



Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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

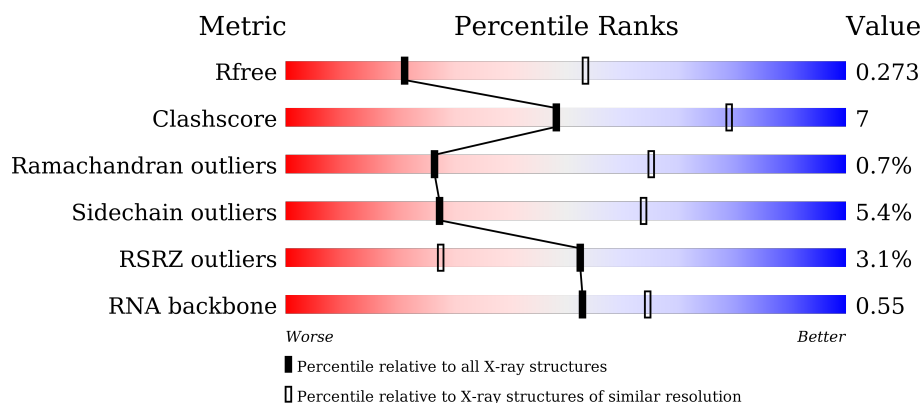
1 Overall quality at a glance

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.









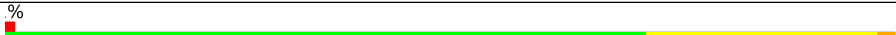
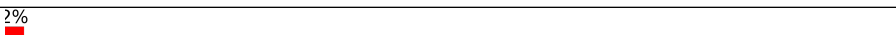
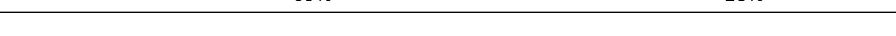
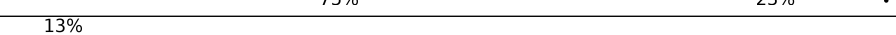
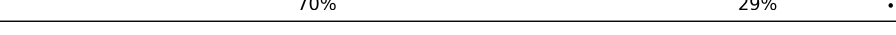
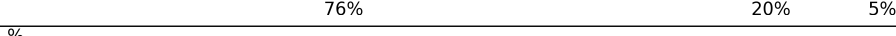













Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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% .





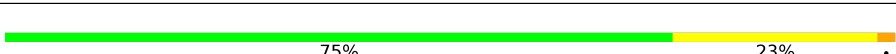
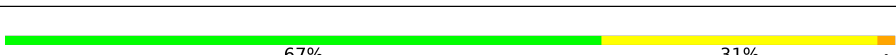
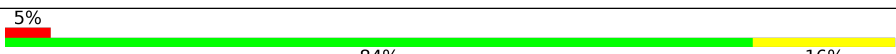
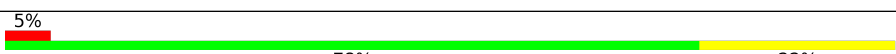
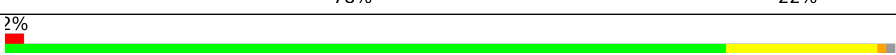

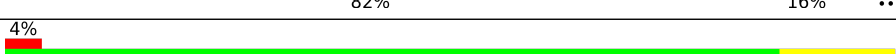
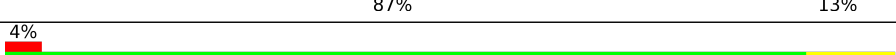
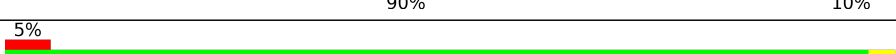
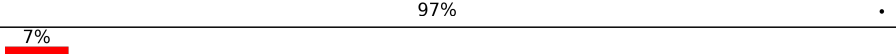
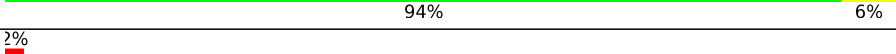
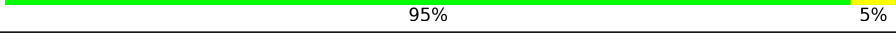
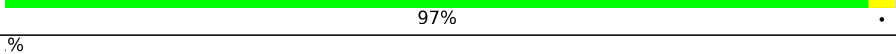
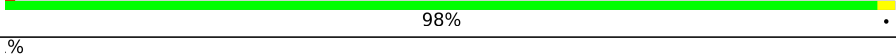
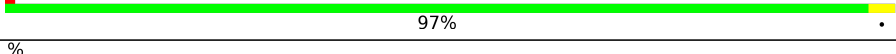
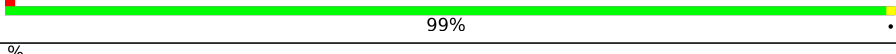
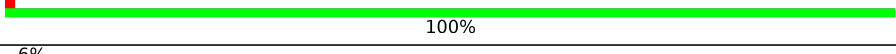
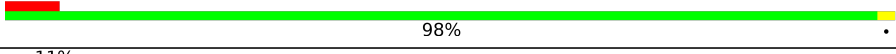
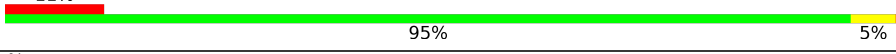
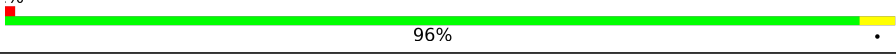
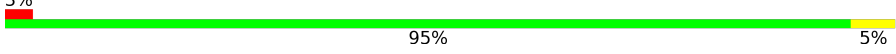
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	131	
16	1U	116	
16	2U	116	
17	1V	101	
17	2V	101	
18	1W	112	
18	2W	112	
19	1X	95	
19	2X	95	
20	1Y	107	
20	2Y	107	
21	1Z	203	
21	2Z	203	
22	10	77	
22	20	77	
23	11	97	
23	21	97	
24	12	70	
24	22	70	
25	13	59	
25	23	59	
26	14	69	
26	24	69	
27	15	59	
27	25	59	

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>
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>
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>
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>
47	1p	82	<div> <div>9%</div> <div>93%</div> <div>7%</div> </div>
47	2p	82	<div> <div>2%</div> <div>93%</div> <div>7%</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>
50	2s	83	<div> <div>24%</div> <div>94%</div> <div>6%</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	0	0	0
			1091	680	225	185			
15	2T	131	Total	C	N	O	0	0	0
			1083	675	224	183			

- 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...

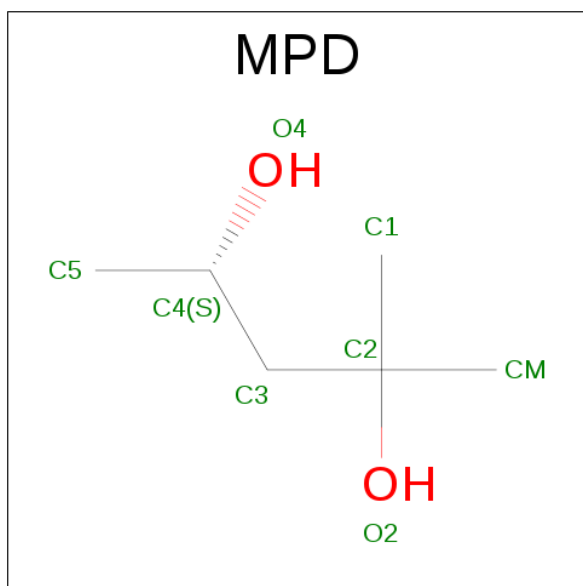
Continued from previous page...

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).

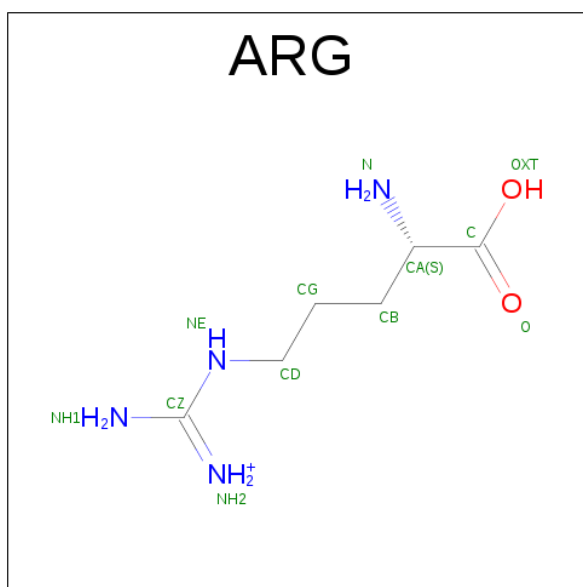
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1	Total	X	0	0
			1	1		
57	2A	1	Total	X	0	0
			1	1		

- 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).

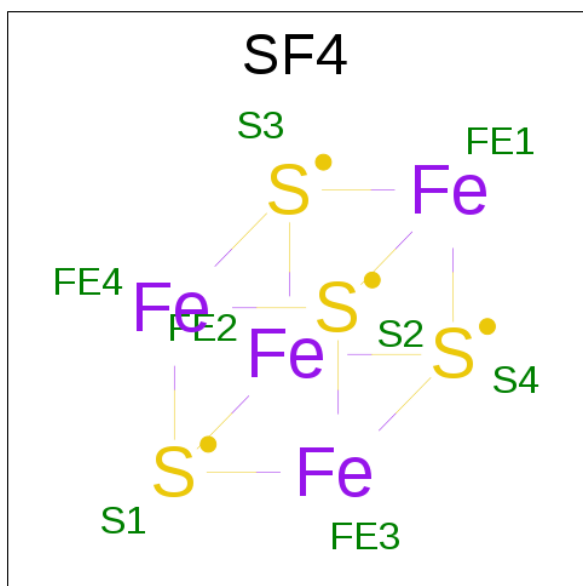
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	29	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	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 17	O 17	0	0
63	1F	14	Total 14	O 14	0	0
63	1G	5	Total 5	O 5	0	0
63	1H	4	Total 4	O 4	0	0
63	1N	7	Total 7	O 7	0	0
63	1O	2	Total 2	O 2	0	0
63	1P	18	Total 18	O 18	0	0
63	1Q	5	Total 5	O 5	0	0
63	1R	7	Total 7	O 7	0	0
63	1T	4	Total 4	O 4	0	0
63	1U	3	Total 3	O 3	0	0
63	1V	3	Total 3	O 3	0	0
63	1X	6	Total 6	O 6	0	0
63	1Y	2	Total 2	O 2	0	0
63	10	4	Total 4	O 4	0	0
63	11	3	Total 3	O 3	0	0
63	13	6	Total 6	O 6	0	0
63	15	2	Total 2	O 2	0	0
63	16	3	Total 3	O 3	0	0
63	18	7	Total 7	O 7	0	0
63	19	3	Total 3	O 3	0	0

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...

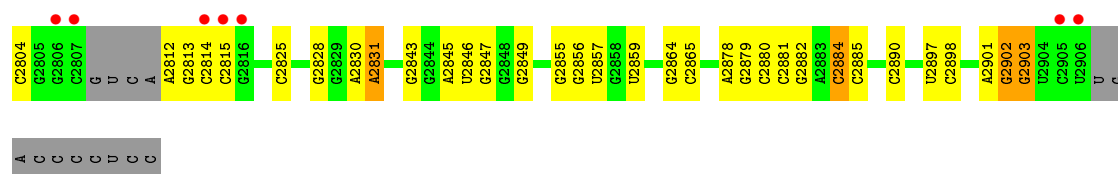
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2Q	5	Total 5	O 5	0	0
63	2R	2	Total 2	O 2	0	0
63	2T	2	Total 2	O 2	0	0
63	2U	3	Total 3	O 3	0	0
63	2X	4	Total 4	O 4	0	0
63	2Y	1	Total 1	O 1	0	0
63	20	2	Total 2	O 2	0	0
63	21	2	Total 2	O 2	0	0
63	23	2	Total 2	O 2	0	0
63	25	1	Total 1	O 1	0	0
63	26	2	Total 2	O 2	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...

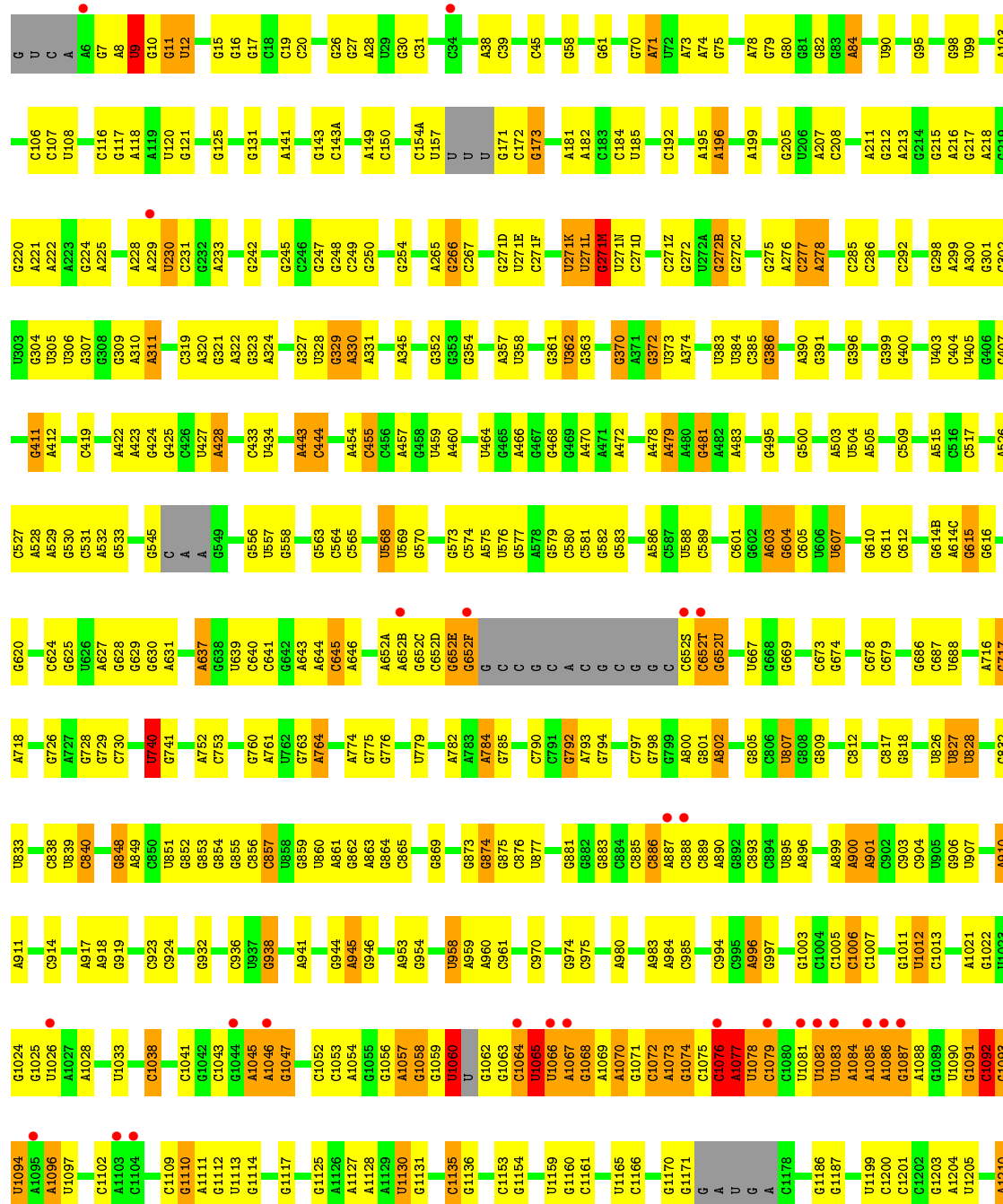
Continued from previous page...

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

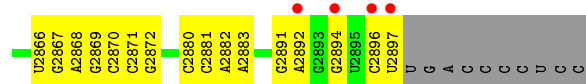
C2692	U2559	A2437	C2338	U2097	U1977	G1854	C1731	G1495	G1401	G1290	A174
U2699	G2560	G2441	C2238	U2101	U1985	G1857	U1735	A1496	G1404	G1291	A175
U2700	G2561	A2442	G2240	U2108	G1986	G1858	A1736	G1497	A1405	U1176	
C2702	U2563	A2446	U2244	G2109	G1989	G1859	A1737	A1500	A1406	A1299	
C2703	G2565	A2447	U2245	U2114	G1990	G1870	G1743	G1506	G1409	G1302	C1180
U2710	U2567	A2450	G2246	G2115	A1991	G1871	A1747	A1507	G1410	C1303	G1181
C2711	C2568	A2451	G2250	C2119	A1992	G1874	A1748	C1514	A1411	G1304	G1184
C2712	G2569	C2452	G2251	U2120	A1993	G1875	G1749	G1517	G1414	G1305	C1185
U2714	C2570	C2453	C2252	U2121	A1994	A1878	G1750	G1518	G1415	U1309	U1186
U2715		C2454	A2253	U2122	G2014	A1879	G1751	G1519	G1416	G1310	U1187
C2715	A2573	C2455	G2122	U2015	U2015	U1753	G1752	C1521	U1418	A1311	A1188
		G2456	C2183	U2016		G1889		G1522	U1419	G1312	
C2721	A2576	G2457	U2123	C2018	G2018	A1890	U1765	G1523	A1425	U1313	G1195
U2724	A2577	G2458	C2126	G2019		A1891	U1766	G1524	A1426	A1314	C1199
A2725	G2578	C2459	C2127	A2023	A2023	G1893	U1767	G1525	G1430	A1315	G1200
A2726	G2579	A2460	G2128	G2024	G2024	G1894	U1768	G1529	A1431	A1316	A1201
G2727	C2580		U2189	C2130		G1895	U1769	G1532	G1432	G1317	A1202
	G2586	C2475	C2190	C2131	G2031	C1897	A1770	G1533	C1433	A1321	G1206
A2734		C2476	A2191	U2131		A1898	G1771	G1534	G1434		
	G2594	A2372	A2192	C2132	G2034	A1899	C1785	C1539	G1435	A1324	U1211
U2739		A2373	C2193	C2133	A2035	G1900	A1788	A1540	U1436		U1212
G2740	U2597	C2376	U2194	G2134	A2036	C1901	U1787	A1541	U1437	G1331	G1217
	C2598	G2377	A2195	A2136			U1788	A1542	A1438		G1218
G2745											A1219
A2746	A2602	G2378	G2289	C2137	G2044	G1905	G1794	C1551	A1441	C1335	U1220
A2747	C2603	C2489	A2290	G2138	U2045	C1904	G1795	A1552	U1442	U1338	G1221
G2748	G2614	G2384	G2291	A2139				A1553		C1339	A1222
	A2615	G2385		U2140	G2049	A1911		A1554	U1451		G1223
U2760	U2616		C2295	A2141	U2050	G1925	A1804	C1555	U1452		C1224
A2761	G2620	A2388	C2296	G2142	G2051	G1922	C1805	C1556	U1453	G1342	G1225
	U2621	C2389	C2297	C2143	A2052	A1922	A1811	A1557	U1454	U1346	
G2768	G2622	A2390	C2298	U2144			G1812	A1558	G1458	A1347	G1231
	U2623	G2391	G2299	G2145	G2054	G1925	G1812	C1559	G1459	A1348	G1232
A2771	U2624	C2392	A2300	G2146	A2055		C1813				
		G2393	G2301	G2147		G1928	A1814	U1560	G1462	U1233	
U2778	C2629	A2394	G2302	A2148	C2058	A1934	A1817	C1561	G1463	A1234	
G2779	G2630	C2397	U2303	C2149	G2059	A1935		U1562	G1464		A1239
C2780	U2513	U2402	C2304	C2150	G2060	C1936	C1821	G1563	A1465	U1357	
	C2640	U2403	G2305	C2151	C2061	U1937	A1822	G1564	U1466	U1359	C1245
C2784	A2641	C2405	C2306	U2152	U2062		G1823	G1565	G1467	C1360	C1246
C2785	G2642	U2307	U2308	G2153	U2063	A1940		U1566	G1471	C1361	C1247
C2786				U2154	C2064	A1941	U1829	G1567	A1472	A1363	G1248
C2787	G2643	G2412	G2316	A2155	C2065	C1942	C1705		A1473		A1255
		A2317	A2317	A2156			C1710	A1575	G1474	A1367	U1256
A2791	C2658	G2416	G2322	C2157	C2077	G1951	A1712	G1579	A1475		C1263
U2792	U2659	G2417	C2222	C2158	G2078	G1952	A1711	G	G1476	G1378	
A2794	C2660	G2422	G2227	C2159	A2081	U1953	A1715	U			
	U2662	C2423	G2228	C2160	A2082	A1954	A1716	A	G1481	U1386	G1281
C2798	G2666	G2426	A2229	C2161	G2083	G1955	U1836	C	G1482	U1387	G1282
U2799			U2230	C2162	A2084	G1956		G1584	C1483	C1391	
U2799	A2674	G2431	C2231	C2163		G1957	A1841	G1585			
C2800		C2432	G2232	C2164	U2090	A1958	G1842	G1586	A1491	U1398	G1285
C2801	G2686	G2433	G2233	C2165	G2091	A1959	A1846	U1587	C1492	A1399	
A2803		A2434	G2235	U2166		A1960	G1947	G1588	G1493	G1286	
		G2337	G2236	C2168	U2096	U1961		A1589	G1494	A1400	



• Molecule 1: 23s ribosomal RNA

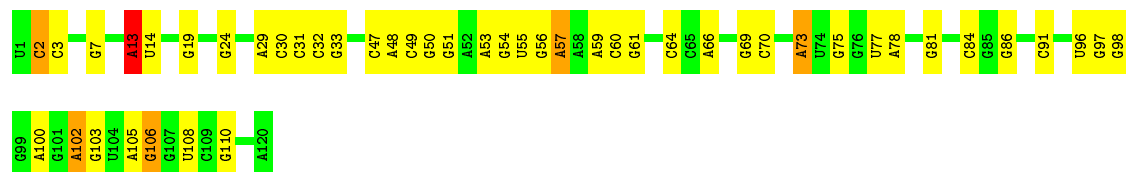


C2745	C2635	G2559	A2430	G2334	U2232	G2148	U2075	C1962	A1812	A1664	G1525	C1428	U1211
U2746	U2636	G2559	A2435	A2335	U2233	G2149	U2076	C1963	A1816	G1667	G1529	G1429	C1297
A2747	G2637	U2537	A2439	A2336	G2234	G2150	U2079	G1964	A1819	A1668	G1529	U1430	C1218
U2756	G2638	C2538	A2441	G2340	G2235	G2151	G2080	U1967	A1820	A1669	U1533	U1431	A1301
A2757	G2639	C2539	C2441	G2343	G2239	G2152	G2081	C1970	A1823	G1674	U1533	C1432	G1220
A2758	G2640	C2540	C2442	U2344	G2240	G2153	A2082	A1971	G1824	C1675	U1533	C1437	C1221A
	G2641	C2541	C2443	G2345	G2241	G2154		A1972	A1825	C1676	A	G1441	G1222
		A2542	C2444	U2347	U2245	G2155	U2086	A1973	G1826	C1677	C1536	G1442	G1223
A2764	G2647	C2543	G2445	U2348	G2246	G2156	G2087	A1974	A1827	U1688	A1542	U1316	A1226
C2648	U2649	G2544	G2446	C2349	G2251	G2157	G2093	C1974	G1828	U1688	C1543	G1443	A1227
			G2447	G2350	G2252	G2158				A1700		G1444	G1227
C2769		U2547	G2448	G2351	A2268	G2159		C1983	G1829	A1701	C1547	G1445	G1228
	A2654	G2548	A2448	G2352	A2269	G2160	G2101		G1835			G1229	G1229
A2776	G2659	G2549	A2451	A2352	A2270	G2161	U2102	U1991	G1836	U1709		G1230	G1230
C2777	A2660	C2550		A2353	A2271	G2162	G2103	G1992	A1839	C1710	A1558	G1231	G1231
A2778	G2661	G2551	U2457	A2360	A2272	G2163	G2104	U1993	G1842	C1711	G1559	C1450A	
A2781	G2662	G2552		A2361	A2273	G2164	G2105		G1843		A1566	G1459	G1335
G2782	G2663	G2553	U2462	A2362	C2275	G2165	G2106	C1996		G1721	A1569	A1460	G1336
		U2554		G2365	G2276	G2166	G2107	G1997	A1847	A1722		A1467	G1337
C2788	U2682	C2556	C2466	G2366	G2277	G2167	C2108	C1999	A1848	U1739	U1578	G1466	G1238
C2789	G2683	U2555	G2467	G2367	G2278	G2168	G2109		A1849	G1740	A1579	G1467	G1239
A				A2369	G2279	G2169	G2110			A1741	A1580	G1468	U1240
C		A2561		G2370	G2280	G2170	G2111	G2004	G1861			G1469	A1241
C	U2687		A2469	G2371	A2281	G2171		A2005		G1746		G1470	G1244
G2792	U2688			G2372	A2282	G2172	U2112		A1877		C1584	A1471	
G2793	G2689	A2564	G2472	G2373	A2283	G2173	U2113	G2010	A1878	C1754	A1586	A1571	A1247
C2794	C2690	A2565	U2473	G2374	G2284	G2174	G2114	G2011		A1755		G1474	
G	C2691	C2566	C2474	U2375	U2285	G2175	G2115	U2011	A1889	G1756	G1593	G1475	G1250
U		G2567	C2475	A2377	G2286	G2176	G2116	G2012				G1476	
C	G2695	C2568	C2476	A2378	G2287	G2177	G2117	A2013			G1594	A1365	
A	U2696		A2477	G2379	G2288	G2178	U2118	A2014	G1899	C1761		G1482	A1253
A2801A	G2697	A2572	G2478	G2380	U2289	G2179	G2119		A1900	A1762	C1598		A1254
C2802	U2698	C2573		G2381	G2290	G2180	G2120	U2022		G1763		G1491	
C2803	G2699	G2574	G2485	G2382	A2291	G2181	U2121	G2023	A1877	G1764	U1602	G1492	G1255
G2804		C2575		G2383	G2292	G2182	G2122		A1878		A1603	C1493	G1256
G2805	U2702	A2576		U2384	G2293	G2183	G2123	A2031	A1914	A1773		A1494	U1263
G2807	C2703		G2488	G2385	A2305	G2184	G2124	G3082	A1919		C1376	A1495	G1264
U2808	A2704	G2582	G2489	G2386	G2306	G2185	G2125	A2033		A1780	A1607	A1496	A1265
A2809	G2705	U2585	U2491	G2387	G2307	G2186	A2126	G2033	A1927	C1781	A1608	A1497	A1266
			G2492	G2388	A2309	G2187	G2127	C2040	A1928	G1782	A1609	G1498	U1267
C2816	G2710		G2493	G2389	A2310	G2188	G2128	G2043	A1929	A1783		C1499	A1268
G2817	A2711	A2602	G2494	U2400	A2311	G2189	U2130		G1930		A1384	G1385	A1269
G2818	U2712		G2495	G2401	U2312	G2190	G2131	C2055	U1931	A1786		G1386	G1270
G2819	A2713	C2606	U2406	G2402	G2313	G2191	U2132	G2056				U1503	G1271
A2820	G2714	G2607	G2410	A2411	G2314	G2192	G2133	G2059	A1932	A1791	C1636	C1504	A1272
G2822		G2608	A2412	G2413	G2315	G2193	A2134	A2060	G1933	U1794	A1637	C1505	U1273
A2823	G2715		G2414	G2414	G2316	G2194	G2135	G2061	C1934	C1795	A1507	C1506	U1406
		U2611	U2503	G2415	C2317	G2195	G2136	A2062	A1935	C1796	U1639	A1508	A1278
G2823	G2716	C2612	U2504	G2416	G2318	G2196	G2137	G2067	A1936	C1797	C1640	C1509	G1279
	G2719	U2613	G2505	G2417	G2319	G2197	G2138	U2068	A1937	U1798	A1641		A1412
G2833		A2614	U2506	G2420	G2320	A2198	G2139	G2069	U1938	U1799	A1509A	G1413	
	C2723		A2422	G2421	G2321	U2203	G2140	G2072	G1945	G1799		G1416	U1282
G2839		C2617	U2511	A2423	A2322	G2205	G2141	G2073	G1946	C1800	G1642	C1417	G1283
G2845	U2726		G2512	G2424		G2206	G2142	G2074	G1801	C1800	C1648	G1417	A1284
G2846	G2727		G2513	A2425		G2207	G2143	G2075	U1947	G1801		G1417	G1285
U2847	U2728	C2620	G2514	G2426	G2325	A2208	G2144	A2071	A1802	A1803		U1420	A1286
				G2427	G2326	G2224	U2145	A2072	A1803		A1652	G1421	A1287
G2732		A2629	U2518	A2428	A2327	G2225	G2146	C2073	A1810		G1653	G1422	U1292
A2733		G2630	G2520	A2328	A2328	G2226	G2147	U2074	U1955		A1655	G1423	C1293



- Molecule 2: 5s ribosomal RNA

Chain 1B: 61% 34% . .



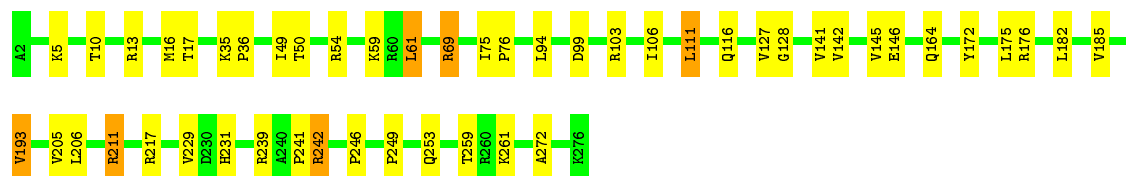
- Molecule 2: 5s ribosomal RNA

Chain 2B: 70% 27% .



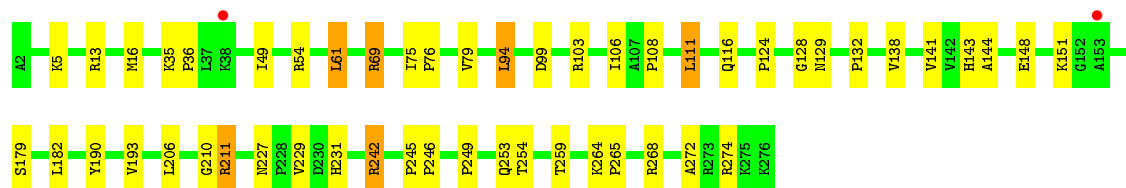
- Molecule 3: 50S ribosomal protein L2

Chain 1D: 82% 16% .



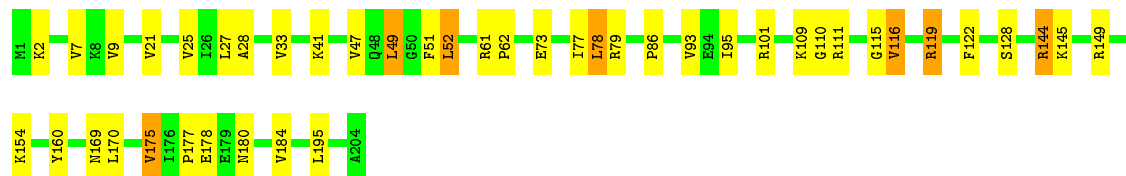
- Molecule 3: 50S ribosomal protein L2

Chain 2D: 81% 16% .

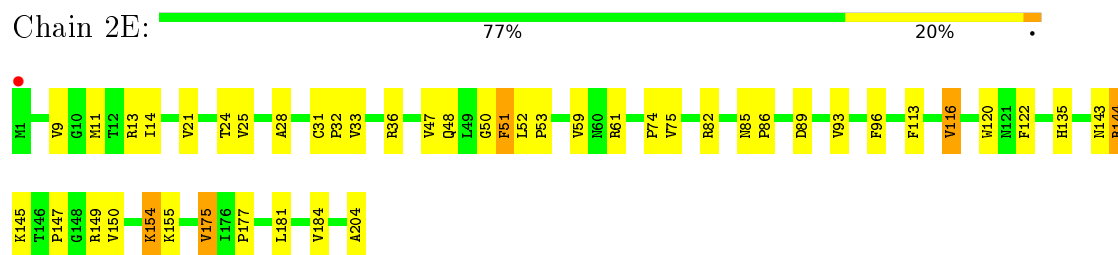


- Molecule 4: 50S ribosomal protein L3

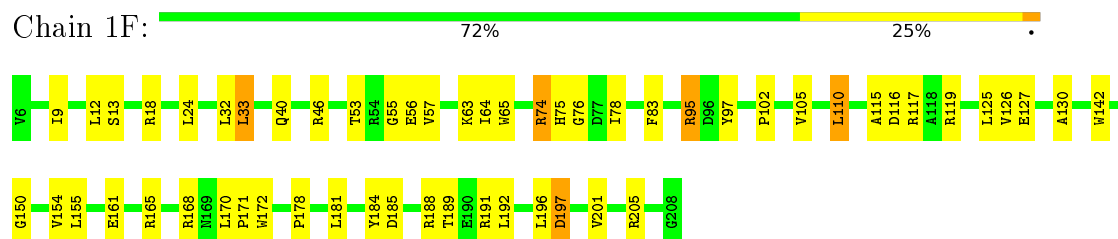
Chain 1E: 78% 18% .



