	0.95	0.25	-	51,51,51,51	0
56	MG	2a	1777	1/1	0.97	0.12	-	66,66,66,66	0
56	MG	2a	1680	1/1	0.93	0.65	-	58,58,58,58	0
56	MG	1A	3124	1/1	0.88	0.19	-	40,40,40,40	0
56	MG	2a	1769	1/1	0.80	0.12	-	73,73,73,73	0
56	MG	2A	3513	1/1	0.96	0.19	-	52,52,52,52	0
56	MG	2A	3451	1/1	0.83	0.12	-	53,53,53,53	0
56	MG	2a	1720	1/1	0.83	0.16	-	57,57,57,57	0
56	MG	1A	3417	1/1	0.98	0.12	-	34,34,34,34	0
56	MG	1a	1855	1/1	0.90	0.58	-	52,52,52,52	0
56	MG	1A	3546	1/1	0.88	0.08	-	41,41,41,41	0
56	MG	1A	3440	1/1	0.96	0.16	-	23,23,23,23	0
56	MG	1A	3398	1/1	0.98	0.05	-	33,33,33,33	0
56	MG	1a	1654	1/1	0.96	0.29	-	71,71,71,71	0
56	MG	1A	3131	1/1	0.97	0.25	-	35,35,35,35	0
56	MG	2A	3343	1/1	0.92	0.11	-	58,58,58,58	0
56	MG	2A	3676	1/1	0.91	0.20	-	54,54,54,54	0
56	MG	1B	223	1/1	0.96	0.17	-	43,43,43,43	0
56	MG	2A	3004	1/1	0.95	0.12	-	52,52,52,52	0
56	MG	2A	3666	1/1	0.88	0.20	-	54,54,54,54	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	2A	3371	1/1	0.97	0.08	-	50,50,50,50	0
56	MG	2A	3166	1/1	0.95	0.32	-	49,49,49,49	0
56	MG	1N	203	1/1	0.91	0.12	-	59,59,59,59	0
56	MG	2A	3108	1/1	0.75	0.22	-	72,72,72,72	0
56	MG	1A	3761	1/1	0.94	0.07	-	45,45,45,45	0
56	MG	1A	3011	1/1	0.94	0.11	-	37,37,37,37	0
56	MG	1A	3258	1/1	0.61	0.15	-	71,71,71,71	0
56	MG	2A	3155	1/1	0.88	0.32	-	46,46,46,46	0
56	MG	1d	504	1/1	0.87	0.10	-	82,82,82,82	0
56	MG	2A	3378	1/1	0.96	0.14	-	50,50,50,50	0
56	MG	1A	3247	1/1	0.89	0.24	-	36,36,36,36	0
56	MG	20	8001	1/1	0.95	0.10	-	60,60,60,60	0
56	MG	1O	8001	1/1	0.97	0.09	-	44,44,44,44	0
56	MG	2A	3462	1/1	0.92	0.23	-	66,66,66,66	0
56	MG	2D	304	1/1	0.98	0.72	-	44,44,44,44	0
56	MG	1A	3700	1/1	0.93	0.18	-	35,35,35,35	0
56	MG	1a	1717	1/1	0.91	0.21	-	67,67,67,67	0
56	MG	1A	3564	1/1	0.84	0.16	-	35,35,35,35	0
56	MG	1A	3843	1/1	0.94	0.12	-	29,29,29,29	0
56	MG	1a	1848	1/1	0.92	0.10	-	69,69,69,69	0
56	MG	2a	1667	1/1	0.92	0.13	-	66,66,66,66	0
56	MG	2A	3506	1/1	0.95	0.32	-	61,61,61,61	0
56	MG	1A	3153	1/1	0.87	0.45	-	49,49,49,49	0
56	MG	2a	1753	1/1	0.92	0.14	-	58,58,58,58	0
56	MG	1A	3526	1/1	0.94	0.16	-	36,36,36,36	0
56	MG	1A	3815	1/1	0.79	0.13	-	27,27,27,27	0
56	MG	1A	3327	1/1	0.98	0.06	-	46,46,46,46	0
56	MG	2A	3536	1/1	0.90	0.11	-	57,57,57,57	0
56	MG	1A	3236	1/1	0.93	0.70	-	47,47,47,47	0
56	MG	2A	3305	1/1	0.97	0.13	-	57,57,57,57	0
56	MG	1a	1790	1/1	0.72	0.11	-	59,59,59,59	0
56	MG	1a	1788	1/1	0.81	0.10	-	67,67,67,67	0
56	MG	2A	3230	1/1	0.90	0.26	-	55,55,55,55	0
56	MG	1A	3158	1/1	0.85	0.33	-	42,42,42,42	0
56	MG	2A	3582	1/1	0.97	0.10	-	60,60,60,60	0
56	MG	1A	3583	1/1	0.78	0.13	-	65,65,65,65	0
56	MG	1A	3347	1/1	0.89	0.12	-	30,30,30,30	0
56	MG	1A	3762	1/1	0.94	0.11	-	45,45,45,45	0
56	MG	2A	3500	1/1	0.85	0.18	-	51,51,51,51	0
56	MG	1A	3486	1/1	0.94	0.18	-	46,46,46,46	0
56	MG	1a	1650	1/1	0.96	0.68	-	51,51,51,51	0
56	MG	1A	3240	1/1	0.99	0.12	-	41,41,41,41	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	1a	1768	1/1	0.82	0.12	-	68,68,68,68	0
