



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2016 – 02:21 AM EDT

PDB ID : 5HCQ  
Title : Crystal structure of antimicrobial peptide Oncocin d15-19 bound to the *Thermus thermophilus* 70S ribosome  
Authors : Gagnon, M.G.; Roy, R.N.; Lomakin, I.B.; Florin, T.; Mankin, A.S.; Steitz, T.A.  
Deposited on : 2016-01-04  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

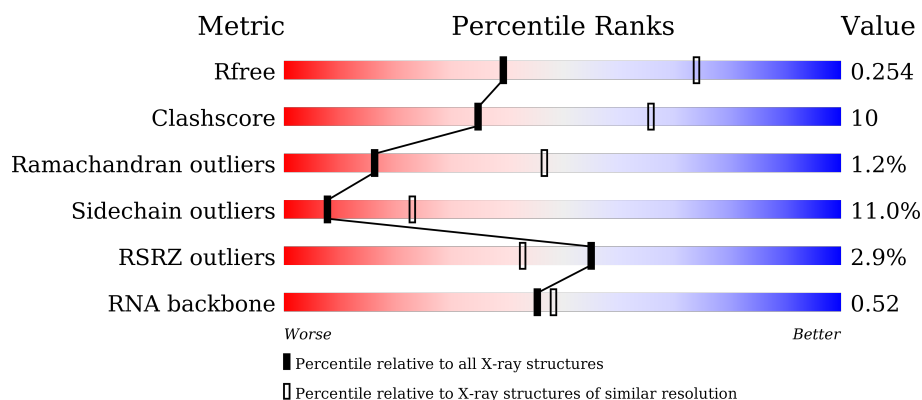
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.
















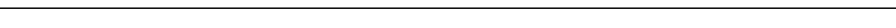











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>2%</div> <div>61% 26% 6% 6%</div> </div>
1	2A	2915	<div> <div>2%</div> <div>51% 36% 8% ..</div> </div>
2	1B	121	<div> <div>66% 31% ..</div> </div>
2	2B	121	<div> <div>2%</div> <div>31% 51% 17% ..</div> </div>


























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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	



















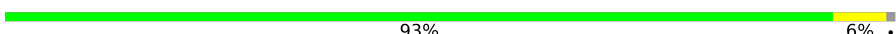






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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1x	77	
54	2x	77	
55	1z	14	
55	2z	14	

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	105	-	-	-	X
56	MG	17	101	-	-	-	X
56	MG	1A	3001	-	-	-	X
56	MG	1A	3002	-	-	-	X
56	MG	1A	3004	-	-	-	X
56	MG	1A	3016	-	-	-	X
56	MG	1A	3026	-	-	-	X
56	MG	1A	3030	-	-	-	X
56	MG	1A	3033	-	-	-	X
56	MG	1A	3041	-	-	-	X
56	MG	1A	3053	-	-	-	X
56	MG	1A	3062	-	-	-	X
56	MG	1A	3075	-	-	-	X
56	MG	1A	3076	-	-	-	X
56	MG	1A	3092	-	-	-	X
56	MG	1A	3094	-	-	-	X
56	MG	1A	3095	-	-	-	X
56	MG	1A	3098	-	-	-	X
56	MG	1A	3102	-	-	-	X
56	MG	1A	3103	-	-	-	X
56	MG	1A	3106	-	-	-	X
56	MG	1A	3107	-	-	-	X
56	MG	1A	3108	-	-	-	X
56	MG	1A	3111	-	-	-	X
56	MG	1A	3112	-	-	-	X
56	MG	1A	3115	-	-	-	X
56	MG	1A	3118	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3119	-	-	-	X
56	MG	1A	3120	-	-	-	X
56	MG	1A	3121	-	-	-	X
56	MG	1A	3123	-	-	-	X
56	MG	1A	3128	-	-	-	X
56	MG	1A	3143	-	-	-	X
56	MG	1A	3146	-	-	-	X
56	MG	1A	3147	-	-	-	X
56	MG	1A	3150	-	-	-	X
56	MG	1A	3152	-	-	-	X
56	MG	1A	3166	-	-	-	X
56	MG	1A	3169	-	-	-	X
56	MG	1A	3170	-	-	-	X
56	MG	1A	3172	-	-	-	X
56	MG	1A	3175	-	-	-	X
56	MG	1A	3189	-	-	-	X
56	MG	1A	3190	-	-	-	X
56	MG	1A	3193	-	-	-	X
56	MG	1A	3209	-	-	-	X
56	MG	1A	3210	-	-	-	X
56	MG	1A	3211	-	-	-	X
56	MG	1A	3214	-	-	-	X
56	MG	1A	3215	-	-	-	X
56	MG	1A	3221	-	-	-	X
56	MG	1A	3231	-	-	-	X
56	MG	1A	3236	-	-	-	X
56	MG	1A	3240	-	-	-	X
56	MG	1A	3263	-	-	-	X
56	MG	1A	3267	-	-	-	X
56	MG	1A	3277	-	-	-	X
56	MG	1A	3279	-	-	-	X
56	MG	1A	3302	-	-	-	X
56	MG	1A	3303	-	-	-	X
56	MG	1A	3346	-	-	-	X
56	MG	1A	3352	-	-	-	X
56	MG	1A	3356	-	-	-	X
56	MG	1A	3373	-	-	-	X
56	MG	1A	3416	-	-	-	X
56	MG	1A	3418	-	-	-	X
56	MG	1A	3419	-	-	-	X
56	MG	1A	3434	-	-	-	X
56	MG	1A	3442	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3449	-	-	-	X
56	MG	1A	3452	-	-	-	X
56	MG	1A	3457	-	-	-	X
56	MG	1A	3463	-	-	-	X
56	MG	1A	3464	-	-	-	X
56	MG	1A	3465	-	-	-	X
56	MG	1A	3498	-	-	-	X
56	MG	1A	3511	-	-	-	X
56	MG	1A	3521	-	-	-	X
56	MG	1A	3528	-	-	-	X
56	MG	1A	3532	-	-	-	X
56	MG	1A	3534	-	-	-	X
56	MG	1A	3540	-	-	-	X
56	MG	1A	3560	-	-	-	X
56	MG	1A	3561	-	-	-	X
56	MG	1A	3569	-	-	-	X
56	MG	1A	3570	-	-	-	X
56	MG	1A	3582	-	-	-	X
56	MG	1A	3583	-	-	-	X
56	MG	1A	3596	-	-	-	X
56	MG	1A	3601	-	-	-	X
56	MG	1A	3605	-	-	-	X
56	MG	1A	3606	-	-	-	X
56	MG	1A	3610	-	-	-	X
56	MG	1A	3611	-	-	-	X
56	MG	1A	3613	-	-	-	X
56	MG	1A	3617	-	-	-	X
56	MG	1A	3627	-	-	-	X
56	MG	1A	3636	-	-	-	X
56	MG	1A	3638	-	-	-	X
56	MG	1A	3651	-	-	-	X
56	MG	1A	3658	-	-	-	X
56	MG	1A	3685	-	-	-	X
56	MG	1A	3699	-	-	-	X
56	MG	1A	3700	-	-	-	X
56	MG	1A	3718	-	-	-	X
56	MG	1A	3719	-	-	-	X
56	MG	1A	3723	-	-	-	X
56	MG	1A	3737	-	-	-	X
56	MG	1A	3738	-	-	-	X
56	MG	1A	3750	-	-	-	X
56	MG	1A	3766	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3767	-	-	-	X
56	MG	1A	3769	-	-	-	X
56	MG	1A	3774	-	-	-	X
56	MG	1A	3789	-	-	-	X
56	MG	1A	3796	-	-	-	X
56	MG	1A	3809	-	-	-	X
56	MG	1A	3813	-	-	-	X
56	MG	1A	3858	-	-	-	X
56	MG	1A	3867	-	-	-	X
56	MG	1A	3881	-	-	-	X
56	MG	1A	3891	-	-	-	X
56	MG	1A	3894	-	-	-	X
56	MG	1A	3896	-	-	-	X
56	MG	1A	3900	-	-	-	X
56	MG	1A	3905	-	-	-	X
56	MG	1A	3918	-	-	-	X
56	MG	1A	3942	-	-	-	X
56	MG	1A	3943	-	-	-	X
56	MG	1A	3945	-	-	-	X
56	MG	1A	3987	-	-	-	X
56	MG	1A	3988	-	-	-	X
56	MG	1A	3991	-	-	-	X
56	MG	1A	3995	-	-	-	X
56	MG	1A	3998	-	-	-	X
56	MG	1A	4000	-	-	-	X
56	MG	1A	4001	-	-	-	X
56	MG	1A	4003	-	-	-	X
56	MG	1A	4010	-	-	-	X
56	MG	1A	4011	-	-	-	X
56	MG	1A	4013	-	-	-	X
56	MG	1A	4017	-	-	-	X
56	MG	1A	4022	-	-	-	X
56	MG	1A	4026	-	-	-	X
56	MG	1A	4029	-	-	-	X
56	MG	1A	4030	-	-	-	X
56	MG	1A	4031	-	-	-	X
56	MG	1A	4032	-	-	-	X
56	MG	1A	4036	-	-	-	X
56	MG	1A	4037	-	-	-	X
56	MG	1A	4040	-	-	-	X
56	MG	1A	4041	-	-	-	X
56	MG	1A	4044	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	4047	-	-	-	X
56	MG	1A	4049	-	-	-	X
56	MG	1B	206	-	-	-	X
56	MG	1B	211	-	-	-	X
56	MG	1D	301	-	-	-	X
56	MG	1D	303	-	-	-	X
56	MG	1D	304	-	-	-	X
56	MG	1D	305	-	-	-	X
56	MG	1D	308	-	-	-	X
56	MG	1D	310	-	-	-	X
56	MG	1D	313	-	-	-	X
56	MG	1D	316	-	-	-	X
56	MG	1E	303	-	-	-	X
56	MG	1E	306	-	-	-	X
56	MG	1E	309	-	-	-	X
56	MG	1F	301	-	-	-	X
56	MG	1F	302	-	-	-	X
56	MG	1F	305	-	-	-	X
56	MG	1N	202	-	-	-	X
56	MG	1N	207	-	-	-	X
56	MG	1P	204	-	-	-	X
56	MG	1P	205	-	-	-	X
56	MG	1Q	3002	-	-	-	X
56	MG	1Q	3004	-	-	-	X
56	MG	1Q	3006	-	-	-	X
56	MG	1R	205	-	-	-	X
56	MG	1U	202	-	-	-	X
56	MG	1U	203	-	-	-	X
56	MG	1U	204	-	-	-	X
56	MG	1U	205	-	-	-	X
56	MG	1W	3003	-	-	-	X
56	MG	1W	3006	-	-	-	X
56	MG	1X	3001	-	-	-	X
56	MG	1a	1602	-	-	-	X
56	MG	1a	1604	-	-	-	X
56	MG	1a	1607	-	-	-	X
56	MG	1a	1643	-	-	-	X
56	MG	1a	1661	-	-	-	X
56	MG	1a	1662	-	-	-	X
56	MG	1a	1670	-	-	-	X
56	MG	1a	1671	-	-	-	X
56	MG	1a	1672	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	1694	-	-	-	X
56	MG	1a	1701	-	-	-	X
56	MG	1a	1707	-	-	-	X
56	MG	1a	1709	-	-	-	X
56	MG	1a	1714	-	-	-	X
56	MG	1a	1719	-	-	-	X
56	MG	1a	1722	-	-	-	X
56	MG	1a	1727	-	-	-	X
56	MG	1a	1730	-	-	-	X
56	MG	1a	1751	-	-	-	X
56	MG	1a	1811	-	-	-	X
56	MG	1a	1820	-	-	-	X
56	MG	1a	1822	-	-	-	X
56	MG	1a	1831	-	-	-	X
56	MG	1a	1833	-	-	-	X
56	MG	1a	1835	-	-	-	X
56	MG	1a	1839	-	-	-	X
56	MG	1a	1847	-	-	-	X
56	MG	1a	1860	-	-	-	X
56	MG	1a	1880	-	-	-	X
56	MG	1a	1882	-	-	-	X
56	MG	1a	1886	-	-	-	X
56	MG	1a	1903	-	-	-	X
56	MG	1e	203	-	-	-	X
56	MG	1h	3003	-	-	-	X
56	MG	1q	201	-	-	-	X
56	MG	1q	203	-	-	-	X
56	MG	1r	3001	-	-	-	X
56	MG	1t	3001	-	-	-	X
56	MG	28	8001	-	-	-	X
56	MG	2A	3009	-	-	-	X
56	MG	2A	3011	-	-	-	X
56	MG	2A	3014	-	-	-	X
56	MG	2A	3036	-	-	-	X
56	MG	2A	3038	-	-	-	X
56	MG	2A	3042	-	-	-	X
56	MG	2A	3046	-	-	-	X
56	MG	2A	3049	-	-	-	X
56	MG	2A	3053	-	-	-	X
56	MG	2A	3055	-	-	-	X
56	MG	2A	3060	-	-	-	X
56	MG	2A	3062	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3069	-	-	-	X
56	MG	2A	3089	-	-	-	X
56	MG	2A	3091	-	-	-	X
56	MG	2A	3092	-	-	-	X
56	MG	2A	3093	-	-	-	X
56	MG	2A	3099	-	-	-	X
56	MG	2A	3102	-	-	-	X
56	MG	2A	3106	-	-	-	X
56	MG	2A	3111	-	-	-	X
56	MG	2A	3114	-	-	-	X
56	MG	2A	3121	-	-	-	X
56	MG	2A	3139	-	-	-	X
56	MG	2A	3141	-	-	-	X
56	MG	2A	3142	-	-	-	X
56	MG	2A	3146	-	-	-	X
56	MG	2A	3147	-	-	-	X
56	MG	2A	3148	-	-	-	X
56	MG	2A	3159	-	-	-	X
56	MG	2A	3160	-	-	-	X
56	MG	2A	3163	-	-	-	X
56	MG	2A	3173	-	-	-	X
56	MG	2A	3176	-	-	-	X
56	MG	2A	3179	-	-	-	X
56	MG	2A	3181	-	-	-	X
56	MG	2A	3182	-	-	-	X
56	MG	2A	3184	-	-	-	X
56	MG	2A	3185	-	-	-	X
56	MG	2A	3189	-	-	-	X
56	MG	2A	3191	-	-	-	X
56	MG	2A	3194	-	-	-	X
56	MG	2A	3200	-	-	-	X
56	MG	2A	3201	-	-	-	X
56	MG	2A	3203	-	-	-	X
56	MG	2A	3207	-	-	-	X
56	MG	2A	3214	-	-	-	X
56	MG	2A	3219	-	-	-	X
56	MG	2A	3221	-	-	-	X
56	MG	2A	3222	-	-	-	X
56	MG	2A	3225	-	-	-	X
56	MG	2A	3231	-	-	-	X
56	MG	2A	3232	-	-	-	X
56	MG	2A	3233	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3238	-	-	-	X
56	MG	2A	3254	-	-	-	X
56	MG	2A	3256	-	-	-	X
56	MG	2A	3264	-	-	-	X
56	MG	2A	3266	-	-	-	X
56	MG	2A	3267	-	-	-	X
56	MG	2A	3272	-	-	-	X
56	MG	2A	3274	-	-	-	X
56	MG	2A	3296	-	-	-	X
56	MG	2A	3297	-	-	-	X
56	MG	2A	3300	-	-	-	X
56	MG	2A	3304	-	-	-	X
56	MG	2A	3305	-	-	-	X
56	MG	2A	3308	-	-	-	X
56	MG	2A	3309	-	-	-	X
56	MG	2A	3311	-	-	-	X
56	MG	2A	3315	-	-	-	X
56	MG	2A	3317	-	-	-	X
56	MG	2A	3331	-	-	-	X
56	MG	2A	3334	-	-	-	X
56	MG	2A	3340	-	-	-	X
56	MG	2A	3342	-	-	-	X
56	MG	2A	3344	-	-	-	X
56	MG	2A	3349	-	-	-	X
56	MG	2A	3350	-	-	-	X
56	MG	2A	3368	-	-	-	X
56	MG	2A	3376	-	-	-	X
56	MG	2A	3377	-	-	-	X
56	MG	2A	3379	-	-	-	X
56	MG	2A	3386	-	-	-	X
56	MG	2A	3387	-	-	-	X
56	MG	2A	3390	-	-	-	X
56	MG	2A	3394	-	-	-	X
56	MG	2A	3400	-	-	-	X
56	MG	2A	3402	-	-	-	X
56	MG	2A	3409	-	-	-	X
56	MG	2A	3410	-	-	-	X
56	MG	2A	3411	-	-	-	X
56	MG	2A	3413	-	-	-	X
56	MG	2A	3419	-	-	-	X
56	MG	2A	3420	-	-	-	X
56	MG	2A	3430	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3441	-	-	-	X
56	MG	2A	3443	-	-	-	X
56	MG	2A	3444	-	-	-	X
56	MG	2A	3450	-	-	-	X
56	MG	2A	3482	-	-	-	X
56	MG	2A	3500	-	-	-	X
56	MG	2A	3513	-	-	-	X
56	MG	2A	3520	-	-	-	X
56	MG	2A	3522	-	-	-	X
56	MG	2A	3547	-	-	-	X
56	MG	2A	3550	-	-	-	X
56	MG	2A	3552	-	-	-	X
56	MG	2A	3553	-	-	-	X
56	MG	2A	3562	-	-	-	X
56	MG	2A	3564	-	-	-	X
56	MG	2A	3567	-	-	-	X
56	MG	2A	3568	-	-	-	X
56	MG	2A	3572	-	-	-	X
56	MG	2A	3573	-	-	-	X
56	MG	2A	3574	-	-	-	X
56	MG	2A	3576	-	-	-	X
56	MG	2A	3577	-	-	-	X
56	MG	2A	3582	-	-	-	X
56	MG	2B	3005	-	-	-	X
56	MG	2D	304	-	-	-	X
56	MG	2E	303	-	-	-	X
56	MG	2E	304	-	-	-	X
56	MG	2P	201	-	-	-	X
56	MG	2U	201	-	-	-	X
56	MG	2V	201	-	-	-	X
56	MG	2a	3005	-	-	-	X
56	MG	2a	3013	-	-	-	X
56	MG	2a	3022	-	-	-	X
56	MG	2a	3026	-	-	-	X
56	MG	2a	3089	-	-	-	X
56	MG	2a	3090	-	-	-	X
56	MG	2a	3097	-	-	-	X
56	MG	2a	3099	-	-	-	X
56	MG	2a	3102	-	-	-	X
56	MG	2a	3116	-	-	-	X
56	MG	2a	3117	-	-	-	X
56	MG	2a	3119	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2a	3123	-	-	-	X
56	MG	2a	3125	-	-	-	X
56	MG	2a	3129	-	-	-	X
56	MG	2a	3130	-	-	-	X
56	MG	2a	3138	-	-	-	X
56	MG	2a	3177	-	-	-	X
56	MG	2a	3178	-	-	-	X
56	MG	2a	3205	-	-	-	X
56	MG	2a	3212	-	-	-	X
56	MG	2a	3225	-	-	-	X
56	MG	2a	3233	-	-	-	X
56	MG	2a	3234	-	-	-	X
56	MG	2a	3239	-	-	-	X
56	MG	2n	502	-	-	-	X



## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 288518 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	2746	Total	C	N	O	P	0	0	0
			59154	26327	11077	19005	2745			
1	2A	2790	Total	C	N	O	P	0	0	0
			60091	26746	11243	19313	2789			

- 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	1146	476	831	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
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2142	1352	426	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
			1425	914	256	251	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	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	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	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
			1117	719	207	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			

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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
			1139	709	231	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
			771	495	140	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
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	186	Total	C	N	O	S	0	0	0
			1470	937	262	269	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			
22	20	75	Total	C	N	O	S	0	0	0
			598	370	127	100	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
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	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
			588	365	118	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
			558	352	102	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	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
			455	285	89	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	1477	Total	C	N	O	P	0	0	0
			31750	14131	5883	10259	1477			
32	2a	1483	Total	C	N	O	P	0	0	0
			31877	14188	5905	10301	1483			

- 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
			1786	1136	321	325	4			
33	2b	231	Total	C	N	O	S	0	0	0
			1697	1079	292	321	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
			1480	932	281	266	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1412	883	269	259	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
			1618	1013	312	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1630	1022	321	280	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
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1095	695	203	193	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
			806	511	143	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			817	516	146	152	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
			1183	732	232	213	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1167	728	220	213	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
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1074	681	202	189	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
			976	620	189	167			
40	2i	127	Total	C	N	O	0	0	0
			932	589	177	166			

- 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
			682	424	130	128			
41	2j	96	Total	C	N	O	0	0	0
			678	424	126	128			