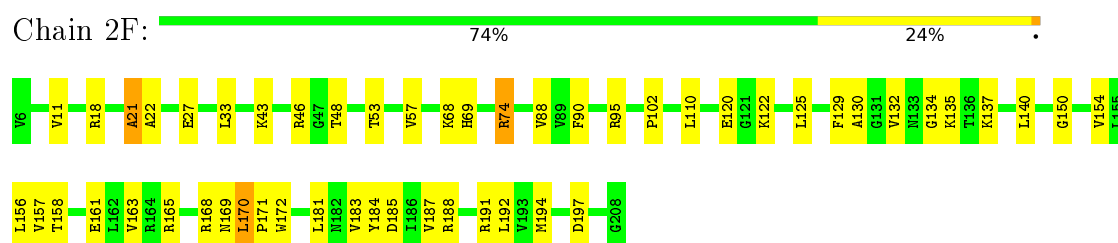
- Molecule 4: 50S ribosomal protein L3



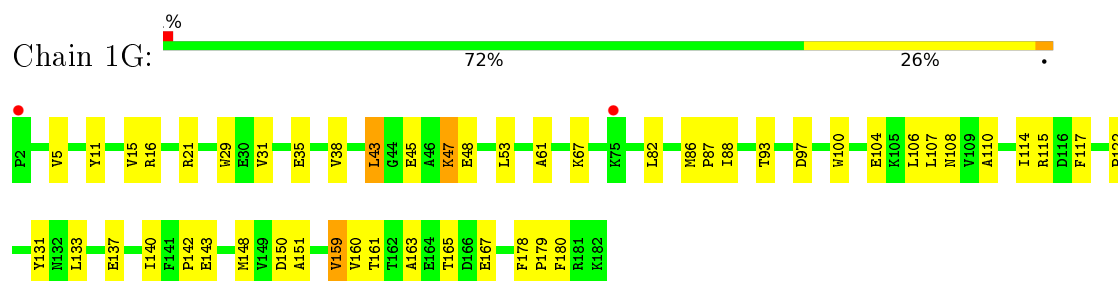
- Molecule 5: 50S ribosomal protein L4



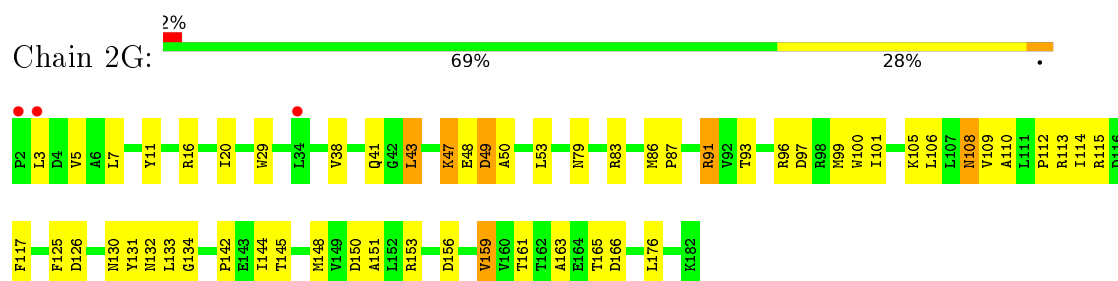
- Molecule 5: 50S ribosomal protein L4



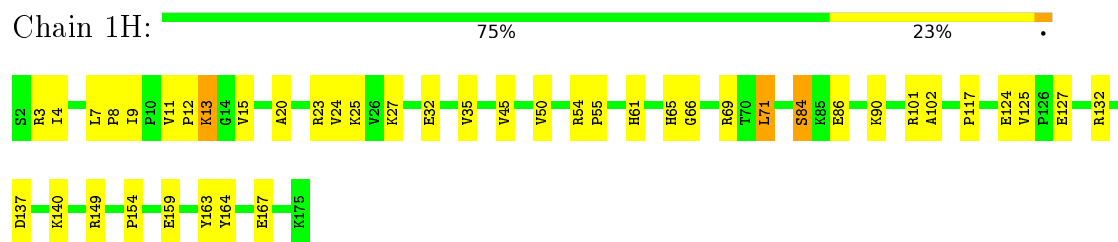
- Molecule 6: 50S ribosomal protein L5



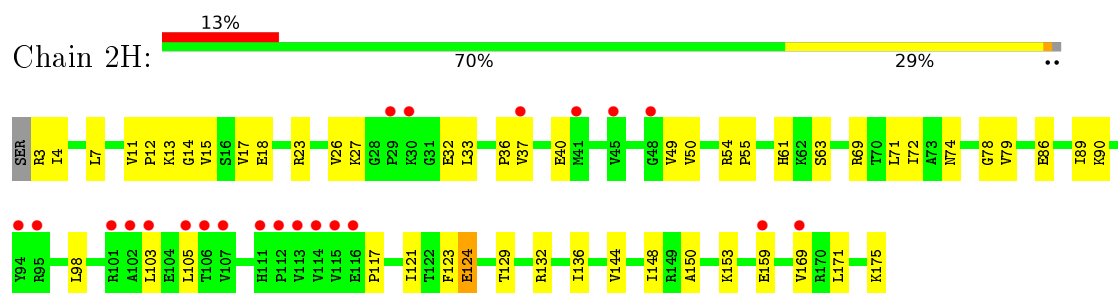
- Molecule 6: 50S ribosomal protein L5



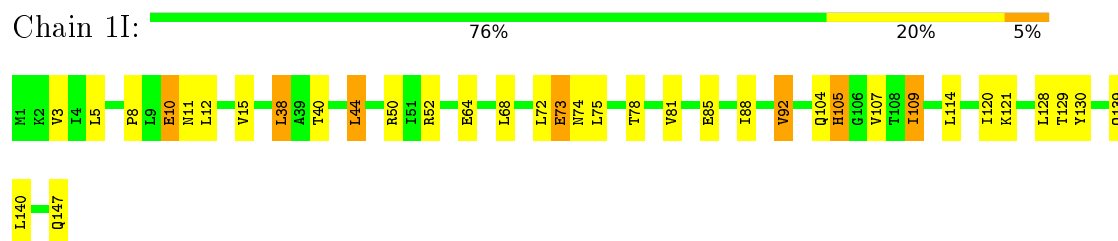
- Molecule 7: 50S ribosomal protein L6



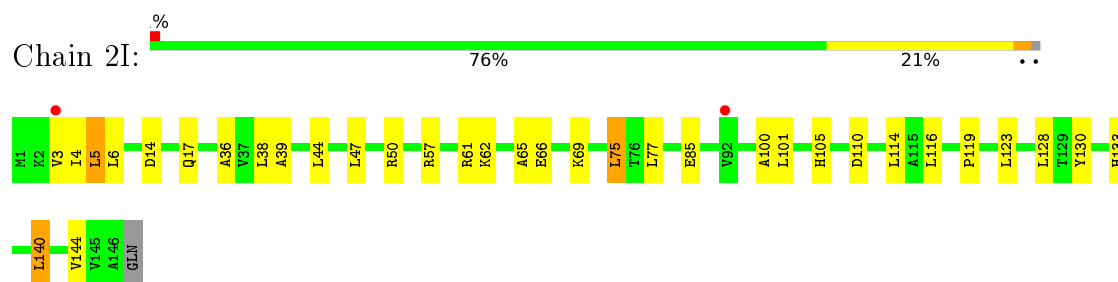
- Molecule 7: 50S ribosomal protein L6



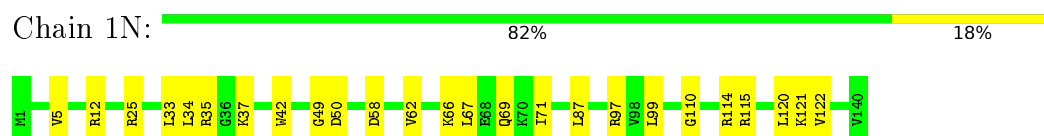
- Molecule 8: 50S ribosomal protein L9



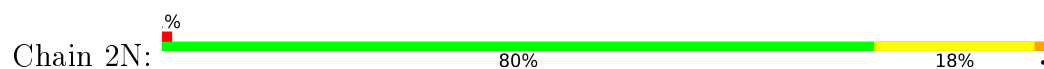
- Molecule 8: 50S ribosomal protein L9

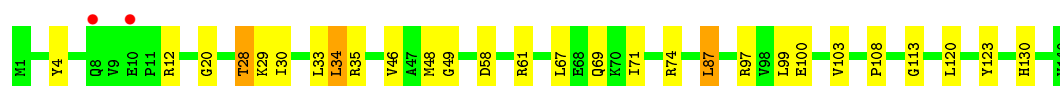


- Molecule 9: 50S ribosomal protein L13

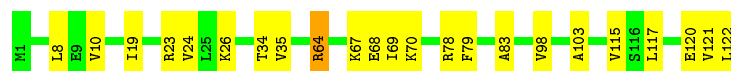
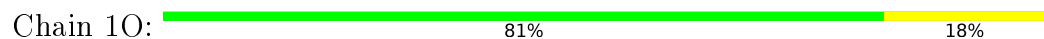


- Molecule 9: 50S ribosomal protein L13

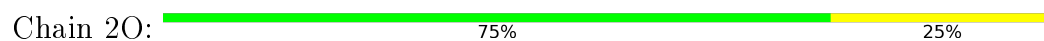




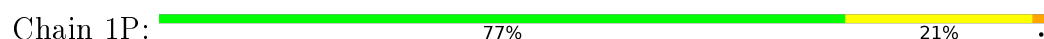
- Molecule 10: 50S ribosomal protein L14



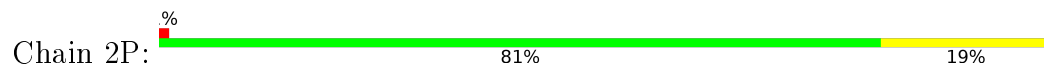
- Molecule 10: 50S ribosomal protein L14



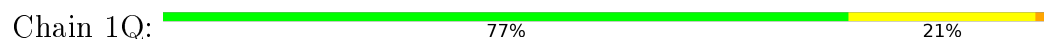
- Molecule 11: 50S ribosomal protein L15



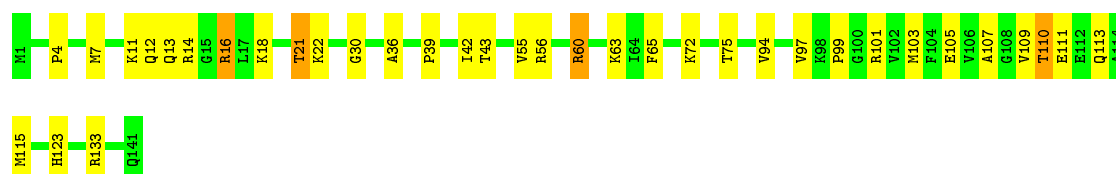
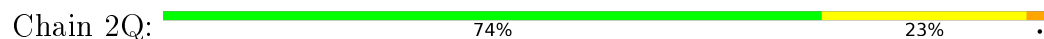
- Molecule 11: 50S ribosomal protein L15




- Molecule 12: 50S ribosomal protein L16

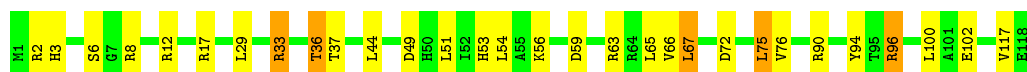


- Molecule 12: 50S ribosomal protein L16



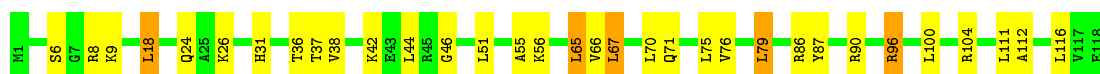
- Molecule 13: 50S ribosomal protein L17

Chain 1R:  75% 21% .



- Molecule 13: 50S ribosomal protein L17

Chain 2R:  72% 24% .




- Molecule 14: 50S ribosomal protein L18

Chain 1S:  75% 23% ..




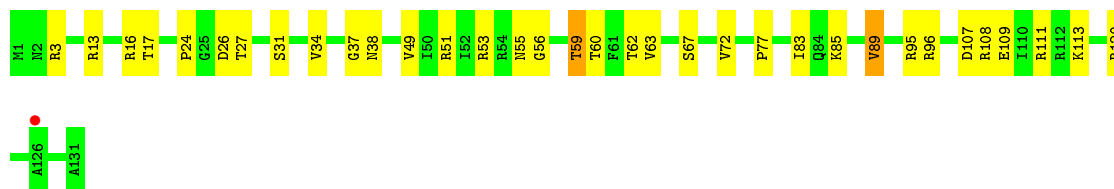
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  5% 75% 24% .




- Molecule 15: 50S ribosomal protein L19

Chain 1T:  % 74% 24% .




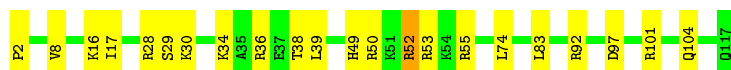
- Molecule 15: 50S ribosomal protein L19

Chain 2T:  77% 23% .




- Molecule 16: 50S ribosomal protein L20

Chain 1U:  81% 18% .



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  81% 18%



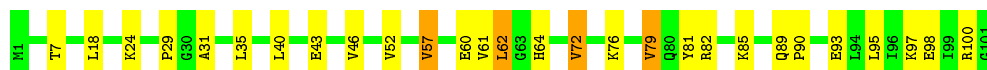
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  70% 28%




- Molecule 17: 50S ribosomal protein L21

Chain 2V:  72% 24%




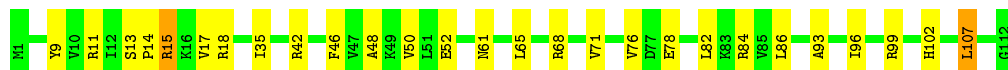
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  85% 14%



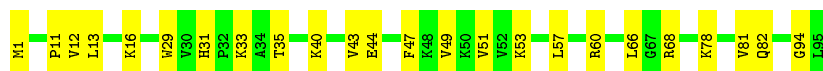
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  76% 22%




- Molecule 19: 50S ribosomal protein L23

Chain 1X:  75% 25%

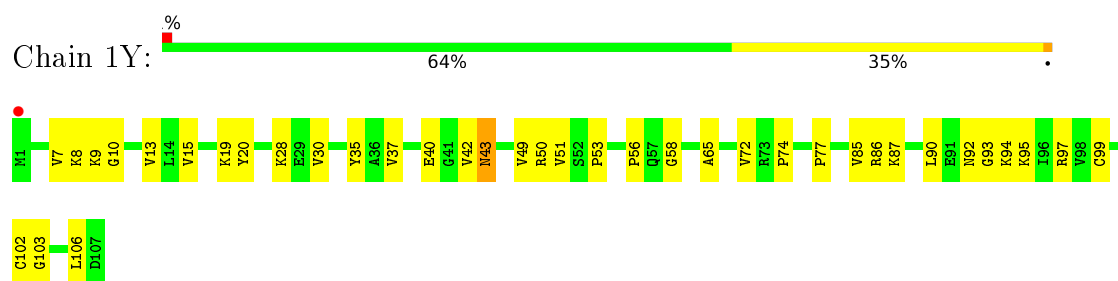


- Molecule 19: 50S ribosomal protein L23

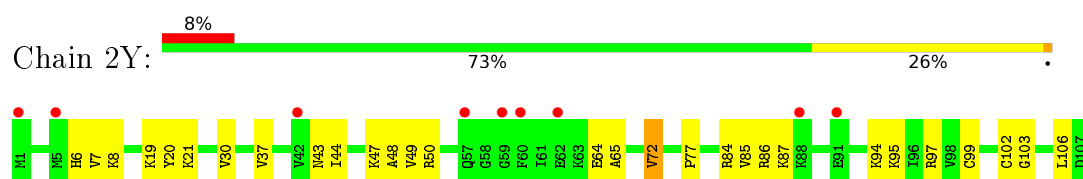
Chain 2X:  78% 21%



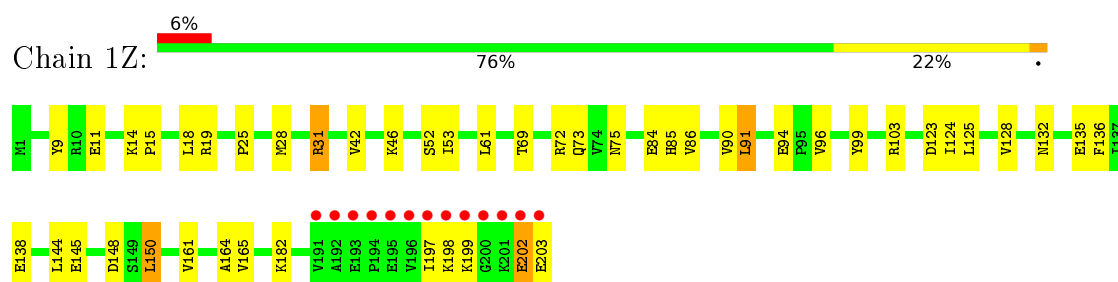
- Molecule 20: 50S ribosomal protein L24



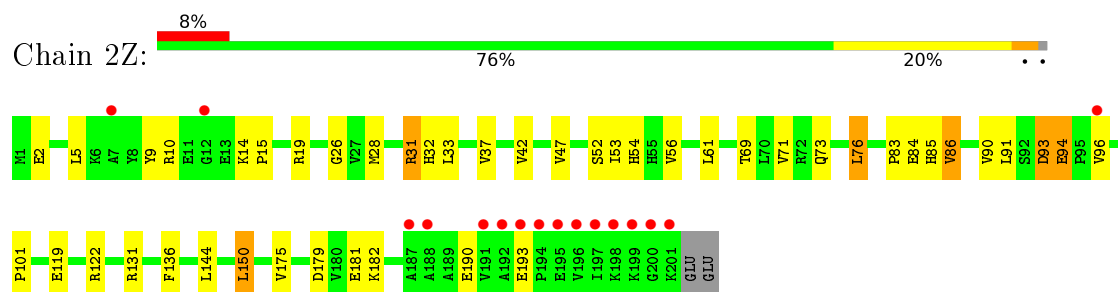
- Molecule 20: 50S ribosomal protein L24



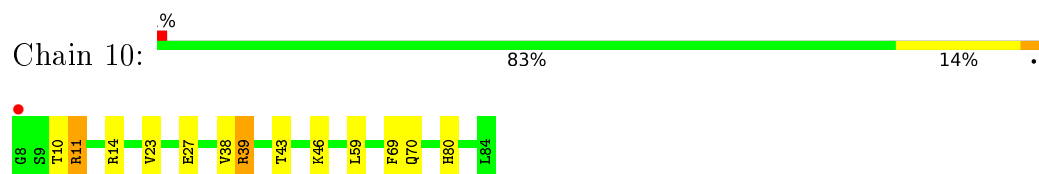
- Molecule 21: 50S ribosomal protein L25



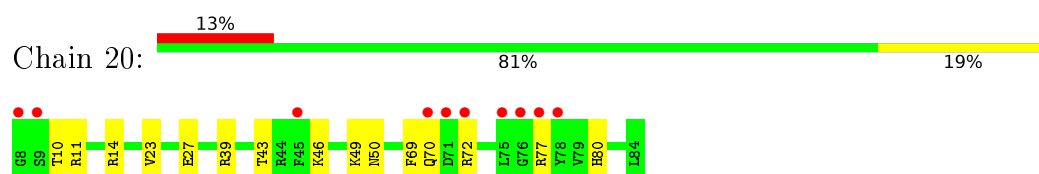
- Molecule 21: 50S ribosomal protein L25



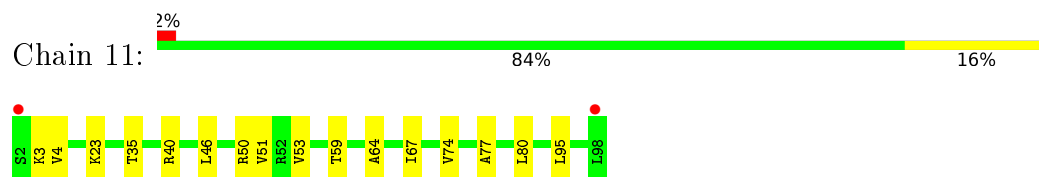
- Molecule 22: 50S ribosomal protein L27



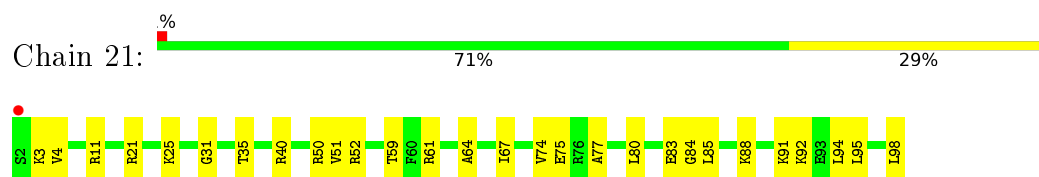
- Molecule 22: 50S ribosomal protein L27



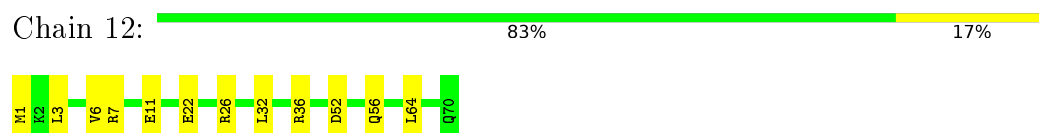
- Molecule 23: 50S ribosomal protein L28



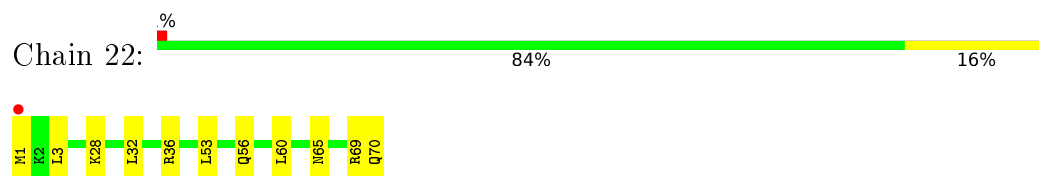
- Molecule 23: 50S ribosomal protein L28



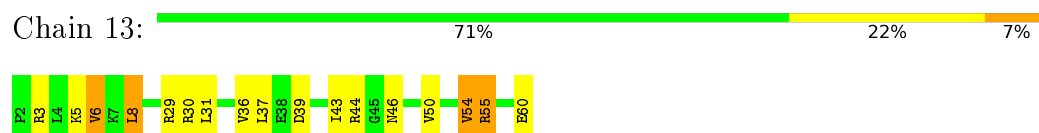
- Molecule 24: 50S ribosomal protein L29



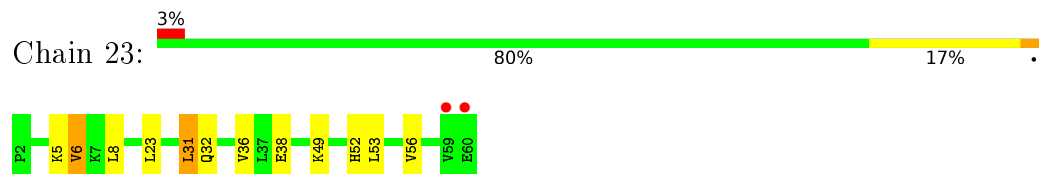
- Molecule 24: 50S ribosomal protein L29



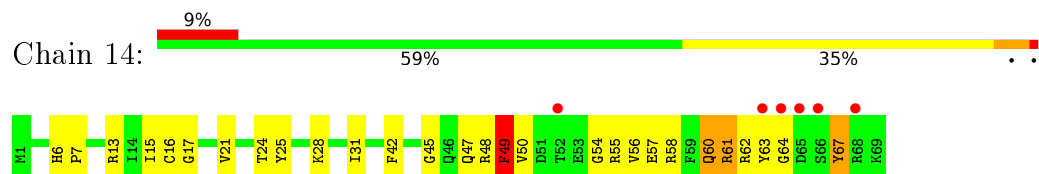
- Molecule 25: 50S ribosomal protein L30



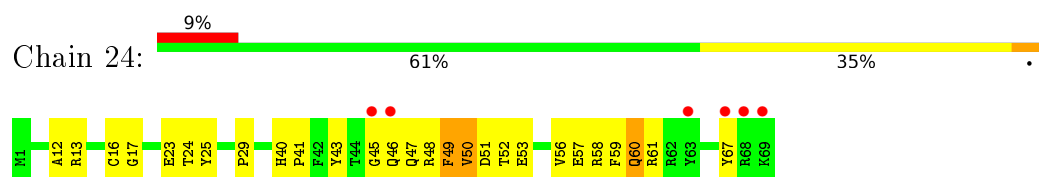
- Molecule 25: 50S ribosomal protein L30



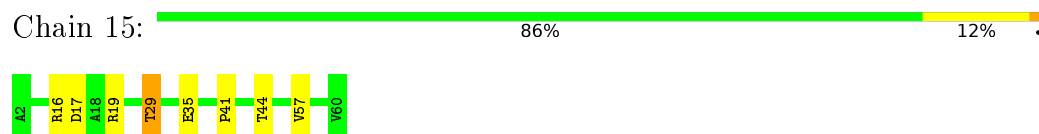
- Molecule 26: 50S ribosomal protein L31



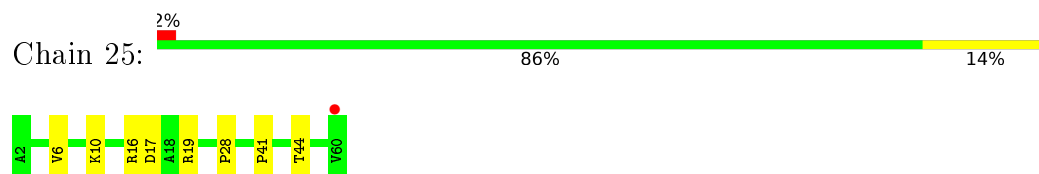
- Molecule 26: 50S ribosomal protein L31



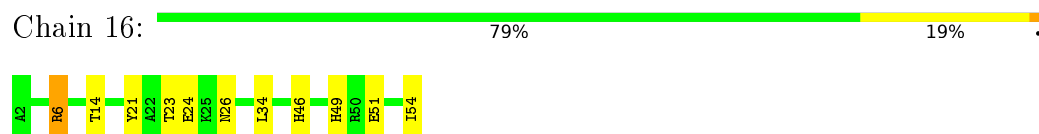
- Molecule 27: 50S ribosomal protein L32



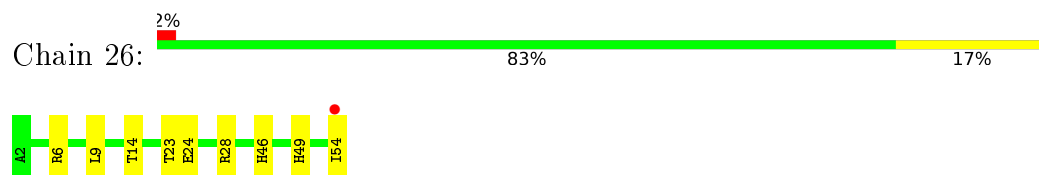
- Molecule 27: 50S ribosomal protein L32



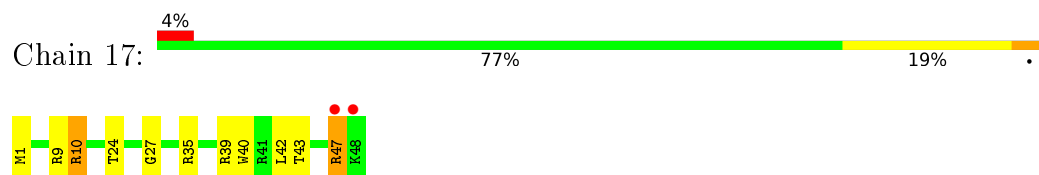
- Molecule 28: 50S ribosomal protein L33



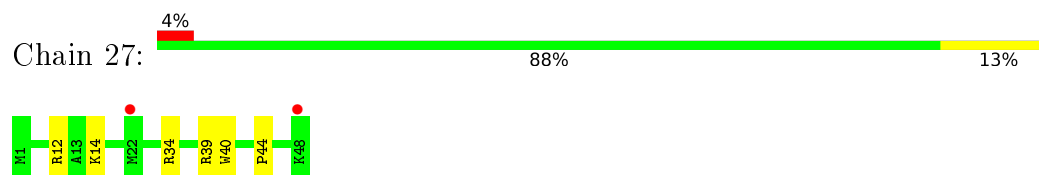
- Molecule 28: 50S ribosomal protein L33




- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



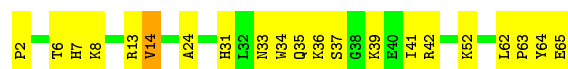
- Molecule 30: 50S ribosomal protein L35

Chain 18:  75% 23% .




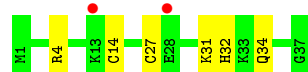
- Molecule 30: 50S ribosomal protein L35

Chain 28:  67% 31% .




- Molecule 31: 50S ribosomal protein L36

Chain 19:  5% 84% 16%




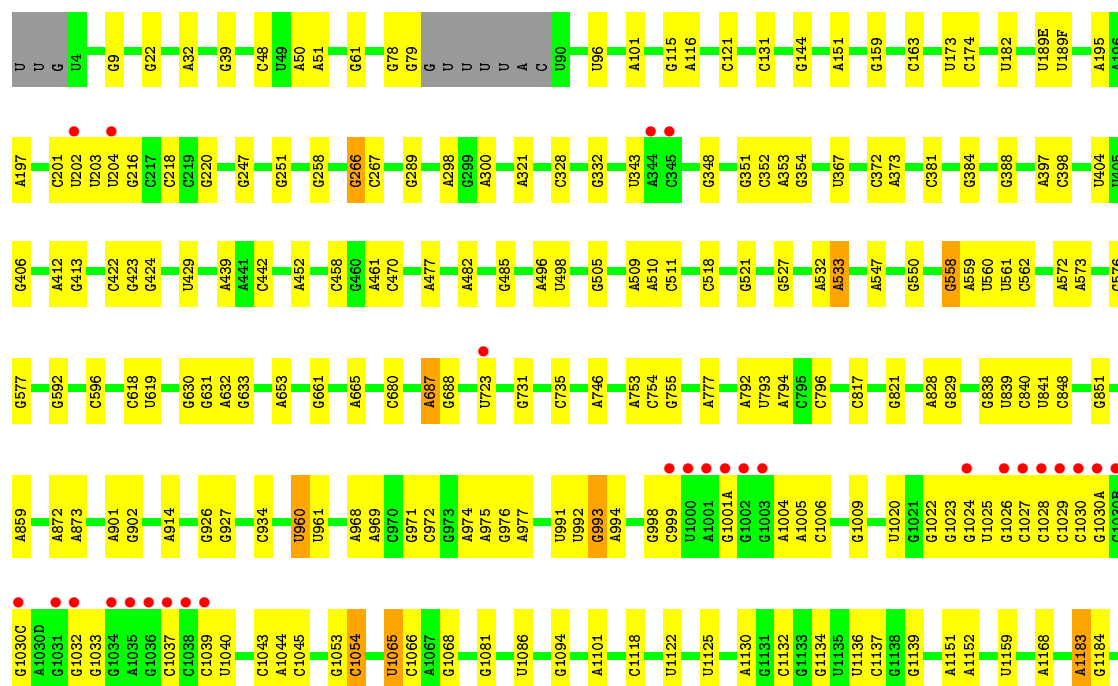
- Molecule 31: 50S ribosomal protein L36

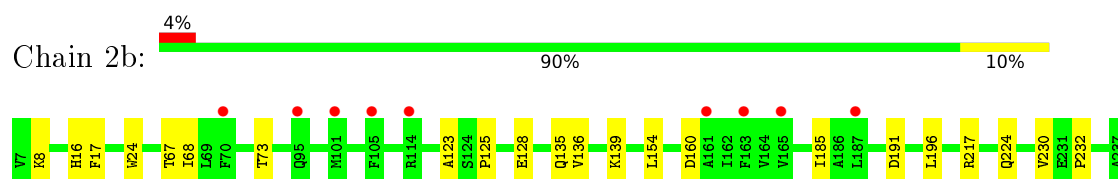
Chain 29:  5% 78% 22%



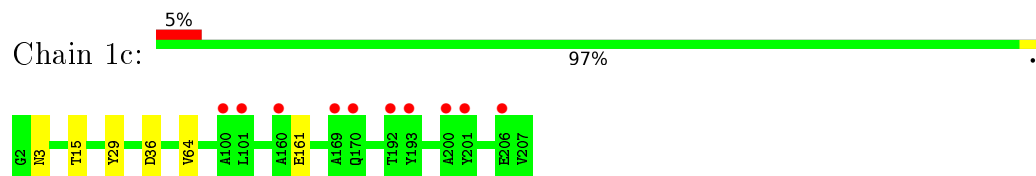
- Molecule 32: 16S ribosomal RNA

Chain 1a:  2% 81% 17% ..

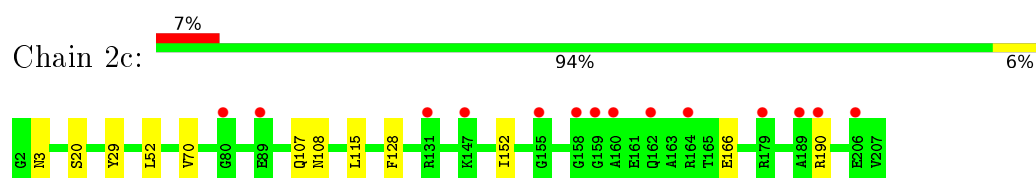




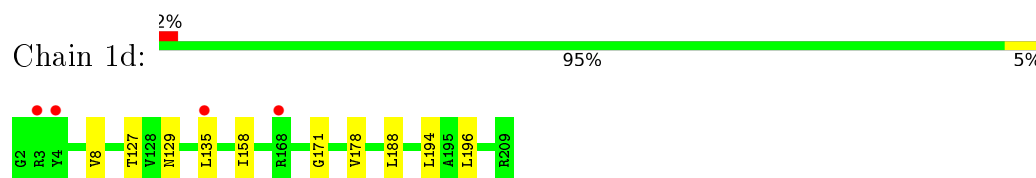
- Molecule 34: 30S ribosomal protein S3



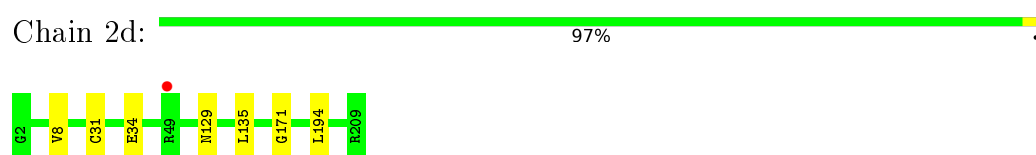
- Molecule 34: 30S ribosomal protein S3



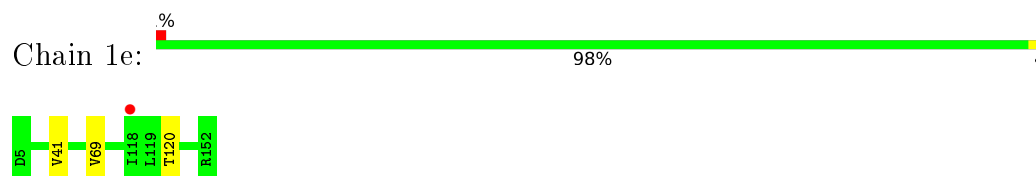
- Molecule 35: 30S ribosomal protein S4



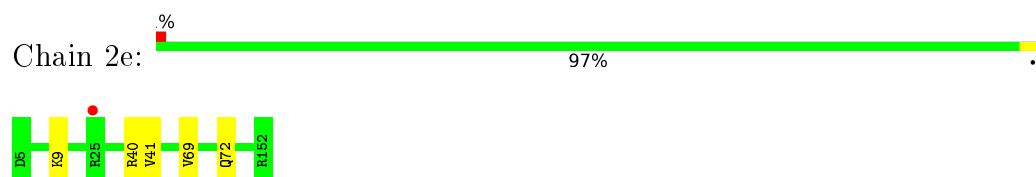
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



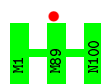
- Molecule 36: 30S ribosomal protein S5



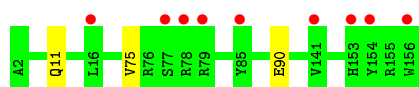
- Molecule 37: 30S ribosomal protein S6



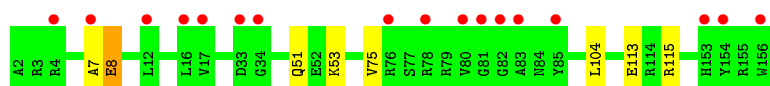
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



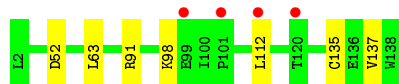
- Molecule 38: 30S ribosomal protein S7



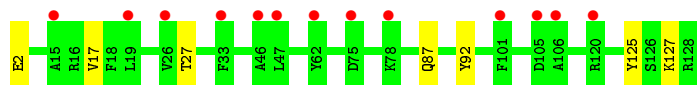
- Molecule 39: 30S ribosomal protein S8



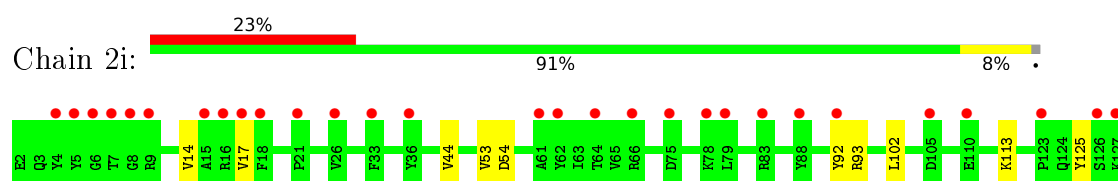
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

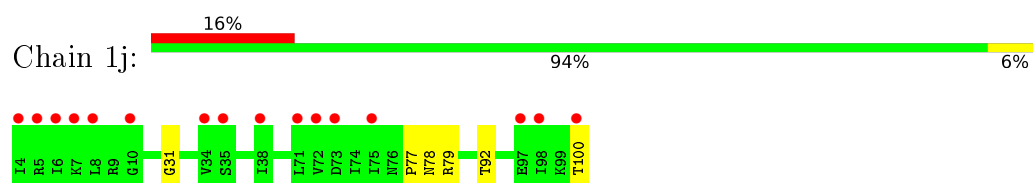


- Molecule 40: 30S ribosomal protein S9

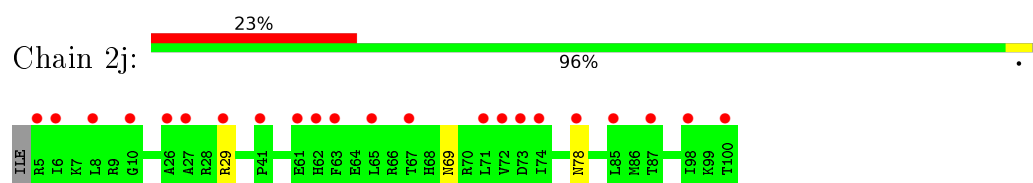


ARG

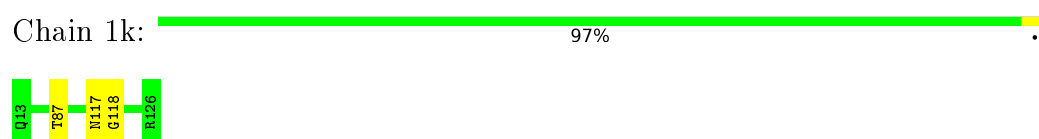
- Molecule 41: 30S ribosomal protein S10



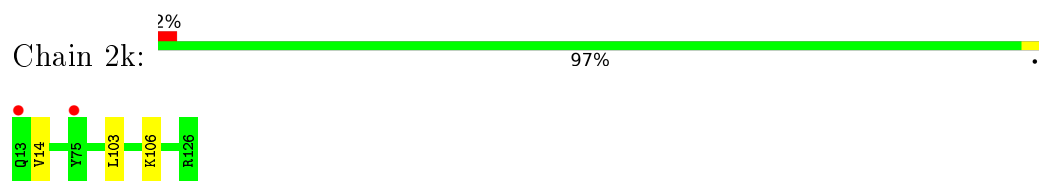
- Molecule 41: 30S ribosomal protein S10



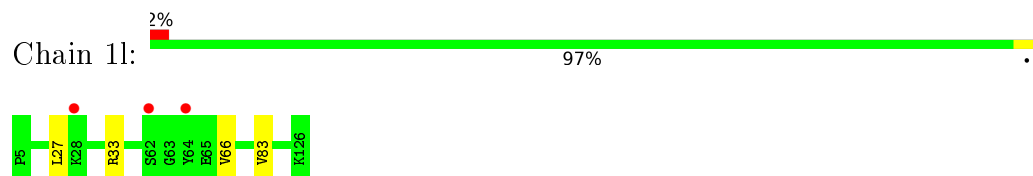
- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11

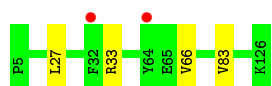


- Molecule 43: 30S ribosomal protein S12

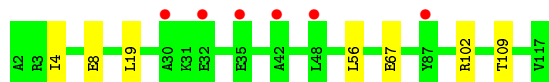


- Molecule 43: 30S ribosomal protein S12

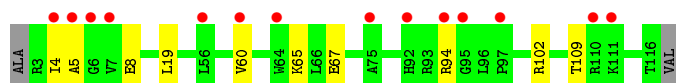
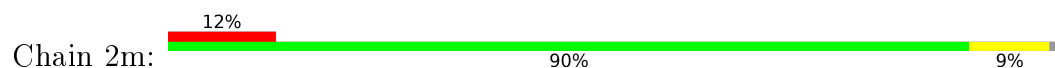




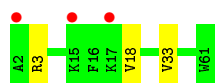
- Molecule 44: 30S ribosomal protein S13



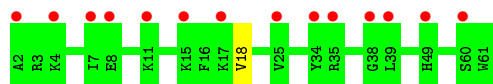
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



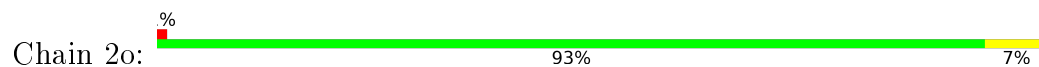
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

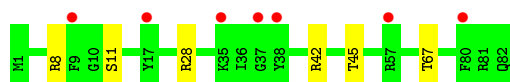


- Molecule 46: 30S ribosomal protein S15

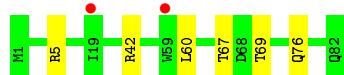


- Molecule 47: 30S ribosomal protein S16





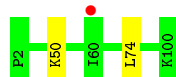
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



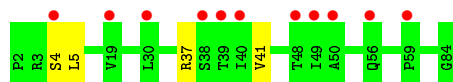
- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

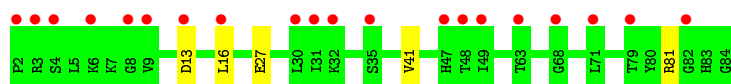


- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

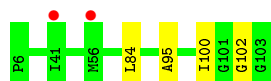




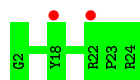
- Molecule 51: 30S ribosomal protein S20



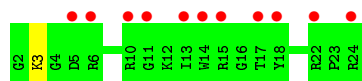
- Molecule 51: 30S ribosomal protein S20



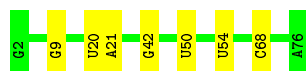
- Molecule 52: 30S ribosomal protein Thx



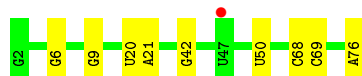
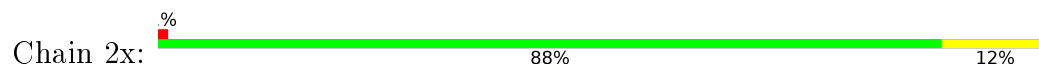
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: tRNA met



- Molecule 53: tRNA met

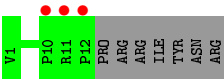


- Molecule 54: Onc112





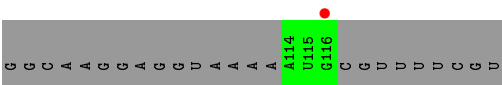
● Molecule 54: Onc112



● Molecule 55: mRNA



● Molecule 55: mRNA



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.