56	MG	1A	3077	1/1	0.93	0.53	-	41,41,41,41	0
56	MG	1A	3268	1/1	0.86	0.28	-	40,40,40,40	0
56	MG	2A	3629	1/1	0.96	0.08	-	57,57,57,57	0
56	MG	1A	3909	1/1	0.95	0.57	-	43,43,43,43	0
56	MG	2a	1650	1/1	0.88	0.40	-	61,61,61,61	0
56	MG	1A	3105	1/1	0.90	0.48	-	42,42,42,42	0
56	MG	2A	3281	1/1	0.98	0.10	-	52,52,52,52	0
56	MG	2A	3567	1/1	0.86	0.12	-	69,69,69,69	0
56	MG	1A	3012	1/1	0.90	0.20	-	35,35,35,35	0
56	MG	1A	3133	1/1	0.82	0.32	-	35,35,35,35	0
56	MG	1A	3750	1/1	0.92	0.11	-	44,44,44,44	0
56	MG	1B	203	1/1	0.91	0.14	-	55,55,55,55	0
56	MG	1a	1744	1/1	0.90	0.13	-	62,62,62,62	0
56	MG	1A	3097	1/1	0.99	0.48	-	34,34,34,34	0
56	MG	1A	3025	1/1	0.79	0.26	-	55,55,55,55	0
56	MG	2A	3547	1/1	0.92	0.07	-	55,55,55,55	0
56	MG	2a	1693	1/1	0.95	0.54	-	63,63,63,63	0
56	MG	1a	1696	1/1	0.93	0.36	-	58,58,58,58	0
56	MG	1A	3064	1/1	0.91	0.31	-	46,46,46,46	0
56	MG	1A	3199	1/1	0.96	0.34	-	37,37,37,37	0
56	MG	1A	3927	1/1	0.74	0.37	-	50,50,50,50	0
56	MG	2A	3348	1/1	0.72	0.21	-	41,41,41,41	0
56	MG	2A	3042	1/1	0.91	0.11	-	57,57,57,57	0
56	MG	1A	3052	1/1	0.98	0.12	-	28,28,28,28	0
56	MG	1A	3167	1/1	0.96	0.15	-	50,50,50,50	0
56	MG	1A	3392	1/1	0.94	0.09	-	57,57,57,57	0
56	MG	2A	3538	1/1	0.93	0.09	-	56,56,56,56	0
56	MG	1a	1715	1/1	0.98	0.18	-	59,59,59,59	0
56	MG	2A	3278	1/1	0.97	0.14	-	61,61,61,61	0
56	MG	1a	1601	1/1	0.88	0.45	-	50,50,50,50	0
56	MG	2a	1726	1/1	0.92	0.10	-	70,70,70,70	0
56	MG	1a	1760	1/1	0.60	0.67	-	65,65,65,65	0
56	MG	2A	3460	1/1	0.95	0.07	-	46,46,46,46	0
56	MG	1a	1725	1/1	0.88	0.34	-	59,59,59,59	0
56	MG	1A	3223	1/1	0.93	0.16	-	46,46,46,46	0
56	MG	1A	3287	1/1	0.96	0.33	-	41,41,41,41	0
56	MG	1A	3633	1/1	0.88	0.59	-	31,31,31,31	0
56	MG	1A	3859	1/1	0.95	0.09	-	35,35,35,35	0
56	MG	1A	3029	1/1	0.90	0.19	-	30,30,30,30	0
56	MG	1A	3384	1/1	0.96	0.12	-	30,30,30,30	0
56	MG	1A	3154	1/1	0.95	0.20	-	45,45,45,45	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	2A	3250	1/1	0.82	0.20	-	48,48,48,48	0
56	MG	1a	1771	1/1	0.84	0.14	-	71,71,71,71	0
56	MG	1A	3407	1/1	0.98	0.08	-	47,47,47,47	0
56	MG	2A	3288	1/1	0.93	0.21	-	41,41,41,41	0
56	MG	1A	3631	1/1	0.84	0.43	-	43,43,43,43	0
56	MG	2A	3620	1/1	0.97	0.11	-	44,44,44,44	0
56	MG	2a	1604	1/1	0.86	0.43	-	72,72,72,72	0
56	MG	1A	3730	1/1	0.88	0.85	-	40,40,40,40	0
56	MG	2A	3146	1/1	0.94	0.56	-	55,55,55,55	0
56	MG	2A	3053	1/1	0.96	0.44	-	58,58,58,58	0
56	MG	1A	3555	1/1	0.86	0.60	-	38,38,38,38	0
56	MG	1A	3590	1/1	0.97	0.20	-	47,47,47,47	0
56	MG	2A	3541	1/1	0.83	0.15	-	49,49,49,49	0
56	MG	1A	3715	1/1	0.96	0.17	-	69,69,69,69	0
56	MG	1A	3738	1/1	0.89	0.53	-	36,36,36,36	0
56	MG	2a	1637	1/1	0.88	0.21	-	60,60,60,60	0
56	MG	2a	1725	1/1	0.98	0.06	-	63,63,63,63	0
56	MG	1U	205	1/1	0.90	0.41	-	40,40,40,40	0
56	MG	2A	3125	1/1	0.81	0.70	-	68,68,68,68	0
56	MG	1A	3262	1/1	0.92	0.24	-	42,42,42,42	0