- 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
			826	513	156	154	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			829	516	155	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
			920	579	181	159	1			
43	2l	122	Total	C	N	O	S	0	0	0
			918	576	182	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			903	555	187	159	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
			482	306	100	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			459	291	93	71	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
			715	447	140	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
			671	424	133	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
			811	519	148	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	84	Total	C	N	O	S	0	0	0
			642	409	119	112	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	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
			712	435	152	123	2			
51	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	124	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
			187	116	42	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			
53	2v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 54 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
54	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 55 is a protein called Oncocin d15-19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	12	Total	C	N	O	0	0	0
			101	67	19	15			
55	2z	12	Total	C	N	O	0	0	0
			101	67	19	15			

- 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	4	Total	Mg	0	0
			4	4		
56	2d	2	Total	Mg	0	0
			2	2		
56	1T	5	Total	Mg	0	0
			5	5		
56	1N	8	Total	Mg	0	0
			8	8		
56	20	1	Total	Mg	0	0
			1	1		
56	18	5	Total	Mg	0	0
			5	5		
56	1o	2	Total	Mg	0	0
			2	2		
56	1Y	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	13	2	Total Mg 2 2	0	0
56	1f	1	Total Mg 1 1	0	0
56	1P	5	Total Mg 5 5	0	0
56	2B	10	Total Mg 10 10	0	0
56	1q	4	Total Mg 4 4	0	0
56	2a	244	Total Mg 244 244	0	0
56	1k	1	Total Mg 1 1	0	0
56	1E	10	Total Mg 10 10	0	0
56	1b	2	Total Mg 2 2	0	0
56	2l	3	Total Mg 3 3	0	0
56	2F	2	Total Mg 2 2	0	0
56	16	2	Total Mg 2 2	0	0
56	28	1	Total Mg 1 1	0	0
56	2e	1	Total Mg 1 1	0	0
56	1W	6	Total Mg 6 6	0	0
56	1A	1051	Total Mg 1051 1051	0	0
56	1t	1	Total Mg 1 1	0	0
56	1n	1	Total Mg 1 1	0	0
56	2P	1	Total Mg 1 1	0	0
56	1X	2	Total Mg 2 2	0	0
56	2p	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	25	1	Total Mg 1 1	0	0
56	1D	17	Total Mg 17 17	0	0
56	2N	1	Total Mg 1 1	0	0
56	1e	4	Total Mg 4 4	0	0
56	2G	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	1V	1	Total Mg 1 1	0	0
56	1a	306	Total Mg 306 306	0	0
56	2Q	5	Total Mg 5 5	0	0
56	15	4	Total Mg 4 4	0	0
56	1x	11	Total Mg 11 11	0	0
56	1R	6	Total Mg 6 6	0	0
56	26	1	Total Mg 1 1	0	0
56	2U	2	Total Mg 2 2	0	0
56	1G	3	Total Mg 3 3	0	0
56	2O	3	Total Mg 3 3	0	0
56	11	1	Total Mg 1 1	0	0
56	1d	2	Total Mg 2 2	0	0
56	2n	2	Total Mg 2 2	0	0
56	1H	4	Total Mg 4 4	0	0
56	2q	1	Total Mg 1 1	0	0

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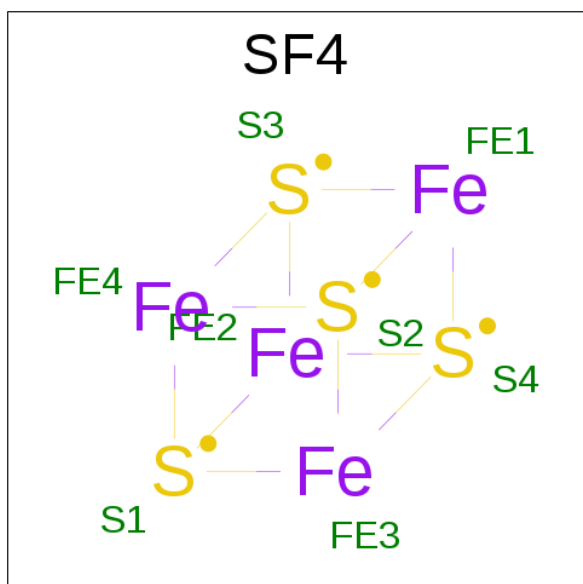
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2Y	1	Total 1	Mg 1	0	0
56	2x	6	Total 6	Mg 6	0	0
56	2R	1	Total 1	Mg 1	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	2D	4	Total 4	Mg 4	0	0
56	14	1	Total 1	Mg 1	0	0
56	2k	2	Total 2	Mg 2	0	0
56	1U	5	Total 5	Mg 5	0	0
56	1O	2	Total 2	Mg 2	0	0
56	1r	3	Total 3	Mg 3	0	0
56	19	3	Total 3	Mg 3	0	0
56	1l	1	Total 1	Mg 1	0	0
56	2V	1	Total 1	Mg 1	0	0
56	1F	7	Total 7	Mg 7	0	0
56	10	7	Total 7	Mg 7	0	0
56	2t	1	Total 1	Mg 1	0	0
56	1Q	6	Total 6	Mg 6	0	0
56	2A	583	Total 583	Mg 583	0	0
56	1h	3	Total 3	Mg 3	0	0
56	1B	26	Total 26	Mg 26	0	0
56	1c	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		
57	14	1	Total	Zn	0	0
			1	1		
57	1n	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	19	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	24	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	2110	Total	O	0	0
			2110	2110		
59	1B	42	Total	O	0	0
			42	42		
59	1D	24	Total	O	0	0
			24	24		
59	1E	30	Total	O	0	0
			30	30		
59	1F	16	Total	O	0	0
			16	16		
59	1G	6	Total	O	0	0
			6	6		
59	1H	3	Total	O	0	0
			3	3		
59	1I	1	Total	O	0	0
			1	1		
59	1N	7	Total	O	0	0
			7	7		
59	1O	4	Total	O	0	0
			4	4		
59	1P	21	Total	O	0	0
			21	21		
59	1Q	11	Total	O	0	0
			11	11		
59	1R	16	Total	O	0	0
			16	16		
59	1S	2	Total	O	0	0
			2	2		
59	1T	7	Total	O	0	0
			7	7		
59	1U	14	Total	O	0	0
			14	14		
59	1V	4	Total	O	0	0
			4	4		
59	1W	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	4	Total 4	O 4	0	0
59	1Y	1	Total 1	O 1	0	0
59	1Z	4	Total 4	O 4	0	0
59	10	8	Total 8	O 8	0	0
59	11	7	Total 7	O 7	0	0
59	12	2	Total 2	O 2	0	0
59	13	4	Total 4	O 4	0	0
59	15	7	Total 7	O 7	0	0
59	16	5	Total 5	O 5	0	0
59	17	8	Total 8	O 8	0	0
59	18	9	Total 9	O 9	0	0
59	19	4	Total 4	O 4	0	0
59	1a	393	Total 393	O 393	0	0
59	1b	1	Total 1	O 1	0	0
59	1c	1	Total 1	O 1	0	0
59	1d	5	Total 5	O 5	0	0
59	1e	3	Total 3	O 3	0	0
59	1f	1	Total 1	O 1	0	0
59	1h	3	Total 3	O 3	0	0
59	1i	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1k	1	Total 1	O 1	0	0
59	1l	3	Total 3	O 3	0	0
59	1m	1	Total 1	O 1	0	0
59	1o	1	Total 1	O 1	0	0
59	1p	1	Total 1	O 1	0	0
59	1q	1	Total 1	O 1	0	0
59	1s	1	Total 1	O 1	0	0
59	1v	1	Total 1	O 1	0	0
59	1x	8	Total 8	O 8	0	0
59	1z	1	Total 1	O 1	0	0
59	2A	813	Total 813	O 813	0	0
59	2B	10	Total 10	O 10	0	0
59	2D	16	Total 16	O 16	0	0
59	2E	9	Total 9	O 9	0	0
59	2F	5	Total 5	O 5	0	0
59	2N	1	Total 1	O 1	0	0
59	2O	3	Total 3	O 3	0	0
59	2P	9	Total 9	O 9	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	3	Total 3	O 3	0	0
59	2T	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2U	3	Total 3	O 3	0	0
59	2W	1	Total 1	O 1	0	0
59	2X	2	Total 2	O 2	0	0
59	2Y	1	Total 1	O 1	0	0
59	2Z	4	Total 4	O 4	0	0
59	20	3	Total 3	O 3	0	0
59	21	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	26	1	Total 1	O 1	0	0
59	27	2	Total 2	O 2	0	0
59	28	2	Total 2	O 2	0	0
59	2a	321	Total 321	O 321	0	0
59	2d	1	Total 1	O 1	0	0
59	2e	1	Total 1	O 1	0	0
59	2i	2	Total 2	O 2	0	0
59	2j	1	Total 1	O 1	0	0
59	2l	1	Total 1	O 1	0	0
59	2m	3	Total 3	O 3	0	0
59	2p	1	Total 1	O 1	0	0
59	2q	1	Total 1	O 1	0	0
59	2t	4	Total 4	O 4	0	0

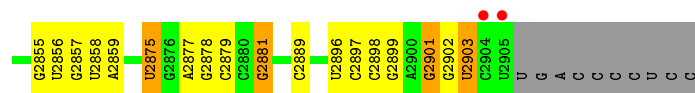
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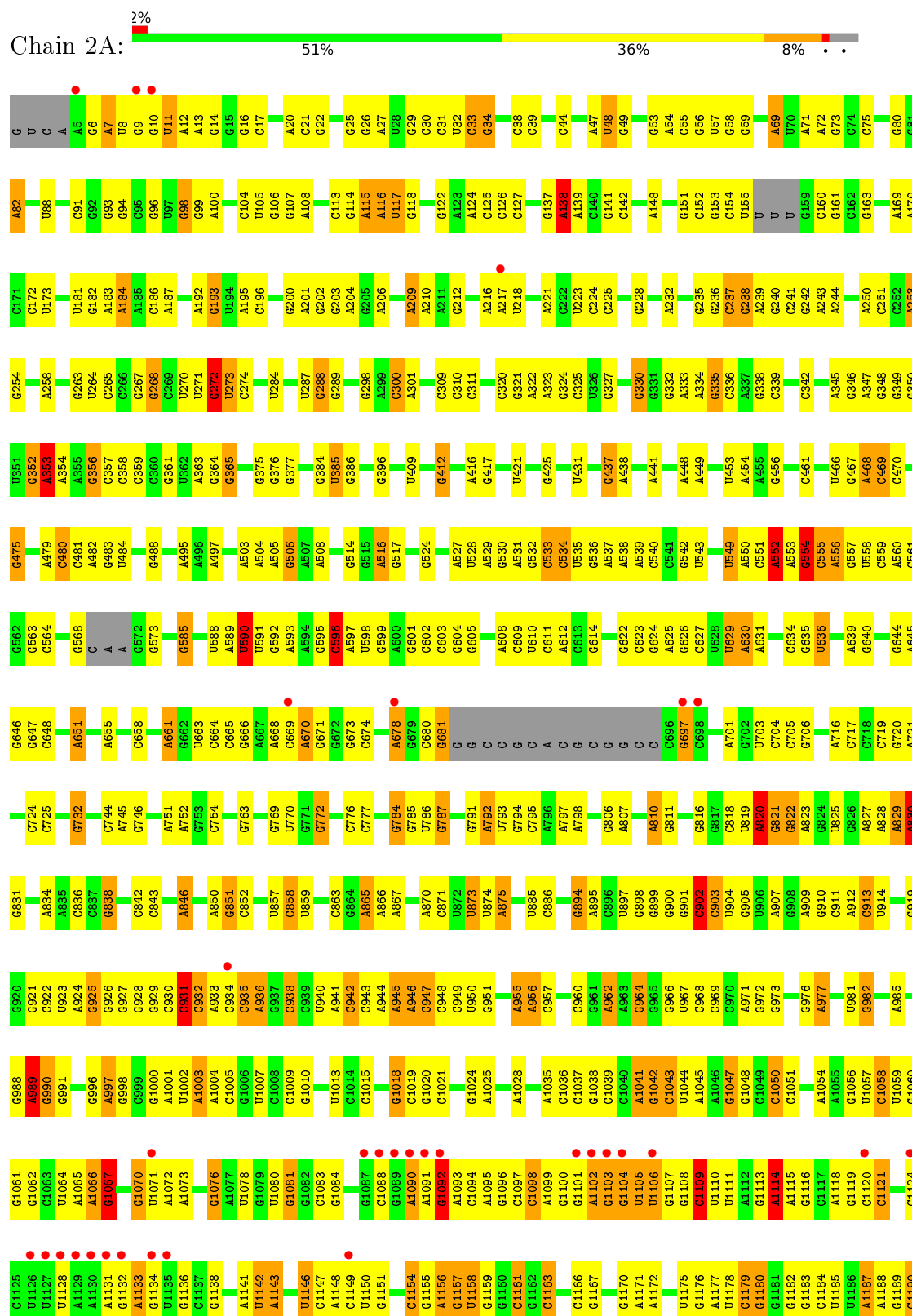
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2x	7	Total	O	0	0
			7	7		
59	2z	1	Total	O	0	0
			1	1		

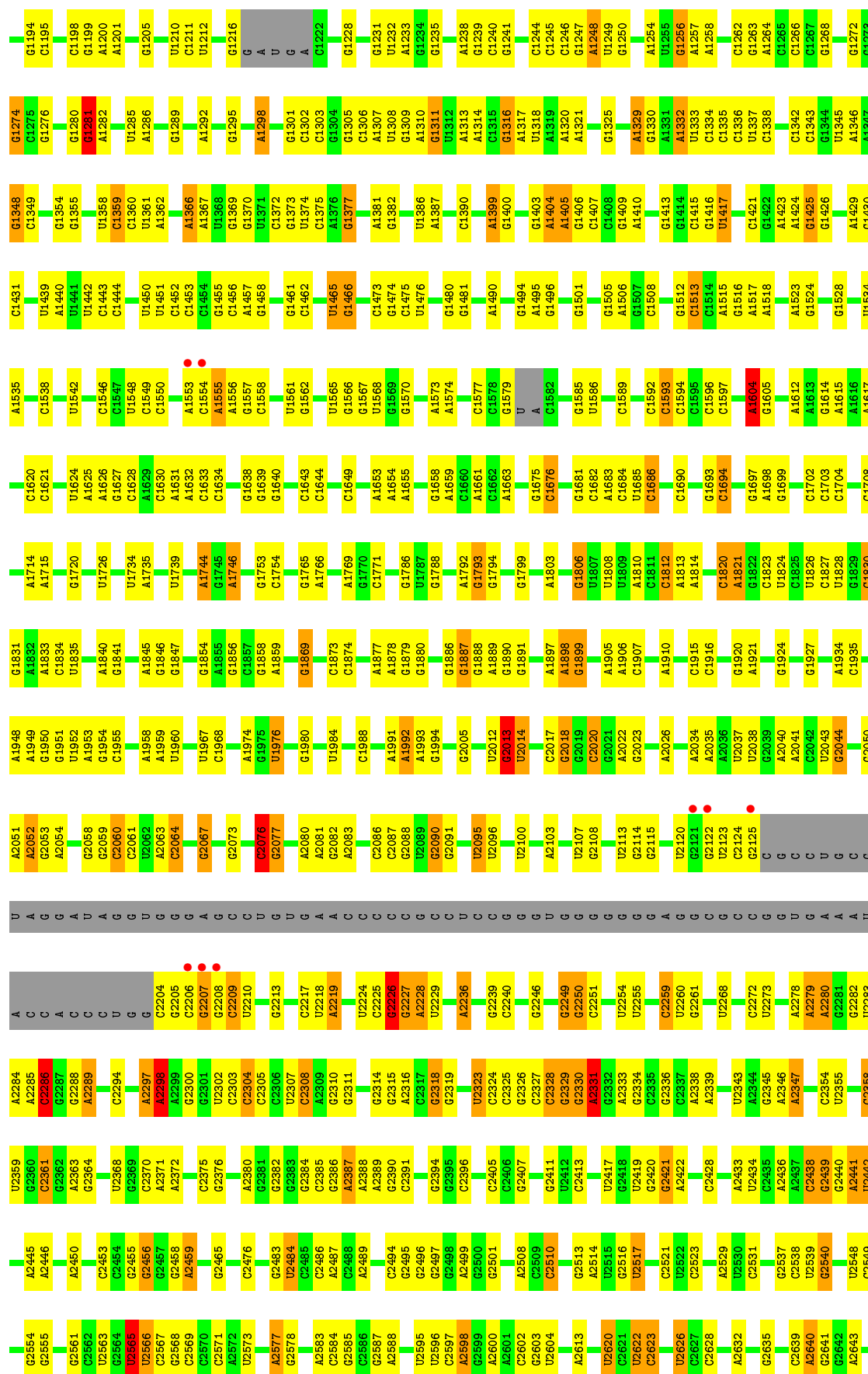




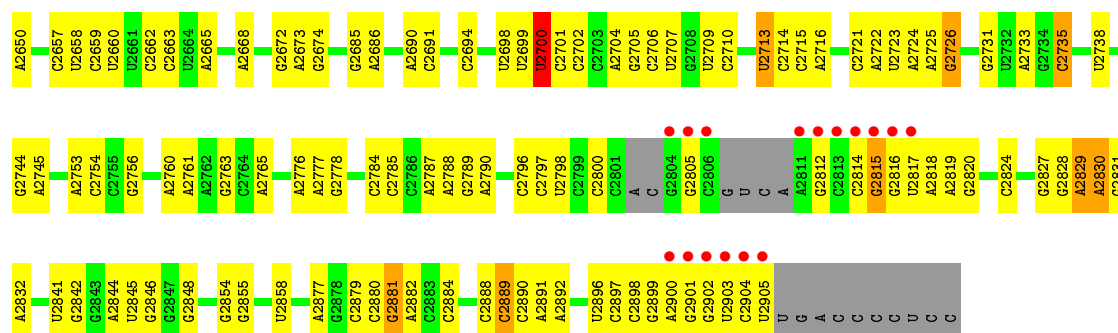


- Molecule 1: 23S Ribosomal RNA

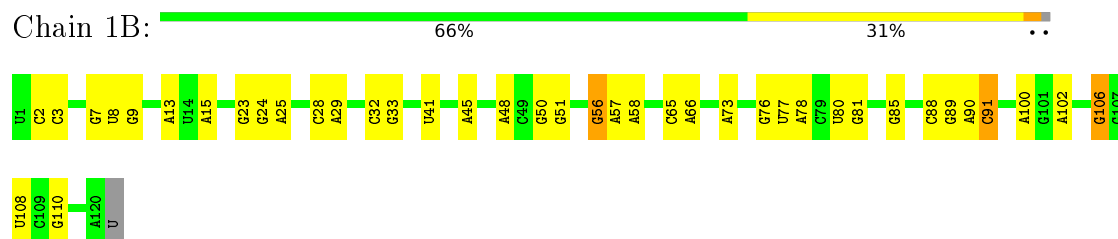




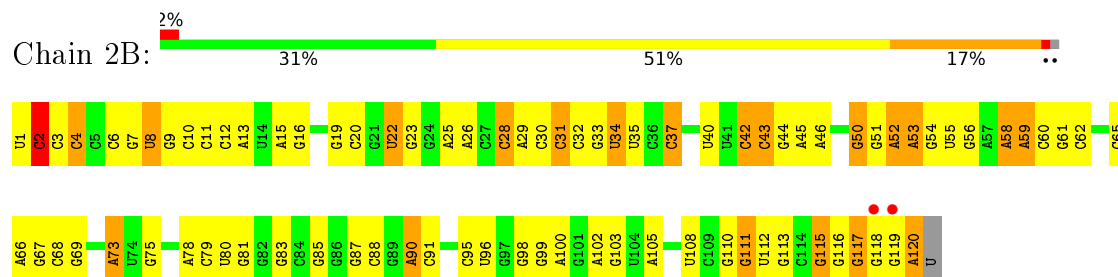




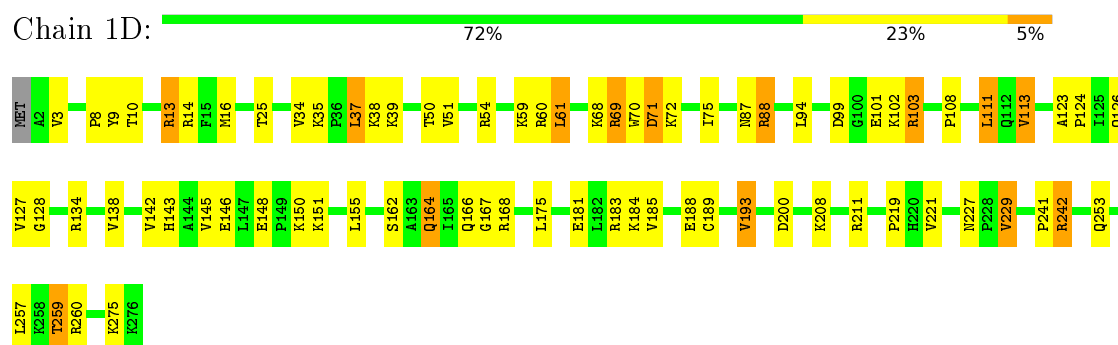
### • Molecule 2: 5S Ribosomal RNA



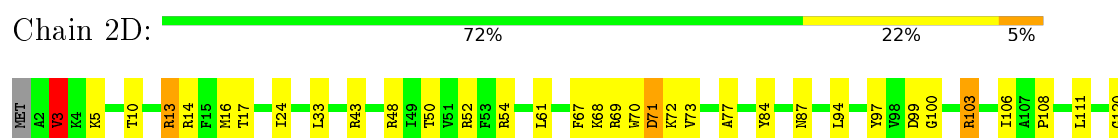
### • Molecule 2: 5S Ribosomal RNA

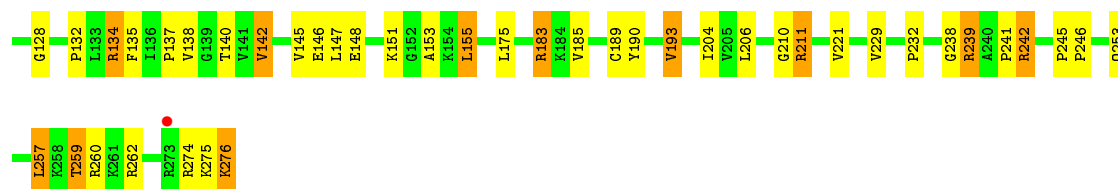


### • Molecule 3: 50S ribosomal protein L2



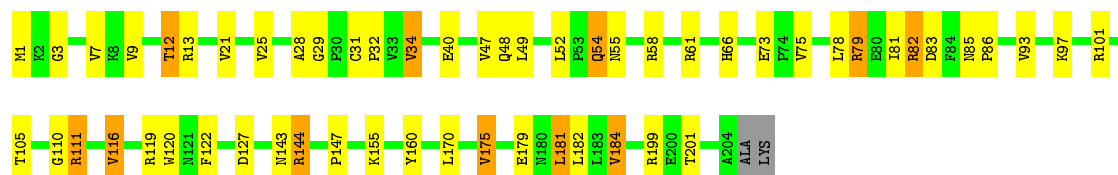
### • Molecule 3: 50S ribosomal protein L2