All (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
1	2A	1092	C	N1-C2-O2	8.72	124.13	118.90
1	1A	854	U	C2-N3-C4	-8.62	121.83	127.00
1	2A	1092	C	C2-N1-C1'	8.18	127.79	118.80
2	1B	75	G	C6-N1-C2	-8.15	120.21	125.10
32	2a	1397	C	C2-N1-C1'	8.09	127.69	118.80
1	2A	1097	U	C2-N1-C1'	8.04	127.35	117.70
32	1a	1495	U	N1-C2-O2	7.98	128.38	122.80
1	2A	673	C	C2-N3-C4	-7.85	115.97	119.90
1	1A	848	G	O5'-P-OP2	-7.77	98.71	105.70
2	1B	102	A	C6-N1-C2	-7.74	113.96	118.60
32	2a	343	U	C2-N1-C1'	-7.69	108.47	117.70
1	1A	2058	C	O5'-P-OP1	-7.67	98.79	105.70
32	2a	343	U	N3-C4-O4	-7.56	114.11	119.40
32	2a	343	U	C5-C4-O4	7.56	130.43	125.90
32	1a	839	U	P-O3'-C3'	7.37	128.55	119.70
1	1A	952	G	C5-C6-O6	7.36	133.01	128.60
32	2a	1397	C	N1-C2-O2	7.32	123.29	118.90
32	2a	1465	C	C2-N3-C4	-7.28	116.26	119.90
32	2a	1158	C	N1-C2-O2	7.28	123.27	118.90
32	2a	1158	C	C2-N1-C1'	7.25	126.77	118.80
32	2a	1495	U	N1-C2-O2	7.24	127.86	122.80
32	1a	1465	C	C2-N3-C4	-7.23	116.29	119.90
1	1A	1045	U	O5'-P-OP2	-7.22	99.20	105.70
1	2A	1060	U	C2-N1-C1'	7.20	126.33	117.70
1	2A	906	G	C5-C6-O6	6.96	132.77	128.60
1	2A	807	U	C2-N3-C4	-6.87	122.88	127.00
1	1A	1358	U	C5-C4-O4	6.83	130.00	125.90
1	1A	1099	C	N1-C2-O2	6.83	123.00	118.90
1	1A	2459	G	C6-N1-C2	-6.82	121.01	125.10
1	2A	1092	C	N3-C2-O2	-6.65	117.25	121.90
32	1a	1436	U	C2-N3-C4	-6.63	123.02	127.00
32	1a	343	U	C2-N1-C1'	-6.52	109.88	117.70
1	2A	2103	C	C2-N1-C1'	6.46	125.90	118.80
32	2a	266	G	P-O3'-C3'	6.39	127.37	119.70
32	1a	266	G	P-O3'-C3'	6.38	127.35	119.70
32	2a	1183	A	P-O3'-C3'	6.37	127.34	119.70
1	2A	1076	C	OP1-P-O3'	6.33	119.13	105.20
1	1A	410	U	N1-C2-O2	6.33	127.23	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	101	A	C4-C5-C6	6.29	120.15	117.00
32	2a	1003	G	N3-C4-C5	-6.29	125.45	128.60
1	1A	1386	U	C2-N3-C4	-6.24	123.26	127.00
1	2A	1077	A	O5'-P-OP1	-6.22	100.10	105.70
1	1A	537	G	O4'-C1'-N9	6.20	113.16	108.20
1	1A	1985	U	C2-N1-C1'	6.19	125.12	117.70
53	2x	6	G	O5'-P-OP2	-6.17	100.15	105.70
32	2a	960	U	C2-N1-C1'	6.14	125.07	117.70
1	1A	31	C	O5'-P-OP1	-6.13	100.18	105.70
1	1A	2390	A	N1-C6-N6	6.13	122.28	118.60
32	1a	1285	A	P-O3'-C3'	6.12	127.04	119.70
1	1A	720	C	N3-C4-C5	6.11	124.34	121.90
32	2a	1054	C	C2-N1-C1'	6.11	125.52	118.80
32	2a	346	G	C6-N1-C2	-6.11	121.44	125.10
1	2A	2103	C	N1-C2-O2	6.08	122.55	118.90
32	2a	1003	G	C2-N3-C4	6.07	114.93	111.90
32	1a	404	U	N1-C2-O2	6.01	127.01	122.80
1	1A	1162	C	C5-C6-N1	6.00	124.00	121.00
1	1A	82	G	N9-C4-C5	-6.00	103.00	105.40
32	1a	1495	U	N3-C2-O2	-5.99	118.00	122.20
32	2a	343	U	C6-N1-C1'	5.97	129.55	121.20
32	1a	558	G	O5'-P-OP1	-5.95	100.34	105.70
1	1A	82	G	C2-N3-C4	-5.90	108.95	111.90
1	2A	1092	C	C6-N1-C2	-5.88	117.95	120.30
1	2A	2103	C	C6-N1-C2	-5.87	117.95	120.30
32	2a	754	C	C2-N1-C1'	5.87	125.25	118.80
1	2A	9	U	C5-C6-N1	5.85	125.63	122.70
32	1a	901	A	N1-C6-N6	5.84	122.11	118.60
1	2A	1097	U	N1-C2-O2	5.82	126.87	122.80
32	1a	1465	C	C5-C4-N4	-5.81	116.13	120.20
32	2a	1397	C	C6-N1-C1'	-5.75	113.90	120.80
1	1A	1162	C	C2-N1-C1'	5.73	125.10	118.80
1	2A	383	U	N1-C2-O2	5.72	126.80	122.80
32	2a	1436	U	C2-N3-C4	-5.72	123.57	127.00
32	2a	346	G	N3-C4-C5	-5.71	125.75	128.60
1	2A	1313	U	C2-N1-C1'	5.70	124.54	117.70
1	1A	720	C	C5-C4-N4	-5.66	116.24	120.20
32	1a	960	U	C2-N1-C1'	5.65	124.48	117.70
1	2A	2447	G	C6-N1-C2	-5.65	121.71	125.10
32	1a	839	U	OP1-P-O3'	5.64	117.62	105.20
32	2a	404	U	N1-C2-O2	5.64	126.75	122.80
1	1A	1346	U	P-O3'-C3'	5.63	126.45	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1158	C	N3-C2-O2	-5.62	117.97	121.90
1	1A	1359	U	C2-N1-C1'	5.60	124.42	117.70
1	1A	1418	U	C5-C4-O4	-5.55	122.57	125.90
32	2a	1281	U	C2-N1-C1'	5.54	124.35	117.70
32	2a	1397	C	N3-C2-O2	-5.53	118.03	121.90
32	2a	1024	G	C2-N3-C4	5.53	114.66	111.90
32	2a	1495	U	C2-N1-C1'	5.52	124.33	117.70
1	1A	1222	A	O5'-P-OP1	-5.52	100.73	105.70
32	1a	1065	U	P-O3'-C3'	5.51	126.32	119.70
2	1B	75	G	C5-C6-N1	5.50	114.25	111.50
32	2a	1028	C	C6-N1-C2	-5.49	118.10	120.30
32	1a	1201	A	P-O3'-C3'	5.48	126.28	119.70
1	2A	271(M)	G	P-O3'-C3'	5.48	126.28	119.70
1	2A	1097	U	C6-N1-C1'	-5.47	113.54	121.20
1	1A	1462	G	O4'-C1'-N9	5.47	112.58	108.20
1	2A	1092	C	C6-N1-C1'	-5.47	114.24	120.80
1	2A	271(M)	G	OP1-P-O3'	5.46	117.22	105.20
32	2a	1491	G	P-O3'-C3'	5.45	126.23	119.70
32	1a	1183	A	P-O3'-C3'	5.43	126.22	119.70
1	1A	1539	C	C2-N1-C1'	5.43	124.77	118.80
32	1a	533	A	N1-C6-N6	5.43	121.86	118.60
1	2A	1083	U	C2-N1-C1'	5.42	124.21	117.70
1	2A	807	U	C5-C4-O4	-5.41	122.65	125.90
32	1a	343	U	O4'-C1'-N1	5.40	112.52	108.20
1	1A	952	G	N1-C6-O6	-5.38	116.67	119.90
1	2A	740	U	O5'-P-OP2	-5.37	100.86	105.70
1	2A	1092	C	C5-C6-N1	5.35	123.68	121.00
1	1A	854	U	N1-C2-N3	5.35	118.11	114.90
32	2a	1054	C	N1-C2-O2	5.32	122.09	118.90
1	1A	1221	G	OP1-P-O3'	5.30	116.86	105.20
1	2A	2451	A	C5-N7-C8	-5.30	101.25	103.90
1	2A	673	C	N3-C4-C5	5.29	124.02	121.90
32	1a	754	C	C2-N1-C1'	5.29	124.61	118.80
1	1A	2597	U	OP1-P-O3'	5.28	116.82	105.20
1	2A	1097	U	C5-C6-N1	5.27	125.33	122.70
32	1a	1183	A	OP1-P-O3'	5.25	116.76	105.20
32	2a	1491	G	OP2-P-O3'	5.25	116.76	105.20
32	1a	533	A	C5-C6-N6	-5.24	119.50	123.70
1	1A	101	A	N1-C6-N6	5.24	121.75	118.60
32	2a	343	U	O4'-C1'-N1	5.24	112.39	108.20
32	1a	1442	G	N3-C4-C5	-5.23	125.98	128.60
32	1a	115	G	P-O3'-C3'	5.22	125.97	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	24	G	C4-N9-C1'	5.22	133.29	126.50
1	2A	1312	U	C5-C4-O4	5.22	129.03	125.90
1	1A	1700	G	P-O3'-C3'	5.21	125.95	119.70
32	2a	993	G	N3-C4-N9	5.21	129.13	126.00
32	1a	300	A	N1-C6-N6	5.20	121.72	118.60
1	2A	801	G	O5'-P-OP2	-5.20	101.02	105.70
32	1a	687	A	P-O3'-C3'	5.19	125.92	119.70
32	1a	991	U	P-O3'-C3'	5.18	125.92	119.70
2	1B	24	G	N3-C4-C5	-5.17	126.02	128.60
32	2a	1065	U	P-O3'-C3'	5.17	125.90	119.70
32	2a	1465	C	C5-C4-N4	-5.16	116.58	120.20
1	1A	847	A	N1-C6-N6	-5.16	115.50	118.60
1	2A	2103	C	N3-C2-O2	-5.16	118.29	121.90
1	2A	1060	U	C6-N1-C1'	-5.15	113.99	121.20
1	1A	952	G	N3-C4-N9	-5.14	122.92	126.00
32	2a	992	U	P-O3'-C3'	5.13	125.85	119.70
32	2a	687	A	P-O3'-C3'	5.11	125.84	119.70
1	1A	1099	C	N3-C2-O2	-5.11	118.32	121.90
1	2A	1210	A	P-O3'-C3'	5.10	125.82	119.70
32	1a	1465	C	N3-C4-C5	5.10	123.94	121.90
2	1B	13	A	O5'-P-OP2	-5.09	101.12	105.70
1	1A	410	U	N3-C2-O2	-5.09	118.64	122.20
32	1a	343	U	C5-C4-O4	5.09	128.95	125.90
1	1A	1085	G	N9-C4-C5	-5.06	103.38	105.40
32	1a	993	G	N3-C4-N9	5.06	129.03	126.00
1	1A	952	G	N9-C4-C5	5.06	107.42	105.40
32	1a	1442	G	P-O3'-C3'	5.06	125.77	119.70
1	2A	1065	U	P-O3'-C3'	5.06	125.77	119.70
2	1B	59	A	C6-N1-C2	-5.05	115.57	118.60
32	2a	533	A	N1-C6-N6	5.05	121.63	118.60
32	1a	1054	C	N1-C2-O2	5.05	121.93	118.90
1	1A	1220	U	P-O3'-C3'	5.04	125.75	119.70
1	1A	1359	U	O4'-C1'-N1	5.03	112.23	108.20
32	2a	1067	A	P-O3'-C3'	5.03	125.74	119.70
1	2A	2157	G	C8-N9-C4	-5.03	104.39	106.40
1	2A	906	G	N9-C4-C5	5.03	107.41	105.40
32	2a	991	U	P-O3'-C3'	5.02	125.72	119.70
2	1B	102	A	N1-C2-N3	5.02	131.81	129.30
1	1A	2201	C	N1-C2-O2	5.01	121.91	118.90
1	1A	952	G	C6-C5-N7	5.01	133.40	130.40