56	MG	1A	3941	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	2A	3401	1/1	0.91	0.08	-	56,56,56,56	0
56	MG	1a	1712	1/1	0.93	0.20	-	70,70,70,70	0
56	MG	2A	3068	1/1	0.92	0.55	-	51,51,51,51	0
56	MG	2A	3355	1/1	0.89	0.39	-	53,53,53,53	0
56	MG	1A	3200	1/1	0.96	0.08	-	46,46,46,46	0
56	MG	2A	3075	1/1	0.92	0.36	-	42,42,42,42	0
56	MG	1A	3470	1/1	0.81	0.11	-	37,37,37,37	0
56	MG	2A	3195	1/1	0.96	0.41	-	43,43,43,43	0
56	MG	1A	3089	1/1	0.79	0.57	-	41,41,41,41	0
56	MG	2A	3607	1/1	0.95	0.08	-	66,66,66,66	0
56	MG	1A	3508	1/1	0.89	0.09	-	53,53,53,53	0
56	MG	1A	3053	1/1	0.88	0.81	-	34,34,34,34	0
56	MG	1A	3749	1/1	0.92	0.11	-	45,45,45,45	0
56	MG	2Q	202	1/1	0.98	0.23	-	61,61,61,61	0
56	MG	1A	3685	1/1	0.92	0.13	-	42,42,42,42	0
56	MG	2a	1766	1/1	0.82	0.21	-	70,70,70,70	0
56	MG	2I	101	1/1	0.93	0.15	-	54,54,54,54	0
56	MG	1A	3706	1/1	0.95	0.13	-	36,36,36,36	0
56	MG	2A	3320	1/1	0.92	0.10	-	56,56,56,56	0
56	MG	2A	3591	1/1	0.97	0.16	-	68,68,68,68	0
56	MG	1A	3156	1/1	0.92	0.21	-	41,41,41,41	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	2x	102	1/1	0.82	0.08	-	73,73,73,73	0
56	MG	1B	212	1/1	0.96	0.05	-	40,40,40,40	0
56	MG	2A	3174	1/1	0.79	0.32	-	55,55,55,55	0
56	MG	1A	3018	1/1	0.99	0.15	-	33,33,33,33	0
56	MG	2A	3202	1/1	0.94	0.63	-	52,52,52,52	0
56	MG	2A	3102	1/1	0.91	0.15	-	48,48,48,48	0
56	MG	1A	3113	1/1	0.95	0.36	-	35,35,35,35	0
56	MG	2A	3088	1/1	0.84	0.26	-	60,60,60,60	0
56	MG	2A	3492	1/1	0.99	0.25	-	45,45,45,45	0
56	MG	2A	3165	1/1	0.84	0.41	-	47,47,47,47	0
56	MG	2A	3419	1/1	0.96	0.57	-	44,44,44,44	0
56	MG	1a	1694	1/1	0.90	0.20	-	64,64,64,64	0
56	MG	1A	3176	1/1	0.91	1.02	-	33,33,33,33	0
56	MG	1A	3180	1/1	0.96	0.16	-	51,51,51,51	0
56	MG	1A	3780	1/1	0.93	0.09	-	44,44,44,44	0
56	MG	1A	3050	1/1	0.95	0.43	-	36,36,36,36	0
56	MG	1A	3863	1/1	0.97	0.10	-	29,29,29,29	0
56	MG	2A	3048	1/1	0.93	0.30	-	51,51,51,51	0
56	MG	2a	1779	1/1	0.91	0.21	-	67,67,67,67	0
56	MG	2A	3597	1/1	0.97	0.07	-	52,52,52,52	0
56	MG	2A	3112	1/1	0.97	0.47	-	56,56,56,56	0
56	MG	1A	3647	1/1	0.93	0.11	-	28,28,28,28	0
56	MG	2a	1740	1/1	0.95	0.07	-	73,73,73,73	0
56	MG	2A	3507	1/1	0.88	0.20	-	72,72,72,72	0
56	MG	2A	3283	1/1	0.89	0.10	-	56,56,56,56	0
56	MG	2X	101	1/1	0.81	0.12	-	61,61,61,61	0
56	MG	1a	1837	1/1	0.94	0.16	-	57,57,57,57	0
56	MG	1a	1854	1/1	0.73	0.14	-	72,72,72,72	0
56	MG	2A	3599	1/1	0.81	0.12	-	59,59,59,59	0
56	MG	2A	3335	1/1	0.86	0.18	-	63,63,63,63	0
56	MG	1A	3217	1/1	0.95	0.73	-	33,33,33,33	0
56	MG	2a	1679	1/1	0.86	0.41	-	62,62,62,62	0
56	MG	2A	3200	1/1	0.91	0.19	-	52,52,52,52	0
56	MG	2A	3231	1/1	0.92	0.10	-	64,64,64,64	0
56	MG	1A	3616	1/1	0.68	0.11	-	67,67,67,67	0
56	MG	1A	3694	1/1	0.93	0.07	-	39,39,39,39	0
56	MG	2a	1643	1/1	0.83	0.28	-	67,67,67,67	0
56	MG	1A	3194	1/1	0.82	0.16	-	40,40,40,40	0
56	MG	1A	3588	1/1	0.93	0.12	-	33,33,33,33	0
56	MG	2A	3397	1/1	0.91	0.20	-	48,48,48,48	0
56	MG	2A	3677	1/1	0.90	0.20	-	57,57,57,57	0