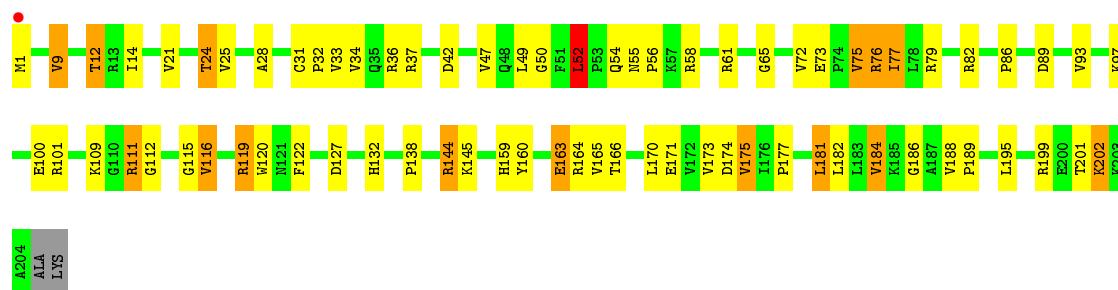
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 72% 22% 5%



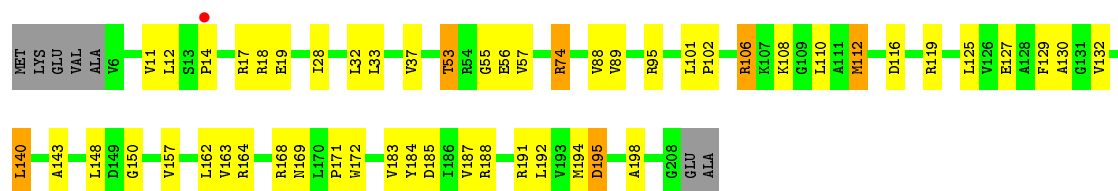
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 64% 28% 7%



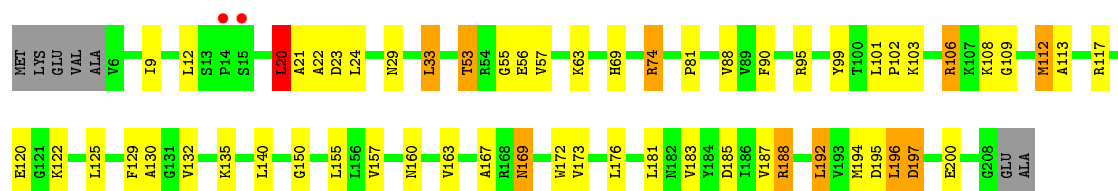
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 71% 22%

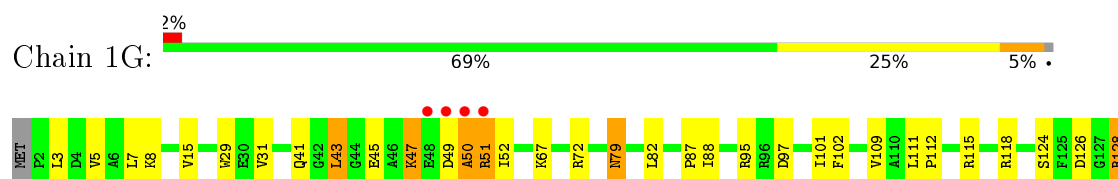


• Molecule 5: 50S ribosomal protein L4

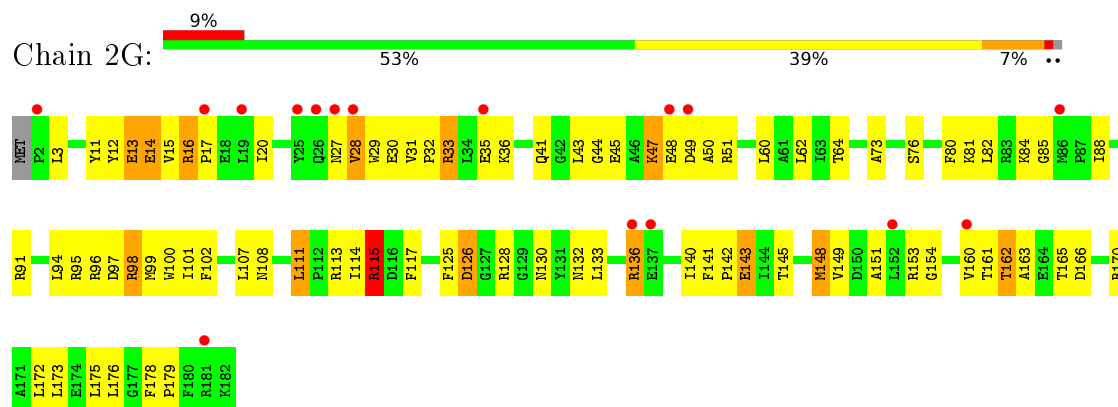
Chain 2F: 69% 23% 5%



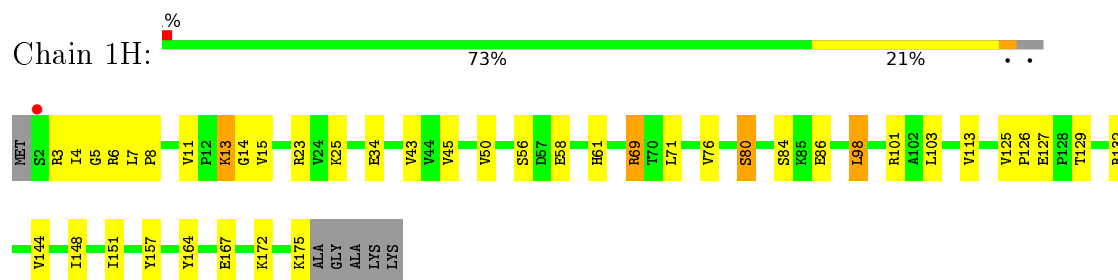
• Molecule 6: 50S ribosomal protein L5



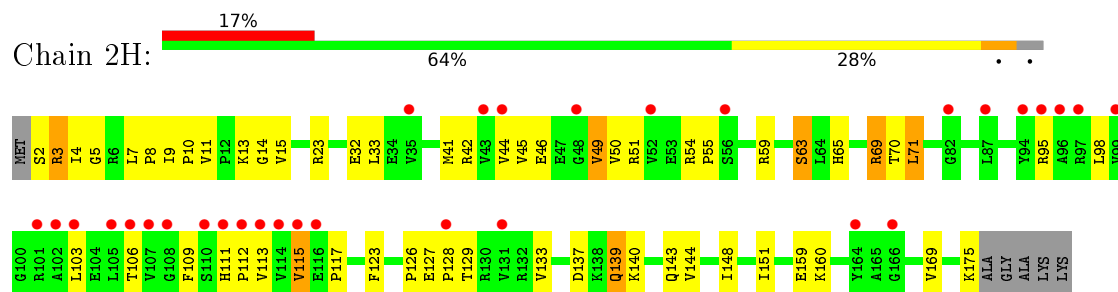
• Molecule 6: 50S ribosomal protein L5



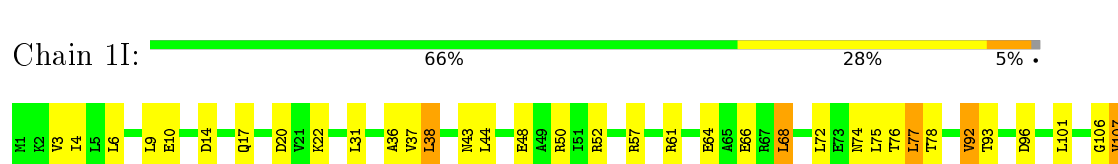
• Molecule 7: 50S ribosomal protein L6

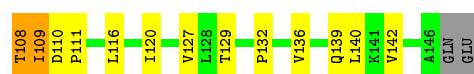


• Molecule 7: 50S ribosomal protein L6

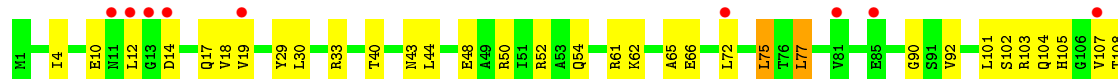


• Molecule 8: 50S ribosomal protein L9

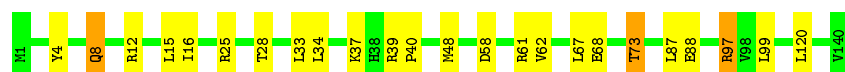
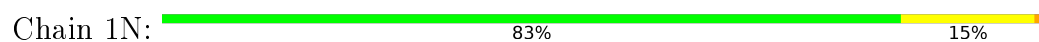




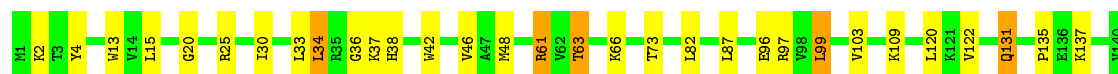
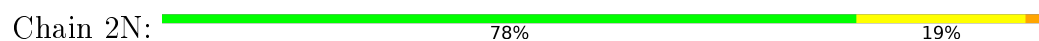
- Molecule 8: 50S ribosomal protein L9



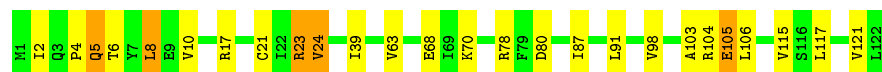
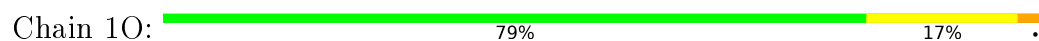
- Molecule 9: 50S ribosomal protein L13



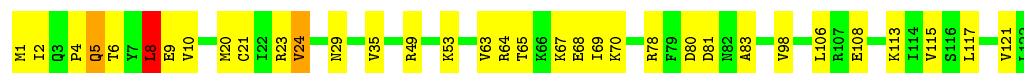
- Molecule 9: 50S ribosomal protein L13



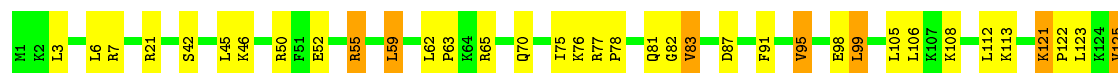
- Molecule 10: 50S ribosomal protein L14



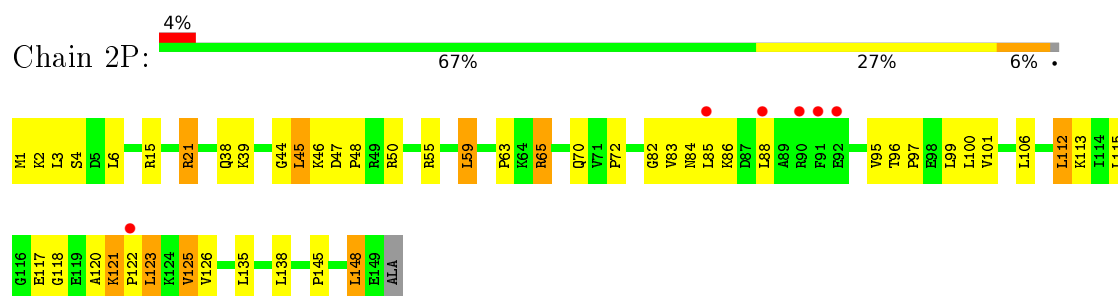
- Molecule 10: 50S ribosomal protein L14



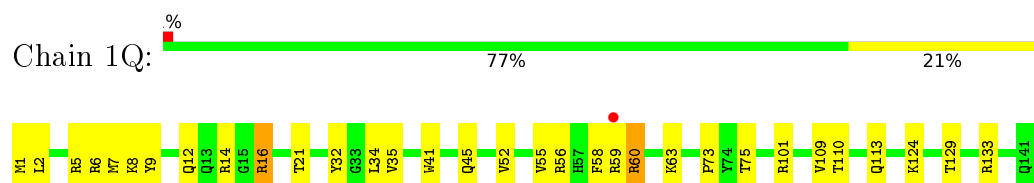
- Molecule 11: 50S ribosomal protein L15



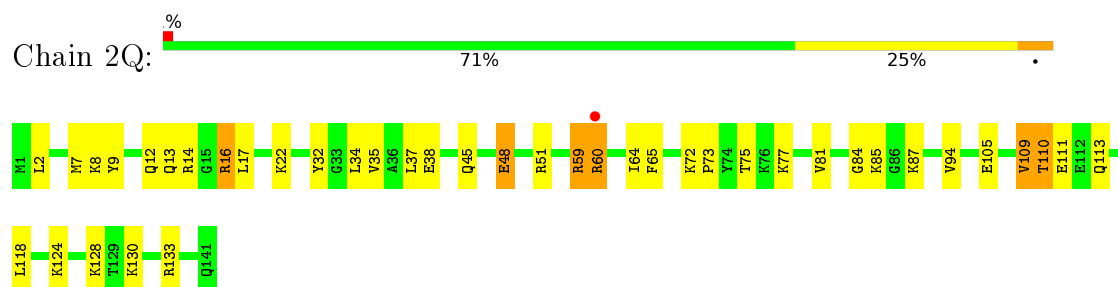
- Molecule 11: 50S ribosomal protein L15



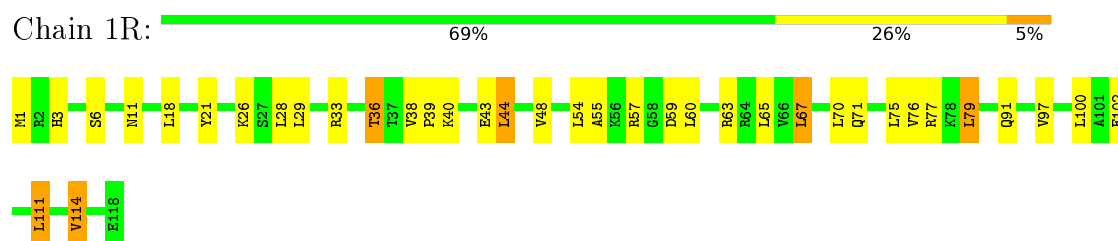
- Molecule 12: 50S ribosomal protein L16



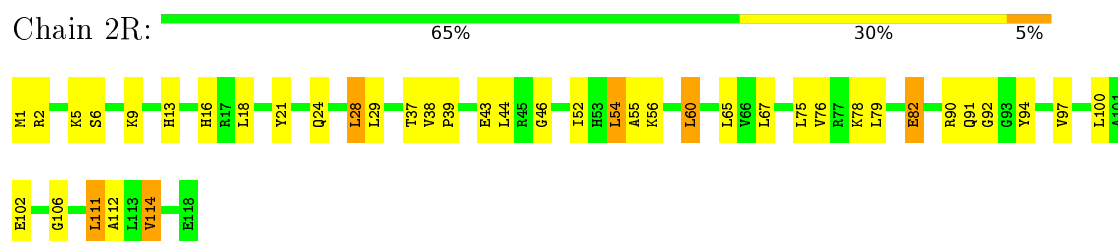
- Molecule 12: 50S ribosomal protein L16



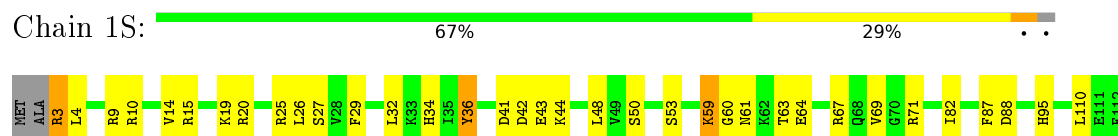
- Molecule 13: 50S ribosomal protein L17



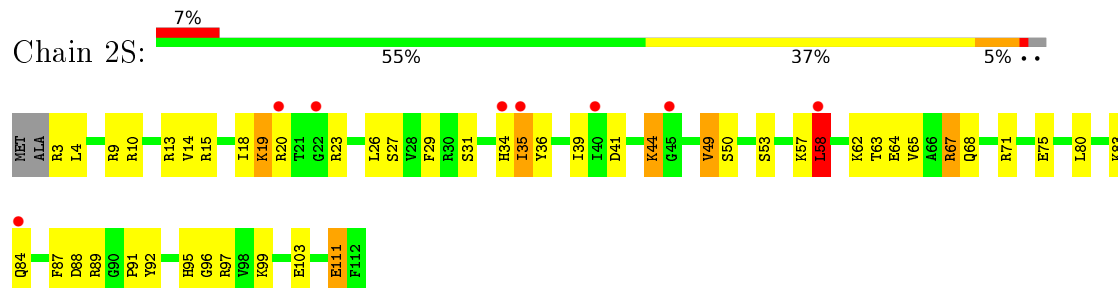
- Molecule 13: 50S ribosomal protein L17



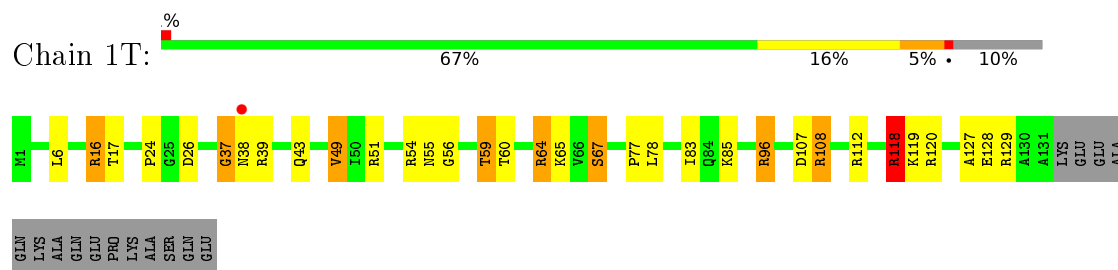
- Molecule 14: 50S ribosomal protein L18