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:1A:1005:A:C6	1:1A:1024:G:N2	29.32	1.00
13:1R:3:HIS:NE2	63:1R:303:HOH:O	1.96	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1405:A:N1	1:1A:1418:U:O4	1.97	0.96
1:2A:1038:C:N4	1:2A:1117:G:H1	1.64	0.95
1:1A:2188:G:O6	1:1A:2194:U:C4	2.21	0.94
1:2A:154(A):C:H42	1:2A:171:G:H1	1.16	0.91
1:2A:1038:C:H42	1:2A:1117:G:H1	0.90	0.90
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.38	0.89
1:1A:1005:A:N6	1:1A:1024:G:N2	29.82	0.88
2:2B:8:U:H3	2:2B:113:G:H1	1.21	0.88
1:1A:2159:C:N3	1:1A:2176:G:N2	2.20	0.88
1:1A:303:C:H42	1:1A:385:G:H1	1.19	0.88
1:2A:1047:G:H21	1:2A:1111:A:H62	1.16	0.88
1:2A:2128:C:H42	1:2A:2160:G:H1	1.19	0.88
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.39	0.87
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.10	0.85
1:1A:1005:A:N6	1:1A:1024:G:C2	30.61	0.85
5:1F:53:THR:HG22	5:1F:56:GLU:HG3	1.58	0.85
1:1A:2188:G:O6	1:1A:2194:U:O4	1.94	0.84
1:2A:2128:C:N4	1:2A:2160:G:H1	1.75	0.83
2:2B:6:C:N4	2:2B:115:G:H1	1.75	0.82
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	99.87	0.82
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.45	0.82
22:10:11:ARG:O	22:10:14:ARG:NH2	2.14	0.81
4:2E:11:MET:HG2	4:2E:24:THR:HG22	1.61	0.81
1:1A:1873:G:O2'	3:1D:253:GLN:NE2	2.14	0.81
1:2A:1842:G:O2'	3:2D:253:GLN:NE2	2.14	0.80
1:2A:1082:U:OP2	1:2A:1085:A:N6	2.15	0.80
21:2Z:2:GLU:HG2	21:2Z:56:VAL:HB	1.64	0.79
26:24:13:ARG:HH22	26:24:23:GLU:HG2	1.47	0.79
1:2A:854:G:H2'	1:2A:855:G:H8	1.49	0.78
1:1A:2297:C:OP2	28:16:6:ARG:NH1	2.16	0.78
1:1A:2133:C:OP2	1:1A:2167:C:N4	2.15	0.78
1:1A:2316:G:H22	1:1A:2324:U:H3	1.31	0.78
1:2A:1482:G:H1	1:2A:1506:C:H42	1.32	0.77
1:1A:2155:G:H3'	1:1A:2179:G:H21	1.50	0.77
1:1A:1556:A:H2'	1:1A:1557:A:O4'	1.83	0.77
1:1A:1310:G:OP1	27:15:19:ARG:NH2	2.16	0.77
1:2A:79:G:N2	1:2A:90:U:O2	30.58	0.77
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.67	0.76
1:2A:2166:G:N2	1:2A:2172:U:O4	2.19	0.76
1:1A:9:U:N3	1:1A:2641:A:C2	2.53	0.76
4:1E:47:VAL:HG21	4:1E:86:PRO:HD2	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:555:G:N1	1:1A:2045:G:OP1	2.18	0.75
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.20	0.75
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.68	0.74
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.20	0.74
18:1W:65:LEU:HD12	18:1W:68:ARG:HE	1.52	0.74
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.69	0.74
1:2A:1087:G:H1	1:2A:1102:C:H42	1.34	0.74
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.23	0.74
1:2A:1441:G:H5''	1:2A:1442:G:H5'	5.69	0.73
1:2A:154(A):C:N4	1:2A:171:G:H1	1.86	0.73
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.53	0.73
1:2A:2059:A:H2'	1:2A:2503:2MA:HM23	1.70	0.73
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.69	0.73
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.52	0.73
1:2A:1038:C:N3	1:2A:1117:G:N2	2.32	0.73
1:1A:1814:A:H5'	1:1A:2620:G:H4'	1.71	0.73
26:24:16:CYS:SG	26:24:17:GLY:N	2.62	0.73
21:2Z:91:LEU:HD11	21:2Z:96:VAL:HG11	1.72	0.72
6:2G:114:ILE:HB	6:2G:117:PHE:HB2	1.70	0.72
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.21	0.72
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.70	0.72
25:23:5:LYS:HG3	25:23:36:VAL:HG22	1.72	0.72
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.71	0.72
1:1A:2188:G:C6	1:1A:2194:U:O4	2.43	0.71
7:1H:101:ARG:HG2	7:1H:117:PRO:HG2	1.72	0.71
1:2A:1041:C:H42	1:2A:1114:G:H1	1.39	0.71
1:2A:427:U:OP1	3:2D:13:ARG:NH2	84.08	0.71
1:1A:929:G:H1	1:1A:940:C:H42	1.39	0.71
1:1A:2081:A:H2'	1:1A:2515:2MA:HM23	1.71	0.71
1:2A:2102:U:O2	1:2A:2187:G:O6	2.08	0.71
1:2A:2469:A:H4'	12:2Q:56:ARG:HG2	1.73	0.71
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.70	0.71
1:2A:2140:C:H2'	1:2A:2141:G:H8	1.54	0.70
9:2N:67:LEU:HD12	9:2N:87:LEU:HD13	1.73	0.70
22:20:49:LYS:H	22:20:80:HIS:HD1	1.38	0.70
1:1A:303:C:N4	1:1A:385:G:H1	1.88	0.70
1:2A:2145:C:O2'	1:2A:2147:G:N2	2.25	0.70
1:2A:984:A:H5''	1:2A:985:C:H5	1.57	0.70
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.73	0.70
1:1A:2457:G:OP1	5:1F:74:ARG:NH2	2.25	0.69
1:1A:656:A:OP1	11:1P:65:ARG:NH1	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	1.73	0.69
1:2A:1569:A:H5'	3:2D:61:LEU:HD21	1.73	0.69
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.74	0.69
1:1A:2355:C:HO2'	1:1A:2385:G:HO2'	1.39	0.69
1:2A:1047:G:N2	1:2A:1111:A:H62	1.90	0.69
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.24	0.69
1:2A:1046:A:N6	1:2A:1211:U:O2	149.57	0.69
1:1A:2134:G:O6	1:1A:2191:A:N7	2.25	0.69
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.75	0.69
1:1A:2359:C:HO2'	28:16:21:TYR:HH	1.41	0.69
1:1A:1246:C:H42	1:1A:1291:G:H1	3.80	0.69
1:2A:857:C:H4'	22:20:23:VAL:HG21	1.74	0.69
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.25	0.69
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.75	0.69
23:21:3:LYS:HB2	23:21:61:ARG:HH12	1.58	0.69
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.75	0.69
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.75	0.68
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.26	0.68
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.26	0.68
26:14:16:CYS:SG	26:14:17:GLY:N	2.66	0.68
1:1A:1431:G:O2'	1:1A:1442:U:O2	2.10	0.68
15:1T:31:SER:OG	15:1T:85:LYS:NZ	2.24	0.68
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.28	0.68
1:1A:1093:G:H2'	1:1A:1156:G:H22	1.59	0.68
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.26	0.68
1:1A:273:G:H21	8:1I:50:ARG:HD3	1.59	0.68
1:2A:1087:G:N2	1:2A:1102:C:N3	2.39	0.68
1:2A:384:U:H2'	1:2A:385:C:H6	1.59	0.68
1:1A:1094:A:OP2	1:1A:1155:C:N4	2.27	0.67
1:1A:1039:G:OP1	16:1U:50:ARG:NH2	2.27	0.67
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.75	0.67
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.27	0.67
1:2A:1286:A:H2'	1:2A:1287:A:H4'	6.25	0.67
10:2O:97:ARG:HA	10:2O:117:LEU:HD22	1.77	0.67
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.76	0.67
1:1A:1305:G:H22	1:1A:1331:G:H1'	39.76	0.67
1:1A:1221:G:N2	1:1A:1223:C:OP2	2.27	0.67
26:24:46:GLN:O	26:24:48:ARG:N	2.28	0.67
1:2A:2103:C:O2	1:2A:2186:G:N2	2.28	0.67
7:2H:40:GLU:OE1	7:2H:61:HIS:NE2	2.27	0.66
1:1A:1219:A:H1'	1:1A:1220:U:H5'	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2640:G:O3'	9:2N:74:ARG:NH2	2.20	0.66
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.29	0.66
16:1U:49:HIS:HA	16:1U:52:ARG:HG2	1.76	0.66
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.77	0.66
8:2I:114:LEU:HD11	8:2I:128:LEU:HB3	1.76	0.66
11:1P:124:LYS:HE3	11:1P:146:VAL:HG21	1.78	0.66
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.29	0.66
1:1A:1305:G:N2	1:1A:1331:G:H1'	39.51	0.66
1:1A:166:G:H2'	1:1A:167:G:H8	3.46	0.66
1:1A:1312:G:O5'	18:1W:15:ARG:NH2	2.29	0.65
1:2A:2134:A:N6	1:2A:2156:G:O2'	2.18	0.65
1:2A:309:G:N3	1:2A:329:G:O2'	2.29	0.65
1:1A:661:G:H1	1:1A:744:C:H42	107.57	0.65
26:24:59:PHE:HA	26:24:60:GLN:C	2.16	0.65
1:2A:2162:G:O3'	1:2A:2172:U:O2'	2.13	0.65
1:2A:2303:G:N2	1:2A:2313:C:O2	2.29	0.65
1:2A:468:G:N7	29:27:39:ARG:NH2	2.45	0.65
1:2A:79:G:H1	1:2A:90:U:H3	29.25	0.65
24:12:32:LEU:HD22	24:12:36:ARG:HH11	1.61	0.65
23:21:77:ALA:HA	23:21:80:LEU:HD13	1.79	0.65
5:2F:135:LYS:HG2	5:2F:137:LYS:HG2	1.79	0.65
1:2A:2343:C:O2'	1:2A:2373:G:O2'	2.13	0.65
24:22:1:MET:SD	24:22:56:GLN:NE2	2.69	0.65
1:1A:1005:A:H5'	1:1A:1038:C:H1'	50.50	0.64
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.31	0.64
1:2A:1062:G:H2'	1:2A:1063:G:H8	1.62	0.64
1:1A:2159:C:H42	1:1A:2176:G:H1	0.74	0.64
1:1A:2355:C:O2'	1:1A:2385:G:O2'	2.15	0.64
1:2A:2103:C:N3	1:2A:2104:G:N2	2.45	0.64
1:1A:2324:U:H5'	6:1G:88:ILE:HD11	1.80	0.64
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.30	0.64
1:2A:1025:G:O2'	63:2A:4446:HOH:O	2.15	0.64
1:2A:852:G:H2'	1:2A:853:G:H8	1.61	0.64
26:14:54:GLY:O	26:14:56:VAL:HA	1.97	0.64
1:2A:1059:G:C2	1:2A:1060:U:O4	2.50	0.64
14:2S:49:VAL:HG21	14:2S:77:ALA:HA	1.79	0.64
1:1A:1218:G:O2'	1:1A:1219:A:O5'	2.15	0.64
1:1A:2138:G:OP2	1:1A:2188:G:N2	2.31	0.64
1:1A:591:U:O2'	63:1A:4764:HOH:O	2.09	0.64
25:13:3:ARG:HD3	25:13:60:GLU:HG3	1.79	0.64
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1073:A:H2'	1:2A:1074:G:C8	2.33	0.64
1:2A:2180:U:H2'	1:2A:2181:G:C8	2.33	0.64
1:1A:2228:G:O2'	1:1A:2229:A:OP1	2.16	0.63
2:1B:106:G:H5'	21:1Z:31:ARG:HB3	1.80	0.63
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.63	0.63
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.80	0.63
1:2A:1360:A:OP2	9:2N:35:ARG:NH2	118.50	0.63
1:1A:1176:U:O2	4:1E:149:ARG:NH2	2.25	0.63
1:1A:1766:G:H8	1:1A:1770:A:H62	1.46	0.63
3:1D:76:PRO:HB2	3:1D:116:GLN:HE21	1.63	0.63
1:2A:1081:U:H3'	1:2A:1085:A:H61	1.62	0.63
1:2A:568:U:O2'	63:2A:4573:HOH:O	2.15	0.63
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.44	0.63
1:2A:2126:A:H4'	1:2A:2127:G:O5'	1.99	0.63
3:1D:13:ARG:NH1	3:1D:16:MET:SD	2.72	0.63
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.79	0.63
1:1A:2564:OMU:C6	1:1A:2564:OMU:C4	2.48	0.63
1:1A:2761:A:H5'	7:1H:4:ILE:HD12	1.81	0.63
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.33	0.63
1:2A:2781:A:H5''	1:2A:2782:G:H5'	1.81	0.63
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.22	0.63
3:2D:76:PRO:HB2	3:2D:116:GLN:HE21	1.63	0.63
1:1A:234:G:O6	30:18:8:LYS:NZ	2.25	0.63
12:2Q:42:ILE:HD12	12:2Q:97:VAL:HG21	1.80	0.63
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.63	0.62
1:2A:247:G:H4'	1:2A:386:G:C5	2.33	0.62
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	1.81	0.62
7:2H:17:VAL:HG13	7:2H:26:VAL:HG22	1.81	0.62
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.31	0.62
14:1S:30:ARG:HG3	14:1S:35:ILE:HD12	1.82	0.62
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.25	0.62
1:1A:555:G:H4'	1:1A:556:C:OP1	1.99	0.62
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	1.80	0.62
17:2V:62:LEU:HD23	17:2V:93:GLU:HG2	1.80	0.62
1:1A:902:G:O2'	22:10:27:GLU:OE2	2.18	0.62
1:1A:673:G:H2'	1:1A:674:G:C8	2.98	0.62
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.80	0.62
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.32	0.62
2:1B:13:A:N1	2:1B:69:G:O2'	2.27	0.62
1:2A:1081:U:H2'	1:2A:1082:U:H5''	1.82	0.62
1:2A:1047:G:H2'	1:2A:1110:G:H22	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:1:MET:HE2	24:12:6:VAL:HG22	1.81	0.61
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.65	0.61
14:2S:23:ARG:NH2	14:2S:84:GLN:OE1	2.33	0.61
1:2A:1057:A:H2'	1:2A:1058:G:H8	1.65	0.61
1:2A:11:G:H2'	1:2A:12:U:H5'	1.80	0.61
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.28	0.61
5:2F:140:LEU:HD11	5:2F:170:LEU:HD11	1.81	0.61
7:1H:90:LYS:HD3	7:1H:159:GLU:HG2	1.81	0.61
1:2A:2185:C:N4	1:2A:2186:G:O6	2.33	0.61
1:2A:2128:C:N3	1:2A:2160:G:N2	2.44	0.61
1:2A:1087:G:H1	1:2A:1102:C:N4	1.98	0.61
25:13:3:ARG:NH1	25:13:60:GLU:OE2	2.34	0.61
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.83	0.61
6:2G:112:PRO:HG3	26:24:43:TYR:HE2	1.65	0.61
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.33	0.61
1:1A:297:C:H2'	1:1A:298:G:H8	1.66	0.61
11:1P:88:LEU:HD11	11:1P:114:ILE:HD12	1.83	0.61
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.34	0.61
1:1A:1218:G:O2'	1:1A:1219:A:O4'	2.18	0.60
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.33	0.60
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.83	0.60
1:1A:1091:A:H5'	1:1A:1092:A:H5''	1.82	0.60
5:1F:165:ARG:HA	5:1F:168:ARG:HD3	1.83	0.60
14:1S:23:ARG:NH2	14:1S:84:GLN:OE1	2.34	0.60
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.83	0.60
1:1A:2156:A:O2'	1:1A:2181:G:N3	2.34	0.60
1:2A:2206:G:H8	1:2A:2207:G:N7	1.99	0.60
1:2A:852:G:H2'	1:2A:853:G:C8	2.36	0.60
1:1A:2137:G:N3	1:1A:2139:A:N6	2.47	0.60
1:2A:1066:U:O2'	1:2A:1068:G:OP2	2.18	0.60
1:1A:1005:A:OP2	1:1A:1006:C:N4	15.01	0.60
1:1A:2149:G:H21	1:1A:2195:A:H1'	1.67	0.60
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.35	0.60
1:2A:1045:A:H8	1:2A:1047:G:N3	1.99	0.60
1:1A:928:G:H1	1:1A:941:U:H3	1.49	0.60
2:1B:86:G:H1	2:1B:91:C:H42	1.49	0.60
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.75	0.60
26:24:48:ARG:O	26:24:50:VAL:N	2.34	0.60
12:2Q:63:LYS:HD2	21:2Z:175:VAL:HG21	1.83	0.60
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.84	0.59
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.67	0.59
25:13:3:ARG:HB2	25:13:60:GLU:HG3	1.84	0.59
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.85	0.59
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.37	0.59
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.85	0.59
1:1A:831:A:H2'	1:1A:839:G:N7	2.17	0.59
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.84	0.59
4:2E:52:LEU:HB3	4:2E:53:PRO:HD2	1.84	0.59
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.13	0.59
12:1Q:35:VAL:HG13	12:1Q:130:LYS:HB3	1.85	0.59
1:2A:2561:A:H2	10:2O:23:ARG:HH21	1.51	0.59
1:1A:2348:A:H61	22:10:43:THR:HG22	1.67	0.59
1:2A:864:G:H1'	1:2A:914:C:H42	1.67	0.59
21:2Z:10:ARG:NH1	21:2Z:26:GLY:O	2.36	0.59
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.35	0.59
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.84	0.59
1:1A:2285:A:H2'	1:1A:2286:A:C8	2.38	0.59
1:2A:323:G:HO2'	1:2A:1205:U:H3	0.67	0.59
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.35	0.59
1:1A:2597:U:H4'	1:1A:2598:C:OP1	2.02	0.58
1:1A:7:G:H2'	1:1A:8:A:O4'	2.03	0.58
1:1A:354:A:H2	1:1A:1255:A:HO2'	1.50	0.58
11:1P:126:VAL:HG12	11:1P:148:LEU:HG	1.86	0.58
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.38	0.58
8:1I:73:GLU:HG2	8:1I:139:GLN:HB2	1.85	0.58
1:2A:2748:A:O2'	7:2H:63:SER:O	2.20	0.58
1:1A:2442:A:H2'	1:1A:2442:A:N3	2.17	0.58
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.39	0.58
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.84	0.58
1:1A:262:C:H42	1:1A:282:G:H1	1.52	0.58
2:1B:91:C:OP2	12:1Q:16:ARG:NH1	2.36	0.58
1:2A:881:G:H1	1:2A:895:U:H3	1.51	0.58
18:2W:65:LEU:HD12	18:2W:68:ARG:HE	1.68	0.58
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.85	0.58
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.68	0.58
1:1A:904:C:H4'	22:10:23:VAL:HG21	1.84	0.58
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.85	0.58
1:1A:2573:A:H2	10:1O:23:ARG:HH21	1.52	0.58
10:1O:68:GLU:OE1	10:1O:78:ARG:NH1	2.36	0.58
1:1A:1003:U:H5''	12:1Q:14:ARG:HD3	1.86	0.58
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.20	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:11:3:LYS:HG3	23:11:4:VAL:H	1.69	0.58
1:1A:1346:U:H4'	1:1A:1347:A:H5''	1.85	0.58
1:2A:1094:U:OP1	1:2A:1096:A:N6	2.37	0.57
1:2A:2108:C:O2	1:2A:2182:G:N2	2.37	0.57
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.86	0.57
1:1A:1699:A:OP1	13:1R:8:ARG:NH1	2.37	0.57
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.37	0.57
15:2T:24:PRO:HA	15:2T:49:VAL:HG23	1.85	0.57
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD23	1.86	0.57
1:2A:2232:U:P	23:21:40:ARG:HH12	2.28	0.57
1:2A:2635:C:O2'	4:2E:48:GLN:NE2	2.37	0.57
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.39	0.57
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.36	0.57
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.84	0.57
29:17:24:THR:HG23	29:17:27:GLY:H	1.69	0.57
1:1A:1087:C:H42	1:1A:1160:G:H1	1.50	0.57
19:1X:60:ARG:HH12	29:17:47:ARG:HH12	1.52	0.57
1:2A:2186:G:N1	1:2A:2187:G:C6	2.72	0.57
2:2B:57:A:H1'	6:2G:29:TRP:HB2	1.87	0.57
7:2H:11:VAL:HG13	7:2H:15:VAL:HG22	1.85	0.57
8:2I:101:LEU:HD11	8:2I:140:LEU:HD11	1.85	0.57
6:1G:114:ILE:HB	6:1G:117:PHE:HB2	1.84	0.57
1:2A:1059:G:C5	1:2A:1060:U:N3	2.73	0.57
1:1A:2402:U:P	30:18:35:GLN:HE22	2.27	0.57
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.35	0.57
10:1O:98:VAL:HG13	10:1O:117:LEU:HB3	1.85	0.57
1:2A:970:C:HO2'	1:2A:984:A:HO2'	1.52	0.57
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.85	0.57
1:1A:238:C:O2	30:18:12:LYS:NZ	2.32	0.57
6:1G:143:GLU:HA	26:14:28:LYS:HD2	1.86	0.57
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.21	0.57
1:2A:2197:U:H1'	1:2A:2198:A:C8	2.39	0.57
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.23	0.57
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	1.86	0.57
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.21	0.57
1:2A:848:G:H2'	1:2A:849:A:C8	2.40	0.57
26:14:57:GLU:HB2	26:14:58:ARG:HA	1.87	0.57
19:1X:43:VAL:HG21	19:1X:81:VAL:HG11	1.87	0.57
22:10:38:VAL:HB	22:10:59:LEU:HB2	1.87	0.57
1:1A:1066:A:N1	1:1A:1186:U:O2'	2.31	0.57
1:1A:173:C:H2'	1:1A:174:U:C6	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.70	0.57
4:2E:9:VAL:HB	15:2T:3:ARG:HG2	1.87	0.57
8:1I:8:PRO:HD3	8:1I:15:VAL:HB	1.87	0.56
12:1Q:42:ILE:HD12	12:1Q:97:VAL:HG21	1.87	0.56
1:2A:479:A:N3	1:2A:481:G:H5''	2.19	0.56
6:2G:41:GLN:HB3	6:2G:43:LEU:HD13	1.85	0.56
7:2H:89:ILE:O	7:2H:129:THR:HG23	2.05	0.56
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.87	0.56
1:1A:2152:U:O2'	1:1A:2155:G:O2'	2.20	0.56
1:1A:1857:G:H4'	3:1D:242:ARG:HH21	1.70	0.56
14:1S:15:ARG:O	14:1S:19:LYS:HG2	2.05	0.56
1:2A:2112:G:H2'	1:2A:2113:U:C6	2.40	0.56
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.86	0.56
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.86	0.56
1:2A:1063:G:H2'	1:2A:1065:U:H6	1.70	0.56
1:1A:1362:U:H2'	1:1A:1363:A:H8	1.70	0.56
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.87	0.56
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	1.88	0.56
20:1Y:28:LYS:HD2	20:1Y:40:GLU:HG3	1.86	0.56
1:2A:1063:G:H1	1:2A:1075:C:H42	1.54	0.56
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.87	0.56
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.37	0.56
1:1A:323:A:H5''	20:1Y:86:ARG:HH21	1.69	0.56
1:2A:1783:A:H5'	1:2A:2608:G:H4'	1.88	0.56
1:2A:2127:G:H2'	1:2A:2128:C:O4'	2.06	0.56
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.40	0.56
1:2A:321:G:OP1	5:2F:135:LYS:NZ	2.38	0.56
1:1A:10:G:N2	1:1A:2812:A:O2'	2.38	0.56
1:1A:1525:G:O2'	1:1A:1605:A:N7	2.37	0.56
1:1A:632:A:H3'	1:1A:633:G:H8	2.50	0.56
7:1H:84:SER:OG	7:1H:132:ARG:NH1	2.39	0.56
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	1.87	0.56
1:2A:1075:C:H2'	1:2A:1076:C:H5'	1.88	0.56
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	1.88	0.56
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.39	0.56
1:1A:186:A:N6	1:1A:2442:A:O2'	2.38	0.56
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.41	0.56
31:19:14:CYS:HA	31:19:27:CYS:HB2	1.87	0.56
1:1A:1957:G:H1'	1:1A:1986:G:N2	2.20	0.56
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.41	0.56
5:1F:155:LEU:HB2	5:1F:189:THR:HG21	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	1.87	0.55
26:24:59:PHE:HA	26:24:61:ARG:N	2.21	0.55
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.89	0.55
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.06	0.55
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH2	2.21	0.55
30:18:14:VAL:HG23	30:18:24:ALA:HB2	1.87	0.55
4:1E:47:VAL:HG12	4:1E:49:LEU:HD13	1.88	0.55
9:1N:12:ARG:NH1	9:1N:50:ASP:OD2	2.39	0.55
26:24:41:PRO:HG3	26:24:49:PHE:CE2	2.41	0.55
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.39	0.55
1:1A:2149:G:N2	1:1A:2195:A:H1'	2.22	0.55
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.20	0.55
1:1A:166:G:H2'	1:1A:167:G:C8	3.83	0.55
1:1A:2240:G:OP1	3:1D:261:LYS:NZ	2.36	0.55
1:1A:181:C:O2'	1:1A:849:A:N3	2.32	0.55
1:1A:2148:A:H4'	1:1A:2149:G:O5'	2.06	0.55
21:1Z:144:LEU:HD11	21:1Z:150:LEU:HD22	1.87	0.55
1:2A:2351:G:HO2'	1:2A:2352:A:H8	1.54	0.55
1:2A:652(E):G:O6	1:2A:652(S):C:N4	2.40	0.55
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.72	0.55
25:13:55:ARG:HD3	63:13:206:HOH:O	2.05	0.55
1:1A:236:G:H4'	1:1A:413:G:C5	2.41	0.55
1:2A:2303:G:O2'	6:2G:132:ASN:HB2	2.07	0.55
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.89	0.55
21:2Z:144:LEU:HD11	21:2Z:150:LEU:HD22	1.89	0.55
1:1A:1199:C:OP1	16:1U:92:ARG:NH2	2.29	0.55
1:1A:1362:U:H2'	1:1A:1363:A:C8	2.42	0.55
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.41	0.55
1:1A:691:G:N2	1:1A:700:A:H1'	2.22	0.55
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.42	0.55
18:1W:18:ARG:NH1	18:1W:76:VAL:O	2.40	0.55
26:24:13:ARG:N	26:24:29:PRO:O	2.37	0.55
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.72	0.55
4:2E:135:HIS:NE2	63:2E:403:HOH:O	2.33	0.55
22:20:11:ARG:O	22:20:14:ARG:NH2	2.40	0.55
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.72	0.55
1:2A:2305:A:H5''	6:2G:134:GLY:HA3	1.89	0.55
1:2A:1482:G:H1	1:2A:1506:C:N4	2.02	0.55
1:1A:976:G:H5'	1:1A:1358:U:O2'	103.11	0.54
1:1A:2740:G:O2'	10:1O:70:LYS:NZ	2.39	0.54
1:2A:1073:A:H2'	1:2A:1074:G:H8	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:624:C:H2'	1:2A:625:G:H8	2.46	0.54
1:1A:532:A:N6	1:1A:1206:G:O2'	79.80	0.54
21:1Z:103:ARG:HD3	21:1Z:136:PHE:CD1	2.42	0.54
1:2A:2319:G:N2	14:2S:3:ARG:HD3	2.21	0.54
1:2A:827:U:O2'	1:2A:2068:U:C2	2.58	0.54
1:1A:2450:U:O2'	1:1A:2452:C:OP1	2.16	0.54
2:1B:78:A:C2	2:1B:100:A:C4	2.96	0.54
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.89	0.54
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.42	0.54
1:2A:2850:A:N7	1:2A:2868:A:O2'	2.38	0.54
1:1A:1829:U:H5'	3:1D:259:THR:CG2	2.36	0.54
6:2G:109:VAL:HG11	6:2G:142:PRO:HB3	1.88	0.54
1:2A:1754:C:H5	15:2T:96:ARG:NH2	2.06	0.54
17:2V:40:LEU:HB2	17:2V:46:VAL:HG12	1.88	0.54
1:2A:2420:C:H5'	28:26:54:ILE:HD11	1.90	0.54
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.43	0.54
1:2A:2577:A:H2'	1:2A:2614:A:N6	2.23	0.54
1:1A:1532:A:H2'	1:1A:1533:G:H8	1.72	0.54
1:1A:2859:U:H4'	1:1A:2878:A:C2	2.43	0.54
2:1B:57:A:H1'	6:1G:29:TRP:HB2	1.89	0.54
7:1H:25:LYS:NZ	7:1H:32:GLU:OE1	2.35	0.54
1:1A:1952:G:O2'	1:1A:1990:G:O6	2.19	0.54
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.41	0.54
1:2A:320:A:H4'	1:2A:322:A:N7	2.22	0.54
1:1A:2902:G:H4'	1:1A:2903:G:O5'	2.08	0.54
6:1G:150:ASP:OD1	6:1G:151:ALA:N	2.41	0.54
1:2A:1076:C:H4'	1:2A:1077:A:OP1	2.08	0.54
1:2A:320:A:H4'	1:2A:322:A:C8	2.42	0.54
1:1A:1899:A:H5'	1:1A:1900:G:OP2	2.07	0.54
1:1A:2298:A:H4'	1:1A:2299:A:O4'	2.08	0.54
1:2A:2156:G:O6	1:2A:2157:G:N2	2.38	0.54
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.43	0.54
26:14:57:GLU:HB2	26:14:58:ARG:HE	1.73	0.54
1:1A:1018:A:H8	1:1A:1018:A:OP1	1.91	0.54
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.73	0.54
15:1T:49:VAL:HG12	15:1T:63:VAL:HG22	1.88	0.54
19:1X:29:TRP:CE3	19:1X:78:LYS:HB3	2.43	0.54
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.40	0.54
1:2A:2112:G:H2'	1:2A:2113:U:H6	1.73	0.54
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.89	0.54
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:964:A:H5''	2:1B:98:G:O2'	2.08	0.53
1:1A:1185:C:O3'	9:1N:25:ARG:NH1	2.41	0.53
15:1T:53:ARG:O	15:1T:59:THR:HB	2.08	0.53
1:2A:1416:G:O2'	1:2A:1417:C:OP2	2.25	0.53
1:2A:2125:G:H22	1:2A:2172:U:H3'	1.72	0.53
1:2A:424:G:H2'	1:2A:425:G:H8	2.72	0.53
7:2H:150:ALA:HA	7:2H:153:LYS:HG3	1.89	0.53
1:1A:171:A:N3	1:1A:460:C:O2'	2.39	0.53
1:1A:2476:C:H1'	63:1A:4823:HOH:O	2.07	0.53
1:1A:275:C:H2'	1:1A:276:C:C6	2.43	0.53
6:1G:97:ASP:HA	6:1G:100:TRP:HD1	1.73	0.53
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.89	0.53
5:2F:156:LEU:HD21	5:2F:163:VAL:HG12	1.90	0.53
8:2I:57:ARG:O	8:2I:61:ARG:HG2	2.08	0.53
7:1H:3:ARG:HH22	7:1H:66:GLY:N	2.07	0.53
26:24:40:HIS:HB3	26:24:43:TYR:CD2	2.43	0.53
1:2A:1024:G:H2'	1:2A:1024:G:N3	3.29	0.53
1:2A:1057:A:N1	1:2A:1081:U:O4	2.40	0.53
5:2F:161:GLU:O	5:2F:165:ARG:HG3	2.08	0.53
1:1A:1098:C:H2'	1:1A:1099:C:O4'	2.08	0.53
1:1A:2144:U:H2'	1:1A:2145:G:C8	2.42	0.53
7:1H:27:LYS:HG2	7:1H:32:GLU:HG2	1.89	0.53
13:1R:59:ASP:N	13:1R:59:ASP:OD1	2.40	0.53
19:1X:44:GLU:HG3	19:1X:51:VAL:HG23	1.90	0.53
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.91	0.53
26:14:15:ILE:HD12	26:14:21:VAL:HG22	1.91	0.53
7:1H:3:ARG:HE	7:1H:54:ARG:HH12	1.57	0.53
21:2Z:179:ASP:H	21:2Z:182:LYS:HE3	1.74	0.53
13:1R:33:ARG:NH2	27:15:57:VAL:O	2.32	0.53
1:1A:2122:G:H1	1:1A:2211:U:H3	1.56	0.53
1:1A:405:C:N4	63:1A:5502:HOH:O	2.42	0.53
1:1A:560:C:O3'	16:1U:53:ARG:NH1	2.42	0.53
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.91	0.53
1:2A:2287:A:H61	1:2A:2344:U:H3	1.56	0.53
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.43	0.53
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.41	0.53
5:1F:110:LEU:HD12	5:1F:205:ARG:HD2	1.91	0.53
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.41	0.53
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.91	0.53
1:2A:2511:U:O4	1:2A:2575:C:N3	2.41	0.53
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	1.91	0.53
26:14:62:ARG:C	26:14:64:GLY:HA2	2.29	0.53
1:1A:1653:C:N4	1:1A:1668:G:OP2	2.38	0.53
1:1A:2188:G:O6	1:1A:2194:U:C5	2.62	0.53
20:1Y:43:ASN:HB3	20:1Y:65:ALA:HB3	1.89	0.53
2:2B:95:C:N4	63:2B:3112:HOH:O	2.41	0.53
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.08	0.53
21:2Z:119:GLU:OE1	21:2Z:122:ARG:NH1	2.42	0.53
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.08	0.53
22:10:70:GLN:HG2	22:10:80:HIS:HE2	1.74	0.53
1:1A:2418:U:H2'	1:1A:2418:U:OP2	2.09	0.53
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.41	0.53
1:1A:70:A:N7	19:1X:31:HIS:HE1	2.07	0.53
1:2A:2184:G:C2	1:2A:2185:C:H1'	2.43	0.53
1:2A:300:A:O2'	1:2A:564:C:N3	74.33	0.53
1:2A:639:U:H2'	1:2A:640:C:C6	2.44	0.53
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.39	0.53
3:2D:75:ILE:HG21	3:2D:99:ASP:HB2	1.90	0.53
1:1A:178:G:O6	1:1A:194:G:O2'	2.24	0.53
1:1A:1836:U:O2	3:1D:50:THR:HB	2.09	0.53
1:1A:664:U:H2'	1:1A:665:C:C6	2.44	0.53
1:1A:2801:C:OP1	4:1E:61:ARG:NH2	2.42	0.53
5:1F:110:LEU:HD21	5:1F:181:LEU:HG	1.91	0.53
21:1Z:198:LYS:HD3	21:1Z:202:GLU:HB2	1.90	0.53
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.90	0.53
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.90	0.53
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.91	0.52
27:15:41:PRO:O	27:15:44:THR:OG1	2.26	0.52
1:1A:714:U:O2	30:18:2:PRO:HD2	2.09	0.52
12:1Q:8:LYS:HA	21:1Z:197:ILE:HB	1.91	0.52
17:1V:43:GLU:N	17:1V:43:GLU:OE1	2.42	0.52
13:2R:36:THR:HG22	13:2R:37:THR:H	1.74	0.52
1:1A:2367:C:H1'	22:10:39:ARG:HH21	1.74	0.52
1:1A:2416:C:O3'	11:1P:77:ARG:NH2	2.42	0.52
2:2B:6:C:N3	2:2B:115:G:N2	2.44	0.52
1:1A:1100:A:H61	1:1A:1151:U:H3	1.58	0.52
1:2A:1710:C:H2'	1:2A:1711:C:H6	1.74	0.52
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.44	0.52
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.09	0.52
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.92	0.52
1:1A:2156:A:OP2	1:1A:2178:G:N1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	1.90	0.52
1:2A:2129:C:H2'	1:2A:2130:U:C2	2.44	0.52
1:2A:876:C:H2'	1:2A:877:U:O4'	2.10	0.52
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.75	0.52
1:1A:1005:A:C5	1:1A:1024:G:N2	28.01	0.52
1:1A:1387:U:O4'	19:1X:57:LEU:HD23	2.10	0.52
1:1A:1900:G:H2'	1:1A:1901:C:C6	2.45	0.52
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.92	0.52
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.90	0.52
17:2V:35:LEU:HB2	17:2V:57:VAL:HG13	1.90	0.52
1:1A:1500:A:H5''	63:1A:5224:HOH:O	2.09	0.52
1:1A:240:A:C5	1:1A:241:G:H1'	2.45	0.52
13:1R:96:ARG:HH12	13:1R:117:VAL:HG13	1.74	0.52
1:2A:1247:A:OP1	5:2F:95:ARG:NH2	2.31	0.52
1:2A:1250:G:H5''	63:2A:4844:HOH:O	2.08	0.52
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.45	0.52
1:2A:2067:G:O2'	1:2A:2069:G:H5'	2.09	0.52
1:2A:2125:G:O2'	1:2A:2173:A:N6	2.41	0.52
1:2A:300:A:H8	1:2A:300:A:O5'	2.85	0.52
7:2H:3:ARG:HE	7:2H:54:ARG:HH12	1.58	0.52
1:2A:2012:G:H4'	18:2W:96:ILE:HD13	1.92	0.52
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.08	0.52
6:1G:110:ALA:HB1	6:1G:140:ILE:HG22	1.92	0.52
1:2A:2146:C:H4'	1:2A:2147:G:C8	2.45	0.52
1:2A:2659:G:O2'	7:2H:175:LYS:NZ	2.42	0.52
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.09	0.52
1:2A:854:G:H2'	1:2A:855:G:C8	2.39	0.52
8:2I:65:ALA:O	8:2I:69:LYS:N	2.41	0.52
13:2R:55:ALA:HB2	13:2R:79:LEU:HD13	1.91	0.52
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.45	0.52
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.44	0.52
1:2A:2638:G:P	4:2E:82:ARG:HH12	2.33	0.52
1:2A:581:C:H2'	1:2A:582:G:C8	2.45	0.52
3:2D:79:VAL:HG21	3:2D:111:LEU:HD11	1.91	0.52
2:1B:19:G:H1	2:1B:64:C:H42	1.57	0.52
9:1N:34:LEU:O	9:1N:49:GLY:HA3	2.10	0.52
13:1R:53:HIS:HD1	13:1R:94:TYR:HH	1.52	0.52
1:2A:2140:C:H2'	1:2A:2141:G:C8	2.41	0.52
1:2A:637:A:OP1	11:2P:133:SER:OG	2.23	0.52
11:2P:138:LEU:HD23	11:2P:145:PRO:HB3	1.90	0.52
1:1A:1091:A:H1'	1:1A:1093:G:N3	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1432:C:H2'	1:1A:1433:C:C6	2.44	0.52
1:1A:953:U:H4'	12:1Q:101:ARG:HH22	1.75	0.52
2:1B:66:A:H61	2:1B:108:U:H2'	1.75	0.52
7:1H:9:ILE:HD11	7:1H:69:ARG:HG2	1.92	0.52
11:1P:17:LYS:HE3	11:1P:27:HIS:CE1	2.45	0.52
1:2A:1063:G:H2'	1:2A:1065:U:C6	2.45	0.52
6:2G:106:LEU:HD12	6:2G:110:ALA:HB3	1.92	0.52
13:2R:38:VAL:HG12	13:2R:42:LYS:HE3	1.92	0.52
18:2W:9:TYR:H	18:2W:102:HIS:CE1	2.27	0.52
26:14:47:GLN:HG2	26:14:49:PHE:H	1.74	0.51
1:1A:1495:G:O2'	1:1A:1575:A:N1	2.36	0.51
1:1A:2389:A:H2'	1:1A:2390:A:C8	2.45	0.51
21:1Z:52:SER:OG	21:1Z:53:ILE:N	2.40	0.51
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.45	0.51
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.45	0.51
8:2I:77:LEU:HD11	8:2I:100:ALA:HB1	1.91	0.51
1:1A:167:G:H2'	1:1A:168:G:H8	2.42	0.51
1:1A:843:C:H2'	1:1A:844:C:C6	2.45	0.51
3:1D:164:GLN:OE1	3:1D:176:ARG:NH2	2.43	0.51
7:1H:124:GLU:OE2	7:1H:132:ARG:HD2	2.09	0.51
1:2A:172:C:H2'	1:2A:173:G:H8	1.75	0.51
1:2A:2224:G:OP1	3:2D:268:ARG:NE	2.43	0.51
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.46	0.51
1:2A:817:C:O2'	1:2A:839:U:H5''	2.10	0.51
1:1A:1023:G:H2'	1:1A:1024:G:C8	3.51	0.51
1:1A:1219:A:H4'	1:1A:1220:U:OP1	2.09	0.51
1:2A:500:G:N1	1:2A:503:A:OP2	2.43	0.51
17:2V:60:GLU:OE1	17:2V:97:LYS:NZ	2.43	0.51
25:13:29:ARG:HG3	25:13:30:ARG:HG3	1.91	0.51
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.93	0.51
1:1A:1263:C:H42	1:1A:1277:G:H1	1.57	0.51
1:1A:2331:G:N2	14:1S:3:ARG:HA	2.25	0.51
1:2A:2172:U:H4'	1:2A:2173:A:OP2	2.10	0.51
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.91	0.51
1:1A:1246:C:N4	1:1A:1291:G:H1	3.65	0.51
1:1A:1834:A:O2'	3:1D:259:THR:HG21	2.09	0.51
1:2A:526:A:O2'	1:2A:2043:C:O2	2.27	0.51
2:2B:49:C:H2'	2:2B:50:G:C8	2.46	0.51
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.92	0.51
6:2G:150:ASP:OD1	6:2G:151:ALA:N	2.43	0.51
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:16:ARG:HG2	12:2Q:18:LYS:HD3	1.93	0.51
20:2Y:19:LYS:HE2	20:2Y:20:TYR:CE2	2.46	0.51
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.32	0.51
15:1T:16:ARG:NH2	15:1T:83:ILE:O	2.42	0.51
30:28:14:VAL:HG23	30:28:24:ALA:HB2	1.92	0.51
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.76	0.51
4:2E:181:LEU:HD11	15:2T:6:LEU:HD23	1.93	0.51
1:2A:2641:G:P	9:2N:74:ARG:HH22	2.32	0.51
10:2O:98:VAL:HG13	10:2O:117:LEU:HB3	1.93	0.51
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.10	0.51
1:1A:2454:C:H2'	1:1A:2455:C:H6	1.75	0.51
1:1A:2579:G:H2'	1:1A:2580:C:C6	2.46	0.51
3:1D:75:ILE:HG21	3:1D:99:ASP:HB2	1.91	0.51
15:1T:56:GLY:O	15:1T:59:THR:HG23	2.11	0.51
1:2A:121:G:H4'	1:2A:149:A:H5'	1.93	0.51
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.26	0.51
1:2A:807:U:O2'	1:2A:2060:A:N1	2.44	0.51
6:2G:96:ARG:O	6:2G:99:MET:HB3	2.10	0.51
25:13:37:LEU:HB3	25:13:43:ILE:HD13	1.92	0.51
1:1A:1750:G:H2'	1:1A:1751:G:H8	1.74	0.51
21:1Z:19:ARG:HH11	21:1Z:84:GLU:HB2	1.76	0.51
1:2A:422:A:H2'	1:2A:423:A:C8	2.46	0.51
1:2A:900:A:H2'	1:2A:901:A:O4'	2.10	0.51
2:2B:2:C:H2'	2:2B:3:C:H6	1.75	0.51
1:1A:2831:A:OP2	4:1E:110:GLY:N	2.39	0.51
1:1A:517:A:H2'	1:1A:518:G:O4'	2.10	0.51
2:2B:112:U:H2'	2:2B:113:G:H8	1.76	0.51
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.11	0.51
1:1A:1560:U:H2'	1:1A:1561:C:C6	2.46	0.50
1:1A:19:C:OP2	16:1U:30:LYS:NZ	2.44	0.50
1:1A:2376:C:H2'	1:1A:2377:G:O4'	2.11	0.50
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.28	0.50
1:2A:1062:G:H2'	1:2A:1063:G:C8	2.46	0.50
1:2A:2133:G:O2'	1:2A:2158:A:N6	2.44	0.50
1:2A:2321:G:O2'	1:2A:2322:A:OP1	2.28	0.50
1:2A:26:G:H1'	1:2A:515:A:H61	1.76	0.50
1:1A:794:U:O2	1:1A:2036:A:H1'	2.12	0.50
1:1A:2171:G:H2'	1:1A:2172:U:O4'	2.11	0.50
1:1A:312:C:H2'	1:1A:313:A:H8	1.76	0.50
5:1F:13:SER:OG	5:1F:127:GLU:OE1	2.24	0.50
10:1O:120:GLU:OE1	15:1T:67:SER:OG	2.23	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.44	0.50
1:2A:1263:U:H1'	27:25:10:LYS:HG3	1.93	0.50
1:2A:1078:U:O2'	1:2A:1079:C:OP2	2.28	0.50
1:2A:277:C:H4'	1:2A:278:A:OP2	2.12	0.50
1:2A:579:G:H2'	1:2A:580:C:C6	2.46	0.50
1:2A:800:A:OP1	1:2A:800:A:H8	1.93	0.50
6:2G:145:THR:HG23	6:2G:148:MET:H	1.75	0.50
1:1A:211:A:H3'	1:1A:448:U:H5'	1.93	0.50
1:2A:16:G:H2'	1:2A:17:G:H8	1.76	0.50
1:2A:1935:G:H1'	1:2A:1964:G:N2	2.27	0.50
12:2Q:60:ARG:NH2	21:2Z:181:GLU:OE2	2.44	0.50
1:1A:1494:G:HO2'	1:1A:1934:A:HO2'	125.70	0.50
1:2A:8:A:H2'	1:2A:9:U:C6	2.46	0.50
1:1A:1557:A:H2'	1:1A:1558:G:O4'	2.11	0.50
1:1A:1588:G:H5''	1:1A:1589:A:OP2	2.12	0.50
1:1A:2879:G:H2'	1:1A:2880:C:O4'	2.12	0.50
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.44	0.50
1:1A:2573:A:H2	10:1O:23:ARG:NH2	2.09	0.50
16:1U:97:ASP:OD1	16:1U:101:ARG:NH1	2.45	0.50
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.11	0.50
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.92	0.50
18:2W:78:GLU:OE2	18:2W:99:ARG:NH1	2.40	0.50
1:1A:1097:G:H2'	1:1A:1098:C:C6	2.47	0.50
1:1A:99:G:O3'	24:12:7:ARG:NH2	2.45	0.50
3:1D:10:THR:OG1	3:1D:13:ARG:HG2	2.11	0.50
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.36	0.50
1:2A:184:C:H2'	1:2A:185:U:C6	2.46	0.50
1:1A:1346:U:H4'	1:1A:1347:A:C5'	2.41	0.50
1:1A:207:A:C2	1:1A:224:U:H4'	2.46	0.50
25:23:8:LEU:O	25:23:32:GLN:N	2.41	0.50
1:1A:1435:G:H2'	1:1A:1436:U:C6	2.87	0.50
1:1A:2308:U:OP2	14:1S:9:ARG:NH2	2.45	0.50
1:1A:2044:U:O2'	1:1A:2629:C:H5'	2.11	0.50
6:1G:107:LEU:HD11	6:1G:178:PHE:CE1	2.46	0.50
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.93	0.50
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.93	0.50
1:2A:116:C:H2'	1:2A:117:G:O4'	2.11	0.50
1:2A:271(Z):C:H1'	1:2A:272(C):G:H1'	1.94	0.50
1:1A:26:G:C6	1:1A:27:G:N1	2.80	0.50
2:1B:103:G:H21	21:1Z:73:GLN:NE2	2.10	0.50
2:1B:14:U:OP2	2:1B:70:C:O2'	2.23	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1442:G:N3	1:2A:1442:G:H2'	2.93	0.50
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.47	0.50
1:2A:19:C:H2'	1:2A:20:C:H6	1.77	0.50
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.47	0.50
1:2A:2816:C:O2	1:2A:2883:A:O2'	2.28	0.50
1:1A:2701:U:H4'	1:1A:2702:C:H5'	1.94	0.49
6:1G:179:PRO:HB2	26:14:42:PHE:HE2	1.76	0.49
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.47	0.49
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.94	0.49
1:1A:1458:A:H2'	1:1A:1459:G:C8	2.48	0.49
5:1F:161:GLU:O	5:1F:165:ARG:HG3	2.12	0.49
23:21:83:GLU:N	23:21:83:GLU:OE1	2.45	0.49
1:1A:2359:C:H2'	1:1A:2360:U:C6	2.47	0.49
1:1A:2724:U:O2'	1:1A:2725:A:OP2	2.25	0.49
1:1A:27:G:N2	1:1A:537:G:H1'	2.28	0.49
1:1A:632:A:H5'	1:1A:633:G:OP2	5.49	0.49
1:1A:906:G:O2'	1:1A:962:G:O6	2.25	0.49
5:1F:154:VAL:HG22	5:1F:191:ARG:HB2	1.94	0.49
26:24:57:GLU:CB	26:24:58:ARG:HD2	2.41	0.49
1:2A:1506:C:H2'	1:2A:1507:A:H5'	1.94	0.49
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.94	0.49
1:2A:2102:U:C2	1:2A:2187:G:O6	2.65	0.49
1:2A:2443:C:H2'	1:2A:2444:G:H8	1.77	0.49
1:2A:588:U:H2'	1:2A:589:C:C6	2.47	0.49
1:1A:1821:C:H5''	1:1A:1822:A:OP1	2.13	0.49
1:1A:2156:A:N6	1:1A:2179:G:H4'	2.28	0.49
1:1A:494:G:N7	29:17:39:ARG:NH2	2.59	0.49
2:1B:48:A:H2'	2:1B:49:C:C6	2.48	0.49
7:1H:125:VAL:HG12	7:1H:127:GLU:O	2.12	0.49
8:1I:38:LEU:HB2	8:1I:40:THR:HG23	1.94	0.49
13:1R:53:HIS:ND1	13:1R:94:TYR:OH	2.29	0.49
1:2A:667:U:O2	30:28:2:PRO:HD2	2.13	0.49
1:2A:1084:A:H3'	1:2A:1085:A:H4'	1.95	0.49
1:2A:2115:G:H4'	1:2A:2167:U:H4'	1.93	0.49
14:2S:15:ARG:HD3	14:2S:25:ARG:HH21	1.77	0.49
1:1A:2377:G:O6	30:18:39:LYS:HE3	2.12	0.49
1:1A:641:G:OP1	5:1F:40:GLN:NE2	2.32	0.49
1:1A:2405:A:O2'	11:1P:60:MET:O	2.22	0.49
25:23:6:VAL:HG12	25:23:56:VAL:HG22	1.95	0.49
1:2A:125:G:OP1	29:27:14:LYS:NZ	2.46	0.49
1:2A:1384:A:O2'	1:2A:1404:C:O2'	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.45	0.49
1:2A:250:G:OP2	30:28:13:ARG:NH1	2.42	0.49
1:2A:740:U:H2'	1:2A:741:G:C8	2.47	0.49
18:2W:65:LEU:HD12	18:2W:68:ARG:NE	2.28	0.49
1:1A:1302:G:H5'	1:1A:1303:C:OP2	2.11	0.49
1:1A:1735:U:O2	1:1A:1747:A:H5'	2.13	0.49
1:2A:2310:A:N1	6:2G:79:ASN:ND2	2.59	0.49
1:2A:958:U:O2	2:2B:90:A:O2'	2.23	0.49
20:2Y:20:TYR:CE2	20:2Y:43:ASN:HA	2.48	0.49
22:10:27:GLU:HB2	22:10:69:PHE:HD1	1.78	0.49
1:1A:1285:G:H2'	1:1A:1286:U:O4'	2.12	0.49
1:1A:997:G:OP1	12:1Q:16:ARG:NH2	2.46	0.49
8:1I:72:LEU:C	8:1I:74:ASN:H	2.16	0.49
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.11	0.49
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.13	0.49
1:2A:2146:C:H4'	1:2A:2147:G:N9	2.28	0.49
1:2A:271(K):U:O2	8:2I:50:ARG:HD2	2.12	0.49
1:2A:2304:G:N2	6:2G:156:ASP:OD2	2.43	0.49
7:2H:117:PRO:HG3	7:2H:123:PHE:CD2	2.47	0.49
10:2O:68:GLU:OE1	10:2O:78:ARG:NH1	2.45	0.49
11:2P:88:LEU:HA	11:2P:91:PHE:HD2	1.78	0.49
1:1A:1150:C:H2'	1:1A:1151:U:C6	2.48	0.49
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.48	0.49
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.94	0.49
1:1A:509:A:H5''	20:1Y:50:ARG:HD3	1.95	0.49
1:2A:1092:C:O2	1:2A:1092:C:H2'	2.12	0.49
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.46	0.49
1:2A:2870:C:H5''	13:2R:65:LEU:HD21	1.95	0.49
1:2A:459:U:H2'	1:2A:460:A:H8	1.77	0.49
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.42	0.49
8:2I:75:LEU:HD11	8:2I:105:HIS:ND1	2.28	0.49
20:2Y:6:HIS:CD2	20:2Y:7:VAL:HG23	2.48	0.49
25:13:8:LEU:HD13	25:13:31:LEU:HD23	1.93	0.49
1:1A:2101:U:O3'	23:11:35:THR:OG1	2.29	0.49
1:1A:602:G:H2'	1:1A:603:C:C6	2.48	0.49
5:1F:197:ASP:OD1	5:1F:197:ASP:N	2.46	0.49
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.93	0.49
24:22:28:LYS:HD2	24:22:60:LEU:HD11	1.95	0.49
1:2A:1420:U:HO2'	1:2A:1421:G:P	2.36	0.49
1:2A:301:G:H1'	1:2A:302:C:C6	2.48	0.49
6:2G:38:VAL:HG13	6:2G:91:ARG:HD3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2825:C:H5'	27:15:29:THR:HG21	1.95	0.49
7:1H:3:ARG:HH21	7:1H:65:HIS:HB3	1.78	0.49
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.94	0.49
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.13	0.49
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.48	0.49
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.28	0.49
1:2A:2295:C:OP1	14:2S:10:ARG:NH1	2.46	0.49
6:2G:144:ILE:HA	6:2G:148:MET:SD	2.53	0.49
23:11:77:ALA:HA	23:11:80:LEU:HD13	1.95	0.48
1:1A:2639:G:O2'	1:1A:2794:A:N1	2.38	0.48
1:2A:2133:G:N3	1:2A:2157:G:H2'	2.28	0.48
1:2A:2170:A:H8	1:2A:2170:A:O5'	1.95	0.48
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.26	0.48
1:2A:277:C:H1'	1:2A:278:A:OP1	2.13	0.48
1:2A:390:A:H4'	1:2A:391:G:H5'	1.95	0.48
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.48	0.48
6:2G:97:ASP:HA	6:2G:100:TRP:CD1	2.40	0.48
7:2H:26:VAL:HG12	7:2H:79:VAL:HG21	1.95	0.48
1:1A:1874:C:H5'	3:1D:253:GLN:NE2	2.29	0.48
1:1A:2188:G:OP2	1:1A:2188:G:H8	1.96	0.48
1:1A:273:G:N2	8:1I:50:ARG:HH21	2.10	0.48
1:2A:1798:U:OP2	3:2D:274:ARG:NH2	2.40	0.48
1:2A:873:G:H1	1:2A:904:C:H42	1.60	0.48
2:2B:91:C:OP2	12:2Q:16:ARG:NH1	2.46	0.48
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH12	1.78	0.48
29:17:47:ARG:HE	29:17:47:ARG:HB3	1.36	0.48
1:1A:167:G:H2'	1:1A:168:G:C8	3.18	0.48
1:1A:1961:5MU:OP1	1:1A:2616:U:O2'	2.31	0.48
3:1D:231:HIS:CD2	3:1D:249:PRO:HG3	2.48	0.48
1:1A:1303:C:H4'	5:1F:83:PHE:CD1	2.48	0.48
16:1U:28:ARG:NH1	16:1U:38:THR:OG1	2.43	0.48
17:1V:95:LEU:HD23	17:1V:97:LYS:HE3	1.95	0.48
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.94	0.48
1:1A:1342:G:OP1	1:1A:2721:G:O2'	2.19	0.48
1:1A:174:U:H4'	1:1A:207:A:H4'	1.96	0.48
1:1A:2227:G:OP2	1:1A:2227:G:H4'	2.14	0.48
1:1A:2253:A:H2'	1:1A:2254:G:C8	2.48	0.48
1:1A:331:G:H21	1:1A:354:A:H62	1.60	0.48
2:1B:30:C:H2'	2:1B:31:C:H5'	1.96	0.48
5:1F:102:PRO:HB2	5:1F:105:VAL:HG23	1.95	0.48
1:2A:1722:A:H1'	1:2A:1739:U:H5	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2206:G:H5'	1:2A:2207:G:C8	2.48	0.48
1:2A:2712:U:H1'	1:2A:2712(A):A:C8	2.48	0.48
1:2A:7:G:H2'	1:2A:8:A:O4'	2.14	0.48
8:2I:114:LEU:HD21	8:2I:128:LEU:HD13	1.95	0.48
1:1A:485:U:OP2	29:17:39:ARG:NH1	2.45	0.48
1:1A:1940:A:O2'	1:1A:1942:OMC:N4	2.47	0.48
1:1A:1985:U:H4'	1:1A:1986:G:OP1	2.14	0.48
1:1A:2244:U:P	23:11:40:ARG:HH12	2.37	0.48
1:1A:2897:U:H2'	1:1A:2898:C:C6	2.48	0.48
1:1A:360:C:O2'	20:1Y:35:TYR:OH	2.25	0.48
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.46	0.48
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	1.95	0.48
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.29	0.48
1:1A:1038:C:OP1	17:1V:74:LYS:NZ	2.38	0.48
1:1A:1566:U:H2'	1:1A:1567:G:O4'	2.13	0.48
1:1A:329:U:H2'	1:1A:330:U:C6	2.49	0.48
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.31	0.48
6:2G:131:TYR:HB3	6:2G:159:VAL:HG13	1.96	0.48
8:2I:6:LEU:HG	8:2I:36:ALA:HA	1.95	0.48
1:2A:84:A:H5'	20:2Y:8:LYS:HB3	1.95	0.48
21:2Z:31:ARG:HD3	21:2Z:32:HIS:NE2	2.29	0.48
1:1A:1324:A:OP1	13:1R:36:THR:HG23	2.14	0.48
1:1A:2370:G:N1	63:1A:5143:HOH:O	2.18	0.48
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.47	0.48
1:2A:2102:U:O2	1:2A:2187:G:C6	2.67	0.48
1:2A:792:G:N3	1:2A:2072:G:O2'	2.38	0.48
3:2D:124:PRO:HG2	3:2D:129:ASN:HD21	1.78	0.48
12:2Q:21:THR:HG21	12:2Q:101:ARG:HB2	1.95	0.48
1:1A:1361:C:O2'	1:1A:1438:A:N3	2.38	0.48
1:1A:1562:U:H2'	1:1A:1563:G:H8	1.79	0.48
2:1B:86:G:H1	2:1B:91:C:N4	2.11	0.48
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.43	0.48
8:1I:114:LEU:HD11	8:1I:128:LEU:HB3	1.94	0.48
21:1Z:28:MET:HE1	21:1Z:61:LEU:HD21	1.96	0.48
1:2A:1041:C:N4	1:2A:1114:G:H1	2.07	0.48
1:2A:1422:G:O3'	10:2O:49:ARG:NH1	99.93	0.48
1:2A:1614:A:C2	18:2W:93:ALA:HB2	2.49	0.48
1:2A:2127:G:N2	1:2A:2173:A:H1'	2.29	0.48
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.96	0.48
1:1A:2108:U:H2'	1:1A:2109:G:C8	2.49	0.48
1:1A:2146:G:H2'	1:1A:2147:G:H5'	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2849:G:O2'	13:1R:49:ASP:OD2	2.30	0.48
9:1N:35:ARG:HH21	9:1N:42:TRP:HZ2	1.61	0.48
13:1R:72:ASP:OD2	13:1R:75:LEU:HB2	2.14	0.48
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.02	0.48
1:2A:565:C:N3	1:2A:576:U:O4	2.47	0.48
2:2B:90:A:N7	2:2B:91:C:H1'	2.29	0.48
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.13	0.48
1:1A:1594:C:H2'	1:1A:1595:C:C6	2.49	0.48
1:1A:2692:C:OP2	4:1E:111:ARG:NH2	2.38	0.48
1:1A:320:C:H2'	1:1A:321:C:H6	1.77	0.48
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.79	0.48
1:1A:999:G:H5''	12:1Q:13:GLN:HB3	1.96	0.48
20:1Y:92:ASN:HB2	20:1Y:94:LYS:N	2.18	0.48
1:2A:1721:G:H8	1:2A:1741:A:H62	1.60	0.48
1:2A:443:A:H5''	1:2A:444:C:OP1	2.14	0.48
1:1A:1405:A:N1	1:1A:1418:U:C4	2.77	0.47
1:1A:655:G:N2	1:1A:658:A:OP2	2.42	0.47
1:2A:1072:C:N4	1:2A:1093:G:H1	2.12	0.47
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.13	0.47
1:2A:2079:U:OP1	23:21:21:ARG:NH1	2.31	0.47
1:2A:2347:C:H2'	1:2A:2348:U:C6	2.49	0.47
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.46	0.47
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.28	0.47
1:1A:1023:G:H2'	1:1A:1024:G:H8	2.78	0.47
1:1A:2031:G:OP1	18:1W:41:LYS:NZ	2.35	0.47
1:1A:1175:A:O2'	1:1A:2527:C:O2	2.31	0.47
22:20:49:LYS:HG2	22:20:50:ASN:ND2	2.29	0.47
1:2A:220:G:O2'	1:2A:233:A:N3	2.40	0.47
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.14	0.47
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.49	0.47
1:2A:918:A:H5''	2:2B:98:G:O2'	2.15	0.47
11:2P:2:LYS:HE3	11:2P:4:SER:OG	2.13	0.47
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.87	0.47
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.49	0.47
1:1A:1347:A:O2'	1:1A:1348:A:H3'	2.14	0.47
14:1S:59:LYS:NZ	14:1S:68:GLN:HE22	2.11	0.47
26:24:48:ARG:HD2	26:24:51:ASP:O	2.14	0.47
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.15	0.47
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.15	0.47
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.28	0.47
1:2A:885:C:H2'	1:2A:886:C:O4'	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:56:VAL:O	26:14:60:GLN:HB2	2.14	0.47
1:1A:388:A:H2'	1:1A:389:G:H8	1.80	0.47
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.49	0.47
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.96	0.47
7:1H:102:ALA:HA	7:1H:117:PRO:HD3	1.96	0.47
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.61	0.47
11:1P:17:LYS:HE3	11:1P:27:HIS:NE2	2.29	0.47
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.15	0.47
1:2A:1300:U:H4'	1:2A:1301:A:H5'	1.95	0.47
1:2A:2115:G:H22	1:2A:2119:A:H5'	1.80	0.47
1:2A:2115:G:H3'	1:2A:2116:G:C5'	2.42	0.47
1:2A:2171:A:H1'	1:2A:2172:U:C6	2.49	0.47
1:1A:1400:A:H2'	1:1A:1401:G:O4'	2.15	0.47
1:1A:2023:A:H2'	1:1A:2024:G:C8	2.49	0.47
1:1A:661:G:H1	1:1A:744:C:N4	107.88	0.47
1:1A:895:G:H2'	1:1A:896:A:C8	2.48	0.47
18:1W:86:LEU:HD22	18:1W:96:ILE:HD11	1.95	0.47
1:1A:324:A:P	20:1Y:86:ARG:HH22	2.37	0.47
21:1Z:19:ARG:NH1	21:1Z:84:GLU:HB2	2.29	0.47
1:2A:245:G:N7	30:28:8:LYS:NZ	2.62	0.47
1:2A:1223:G:N2	1:2A:1226:A:OP2	2.40	0.47
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.15	0.47
1:2A:528:A:O2'	1:2A:529:A:H5'	2.15	0.47
1:1A:2147:G:O2'	1:1A:2195:A:N6	2.47	0.47
11:1P:121:LYS:O	11:1P:123:LEU:N	2.48	0.47
5:1F:117:ARG:HH12	11:1P:1:MET:N	2.13	0.47
20:1Y:7:VAL:HG21	20:1Y:72:VAL:HG12	1.96	0.47
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.48	0.47
1:2A:184:C:H2'	1:2A:185:U:H6	1.80	0.47
1:2A:2133:G:C2	1:2A:2157:G:H2'	2.50	0.47
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.50	0.47
4:2E:13:ARG:HG2	15:2T:58:ASN:HD21	1.78	0.47
1:2A:1279:G:H4'	13:2R:31:HIS:CD2	2.50	0.47
1:1A:2258:G:H2'	1:1A:2259:A:C8	2.49	0.47
1:1A:310:C:H2'	1:1A:311:C:C6	2.49	0.47
5:1F:9:ILE:HG21	5:1F:125:LEU:HD13	1.96	0.47
7:1H:3:ARG:NH1	7:1H:4:ILE:H	2.12	0.47
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.29	0.47
1:2A:11:G:C2'	1:2A:12:U:H5'	2.45	0.47
1:2A:1508:A:H5'	1:2A:1509(A):A:C8	2.49	0.47
1:2A:2728:U:H5'	10:2O:70:LYS:NZ	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:275:G:H2'	1:2A:276:A:C8	2.49	0.47
1:2A:2808:U:H5''	1:2A:2891:G:O6	2.15	0.47
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.14	0.47
1:2A:323:G:C8	5:2F:171:PRO:HG3	2.48	0.47
9:2N:69:GLN:O	9:2N:71:ILE:HD12	2.15	0.47
12:2Q:39:PRO:HD3	12:2Q:99:PRO:HG3	1.97	0.47
1:1A:1046:A:N6	1:1A:1211:U:O2	28.32	0.47
1:1A:1532:A:H2'	1:1A:1533:G:C8	2.49	0.47
1:1A:2661:U:H2'	1:1A:2662:U:C6	2.50	0.47
1:1A:424:G:H2'	1:1A:425:G:H8	2.39	0.47
5:1F:126:VAL:HG11	5:1F:142:TRP:HZ2	1.80	0.47
10:1O:8:LEU:HB2	10:1O:19:ILE:HG13	1.95	0.47
19:1X:40:LYS:HG3	19:1X:51:VAL:HB	1.96	0.47
1:2A:1199:U:O2'	63:2A:3751:HOH:O	2.20	0.47
1:2A:1359:A:N3	1:2A:1359:A:H5'	2.30	0.47
19:2X:57:LEU:HD13	19:2X:78:LYS:HG3	1.96	0.47
25:13:6:VAL:HG12	25:13:54:VAL:HG21	1.97	0.47
1:1A:2747:A:H2'	1:1A:2748:G:O4'	2.15	0.47
1:1A:768:C:H2'	1:1A:769:A:C8	2.50	0.47
7:1H:13:LYS:HB3	7:1H:13:LYS:HE2	1.65	0.47
8:1I:104:GLN:HE21	8:1I:105:HIS:CE1	2.33	0.47
12:1Q:57:HIS:HD2	12:1Q:117:ALA:HB2	1.79	0.47
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.49	0.47
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.50	0.47
1:2A:1655:A:N6	1:2A:2005:A:O2'	2.48	0.47
1:2A:2336:A:H61	22:20:43:THR:CG2	2.26	0.47
1:2A:1983:C:H4'	1:2A:2606:C:H4'	1.96	0.47
6:2G:7:LEU:HD23	6:2G:100:TRP:HE3	1.79	0.47
1:2A:1443:G:H5'	15:2T:125:ARG:NH1	54.97	0.47
1:1A:1091:A:H1'	1:1A:1093:G:C2	2.49	0.47
1:1A:1554:A:H4'	1:1A:1556:A:C5	2.50	0.47
1:1A:1604:C:H5''	1:1A:1605:A:OP2	2.15	0.47
1:1A:2222:C:O2	1:1A:2238:C:N4	2.48	0.47
1:1A:2686:G:H5'	10:1O:26:LYS:HE3	1.97	0.47
17:1V:16:PRO:HD3	17:1V:99:ILE:HD11	1.97	0.47
1:2A:1761:C:H3'	1:2A:1762:A:H5''	1.96	0.47
1:2A:2128:C:H5'	1:2A:2129:C:OP2	2.15	0.47
1:2A:774:A:N3	1:2A:774:A:H2'	2.30	0.47
2:2B:48:A:H4'	14:2S:95:HIS:CD2	2.47	0.47
7:2H:7:LEU:HB3	7:2H:69:ARG:HH21	1.80	0.47
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:12:GLN:HE21	12:2Q:72:LYS:HG3	1.79	0.47
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.50	0.47
1:1A:1904:C:H2'	1:1A:1905:G:O4'	2.15	0.47
1:1A:745:C:O2'	1:1A:781:A:N6	2.48	0.47
6:1G:16:ARG:CZ	6:1G:31:VAL:HG21	2.45	0.47
1:2A:1474:C:H2'	1:2A:1475:G:C8	2.50	0.47
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.50	0.47
1:2A:1639:U:H4'	1:2A:2699:C:H4'	1.97	0.47
1:2A:641:C:O2'	1:2A:2350:C:OP1	2.31	0.47
1:2A:298:G:H5''	1:2A:299:A:OP1	2.15	0.47
8:2I:5:LEU:HD12	8:2I:36:ALA:HB2	1.97	0.47
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.30	0.46
1:1A:2569:G:H2'	1:1A:2570:C:C6	2.50	0.46
1:1A:626:A:H4'	1:1A:627:G:H5'	1.96	0.46
4:1E:175:VAL:O	4:1E:177:PRO:HD3	2.16	0.46
5:1F:178:PRO:HB2	5:1F:201:VAL:HG21	1.97	0.46
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.97	0.46
1:2A:1359:A:H2'	1:2A:1360:A:H5'	1.98	0.46
1:2A:1641:A:H2'	1:2A:1642:G:O4'	2.15	0.46
1:2A:196:A:N3	1:2A:196:A:H2'	2.30	0.46
1:2A:2371:G:H21	28:26:46:HIS:CE1	2.33	0.46
1:2A:2733:A:H2	4:2E:204:ALA:H	1.63	0.46
1:2A:729:G:O2'	1:2A:763:G:H4'	2.15	0.46
1:1A:1338:U:H2'	1:1A:1339:C:C6	2.50	0.46
1:1A:210:A:N1	1:1A:254:A:O2'	2.46	0.46
1:1A:848:G:O6	5:1F:53:THR:OG1	2.32	0.46
13:1R:54:LEU:HA	13:1R:54:LEU:HD12	1.77	0.46
21:1Z:136:PHE:HE1	21:1Z:138:GLU:HG3	1.79	0.46
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.14	0.46
4:2E:150:VAL:HG13	4:2E:154:LYS:HD2	1.98	0.46
1:1A:1494:G:O2'	1:1A:1934:A:O2'	125.97	0.46
1:1A:2602:A:H5''	3:1D:239:ARG:HG3	1.97	0.46
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.50	0.46
9:2N:30:ILE:HG22	9:2N:34:LEU:HD22	1.98	0.46
10:2O:107:ARG:HH21	10:2O:115:VAL:HG11	1.79	0.46
18:2W:65:LEU:HB2	18:2W:68:ARG:HD2	1.98	0.46
1:1A:1356:G:OP2	29:17:9:ARG:NE	2.42	0.46
1:1A:1409:C:H2'	1:1A:1410:G:H8	2.41	0.46
1:1A:2135:U:H3	1:1A:2190:G:H4'	1.80	0.46
1:1A:324:A:H2'	1:1A:358:C:H1'	1.98	0.46
7:1H:20:ALA:HB3	7:1H:23:ARG:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1047:G:H21	1:2A:1111:A:N6	1.97	0.46
1:2A:411:G:OP2	1:2A:2406:U:O2'	2.32	0.46
1:2A:58:G:O2'	1:2A:73:A:N1	2.46	0.46
2:2B:59:A:H2'	2:2B:60:C:O4'	2.15	0.46
1:1A:1073:A:C2	1:1A:2500:A:H5'	2.50	0.46
1:1A:1314:A:H2'	1:1A:1315:A:O4'	2.16	0.46
1:1A:1700:G:H3'	13:1R:2:ARG:HD3	1.98	0.46
1:1A:1921:G:H2'	1:1A:1921:G:N3	2.31	0.46
1:1A:2181:G:H2'	1:1A:2182:G:H8	1.80	0.46
2:1B:103:G:N2	21:1Z:73:GLN:HE22	2.13	0.46
1:2A:1045:A:H5'	1:2A:1047:G:OP1	2.15	0.46
1:2A:1056:G:O2'	1:2A:1086:A:H1'	2.15	0.46
1:2A:1218:C:H42	1:2A:1231:G:H1	1.63	0.46
1:2A:2118:U:O2'	1:2A:2119:A:H5''	2.15	0.46
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.50	0.46
1:2A:586:A:N1	1:2A:809:G:O2'	2.39	0.46
1:2A:959:A:N3	1:2A:2457:U:O2'	2.42	0.46
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.50	0.46
1:1A:1248:G:H5'	11:1P:3:LEU:HD23	1.98	0.46
1:1A:1750:G:H2'	1:1A:1751:G:C8	2.50	0.46
1:1A:596:G:O2'	1:1A:597:C:H3'	2.15	0.46
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.53	0.46
16:1U:16:LYS:HB3	16:1U:16:LYS:HE2	1.74	0.46
21:1Z:31:ARG:NH1	21:1Z:94:GLU:OE2	2.49	0.46
23:21:3:LYS:HB3	23:21:4:VAL:H	1.53	0.46
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.16	0.46
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.27	0.46
1:2A:718:A:H8	1:2A:718:A:O5'	1.99	0.46
6:2G:108:ASN:OD1	6:2G:108:ASN:N	2.48	0.46
7:2H:124:GLU:HG3	7:2H:132:ARG:HB3	1.98	0.46
9:2N:20:GLY:HA2	9:2N:61:ARG:HG3	1.96	0.46
15:2T:53:ARG:O	15:2T:59:THR:HG23	2.15	0.46
19:2X:26:TYR:HB3	19:2X:92:LEU:HD22	1.97	0.46
1:1A:2015:U:H4'	4:1E:128:SER:OG	2.16	0.46
1:1A:821:A:H2'	1:1A:821:A:N3	2.31	0.46
11:1P:140:ALA:O	25:23:38:GLU:HG2	2.16	0.46
1:2A:1056:G:H4'	1:2A:1086:A:H8	1.80	0.46
1:2A:1517:G:H1'	1:2A:1919:A:O3'	102.74	0.46
1:2A:299:A:N1	1:2A:322:A:O2'	2.35	0.46
1:2A:901:A:H8	1:2A:901:A:O5'	2.90	0.46
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:61:LEU:HD13	3:2D:61:LEU:HA	1.85	0.46
1:1A:142:G:H2'	1:1A:143:C:C6	2.51	0.46
1:1A:269:G:H2'	1:1A:270:C:C6	2.50	0.46
4:1E:109:LYS:O	4:1E:111:ARG:NH1	2.49	0.46
4:1E:170:LEU:HB3	4:1E:184:VAL:CG2	2.46	0.46
1:1A:2799:U:O2'	4:1E:62:PRO:O	2.25	0.46
8:1I:72:LEU:O	8:1I:74:ASN:N	2.43	0.46
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.98	0.46
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.28	0.46
1:2A:2287:A:O2'	1:2A:2288:A:H3'	2.16	0.46
1:2A:403:U:H4'	1:2A:404:C:H5'	1.97	0.46
1:2A:527:C:H3'	63:2A:4002:HOH:O	2.15	0.46
1:2A:643:A:N1	1:2A:2369:A:O2'	2.39	0.46
1:2A:652(E):G:H2'	1:2A:652(F):G:C8	2.51	0.46
1:2A:716:A:C2	1:2A:717:G:H1'	2.51	0.46
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.50	0.46
10:2O:98:VAL:HG22	10:2O:118:ALA:HA	1.97	0.46
17:2V:24:LYS:HG3	17:2V:64:HIS:HD2	1.81	0.46
1:2A:299:A:H5''	20:2Y:86:ARG:HH21	1.81	0.46
28:16:23:THR:OG1	28:16:24:GLU:N	2.48	0.46
1:1A:2160:C:H2'	1:1A:2161:C:C5	2.51	0.46
1:1A:864:C:O2'	1:1A:886:U:H5''	2.14	0.46
30:28:6:THR:HG23	30:28:64:TYR:HD2	1.81	0.46
1:2A:1364:G:P	23:21:3:LYS:HG3	2.56	0.46
1:2A:2109:U:H1'	1:2A:2181:G:H22	1.80	0.46
1:2A:2803:C:H2'	1:2A:2804:C:H6	1.80	0.46
1:2A:307:G:N1	1:2A:310:A:OP2	2.48	0.46
1:2A:192:C:O2'	1:2A:802:A:N3	2.47	0.46
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.31	0.46
1:1A:1704:C:H2'	1:1A:1705:C:C6	2.51	0.46
1:1A:2062:C:H2'	1:1A:2063:U:O4'	2.16	0.46
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.98	0.46
13:1R:36:THR:HG22	13:1R:37:THR:H	1.80	0.46
1:2A:1069:A:H2'	1:2A:1073:A:N7	2.31	0.46
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.50	0.46
8:2I:62:LYS:HE2	8:2I:133:HIS:NE2	2.31	0.46
5:2F:187:VAL:HG12	11:2P:3:LEU:HD12	1.98	0.46
1:1A:310:C:H2'	1:1A:311:C:H6	1.80	0.45
1:1A:465:G:H2'	1:1A:466:G:C8	2.51	0.45
1:1A:694:G:N2	1:1A:697:C:H1'	2.31	0.45
2:1B:60:C:H2'	2:1B:61:G:H8	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1V:21:ARG:HG2	17:1V:91:TYR:CD1	2.51	0.45
27:25:41:PRO:O	27:25:44:THR:OG1	2.33	0.45
1:2A:1081:U:C2'	1:2A:1082:U:H5''	2.45	0.45
1:2A:1159:U:O2	1:2A:1161:C:N4	7.87	0.45
1:2A:1466:G:H2'	1:2A:1547:C:H41	1.79	0.45
1:2A:1799:G:N7	3:2D:179:SER:OG	2.42	0.45
1:2A:1823:G:OP1	3:2D:54:ARG:NH1	2.49	0.45
1:2A:2130:U:H2'	1:2A:2158:A:N1	2.32	0.45
1:2A:2756:U:H1'	1:2A:2757:A:H5''	1.98	0.45
1:2A:384:U:H2'	1:2A:385:C:C6	2.44	0.45
1:2A:629:G:H2'	1:2A:630:G:O4'	2.51	0.45
1:2A:728:G:H4'	3:2D:13:ARG:HE	1.81	0.45
7:2H:121:ILE:HG13	7:2H:144:VAL:HG21	1.98	0.45
13:2R:26:LYS:HE2	13:2R:70:LEU:O	2.16	0.45
1:1A:260:A:N6	1:1A:284:G:H1'	2.31	0.45
1:1A:77:A:H2'	1:1A:78:G:C8	2.52	0.45
1:1A:1823:G:H5'	3:1D:205:VAL:HG13	1.99	0.45
6:1G:11:TYR:O	6:1G:16:ARG:N	2.40	0.45
8:1I:88:ILE:O	8:1I:121:LYS:NZ	2.48	0.45
21:1Z:19:ARG:HG3	21:1Z:25:PRO:HD3	1.99	0.45
26:24:24:THR:OG1	26:24:25:TYR:N	2.46	0.45
1:2A:1091:G:N3	1:2A:1091:G:H2'	2.31	0.45
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.16	0.45
1:2A:2136:C:H5	1:2A:2137:C:H41	1.65	0.45
1:2A:300:A:N3	1:2A:319:C:H1'	2.30	0.45
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.97	0.45
7:2H:23:ARG:HG3	7:2H:36:PRO:HA	1.97	0.45
9:2N:34:LEU:O	9:2N:49:GLY:HA3	2.16	0.45
10:2O:63:VAL:HG23	10:2O:64:ARG:HG3	1.98	0.45
18:2W:48:ALA:O	18:2W:52:GLU:HG2	2.16	0.45
1:1A:1462:G:O2'	1:1A:1463:C:OP2	2.30	0.45
1:1A:1846:A:H8	1:1A:1846:A:OP1	1.99	0.45
1:1A:2855:G:H2'	1:1A:2856:G:C8	2.51	0.45
5:1F:188:ARG:NH2	63:1F:412:HOH:O	2.48	0.45
1:2A:1431:U:H2'	1:2A:1432:C:C6	2.51	0.45
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.16	0.45
1:2A:797:C:H2'	1:2A:798:G:O4'	2.17	0.45
1:2A:779:U:OP1	3:2D:49:ILE:HG13	2.16	0.45
1:1A:1889:G:N2	1:1A:1905:G:H2'	2.31	0.45
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.52	0.45
1:1A:2121:U:H3	1:1A:2212:G:H1	1.62	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2245:U:H2'	1:1A:2246:G:C8	2.52	0.45
1:1A:2303:U:H2'	1:1A:2304:C:C6	2.52	0.45
1:1A:2331:G:N2	14:1S:3:ARG:HD3	2.31	0.45
26:24:48:ARG:HG3	26:24:52:THR:HG23	1.98	0.45
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.52	0.45
1:2A:2113:U:H2'	1:2A:2114:A:O4'	2.16	0.45
1:2A:2573:C:OP1	1:2A:2574:G:H5''	2.16	0.45
10:2O:122:LEU:HD13	15:2T:72:VAL:HG11	1.98	0.45
1:1A:1471:G:H2'	1:1A:1472:G:C8	2.52	0.45
12:1Q:2:LEU:HG	12:1Q:69:PHE:CE1	2.52	0.45
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.99	0.45
20:1Y:19:LYS:HE2	20:1Y:20:TYR:CE2	2.51	0.45
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	2.00	0.45
1:2A:2167:U:H2'	1:2A:2168:G:C4	2.51	0.45
1:2A:581:C:H2'	1:2A:582:G:H8	1.80	0.45
1:2A:674:G:O2'	5:2F:74:ARG:HD3	2.16	0.45
21:2Z:10:ARG:HD3	21:2Z:37:VAL:O	2.17	0.45
25:13:39:ASP:OD2	25:13:44:ARG:NH2	2.47	0.45
31:19:32:HIS:O	31:19:34:GLN:HG3	2.16	0.45
1:1A:1521:C:H2'	1:1A:1522:G:C8	2.51	0.45
1:1A:2332:A:H2'	1:1A:2332:A:N3	2.31	0.45
1:1A:265:U:H2'	1:1A:266:C:C6	2.51	0.45
1:1A:394:C:H3'	63:1A:5451:HOH:O	2.17	0.45
11:1P:39:LYS:HD2	11:1P:45:LEU:HD11	1.98	0.45
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.17	0.45
28:26:23:THR:OG1	28:26:24:GLU:N	2.49	0.45
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.16	0.45
1:2A:1200:C:H5'	63:2A:3751:HOH:O	2.15	0.45
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.99	0.45
1:2A:2869:G:H2'	1:2A:2870:C:O4'	2.16	0.45
8:2I:116:LEU:HD11	8:2I:119:PRO:HA	1.99	0.45
26:14:24:THR:OG1	26:14:25:TYR:N	2.50	0.45
1:1A:2490:A:H5'	31:19:31:LYS:HE2	1.99	0.45
1:1A:215:G:N2	1:1A:217:A:H62	2.15	0.45
1:1A:2327:G:H2'	1:1A:2328:C:C6	2.51	0.45
1:1A:829:A:H5'	1:1A:830:A:N7	2.31	0.45
8:1I:68:LEU:HD21	8:1I:109:ILE:HD11	1.98	0.45
14:1S:110:LEU:HA	14:1S:110:LEU:HD12	1.84	0.45
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.65	0.45
1:2A:1003:G:H2'	1:2A:1003:G:N3	2.75	0.45
1:2A:728:G:H5''	3:2D:13:ARG:HH21	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:839:U:H3'	1:2A:840:C:C5	4.14	0.45
1:2A:903:C:H2'	1:2A:904:C:H6	1.81	0.45
14:2S:93:LYS:HE3	14:2S:95:HIS:HB2	1.97	0.45
1:1A:2235:G:OP1	3:1D:172:TYR:OH	2.29	0.45
1:1A:765:A:O5'	1:1A:765:A:H8	1.99	0.45
1:1A:909:G:H2'	1:1A:910:A:O4'	2.17	0.45
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.52	0.45
21:1Z:103:ARG:HD3	21:1Z:136:PHE:CG	2.52	0.45
21:1Z:128:VAL:HG21	21:1Z:161:VAL:HG12	1.98	0.45
1:2A:1057:A:O2'	1:2A:1058:G:OP1	2.34	0.45
1:2A:149:A:H2'	1:2A:150:C:C6	2.85	0.45
1:2A:212:G:H2'	1:2A:213:A:O4'	2.17	0.45
1:2A:2662:A:O5'	1:2A:2662:A:H8	1.99	0.45
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.17	0.45
1:2A:574:C:N3	4:2E:145:LYS:NZ	2.61	0.45
8:2I:62:LYS:HB3	8:2I:133:HIS:CE1	2.52	0.45
9:2N:46:VAL:HG23	9:2N:48:MET:HG2	1.99	0.45
10:2O:98:VAL:HG11	10:2O:114:ILE:HG23	1.97	0.45
10:2O:17:ARG:HA	10:2O:17:ARG:HD3	1.83	0.45
21:2Z:28:MET:HB3	21:2Z:28:MET:HE2	1.92	0.45
26:14:61:ARG:HG3	26:14:62:ARG:H	1.80	0.45
1:1A:138:G:N3	1:1A:140:A:N6	2.57	0.45
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.52	0.45
1:1A:2263:OMG:HM23	1:1A:2263:OMG:H1'	1.72	0.45
1:2A:1384:A:N3	1:2A:1405:U:H1'	2.32	0.45
1:2A:2410:G:C2	1:2A:2411:A:H1'	2.52	0.45
1:2A:2848:G:H1'	1:2A:2867:G:N2	2.31	0.45
3:2D:124:PRO:HG2	3:2D:129:ASN:ND2	2.31	0.45
1:2A:2512:C:H4'	4:2E:122:PHE:CE2	2.52	0.45
6:2G:126:ASP:HB3	6:2G:130:ASN:H	1.80	0.45
8:2I:14:ASP:O	8:2I:17:GLN:HB3	2.17	0.45
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.98	0.45
18:2W:35:ILE:HG23	27:25:28:PRO:HD2	1.98	0.45
1:1A:1898:A:H2'	1:1A:1899:A:C8	2.52	0.45
1:1A:630:U:OP1	5:1F:102:PRO:HA	2.17	0.45
7:1H:55:PRO:HG2	7:1H:61:HIS:ND1	2.31	0.45
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.53	0.45
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.99	0.45
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.52	0.45
1:2A:2405:G:H5'	11:2P:75:ILE:HD13	1.99	0.45
1:2A:26:G:C6	1:2A:27:G:N1	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2845:G:H2'	1:2A:2846:G:C8	2.51	0.45
1:2A:311:A:C6	1:2A:328:U:C4	3.05	0.45
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.17	0.45
1:2A:620:G:H5'	1:2A:620:G:N3	2.32	0.45
3:2D:13:ARG:NH1	3:2D:16:MET:SD	2.90	0.45
1:2A:1843:C:H5'	3:2D:253:GLN:NE2	2.32	0.45
8:2I:5:LEU:HD12	8:2I:5:LEU:HA	1.77	0.45
1:2A:911:A:N6	12:2Q:11:LYS:O	2.48	0.45
14:2S:26:LEU:HD22	14:2S:87:PHE:CD1	2.52	0.45
19:2X:11:PRO:HG2	19:2X:13:LEU:HD21	1.98	0.45
20:2Y:44:ILE:HD13	20:2Y:64:GLU:HG3	1.99	0.45
26:14:63:TYR:N	26:14:64:GLY:HA2	2.32	0.44
1:1A:1405:A:H2'	1:1A:1406:A:H5'	1.98	0.44
1:1A:1464:G:H8	1:1A:1464:G:O5'	1.99	0.44
1:1A:535:C:H2'	1:1A:536:U:O4'	2.16	0.44
1:1A:842:C:H2'	1:1A:843:C:C6	2.52	0.44
3:1D:142:VAL:HG23	3:1D:193:VAL:HA	1.98	0.44
4:1E:51:PHE:CD2	4:1E:52:LEU:HG	2.51	0.44
15:1T:51:ARG:HB3	15:1T:62:THR:HB	1.99	0.44
1:2A:1722:A:H1'	1:2A:1739:U:C5	2.51	0.44
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.49	0.44
2:2B:14:U:OP2	2:2B:70:C:O2'	2.31	0.44
2:2B:95:C:H2'	2:2B:96:U:C6	2.52	0.44
1:2A:1654:A:O2'	4:2E:113:PHE:O	2.29	0.44
7:2H:26:VAL:O	7:2H:79:VAL:HG11	2.18	0.44
1:1A:1004:A:C5	1:1A:1037:C:C2	54.05	0.44
1:1A:1096:A:H2'	1:1A:1097:G:O4'	2.17	0.44
1:1A:1993:A:C4	3:1D:241:PRO:HD3	2.52	0.44
1:1A:956:A:N1	1:1A:2289:G:H1'	2.32	0.44
58:1A:3907:MPD:H4	58:1A:3907:MPD:HM2	1.77	0.44
1:1A:662:A:OP1	11:1P:133:SER:OG	2.34	0.44
1:1A:1053:C:H5''	9:1N:35:ARG:NH1	2.32	0.44
1:2A:2104:G:O6	1:2A:2185:C:H2'	2.17	0.44
1:2A:1297:C:OP1	1:2A:2710:C:H4'	2.17	0.44
1:2A:27:G:HO2'	1:2A:28:A:P	2.39	0.44
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.52	0.44
5:2F:120:GLU:HB3	5:2F:122:LYS:HG2	2.00	0.44
6:2G:86:MET:HA	6:2G:87:PRO:HD3	1.87	0.44
7:2H:33:LEU:HD21	7:2H:136:ILE:HG13	2.00	0.44
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.50	0.44
21:2Z:53:ILE:HG22	21:2Z:71:VAL:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2144:U:H2'	1:1A:2145:G:H8	1.82	0.44
1:1A:559:U:H2'	1:1A:560:C:C6	2.52	0.44
1:1A:741:U:OP1	3:1D:59:LYS:NZ	2.40	0.44
2:1B:77:U:O2'	2:1B:78:A:H5'	2.17	0.44
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.18	0.44
16:1U:34:LYS:HD3	16:1U:34:LYS:HA	1.57	0.44
1:2A:1067:A:H4'	1:2A:1068:G:OP2	2.17	0.44
1:2A:1754:C:H2'	1:2A:1755:A:O4'	2.17	0.44
1:2A:27:G:O2'	1:2A:28:A:OP2	2.28	0.44
1:2A:826:U:H2'	1:2A:828:U:O4'	2.18	0.44
4:2E:96:PHE:O	4:2E:175:VAL:HG11	2.16	0.44
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.52	0.44
7:2H:98:LEU:HD12	7:2H:103:LEU:HA	2.00	0.44
19:2X:9:LEU:HA	24:22:36:ARG:HH21	1.82	0.44
1:1A:1231:G:H2'	1:1A:1232:G:O4'	2.17	0.44
1:1A:1562:U:H2'	1:1A:1563:G:C8	2.52	0.44
1:1A:1854:G:OP1	3:1D:54:ARG:NH1	2.50	0.44
1:1A:2123:G:H2'	1:1A:2124:U:O4'	2.16	0.44
1:1A:2559:U:O2	10:1O:23:ARG:NH2	2.39	0.44
1:1A:929:G:H1	1:1A:940:C:N4	2.10	0.44
8:1I:129:THR:HG22	8:1I:139:GLN:OE1	2.18	0.44
1:2A:1328:G:H2'	1:2A:1330:C:C5	2.53	0.44
1:2A:2193:G:H2'	1:2A:2194:G:O4'	2.17	0.44
6:2G:113:ARG:HH22	6:2G:142:PRO:HA	1.82	0.44
12:2Q:110:THR:HG23	12:2Q:113:GLN:HB2	1.99	0.44
1:1A:1100:A:O4'	1:1A:1100:A:P	2.75	0.44
1:1A:1690:G:H2'	1:1A:1691:C:O4'	2.17	0.44
1:1A:2096:U:H2'	1:1A:2097:U:C6	2.52	0.44
1:1A:2156:A:H62	1:1A:2179:G:H4'	1.83	0.44
1:1A:2390:A:C5	1:1A:2391:G:H1'	2.53	0.44
3:1D:175:LEU:HD12	3:1D:185:VAL:HG21	1.99	0.44
4:1E:119:ARG:HG2	4:1E:160:TYR:CG	2.53	0.44
6:1G:35:GLU:HB3	6:1G:160:VAL:HB	2.00	0.44
1:2A:2128:C:N4	1:2A:2160:G:N1	2.54	0.44
1:2A:2238:G:N3	1:2A:2238:G:H2'	2.32	0.44
1:2A:271(L):U:H5'	8:2I:50:ARG:HH22	1.83	0.44
14:2S:23:ARG:NH2	14:2S:84:GLN:HB3	2.33	0.44
1:1A:925:A:H2'	1:1A:926:G:H5'	1.98	0.44
1:1A:936:C:H2'	1:1A:937:A:O4'	4.14	0.44
5:1F:196:LEU:HA	5:1F:196:LEU:HD23	1.90	0.44
19:1X:68:ARG:CZ	19:1X:68:ARG:HB3	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:198:LYS:HB2	21:1Z:202:GLU:C	2.38	0.44
1:2A:1056:G:H4'	1:2A:1086:A:C8	2.52	0.44
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.33	0.44
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.99	0.44
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.53	0.44
1:2A:612:C:O2	1:2A:629:G:N2	50.60	0.44
6:2G:115:ARG:CZ	6:2G:115:ARG:H	5.69	0.44
19:2X:44:GLU:HG3	19:2X:51:VAL:HG23	1.99	0.44
21:2Z:94:GLU:HG3	21:2Z:94:GLU:H	1.56	0.44
1:1A:155:C:H42	1:1A:160:G:H1	1.65	0.44
1:1A:874:U:O2'	1:1A:2090:U:C2	2.66	0.44
1:1A:2745:G:H3'	1:1A:2746:A:O4'	2.17	0.44
1:1A:549:U:H2'	1:1A:550:U:C6	2.53	0.44
2:1B:50:G:H5''	14:1S:61:ASN:ND2	2.33	0.44
23:21:88:LYS:O	23:21:92:LYS:HG3	2.16	0.44
26:24:12:ALA:HA	26:24:29:PRO:HA	2.00	0.44
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.99	0.44
1:2A:1810:A:O5'	1:2A:1810:A:H8	2.01	0.44
1:2A:19:C:H2'	1:2A:20:C:C6	2.52	0.44
1:2A:2405:G:O2'	1:2A:2411:A:N6	2.50	0.44
12:2Q:43:THR:HG22	12:2Q:94:VAL:HG12	2.00	0.44
14:2S:19:LYS:HG2	14:2S:19:LYS:H	1.61	0.44
17:2V:62:LEU:HD21	17:2V:95:LEU:HB2	2.00	0.44
19:2X:29:TRP:CE3	19:2X:78:LYS:HB3	2.52	0.44
21:2Z:5:LEU:HD13	21:2Z:47:VAL:HG21	1.99	0.44
19:1X:1:MET:HE1	24:12:26:ARG:HH21	1.83	0.44
26:14:48:ARG:O	26:14:50:VAL:N	2.51	0.44
1:1A:1263:C:N4	1:1A:1277:G:H1	2.15	0.44
1:1A:1491:A:H8	1:1A:1507:A:C4	2.36	0.44
1:1A:2699:U:H2'	1:1A:2700:U:O4'	2.16	0.44
4:1E:77:ILE:HG21	4:1E:195:LEU:HD11	2.00	0.44
5:1F:24:LEU:HB3	5:1F:115:ALA:HB2	1.98	0.44
6:1G:122:PRO:HG3	6:1G:180:PHE:HB3	2.00	0.44
13:1R:56:LYS:NZ	13:1R:90:ARG:O	2.50	0.44
21:1Z:128:VAL:HG22	21:1Z:132:ASN:HB3	1.99	0.44
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.53	0.44
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.53	0.44
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.81	0.44
1:2A:2317:C:N4	1:2A:2318:G:O6	2.51	0.44
1:2A:271(L):U:H4'	1:2A:271(M):G:H5'	1.99	0.44
1:2A:2788:C:O2'	1:2A:2809:A:N3	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.18	0.44
4:2E:143:ASN:HD22	4:2E:147:PRO:CD	2.31	0.44
5:2F:165:ARG:HG2	5:2F:168:ARG:HH21	1.82	0.44
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.18	0.44
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	2.00	0.44
14:2S:15:ARG:HD3	14:2S:25:ARG:NH2	2.33	0.44
14:2S:34:HIS:ND1	14:2S:53:SER:OG	2.40	0.44
16:2U:85:LYS:HB3	16:2U:116:ALA:HB1	2.00	0.44
21:2Z:76:LEU:HD12	21:2Z:83:PRO:HA	1.99	0.44
1:1A:1451:U:H2'	1:1A:1452:U:C6	2.52	0.44
1:1A:2187:G:O2'	1:1A:2188:G:H5'	2.18	0.44
1:1A:469:A:H1'	1:1A:1246:C:O4'	2.18	0.44
1:1A:484:G:O2'	1:1A:495:G:O6	2.34	0.44
6:1G:115:ARG:NH1	6:1G:137:GLU:OE2	2.51	0.44
17:1V:60:GLU:OE1	17:1V:97:LYS:NZ	2.37	0.44
28:26:9:LEU:HA	28:26:54:ILE:HB	2.00	0.44
1:2A:1450:G:H2'	1:2A:1450(A):C:H6	1.82	0.44
1:2A:1819:A:H4'	1:2A:1820:U:H5''	2.00	0.44
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.53	0.44
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.52	0.44
1:2A:2689:U:P	1:2A:2719:G:H22	2.40	0.44
1:2A:483:A:H5''	20:2Y:50:ARG:HD3	1.98	0.44
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.16	0.44
7:2H:55:PRO:HG2	7:2H:61:HIS:ND1	2.32	0.44
14:2S:11:LYS:HE2	14:2S:91:PRO:HD3	2.00	0.44
25:13:46:ASN:O	25:13:50:VAL:HG22	2.17	0.43
1:1A:1068:G:N7	9:1N:66:LYS:HE2	2.33	0.43
1:1A:1309:U:C4	1:1A:1310:G:C6	3.06	0.43
1:1A:1753:U:O2	1:1A:1788:U:H5'	2.18	0.43
1:1A:2034:G:OP2	18:1W:16:LYS:NZ	2.49	0.43
1:1A:2163:G:H3'	1:1A:2164:C:C6	2.54	0.43
1:1A:2474:U:H1'	1:1A:2503:U:O4	2.17	0.43
1:1A:383:A:H2'	1:1A:384:G:O4'	2.17	0.43
1:1A:611:U:H2'	1:1A:612:C:C6	2.53	0.43
1:1A:950:C:H2'	1:1A:951:U:C6	2.52	0.43
1:1A:1857:G:H4'	3:1D:242:ARG:NH2	2.32	0.43
1:1A:1834:A:H4'	3:1D:259:THR:HG23	1.99	0.43
14:1S:59:LYS:HB2	14:1S:60:GLY:H	1.51	0.43
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.53	0.43
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.29	0.43
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:242:G:O2'	1:2A:254:G:O6	2.31	0.43
1:2A:1999:C:H4'	1:2A:2723:C:O2	2.18	0.43
3:2D:231:HIS:CD2	3:2D:249:PRO:HG3	2.52	0.43
7:2H:90:LYS:HD3	7:2H:159:GLU:HG2	1.99	0.43
16:2U:27:LEU:HA	16:2U:30:LYS:HB2	1.99	0.43
29:17:35:ARG:HG3	29:17:42:LEU:HD11	1.99	0.43
1:1A:1405:A:H61	1:1A:1418:U:H3	0.57	0.43
1:1A:274:U:H5	8:1I:52:ARG:HD2	1.83	0.43
1:1A:834:U:H5''	1:1A:835:A:H5'	2.00	0.43
2:1B:53:A:H2'	2:1B:54:G:O4'	2.18	0.43
4:1E:115:GLY:O	4:1E:119:ARG:HB2	2.18	0.43
13:1R:63:ARG:O	13:1R:67:LEU:HB2	2.18	0.43
20:1Y:51:VAL:HG22	20:1Y:58:GLY:HA3	2.00	0.43
1:2A:1422:G:H2'	1:2A:1423:G:H8	2.40	0.43
1:2A:2130:U:H2'	1:2A:2158:A:N6	2.30	0.43
1:2A:30:G:H2'	1:2A:31:C:C6	2.53	0.43
1:2A:864:G:H1'	1:2A:914:C:N4	2.31	0.43
2:2B:2:C:H2'	2:2B:3:C:C6	2.52	0.43
1:2A:2882:A:OP1	13:2R:96:ARG:NH1	2.51	0.43
20:2Y:30:VAL:HG22	20:2Y:37:VAL:HG12	1.98	0.43
1:1A:1199:C:H2'	1:1A:1200:G:O4'	2.18	0.43
1:1A:1785:C:H5	15:1T:96:ARG:NH2	2.16	0.43
1:1A:598:A:H4'	1:1A:2512:U:H4'	2.00	0.43
1:1A:2710:U:H2'	1:1A:2711:C:C6	2.52	0.43
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	2.00	0.43
4:1E:2:LYS:HB2	4:1E:95:ILE:HD12	2.00	0.43
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.81	0.43
1:2A:149:A:H2'	1:2A:150:C:H6	2.28	0.43
1:2A:1710:C:H2'	1:2A:1711:C:C6	2.52	0.43
4:2E:51:PHE:H	4:2E:75:VAL:CG1	2.31	0.43
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.49	0.43
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.38	0.43
23:11:3:LYS:H	23:11:46:LEU:HD12	1.83	0.43
1:1A:2299:A:O2'	1:1A:2300:A:H3'	2.18	0.43
1:1A:354:A:HO2'	1:1A:355:A:H8	1.63	0.43
1:1A:460:C:H2'	1:1A:461:U:C6	2.54	0.43
1:1A:936:C:O2'	1:1A:937:A:O5'	2.34	0.43
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	2.00	0.43
20:1Y:13:VAL:HG12	20:1Y:74:PRO:HA	2.00	0.43
20:1Y:87:LYS:HB3	20:1Y:95:LYS:HD2	2.00	0.43
1:2A:1235:G:C6	1:2A:1236:G:N1	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.42	0.43
1:2A:1499:C:H2'	1:2A:1500:G:C8	2.54	0.43
1:2A:2148:G:C2	1:2A:2149:G:H1'	2.54	0.43
1:2A:2309:A:H2'	1:2A:2310:A:C8	2.52	0.43
1:2A:30:G:C5	1:2A:31:C:C4	3.07	0.43
1:2A:373:U:H2'	1:2A:374:A:H8	1.84	0.43
3:2D:35:LYS:HB2	3:2D:36:PRO:HD2	2.01	0.43
7:2H:37:VAL:HG21	7:2H:72:ILE:HD11	2.00	0.43
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.38	0.43
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	2.00	0.43
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	2.00	0.43
1:1A:933:C:H3'	1:1A:934:A:H5''	2.00	0.43
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.99	0.43
6:1G:104:GLU:O	6:1G:108:ASN:ND2	2.30	0.43
4:1E:9:VAL:HB	15:1T:3:ARG:HG2	1.98	0.43
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.81	0.43
1:2A:207:A:H2'	1:2A:208:C:O4'	2.18	0.43
1:2A:272:G:N3	1:2A:272(B):G:H1'	2.33	0.43
1:2A:330:A:HO2'	1:2A:331:A:H8	1.63	0.43
1:2A:370:G:OP2	1:2A:370:G:H8	2.02	0.43
1:2A:265:A:N6	1:2A:428:A:H1'	2.33	0.43
2:2B:30:C:H2'	2:2B:31:C:H5'	1.99	0.43
3:2D:16:MET:HG3	3:2D:206:LEU:O	2.19	0.43
31:19:4:ARG:NH2	63:19:201:HOH:O	2.51	0.43
1:1A:1858:C:O2'	1:1A:1992:A:N3	2.44	0.43
1:1A:2155:G:C2	1:1A:2179:G:H2'	2.53	0.43
1:1A:2346:G:H5'	14:1S:9:ARG:HG2	1.99	0.43
1:1A:2642:G:H2'	1:1A:2643:G:C8	2.54	0.43
1:1A:324:A:OP2	20:1Y:86:ARG:NH2	2.52	0.43
1:1A:982:U:H2'	1:1A:983:G:O4'	2.19	0.43
2:1B:73:A:C4	2:1B:105:A:C2	3.07	0.43
4:1E:78:LEU:O	4:1E:79:ARG:NH1	2.51	0.43
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	2.00	0.43
21:1Z:9:TYR:OH	21:1Z:61:LEU:HD23	2.19	0.43
1:2A:1945:G:H2'	1:2A:1946:U:C6	2.54	0.43
1:2A:2689:U:H4'	1:2A:2690:C:H5'	2.00	0.43
1:2A:818:G:H4'	1:2A:838:C:O3'	2.18	0.43
1:2A:959:A:N6	1:2A:960:A:N1	2.67	0.43
15:2T:65:LYS:HE2	15:2T:67:SER:HB2	2.00	0.43
1:1A:2060:G:H2'	1:1A:2061:C:O4'	2.19	0.43
1:1A:2846:U:H2'	1:1A:2847:G:C8	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2864:G:H2'	1:1A:2865:C:C6	2.53	0.43
1:1A:572:A:O2'	1:1A:573:G:OP1	2.28	0.43
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.19	0.43
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.32	0.43
12:1Q:21:THR:HG21	12:1Q:101:ARG:HB2	2.01	0.43
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	2.00	0.43
1:1A:1245:C:H1'	16:1U:2:PRO:HG3	2.00	0.43
16:1U:52:ARG:HA	16:1U:55:ARG:HG3	1.99	0.43
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.74	0.43
21:1Z:75:ASN:HB2	21:1Z:85:HIS:HB3	2.00	0.43
1:2A:2728:U:H5'	10:2O:70:LYS:HZ3	1.83	0.43
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.58	0.43
9:2N:4:TYR:HB2	16:2U:101:ARG:NH2	2.33	0.43
17:2V:31:ALA:O	17:2V:61:VAL:HG22	2.19	0.43
1:1A:1186:U:H4'	1:1A:1188:A:O4'	2.19	0.43
1:1A:2161:C:N4	1:1A:2174:G:H1	2.16	0.43
1:1A:589:U:H5''	11:1P:29:LYS:HE3	2.01	0.43
1:1A:77:A:H2'	1:1A:78:G:H8	1.84	0.43
2:1B:29:A:H2'	2:1B:30:C:C6	2.54	0.43
6:1G:61:ALA:HB1	26:14:7:PRO:HG2	2.00	0.43
16:1U:29:SER:C	16:1U:30:LYS:HD2	2.39	0.43
20:1Y:56:PRO:C	20:1Y:58:GLY:H	2.22	0.43
1:2A:80:G:H1	1:2A:106:C:H42	1.67	0.43
1:2A:107:C:H2'	1:2A:108:U:H6	1.84	0.43
1:2A:1973:G:H2'	1:2A:1974:C:C6	2.54	0.43
1:2A:2233:U:H2'	1:2A:2234:G:C8	2.54	0.43
3:2D:106:ILE:HD11	3:2D:144:ALA:HB2	2.00	0.43
3:2D:264:LYS:HA	3:2D:265:PRO:HD3	1.90	0.43
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	1.99	0.43
21:2Z:54:HIS:CG	21:2Z:101:PRO:HG3	2.54	0.43
21:2Z:26:GLY:HA2	21:2Z:85:HIS:CD2	2.54	0.43
1:1A:1220:U:H1'	1:1A:1221:G:OP1	2.18	0.43
1:1A:1736:A:H2'	1:1A:1737:A:C8	2.54	0.43
1:1A:2014:G:C2	1:1A:2019:G:C5	3.07	0.43
1:1A:2702:C:OP1	13:1R:17:ARG:NH2	2.46	0.43
1:1A:2713:C:H2'	1:1A:2714:U:H2'	1.99	0.43
1:1A:2859:U:OP2	15:1T:95:ARG:NH1	2.52	0.43
4:1E:9:VAL:HG22	4:1E:25:VAL:HB	1.99	0.43
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.37	0.43
20:1Y:77:PRO:HD2	20:1Y:106:LEU:HD23	2.01	0.43
21:1Z:91:LEU:HD11	21:1Z:96:VAL:HG11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:21:91:LYS:HA	23:21:94:LEU:HD12	2.00	0.43
1:2A:1068:G:H8	1:2A:1068:G:OP2	7.03	0.43
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.18	0.43
1:2A:2492:U:H2'	1:2A:2493:U:C6	2.54	0.43
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.54	0.43
1:2A:569:U:C4	1:2A:570:G:C6	3.07	0.43
3:2D:94:LEU:HD23	3:2D:94:LEU:HA	1.89	0.43
6:2G:49:ASP:OD2	6:2G:49:ASP:N	2.52	0.43
6:2G:83:ARG:H	6:2G:86:MET:CE	2.31	0.43
16:2U:34:LYS:HA	16:2U:34:LYS:HD3	1.61	0.43
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.19	0.43
1:1A:1224:C:H2'	1:1A:1225:C:H6	1.84	0.43
1:1A:1586:G:H2'	1:1A:1587:U:O4'	2.19	0.43
1:1A:2161:C:H42	1:1A:2174:G:H1	1.67	0.43
1:1A:23:G:OP1	1:1A:529:U:N3	2.51	0.43
1:1A:590:A:OP2	11:1P:29:LYS:NZ	2.35	0.43
1:1A:636:G:N2	1:1A:640:A:O2'	2.51	0.43
8:1I:44:LEU:HD12	8:1I:44:LEU:HA	1.85	0.43
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.99	0.43
21:1Z:125:LEU:HG	21:1Z:164:ALA:HB3	2.01	0.43
21:1Z:124:ILE:HD11	21:1Z:165:VAL:HG21	2.01	0.43
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.54	0.43
1:2A:1064:C:H3'	1:2A:1065:U:C5'	2.49	0.43
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.45	0.43
1:2A:1669:A:H5''	1:2A:2550:G:OP1	2.18	0.43
1:2A:687:C:H2'	1:2A:688:U:O4'	2.18	0.43
1:2A:874:G:H2'	1:2A:875:G:O4'	2.18	0.43
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.53	0.43
8:2I:140:LEU:HA	8:2I:140:LEU:HD23	1.83	0.43
13:2R:87:TYR:OH	13:2R:116:LEU:HB3	2.18	0.43
17:2V:89:GLN:HA	17:2V:90:PRO:HD3	1.88	0.43
1:1A:1239:A:H62	1:1A:1299:A:N6	21.38	0.42
1:1A:1639:G:H2'	1:1A:1640:G:C8	2.54	0.42
1:1A:823:G:N7	1:1A:840:A:O2'	2.46	0.42
6:1G:107:LEU:HD11	6:1G:178:PHE:HE1	1.82	0.42
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.54	0.42
31:29:10:ILE:HD12	31:29:32:HIS:HA	2.00	0.42
1:2A:1360:A:OP1	1:2A:1360:A:H8	5.17	0.42
1:2A:2689:U:OP2	1:2A:2719:G:N2	2.49	0.42
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.54	0.42
1:2A:576:U:H2'	1:2A:577:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:610:G:H2'	1:2A:611:C:C6	2.54	0.42
1:2A:628:G:H2'	1:2A:629:G:C8	3.02	0.42
4:2E:144:ARG:HB3	4:2E:145:LYS:H	1.49	0.42
4:2E:120:TRP:CD1	4:2E:155:LYS:HB3	2.54	0.42
7:2H:17:VAL:HG11	7:2H:50:VAL:HG21	2.01	0.42
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	2.01	0.42
24:12:32:LEU:HD22	24:12:36:ARG:NH1	2.32	0.42
28:16:34:LEU:HB2	28:16:51:GLU:HB2	2.01	0.42
1:1A:2724:U:OP1	1:1A:2727:G:H4'	2.20	0.42
1:1A:2760:G:O6	1:1A:2768:C:H5''	2.18	0.42
1:1A:399:G:O2'	1:1A:427:G:O6	2.36	0.42
1:1A:766:C:H2'	1:1A:767:C:C6	2.55	0.42
1:1A:923:C:H2'	1:1A:924:U:O4'	2.19	0.42
1:1A:939:C:H2'	1:1A:940:C:C6	2.54	0.42
20:1Y:53:PRO:O	20:1Y:56:PRO:HD3	2.20	0.42
1:2A:1160:G:C6	1:2A:1161:C:C4	3.06	0.42
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.53	0.42
1:2A:1450:G:H2'	1:2A:1450(A):C:C6	2.54	0.42
1:2A:2166:G:H2'	1:2A:2167:U:O4'	2.19	0.42
1:2A:224:G:H2'	1:2A:225:A:O4'	2.19	0.42
1:2A:2318:G:N2	14:2S:3:ARG:HE	2.17	0.42
3:2D:245:PRO:HA	3:2D:246:PRO:HD3	1.91	0.42
4:2E:50:GLY:O	4:2E:51:PHE:HB2	2.18	0.42
21:2Z:14:LYS:HA	21:2Z:15:PRO:HD3	1.88	0.42
1:1A:1386:U:OP1	19:1X:16:LYS:NZ	2.46	0.42
1:1A:593:G:H2'	1:1A:2052:A:C5	2.53	0.42
1:1A:2856:G:H2'	1:1A:2857:U:O4'	2.20	0.42
1:1A:756:U:H2'	1:1A:757:G:C8	2.54	0.42
1:1A:762:G:H2'	1:1A:763:A:O4'	2.19	0.42
1:1A:956:A:H2'	1:1A:957:A:C8	2.53	0.42
2:1B:102:A:H2'	2:1B:103:G:O4'	2.19	0.42
5:1F:63:LYS:HA	5:1F:76:GLY:O	2.19	0.42
1:2A:1085:A:H2'	1:2A:1086:A:C2	2.54	0.42
1:2A:2075:U:OP2	1:2A:2238:G:O2'	2.35	0.42
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.19	0.42
1:2A:305:U:H2'	1:2A:306:U:C6	2.54	0.42
1:2A:601:C:O2	1:2A:605:C:H4'	2.19	0.42
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.52	0.42
9:2N:103:VAL:HG11	9:2N:120:LEU:HD22	2.00	0.42
14:2S:49:VAL:HG12	14:2S:73:LEU:HD12	2.01	0.42
21:2Z:93:ASP:HB3	21:2Z:131:ARG:HH22	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2432:C:H5'	28:16:54:ILE:HD11	2.01	0.42
1:1A:1093:G:H2'	1:1A:1156:G:N2	2.31	0.42
1:1A:1686:U:H4'	1:1A:2711:C:H4'	2.01	0.42
1:1A:485:U:H4'	29:17:40:TRP:CZ3	2.55	0.42
4:1E:9:VAL:HG13	4:1E:25:VAL:O	2.20	0.42
19:1X:11:PRO:HG2	19:1X:13:LEU:HD21	2.01	0.42
1:2A:2154:G:C6	1:2A:2155:G:C6	3.07	0.42
1:2A:2378:A:O5'	1:2A:2378:A:H8	2.02	0.42
1:2A:266:G:O2'	1:2A:267:C:OP2	4.85	0.42
1:2A:459:U:OP2	29:27:39:ARG:NH1	2.52	0.42
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.20	0.42
13:2R:65:LEU:HD12	13:2R:65:LEU:HA	1.82	0.42
1:1A:1857:G:H2'	1:1A:1858:C:O4'	2.19	0.42
1:1A:1897:C:H2'	1:1A:1898:A:O4'	2.19	0.42
1:1A:2203:G:H2'	1:1A:2204:G:C8	2.55	0.42
1:1A:2524:C:H2'	1:1A:2525:G:O4'	2.19	0.42
1:1A:933:C:H4'	1:1A:933:C:OP1	2.18	0.42
4:1E:27:LEU:HD12	4:1E:180:ASN:O	2.19	0.42
12:1Q:135:ASP:O	12:1Q:139:GLU:HG3	2.20	0.42
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.20	0.42
17:1V:28:GLU:HG3	17:1V:29:PRO:HD2	2.00	0.42
22:20:43:THR:OG1	22:20:46:LYS:HG2	2.19	0.42
1:2A:1127:A:N7	1:2A:2488:A:O2'	2.50	0.42
1:2A:433:C:H2'	1:2A:434:U:H6	3.05	0.42
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.53	0.42
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.47	0.42
19:2X:31:HIS:HA	19:2X:32:PRO:HD3	1.83	0.42
28:16:6:ARG:HH12	28:16:26:ASN:HB2	1.85	0.42
1:1A:1517:G:H1'	1:1A:1941:A:O3'	111.22	0.42
1:1A:1686:U:O2'	1:1A:1687:C:H5'	2.20	0.42
1:1A:2368:C:H2'	1:1A:2369:U:O4'	2.20	0.42
1:1A:2388:A:H2'	1:1A:2389:A:O4'	2.19	0.42
1:1A:2880:C:H2'	1:1A:2881:C:O4'	2.19	0.42
1:1A:518:G:H2'	1:1A:519:G:O4'	2.19	0.42
1:1A:766:C:H2'	1:1A:767:C:H6	1.83	0.42
1:1A:826:U:OP1	3:1D:49:ILE:HG13	2.19	0.42
8:1I:38:LEU:H	8:1I:38:LEU:HD22	1.85	0.42
20:1Y:30:VAL:HG22	20:1Y:37:VAL:HG12	2.01	0.42
1:2A:1062:G:H5'	1:2A:1070:A:H5'	2.00	0.42
1:2A:495:G:H21	18:2W:61:ASN:HD21	1.68	0.42
1:2A:760:G:H2'	1:2A:761:A:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:14:ILE:HB	15:2T:14:TYR:CZ	2.55	0.42
1:2A:321:G:H5'	5:2F:134:GLY:O	2.19	0.42
7:2H:74:ASN:O	7:2H:78:GLY:N	2.52	0.42
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.34	0.42
16:2U:83:LEU:HD21	16:2U:95:LEU:HD21	2.01	0.42
18:2W:82:LEU:HD22	18:2W:84:ARG:NH2	2.34	0.42
20:2Y:94:LYS:HA	20:2Y:94:LYS:HD3	1.92	0.42
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.19	0.42
1:1A:1481:G:H2'	1:1A:1482:G:O4'	2.20	0.42
1:1A:1710:C:HO2'	1:1A:1711:A:P	2.43	0.42
1:1A:1712:A:H4'	10:1O:67:LYS:HB2	2.00	0.42
1:1A:1715:A:H4'	1:1A:1716:A:O5'	2.19	0.42
1:1A:1992:A:H4'	1:1A:1993:A:OP1	2.20	0.42
1:1A:397:G:H8	1:1A:397:G:OP2	2.02	0.42
1:1A:629:U:H4'	1:1A:705:C:H4'	2.00	0.42
14:1S:35:ILE:HG12	14:1S:101:LEU:HD12	2.02	0.42
15:1T:26:ASP:OD1	15:1T:120:ARG:NH2	2.37	0.42
17:1V:98:GLU:OE2	17:1V:100:ARG:NH1	2.42	0.42
1:2A:1057:A:H2'	1:2A:1058:G:C8	2.51	0.42
1:2A:1739:U:O2'	1:2A:1740:G:H8	2.02	0.42
1:2A:459:U:H2'	1:2A:460:A:C8	2.54	0.42
1:2A:864:G:C6	1:2A:865:C:N4	2.88	0.42
11:2P:101:VAL:HA	11:2P:106:LEU:O	2.20	0.42
24:12:7:ARG:O	24:12:11:GLU:HG3	2.20	0.42
1:1A:1159:U:H2'	1:1A:1160:G:C8	2.54	0.42
1:1A:1710:C:O2'	1:1A:1711:A:O5'	2.32	0.42
2:1B:81:G:N7	59:1B:229:ARG:NH2	2.57	0.42
5:1F:95:ARG:HB3	5:1F:97:TYR:CE2	2.55	0.42
10:1O:64:ARG:HB2	10:1O:79:PHE:CD2	2.55	0.42
12:1Q:110:THR:HG23	12:1Q:113:GLN:OE1	2.20	0.42
1:2A:1128:A:O2'	1:2A:2490:G:OP1	2.30	0.42
1:2A:419:C:N3	1:2A:425:G:N1	23.74	0.42
1:2A:478:A:N1	1:2A:500:G:H4'	2.35	0.42
1:2A:678:C:H2'	1:2A:679:C:C6	2.55	0.42
3:2D:5:LYS:HB3	3:2D:5:LYS:HE3	1.90	0.42
1:2A:1227:G:OP1	16:2U:13:LYS:HE3	2.19	0.42
1:1A:1159:U:H2'	1:1A:1160:G:H8	1.85	0.42
1:1A:2495:C:N3	12:1Q:124:LYS:NZ	2.62	0.42
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.54	0.42
1:1A:2814:C:H2'	1:1A:2815:C:C6	2.55	0.42
21:1Z:14:LYS:HA	21:1Z:15:PRO:HD3	1.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:29:32:HIS:O	31:29:34:GLN:HG3	2.20	0.42
1:2A:1007:C:H5''	9:2N:35:ARG:NH1	2.35	0.42
1:2A:1186:G:C2	1:2A:1187:G:H1'	2.54	0.42
1:2A:1499:C:H2'	1:2A:1500:G:H8	1.85	0.42
1:2A:2134:A:H5''	1:2A:2156:G:N2	2.34	0.42
1:2A:2157:G:H8	1:2A:2157:G:H3'	1.85	0.42
1:2A:960:A:H5'	1:2A:2457:U:H4'	2.02	0.42
1:2A:2494:G:C4	1:2A:2495:G:C8	3.08	0.42
2:2B:3:C:H2'	2:2B:4:C:C6	2.55	0.42
15:2T:81:PRO:HG2	15:2T:82:LEU:HD12	2.02	0.42
1:1A:1404:G:O2'	1:1A:1405:A:H5''	2.20	0.42
1:1A:1765:U:H2'	1:1A:1766:G:O4'	2.20	0.42
1:1A:196:A:H2'	1:1A:197:C:O4'	2.19	0.42
1:1A:2372:A:H2'	1:1A:2373:A:O4'	2.20	0.42
1:1A:2762:A:OP1	7:1H:3:ARG:NH1	2.53	0.42
1:1A:926:G:H2'	1:1A:927:G:O4'	2.19	0.42
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.53	0.42
1:2A:1130:U:O2	4:2E:149:ARG:NH2	2.48	0.42
1:2A:2081:C:H2'	1:2A:2082:A:C8	2.55	0.42
1:2A:1889:A:N1	1:2A:2234:G:H1'	2.34	0.42
1:2A:1637:A:H4'	1:2A:2711:A:O2'	2.20	0.42
7:2H:105:LEU:HD12	7:2H:105:LEU:HA	1.90	0.42
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.55	0.42
15:2T:49:VAL:HG12	15:2T:63:VAL:HG22	2.01	0.42
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.55	0.42
20:2Y:47:LYS:NZ	20:2Y:48:ALA:O	2.43	0.42
23:11:53:VAL:HG22	23:11:74:VAL:HG13	2.02	0.41
1:1A:1541:A:H2'	1:1A:1542:A:C8	2.54	0.41
1:1A:1560:U:H2'	1:1A:1561:C:H6	1.85	0.41
1:1A:312:C:H2'	1:1A:313:A:C8	2.55	0.41
4:1E:144:ARG:HB3	4:1E:145:LYS:H	1.44	0.41
1:1A:142:G:H4'	19:1X:35:THR:HG21	2.02	0.41
19:1X:47:PHE:O	19:1X:49:VAL:HG13	2.20	0.41
19:1X:60:ARG:HH22	29:17:47:ARG:NH1	2.17	0.41
20:1Y:8:LYS:HE2	20:1Y:97:ARG:NH2	2.34	0.41
1:2A:1336:A:H2'	1:2A:1337:G:H8	1.85	0.41
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.45	0.41
1:2A:2245:U:H5''	1:2A:2246:G:H5'	2.01	0.41
1:2A:2399:G:H2'	1:2A:2400:G:O4'	2.20	0.41
1:2A:70:G:H1	1:2A:99:U:H3	37.74	0.41
1:2A:1653:G:C6	13:2R:9:LYS:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:27:THR:HB	15:2T:90:GLN:HB3	2.02	0.41
25:13:5:LYS:HG3	25:13:36:VAL:HG22	2.01	0.41
1:1A:1217:G:N3	1:1A:1217:G:H2'	2.35	0.41
1:1A:2114:U:H4'	1:1A:2115:G:O5'	2.20	0.41
3:1D:61:LEU:HD12	3:1D:61:LEU:HA	1.90	0.41
4:1E:101:ARG:HG3	4:1E:169:ASN:HA	2.02	0.41
6:1G:86:MET:HA	6:1G:87:PRO:HD3	1.81	0.41
7:1H:3:ARG:HE	7:1H:54:ARG:NH1	2.18	0.41
12:1Q:58:PHE:O	12:1Q:60:ARG:N	2.53	0.41
13:1R:51:LEU:HD22	13:1R:66:VAL:HG13	2.02	0.41
14:1S:66:ALA:HA	14:1S:69:VAL:HG13	2.02	0.41
15:1T:27:THR:HB	15:1T:89:VAL:HG22	2.02	0.41
1:1A:795:G:C8	18:1W:89:ALA:HB1	2.55	0.41
28:26:28:ARG:HB2	28:26:28:ARG:HE	1.59	0.41
1:2A:455:C:N3	1:2A:472:A:H2'	2.35	0.41
1:2A:652(A):A:N3	1:2A:652(A):A:H2'	2.35	0.41
1:2A:652(D):C:H2'	1:2A:652(E):G:O4'	2.20	0.41
1:2A:78:A:H2'	1:2A:79:G:C8	2.55	0.41
1:2A:903:C:H2'	1:2A:904:C:C6	2.54	0.41
20:2Y:21:LYS:HB2	20:2Y:21:LYS:HE3	1.87	0.41
1:1A:1093:G:O2'	1:1A:1094:A:H8	2.03	0.41
1:1A:1305:G:C2	1:1A:1331:G:N3	38.80	0.41
1:1A:268:G:O2'	1:1A:269:G:H8	2.03	0.41
1:1A:752:A:H2'	1:1A:753:A:O4'	2.20	0.41
1:1A:768:C:H2'	1:1A:769:A:H8	1.85	0.41
1:1A:901:G:H2'	1:1A:902:G:C8	2.56	0.41
2:1B:2:C:H2'	2:1B:3:C:H6	1.84	0.41
8:1I:107:VAL:HG12	8:1I:109:ILE:HD13	2.02	0.41
9:1N:110:GLY:O	9:1N:114:ARG:HB2	2.20	0.41
12:1Q:109:VAL:HG22	12:1Q:113:GLN:OE1	2.21	0.41
16:1U:17:ILE:HG23	16:1U:39:LEU:HD12	2.01	0.41
25:23:52:HIS:CD2	25:23:53:LEU:HG	2.55	0.41
25:23:8:LEU:HG	25:23:31:LEU:HD22	2.01	0.41
26:24:56:VAL:O	26:24:60:GLN:HB3	2.20	0.41
30:28:39:LYS:HA	30:28:42:ARG:NH1	2.35	0.41
1:2A:1614:A:P	1:2A:1614:A:H8	2.42	0.41
1:2A:428:A:OP2	1:2A:428:A:H8	2.03	0.41
1:2A:582:G:H2'	1:2A:583:G:C8	2.55	0.41
1:2A:862:G:O2'	2:2B:78:A:N3	2.53	0.41
1:2A:615:G:OP2	5:2F:43:LYS:HE3	2.20	0.41
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.55	0.41
1:1A:1087:C:N4	1:1A:1160:G:H1	2.17	0.41
1:1A:716:G:H5''	1:1A:716:G:C8	2.56	0.41
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.55	0.41
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.03	0.41
13:1R:102:GLU:OE2	18:1W:37:ARG:NH2	2.48	0.41
21:1Z:145:GLU:O	21:1Z:148:ASP:N	2.42	0.41
1:1A:2291:G:H4'	21:1Z:199:LYS:O	2.20	0.41
22:20:70:GLN:NE2	22:20:72:ARG:HD2	2.35	0.41
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.55	0.41
1:2A:2160:G:OP2	1:2A:2160:G:H8	2.03	0.41
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.21	0.41
1:2A:372:G:O2'	1:2A:400:G:O6	2.38	0.41
1:2A:764:A:H5'	3:2D:210:GLY:HA2	2.02	0.41
7:2H:27:LYS:HA	7:2H:32:GLU:HA	2.02	0.41
1:2A:863:A:P	12:2Q:22:LYS:HG3	2.61	0.41
13:2R:18:LEU:HA	13:2R:18:LEU:HD23	1.89	0.41
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.20	0.41
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.56	0.41
26:14:56:VAL:HB	26:14:60:GLN:HG2	2.03	0.41
1:1A:1432:C:H2'	1:1A:1433:C:H6	1.84	0.41
1:1A:1682:G:C6	1:1A:1683:C:C4	3.07	0.41
1:1A:1893:G:H2'	1:1A:1894:G:H8	1.85	0.41
1:1A:2227:G:H5''	1:1A:2228:G:C5	2.56	0.41
1:1A:2798:C:OP1	4:1E:41:LYS:NZ	2.51	0.41
3:1D:111:LEU:HA	3:1D:111:LEU:HD23	1.79	0.41
5:1F:33:LEU:HA	5:1F:33:LEU:HD12	1.85	0.41
8:1I:10:GLU:HG2	8:1I:10:GLU:O	2.21	0.41
9:1N:120:LEU:HG	9:1N:122:VAL:HG23	2.02	0.41
31:29:27:CYS:SG	31:29:28:GLU:N	2.92	0.41
1:2A:1278:A:H2'	1:2A:1279:G:C8	2.55	0.41
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.85	0.41
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.36	0.41
1:2A:38:A:H2'	1:2A:39:C:C6	2.55	0.41
1:2A:466:A:P	29:27:34:ARG:HH21	2.43	0.41
1:2A:839:U:H2'	1:2A:840:C:C6	2.55	0.41
1:2A:860:U:H2'	1:2A:861:A:H8	1.85	0.41
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.41	0.41
12:2Q:63:LYS:HD3	12:2Q:65:PHE:CZ	2.55	0.41
1:2A:1287:A:H8	13:2R:104:ARG:HD3	1.84	0.41
1:1A:10:G:C4	1:1A:2641:A:C6	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1170:C:H2'	1:1A:1171:G:O4'	2.20	0.41
1:1A:2119:C:H2'	1:1A:2120:U:O4'	2.21	0.41
1:1A:2803:A:N3	1:1A:2803:A:H2'	2.35	0.41
1:1A:801:C:H2'	1:1A:802:C:C6	2.56	0.41
3:1D:242:ARG:HD3	3:1D:246:PRO:HG3	2.03	0.41
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	2.03	0.41
1:1A:509:A:O2'	20:1Y:49:VAL:O	2.28	0.41
21:1Z:99:TYR:HB3	21:1Z:123:ASP:OD2	2.21	0.41
1:2A:1349:A:H61	1:2A:1598:C:N4	2.19	0.41
1:2A:2637:U:H5''	4:2E:82:ARG:NH1	2.35	0.41
1:2A:357:A:H2'	1:2A:358:U:C6	2.55	0.41
11:2P:39:LYS:HB2	11:2P:45:LEU:HD21	2.01	0.41
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.38	0.41
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.20	0.41
17:2V:29:PRO:HA	17:2V:61:VAL:HG23	2.01	0.41
24:12:52:ASP:O	24:12:56:GLN:HG3	2.20	0.41
26:14:67:TYR:CD2	26:14:67:TYR:N	2.89	0.41
1:1A:1688:A:H2'	1:1A:1689:G:O4'	2.21	0.41
1:1A:2568:C:H2'	1:1A:2569:G:O4'	2.21	0.41
1:1A:2659:U:H2'	1:1A:2660:C:C6	2.55	0.41
1:1A:868:A:H2'	1:1A:991:G:H5''	2.02	0.41
2:1B:33:G:C2	2:1B:50:G:C2	3.08	0.41
6:1G:107:LEU:HD21	6:1G:178:PHE:CD1	2.56	0.41
9:1N:69:GLN:O	9:1N:71:ILE:HD12	2.21	0.41
10:1O:64:ARG:HD3	10:1O:79:PHE:CD1	2.56	0.41
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	2.01	0.41
30:28:37:SER:O	30:28:41:ILE:HG12	2.20	0.41
1:2A:1504:C:H2'	1:2A:1505:C:C6	2.55	0.41
1:2A:2379:G:H4'	14:2S:21:THR:HG21	2.02	0.41
1:2A:2390:U:P	30:28:35:GLN:HE22	2.43	0.41
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.21	0.41
1:2A:603:A:H4'	1:2A:604:G:H5'	2.02	0.41
1:2A:644:A:H4'	1:2A:645:C:H5	1.85	0.41
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.21	0.41
9:2N:28:THR:HG22	9:2N:29:LYS:N	2.36	0.41
1:1A:1247:C:N4	1:1A:1248:G:C6	2.88	0.41
1:1A:1281:G:C6	1:1A:1282:G:N1	2.89	0.41
1:1A:1771:G:H8	1:1A:1771:G:O5'	2.03	0.41
1:1A:1954:A:H2'	1:1A:1955:G:O4'	2.21	0.41
1:1A:2050:U:H2'	1:1A:2051:G:O4'	2.21	0.41
1:1A:2231:G:H2'	1:1A:2232:G:H8	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2383:G:H21	28:16:46:HIS:HE1	1.69	0.41
1:1A:637:U:H5'	1:1A:640:A:N6	2.36	0.41
1:1A:752:A:C2	1:1A:774:A:H1'	2.56	0.41
1:1A:9:U:C2	1:1A:2641:A:N1	2.89	0.41
22:20:27:GLU:HB2	22:20:69:PHE:HD1	1.85	0.41
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.56	0.41
1:2A:1962:5MC:O2'	1:2A:1964:G:OP2	2.31	0.41
1:2A:278:A:OP2	1:2A:278:A:H8	2.04	0.41
1:2A:2839:G:H5'	13:2R:46:GLY:CA	2.51	0.41
1:2A:568:U:H5'	1:2A:945:A:N6	2.36	0.41
6:2G:151:ALA:O	6:2G:153:ARG:NH1	2.54	0.41
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	2.03	0.41
7:2H:55:PRO:HG2	7:2H:61:HIS:CE1	2.56	0.41
1:1A:1068:G:OP2	1:1A:1068:G:H8	6.96	0.41
1:1A:1220:U:O2'	1:1A:1221:G:O5'	2.31	0.41
1:1A:1747:A:H5'	1:1A:1747:A:H8	1.86	0.41
1:1A:2136:A:O2'	1:1A:2190:G:OP1	2.39	0.41
1:1A:209:G:O2'	1:1A:222:A:N3	2.43	0.41
1:1A:339:G:H2'	1:1A:340:C:C6	2.55	0.41
2:1B:91:C:P	12:1Q:16:ARG:HH11	2.43	0.41
7:1H:71:LEU:HD12	7:1H:71:LEU:HA	1.86	0.41
1:2A:98:G:H5''	24:22:3:LEU:HG	2.03	0.41
30:28:63:PRO:HG2	30:28:64:TYR:CD2	2.55	0.41
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.56	0.41
1:2A:2555:U:H5''	1:2A:2556:C:OP2	2.20	0.41
1:2A:2745:C:C4	1:2A:2746:U:C4	3.09	0.41
4:2E:175:VAL:O	4:2E:177:PRO:HD3	2.21	0.41
5:2F:46:ARG:HB3	5:2F:48:THR:HG23	2.03	0.41
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	2.02	0.41
1:2A:483:A:O4'	20:2Y:48:ALA:HB1	2.20	0.41
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.29	0.41
25:13:3:ARG:HD3	25:13:60:GLU:CG	2.49	0.41
1:1A:1098:C:H42	1:1A:1153:G:H1	1.68	0.41
1:1A:1565:G:C6	1:1A:1566:U:C4	3.08	0.41
1:1A:2734:A:O2'	1:1A:2884:C:H5'	2.20	0.41
1:1A:619:G:H2'	1:1A:620:U:O4'	2.20	0.41
1:1A:659:C:H2'	1:1A:660:C:C6	2.56	0.41
1:1A:747:G:H2'	1:1A:748:G:O4'	2.21	0.41
2:1B:96:U:H2'	2:1B:97:G:C8	2.55	0.41
1:1A:956:A:C5	12:1Q:13:GLN:HG3	2.56	0.41
17:1V:25:LEU:O	17:1V:64:HIS:HE1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:13:ARG:NH2	26:24:23:GLU:HG2	2.26	0.41
1:2A:1203:G:H2'	1:2A:1241:A:N6	2.35	0.41
1:2A:1282:U:H2'	1:2A:1283:G:O4'	2.21	0.41
1:2A:557:U:H2'	1:2A:558:G:C8	2.56	0.41
4:2E:51:PHE:H	4:2E:75:VAL:HG11	1.86	0.41
14:2S:64:GLU:HB2	26:24:59:PHE:HE2	84.65	0.41
24:12:1:MET:SD	24:12:56:GLN:NE2	2.94	0.41
1:1A:1730:C:H2'	1:1A:1731:C:C6	2.55	0.41
1:1A:1895:U:OP1	1:1A:2422:G:O2'	2.26	0.41
1:1A:1312:G:O2'	1:1A:2034:G:O6	2.31	0.41
1:1A:2202:U:H2'	1:1A:2203:G:O4'	2.21	0.41
1:1A:230:A:H5''	63:1A:4740:HOH:O	2.19	0.41
1:1A:901:G:H2'	1:1A:902:G:H8	1.86	0.41
3:1D:5:LYS:HB3	3:1D:5:LYS:HE3	1.85	0.41
10:1O:34:THR:OG1	10:1O:35:VAL:N	2.53	0.41
12:1Q:31:ASP:HA	12:1Q:134:ARG:NH1	2.36	0.41
14:1S:61:ASN:O	14:1S:65:VAL:HG23	2.21	0.41
23:21:98:LEU:HA	23:21:98:LEU:HD23	1.96	0.41
1:2A:82:G:N1	1:2A:103:A:OP2	2.45	0.41
1:2A:1203:G:C6	1:2A:1204:A:N6	2.89	0.41
1:2A:2466:C:C2	1:2A:2485:G:C2	3.08	0.41
1:2A:588:U:H1'	5:2F:90:PHE:HB3	2.03	0.41
1:2A:71:A:H5''	1:2A:73:A:C8	2.56	0.41
1:2A:919:G:N2	1:2A:2269:A:OP2	2.54	0.41
2:2B:6:C:H2'	2:2B:7:G:O4'	2.21	0.41
3:2D:206:LEU:HA	3:2D:206:LEU:HD23	1.90	0.41
4:2E:31:CYS:HA	4:2E:32:PRO:HD2	1.96	0.41
8:2I:3:VAL:HA	8:2I:39:ALA:H	1.86	0.41
10:2O:63:VAL:HB	10:2O:102:VAL:HG12	2.02	0.41
16:2U:32:PHE:HZ	16:2U:36:ARG:HH21	1.68	0.41
1:1A:1024:G:H2'	1:1A:1024:G:N3	2.90	0.40
1:1A:1074:A:N6	1:1A:1171:G:H2'	2.36	0.40
1:1A:2018:C:H4'	1:1A:2019:G:OP1	2.20	0.40
1:1A:783:C:H5''	63:1A:4849:HOH:O	2.19	0.40
1:1A:993:G:H2'	1:1A:993:G:N3	2.91	0.40
4:1E:119:ARG:HG2	4:1E:160:TYR:CD2	2.56	0.40
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.39	0.40
7:1H:11:VAL:HA	7:1H:12:PRO:HD2	1.95	0.40
1:2A:1638:C:O2	1:2A:2698:U:O2'	2.35	0.40
1:2A:2081:C:H2'	1:2A:2082:A:H8	1.86	0.40
1:2A:230:U:H2'	1:2A:231:C:C6	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:285:C:H2'	1:2A:286:C:C6	2.55	0.40
2:2B:106:G:H5'	21:2Z:31:ARG:HB3	2.04	0.40
1:2A:2443:C:OP1	5:2F:68:LYS:HD3	2.20	0.40
10:2O:64:ARG:HD3	10:2O:101:PRO:O	2.21	0.40
11:2P:121:LYS:O	11:2P:123:LEU:N	2.54	0.40
6:1G:61:ALA:O	26:14:7:PRO:HG2	2.21	0.40
1:1A:2190:G:H8	1:1A:2190:G:O5'	2.04	0.40
1:1A:2391:G:O2'	14:1S:17:ARG:NH1	2.39	0.40
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.56	0.40
14:1S:19:LYS:HE2	14:1S:25:ARG:NH1	2.37	0.40
17:1V:35:LEU:HA	17:1V:36:PRO:HD3	1.97	0.40
24:22:53:LEU:HA	24:22:53:LEU:HD23	1.91	0.40
1:2A:1466:G:H2'	1:2A:1547:C:N4	2.36	0.40
1:2A:2443:C:H2'	1:2A:2444:G:C8	2.55	0.40
1:2A:2711:A:OP1	1:2A:2712:U:H3'	2.21	0.40
1:2A:907:U:O2'	12:2Q:101:ARG:NH2	2.53	0.40
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.67	0.40
18:2W:82:LEU:HD22	18:2W:84:ARG:HH22	1.86	0.40
1:1A:1841:A:H2'	1:1A:1842:G:O4'	2.21	0.40
1:1A:2227:G:H2'	1:1A:2228:G:C2	2.57	0.40
1:1A:2304:C:OP1	14:1S:17:ARG:NH2	2.40	0.40
1:1A:635:C:H2'	1:1A:636:G:O4'	2.21	0.40
1:1A:818:G:OP1	29:17:10:ARG:NH1	2.52	0.40
1:2A:1125:G:H5'	31:29:37:GLY:HA2	2.04	0.40
1:2A:1021:A:H3'	1:2A:1021:A:N3	2.37	0.40
1:2A:2776:A:H4'	1:2A:2777:G:H5''	2.04	0.40
1:2A:361:G:O2'	1:2A:362:U:H5'	2.22	0.40
1:2A:833:U:O2	11:2P:55:ARG:NH1	2.50	0.40
1:2A:923:C:H2'	1:2A:924:C:C6	2.56	0.40
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.54	0.40
10:2O:18:LYS:HB2	10:2O:45:GLU:HB3	2.03	0.40
15:2T:99:LEU:HD22	15:2T:101:PHE:HE2	1.86	0.40
1:1A:1551:C:H2'	1:1A:1552:C:C6	2.57	0.40
1:1A:1890:A:N6	1:1A:1905:G:O2'	2.55	0.40
1:1A:2342:G:H2'	1:1A:2343:G:O4'	2.21	0.40
1:1A:2724:U:O2'	1:1A:2726:A:H5'	2.22	0.40
1:1A:2784:C:H2'	1:1A:2785:C:C6	2.57	0.40
1:1A:721:G:H4'	1:1A:722:A:O4'	5.96	0.40
2:1B:32:C:C2	2:1B:51:G:N2	2.89	0.40
2:1B:54:G:H2'	2:1B:55:U:H6	1.86	0.40
15:1T:107:ASP:O	15:1T:111:ARG:HG3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2371:G:N3	28:26:46:HIS:HE1	2.19	0.40
1:2A:1513:C:H2'	1:2A:1514:U:C6	2.56	0.40
1:2A:1991:U:H2'	1:2A:1992:G:H5''	2.03	0.40
1:2A:2661:G:H2'	1:2A:2662:A:C8	2.56	0.40
1:2A:304:G:H2'	1:2A:305:U:C6	2.57	0.40
1:2A:784:A:O4'	3:2D:227:ASN:ND2	2.54	0.40
21:2Z:26:GLY:HA3	21:2Z:86:VAL:HG23	2.02	0.40
24:12:22:GLU:HG3	24:12:64:LEU:HD11	2.03	0.40
1:1A:1725:G:N3	1:1A:1725:G:H5''	2.36	0.40
1:1A:1735:U:H1'	1:1A:1748:A:C6	2.57	0.40
1:1A:233:A:C2	1:1A:244:A:C4	3.10	0.40
1:1A:2786:C:H2'	1:1A:2787:C:H6	1.86	0.40
3:1D:127:VAL:HA	3:1D:193:VAL:HG22	2.03	0.40
1:1A:1925:G:OP1	3:1D:241:PRO:HB2	2.21	0.40
3:1D:182:LEU:HB2	3:1D:272:ALA:HB3	2.04	0.40
8:1I:81:VAL:O	8:1I:147:GLN:N	2.53	0.40
23:21:25:LYS:HG3	23:21:31:GLY:HA2	2.03	0.40
1:2A:1421:G:C2	1:2A:1422:G:C8	3.09	0.40
1:2A:217:G:H2'	1:2A:218:A:O4'	2.21	0.40
1:2A:954:G:O2'	1:2A:2274:A:N1	2.40	0.40
1:2A:2462:U:H1'	1:2A:2491:U:O4	2.22	0.40
1:2A:275:G:C6	1:2A:276:A:C6	3.09	0.40
2:2B:7:G:H3'	2:2B:8:U:H5''	2.03	0.40
7:2H:11:VAL:HA	7:2H:12:PRO:HD2	1.98	0.40
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.64	0.40
12:2Q:4:PRO:HB2	12:2Q:7:MET:HE1	2.03	0.40
18:2W:13:SER:HA	18:2W:14:PRO:HD3	1.93	0.40
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	2.02	0.40