56	MG	1A	3820	1/1	0.87	0.48	-	33,33,33,33	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	1A	3322	1/1	0.92	0.08	-	68,68,68,68	0
56	MG	1A	3559	1/1	0.97	0.15	-	39,39,39,39	0
56	MG	1a	1762	1/1	0.94	0.16	-	71,71,71,71	0
56	MG	1A	3671	1/1	0.95	0.06	-	62,62,62,62	0
56	MG	2E	303	1/1	0.97	0.17	-	51,51,51,51	0
56	MG	2A	3128	1/1	0.95	0.18	-	51,51,51,51	0
56	MG	2a	1731	1/1	0.89	0.08	-	69,69,69,69	0
56	MG	2A	3381	1/1	0.87	0.36	-	53,53,53,53	0
56	MG	1a	1699	1/1	0.90	0.11	-	68,68,68,68	0
56	MG	2A	3040	1/1	0.98	0.47	-	42,42,42,42	0
56	MG	2A	3240	1/1	0.76	0.31	-	60,60,60,60	0
56	MG	1A	3009	1/1	0.93	0.22	-	27,27,27,27	0
56	MG	1a	1755	1/1	0.88	0.32	-	68,68,68,68	0
56	MG	1A	3015	1/1	0.94	0.31	-	37,37,37,37	0
56	MG	2a	1781	1/1	0.97	0.44	-	50,50,50,50	0
56	MG	1A	3603	1/1	0.95	0.12	-	48,48,48,48	0
56	MG	1A	3447	1/1	0.98	0.12	-	34,34,34,34	0
56	MG	1A	3435	1/1	0.79	0.23	-	35,35,35,35	0
56	MG	1B	226	1/1	0.88	0.18	-	48,48,48,48	0
56	MG	1A	3521	1/1	0.93	0.11	-	44,44,44,44	0
56	MG	1A	3661	1/1	0.89	0.30	-	40,40,40,40	0
56	MG	2A	3060	1/1	0.95	0.20	-	48,48,48,48	0
56	MG	1A	3500	1/1	0.85	0.35	-	39,39,39,39	0
56	MG	1A	3353	1/1	0.96	0.09	-	43,43,43,43	0
56	MG	1a	1853	1/1	0.95	0.08	-	66,66,66,66	0
56	MG	1A	3232	1/1	0.96	0.10	-	56,56,56,56	0
56	MG	2A	3217	1/1	0.85	0.33	-	53,53,53,53	0
56	MG	2A	3623	1/1	0.81	0.12	-	51,51,51,51	0
56	MG	1A	3744	1/1	0.85	0.16	-	46,46,46,46	0
56	MG	1A	3653	1/1	0.94	0.13	-	47,47,47,47	0
56	MG	2a	1660	1/1	0.94	0.33	-	81,81,81,81	0
56	MG	1A	3866	1/1	0.94	0.26	-	36,36,36,36	0
56	MG	1A	3476	1/1	0.97	0.04	-	38,38,38,38	0
56	MG	2A	3573	1/1	0.99	0.20	-	59,59,59,59	0
56	MG	1A	3827	1/1	0.90	0.07	-	47,47,47,47	0
56	MG	1A	3102	1/1	0.93	0.33	-	31,31,31,31	0
56	MG	2a	1745	1/1	0.86	0.14	-	71,71,71,71	0
56	MG	1A	3777	1/1	0.94	0.35	-	39,39,39,39	0
56	MG	1A	3065	1/1	0.93	0.26	-	37,37,37,37	0
56	MG	1a	1824	1/1	0.97	0.24	-	54,54,54,54	0
56	MG	1A	3250	1/1	0.94	0.34	-	48,48,48,48	0
56	MG	1a	1626	1/1	0.92	0.11	-	60,60,60,60	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	1A	3890	1/1	0.84	0.47	-	32,32,32,32	0
56	MG	1A	3850	1/1	0.91	0.19	-	44,44,44,44	0
56	MG	2A	3350	1/1	0.95	0.20	-	65,65,65,65	0
56	MG	1a	1806	1/1	0.96	0.28	-	68,68,68,68	0
56	MG	2a	1752	1/1	0.81	0.19	-	64,64,64,64	0
56	MG	2A	3467	1/1	0.97	0.24	-	62,62,62,62	0
56	MG	1A	3401	1/1	0.95	0.13	-	56,56,56,56	0
56	MG	1A	3548	1/1	0.96	0.19	-	47,47,47,47	0
56	MG	2A	3383	1/1	0.83	0.41	-	57,57,57,57	0
56	MG	1A	3304	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	1A	3244	1/1	0.81	0.24	-	31,31,31,31	0
56	MG	2A	3584	1/1	0.77	0.19	-	64,64,64,64	0
56	MG	1A	3635	1/1	0.95	0.09	-	35,35,35,35	0
56	MG	1A	3888	1/1	0.91	1.04	-	32,32,32,32	0
56	MG	1A	3728	1/1	0.92	0.15	-	38,38,38,38	0
56	MG	1A	3678	1/1	0.95	0.09	-	44,44,44,44	0
56	MG	1a	1814	1/1	0.83	0.19	-	64,64,64,64	0
56	MG	1A	3871	1/1	0.88	0.15	-	43,43,43,43	0