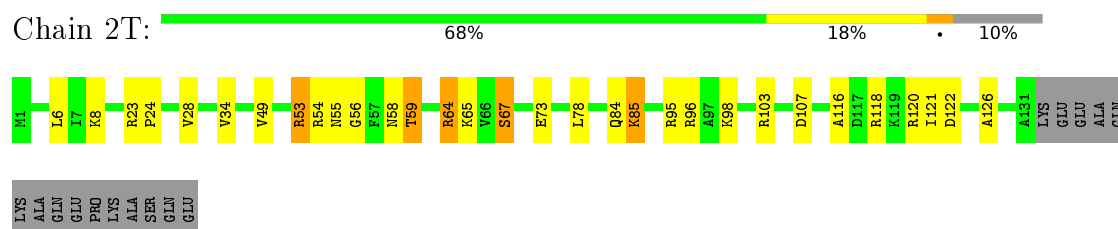
- Molecule 14: 50S ribosomal protein L18



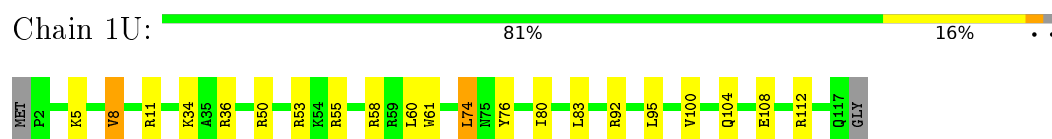
- Molecule 15: 50S ribosomal protein L19



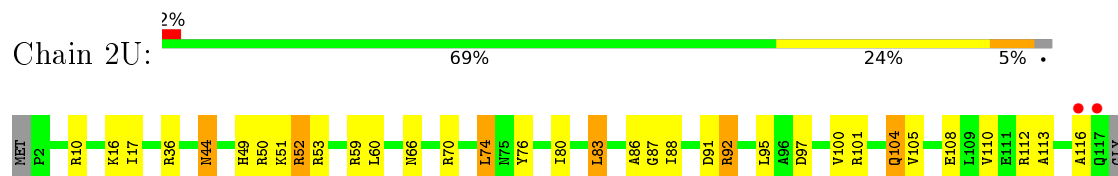
- Molecule 15: 50S ribosomal protein L19



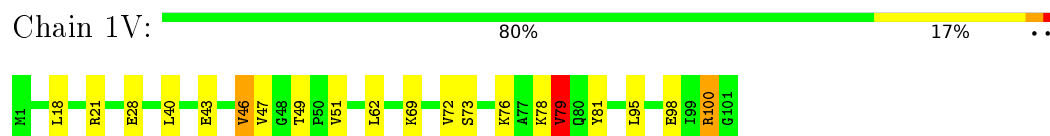
- Molecule 16: 50S ribosomal protein L20



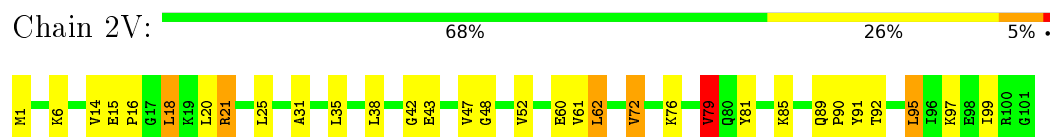
- Molecule 16: 50S ribosomal protein L20



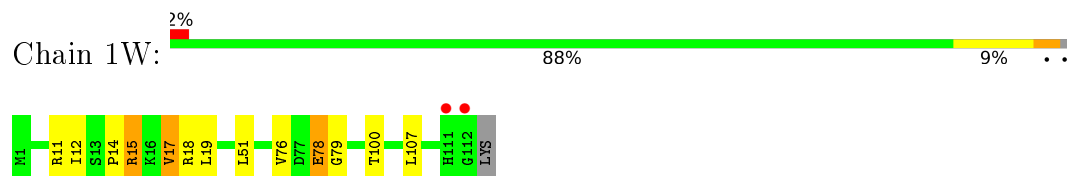
- Molecule 17: 50S ribosomal protein L21



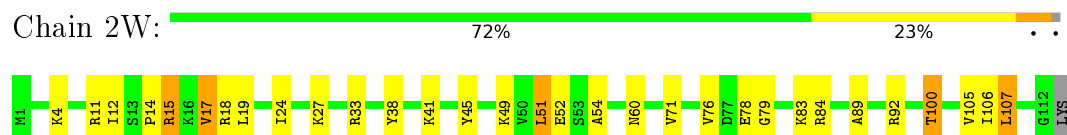
- Molecule 17: 50S ribosomal protein L21



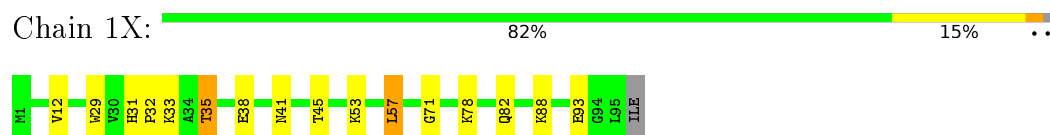
- Molecule 18: 50S ribosomal protein L22



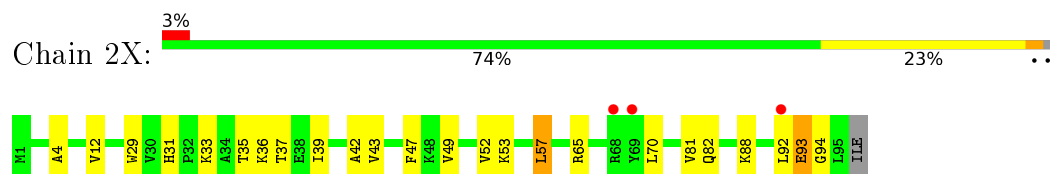
- Molecule 18: 50S ribosomal protein L22



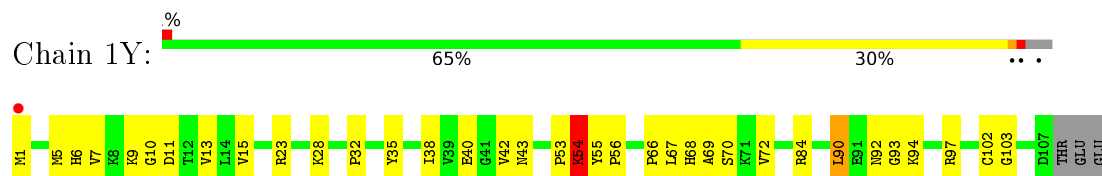
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23

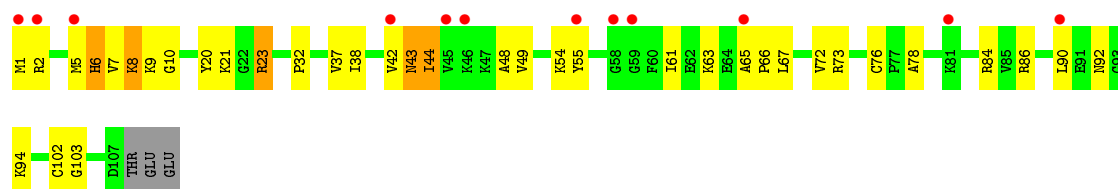


- Molecule 20: 50S ribosomal protein L24



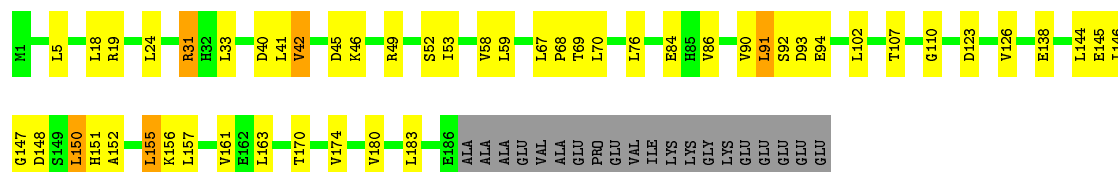
- Molecule 20: 50S ribosomal protein L24





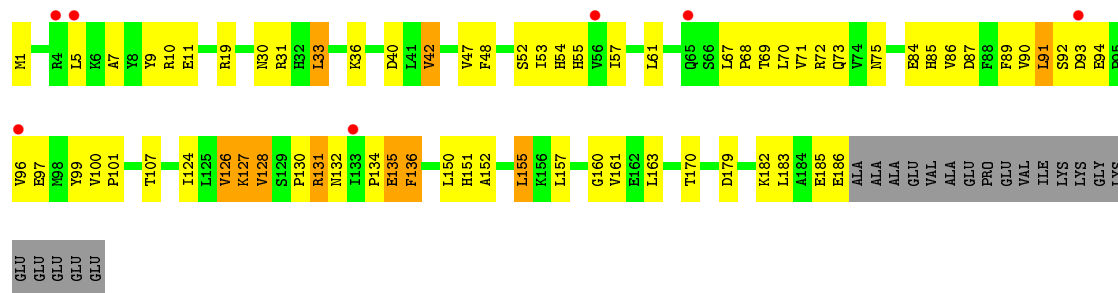
- Molecule 21: 50S ribosomal protein L25

Chain 1Z: 66% 22% 10%



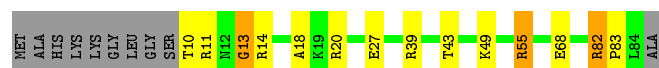
- Molecule 21: 50S ribosomal protein L25

Chain 2Z: 3% 57% 29% 5% 10%



- Molecule 22: 50S ribosomal protein L27

Chain 10: 72% 13% 12%



- Molecule 22: 50S ribosomal protein L27

Chain 20: 7% 73% 12% 12%



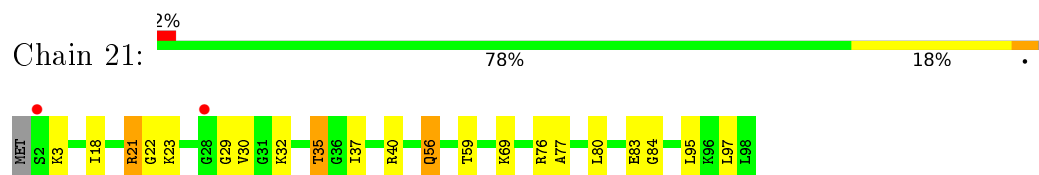
- Molecule 23: 50S ribosomal protein L28

Chain 11: 81% 16% 3%

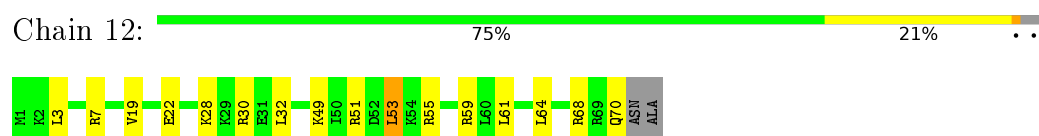




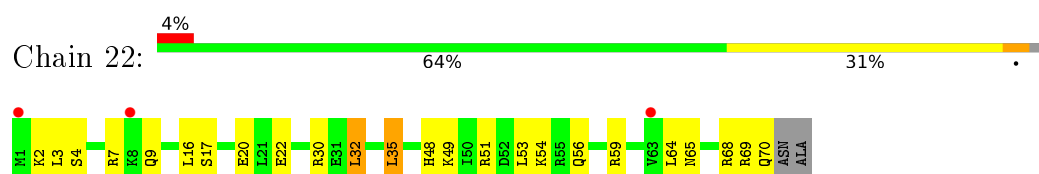
- Molecule 23: 50S ribosomal protein L28



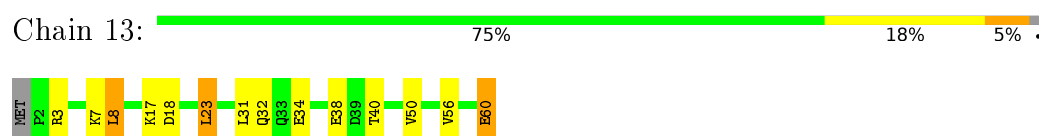
- Molecule 24: 50S ribosomal protein L29



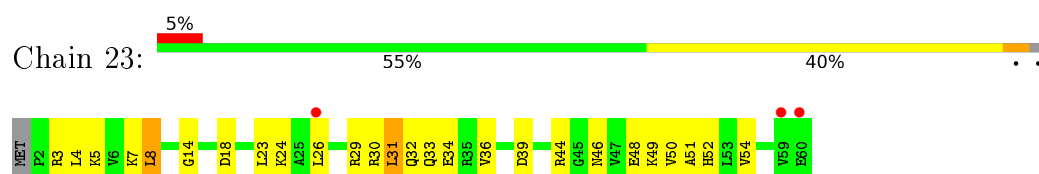
- Molecule 24: 50S ribosomal protein L29



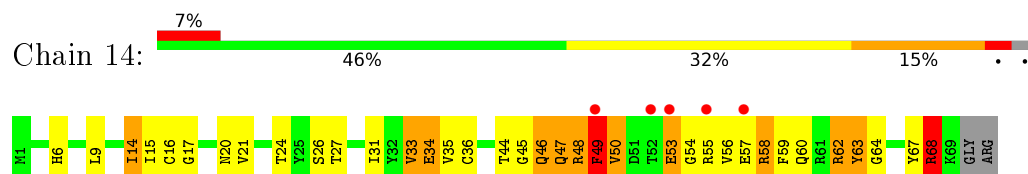
- Molecule 25: 50S ribosomal protein L30



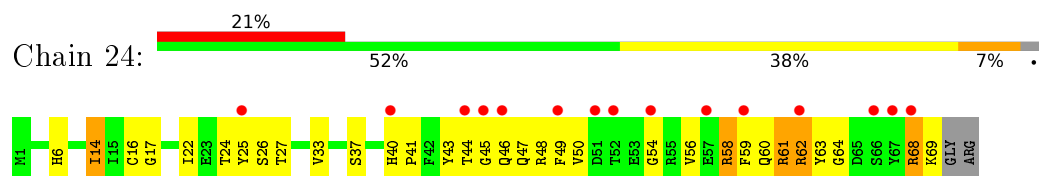
- Molecule 25: 50S ribosomal protein L30




- Molecule 26: 50S ribosomal protein L31

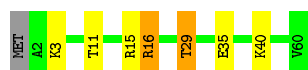


- Molecule 26: 50S ribosomal protein L31




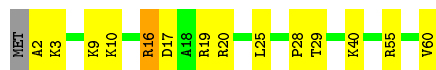
- Molecule 27: 50S ribosomal protein L32

Chain 15:  87% 8% ..




- Molecule 27: 50S ribosomal protein L32

Chain 25:  75% 22% ..



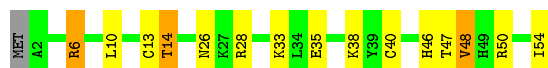
- Molecule 28: 50S ribosomal protein L33

Chain 16:  74% 22% ..




- Molecule 28: 50S ribosomal protein L33

Chain 26:  70% 22% 6% .



- Molecule 29: 50S ribosomal protein L34

Chain 17:  2% 73% 20% ..



- Molecule 29: 50S ribosomal protein L34

Chain 27:  6% 65% 31% ..



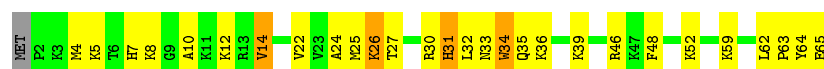
- Molecule 30: 50S ribosomal protein L35

Chain 18:  66% 29% ..

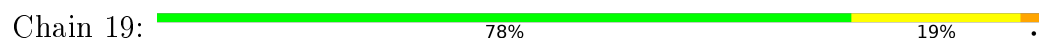


- Molecule 30: 50S ribosomal protein L35

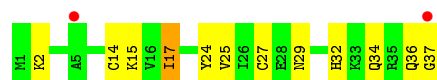
Chain 28:  55% 37% 6% .



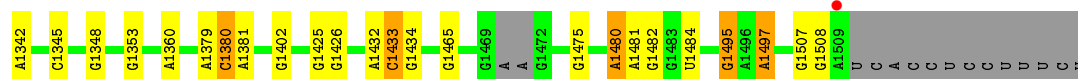
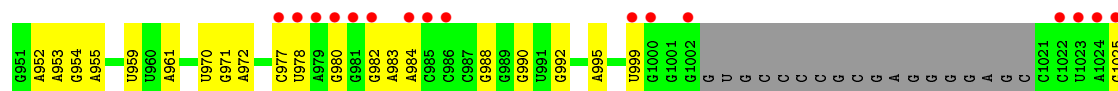
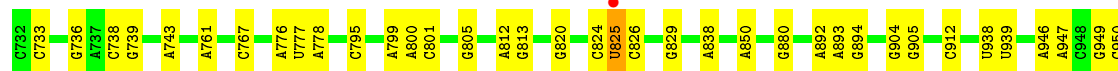
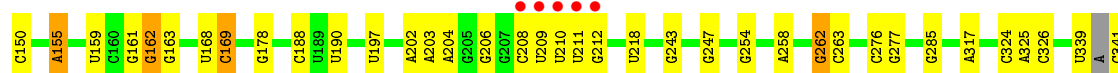
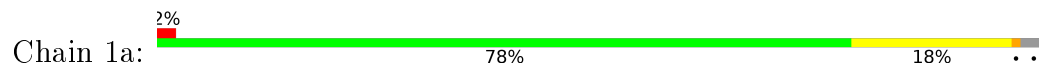
- Molecule 31: 50S ribosomal protein L36



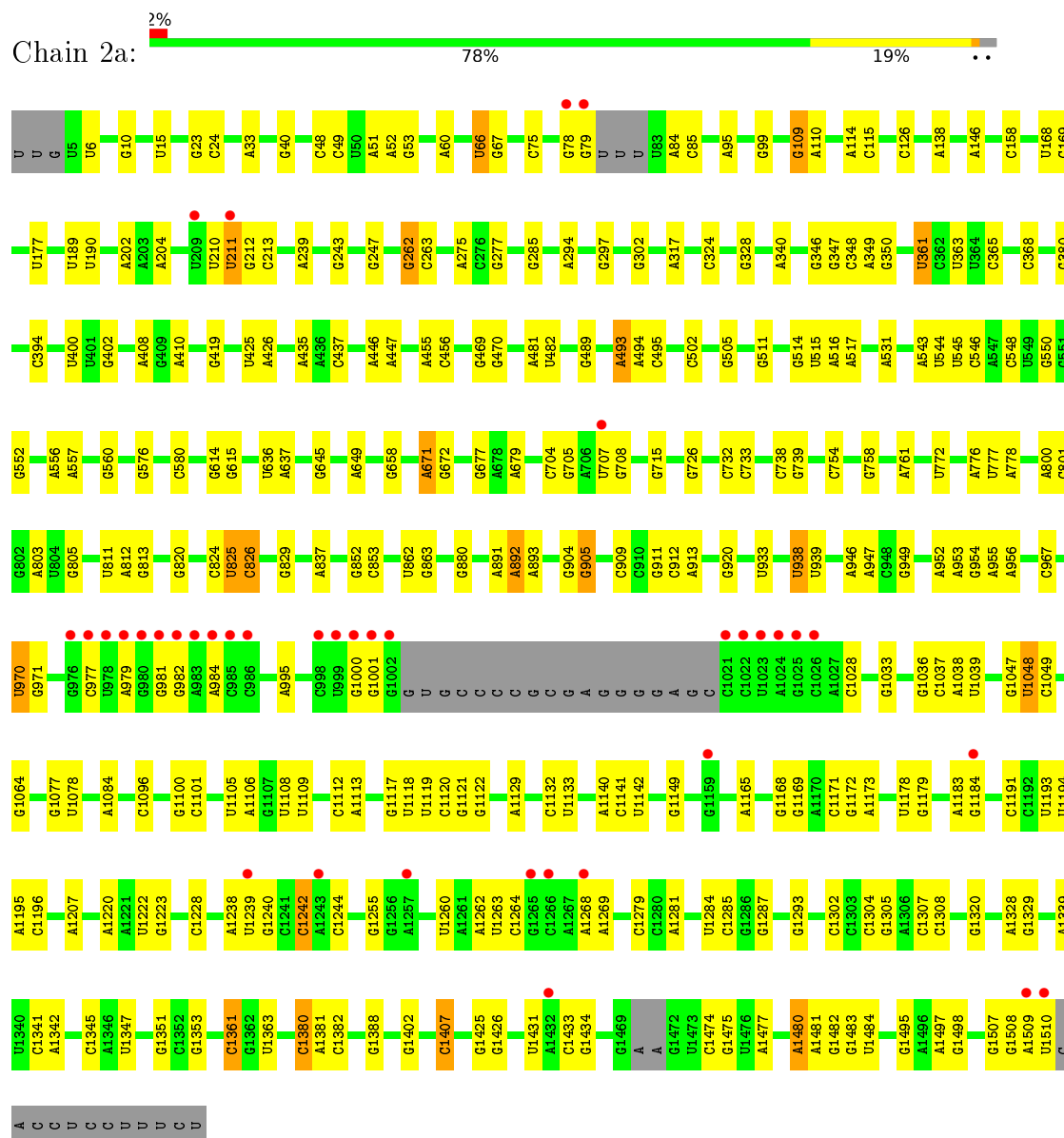
- Molecule 31: 50S ribosomal protein L36