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
41	1j	77	PRO
41	1j	79	ARG
44	1m	67	GLU
48	1q	68	ARG
5	2F	21	ALA
5	2F	130	ALA
6	2G	50	ALA
19	2X	94	GLY
26	24	49	PHE
33	2b	8	LYS
33	2b	16	HIS
33	2b	17	PHE
38	2g	8	GLU
40	2i	44	VAL
40	2i	54	ASP
44	2m	67	GLU
8	1I	11	ASN
19	1X	94	GLY
26	14	45	GLY
33	1b	17	PHE
33	1b	126	GLU
42	1k	118	GLY
4	2E	51	PHE
6	2G	43	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	107	GLN
35	2d	171	GLY
38	2g	7	ALA
6	1G	43	LEU
8	1I	73	GLU
14	1S	59	LYS
33	1b	20	GLU
35	1d	129	ASN
41	1j	78	ASN
26	24	47	GLN
26	24	60	GLN
46	2o	88	ARG
51	2t	100	ILE
51	2t	102	GLY
4	1E	52	LEU
8	1I	85	GLU
33	1b	8	LYS
51	1t	95	ALA
8	2I	85	GLU
33	2b	125	PRO
34	2c	108	ASN
35	2d	129	ASN
41	2j	78	ASN
46	2o	23	GLY
51	2t	95	ALA
11	1P	122	PRO
33	1b	125	PRO
11	2P	122	PRO
17	2V	79	VAL
33	2b	123	ALA
52	2u	3	LYS
6	1G	47	LYS
26	14	55	ARG
33	1b	21	ARG
46	1o	23	GLY
6	2G	47	LYS
44	2m	5	ALA
41	1j	31	GLY
17	1V	79	VAL
33	1b	124	SER
33	1b	127	ILE
26	24	45	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	232	PRO
51	1t	100	ILE
33	1b	232	PRO
51	1t	98	PRO