56	MG	2A	3375	1/1	0.96	0.17	-	50,50,50,50	0
56	MG	2a	1778	1/1	0.89	0.17	-	77,77,77,77	0
56	MG	1A	3290	1/1	0.94	0.11	-	34,34,34,34	0
56	MG	1A	3010	1/1	0.91	0.29	-	45,45,45,45	0
56	MG	1A	3178	1/1	0.94	0.34	-	37,37,37,37	0
56	MG	1A	3498	1/1	0.98	0.06	-	56,56,56,56	0
56	MG	2a	1759	1/1	0.81	0.14	-	78,78,78,78	0
56	MG	2B	3006	1/1	0.94	0.45	-	69,69,69,69	0
56	MG	1a	1810	1/1	0.86	0.23	-	74,74,74,74	0
56	MG	2A	3119	1/1	0.94	0.20	-	49,49,49,49	0
56	MG	10	104	1/1	0.96	0.15	-	47,47,47,47	0
56	MG	1A	3696	1/1	0.79	0.10	-	40,40,40,40	0
56	MG	1A	3770	1/1	0.90	0.07	-	50,50,50,50	0
56	MG	2A	3430	1/1	0.93	0.07	-	56,56,56,56	0
56	MG	2O	202	1/1	0.84	0.13	-	63,63,63,63	0
56	MG	2A	3576	1/1	0.94	0.11	-	70,70,70,70	0
56	MG	1A	3402	1/1	0.98	0.05	-	36,36,36,36	0
56	MG	2a	1758	1/1	0.84	0.14	-	66,66,66,66	0
56	MG	1A	3382	1/1	0.90	0.15	-	30,30,30,30	0
56	MG	2B	3008	1/1	0.98	0.27	-	64,64,64,64	0
56	MG	1A	3882	1/1	0.96	0.12	-	57,57,57,57	0
56	MG	1A	3283	1/1	0.89	0.15	-	32,32,32,32	0
56	MG	1A	3705	1/1	0.86	0.16	-	45,45,45,45	0
56	MG	1A	3277	1/1	0.69	0.66	-	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	1a	1834	1/1	0.95	0.12	-	57,57,57,57	0
56	MG	2A	3044	1/1	0.94	0.17	-	61,61,61,61	0
56	MG	2A	3562	1/1	0.95	0.10	-	43,43,43,43	0
56	MG	1A	3560	1/1	0.94	0.30	-	35,35,35,35	0
56	MG	2A	3339	1/1	0.86	0.09	-	65,65,65,65	0
56	MG	1A	3687	1/1	0.94	0.11	-	46,46,46,46	0
56	MG	1A	3880	1/1	0.93	0.24	-	35,35,35,35	0
56	MG	1A	3760	1/1	0.90	0.19	-	58,58,58,58	0
56	MG	1a	1833	1/1	0.94	0.09	-	73,73,73,73	0
56	MG	2A	3405	1/1	0.95	0.09	-	66,66,66,66	0
56	MG	2A	3223	1/1	0.85	0.56	-	60,60,60,60	0
56	MG	2x	109	1/1	0.87	0.15	-	69,69,69,69	0
56	MG	1A	3272	1/1	0.88	0.15	-	52,52,52,52	0
56	MG	2B	3005	1/1	0.90	0.47	-	77,77,77,77	0
56	MG	2A	3609	1/1	0.95	0.13	-	58,58,58,58	0
56	MG	1U	202	1/1	0.94	0.43	-	42,42,42,42	0
56	MG	2A	3143	1/1	0.79	0.27	-	56,56,56,56	0
56	MG	1A	3143	1/1	0.88	0.08	-	63,63,63,63	0
56	MG	1A	3117	1/1	0.98	0.30	-	45,45,45,45	0
56	MG	2A	3434	1/1	0.90	0.21	-	58,58,58,58	0
56	MG	1A	3175	1/1	0.57	0.19	-	57,57,57,57	0
56	MG	1A	3061	1/1	0.91	0.18	-	43,43,43,43	0
56	MG	2A	3634	1/1	0.97	0.14	-	48,48,48,48	0
56	MG	1x	105	1/1	0.92	0.17	-	64,64,64,64	0
56	MG	2a	1755	1/1	0.89	0.10	-	72,72,72,72	0
56	MG	1B	219	1/1	0.91	0.08	-	42,42,42,42	0
56	MG	1A	3674	1/1	0.89	0.16	-	39,39,39,39	0
56	MG	1a	1724	1/1	0.83	0.39	-	78,78,78,78	0
56	MG	1A	3904	1/1	0.90	0.18	-	53,53,53,53	0
56	MG	2A	3458	1/1	0.94	0.26	-	42,42,42,42	0
56	MG	2A	3009	1/1	0.71	0.52	-	59,59,59,59	0
56	MG	1A	3379	1/1	0.89	0.16	-	43,43,43,43	0
56	MG	1a	1647	1/1	0.82	0.43	-	66,66,66,66	0
56	MG	1A	3709	1/1	0.91	0.18	-	37,37,37,37	0
56	MG	2a	1615	1/1	0.90	0.13	-	63,63,63,63	0
56	MG	2A	3680	1/1	0.98	0.05	-	65,65,65,65	0
56	MG	1a	1781	1/1	0.87	0.35	-	58,58,58,58	0
56	MG	2B	3007	1/1	0.94	0.22	-	63,63,63,63	0
56	MG	1A	3757	1/1	0.95	0.12	-	38,38,38,38	0