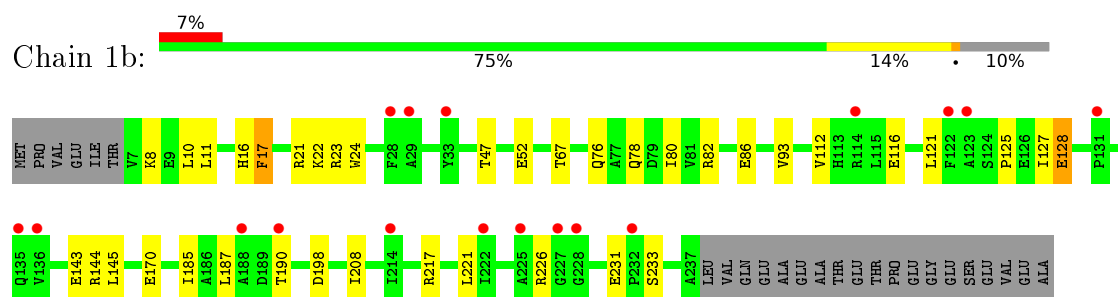
- Molecule 32: 16S Ribosomal RNA



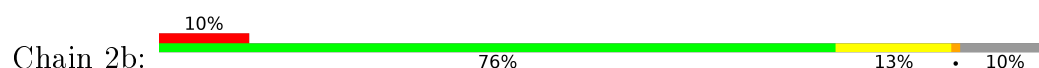
- Molecule 32: 16S Ribosomal RNA

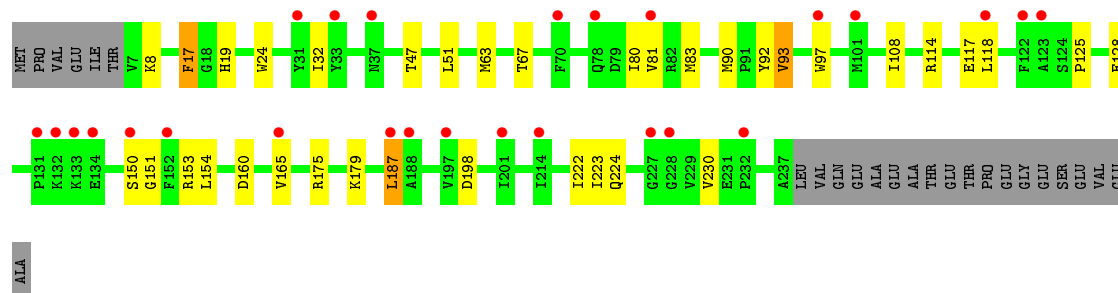


- Molecule 33: 30S ribosomal protein S2

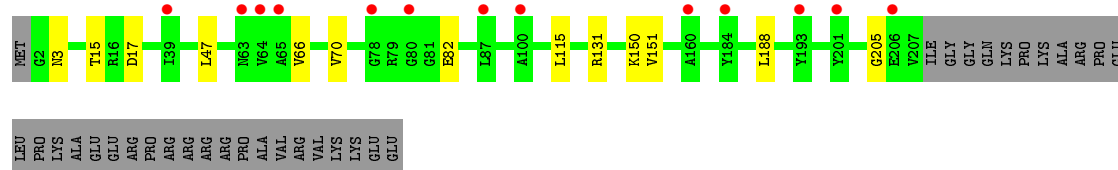
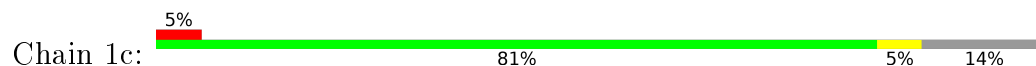


- Molecule 33: 30S ribosomal protein S2

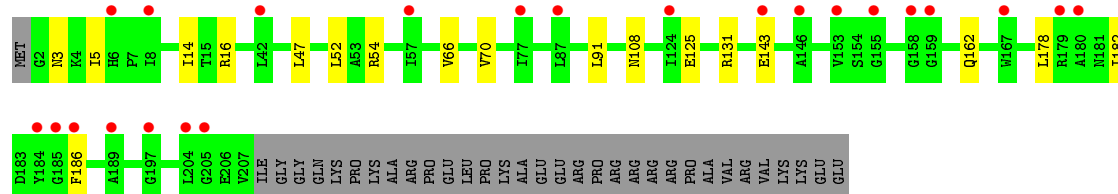
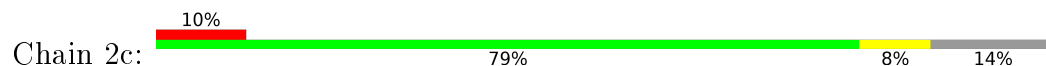




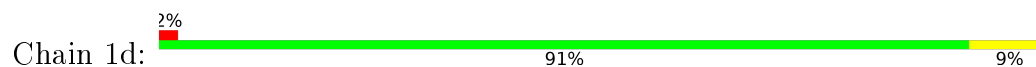
- Molecule 34: 30S ribosomal protein S3



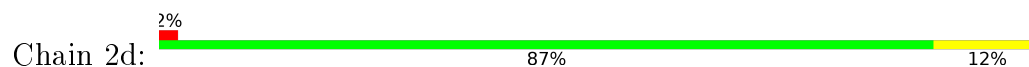
- Molecule 34: 30S ribosomal protein S3



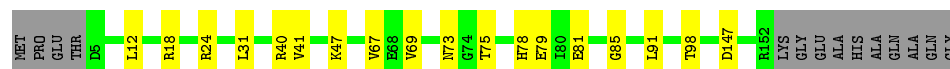
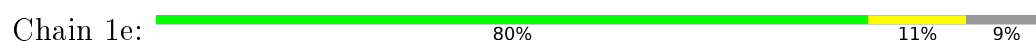
- Molecule 35: 30S ribosomal protein S4



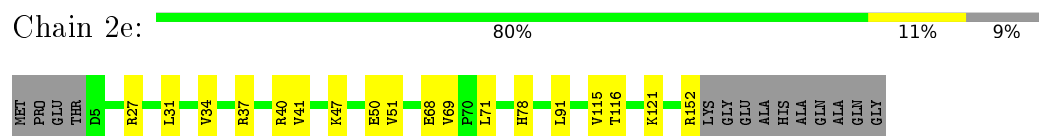
- Molecule 35: 30S ribosomal protein S4



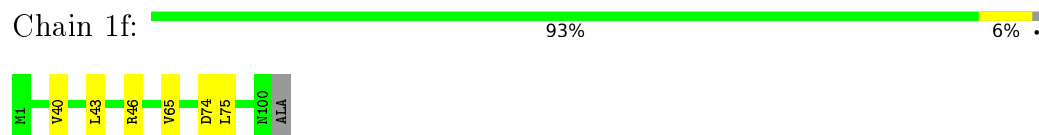
- Molecule 36: 30S ribosomal protein S5



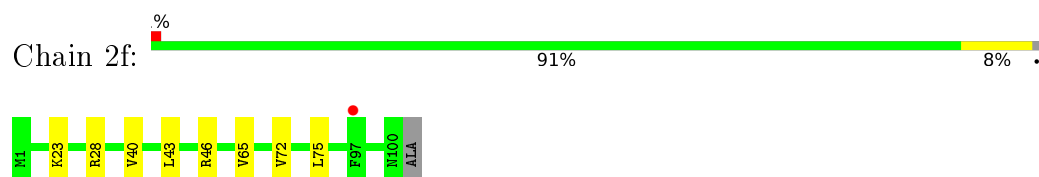
- Molecule 36: 30S ribosomal protein S5



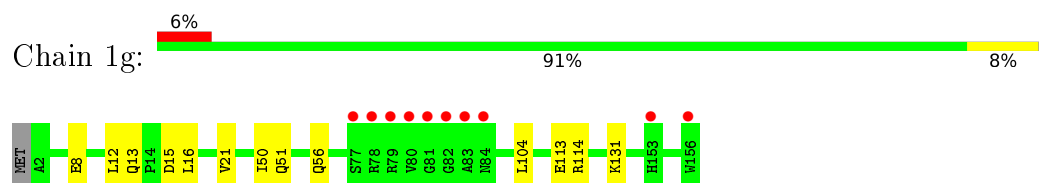
- Molecule 37: 30S ribosomal protein S6



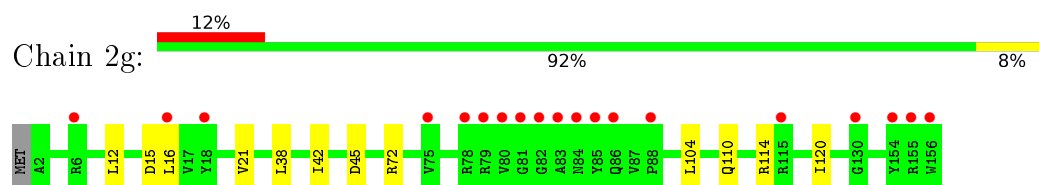
- Molecule 37: 30S ribosomal protein S6



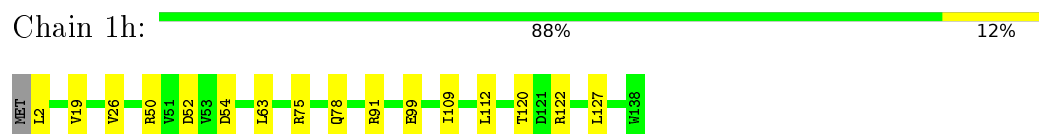
- Molecule 38: 30S ribosomal protein S7



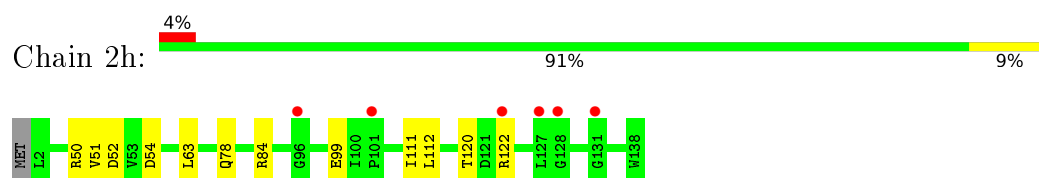
- Molecule 38: 30S ribosomal protein S7



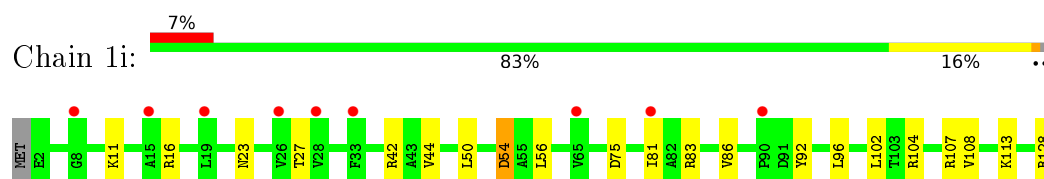
- Molecule 39: 30S ribosomal protein S8



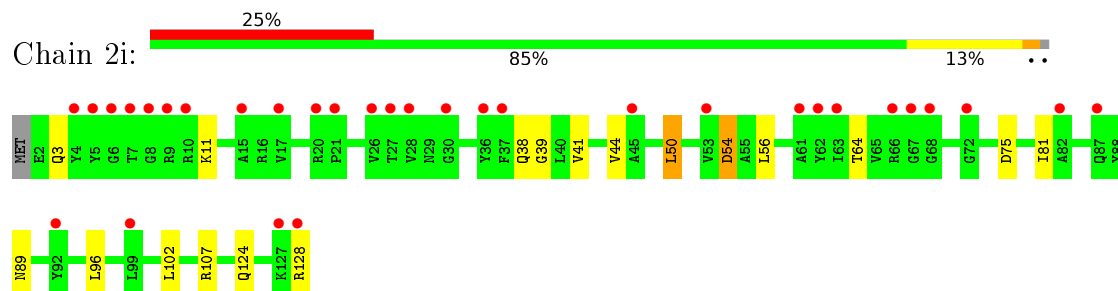
- Molecule 39: 30S ribosomal protein S8



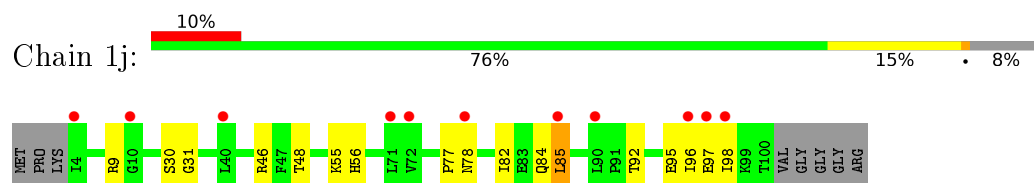
- Molecule 40: 30S ribosomal protein S9



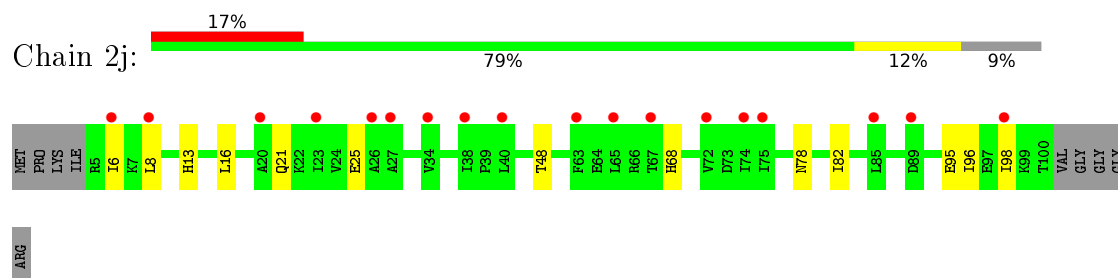
- Molecule 40: 30S ribosomal protein S9



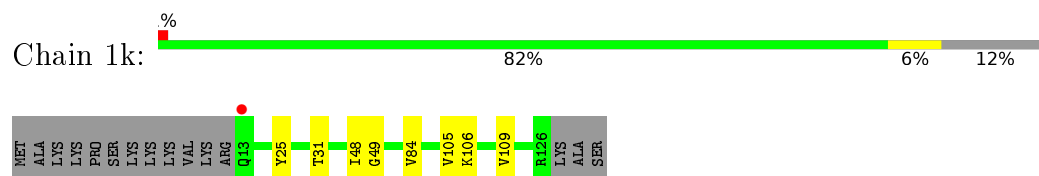
- Molecule 41: 30S ribosomal protein S10



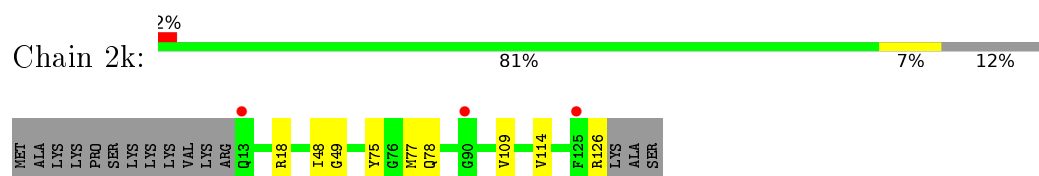
- Molecule 41: 30S ribosomal protein S10



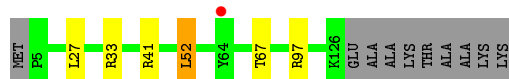
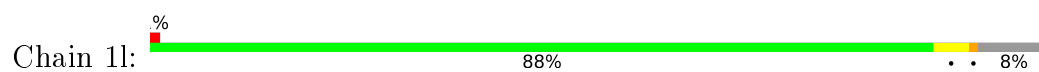
- Molecule 42: 30S ribosomal protein S11



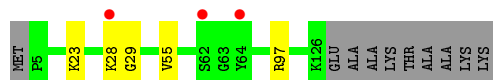
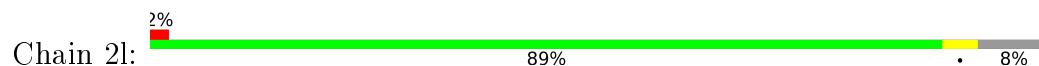
- Molecule 42: 30S ribosomal protein S11



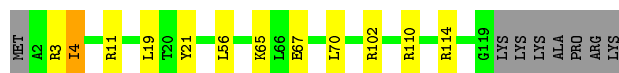
- Molecule 43: 30S ribosomal protein S12



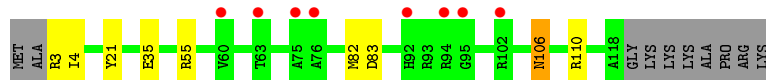
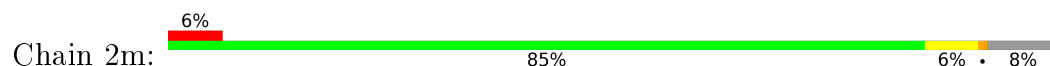
- Molecule 43: 30S ribosomal protein S12



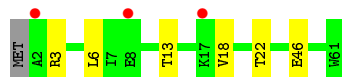
- Molecule 44: 30S ribosomal protein S13



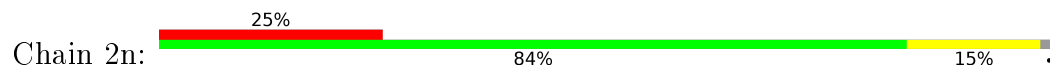
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z




- Molecule 46: 30S ribosomal protein S15




- Molecule 46: 30S ribosomal protein S15

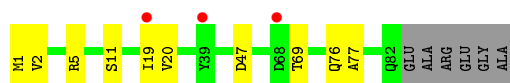


Chain 2o:  87% 12% .