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (507) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	61	LEU
3	1D	69	ARG
3	1D	94	LEU
3	1D	103	ARG
3	1D	106	ILE
3	1D	111	LEU
3	1D	141	VAL
3	1D	193	VAL
3	1D	211	ARG
3	1D	217	ARG
3	1D	229	VAL
3	1D	242	ARG
4	1E	7	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	1E	21	VAL
4	1E	33	VAL
4	1E	49	LEU
4	1E	73	GLU
4	1E	78	LEU
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	154	LYS
4	1E	175	VAL
4	1E	178	GLU
5	1F	12	LEU
5	1F	18	ARG
5	1F	32	LEU
5	1F	33	LEU
5	1F	57	VAL
5	1F	74	ARG
5	1F	95	ARG
5	1F	110	LEU
5	1F	170	LEU
5	1F	192	LEU
5	1F	197	ASP
6	1G	5	VAL
6	1G	21	ARG
6	1G	43	LEU
6	1G	45	GLU
6	1G	53	LEU
6	1G	82	LEU
6	1G	133	LEU
6	1G	148	MET
6	1G	159	VAL
6	1G	165	THR
6	1G	167	GLU
7	1H	13	LYS
7	1H	15	VAL
7	1H	45	VAL
7	1H	71	LEU
7	1H	84	SER
8	1I	5	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	38	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1I	44	LEU
8	1I	64	GLU
8	1I	75	LEU
8	1I	78	THR
8	1I	92	VAL
8	1I	109	ILE
8	1I	140	LEU
9	1N	5	VAL
9	1N	33	LEU
9	1N	62	VAL
9	1N	67	LEU
9	1N	87	LEU
9	1N	97	ARG
9	1N	99	LEU
9	1N	115	ARG
9	1N	121	LYS
10	1O	10	VAL
10	1O	24	VAL
10	1O	64	ARG
10	1O	69	ILE
11	1P	2	LYS
11	1P	3	LEU
11	1P	59	LEU
11	1P	83	VAL
11	1P	98	GLU
11	1P	99	LEU
11	1P	112	LEU
11	1P	125	VAL
11	1P	147	LEU
12	1Q	2	LEU
12	1Q	7	MET
12	1Q	21	THR
12	1Q	55	VAL
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	110	THR
13	1R	6	SER
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	65	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1R	67	LEU
13	1R	75	LEU
13	1R	96	ARG
13	1R	100	LEU
14	1S	36	TYR
14	1S	59	LYS
14	1S	69	VAL
15	1T	13	ARG
15	1T	17	THR
15	1T	34	VAL
15	1T	59	THR
15	1T	89	VAL
15	1T	108	ARG
16	1U	8	VAL
16	1U	36	ARG
16	1U	52	ARG
16	1U	74	LEU
16	1U	83	LEU
16	1U	104	GLN
17	1V	46	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
17	1V	85	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	60	ASN
18	1W	107	LEU
19	1X	66	LEU
20	1Y	43	ASN
20	1Y	85	VAL
20	1Y	90	LEU
20	1Y	99	CYS
21	1Z	11	GLU
21	1Z	18	LEU
21	1Z	31	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	42	VAL
21	1Z	46	LYS
21	1Z	72	ARG
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	135	GLU
21	1Z	150	LEU
21	1Z	182	LYS
21	1Z	202	GLU
21	1Z	203	GLU
22	10	10	THR
22	10	11	ARG
22	10	39	ARG
23	11	23	LYS
23	11	95	LEU
24	12	3	LEU
25	13	6	VAL
25	13	8	LEU
25	13	54	VAL
25	13	55	ARG
26	14	13	ARG
26	14	49	PHE
26	14	60	GLN
26	14	61	ARG
26	14	67	TYR
27	15	29	THR
27	15	35	GLU
28	16	6	ARG
28	16	14	THR
28	16	49	HIS
29	17	1	MET
29	17	10	ARG
29	17	43	THR
29	17	47	ARG
30	18	14	VAL
30	18	30	ARG
30	18	31	HIS
30	18	34	TRP
33	1b	15	VAL
33	1b	19	HIS
33	1b	21	ARG
33	1b	24	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	45	GLN
33	1b	67	THR
33	1b	68	ILE
33	1b	73	THR
33	1b	81	VAL
33	1b	106	LYS
33	1b	111	ARG
33	1b	112	VAL
33	1b	114	ARG
33	1b	122	PHE
33	1b	128	GLU
33	1b	158	LEU
33	1b	160	ASP
33	1b	172	ILE
33	1b	178	ARG
33	1b	200	ILE
33	1b	221	LEU
33	1b	224	GLN
34	1c	3	ASN
34	1c	15	THR
34	1c	29	TYR
34	1c	36	ASP
34	1c	64	VAL
34	1c	161	GLU
35	1d	8	VAL
35	1d	127	THR
35	1d	135	LEU
35	1d	158	ILE
35	1d	178	VAL
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
36	1e	41	VAL
36	1e	69	VAL
36	1e	120	THR
37	1f	92	LYS
38	1g	11	GLN
38	1g	75	VAL
38	1g	90	GLU
39	1h	26	VAL
39	1h	51	VAL
39	1h	52	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	1h	63	LEU
39	1h	95	VAL
40	1i	2	GLU
40	1i	17	VAL
40	1i	27	THR
40	1i	87	GLN
40	1i	92	TYR
40	1i	125	TYR
41	1j	92	THR
41	1j	100	THR
42	1k	87	THR
42	1k	117	ASN
43	1l	27	LEU
43	1l	33	ARG
43	1l	66	VAL
43	1l	83	VAL
44	1m	4	ILE
44	1m	8	GLU
44	1m	19	LEU
44	1m	56	LEU
44	1m	102	ARG
44	1m	109	THR
45	1n	3	ARG
45	1n	18	VAL
45	1n	33	VAL
46	1o	3	ILE
46	1o	39	LEU
47	1p	8	ARG
47	1p	11	SER
47	1p	28	ARG
47	1p	42	ARG
47	1p	45	THR
47	1p	67	THR
48	1q	93	GLN
49	1r	76	LEU
50	1s	4	SER
50	1s	5	LEU
50	1s	37	ARG
50	1s	41	VAL
51	1t	84	LEU
51	1t	100	ILE
3	2D	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2D	69	ARG
3	2D	94	LEU
3	2D	103	ARG
3	2D	111	LEU
3	2D	138	VAL
3	2D	141	VAL
3	2D	193	VAL
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
4	2E	21	VAL
4	2E	33	VAL
4	2E	89	ASP
4	2E	116	VAL
4	2E	144	ARG
4	2E	154	LYS
4	2E	175	VAL
4	2E	184	VAL
5	2F	18	ARG
5	2F	27	GLU
5	2F	33	LEU
5	2F	53	THR
5	2F	57	VAL
5	2F	74	ARG
5	2F	88	VAL
5	2F	158	THR
5	2F	170	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
6	2G	3	LEU
6	2G	5	VAL
6	2G	49	ASP
6	2G	53	LEU
6	2G	91	ARG
6	2G	108	ASN
6	2G	133	LEU
6	2G	159	VAL
6	2G	165	THR
7	2H	18	GLU
7	2H	49	VAL
7	2H	71	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	2H	124	GLU
7	2H	171	LEU
8	2I	5	LEU
8	2I	47	LEU
8	2I	66	GLU
8	2I	75	LEU
8	2I	123	LEU
8	2I	140	LEU
8	2I	144	VAL
9	2N	12	ARG
9	2N	28	THR
9	2N	33	LEU
9	2N	34	LEU
9	2N	87	LEU
9	2N	99	LEU
10	2O	10	VAL
10	2O	24	VAL
10	2O	53	LYS
10	2O	69	ILE
11	2P	59	LEU
11	2P	83	VAL
11	2P	112	LEU
11	2P	125	VAL
12	2Q	16	ARG
12	2Q	21	THR
12	2Q	55	VAL
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	109	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	18	LEU
13	2R	24	GLN
13	2R	44	LEU
13	2R	65	LEU
13	2R	67	LEU
13	2R	71	GLN
13	2R	75	LEU
13	2R	79	LEU
13	2R	86	ARG
13	2R	96	ARG
13	2R	100	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	2R	111	LEU
14	2S	13	ARG
14	2S	14	VAL
14	2S	25	ARG
14	2S	75	GLU
15	2T	16	ARG
15	2T	74	ARG
15	2T	89	VAL
16	2U	8	VAL
16	2U	60	LEU
16	2U	74	LEU
16	2U	95	LEU
16	2U	112	ARG
16	2U	117	GLN
17	2V	7	THR
17	2V	18	LEU
17	2V	52	VAL
17	2V	57	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	107	LEU
19	2X	8	ILE
19	2X	57	LEU
19	2X	66	LEU
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	99	CYS
21	2Z	31	ARG
21	2Z	42	VAL
21	2Z	76	LEU
21	2Z	86	VAL
21	2Z	93	ASP
21	2Z	94	GLU
21	2Z	136	PHE
21	2Z	150	LEU
21	2Z	190	GLU
21	2Z	193	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	20	10	THR
22	20	39	ARG
23	21	52	ARG
23	21	75	GLU
23	21	85	LEU
23	21	95	LEU
24	22	32	LEU
24	22	70	GLN
25	23	6	VAL
25	23	23	LEU
25	23	31	LEU
26	24	50	VAL
26	24	53	GLU
26	24	67	TYR
27	25	6	VAL
28	26	6	ARG
28	26	14	THR
28	26	49	HIS
30	28	14	VAL
30	28	31	HIS
30	28	34	TRP
33	2b	24	TRP
33	2b	67	THR
33	2b	68	ILE
33	2b	73	THR
33	2b	128	GLU
33	2b	135	GLN
33	2b	136	VAL
33	2b	139	LYS
33	2b	154	LEU
33	2b	160	ASP
33	2b	185	ILE
33	2b	191	ASP
33	2b	196	LEU
33	2b	217	ARG
33	2b	224	GLN
33	2b	230	VAL
34	2c	3	ASN
34	2c	20	SER
34	2c	29	TYR
34	2c	52	LEU
34	2c	70	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	115	LEU
34	2c	128	PHE
34	2c	152	ILE
34	2c	166	GLU
34	2c	190	ARG
35	2d	8	VAL
35	2d	31	CYS
35	2d	34	GLU
35	2d	135	LEU
35	2d	194	LEU
36	2e	9	LYS
36	2e	40	ARG
36	2e	41	VAL
36	2e	69	VAL
36	2e	72	GLN
38	2g	8	GLU
38	2g	51	GLN
38	2g	53	LYS
38	2g	75	VAL
38	2g	104	LEU
38	2g	113	GLU
38	2g	115	ARG
39	2h	52	ASP
39	2h	63	LEU
39	2h	91	ARG
39	2h	98	LYS
39	2h	112	LEU
39	2h	135	CYS
39	2h	137	VAL
40	2i	14	VAL
40	2i	17	VAL
40	2i	53	VAL
40	2i	92	TYR
40	2i	93	ARG
40	2i	102	LEU
40	2i	113	LYS
40	2i	125	TYR
41	2j	29	ARG
41	2j	69	ASN
42	2k	14	VAL
42	2k	103	LEU
42	2k	106	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	2l	27	LEU
43	2l	33	ARG
43	2l	66	VAL
43	2l	83	VAL
44	2m	4	ILE
44	2m	8	GLU
44	2m	19	LEU
44	2m	60	VAL
44	2m	65	LYS
44	2m	94	ARG
44	2m	102	ARG
44	2m	109	THR
45	2n	18	VAL
46	2o	5	LYS
46	2o	10	LYS
46	2o	28	GLN
46	2o	83	GLU
47	2p	5	ARG
47	2p	42	ARG
47	2p	60	LEU
47	2p	67	THR
47	2p	69	THR
47	2p	76	GLN
48	2q	50	LYS
48	2q	74	LEU
49	2r	25	THR
50	2s	13	ASP
50	2s	16	LEU
50	2s	27	GLU
50	2s	41	VAL
50	2s	81	ARG
51	2t	84	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	143	HIS
3	1D	253	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	75	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	203	GLN
6	1G	79	ASN
8	1I	54	GLN
8	1I	105	HIS
9	1N	8	GLN
10	1O	3	GLN
10	1O	5	GLN
12	1Q	123	HIS
14	1S	68	GLN
14	1S	95	HIS
15	1T	58	ASN
16	1U	104	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	92	ASN
21	1Z	32	HIS
21	1Z	73	GLN
30	18	35	GLN
34	1c	6	HIS
34	1c	181	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	129	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	109	ASN
40	1i	3	GLN
41	1j	56	HIS
41	1j	62	HIS
46	1o	28	GLN
48	1q	26	GLN
50	1s	47	HIS
50	1s	56	GLN
3	2D	116	GLN
3	2D	253	GLN
5	2F	69	HIS
5	2F	203	GLN
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	123	HIS
13	2R	13	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	2S	95	HIS
15	2T	58	ASN
18	2W	61	ASN
19	2X	31	HIS
21	2Z	54	HIS
21	2Z	73	GLN
21	2Z	151	HIS
22	20	50	ASN
22	20	70	GLN
26	24	46	GLN
31	29	20	HIS
33	2b	40	HIS
34	2c	6	HIS
34	2c	176	HIS
34	2c	181	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	129	ASN
36	2e	78	HIS
37	2f	94	GLN
38	2g	11	GLN
38	2g	86	GLN
40	2i	3	GLN
40	2i	124	GLN
41	2j	13	HIS
41	2j	69	ASN
44	2m	92	HIS
46	2o	62	GLN
47	2p	76	GLN
48	2q	16	GLN
48	2q	26	GLN
50	2s	23	ASN
50	2s	57	HIS
50	2s	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2814/2915 (96%)	427 (15%)	31 (1%)
1	2A	2859/2915 (98%)	486 (16%)	28 (0%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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%)