56	MG	2A	3156	1/1	0.57	0.27	-	58,58,58,58	0
56	MG	1a	1827	1/1	0.81	0.34	-	77,77,77,77	0
56	MG	1a	1758	1/1	0.90	0.18	-	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	2F	302	1/1	0.88	0.19	-	47,47,47,47	0
56	MG	1A	3831	1/1	0.86	0.10	-	58,58,58,58	0
56	MG	2A	3581	1/1	0.92	0.18	-	67,67,67,67	0
56	MG	1A	3501	1/1	0.78	0.11	-	43,43,43,43	0
56	MG	2a	1654	1/1	0.85	0.47	-	62,62,62,62	0
56	MG	1A	3208	1/1	0.90	0.23	-	45,45,45,45	0
56	MG	2A	3431	1/1	0.67	0.25	-	61,61,61,61	0
56	MG	1A	3778	1/1	0.87	0.22	-	53,53,53,53	0
56	MG	1A	3043	1/1	0.89	0.61	-	29,29,29,29	0
56	MG	2x	110	1/1	0.86	0.11	-	70,70,70,70	0
56	MG	2A	3443	1/1	0.96	0.27	-	53,53,53,53	0
56	MG	2A	3294	1/1	0.78	0.14	-	50,50,50,50	0
56	MG	1D	319	1/1	0.89	0.15	-	66,66,66,66	0
56	MG	1A	3895	1/1	0.93	0.18	-	35,35,35,35	0
56	MG	2A	3445	1/1	0.89	0.27	-	61,61,61,61	0
56	MG	1A	3847	1/1	0.87	0.13	-	46,46,46,46	0
56	MG	1A	3503	1/1	0.98	0.10	-	38,38,38,38	0
56	MG	1A	3079	1/1	0.92	0.22	-	39,39,39,39	0
56	MG	1A	3518	1/1	0.92	0.18	-	37,37,37,37	0
56	MG	2A	3065	1/1	0.93	0.23	-	47,47,47,47	0
56	MG	2A	3123	1/1	0.91	0.30	-	69,69,69,69	0
56	MG	2A	3085	1/1	0.93	0.30	-	62,62,62,62	0
56	MG	1A	3003	1/1	0.91	0.18	-	40,40,40,40	0
56	MG	1A	3267	1/1	0.86	0.34	-	52,52,52,52	0
56	MG	2A	3361	1/1	0.96	0.17	-	60,60,60,60	0
56	MG	1A	3793	1/1	0.86	0.17	-	37,37,37,37	0
56	MG	2A	3078	1/1	0.56	0.19	-	67,67,67,67	0
56	MG	1Y	502	1/1	0.96	0.12	-	56,56,56,56	0
56	MG	1A	3246	1/1	0.72	0.24	-	59,59,59,59	0
56	MG	2A	3454	1/1	0.93	0.12	-	60,60,60,60	0
56	MG	2A	3337	1/1	0.94	0.07	-	60,60,60,60	0
56	MG	2a	1668	1/1	0.53	0.59	-	60,60,60,60	0
56	MG	2A	3136	1/1	0.84	0.22	-	54,54,54,54	0
56	MG	2A	3111	1/1	0.95	0.45	-	48,48,48,48	0
56	MG	2A	3319	1/1	0.85	0.12	-	51,51,51,51	0
56	MG	2a	1629	1/1	0.95	0.10	-	78,78,78,78	0
56	MG	1A	3528	1/1	0.98	0.17	-	45,45,45,45	0
56	MG	1A	3751	1/1	0.72	0.25	-	43,43,43,43	0
56	MG	1A	3241	1/1	0.83	0.51	-	30,30,30,30	0
56	MG	1A	3495	1/1	0.84	0.25	-	37,37,37,37	0
56	MG	2a	1697	1/1	0.96	0.15	-	65,65,65,65	0
56	MG	2a	1732	1/1	0.93	0.10	-	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	2B	3010	1/1	0.86	0.21	-	69,69,69,69	0
56	MG	1A	3660	1/1	0.71	0.14	-	38,38,38,38	0
56	MG	1a	1651	1/1	0.79	0.28	-	52,52,52,52	0
56	MG	1A	3932	1/1	0.92	0.26	-	51,51,51,51	0
56	MG	2A	3023	1/1	0.91	0.17	-	53,53,53,53	0
56	MG	1A	3191	1/1	0.86	0.28	-	40,40,40,40	0
56	MG	1A	3438	1/1	0.97	0.07	-	46,46,46,46	0
56	MG	1A	3145	1/1	0.95	0.17	-	38,38,38,38	0
56	MG	2A	3646	1/1	0.88	0.15	-	66,66,66,66	0
56	MG	1A	3775	1/1	0.94	0.13	-	36,36,36,36	0
56	MG	1W	3002	1/1	0.94	0.20	-	41,41,41,41	0
56	MG	1A	3183	1/1	0.83	0.46	-	42,42,42,42	0
56	MG	1A	3768	1/1	0.86	0.22	-	27,27,27,27	0
56	MG	2a	1649	1/1	0.76	0.24	-	68,68,68,68	0
56	MG	1A	3008	1/1	0.83	0.32	-	47,47,47,47	0
56	MG	1A	3344	1/1	0.91	0.10	-	31,31,31,31	0
56	MG	1A	3449	1/1	0.92	0.09	-	53,53,53,53	0