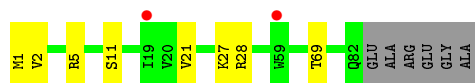
- Molecule 47: 30S ribosomal protein S16

Chain 1p:  3% 82% 11% 7%



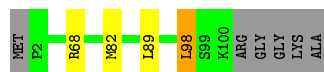
- Molecule 47: 30S ribosomal protein S16

Chain 2p:  2% 84% 9% 7%

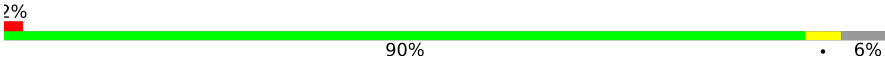


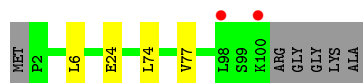
- Molecule 48: 30S ribosomal protein S17

Chain 1q:  90% . . 6%



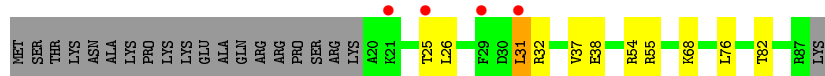
- Molecule 48: 30S ribosomal protein S17

Chain 2q:  2% 90% . 6%



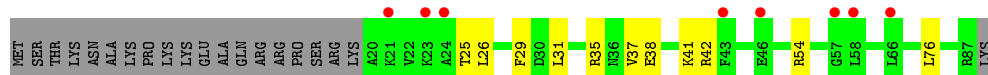
- Molecule 49: 30S ribosomal protein S18

Chain 1r:  5% 65% 11% . 23%

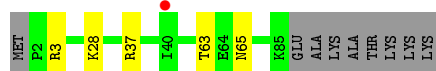
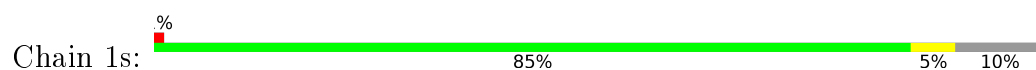


- Molecule 49: 30S ribosomal protein S18

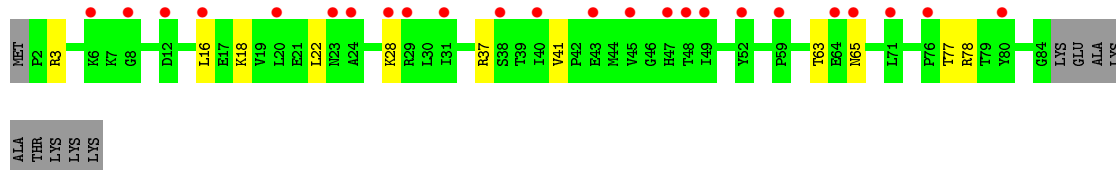
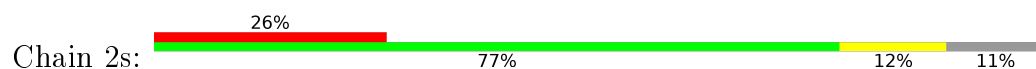
Chain 2r:  9% 65% 13% 23%



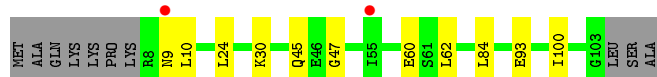
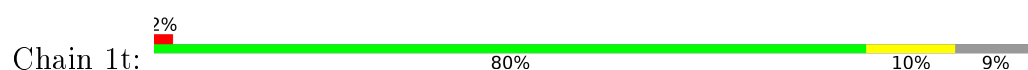
- Molecule 50: 30S ribosomal protein S19



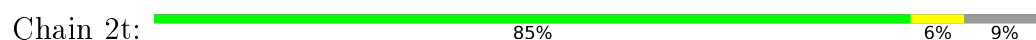
- Molecule 50: 30S ribosomal protein S19



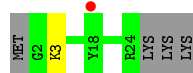
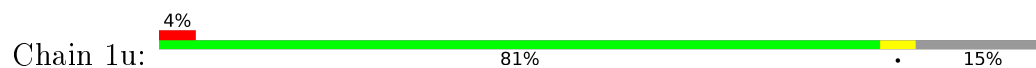
- Molecule 51: 30S ribosomal protein S20



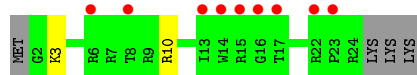
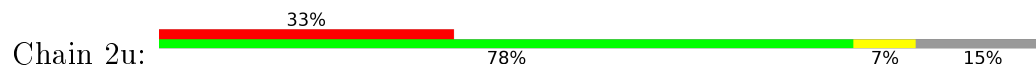
- Molecule 51: 30S ribosomal protein S20



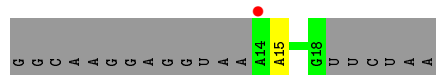
- Molecule 52: 30S ribosomal protein Thx



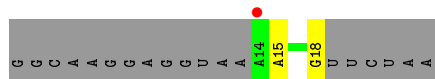
- Molecule 52: 30S ribosomal protein Thx



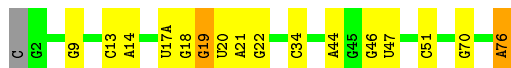
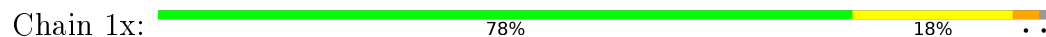
- Molecule 53: mRNA



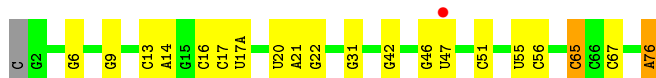
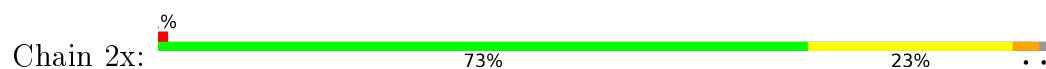
- Molecule 53: mRNA



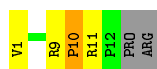
- Molecule 54: P-site tRNA



- Molecule 54: P-site tRNA



- Molecule 55: Oncocin d15-19



- Molecule 55: Oncocin d15-19



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.05Å 450.75Å 623.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.80 49.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.92-2.80) 99.7 (49.92-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.200 , 0.251 0.206 , 0.254	Depositor DCC
$R_{free}$ test set	71597 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.7	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1426338 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	288518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: 5MU, ZN, SF4, MG, 5MC, 4SU, 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	0.87	14/66249 (0.0%)	1.19	268/103407 (0.3%)
1	2A	0.65	4/67298 (0.0%)	1.16	185/105044 (0.2%)
2	1B	0.64	0/2877	1.02	2/4488 (0.0%)
2	2B	0.81	0/2878	1.22	7/4490 (0.2%)
3	1D	0.55	0/2186	0.65	0/2944
3	2D	0.48	0/2192	0.65	0/2951
4	1E	0.56	0/1592	0.66	0/2149
4	2E	0.47	0/1592	0.66	0/2149
5	1F	0.52	0/1619	0.65	0/2193
5	2F	0.42	0/1615	0.65	0/2188
6	1G	0.40	0/1450	0.62	0/1959
6	2G	0.47	0/1449	0.70	1/1958 (0.1%)
7	1H	0.47	0/1356	0.59	0/1834
7	2H	0.45	0/1356	0.63	0/1834
8	1I	0.41	0/1100	0.63	0/1501
8	2I	0.38	0/1076	0.64	1/1471 (0.1%)
9	1N	0.52	0/1144	0.60	0/1543
9	2N	0.43	0/1144	0.62	0/1543
10	1O	0.54	0/943	0.63	1/1269 (0.1%)
10	2O	0.47	0/943	0.69	1/1269 (0.1%)
11	1P	0.51	0/1156	0.68	0/1537
11	2P	0.45	0/1152	0.67	1/1533 (0.1%)
12	1Q	0.56	0/1143	0.66	0/1527
12	2Q	0.45	0/1143	0.64	0/1527
13	1R	0.54	0/982	0.67	0/1312
13	2R	0.41	0/982	0.66	0/1312
14	1S	0.43	0/887	0.63	0/1180
14	2S	0.51	0/880	0.71	1/1172 (0.1%)
15	1T	0.49	0/1105	0.67	1/1477 (0.1%)
15	2T	0.42	0/1097	0.61	0/1468
16	1U	0.60	0/977	0.66	1/1301 (0.1%)
16	2U	0.49	0/977	0.67	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1V	0.54	0/782	0.62	0/1049
17	2V	0.48	0/782	0.59	0/1049
18	1W	0.59	0/897	0.67	0/1205
18	2W	0.50	0/897	0.66	0/1205
19	1X	0.53	0/764	0.62	0/1025
19	2X	0.49	0/764	0.63	1/1025 (0.1%)
20	1Y	0.55	0/819	0.67	0/1095
20	2Y	0.46	0/819	0.65	0/1095
21	1Z	0.41	0/1502	0.59	0/2041
21	2Z	0.45	0/1486	0.61	0/2022
22	10	0.53	0/606	0.71	1/808 (0.1%)
22	20	0.38	0/606	0.61	0/808
23	11	0.52	0/762	0.68	2/1014 (0.2%)
23	21	0.46	0/762	0.59	0/1014
24	12	0.47	0/590	0.58	0/781
24	22	0.47	0/590	0.58	0/781
25	13	0.54	0/474	0.63	0/635
25	23	0.42	0/469	0.59	0/630
26	14	0.45	0/571	0.70	0/768
26	24	0.51	0/545	0.76	0/737
27	15	0.57	0/469	0.71	0/635
27	25	0.48	0/469	0.61	0/635
28	16	0.53	0/460	0.61	0/613
28	26	0.48	0/456	0.61	0/608
29	17	0.59	0/426	0.68	0/561
29	27	0.49	0/426	0.68	0/561
30	18	0.56	0/525	0.67	0/691
30	28	0.47	0/525	0.62	0/691
31	19	0.60	0/310	0.65	0/407
31	29	0.46	0/310	0.66	0/407
32	1a	0.56	1/35537 (0.0%)	1.05	68/55456 (0.1%)
32	2a	0.52	0/35680	1.02	51/55681 (0.1%)
33	1b	0.40	0/1820	0.63	0/2468
33	2b	2.74	8/1728 (0.5%)	0.77	4/2352 (0.2%)
34	1c	0.38	0/1504	0.56	0/2047
34	2c	0.42	0/1435	0.62	0/1960
35	1d	0.40	0/1648	0.60	0/2222
35	2d	0.38	0/1659	0.59	0/2230
36	1e	0.39	0/1145	0.62	0/1543
36	2e	0.38	0/1111	0.65	0/1504
37	1f	0.38	0/819	0.60	0/1111
37	2f	0.39	0/830	0.55	0/1125
38	1g	0.36	0/1198	0.56	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	2g	0.40	0/1185	0.55	0/1602
39	1h	0.35	0/1108	0.59	0/1494
39	2h	0.35	0/1094	0.57	0/1478
40	1i	0.37	0/995	0.64	0/1339
40	2i	0.43	0/949	0.64	1/1284 (0.1%)
41	1j	0.40	0/695	0.67	1/950 (0.1%)
41	2j	0.42	0/690	0.64	0/943
42	1k	0.38	0/840	0.60	0/1138
42	2k	0.38	0/844	0.57	0/1145
43	1l	0.43	0/936	0.67	1/1263 (0.1%)
43	2l	0.41	0/934	0.66	1/1262 (0.1%)
44	1m	0.37	0/933	0.63	0/1254
44	2m	0.42	0/913	0.58	0/1230
45	1n	0.43	0/491	0.66	0/653
45	2n	0.43	0/467	0.55	0/624
46	1o	0.38	0/726	0.59	0/970
46	2o	0.38	0/739	0.57	0/985
47	1p	0.36	0/686	0.61	0/926
47	2p	0.38	0/693	0.61	0/935
48	1q	0.39	0/824	0.60	1/1105 (0.1%)
48	2q	0.38	0/836	0.55	0/1117
49	1r	0.39	0/560	0.63	1/746 (0.1%)
49	2r	0.38	0/560	0.59	0/746
50	1s	0.36	0/657	0.62	0/890
50	2s	0.40	0/661	0.63	1/893 (0.1%)
51	1t	0.38	0/714	0.66	0/948
51	2t	0.35	0/733	0.58	0/969
52	1u	0.32	0/191	0.57	0/252
52	2u	0.44	0/203	0.58	0/266
53	1v	0.70	0/122	1.30	0/188
53	2v	0.87	0/122	1.35	1/188 (0.5%)
54	1x	0.76	5/1725 (0.3%)	1.40	28/2689 (1.0%)
54	2x	0.65	1/1725 (0.1%)	1.34	24/2689 (0.9%)
55	1z	0.79	0/106	1.00	1/146 (0.7%)
55	2z	0.55	0/106	0.96	0/146
All	All	0.67	33/306280 (0.0%)	1.02	659/458192 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1
19	1X	0	1
19	2X	0	1
20	1Y	0	1
34	2c	0	1
All	All	0	5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	60.02	2.29	1.39
33	2b	92	TYR	CD2-CE2	52.66	2.18	1.39
33	2b	92	TYR	CE1-CZ	41.90	1.93	1.38
33	2b	92	TYR	CE2-CZ	41.41	1.92	1.38
33	2b	92	TYR	CG-CD1	33.83	1.83	1.39
33	2b	92	TYR	CG-CD2	32.20	1.81	1.39
33	2b	151	GLY	N-CA	22.69	1.80	1.46
1	1A	1066	A	N9-C4	-10.43	1.31	1.37
33	2b	150	SER	C-N	10.37	1.51	1.33
1	1A	552	A	N9-C4	-10.20	1.31	1.37
1	1A	1187	A	N9-C4	-9.50	1.32	1.37
1	1A	2298	A	N9-C4	-9.47	1.32	1.37
1	2A	552	A	N9-C4	-9.37	1.32	1.37
1	1A	353	A	N9-C4	-8.97	1.32	1.37
1	1A	989	A	N9-C4	-8.44	1.32	1.37
54	1x	22	G	N7-C5	7.80	1.44	1.39
1	1A	1934	A	N9-C4	7.00	1.42	1.37
32	1a	155	A	N9-C4	7.00	1.42	1.37
54	1x	22	G	C8-N7	6.53	1.34	1.30
54	1x	14	A	N7-C5	-6.52	1.35	1.39
1	1A	989	A	C5-C6	-6.26	1.35	1.41
1	2A	2298	A	N9-C4	-5.98	1.34	1.37
54	1x	46	G	C6-N1	5.86	1.43	1.39
54	1x	14	A	C8-N7	-5.86	1.27	1.31
1	1A	1806	G	C8-N7	-5.74	1.27	1.30
1	1A	977	A	N9-C4	-5.66	1.34	1.37
1	2A	1066	A	N9-C4	-5.64	1.34	1.37
1	2A	1187	A	N9-C4	-5.50	1.34	1.37
1	1A	551	C	N3-C4	-5.29	1.30	1.33
1	1A	1604	A	N9-C4	-5.26	1.34	1.37
1	1A	553	A	N9-C4	-5.19	1.34	1.37
1	1A	2618	G	N7-C5	-5.07	1.36	1.39
54	2x	22	G	C8-N7	5.05	1.33	1.30