All (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
1	1A	60	G
1	1A	63	A
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	121	G
1	1A	123	G
1	1A	170	A
1	1A	171	A
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	206	G
1	1A	211	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	269	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	275	C
1	1A	288	U
1	1A	289	G
1	1A	296	U
1	1A	299	G
1	1A	303	C
1	1A	335	A
1	1A	348	A
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	397	G
1	1A	398	A
1	1A	399	G
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	448	U
1	1A	455	A
1	1A	474	U
1	1A	480	A
1	1A	481	C
1	1A	483	A
1	1A	507	G
1	1A	510	C
1	1A	530	A
1	1A	534	C
1	1A	554	A
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	598	A
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	638	U
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	692	C
1	1A	693	G
1	1A	694	G
1	1A	697	C
1	1A	698	G
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	787	U
1	1A	800	C
1	1A	809	U
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	847	A
1	1A	852	G
1	1A	858	U
1	1A	859	C
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	926	G
1	1A	927	G
1	1A	931	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	932	C
1	1A	933	C
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	938	G
1	1A	942	A
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	998	A
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1036	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U
1	1A	1059	C
1	1A	1067	A
1	1A	1072	U
1	1A	1079	U
1	1A	1088	G
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1098	C
1	1A	1099	C
1	1A	1100	A
1	1A	1155	C
1	1A	1156	G
1	1A	1158	G
1	1A	1162	C
1	1A	1174	A
1	1A	1175	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1184	G
1	1A	1186	U
1	1A	1195	G
1	1A	1201	A
1	1A	1202	A
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1234	A
1	1A	1255	A
1	1A	1256	U
1	1A	1263	C
1	1A	1290	G
1	1A	1299	A
1	1A	1302	G
1	1A	1314	A
1	1A	1317	G
1	1A	1318	A
1	1A	1321	A
1	1A	1335	C
1	1A	1346	U
1	1A	1347	A
1	1A	1359	U
1	1A	1367	A
1	1A	1378	G
1	1A	1391	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1414	G
1	1A	1416	C
1	1A	1425	A
1	1A	1430	A
1	1A	1431	G
1	1A	1432	C
1	1A	1441	A
1	1A	1462	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1483	C
1	1A	1491	A
1	1A	1492	C
1	1A	1497	G
1	1A	1500	A
1	1A	1506	G
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1539	C
1	1A	1542	A
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1589	A
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1626	A
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1662	A
1	1A	1686	U
1	1A	1695	C
1	1A	1701	A
1	1A	1711	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1766	G
1	1A	1767	A
1	1A	1768	U
1	1A	1769	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1787	G
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1805	C
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1859	G
1	1A	1870	G
1	1A	1878	A
1	1A	1879	A
1	1A	1896	G
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1935	A
1	1A	1936	C
1	1A	1937	5MU
1	1A	1942	OMC
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2045	G
1	1A	2049	G
1	1A	2053	A
1	1A	2054	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2121	U
1	1A	2124	U
1	1A	2125	C
1	1A	2126	G
1	1A	2129	C
1	1A	2130	C
1	1A	2132	G
1	1A	2137	G
1	1A	2138	G
1	1A	2139	A
1	1A	2141	A
1	1A	2142	G
1	1A	2144	U
1	1A	2147	G
1	1A	2148	A
1	1A	2149	G
1	1A	2150	C
1	1A	2152	U
1	1A	2153	G
1	1A	2155	G
1	1A	2158	C
1	1A	2159	C
1	1A	2160	C
1	1A	2168	C
1	1A	2174	G
1	1A	2180	A
1	1A	2181	G
1	1A	2184	G
1	1A	2187	G
1	1A	2188	G
1	1A	2191	A
1	1A	2192	A
1	1A	2202	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2205	C
1	1A	2206	G
1	1A	2208	G
1	1A	2209	G
1	1A	2212	G
1	1A	2214	G
1	1A	2220	A
1	1A	2226	C
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2231	G
1	1A	2237	A
1	1A	2246	G
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2290	A
1	1A	2295	C
1	1A	2299	A
1	1A	2301	G
1	1A	2306	C
1	1A	2317	A
1	1A	2324	U
1	1A	2332	A
1	1A	2333	G
1	1A	2337	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2395	G
1	1A	2397	C
1	1A	2412	G
1	1A	2418	U
1	1A	2426	G
1	1A	2434	A
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2446	A
1	1A	2447	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2451	A
1	1A	2453	C
1	1A	2457	G
1	1A	2460	A
1	1A	2480	G
1	1A	2481	A
1	1A	2488	A
1	1A	2514	G
1	1A	2516	U
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2532	C
1	1A	2541	G
1	1A	2547	G
1	1A	2561	G
1	1A	2562	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2586	G
1	1A	2594	G
1	1A	2597	U
1	1A	2598	C
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2674	A
1	1A	2701	U
1	1A	2702	C
1	1A	2703	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2771	A
1	1A	2778	A
1	1A	2779	G
1	1A	2780	C
1	1A	2791	A
1	1A	2793	G
1	1A	2803	A
1	1A	2804	C
1	1A	2813	G
1	1A	2828	G
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2882	G
1	1A	2884	C
1	1A	2885	C
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	47	C
2	1B	56	G
2	1B	57	A
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	96	U
32	1a	101	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	151	A
32	1a	159	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(E)	U
32	1a	189(F)	U
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	218	C
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	298	A
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	381	C
32	1a	384	G
32	1a	388	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	477	A
32	1a	482	A
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	527	G7M
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	550	G
32	1a	558	G
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	618	C
32	1a	619	U
32	1a	630	G
32	1a	631	G
32	1a	632	A
32	1a	633	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	680	C
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	735	C
32	1a	746	A
32	1a	753	A
32	1a	755	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	796	C
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	838	G
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	859	A
32	1a	872	A
32	1a	873	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	960	U
32	1a	961	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	998	G
32	1a	999	C
32	1a	1001(A)	G
32	1a	1004	A
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1039	C
32	1a	1040	U
32	1a	1043	C
32	1a	1044	A
32	1a	1045	C
32	1a	1053	G
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1101	A
32	1a	1118	C
32	1a	1122	U
32	1a	1125	U
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1151	A
32	1a	1152	A
32	1a	1159	U
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1240	U
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1278	U
32	1a	1280	A
32	1a	1281	U
32	1a	1282	C
32	1a	1286	A
32	1a	1287	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1312	G
32	1a	1315	U
32	1a	1317	C
32	1a	1319	A
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
53	1x	9	G
53	1x	20	U
53	1x	21	A
53	1x	42	G
53	1x	50	U
53	1x	54	5MU
53	1x	68	C
1	2A	10	G
1	2A	11	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	12	U
1	2A	15	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	95	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	211	A
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	249	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	292	C
1	2A	311	A
1	2A	324	A
1	2A	327	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	329	G
1	2A	330	A
1	2A	345	A
1	2A	352	G
1	2A	354	G
1	2A	362	U
1	2A	363	G
1	2A	370	G
1	2A	372	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	464	U
1	2A	470	A
1	2A	479	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(F)	G
1	2A	652(T)	C
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	740	U
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	793	A
1	2A	794	G
1	2A	802	A
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	848	G
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	874	G
1	2A	883	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	899	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	936	C
1	2A	938	G
1	2A	941	A
1	2A	944	G
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1043	C
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1058	G
1	2A	1060	U
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1070	A
1	2A	1071	G
1	2A	1072	C
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1087	G
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1096	A
1	2A	1109	C
1	2A	1110	G
1	2A	1112	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1170	G
1	2A	1171	G
1	2A	1211	U
1	2A	1220	A
1	2A	1229	G
1	2A	1236	G
1	2A	1237	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1268	A
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1313	U
1	2A	1314	C
1	2A	1342	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1373	A
1	2A	1376	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1459	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1602	U
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1639	U
1	2A	1648	C
1	2A	1664	A
1	2A	1674	G
1	2A	1675	C
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1820	U
1	2A	1828	G
1	2A	1835	G
1	2A	1847	A
1	2A	1861	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1937	A
1	2A	1947	C
1	2A	1955	U
1	2A	1962	5MC
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2004	G
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2070	G
1	2A	2076	U
1	2A	2093	G
1	2A	2101	G
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2121	G
1	2A	2123	G
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2141	G
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2151	G
1	2A	2159	G
1	2A	2162	G
1	2A	2163	C
1	2A	2164	C
1	2A	2172	U
1	2A	2173	A
1	2A	2180	U
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2191	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2225	A
1	2A	2235	G
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2273	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2297	C
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2316	C
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2340	G
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2427	C
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2445	G
1	2A	2448	A
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2549	G
1	2A	2553	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2572	A
1	2A	2574	G
1	2A	2576	G
1	2A	2577	A
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2620	C
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2769	C
1	2A	2778	A
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2823	A
1	2A	2833	G
1	2A	2866	U
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U
2	2B	2	C
2	2B	7	G
2	2B	8	U
2	2B	13	A
2	2B	15	A
2	2B	33	G
2	2B	42	C
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	106	G
2	2B	110	G
32	2a	5	U
32	2a	9	G
32	2a	10	A
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	48	C
32	2a	50	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	51	A
32	2a	66	G
32	2a	89	C
32	2a	96	U
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	151	A
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	218	C
32	2a	220	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	298	A
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	348	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	388	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	422	C
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	477	A
32	2a	482	A
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	527	G7M
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	550	G
32	2a	558	G
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	562	C
32	2a	572	A
32	2a	573	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	576	G
32	2a	592	G
32	2a	596	C
32	2a	618	C
32	2a	619	U
32	2a	630	G
32	2a	631	G
32	2a	632	A
32	2a	633	G
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	746	A
32	2a	753	A
32	2a	755	G
32	2a	766	A
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	796	C
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	838	G
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	859	A
32	2a	872	A
32	2a	873	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	1005	A
32	2a	1009	G
32	2a	1022	G
32	2a	1023	G
32	2a	1024	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(C)	G
32	2a	1032	G
32	2a	1033	G
32	2a	1034	G
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1045	C
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1101	A
32	2a	1117	G
32	2a	1118	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1147	C
32	2a	1151	A
32	2a	1152	A
32	2a	1158	C
32	2a	1159	U
32	2a	1168	A
32	2a	1183	A
32	2a	1184	G
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1299	A
32	2a	1300	G
32	2a	1305	G
32	2a	1312	G
32	2a	1315	U
32	2a	1317	C
32	2a	1319	A
32	2a	1320	C
32	2a	1340	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1456	G
32	2a	1487	G
32	2a	1492	A
32	2a	1493	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
53	2x	9	G
53	2x	20	U
53	2x	21	A
53	2x	42	G
53	2x	50	U
53	2x	68	C
53	2x	69	C
53	2x	76	A

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	78	G
1	1A	115	G
1	1A	185	A
1	1A	302	A
1	1A	509	A
1	1A	532	A
1	1A	831	A
1	1A	874	U
1	1A	913	A
1	1A	941	U
1	1A	1003	U
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1097	G
1	1A	1099	C
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1299	A
1	1A	1346	U
1	1A	1700	G
1	1A	1710	C
1	1A	2300	A
1	1A	2434	A
1	1A	2442	A
1	1A	2597	U
1	1A	2701	U
1	1A	2902	G
1	2A	9	U
1	2A	195	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	532	A
1	2A	652(E)	G
1	2A	752	A
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1053	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2689	U
1	2A	2756	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	OMU	C3'-C2'	-8.86	1.33	1.53
1	2A	2552	OMU	C3'-C2'	-8.58	1.33	1.53
32	2a	516	PSU	C5-C1'	-6.44	1.46	1.52
1	2A	2552	OMU	O4'-C4'	-6.13	1.31	1.45
1	1A	2564	OMU	O4'-C4'	-5.64	1.32	1.45
32	1a	516	PSU	C5-C1'	-5.08	1.47	1.52
1	1A	2617	PSU	C5-C1'	-4.42	1.48	1.52
1	2A	2605	PSU	C5-C1'	-3.91	1.48	1.52
43	1l	92	0TD	CB-SB	-2.93	1.76	1.84
1	1A	2617	PSU	C6-C5	-2.91	1.34	1.38
32	2a	516	PSU	O4'-C1'	-2.83	1.40	1.44
32	1a	516	PSU	O4'-C1'	-2.70	1.40	1.44
53	2x	55	PSU	C5-C1'	-2.69	1.49	1.52
32	2a	1402	4OC	CM4-N4	-2.54	1.40	1.45
1	2A	1917	PSU	C6-C5	-2.53	1.34	1.38
1	2A	2605	PSU	C6-C5	-2.48	1.35	1.38
32	2a	516	PSU	C6-C5	-2.47	1.35	1.38
53	2x	55	PSU	C6-C5	-2.46	1.35	1.38
43	2l	92	0TD	CB-SB	-2.42	1.78	1.84
1	1A	1939	PSU	C6-C5	-2.41	1.35	1.38
32	1a	1518	MA6	C5-C4	-2.37	1.35	1.40
32	1a	516	PSU	C6-C5	-2.36	1.35	1.38
1	1A	2515	2MA	C5-C4	-2.33	1.35	1.40
1	1A	1933	PSU	C6-C5	-2.30	1.35	1.38
1	2A	2503	2MA	C5-C4	-2.27	1.35	1.40
32	1a	1519	MA6	C5-C4	-2.27	1.35	1.40
32	2a	1519	MA6	C5-C4	-2.23	1.35	1.40
1	1A	1961	5MU	C5M-C5	-2.23	1.46	1.51
43	1l	92	0TD	CA-N	-2.21	1.41	1.47
32	2a	1518	MA6	C5-C4	-2.21	1.35	1.40
53	1x	55	PSU	C6-C5	-2.21	1.35	1.38
1	2A	1911	PSU	C6-C5	-2.18	1.35	1.38
32	1a	1402	4OC	CM4-N4	-2.17	1.41	1.45
43	2l	92	0TD	CA-N	-2.12	1.41	1.47
1	1A	1984	5MC	CM5-C5	-2.10	1.46	1.51
1	2A	2251	OMG	C5-C4	-2.10	1.35	1.40
1	2A	1917	PSU	C5-C1'	-2.09	1.50	1.52
32	1a	966	M2G	CM2-N2	-2.07	1.40	1.45
1	1A	2263	OMG	C5-C4	-2.06	1.35	1.40
32	2a	966	M2G	CM2-N2	-2.04	1.40	1.45
1	2A	1915	5MU	C2-N3	2.07	1.42	1.38
53	2x	55	PSU	C2-N1	2.09	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1207	2MG	C2-N3	2.10	1.42	1.34
53	1x	8	4SU	C6-N1	2.14	1.38	1.35
1	1A	2564	OMU	O2'-C2'	2.15	1.48	1.42
32	1a	1207	2MG	C2-N3	2.17	1.42	1.34
1	2A	2251	OMG	C2-N2	2.25	1.38	1.34
32	1a	1518	MA6	C2-N3	2.29	1.36	1.32
53	2x	8	4SU	C6-N1	2.29	1.38	1.35
32	2a	516	PSU	C6-N1	2.31	1.39	1.34
32	1a	1498	UR3	C4-N3	2.35	1.41	1.38
53	2x	8	4SU	C2-N3	2.35	1.43	1.38
1	2A	2552	OMU	O2'-C2'	2.39	1.49	1.42
32	2a	1518	MA6	C2-N3	2.40	1.36	1.32
32	1a	1519	MA6	C2-N3	2.48	1.36	1.32
32	2a	1519	MA6	C2-N3	2.49	1.36	1.32
1	1A	1939	PSU	C6-N1	2.55	1.39	1.34
32	2a	1498	UR3	C4-N3	2.59	1.42	1.38
1	1A	2263	OMG	C2-N2	2.62	1.39	1.34
1	1A	2617	PSU	C6-N1	2.63	1.39	1.34
1	2A	1917	PSU	C6-N1	2.64	1.40	1.34
1	1A	1933	PSU	C6-N1	2.64	1.40	1.34
1	2A	1920	OMC	C4-N3	2.66	1.40	1.35
1	2A	1911	PSU	C6-N1	2.69	1.40	1.34
32	1a	516	PSU	C6-N1	2.69	1.40	1.34
32	2a	1207	2MG	C2-N1	2.69	1.44	1.34
1	2A	2503	2MA	C6-N1	2.76	1.40	1.34
1	1A	1942	OMC	C4-N3	2.81	1.40	1.35
1	2A	2605	PSU	C6-N1	2.83	1.40	1.34
32	1a	1207	2MG	C2-N1	2.87	1.44	1.34
1	1A	2515	2MA	C6-N1	2.88	1.40	1.34
53	1x	55	PSU	C6-N1	2.88	1.40	1.34
53	2x	55	PSU	C6-N1	2.92	1.40	1.34
32	2a	1402	4OC	C4-N3	2.92	1.39	1.34
53	1x	8	4SU	C5-C4	3.11	1.42	1.38
1	1A	1942	OMC	C5-C4	3.30	1.48	1.41
32	2a	1402	4OC	C2-N3	3.37	1.45	1.38
1	1A	1942	OMC	C6-C5	3.41	1.45	1.38
32	1a	1402	4OC	C4-N3	3.42	1.40	1.34
1	2A	1920	OMC	C2-N3	3.51	1.45	1.38
32	1a	1402	4OC	C2-N3	3.53	1.45	1.38
32	2a	1207	2MG	C6-N1	3.58	1.39	1.33
32	1a	1207	2MG	C6-N1	3.58	1.39	1.33
32	1a	1402	4OC	C6-C5	3.58	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1920	OMC	C5-C4	3.60	1.49	1.41
1	1A	1942	OMC	C2-N3	3.60	1.45	1.38
32	1a	527	G7M	C2-N2	3.65	1.41	1.34
32	2a	527	G7M	C2-N2	3.66	1.41	1.34
32	2a	1402	4OC	C6-C5	3.72	1.46	1.38
1	2A	1920	OMC	C6-C5	3.72	1.46	1.38
1	2A	2251	OMG	C2-N1	3.74	1.42	1.35
1	1A	2263	OMG	C2-N1	3.82	1.42	1.35
1	1A	1961	5MU	C4-N3	3.83	1.39	1.33
1	2A	2552	OMU	C3'-C4'	3.91	1.63	1.53
1	1A	2564	OMU	C3'-C4'	3.94	1.63	1.53
1	2A	1939	5MU	C4-N3	3.94	1.40	1.33
32	1a	1207	2MG	C6-C5	4.03	1.49	1.41
32	1a	1498	UR3	C6-C5	4.05	1.46	1.38
32	2a	1207	2MG	C6-C5	4.06	1.49	1.41
32	2a	1498	UR3	C6-C5	4.09	1.47	1.38
32	1a	1402	4OC	C6-N1	4.13	1.41	1.35
1	1A	1942	OMC	C6-N1	4.17	1.41	1.35
1	2A	2251	OMG	C6-C5	4.24	1.49	1.41
32	1a	1402	4OC	C5-C4	4.28	1.49	1.39
32	1a	527	G7M	C6-N1	4.35	1.40	1.33
53	2x	54	5MU	C4-N3	4.36	1.40	1.33
32	2a	1402	4OC	C5-C4	4.36	1.49	1.39
1	1A	1942	OMC	C4-N4	4.38	1.47	1.35
32	2a	1402	4OC	C6-N1	4.39	1.41	1.35
32	1a	966	M2G	C6-N1	4.42	1.41	1.33
1	1A	2263	OMG	C6-N1	4.43	1.41	1.33
32	2a	527	G7M	C6-N1	4.43	1.41	1.33
1	2A	2251	OMG	C6-N1	4.44	1.41	1.33
1	2A	1920	OMC	C4-N4	4.46	1.47	1.35
1	1A	1937	5MU	C4-N3	4.48	1.41	1.33
53	1x	54	5MU	C4-N3	4.48	1.41	1.33
1	2A	1920	OMC	C6-N1	4.48	1.41	1.35
53	2x	8	4SU	C5-C4	4.50	1.44	1.38
1	1A	2263	OMG	C6-C5	4.55	1.50	1.41
32	1a	1498	UR3	C6-N1	4.58	1.41	1.35
32	2a	516	PSU	C4-N3	4.60	1.41	1.33
32	2a	966	M2G	C6-N1	4.60	1.41	1.33
1	2A	1915	5MU	C4-N3	4.60	1.41	1.33
1	1A	2515	2MA	C2-N3	4.63	1.42	1.34
1	2A	2503	2MA	C2-N1	4.66	1.42	1.34
32	1a	527	G7M	C2-N1	4.72	1.44	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2515	2MA	C2-N1	4.74	1.42	1.34
32	2a	527	G7M	C2-N1	4.75	1.44	1.35
32	2a	1498	UR3	C6-N1	4.79	1.41	1.35
1	1A	2515	2MA	C6-C5	4.83	1.49	1.40
32	2a	527	G7M	C6-C5	4.92	1.51	1.41
1	2A	2503	2MA	C2-N3	4.93	1.43	1.34
32	1a	527	G7M	C6-C5	5.00	1.51	1.41
1	2A	2503	2MA	C6-C5	5.05	1.50	1.40
32	1a	516	PSU	C4-N3	5.13	1.42	1.33
32	2a	966	M2G	C2-N1	5.27	1.43	1.34
32	2a	966	M2G	C6-C5	5.29	1.52	1.41
1	2A	2503	2MA	C4-N3	5.36	1.44	1.35
32	1a	966	M2G	C2-N1	5.38	1.43	1.34
32	1a	966	M2G	C6-C5	5.43	1.52	1.41
1	2A	1917	PSU	C4-N3	5.50	1.43	1.33
1	1A	2515	2MA	C4-N3	5.51	1.44	1.35
1	1A	2617	PSU	C4-N3	5.58	1.43	1.33
32	2a	1207	2MG	C4-N3	5.60	1.44	1.35
1	2A	1911	PSU	C4-N3	5.63	1.43	1.33
32	1a	1207	2MG	C4-N3	5.65	1.44	1.35
1	1A	1939	PSU	C4-N3	5.72	1.43	1.33
32	1a	966	M2G	C2-N2	5.74	1.44	1.34
32	2a	966	M2G	C2-N2	5.94	1.44	1.34
53	1x	55	PSU	C4-N3	5.95	1.43	1.33
32	2a	527	G7M	C4-N3	6.09	1.45	1.35
1	1A	1933	PSU	C4-N3	6.15	1.44	1.33
32	1a	527	G7M	C4-N3	6.21	1.45	1.35
1	1A	2263	OMG	C4-N3	6.22	1.45	1.35
1	2A	2605	PSU	C4-N3	6.25	1.44	1.33
1	2A	2251	OMG	C4-N3	6.36	1.45	1.35
53	2x	55	PSU	C4-N3	6.44	1.44	1.33
32	1a	966	M2G	C4-N3	6.62	1.46	1.35
32	2a	966	M2G	C4-N3	7.09	1.47	1.35
32	2a	1207	2MG	C2-N2	7.19	1.42	1.34
32	1a	1207	2MG	C2-N2	7.41	1.42	1.34
32	1a	527	G7M	C8-N7	7.73	1.47	1.33
32	2a	527	G7M	C8-N7	7.90	1.47	1.33
32	2a	527	G7M	C8-N9	8.27	1.48	1.33
32	1a	527	G7M	C8-N9	8.32	1.48	1.33
1	1A	2564	OMU	O4'-C1'	11.04	1.57	1.41
1	2A	2552	OMU	O4'-C1'	11.33	1.57	1.41
1	1A	2564	OMU	C6-N1	17.44	1.58	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C6-N1	18.06	1.59	1.35