56	MG	2A	3311	1/1	0.57	0.20	-	45,45,45,45	0
56	MG	1a	1682	1/1	0.64	0.47	-	55,55,55,55	0
56	MG	2A	3423	1/1	0.89	0.09	-	56,56,56,56	0
56	MG	2A	3456	1/1	0.93	0.20	-	63,63,63,63	0
56	MG	2A	3333	1/1	0.90	0.32	-	58,58,58,58	0
56	MG	1D	311	1/1	0.86	0.25	-	47,47,47,47	0
56	MG	2A	3346	1/1	0.96	0.25	-	60,60,60,60	0
56	MG	1A	3464	1/1	0.80	0.17	-	26,26,26,26	0
56	MG	1a	1629	1/1	0.73	0.33	-	54,54,54,54	0
56	MG	13	103	1/1	0.87	0.79	-	42,42,42,42	0
56	MG	1a	1613	1/1	0.89	0.14	-	75,75,75,75	0
56	MG	1A	3427	1/1	0.95	0.05	-	53,53,53,53	0
56	MG	1a	1688	1/1	0.82	0.45	-	58,58,58,58	0
56	MG	1A	3114	1/1	0.96	0.34	-	34,34,34,34	0
56	MG	1A	3665	1/1	0.93	0.07	-	46,46,46,46	0
56	MG	1A	3853	1/1	0.98	0.08	-	43,43,43,43	0
56	MG	2a	1706	1/1	0.98	0.09	-	56,56,56,56	0
56	MG	2A	3543	1/1	0.98	0.11	-	45,45,45,45	0
56	MG	1A	3625	1/1	0.97	0.24	-	36,36,36,36	0
56	MG	1A	3765	1/1	0.95	0.17	-	54,54,54,54	0
56	MG	1A	3278	1/1	0.84	0.12	-	28,28,28,28	0
56	MG	1a	1749	1/1	0.96	0.06	-	59,59,59,59	0
56	MG	2A	3565	1/1	0.80	0.22	-	48,48,48,48	0
56	MG	2a	1713	1/1	0.81	0.12	-	67,67,67,67	0
56	MG	2a	1734	1/1	0.91	0.23	-	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	2A	3095	1/1	0.96	0.24	-	47,47,47,47	0
56	MG	1A	3622	1/1	0.93	0.12	-	56,56,56,56	0
56	MG	2A	3170	1/1	0.85	0.34	-	52,52,52,52	0
56	MG	1Q	204	1/1	0.93	0.16	-	44,44,44,44	0
56	MG	1A	3185	1/1	0.74	0.58	-	42,42,42,42	0
56	MG	2A	3558	1/1	0.83	0.26	-	50,50,50,50	0
56	MG	2A	3612	1/1	0.93	0.09	-	51,51,51,51	0
56	MG	2A	3382	1/1	0.95	0.22	-	56,56,56,56	0
56	MG	1A	3561	1/1	0.96	0.13	-	54,54,54,54	0
56	MG	1a	1839	1/1	0.85	0.19	-	63,63,63,63	0
56	MG	1a	1670	1/1	0.78	0.14	-	59,59,59,59	0
56	MG	1a	1720	1/1	0.98	0.09	-	52,52,52,52	0
56	MG	1a	1807	1/1	0.94	0.14	-	56,56,56,56	0
56	MG	2B	3013	1/1	0.83	0.14	-	72,72,72,72	0
56	MG	1A	3856	1/1	0.98	0.15	-	46,46,46,46	0
56	MG	1A	3846	1/1	0.94	0.17	-	31,31,31,31	0
56	MG	1A	3373	1/1	0.97	0.10	-	60,60,60,60	0
56	MG	1A	3641	1/1	0.92	0.15	-	40,40,40,40	0
56	MG	2a	1647	1/1	0.92	0.12	-	73,73,73,73	0
56	MG	1a	1627	1/1	0.89	0.19	-	57,57,57,57	0
56	MG	1a	1669	1/1	0.91	0.34	-	57,57,57,57	0
56	MG	2A	3316	1/1	0.87	0.30	-	67,67,67,67	0
56	MG	2A	3366	1/1	0.87	0.18	-	44,44,44,44	0
56	MG	1a	1813	1/1	0.74	0.11	-	72,72,72,72	0
56	MG	2A	3062	1/1	0.89	0.49	-	44,44,44,44	0
56	MG	1B	202	1/1	0.87	0.19	-	61,61,61,61	0
56	MG	1A	3340	1/1	0.89	0.21	-	53,53,53,53	0
56	MG	1A	3883	1/1	0.89	0.23	-	47,47,47,47	0
56	MG	2A	3413	1/1	0.95	0.28	-	62,62,62,62	0
56	MG	1A	3055	1/1	0.98	0.38	-	37,37,37,37	0
56	MG	1A	3063	1/1	0.95	0.22	-	37,37,37,37	0
56	MG	2A	3208	1/1	0.92	0.24	-	50,50,50,50	0
56	MG	1A	3874	1/1	0.94	0.19	-	47,47,47,47	0
56	MG	1A	3912	1/1	0.97	0.07	-	54,54,54,54	0
56	MG	2a	1613	1/1	0.97	0.40	-	61,61,61,61	0
56	MG	2a	1682	1/1	0.92	0.28	-	58,58,58,58	0
56	MG	1A	3231	1/1	0.97	0.15	-	36,36,36,36	0