All (659) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	C-N-CA	16.37	156.68	122.30
1	1A	552	A	C2-N3-C4	-16.26	102.47	110.60
1	1A	1066	A	C2-N3-C4	-14.19	103.50	110.60
54	1x	46	G	C6-N1-C2	-14.02	116.69	125.10
1	1A	353	A	C2-N3-C4	-13.24	103.98	110.60
1	1A	552	A	N3-C4-C5	12.94	135.85	126.80
1	1A	552	A	N3-C4-N9	-12.85	117.12	127.40
1	1A	989	A	C5-N7-C8	-12.77	97.52	103.90
1	2A	552	A	C2-N3-C4	-12.38	104.41	110.60
1	1A	1187	A	C2-N3-C4	-12.21	104.50	110.60
1	1A	2298	A	C2-N3-C4	-11.71	104.74	110.60
54	2x	46	G	C6-N1-C2	-11.64	118.12	125.10
1	1A	2083	A	C2-N3-C4	-11.57	104.81	110.60
54	1x	22	G	C5-N7-C8	-11.53	98.53	104.30
54	1x	14	A	C5-N7-C8	11.48	109.64	103.90
1	2A	2565	U	O5'-P-OP1	-10.84	95.95	105.70
54	2x	22	G	C5-N7-C8	-10.76	98.92	104.30
1	1A	989	A	C2-N3-C4	-10.55	105.32	110.60
54	1x	14	A	C4-C5-C6	10.47	122.23	117.00
1	1A	138	A	N7-C8-N9	10.44	119.02	113.80
1	1A	138	A	C5-N7-C8	-10.13	98.83	103.90
1	1A	989	A	C4-C5-N7	9.87	115.63	110.70
1	2A	552	A	N3-C4-C5	9.81	133.67	126.80
54	1x	46	G	C5-C6-N1	9.70	116.35	111.50
1	1A	990	G	O5'-P-OP1	-9.68	96.99	105.70
1	1A	1187	A	N3-C4-C5	9.53	133.47	126.80
1	1A	536	G	O4'-C1'-N9	9.47	115.78	108.20
32	1a	341	C	N1-C2-O2	9.38	124.53	118.90
1	1A	542	G	O5'-P-OP2	-9.29	97.33	105.70
2	2B	115	G	C8-N9-C4	9.01	110.00	106.40
33	2b	151	GLY	N-CA-C	8.99	135.57	113.10
1	1A	977	A	C5-N7-C8	-8.92	99.44	103.90
1	1A	138	A	C8-N9-C4	-8.80	102.28	105.80
32	2a	1380	C	N1-C2-O2	8.78	124.17	118.90
1	2A	1248	A	C2-N3-C4	-8.77	106.21	110.60
1	1A	1066	A	N3-C4-C5	8.75	132.92	126.80
1	1A	214	G	O4'-C1'-N9	8.71	115.17	108.20
1	1A	989	A	N1-C6-N6	8.71	123.82	118.60
54	1x	22	G	C4-C5-C6	-8.65	113.61	118.80
1	1A	1044	U	O5'-P-OP2	-8.62	97.94	105.70
1	1A	1066	A	C5-N7-C8	-8.53	99.64	103.90
1	2A	1281	G	O5'-P-OP1	-8.46	98.08	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	825	U	C5-C6-N1	8.46	126.93	122.70
54	2x	22	G	N7-C8-N9	8.40	117.30	113.10
1	1A	597	A	O5'-P-OP1	-8.37	98.17	105.70
1	2A	1187	A	C2-N3-C4	-8.37	106.42	110.60
1	1A	1744	A	C2-N3-C4	-8.34	106.43	110.60
1	2A	1066	A	C2-N3-C4	-8.33	106.43	110.60
32	1a	1120	C	C6-N1-C2	-8.32	116.97	120.30
1	1A	2298	A	N3-C4-C5	8.32	132.62	126.80
32	1a	341	C	C6-N1-C2	-8.29	116.98	120.30
1	2A	1659	A	O5'-P-OP1	-8.22	98.30	105.70
32	1a	361	U	C5-C6-N1	-8.19	118.61	122.70
1	2A	787	G	O5'-P-OP1	-8.17	98.35	105.70
54	1x	22	G	N7-C8-N9	8.15	117.18	113.10
32	1a	341	C	C2-N1-C1'	8.11	127.72	118.80
1	2A	475	G	N1-C6-O6	-8.09	115.05	119.90
1	1A	2091	G	O5'-P-OP2	-8.08	98.43	105.70
54	2x	46	G	N3-C2-N2	-8.06	114.26	119.90
1	1A	1066	A	N3-C4-N9	-8.05	120.96	127.40
1	1A	552	A	C5-C6-N1	-7.90	113.75	117.70
32	1a	150	C	N1-C2-O2	7.89	123.64	118.90
1	1A	989	A	N7-C8-N9	7.88	117.74	113.80
1	1A	1397	U	O5'-P-OP1	-7.88	98.61	105.70
1	1A	2013	G	P-O3'-C3'	7.88	129.16	119.70
1	1A	1187	A	N3-C4-N9	-7.88	121.10	127.40
1	2A	2587	G	O5'-P-OP1	-7.87	98.62	105.70
54	2x	46	G	C5-C6-N1	7.87	115.43	111.50
1	1A	495	A	O5'-P-OP1	-7.84	98.64	105.70
1	1A	985	A	O5'-P-OP1	-7.83	98.66	105.70
1	1A	11	U	C2-N1-C1'	7.82	127.09	117.70
1	2A	1109	C	C2-N1-C1'	7.78	127.36	118.80
1	1A	353	A	N1-C2-N3	7.78	133.19	129.30
1	1A	398	G	O4'-C1'-N9	7.77	114.41	108.20
1	2A	552	A	N3-C4-N9	-7.73	121.22	127.40
54	1x	46	G	C5-C6-O6	-7.71	123.98	128.60
1	2A	989	A	N1-C6-N6	7.70	123.22	118.60
1	1A	1694	C	O5'-P-OP1	-7.70	98.77	105.70
1	1A	808	U	C5-C4-O4	-7.68	121.29	125.90
54	2x	14	A	C5-N7-C8	7.67	107.74	103.90
32	2a	514	G	C4-N9-C1'	7.65	136.44	126.50
1	1A	592	G	C5-C6-O6	-7.61	124.03	128.60
1	1A	1806	G	O5'-P-OP2	-7.59	98.87	105.70
32	1a	341	C	N3-C2-O2	-7.58	116.59	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	353	A	N3-C4-C5	7.58	132.11	126.80
32	2a	1380	C	C2-N1-C1'	7.58	127.14	118.80
1	1A	253	A	C5-N7-C8	-7.57	100.12	103.90
32	2a	1207	A	C5-C6-N6	7.57	129.75	123.70
1	1A	989	A	N3-C4-C5	7.56	132.09	126.80
1	1A	2565	U	O5'-P-OP1	-7.56	98.89	105.70
1	2A	1248	A	O4'-C1'-N9	7.55	114.24	108.20
1	2A	1744	A	C2-N3-C4	-7.53	106.83	110.60
1	1A	833	U	O5'-P-OP1	-7.51	98.94	105.70
32	1a	1480	A	C2-N3-C4	-7.50	106.85	110.60
1	1A	1066	A	C5-C6-N1	-7.49	113.96	117.70
32	2a	361	U	C5-C6-N1	-7.48	118.96	122.70
1	2A	536	G	O4'-C1'-N9	7.45	114.16	108.20
1	1A	2514	A	N1-C2-N3	-7.45	125.57	129.30
32	1a	1495	G	O5'-P-OP2	-7.44	99.01	105.70
54	1x	22	G	N3-C4-N9	-7.43	121.54	126.00
32	1a	1480	A	N1-C2-N3	7.42	133.01	129.30
32	1a	361	U	C2-N1-C1'	-7.39	108.83	117.70
54	2x	76	A	N1-C6-N6	7.38	123.03	118.60
1	1A	353	A	C5-N7-C8	-7.36	100.22	103.90
32	2a	933	U	C2-N3-C4	7.36	131.41	127.00
1	1A	253	A	N7-C8-N9	7.32	117.46	113.80
1	1A	977	A	N7-C8-N9	7.30	117.45	113.80
1	1A	2297	A	N7-C8-N9	7.30	117.45	113.80
1	2A	192	A	O5'-P-OP2	-7.28	99.15	105.70
1	2A	2442	U	O5'-P-OP2	-7.28	99.15	105.70
1	1A	551	C	C5-C4-N4	7.25	125.27	120.20
1	1A	2857	G	O4'-C1'-N9	7.25	114.00	108.20
1	2A	2484	U	C2-N1-C1'	7.22	126.36	117.70
1	2A	1109	C	C6-N1-C2	-7.19	117.42	120.30
1	1A	2801	C	C2-N1-C1'	-7.18	110.90	118.80
32	2a	1380	C	N3-C2-O2	-7.17	116.88	121.90
1	1A	30	C	O5'-P-OP1	-7.17	99.25	105.70
1	1A	2640	A	O4'-C1'-N9	7.16	113.93	108.20
1	1A	2083	A	O4'-C1'-N9	7.15	113.92	108.20
1	2A	138	A	N7-C8-N9	7.15	117.38	113.80
54	1x	22	G	C8-N9-C1'	7.15	136.30	127.00
1	2A	989	A	C2-N3-C4	-7.15	107.03	110.60
1	2A	1676	C	N1-C2-O2	-7.11	114.64	118.90
1	2A	138	A	C8-N9-C4	-7.10	102.96	105.80
1	1A	418	C	O5'-P-OP1	-7.07	99.34	105.70
1	2A	2226	G	C4-N9-C1'	-7.07	117.31	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	598	U	O5'-P-OP1	-7.05	99.35	105.70
32	1a	1107	G	N3-C4-C5	-7.05	125.07	128.60
1	1A	1153	U	C5-C6-N1	7.04	126.22	122.70
54	2x	14	A	C4-C5-C6	7.02	120.51	117.00
1	2A	989	A	O4'-C1'-N9	7.01	113.81	108.20
1	2A	2298	A	C2-N3-C4	-7.01	107.10	110.60
32	1a	341	C	C5-C6-N1	6.98	124.49	121.00
1	2A	2510	C	N1-C2-O2	-6.93	114.74	118.90
1	1A	1196	G	O5'-P-OP2	-6.93	99.47	105.70
1	1A	1404	A	C2-N3-C4	6.92	114.06	110.60
1	2A	2484	U	N1-C2-O2	6.91	127.64	122.80
1	1A	552	A	C8-N9-C1'	6.87	140.06	127.70
1	2A	1744	A	C5-N7-C8	-6.87	100.47	103.90
1	1A	1153	U	C2-N1-C1'	6.86	125.93	117.70
32	1a	87	C	N1-C2-O2	6.86	123.01	118.90
1	1A	2726	G	O5'-P-OP2	-6.84	99.54	105.70
1	1A	2298	A	N3-C4-N9	-6.83	121.93	127.40
1	2A	193	G	O5'-P-OP2	-6.83	99.55	105.70
32	1a	1120	C	C5-C6-N1	6.83	124.42	121.00
1	1A	1067	G	N3-C2-N2	-6.82	115.13	119.90
1	1A	1659	A	O5'-P-OP1	-6.81	99.57	105.70
1	1A	2439	G	N1-C6-O6	-6.80	115.82	119.90
1	1A	1248	A	O4'-C1'-N9	6.79	113.64	108.20
32	1a	738	C	N1-C2-O2	6.78	122.97	118.90
33	2b	187	LEU	CA-CB-CG	6.77	130.87	115.30
19	2X	57	LEU	CA-CB-CG	6.77	130.86	115.30
14	2S	58	LEU	CA-CB-CG	6.75	130.84	115.30
1	1A	1604	A	C2-N3-C4	-6.75	107.23	110.60
1	1A	2330	G	C6-C5-N7	-6.75	126.35	130.40
1	1A	2724	A	C8-N9-C4	6.74	108.50	105.80
32	2a	1133	U	C5-C4-O4	6.74	129.94	125.90
32	1a	1480	A	O5'-P-OP2	-6.73	99.64	105.70
1	1A	552	A	C4-N9-C1'	-6.73	114.19	126.30
1	1A	2441	A	O5'-P-OP2	-6.71	99.66	105.70
1	1A	2330	G	O4'-C1'-N9	6.69	113.55	108.20
1	2A	989	A	C6-C5-N7	-6.67	127.63	132.30
1	1A	138	A	C6-C5-N7	-6.66	127.64	132.30
1	1A	138	A	C4-C5-N7	6.65	114.03	110.70
1	1A	409	U	C2-N1-C1'	-6.65	109.72	117.70
23	11	21	ARG	NE-CZ-NH1	6.65	123.62	120.30
32	2a	1480	A	N1-C2-N3	6.65	132.62	129.30
32	1a	825	U	C6-N1-C2	-6.62	117.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	353	A	C2-N3-C4	-6.61	107.29	110.60
1	1A	469	C	O5'-P-OP1	6.61	118.63	110.70
1	1A	1067	G	N3-C4-N9	-6.60	122.04	126.00
54	2x	22	G	C8-N9-C4	-6.58	103.77	106.40
1	2A	2905	U	C2-N1-C1'	6.58	125.59	117.70
1	1A	2249	G	OP1-P-OP2	6.55	129.43	119.60
1	2A	1021	C	N1-C2-O2	6.55	122.83	118.90
33	2b	118	LEU	CA-CB-CG	6.53	130.33	115.30
32	1a	1048	U	P-O3'-C3'	6.52	127.53	119.70
1	1A	2297	A	C2-N3-C4	-6.52	107.34	110.60
54	1x	14	A	C4-C5-N7	-6.52	107.44	110.70
54	2x	22	G	C4-C5-N7	6.51	113.40	110.80
1	1A	2297	A	N1-C2-N3	6.50	132.55	129.30
1	2A	2484	U	N3-C2-O2	-6.49	117.66	122.20
32	2a	211	U	C2-N1-C1'	6.48	125.47	117.70
1	2A	1377	G	O5'-P-OP2	-6.48	99.87	105.70
1	2A	2204	C	N1-C2-O2	6.46	122.78	118.90
1	1A	2297	A	C5-N7-C8	-6.46	100.67	103.90
1	1A	1957	A	O4'-C1'-N9	6.46	113.37	108.20
54	1x	14	A	C8-N9-C1'	-6.45	116.09	127.70
1	2A	2458	G	N3-C4-C5	6.43	131.82	128.60
1	1A	893	U	C2-N1-C1'	-6.43	109.98	117.70
32	1a	188	C	N1-C2-O2	-6.41	115.05	118.90
1	1A	2083	A	N1-C2-N3	6.41	132.50	129.30
1	1A	891	G	O4'-C1'-N9	6.40	113.32	108.20
1	2A	409	U	O4'-C1'-N1	6.39	113.31	108.20
32	2a	66	U	P-O3'-C3'	6.39	127.37	119.70
1	2A	1744	A	C6-C5-N7	-6.38	127.84	132.30
1	1A	138	A	O4'-C1'-N9	6.37	113.30	108.20
1	2A	1248	A	C5-N7-C8	-6.37	100.71	103.90
32	2a	826	C	C5-C6-N1	6.37	124.19	121.00
32	1a	493	A	C8-N9-C4	-6.37	103.25	105.80
2	2B	2	C	N1-C2-O2	6.37	122.72	118.90
32	1a	1480	A	C6-C5-N7	-6.36	127.85	132.30
1	1A	830	A	O4'-C1'-N9	6.36	113.28	108.20
54	1x	14	A	C5-C6-N1	-6.36	114.52	117.70
1	1A	551	C	N3-C2-O2	-6.35	117.45	121.90
1	1A	1538	C	C2-N1-C1'	6.35	125.78	118.80
1	1A	1482	C	C6-N1-C2	-6.34	117.76	120.30
1	2A	852	C	N1-C2-O2	-6.33	115.10	118.90
2	2B	115	G	N7-C8-N9	-6.33	109.94	113.10
1	1A	552	A	C6-N1-C2	6.31	122.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	22	G	N1-C6-O6	-6.31	116.11	119.90
54	1x	14	A	C4-N9-C1'	6.30	137.63	126.30
1	1A	2297	A	C8-N9-C4	-6.29	103.28	105.80
1	1A	125	C	N1-C2-O2	-6.29	115.13	118.90
2	2B	37	C	C6-N1-C2	-6.29	117.78	120.30
1	2A	1506	A	O4'-C1'-N9	6.28	113.22	108.20
1	2A	1744	A	N1-C6-N6	6.27	122.36	118.60
1	1A	893	U	C5-C6-N1	-6.27	119.56	122.70
1	1A	592	G	C4-C5-N7	6.27	113.31	110.80
32	1a	262	G	P-O3'-C3'	6.25	127.21	119.70
1	2A	1109	C	N1-C2-O2	6.25	122.65	118.90
32	2a	514	G	C8-N9-C1'	-6.25	118.88	127.00
1	1A	977	A	C4-C5-N7	6.24	113.82	110.70
1	2A	1676	C	N3-C2-O2	6.23	126.26	121.90
1	2A	1076	G	N1-C6-O6	6.22	123.63	119.90
1	1A	138	A	N1-C6-N6	6.22	122.33	118.60
1	2A	902	C	C6-N1-C2	-6.21	117.82	120.30
54	2x	46	G	N9-C4-C5	6.21	107.88	105.40
1	1A	353	A	N3-C4-N9	-6.20	122.44	127.40
1	1A	1097	C	C6-N1-C2	-6.20	117.82	120.30
32	1a	603	U	C2-N1-C1'	6.20	125.14	117.70
54	1x	70	G	N9-C4-C5	6.20	107.88	105.40
1	1A	2701	C	O5'-P-OP1	-6.19	100.13	105.70
1	2A	2458	G	C4-N9-C1'	-6.19	118.45	126.50
1	2A	989	A	C5-N7-C8	-6.19	100.81	103.90
1	2A	1806	G	O5'-P-OP2	-6.18	100.13	105.70
32	2a	1380	C	C6-N1-C2	-6.18	117.83	120.30
32	1a	825	U	C2-N1-C1'	6.18	125.12	117.70
1	1A	1066	A	N1-C2-N3	6.18	132.39	129.30
32	1a	150	C	C2-N1-C1'	6.18	125.60	118.80
54	1x	46	G	N3-C2-N2	-6.18	115.58	119.90
1	2A	2700	U	P-O3'-C3'	6.16	127.09	119.70
1	2A	253	A	N1-C6-N6	6.16	122.29	118.60
1	2A	1744	A	C4-C5-N7	6.14	113.77	110.70
1	2A	792	A	O4'-C1'-N9	6.12	113.10	108.20
1	1A	2013	G	C2'-C3'-O3'	6.12	123.50	113.70
10	1O	8	LEU	CA-CB-CG	6.09	129.32	115.30
1	1A	905	G	N3-C4-C5	6.09	131.65	128.60
1	1A	183	A	P-O3'-C3'	6.08	127.00	119.70
49	1r	31	LEU	CA-CB-CG	6.08	129.29	115.30
1	2A	534	C	O5'-P-OP2	-6.08	100.23	105.70
1	2A	1958	A	O4'-C1'-N9	6.07	113.06	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	551	C	N3-C4-N4	-6.07	113.75	118.00
2	2B	2	C	C2-N1-C1'	6.06	125.47	118.80
1	1A	1066	A	N7-C8-N9	6.06	116.83	113.80
54	1x	22	G	C5-C6-N1	6.06	114.53	111.50
1	2A	977	A	C5-N7-C8	-6.05	100.88	103.90
1	2A	2455	G	C4-C5-N7	-6.04	108.38	110.80
8	2I	116	LEU	CA-CB-CG	6.04	129.20	115.30
1	1A	2640	A	N1-C2-N3	6.02	132.31	129.30
1	1A	989	A	N3-C4-N9	-6.02	122.59	127.40
1	1A	1430	G	O4'-C1'-N9	6.01	113.01	108.20
1	2A	2226	G	C8-N9-C1'	6.01	134.81	127.00
32	2a	825	U	C5-C6-N1	6.01	125.70	122.70
1	1A	1187	A	O5'-P-OP1	-6.01	100.29	105.70
1	1A	1859	A	O5'-P-OP2	-6.00	100.30	105.70
16	2U	74	LEU	CA-CB-CG	6.00	129.10	115.30
1	1A	2083	A	N3-C4-C5	5.98	130.99	126.80
1	2A	2640	A	O4'-C1'-N9	5.98	112.98	108.20
32	1a	1480	A	C5-N7-C8	-5.97	100.91	103.90
1	1A	2801	C	O4'-C1'-N1	5.97	112.98	108.20
54	2x	76	A	C5-N7-C8	-5.96	100.92	103.90
32	1a	978	U	C5-C4-O4	5.95	129.47	125.90
1	2A	960	C	N1-C2-O2	5.95	122.47	118.90
1	2A	989	A	C4-C5-N7	5.95	113.67	110.70
1	1A	2449	U	OP2-P-O3'	5.95	118.28	105.20
2	2B	37	C	C5-C6-N1	5.94	123.97	121.00
32	2a	1207	A	N1-C6-N6	-5.94	115.04	118.60
32	2a	493	A	C8-N9-C4	-5.94	103.42	105.80
1	2A	470	C	N1-C2-O2	-5.93	115.34	118.90
1	1A	792	A	O4'-C1'-N9	5.93	112.94	108.20
54	1x	70	G	N3-C4-N9	-5.92	122.45	126.00
1	2A	2814	C	C6-N1-C2	-5.92	117.93	120.30
1	1A	1281	G	C8-N9-C4	5.91	108.77	106.40
32	1a	1497	A	C8-N9-C4	-5.91	103.44	105.80
1	2A	1109	C	C5-C6-N1	5.89	123.95	121.00
1	2A	2298	A	N3-C4-C5	5.89	130.92	126.80
1	2A	2261	G	OP1-P-OP2	5.89	128.43	119.60
1	2A	596	C	O5'-P-OP1	-5.88	100.41	105.70
1	1A	253	A	N1-C6-N6	5.87	122.12	118.60
1	2A	2095	U	O5'-P-OP1	-5.87	100.42	105.70
43	2I	29	GLY	N-CA-C	-5.87	98.43	113.10
1	1A	35	G	O5'-P-OP2	-5.87	100.42	105.70
1	2A	2226	G	N3-C4-C5	5.87	131.53	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1248	A	N1-C6-N6	5.86	122.11	118.60
32	1a	1106	A	C5-C6-N6	5.85	128.38	123.70
1	2A	1417	U	C5-C4-O4	-5.84	122.39	125.90
1	1A	1744	A	C5-N7-C8	-5.84	100.98	103.90
32	2a	1207	A	C6-N1-C2	5.84	122.10	118.60
32	2a	933	U	C5-C4-O4	5.83	129.40	125.90
32	1a	1133	U	C2-N3-C4	5.83	130.50	127.00
1	1A	552	A	C4-C5-C6	-5.82	114.09	117.00
1	1A	2700	U	N3-C2-O2	-5.82	118.13	122.20
1	2A	253	A	C6-C5-N7	-5.82	128.23	132.30
1	2A	1067	G	C4-C5-N7	-5.81	108.48	110.80
1	1A	778	C	N3-C4-C5	-5.81	119.58	121.90
41	1j	85	LEU	CA-CB-CG	5.81	128.65	115.30
1	1A	1857	C	O5'-P-OP1	-5.80	100.48	105.70
1	2A	2632	A	C2-N3-C4	-5.79	107.70	110.60
1	1A	253	A	C4-C5-N7	5.79	113.59	110.70
1	2A	2260	U	C6-N1-C2	5.78	124.47	121.00
1	1A	580	G	C5-C6-O6	5.78	132.07	128.60
1	2A	2604	U	N3-C4-O4	-5.78	115.36	119.40
1	1A	854	G	O5'-P-OP2	-5.78	100.50	105.70
1	1A	2711	C	C6-N1-C2	5.78	122.61	120.30
1	2A	2905	U	N1-C2-O2	5.77	126.84	122.80
1	1A	586	C	N1-C2-O2	-5.77	115.44	118.90
1	1A	1812	C	OP1-P-O3'	5.76	117.86	105.20
1	1A	2330	G	C4-C5-N7	5.76	113.10	110.80
1	2A	551	C	O4'-C1'-N1	5.75	112.80	108.20
1	2A	590	U	C5-C4-O4	5.75	129.35	125.90
1	2A	2331	A	C2-N3-C4	5.75	113.47	110.60
1	2A	552	A	C5-C6-N1	-5.74	114.83	117.70
1	1A	2374	C	N3-C4-N4	-5.73	113.99	118.00
32	1a	150	C	N3-C2-O2	-5.73	117.89	121.90
1	1A	580	G	N1-C6-O6	-5.73	116.46	119.90
1	2A	2523	C	N1-C2-O2	-5.73	115.46	118.90
1	2A	1974	A	C8-N9-C4	5.72	108.09	105.80
1	1A	1846	G	O5'-P-OP1	-5.72	100.55	105.70