All (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
32	1a	1207	2MG	C1'-N9-C4	-10.71	114.85	126.81
53	2x	54	5MU	C5-C4-N3	-10.65	116.41	125.35
32	1a	1518	MA6	N3-C2-N1	-10.54	120.59	128.87
1	2A	1915	5MU	C5-C4-N3	-10.44	116.58	125.35
1	1A	1961	5MU	C5-C4-N3	-10.24	116.75	125.35
32	2a	1207	2MG	C1'-N9-C4	-10.23	115.38	126.81
1	1A	1937	5MU	C5-C4-N3	-9.96	116.99	125.35
32	2a	1518	MA6	C1'-N9-C4	-9.89	115.77	126.81
32	1a	1518	MA6	C1'-N9-C4	-9.45	116.26	126.81
32	2a	1519	MA6	C1'-N9-C4	-8.82	116.97	126.81
32	1a	1519	MA6	C1'-N9-C4	-8.63	117.17	126.81
53	2x	8	4SU	C5-C4-N3	-8.48	114.57	123.56
53	1x	8	4SU	C5-C4-N3	-7.32	115.79	123.56
32	2a	527	G7M	N3-C2-N1	-5.95	119.46	127.56
32	1a	527	G7M	N3-C2-N1	-5.55	120.01	127.56
1	1A	2263	OMG	N3-C2-N1	-5.45	120.14	127.56
1	2A	2251	OMG	N3-C2-N1	-4.98	120.78	127.56
32	1a	516	PSU	C5-C1'-C2'	-4.94	107.05	115.44
32	1a	1402	4OC	CM4-N4-C4	-4.49	119.09	122.87
32	2a	1207	2MG	N3-C2-N1	-4.05	120.12	126.19
32	1a	1207	2MG	N3-C2-N1	-3.99	120.22	126.19
1	2A	1917	PSU	C5-C1'-C2'	-3.88	108.85	115.44
43	1l	92	0TD	CB-CA-N	-3.80	102.22	109.83
32	1a	516	PSU	C4-C5-C1'	-3.79	114.84	121.22
32	2a	516	PSU	C4-C5-C1'	-3.71	114.97	121.22
1	2A	2552	OMU	C4'-O4'-C1'	-3.69	105.73	109.64
32	1a	1207	2MG	CM2-N2-C2	-3.53	119.07	123.03
32	2a	966	M2G	N3-C2-N1	-3.51	120.38	126.35
32	1a	966	M2G	N3-C2-N1	-3.31	120.73	126.35
32	2a	1207	2MG	C5-C6-N1	-3.26	119.25	123.52
1	2A	2605	PSU	C4-C5-C1'	-3.24	115.77	121.22
32	2a	516	PSU	C5-C6-N1	-3.23	119.87	124.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1x	55	PSU	C4-C5-C1'	-3.22	115.80	121.22
32	1a	516	PSU	C5-C6-N1	-3.22	119.90	124.38
32	2a	527	G7M	C5-C6-N1	-3.16	119.39	123.52
32	1a	1207	2MG	C5-C6-N1	-3.15	119.41	123.52
32	1a	527	G7M	C5-C6-N1	-3.12	119.45	123.52
1	2A	2605	PSU	C5-C1'-C2'	-3.09	110.19	115.44
32	1a	966	M2G	C5-C6-N1	-3.05	119.54	123.52
1	1A	2564	OMU	C4'-O4'-C1'	-3.01	106.45	109.64
32	2a	527	G7M	C1'-N9-C4	-3.01	123.44	126.81
32	2a	1207	2MG	CM2-N2-C2	-2.97	119.69	123.03
53	2x	55	PSU	C5-C1'-C2'	-2.90	110.51	115.44
1	1A	2617	PSU	C4-C5-C1'	-2.88	116.36	121.22
1	2A	2251	OMG	C5-C6-N1	-2.82	119.84	123.52
1	1A	2617	PSU	C5-C1'-C2'	-2.79	110.70	115.44
32	2a	966	M2G	C5-C6-N1	-2.77	119.90	123.52
1	2A	1917	PSU	C5-C6-N1	-2.73	120.58	124.38
1	2A	1917	PSU	C4-C5-C1'	-2.70	116.66	121.22
32	2a	1402	4OC	CM4-N4-C4	-2.64	120.64	122.87
53	1x	55	PSU	C5-C6-N1	-2.63	120.71	124.38
1	1A	2515	2MA	N3-C2-N1	-2.59	120.51	125.60
32	2a	516	PSU	C5-C1'-C2'	-2.56	111.09	115.44
1	2A	2605	PSU	C5-C6-N1	-2.54	120.83	124.38
1	1A	2617	PSU	C5-C6-N1	-2.49	120.91	124.38
53	2x	55	PSU	C4-C5-C1'	-2.46	117.08	121.22
1	1A	2263	OMG	C5-C6-N1	-2.45	120.32	123.52
1	2A	2503	2MA	N3-C2-N1	-2.42	120.85	125.60
53	2x	55	PSU	C5-C6-N1	-2.32	121.15	124.38
1	1A	1933	PSU	C5-C6-N1	-2.20	121.31	124.38
43	2l	92	0TD	CB-CA-N	-2.19	105.45	109.83
1	2A	1911	PSU	C5-C1'-C2'	-2.13	111.83	115.44
53	1x	55	PSU	C5-C1'-C2'	-2.12	111.84	115.44
1	2A	1911	PSU	C5-C6-N1	-2.11	121.44	124.38
1	2A	1911	PSU	C4-C5-C1'	-2.10	117.69	121.22
1	1A	2617	PSU	O2'-C2'-C1'	-2.02	107.54	111.93
1	1A	2263	OMG	N2-C2-N1	2.06	120.61	117.20
32	1a	1207	2MG	N2-C2-N3	2.09	119.36	116.94
1	1A	2564	OMU	O4'-C1'-N1	2.09	112.08	108.10
32	1a	1404	5MC	C5-C4-N3	2.09	124.81	121.26
32	2a	1404	5MC	C5-C4-N3	2.11	124.84	121.26
53	1x	32	5MC	C5-C4-N3	2.11	124.84	121.26
1	2A	1942	5MC	C5-C4-N3	2.20	125.00	121.26
32	1a	1207	2MG	O3'-C3'-C2'	2.21	118.99	111.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1407	5MC	C5-C4-N3	2.22	125.02	121.26
32	2a	1407	5MC	C5-C4-N3	2.23	125.05	121.26
1	2A	2503	2MA	CM2-C2-N1	2.27	121.08	117.20
1	1A	1942	OMC	N4-C4-N3	2.28	120.49	116.50
32	2a	966	M2G	N3-C2-N2	2.32	119.69	117.14
1	1A	2617	PSU	O4'-C1'-C2'	2.34	107.22	104.69
32	1a	967	5MC	C5-C4-N3	2.38	125.30	121.26
1	2A	1962	5MC	C5-C4-N3	2.38	125.30	121.26
32	2a	1207	2MG	N2-C2-N3	2.40	119.72	116.94
32	2a	967	5MC	C5-C4-N3	2.41	125.36	121.26
32	2a	527	G7M	N2-C2-N1	2.43	121.20	117.20
53	2x	55	PSU	O4'-C1'-C2'	2.48	107.37	104.69
53	2x	32	5MC	C5-C4-N3	2.50	125.51	121.26
1	1A	1984	5MC	C5-C4-N3	2.51	125.51	121.26
1	1A	1964	5MC	C5-C4-N3	2.54	125.58	121.26
32	1a	1400	5MC	C5-C4-N3	2.54	125.58	121.26
32	2a	966	M2G	N1-C2-N2	2.56	119.93	117.14
32	2a	1400	5MC	C5-C4-N3	2.56	125.61	121.26
1	1A	1939	PSU	O4'-C1'-C2'	2.57	107.47	104.69
1	2A	1917	PSU	O4'-C1'-C2'	2.64	107.55	104.69
1	2A	2605	PSU	O4'-C1'-C2'	2.67	107.57	104.69
1	1A	1933	PSU	O4'-C1'-C2'	2.67	107.58	104.69
53	1x	55	PSU	O4'-C1'-C2'	2.70	107.61	104.69
1	2A	1911	PSU	O4'-C1'-C2'	2.73	107.64	104.69
32	2a	1207	2MG	N2-C2-N1	2.77	120.15	116.94
1	1A	2263	OMG	C6-N1-C2	2.93	119.32	115.88
1	2A	2251	OMG	C6-N1-C2	2.96	119.36	115.88
1	1A	2515	2MA	CM2-C2-N1	2.98	122.28	117.20
32	1a	516	PSU	O4'-C1'-C2'	2.98	107.92	104.69
32	1a	1207	2MG	N2-C2-N1	2.99	120.41	116.94
32	1a	966	M2G	N1-C2-N2	3.17	120.60	117.14
32	2a	516	PSU	O4'-C1'-C2'	3.26	108.22	104.69
32	1a	1207	2MG	C6-N1-C2	3.33	120.01	115.24
32	2a	1519	MA6	C2-N1-C6	3.56	120.03	111.64
32	2a	1207	2MG	C6-N1-C2	3.59	120.38	115.24
32	1a	1519	MA6	C2-N1-C6	3.63	120.19	111.64
32	1a	1518	MA6	C2-N1-C6	3.64	120.22	111.64
32	2a	1518	MA6	C2-N1-C6	3.70	120.38	111.64
32	1a	1402	4OC	C2-N3-C4	3.73	120.17	115.43
32	2a	1402	4OC	C2-N3-C4	3.88	120.36	115.43
1	1A	2564	OMU	C4-N3-C2	3.88	118.30	114.21
1	1A	1942	OMC	C6-C5-C4	3.93	118.98	117.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	527	G7M	C6-N1-C2	4.19	120.80	115.88
32	1a	966	M2G	C2-N3-C4	4.21	119.61	114.99
32	1a	1402	4OC	C6-C5-C4	4.34	119.12	117.42
43	1l	92	0TD	CSB-SB-CB	4.44	109.75	101.44
32	1a	1207	2MG	C2-N3-C4	4.46	119.88	114.99
32	2a	966	M2G	C2-N3-C4	4.48	119.90	114.99
32	2a	1207	2MG	C2-N3-C4	4.50	119.93	114.99
32	2a	527	G7M	C6-N1-C2	4.52	121.18	115.88
1	2A	2552	OMU	C4-N3-C2	4.53	118.99	114.21
43	2l	92	0TD	CSB-SB-CB	4.65	110.13	101.44
1	2A	1920	OMC	C6-C5-C4	4.86	119.34	117.44
32	2a	1402	4OC	C6-C5-C4	5.04	119.40	117.42
1	1A	2515	2MA	C2-N3-C4	7.21	118.76	115.29
1	2A	2503	2MA	C2-N3-C4	7.40	118.85	115.29
32	1a	516	PSU	C4-N3-C2	9.39	122.99	115.16
1	1A	1961	5MU	C4-N3-C2	9.50	123.08	115.16
32	2a	516	PSU	C4-N3-C2	9.50	123.08	115.16
1	1A	1937	5MU	C4-N3-C2	9.65	123.21	115.16
1	2A	1939	5MU	C4-N3-C2	9.79	123.33	115.16
53	2x	55	PSU	C4-N3-C2	9.81	123.34	115.16
1	2A	1915	5MU	C4-N3-C2	9.87	123.39	115.16
53	1x	55	PSU	C4-N3-C2	9.91	123.42	115.16
1	2A	1917	PSU	C4-N3-C2	9.92	123.44	115.16
1	2A	2605	PSU	C4-N3-C2	10.00	123.50	115.16
53	2x	54	5MU	C4-N3-C2	10.00	123.50	115.16
1	1A	1933	PSU	C4-N3-C2	10.03	123.53	115.16
1	1A	2617	PSU	C4-N3-C2	10.18	123.65	115.16
53	1x	54	5MU	C4-N3-C2	10.29	123.75	115.16
1	2A	1911	PSU	C4-N3-C2	10.30	123.75	115.16
1	1A	1939	PSU	C4-N3-C2	10.39	123.83	115.16
1	1A	2263	OMG	C1'-N9-C4	10.79	138.85	126.81
1	2A	2251	OMG	C1'-N9-C4	10.91	138.98	126.81
1	1A	2515	2MA	C1'-N9-C4	17.17	145.97	126.81
1	2A	2503	2MA	C1'-N9-C4	18.71	147.69	126.81

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	1Z	203	GLU	7.4
32	2a	1030(A)	G	6.9
21	2Z	193	GLU	6.8
1	2A	2125	G	6.7
21	1Z	197	ILE	6.5
32	1a	1036	G	6.2
38	1g	156	TRP	6.2
41	1j	98	ILE	6.1
22	20	8	GLY	6.0
32	2a	1036	G	5.8
40	2i	6	GLY	5.7
21	2Z	191	VAL	5.7
1	2A	2173	A	5.7
21	2Z	200	GLY	5.6
44	2m	7	VAL	5.6
23	2l	2	SER	5.5
1	2A	2148	G	5.5
32	1a	1034	G	5.5
1	2A	2162	G	5.4
22	10	8	GLY	5.4
21	1Z	194	PRO	5.3
41	1j	10	GLY	5.3
40	2i	7	THR	5.2
41	1j	35	SER	5.2
1	2A	2146	C	5.1
38	2g	156	TRP	5.1
21	2Z	194	PRO	5.1
21	1Z	196	VAL	5.1
32	2a	1034	G	5.0
1	2A	2147	G	5.0
1	2A	2110	G	4.9
32	2a	1026	G	4.9
34	1c	206	GLU	4.9
1	1A	2145	G	4.9
50	1s	39	THR	4.9
55	A	113	G	4.8
1	1A	1555	C	4.8
21	1Z	202	GLU	4.7
21	1Z	201	LYS	4.7
1	2A	2109	U	4.7
26	24	68	ARG	4.7
50	2s	31	ILE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	1s	4	SER	4.7
1	2A	2124	G	4.6
1	1A	2154	U	4.6
6	2G	2	PRO	4.5
1	2A	2174	C	4.5
1	2A	2802	G	4.5
1	2A	2133	G	4.5
32	1a	1030(B)	C	4.5
21	2Z	196	VAL	4.5
21	2Z	197	ILE	4.4
21	1Z	195	GLU	4.4
21	2Z	198	LYS	4.4
40	1i	106	ALA	4.3
38	2g	16	LEU	4.3
40	2i	62	TYR	4.3
1	1A	2139	A	4.3
21	2Z	192	ALA	4.3
28	26	54	ILE	4.3
41	2j	6	ILE	4.3
1	2A	1082	U	4.3
32	1a	1037	C	4.3
1	2A	229	A	4.3
32	1a	1035	A	4.3
45	1n	2	ALA	4.2
1	1A	2165	C	4.2
1	1A	2169	G	4.2
1	2A	2154	G	4.2
21	1Z	199	LYS	4.2
1	2A	2169	A	4.2
1	2A	2897	U	4.2
1	2A	1085	A	4.2
40	2i	15	ALA	4.2
32	1a	1286	A	4.1
1	2A	2143	C	4.1
7	2H	112	PRO	4.1
29	17	48	LYS	4.1
32	2a	1030	C	4.1
1	1A	2183	C	4.1
40	2i	5	TYR	4.1
22	20	9	SER	4.1
52	2u	11	GLY	4.0
41	1j	72	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2166	U	4.0
32	2a	1030(C)	G	4.0
1	2A	2134	A	4.0
1	2A	2159	G	4.0
31	29	37	GLY	4.0
1	1A	2163	G	4.0
45	2n	39	LEU	3.9
1	2A	2139	C	3.9
32	2a	1035	A	3.9
45	2n	2	ALA	3.9
26	24	69	LYS	3.9
21	2Z	195	GLU	3.9
32	1a	1001	A	3.9
32	1a	1026	G	3.9
32	1a	1030(C)	G	3.9
33	1b	130	ARG	3.9
1	2A	2801(A)	A	3.9
1	2A	2176	A	3.8
32	2a	1027	C	3.8
51	1t	18	GLN	3.8
1	2A	2803	C	3.8
44	2m	92	HIS	3.8
1	2A	2108	C	3.8
1	2A	2896	C	3.8
7	2H	105	LEU	3.8
1	2A	2155	G	3.8
1	1A	2180	A	3.8
1	2A	1067	A	3.8
1	1A	2175	G	3.8
41	1j	97	GLU	3.7
20	1Y	1	MET	3.7
1	2A	2144	U	3.7
1	2A	1509	C	3.7
32	1a	202	U	3.7
32	1a	1030	C	3.7
43	1l	28	LYS	3.7
38	2g	82	GLY	3.7
1	1A	2138	G	3.7
7	2H	113	VAL	3.7
32	1a	1028	C	3.7
1	2A	2123	G	3.7
38	2g	154	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	652(F)	G	3.6
21	2Z	201	LYS	3.6
32	2a	1001(A)	G	3.6
1	1A	2164	C	3.6
1	2A	1076	C	3.6
1	2A	2127	G	3.6
41	1j	8	LEU	3.6
1	2A	2179	C	3.6
23	11	2	SER	3.6
1	1A	2187	G	3.6
40	2i	26	VAL	3.6
1	2A	652(B)	A	3.6
40	2i	33	PHE	3.6
41	2j	85	LEU	3.6
1	2A	2132	U	3.6
20	2Y	60	PHE	3.6
32	1a	1533	C	3.6
50	2s	49	ILE	3.6
1	2A	2153	G	3.5
20	2Y	1	MET	3.5
20	2Y	5	MET	3.5
33	2b	101	MET	3.5
47	1p	35	LYS	3.5
1	2A	1046	A	3.5
32	1a	1000	U	3.5
1	1A	2182	G	3.5
50	1s	40	ILE	3.5
1	2A	1083	U	3.5
43	1l	64	TYR	3.5
41	1j	5	ARG	3.4
45	2n	34	TYR	3.4
1	1A	1221	G	3.4
1	1A	2181	G	3.4
45	1n	17	LYS	3.4
1	1A	2173	G	3.4
50	2s	4	SER	3.4
32	2a	1286	A	3.4
52	2u	5	ASP	3.4
1	2A	2130	U	3.4
34	1c	192	THR	3.4
26	14	64	GLY	3.3
34	2c	155	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1030(A)	G	3.3
40	2i	8	GLY	3.3
43	1l	62	SER	3.3
1	2A	2128	C	3.3
1	2A	2178	C	3.3
52	2u	6	ARG	3.3
1	2A	2152	G	3.3
1	2A	2137	C	3.3
1	2A	2138	C	3.3
38	2g	17	VAL	3.3
45	2n	25	VAL	3.3
1	2A	1087	G	3.3
32	1a	344	A	3.3
47	2p	19	ILE	3.3
32	1a	1027	C	3.3
1	2A	2120	G	3.3
1	1A	2906	U	3.3
1	2A	2118	U	3.3
32	1a	1002	G	3.3
41	2j	10	GLY	3.3
44	2m	75	ALA	3.3
1	2A	2160	G	3.3
1	1A	2129	C	3.3
1	2A	2172	U	3.3
1	1A	2193	A	3.3
1	2A	2126	A	3.2
50	1s	50	ALA	3.2
50	2s	30	LEU	3.2
50	2s	79	THR	3.2
1	1A	2195	A	3.2
1	2A	2131	G	3.2
40	2i	18	PHE	3.2
7	2H	103	LEU	3.2
32	1a	1257	U	3.2
22	20	76	GLY	3.2
50	1s	56	GLN	3.2
1	2A	887	A	3.2
1	2A	1103	A	3.2
40	2i	127	LYS	3.2
6	1G	2	PRO	3.2
52	1u	18	TYR	3.2
38	1g	79	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	1064	C	3.2
1	1A	2189	U	3.2
32	2a	1001	A	3.2
1	1A	2186	C	3.1
44	2m	6	GLY	3.1
7	2H	159	GLU	3.1
50	2s	71	LEU	3.1
41	2j	74	ILE	3.1
1	2A	1095	A	3.1
41	2j	72	VAL	3.1
1	2A	2175	C	3.1
40	2i	79	LEU	3.1
32	2a	1257	U	3.1
1	1A	2188	G	3.1
34	2c	189	ALA	3.1
32	2a	1531	A	3.1
7	2H	114	VAL	3.1
1	2A	1026	U	3.1
21	1Z	191	VAL	3.1
50	2s	16	LEU	3.1
51	1t	9	ASN	3.1
34	2c	190	ARG	3.1
1	1A	2134	G	3.1
35	1d	3	ARG	3.1
26	14	66	SER	3.0
1	1A	2152	U	3.0
1	2A	2161	C	3.0
44	1m	87	TYR	3.0
38	2g	80	VAL	3.0
41	2j	65	LEU	3.0
7	2H	111	HIS	3.0
36	1e	118	ILE	3.0
40	1i	75	ASP	3.0
1	1A	2190	G	3.0
1	1A	2816	G	3.0
44	2m	95	GLY	3.0
44	2m	4	ILE	3.0
1	1A	2137	G	3.0
1	2A	2121	G	3.0
1	2A	2164	C	3.0
26	24	46	GLN	3.0
38	1g	16	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2168	G	3.0
32	1a	1001(A)	G	3.0
41	1j	75	ILE	3.0
22	20	77	ARG	2.9
32	2a	1028	C	2.9
34	1c	193	TYR	2.9
40	2i	36	TYR	2.9
32	2a	80	G	2.9
32	2a	1002	G	2.9
32	2a	1042	G	2.9
45	2n	35	ARG	2.9
50	2s	35	SER	2.9
33	1b	131	PRO	2.9
1	2A	2165	G	2.9
50	2s	32	LYS	2.9
6	2G	34	LEU	2.9
14	2S	5	THR	2.9
50	2s	3	ARG	2.9
41	2j	41	PRO	2.9
1	2A	1104	C	2.9
32	1a	1029	C	2.9
38	1g	78	ARG	2.9
1	1A	2194	U	2.9
7	2H	94	TYR	2.9
33	2b	70	PHE	2.9
1	1A	935	C	2.9
26	24	67	TYR	2.9
7	2H	115	VAL	2.9
40	2i	78	LYS	2.9
22	20	45	PHE	2.9
41	2j	73	ASP	2.9
37	1f	55	ASP	2.9
41	2j	63	PHE	2.8
40	1i	47	LEU	2.8
33	1b	123	ALA	2.8
1	2A	888	C	2.8
38	1g	153	HIS	2.8
43	2l	64	TYR	2.8
40	1i	33	PHE	2.8
22	20	72	ARG	2.8
32	1a	204	U	2.8
1	2A	2111	C	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2145	C	2.8
32	1a	1038	C	2.8
40	2i	21	PRO	2.8
38	2g	34	GLY	2.8
29	27	48	LYS	2.8
45	2n	8	GLU	2.8
1	2A	2129	C	2.8
7	2H	102	ALA	2.8
1	1A	2153	G	2.8
41	2j	62	HIS	2.8
50	2s	2	PRO	2.8
22	20	71	ASP	2.8
1	1A	2128	G	2.7
34	2c	206	GLU	2.7
1	1A	2149	G	2.7
1	2A	2151	G	2.7
1	2A	2157	G	2.7
34	2c	164	ARG	2.7
7	2H	169	VAL	2.7
26	14	52	THR	2.7
1	1A	2126	G	2.7
1	1A	2156	A	2.7
1	2A	2107	C	2.7
50	2s	47	HIS	2.7
50	1s	19	VAL	2.7
47	1p	37	GLY	2.7
14	2S	111	GLU	2.7
44	2m	111	LYS	2.7
34	1c	170	GLN	2.7
38	2g	78	ARG	2.7
40	2i	66	ARG	2.7
40	1i	15	ALA	2.7
32	1a	723	U	2.7
32	2a	1030(D)	A	2.7
1	2A	2136	C	2.7
34	2c	159	GLY	2.7
32	2a	90	U	2.6
32	2a	1031	G	2.6
45	2n	15	LYS	2.6
33	1b	133	LYS	2.6
44	2m	94	ARG	2.6
1	1A	2141	A	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	2N	10	GLU	2.6
47	1p	17	TYR	2.6
1	2A	2140	C	2.6
32	2a	1037	C	2.6
7	2H	30	LYS	2.6
34	1c	160	ALA	2.6
40	1i	46	ALA	2.6
26	14	68	ARG	2.6
52	2u	10	ARG	2.6
40	1i	26	VAL	2.6
1	2A	2158	A	2.6
11	2P	109	GLY	2.6
45	2n	38	GLY	2.6
34	2c	147	LYS	2.6
38	2g	85	TYR	2.6
50	1s	48	THR	2.6
1	1A	2815	C	2.6
45	1n	15	LYS	2.6
41	1j	73	ASP	2.6
31	29	16	VAL	2.6
50	1s	30	LEU	2.6
7	2H	29	PRO	2.6
33	1b	232	PRO	2.6
41	1j	71	LEU	2.6
41	2j	87	THR	2.6
33	1b	201	ILE	2.6
32	2a	1041	A	2.6
1	2A	2142	C	2.6
54	2y	10	PRO	2.6
1	1A	1099	C	2.5
1	1A	2814	C	2.5
14	2S	58	LEU	2.5
1	2A	2119	A	2.5
1	1A	2177	G	2.5
32	1a	1003	G	2.5
32	2a	1032	G	2.5
41	2j	29	ARG	2.5
52	2u	15	ARG	2.5
32	2a	1533	C	2.5
32	1a	1031	G	2.5
33	1b	122	PHE	2.5
33	2b	161	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	201	TYR	2.5
38	2g	153	HIS	2.5
50	2s	8	GLY	2.5
20	2Y	91	GLU	2.5
7	2H	116	GLU	2.5
25	23	59	VAL	2.5
1	1A	2155	G	2.5
41	2j	100	THR	2.5
33	1b	129	GLU	2.5
53	2x	47	U	2.5
1	2A	1044	G	2.5
32	2a	1023	G	2.5
38	1g	154	TYR	2.5
1	2A	6	A	2.5
35	1d	135	LEU	2.5
41	1j	34	VAL	2.5
1	2A	2150	U	2.4
41	1j	6	ILE	2.4
52	2u	22	ARG	2.4
39	2h	99	GLU	2.4
4	2E	1	MET	2.4
40	2i	88	TYR	2.4
1	1A	2185	C	2.4
32	1a	999	C	2.4
29	27	22	MET	2.4
51	2t	56	MET	2.4
35	1d	168	ARG	2.4
41	2j	98	ILE	2.4
1	1A	2130	C	2.4
1	1A	2142	G	2.4
1	1A	2147	G	2.4
1	1A	2184	G	2.4
1	2A	2793	G	2.4
1	2A	2894	G	2.4
34	1c	200	ALA	2.4
41	2j	71	LEU	2.4
20	2Y	59	GLY	2.4
40	2i	92	TYR	2.4
25	23	60	GLU	2.4
33	2b	187	LEU	2.4
50	2s	6	LYS	2.4
32	1a	1212	U	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	7	ALA	2.4
40	1i	62	TYR	2.4
32	1a	345	C	2.4
21	2Z	199	LYS	2.4
21	2Z	188	ALA	2.4
41	1j	4	ILE	2.4
32	2a	1006	C	2.4
33	1b	135	GLN	2.4
32	1a	1531	A	2.4
35	1d	4	TYR	2.4
41	2j	5	ARG	2.4
32	2a	1117	G	2.4
1	1A	2140	U	2.4
34	1c	101	LEU	2.4
1	1A	2151	C	2.4
1	1A	2161	C	2.4
1	1A	2905	C	2.4
1	1A	2198	A	2.4
27	25	60	VAL	2.4
7	2H	101	ARG	2.4
32	2a	91	C	2.4
39	2h	112	LEU	2.4
7	2H	48	GLY	2.3
38	2g	33	ASP	2.3
47	1p	9	PHE	2.3
1	2A	1066	U	2.3
1	2A	2319	G	2.3
54	2y	12	PRO	2.3
1	1A	696	C	2.3
46	2o	86	GLY	2.3
45	2n	4	LYS	2.3
44	1m	42	ALA	2.3
29	17	47	ARG	2.3
1	2A	2805	G	2.3
51	1t	21	LYS	2.3
37	2f	89	MET	2.3
40	2i	9	ARG	2.3
31	19	28	GLU	2.3
52	2u	14	TRP	2.3
41	2j	8	LEU	2.3
41	2j	26	ALA	2.3
1	2A	2122	U	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1532	U	2.3
22	20	70	GLN	2.3
44	2m	110	ARG	2.3
11	2P	110	TYR	2.3
1	2A	1079	C	2.3
1	1A	2170	G	2.3
54	2y	11	ARG	2.3
1	1A	2136	A	2.3
42	2k	13	GLN	2.3
3	2D	153	ALA	2.3
41	1j	7	LYS	2.3
1	1A	2178	G	2.3
1	2A	2167	U	2.3
36	2e	25	ARG	2.3
46	1o	6	GLU	2.3
1	2A	652(T)	C	2.3
32	2a	204	U	2.3
41	2j	27	ALA	2.3
7	2H	106	THR	2.3
40	2i	64	THR	2.3
50	2s	63	THR	2.3
50	2s	82	GLY	2.3
52	2u	24	ARG	2.3
39	2h	101	PRO	2.3
50	1s	59	PRO	2.3
20	2Y	57	GLN	2.3
33	1b	214	ILE	2.3
40	1i	105	ASP	2.3
40	2i	126	SER	2.3
31	19	13	LYS	2.3
38	1g	141	VAL	2.3
45	2n	17	LYS	2.3
50	2s	13	ASP	2.3
40	2i	83	ARG	2.2
1	1A	2200	C	2.2
1	2A	34	C	2.2
40	2i	123	PRO	2.2
34	2c	89	GLU	2.2
1	2A	2171	A	2.2
1	1A	2176	G	2.2
1	1A	2807	C	2.2
1	2A	2804	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	16	ARG	2.2
7	2H	37	VAL	2.2
21	2Z	96	VAL	2.2
41	1j	100	THR	2.2
1	1A	2174	G	2.2
38	2g	4	ARG	2.2
47	1p	38	TYR	2.2
40	1i	19	LEU	2.2
49	2r	58	LEU	2.2
8	2I	92	VAL	2.2
32	2a	1248	A	2.2
45	2n	49	HIS	2.2
1	1A	2806	G	2.2
1	1A	933	C	2.2
1	1A	2150	C	2.2
24	22	1	MET	2.2
9	2N	8	GLN	2.2
40	1i	78	LYS	2.2
1	1A	2160	C	2.2
44	1m	32	GLU	2.2
34	2c	162	GLN	2.2
52	2u	13	ILE	2.2
40	2i	61	ALA	2.2
1	2A	2177	C	2.2
6	2G	3	LEU	2.2
32	2a	89	C	2.2
1	2A	2141	G	2.2
1	2A	2156	G	2.2
44	2m	5	ALA	2.2
34	2c	179	ARG	2.2
7	2H	41	MET	2.2
32	1a	1039	C	2.2
32	2a	1029	C	2.2
1	1A	2179	G	2.2
55	B	116	G	2.2
38	1g	77	SER	2.2
44	1m	48	LEU	2.2
41	2j	61	GLU	2.2
1	1A	2162	C	2.2
7	2H	95	ARG	2.2
15	1T	126	ALA	2.2
22	20	78	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	11	LYS	2.2
1	2A	1081	U	2.2
1	1A	2148	A	2.2
1	2A	2170	A	2.2
40	1i	120	ARG	2.2
41	2j	78	ASN	2.2
50	2s	48	THR	2.2
50	2s	68	GLY	2.2
22	20	75	LEU	2.1
47	1p	80	PHE	2.1
1	2A	1086	A	2.1
21	2Z	12	GLY	2.1
44	2m	56	LEU	2.1
34	1c	100	ALA	2.1
45	2n	7	ILE	2.1
26	24	45	GLY	2.1
1	1A	2131	U	2.1
1	2A	2180	U	2.1
21	2Z	7	ALA	2.1
33	2b	114	ARG	2.1
33	2b	163	PHE	2.1
34	2c	131	ARG	2.1
48	2q	60	ILE	2.1
14	2S	26	LEU	2.1
34	2c	80	GLY	2.1
26	14	65	ASP	2.1
7	2H	45	VAL	2.1
33	2b	165	VAL	2.1
50	1s	49	ILE	2.1
44	2m	97	PRO	2.1
52	1u	22	ARG	2.1
26	24	63	TYR	2.1
32	2a	1044	A	2.1
44	2m	60	VAL	2.1
39	2h	120	THR	2.1
3	2D	38	LYS	2.1
38	1g	85	TYR	2.1
38	2g	83	ALA	2.1
44	1m	35	GLU	2.1
1	2A	2892	A	2.1
50	2s	9	VAL	2.1
51	2t	41	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	95	GLN	2.1
1	1A	2168	C	2.1
45	2n	60	SER	2.1
52	2u	18	TYR	2.1
1	1A	2144	U	2.1
32	1a	1032	G	2.1
40	2i	4	TYR	2.1
42	2k	75	TYR	2.1
44	1m	30	ALA	2.1
40	2i	105	ASP	2.1
41	1j	38	ILE	2.1
32	2a	723	U	2.1
38	2g	76	ARG	2.1
52	2u	17	THR	2.1
32	2a	1270	C	2.1
20	2Y	88	LYS	2.0
44	2m	64	TRP	2.0
32	2a	1024	G	2.0
34	2c	160	ALA	2.0
38	2g	81	GLY	2.0
1	2A	2135	A	2.0
47	1p	57	ARG	2.0
1	1A	2167	C	2.0
1	2A	652(S)	C	2.0
32	2a	1043	C	2.0
20	2Y	42	VAL	2.0
21	2Z	187	ALA	2.0
6	1G	75	LYS	2.0
32	1a	1024	G	2.0
32	1a	1532	U	2.0
33	2b	105	PHE	2.0
39	1h	4	ASP	2.0
40	2i	110	GLU	2.0
1	1A	2157	A	2.0
7	2H	107	VAL	2.0
8	2I	3	VAL	2.0
40	2i	75	ASP	2.0
47	2p	59	TRP	2.0
50	1s	38	SER	2.0
14	2S	35	ILE	2.0
23	11	98	LEU	2.0
34	1c	169	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	158	GLY	2.0
1	1A	2201	C	2.0
41	2j	67	THR	2.0
20	2Y	62	GLU	2.0
26	14	63	TYR	2.0
40	2i	17	VAL	2.0
35	2d	49	ARG	2.0
38	2g	12	LEU	2.0
32	2a	1131	G	2.0
40	1i	101	PHE	2.0
43	2l	32	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
56	MG	2A	3561	1/1	0.89	0.08	-3.51	58,58,58,58	0
56	MG	11	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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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	1l	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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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

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	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
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.