56	MG	1A	3902	1/1	0.89	0.59	-	35,35,35,35	0
56	MG	1A	3544	1/1	0.94	0.15	-	59,59,59,59	0
56	MG	2A	3641	1/1	0.78	0.11	-	61,61,61,61	0
56	MG	1A	3396	1/1	0.98	0.11	-	41,41,41,41	0
56	MG	2A	3473	1/1	0.96	0.10	-	57,57,57,57	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	2a	1605	1/1	0.90	0.08	-	73,73,73,73	0
56	MG	1B	206	1/1	0.87	0.16	-	49,49,49,49	0
56	MG	1A	3594	1/1	0.82	0.43	-	48,48,48,48	0
56	MG	2A	3518	1/1	0.75	0.14	-	63,63,63,63	0
56	MG	1A	3716	1/1	0.92	0.15	-	60,60,60,60	0
56	MG	1a	1673	1/1	0.94	0.17	-	53,53,53,53	0
56	MG	1A	3483	1/1	0.96	0.11	-	39,39,39,39	0
56	MG	1a	1820	1/1	0.95	0.31	-	63,63,63,63	0
56	MG	2a	1631	1/1	0.94	0.61	-	64,64,64,64	0
56	MG	1A	3867	1/1	0.95	0.13	-	52,52,52,52	0
56	MG	1a	1843	1/1	0.86	0.58	-	62,62,62,62	0
56	MG	1a	1828	1/1	0.81	0.28	-	60,60,60,60	0
56	MG	2A	3327	1/1	0.97	0.14	-	58,58,58,58	0
56	MG	2A	3476	1/1	0.91	0.17	-	57,57,57,57	0
56	MG	2A	3472	1/1	0.93	0.14	-	68,68,68,68	0
56	MG	2A	3624	1/1	0.96	0.09	-	48,48,48,48	0
56	MG	1A	3655	1/1	0.96	0.05	-	49,49,49,49	0
56	MG	1A	3547	1/1	0.93	0.09	-	38,38,38,38	0
56	MG	2a	1709	1/1	0.95	0.15	-	63,63,63,63	0
56	MG	1A	3529	1/1	0.98	0.12	-	44,44,44,44	0
56	MG	2A	3076	1/1	0.94	0.78	-	49,49,49,49	0
56	MG	2A	3626	1/1	0.86	0.16	-	49,49,49,49	0
56	MG	2l	201	1/1	0.83	0.17	-	71,71,71,71	0
56	MG	1A	3324	1/1	0.90	0.14	-	34,34,34,34	0
56	MG	1A	3790	1/1	0.81	0.13	-	32,32,32,32	0
56	MG	2A	3415	1/1	0.97	0.12	-	52,52,52,52	0
56	MG	1A	3722	1/1	0.83	0.07	-	36,36,36,36	0
56	MG	2A	3583	1/1	0.93	0.13	-	68,68,68,68	0
56	MG	2A	3377	1/1	0.92	0.10	-	49,49,49,49	0
56	MG	2A	3211	1/1	0.82	0.56	-	60,60,60,60	0
56	MG	2a	1733	1/1	0.86	0.13	-	75,75,75,75	0
56	MG	2A	3334	1/1	0.92	0.12	-	61,61,61,61	0
56	MG	1A	3365	1/1	0.95	0.16	-	43,43,43,43	0
56	MG	1A	3418	1/1	0.85	0.08	-	52,52,52,52	0
56	MG	2A	3233	1/1	0.73	0.52	-	49,49,49,49	0
56	MG	2A	3190	1/1	0.69	0.45	-	52,52,52,52	0
56	MG	2A	3219	1/1	0.93	0.26	-	45,45,45,45	0
56	MG	1A	3557	1/1	0.85	0.27	-	42,42,42,42	0
56	MG	2A	3001	1/1	0.85	0.29	-	60,60,60,60	0
56	MG	1a	1850	1/1	0.98	0.12	-	72,72,72,72	0
56	MG	2A	3555	1/1	0.86	0.11	-	59,59,59,59	0
56	MG	2A	3030	1/1	0.78	0.31	-	51,51,51,51	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	1A	3459	1/1	0.96	0.16	-	46,46,46,46	0
56	MG	1A	3849	1/1	0.86	0.21	-	60,60,60,60	0
56	MG	1A	3455	1/1	0.97	0.18	-	37,37,37,37	0
56	MG	1D	320	1/1	0.97	0.23	-	46,46,46,46	0
56	MG	1A	3766	1/1	0.93	0.29	-	42,42,42,42	0
56	MG	2A	3594	1/1	0.94	0.20	-	82,82,82,82	0
56	MG	1A	3507	1/1	0.79	0.57	-	52,52,52,52	0
56	MG	1A	3878	1/1	0.92	0.33	-	51,51,51,51	0
56	MG	2A	3301	1/1	0.82	0.13	-	52,52,52,52	0
56	MG	2A	3227	1/1	0.87	0.17	-	58,58,58,58	0
56	MG	1a	1817	1/1	0.85	0.27	-	72,72,72,72	0
56	MG	2A	3604	1/1	0.83	0.12	-	49,49,49,49	0
56	MG	1A	3825	1/1	0.82	0.07	-	46,46,46,46	0
56	MG	1A	3595	1/1	0.95	0.26	-	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.