1	1A	352	G	O5'-P-OP2	-5.71	100.56	105.70
1	1A	1017	A	OP1-P-OP2	-5.71	111.04	119.60
54	2x	14	A	C4-C5-N7	-5.71	107.85	110.70
32	2a	1047	G	P-O3'-C3'	5.70	126.54	119.70
1	1A	2298	A	C5-N7-C8	-5.70	101.05	103.90
1	2A	552	A	C5-N7-C8	-5.70	101.05	103.90
10	2O	8	LEU	CA-CB-CG	5.70	128.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1285	U	P-O3'-C3'	5.70	126.54	119.70
32	2a	1363	U	N1-C2-O2	5.70	126.79	122.80
1	2A	1976	U	C5-C6-N1	-5.70	119.85	122.70
1	1A	2330	G	C4-N9-C1'	5.70	133.90	126.50
54	1x	22	G	C8-N9-C4	-5.69	104.12	106.40
1	1A	1066	A	N1-C6-N6	5.68	122.01	118.60
1	2A	300	C	C2-N1-C1'	5.68	125.05	118.80
1	2A	193	G	OP1-P-OP2	5.67	128.10	119.60
32	2a	1106	A	C5-C6-N6	5.67	128.23	123.70
1	1A	2056	G	O4'-C1'-N9	5.66	112.73	108.20
16	1U	74	LEU	CA-CB-CG	5.66	128.32	115.30
1	2A	2598	A	N1-C6-N6	5.66	122.00	118.60
32	1a	155	A	C8-N9-C4	-5.66	103.54	105.80
1	1A	1810	A	N1-C6-N6	-5.65	115.21	118.60
1	2A	2297	A	N1-C6-N6	5.65	121.99	118.60
1	1A	253	A	C6-C5-N7	-5.65	128.35	132.30
1	1A	106	G	C5-C6-O6	5.64	131.99	128.60
1	1A	1743	G	C5-C6-O6	-5.64	125.22	128.60
1	1A	2053	G	N7-C8-N9	-5.64	110.28	113.10
1	1A	106	G	N1-C6-O6	-5.63	116.52	119.90
1	2A	552	A	N1-C6-N6	5.63	121.98	118.60
1	2A	1820	C	P-O3'-C3'	5.63	126.46	119.70
1	1A	1430	G	N3-C4-N9	-5.63	122.62	126.00
1	1A	2124	C	C2-N3-C4	5.62	122.71	119.90
1	2A	1681	G	N1-C6-O6	5.62	123.27	119.90
32	1a	795	C	C6-N1-C2	5.62	122.55	120.30
1	2A	1311	G	C8-N9-C4	5.62	108.65	106.40
1	1A	2444	A	N1-C6-N6	5.62	121.97	118.60
1	2A	830	A	N1-C6-N6	5.61	121.96	118.60
1	1A	1809	U	O4'-C1'-N1	5.60	112.68	108.20
1	2A	2013	G	P-O3'-C3'	5.59	126.41	119.70
32	2a	1132	C	N1-C2-O2	5.59	122.25	118.90
1	1A	1187	A	C5-N7-C8	-5.59	101.11	103.90
1	2A	1076	G	C5-C6-O6	-5.59	125.25	128.60
1	1A	253	A	O4'-C1'-N9	5.58	112.67	108.20
1	1A	989	A	C6-C5-N7	-5.58	128.39	132.30
1	2A	902	C	O5'-P-OP1	-5.58	100.68	105.70
54	2x	76	A	C6-C5-N7	-5.58	128.40	132.30
1	1A	1281	G	N3-C4-C5	5.57	131.39	128.60
1	1A	1990	A	OP1-P-O3'	5.57	117.46	105.20
1	1A	68	G	N1-C6-O6	-5.57	116.56	119.90
1	2A	253	A	O4'-C1'-N9	5.57	112.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1461	G	O4'-C1'-N9	5.57	112.66	108.20
1	2A	1007	U	O5'-P-OP1	-5.57	100.69	105.70
1	2A	2014	U	O5'-P-OP1	-5.57	100.69	105.70
32	2a	1480	A	N7-C8-N9	5.57	116.58	113.80
1	1A	114	G	C8-N9-C4	5.56	108.62	106.40
32	1a	599	C	C6-N1-C2	-5.56	118.08	120.30
1	1A	219	C	C6-N1-C2	-5.55	118.08	120.30
1	1A	838	G	O4'-C1'-N9	-5.55	103.76	108.20
32	2a	738	C	C2-N1-C1'	5.54	124.90	118.80
1	2A	744	C	O5'-P-OP2	-5.54	100.71	105.70
54	2x	22	G	C4-C5-C6	-5.54	115.48	118.80
1	1A	2524	G	N7-C8-N9	5.54	115.87	113.10
54	1x	46	G	N1-C2-N3	5.54	127.22	123.90
1	1A	1187	A	C5-C6-N1	-5.53	114.93	117.70
6	2G	115	ARG	NE-CZ-NH1	5.53	123.07	120.30
50	2s	16	LEU	CA-CB-CG	5.53	128.03	115.30
1	1A	253	A	C8-N9-C4	-5.53	103.59	105.80
1	2A	846	A	O5'-P-OP1	-5.53	100.72	105.70
1	1A	554	G	N3-C4-N9	-5.53	122.68	126.00
1	2A	2076	C	C6-N1-C2	5.53	122.51	120.30
1	2A	2438	C	C6-N1-C2	5.52	122.51	120.30
1	1A	2514	A	N9-C4-C5	-5.52	103.59	105.80
54	1x	22	G	C4-C5-N7	5.52	113.01	110.80
54	2x	76	A	C4-C5-N7	5.52	113.46	110.70
1	2A	1114	A	P-O3'-C3'	5.52	126.32	119.70
2	1B	41	U	C5-C6-N1	-5.51	119.94	122.70
1	2A	1847	G	C5-C6-O6	5.51	131.91	128.60
1	2A	1248	A	C4-C5-N7	5.51	113.46	110.70
32	2a	1361	C	C2-N1-C1'	5.51	124.86	118.80
1	1A	1218	A	P-O3'-C3'	5.51	126.31	119.70
1	2A	1661	A	N1-C6-N6	5.51	121.91	118.60
53	2v	18	G	N3-C4-C5	-5.51	125.84	128.60
32	1a	671	A	P-O3'-C3'	5.50	126.31	119.70
1	1A	785	G	O5'-P-OP2	-5.50	100.75	105.70
1	1A	592	G	C5-C6-N1	5.49	114.25	111.50
1	1A	1002	U	C6-N1-C2	-5.49	117.71	121.00
1	1A	1983	C	C5-C6-N1	5.49	123.74	121.00
1	1A	2083	A	C5-C6-N1	-5.48	114.96	117.70
1	1A	1020	G	O5'-P-OP1	-5.47	100.78	105.70
32	1a	738	C	N3-C2-O2	-5.47	118.07	121.90
1	1A	2330	G	C8-N9-C1'	-5.46	119.90	127.00
1	2A	138	A	C5-N7-C8	-5.46	101.17	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	46	G	C4-C5-N7	-5.46	108.62	110.80
32	1a	767	C	N1-C2-O2	5.46	122.17	118.90
32	1a	169	C	C6-N1-C2	-5.45	118.12	120.30
1	2A	1172	A	O5'-P-OP1	-5.45	100.79	105.70
1	1A	2696	G	N1-C6-O6	-5.45	116.63	119.90
54	2x	65	C	C2-N1-C1'	5.45	124.79	118.80
1	1A	1984	U	C2-N1-C1'	5.45	124.23	117.70
1	2A	2577	A	O5'-P-OP2	-5.45	100.80	105.70
32	1a	197	U	C5-C6-N1	5.44	125.42	122.70
23	1l	21	ARG	NE-CZ-NH2	-5.44	117.58	120.30
32	2a	1480	A	C5-N7-C8	-5.44	101.18	103.90
1	1A	839	A	O5'-P-OP2	-5.43	100.81	105.70
1	1A	750	G	O4'-C1'-N9	5.43	112.54	108.20
1	1A	798	A	C8-N9-C4	5.43	107.97	105.80
1	1A	2080	A	O4'-C1'-N9	5.42	112.54	108.20
2	1B	91	C	C6-N1-C2	5.42	122.47	120.30
32	1a	1480	A	N1-C6-N6	5.42	121.85	118.60
32	2a	1474	C	O5'-P-OP2	-5.41	100.83	105.70
32	1a	738	C	C2-N1-C1'	5.41	124.75	118.80
1	2A	960	C	N3-C2-O2	-5.40	118.12	121.90
54	1x	22	G	N3-C4-C5	5.40	131.30	128.60
54	2x	6	G	C4-C5-N7	5.40	112.96	110.80
1	1A	1744	A	O4'-C1'-N9	5.39	112.52	108.20
1	2A	636	U	N3-C2-O2	-5.39	118.43	122.20
1	2A	253	A	C5-N7-C8	-5.39	101.21	103.90
1	1A	1744	A	N1-C2-N3	5.38	131.99	129.30
1	1A	2514	A	C8-N9-C4	5.38	107.95	105.80
32	1a	1380	C	N1-C2-O2	5.38	122.13	118.90
32	1a	1433	C	C6-N1-C2	-5.38	118.15	120.30
1	2A	1744	A	N7-C8-N9	5.38	116.49	113.80
32	1a	1480	A	N7-C8-N9	5.37	116.49	113.80
11	2P	44	GLY	C-N-CA	5.37	135.13	121.70
1	2A	253	A	N7-C8-N9	5.37	116.49	113.80
1	2A	481	C	C6-N1-C2	5.37	122.45	120.30
1	1A	830	A	C5-N7-C8	5.37	106.58	103.90
1	2A	2250	G	C5-C6-O6	5.37	131.82	128.60
32	1a	767	C	N3-C2-O2	-5.36	118.15	121.90
1	1A	731	A	C8-N9-C4	-5.36	103.66	105.80
1	2A	1690	C	N1-C2-O2	5.35	122.11	118.90
32	2a	1407	C	C6-N1-C2	-5.35	118.16	120.30
1	1A	2040	A	N1-C6-N6	-5.35	115.39	118.60
1	1A	1744	A	C6-C5-N7	-5.35	128.56	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	46	G	N3-C4-C5	-5.35	125.93	128.60
54	1x	22	G	C4-N9-C1'	-5.34	119.56	126.50
1	1A	554	G	N3-C4-C5	5.33	131.27	128.60
1	1A	1076	G	N1-C6-O6	-5.33	116.70	119.90
1	2A	875	A	OP1-P-OP2	5.33	127.60	119.60
1	2A	2735	C	N1-C2-O2	-5.33	115.70	118.90
32	1a	361	U	C6-N1-C1'	5.33	128.66	121.20
1	1A	2013	G	O4'-C1'-N9	-5.33	103.94	108.20
1	2A	2259	C	O5'-P-OP2	-5.33	100.91	105.70
1	2A	977	A	N7-C8-N9	5.32	116.46	113.80
1	2A	931	C	C6-N1-C2	-5.32	118.17	120.30
1	1A	2298	A	C5-C6-N1	-5.32	115.04	117.70
32	1a	162	G	N3-C4-N9	5.32	129.19	126.00
32	2a	732	C	P-O3'-C3'	5.32	126.08	119.70
2	2B	37	C	C2-N1-C1'	5.32	124.65	118.80
32	1a	1037	C	C2-N1-C1'	5.31	124.64	118.80
1	1A	614	G	O5'-P-OP2	-5.31	100.92	105.70
1	1A	2319	G	C5-N7-C8	-5.31	101.64	104.30
32	2a	1106	A	N1-C6-N6	-5.31	115.41	118.60
32	1a	722	C	C6-N1-C2	-5.31	118.18	120.30
1	2A	2635	G	N7-C8-N9	-5.31	110.45	113.10
32	2a	891	A	P-O3'-C3'	5.31	126.07	119.70
1	1A	977	A	O4'-C1'-N9	5.30	112.44	108.20
1	1A	2283	U	O5'-P-OP2	-5.30	100.93	105.70
1	1A	2514	A	C2-N3-C4	5.30	113.25	110.60
55	1z	10	PRO	CA-N-CD	-5.30	104.08	111.50
1	2A	857	U	C2-N1-C1'	-5.30	111.33	117.70
32	2a	892	A	O5'-P-OP1	-5.30	100.93	105.70
1	2A	202	G	O4'-C1'-N9	5.30	112.44	108.20
1	2A	1359	C	C2-N1-C1'	5.30	124.63	118.80
32	2a	78	G	C5-C6-O6	5.30	131.78	128.60
1	2A	330	G	O5'-P-OP2	-5.30	100.93	105.70
32	2a	1048	U	P-O3'-C3'	5.30	126.06	119.70
1	2A	272	G	C4-N9-C1'	5.30	133.39	126.50
1	2A	1187	A	N1-C2-N3	5.29	131.95	129.30
32	2a	853	C	N3-C2-O2	-5.29	118.20	121.90
1	2A	475	G	C5-C6-O6	5.29	131.77	128.60
32	1a	1048	U	OP2-P-O3'	5.28	116.81	105.20
32	2a	671	A	P-O3'-C3'	5.28	126.03	119.70
1	1A	2875	U	C5-C6-N1	-5.28	120.06	122.70
1	2A	977	A	C4-C5-N7	5.28	113.34	110.70
1	2A	977	A	O4'-C1'-N9	5.28	112.42	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	725	C	C5-C6-N1	-5.27	118.36	121.00
1	1A	2700	U	P-O3'-C3'	5.27	126.03	119.70
40	2i	50	LEU	CA-CB-CG	5.27	127.43	115.30
1	1A	2801	C	C6-N1-C1'	5.27	127.12	120.80
1	2A	2583	A	C8-N9-C4	5.27	107.91	105.80
1	2A	2013	G	N3-C4-C5	-5.26	125.97	128.60
1	1A	2735	C	N3-C2-O2	-5.26	118.22	121.90
1	1A	1211	C	C5-C4-N4	-5.26	116.52	120.20
1	1A	1983	C	C4-C5-C6	-5.26	114.77	117.40
1	2A	1614	G	C4-N9-C1'	-5.25	119.67	126.50
1	1A	193	G	C8-N9-C4	5.25	108.50	106.40
1	1A	2209	C	C5-C6-N1	5.25	123.62	121.00
1	2A	630	A	C8-N9-C4	-5.25	103.70	105.80
48	1q	98	LEU	CA-CB-CG	5.24	127.36	115.30
1	1A	1693	G	O5'-P-OP1	-5.24	100.98	105.70
32	1a	1179	G	N3-C4-N9	5.24	129.15	126.00
1	1A	1862	C	C6-N1-C2	-5.24	118.20	120.30
1	2A	284	U	O4'-C1'-N1	5.24	112.39	108.20
1	1A	409	U	C5-C6-N1	-5.24	120.08	122.70
1	2A	1138	G	C4-N9-C1'	5.24	133.31	126.50
1	1A	1154	C	C6-N1-C2	-5.24	118.21	120.30
54	2x	76	A	C2-N3-C4	-5.24	107.98	110.60
32	1a	1039	U	C2-N3-C4	5.23	130.14	127.00
1	2A	1066	A	N3-C4-C5	5.23	130.46	126.80
1	2A	1066	A	C5-N7-C8	-5.23	101.28	103.90
1	2A	1708	C	C2-N3-C4	-5.23	117.29	119.90
32	2a	905	G	C5-C6-O6	5.23	131.74	128.60
1	1A	889	G	N1-C6-O6	-5.22	116.77	119.90
1	1A	2457	G	C8-N9-C4	-5.22	104.31	106.40
32	1a	262	G	O4'-C1'-N9	-5.22	104.02	108.20
54	2x	22	G	C8-N9-C1'	5.22	133.78	127.00
1	1A	1248	A	C5-N7-C8	-5.21	101.29	103.90
1	1A	409	U	O4'-C1'-N1	5.21	112.37	108.20
32	2a	1141	C	C6-N1-C2	-5.21	118.22	120.30
1	1A	2053	G	C5-N7-C8	5.21	106.91	104.30
1	1A	11	U	C6-N1-C2	-5.21	117.88	121.00
1	1A	830	A	N1-C6-N6	-5.21	115.48	118.60
1	1A	794	G	C8-N9-C1'	5.20	133.76	127.00
1	1A	1508	C	C6-N1-C2	-5.20	118.22	120.30
32	1a	1317	C	C6-N1-C2	5.20	122.38	120.30
1	1A	106	G	C6-C5-N7	5.20	133.52	130.40
1	1A	1234	G	C5-N7-C8	5.20	106.90	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1686	C	N1-C2-O2	5.20	122.02	118.90
1	2A	2286	C	OP1-P-O3'	5.19	116.62	105.20
43	1l	52	LEU	CA-CB-CG	5.19	127.24	115.30
32	2a	1382	C	N1-C2-O2	-5.19	115.79	118.90
1	2A	1190	C	C6-N1-C2	-5.18	118.23	120.30
54	1x	46	G	N9-C4-C5	5.18	107.47	105.40
1	1A	990	G	C5-C6-O6	5.18	131.71	128.60
32	1a	162	G	N9-C4-C5	-5.18	103.33	105.40
1	2A	1960	U	N3-C4-O4	-5.17	115.78	119.40
1	2A	2204	C	C2-N1-C1'	5.17	124.49	118.80
1	2A	1614	G	C8-N9-C1'	5.17	133.72	127.00
1	1A	905	G	C4-N9-C1'	-5.17	119.78	126.50
1	2A	2521	C	C6-N1-C2	-5.17	118.23	120.30
32	2a	1169	G	N3-C2-N2	-5.17	116.28	119.90
1	1A	893	U	N3-C4-O4	-5.17	115.78	119.40
32	1a	1070	G	N3-C4-C5	-5.16	126.02	128.60
1	1A	977	A	C8-N9-C4	-5.16	103.74	105.80
1	1A	988	G	C4-N9-C1'	5.15	133.20	126.50
1	2A	469	C	N1-C2-O2	-5.15	115.81	118.90
1	2A	2455	G	C5-C6-O6	5.15	131.69	128.60
32	2a	754	C	C6-N1-C2	5.15	122.36	120.30
32	1a	714	G	N1-C6-O6	-5.15	116.81	119.90
1	1A	1806	G	N9-C4-C5	-5.15	103.34	105.40
1	1A	2693	U	O5'-P-OP2	-5.14	101.07	105.70
1	1A	81	G	N9-C4-C5	-5.14	103.34	105.40
1	1A	2875	U	C4-C5-C6	5.14	122.79	119.70
32	2a	1475	G	O5'-P-OP2	-5.14	101.07	105.70
32	2a	1242	C	C6-N1-C2	-5.14	118.25	120.30
32	1a	109	G	P-O3'-C3'	5.13	125.86	119.70
32	1a	155	A	N7-C8-N9	5.13	116.36	113.80
1	1A	11	U	N3-C2-O2	-5.13	118.61	122.20
1	1A	830	A	C4-C5-N7	-5.13	108.14	110.70
1	1A	2464	A	O5'-P-OP2	-5.13	101.09	105.70
22	10	13	GLY	N-CA-C	5.12	125.91	113.10
1	1A	1067	G	N3-C4-C5	5.12	131.16	128.60
1	1A	640	G	O5'-P-OP2	-5.12	101.09	105.70
1	1A	2222	C	N3-C2-O2	-5.12	118.32	121.90
1	1A	2385	C	C2-N3-C4	-5.12	117.34	119.90
1	2A	2514	A	C5-C6-N6	-5.12	119.61	123.70
1	1A	1724	G	C8-N9-C4	-5.12	104.35	106.40
1	1A	2297	A	N9-C1'-C2'	5.11	120.65	114.00
1	2A	1824	U	C5-C6-N1	-5.11	120.14	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1480	A	C4-C5-N7	5.11	113.25	110.70
1	2A	1298	A	N1-C6-N6	-5.10	115.54	118.60
1	2A	2020	C	OP2-P-O3'	5.10	116.43	105.20
1	2A	2571	C	C6-N1-C2	5.10	122.34	120.30
32	2a	262	G	P-O3'-C3'	5.10	125.82	119.70
32	2a	970	U	P-O3'-C3'	5.10	125.82	119.70
32	1a	1133	U	N3-C4-C5	-5.10	111.54	114.60
1	1A	590	U	N3-C4-C5	5.10	117.66	114.60
32	1a	1039	U	C5-C4-O4	5.09	128.96	125.90
1	2A	1121	C	N1-C2-O2	5.09	121.96	118.90
1	1A	1098	C	N1-C1'-C2'	-5.09	106.40	112.00
1	2A	1021	C	N3-C2-O2	-5.09	118.34	121.90
1	2A	1604	A	P-O3'-C3'	5.09	125.81	119.70
1	1A	1984	U	C5-C6-N1	5.09	125.24	122.70
1	2A	2723	U	O4'-C1'-N1	5.09	112.27	108.20
1	2A	2815	G	O4'-C1'-N9	5.09	112.27	108.20
1	1A	2801	C	C5-C6-N1	-5.08	118.46	121.00
1	2A	534	C	N3-C2-O2	-5.08	118.34	121.90
1	1A	1358	U	C2-N1-C1'	5.08	123.80	117.70
54	2x	67	C	C2-N1-C1'	5.08	124.39	118.80
32	1a	1133	U	C5-C4-O4	5.08	128.95	125.90
1	1A	1538	C	C6-N1-C1'	-5.08	114.71	120.80
1	2A	1329	A	N1-C6-N6	5.08	121.65	118.60
1	1A	2607	U	N3-C2-O2	5.08	125.75	122.20
1	2A	1092	G	C4-N9-C1'	5.07	133.09	126.50
1	1A	1559	U	O5'-P-OP1	-5.07	101.14	105.70
32	2a	109	G	P-O3'-C3'	5.07	125.78	119.70
1	1A	2881	G	N3-C4-C5	-5.07	126.07	128.60
15	1T	118	ARG	NE-CZ-NH1	5.07	122.83	120.30
54	1x	76	A	C2-N3-C4	-5.07	108.07	110.60
32	1a	516	A	OP1-P-O3'	5.06	116.34	105.20
1	1A	1156	A	O4'-C1'-N9	5.06	112.25	108.20
1	1A	2464	A	OP2-P-O3'	5.06	116.33	105.20
1	1A	2901	G	N3-C4-C5	5.06	131.13	128.60
1	2A	797	A	O5'-P-OP1	-5.05	101.15	105.70
1	2A	1138	G	N3-C4-N9	5.05	129.03	126.00
1	1A	2439	G	C5-C6-O6	5.05	131.63	128.60
1	1A	787	G	O5'-P-OP1	-5.05	101.16	105.70
32	1a	341	C	C2-N3-C4	5.05	122.42	119.90
1	1A	2512	C	C6-N1-C2	5.04	122.32	120.30
1	1A	2530	U	C5-C4-O4	-5.04	122.88	125.90
1	2A	421	U	N1-C2-O2	5.04	126.33	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1900	C	C6-N1-C2	-5.04	118.28	120.30
1	2A	787	G	O5'-P-OP2	5.04	116.75	110.70
1	2A	1138	G	N3-C4-C5	-5.04	126.08	128.60
1	2A	1163	C	C6-N1-C2	-5.04	118.28	120.30
32	2a	938	U	C2-N1-C1'	5.04	123.75	117.70
1	2A	1067	G	N9-C4-C5	5.04	107.41	105.40
32	2a	24	C	O5'-P-OP2	5.04	116.74	110.70
1	1A	552	A	C5-N7-C8	-5.03	101.38	103.90
1	2A	2639	C	N1-C2-O2	5.03	121.92	118.90
1	1A	714	G	OP2-P-O3'	5.03	116.27	105.20
1	2A	2286	C	O4'-C1'-N1	-5.03	104.17	108.20
32	2a	1183	A	P-O3'-C3'	5.03	125.74	119.70
54	2x	14	A	C4-N9-C1'	5.03	135.36	126.30
1	1A	2456	G	C5-C6-O6	5.03	131.62	128.60
32	1a	1313	G	O4'-C1'-N9	5.03	112.22	108.20
1	1A	820	A	C8-N9-C4	-5.02	103.79	105.80
1	2A	1358	U	C5-C6-N1	5.02	125.21	122.70
54	1x	19	G	O4'-C1'-N9	-5.02	104.18	108.20
1	2A	554	G	N3-C4-N9	-5.02	122.99	126.00
1	2A	1066	A	N3-C4-N9	-5.02	123.38	127.40
32	2a	826	C	C6-N1-C2	-5.02	118.29	120.30
1	2A	2841	U	C5-C6-N1	-5.02	120.19	122.70
54	2x	46	G	N1-C2-N3	5.02	126.91	123.90
1	2A	1009	C	C6-N1-C2	-5.02	118.29	120.30
1	2A	1994	G	N1-C6-O6	-5.02	116.89	119.90
1	1A	1810	A	C5-C6-N6	5.02	127.71	123.70
1	2A	549	U	N3-C2-O2	5.01	125.71	122.20
1	1A	580	G	N3-C2-N2	5.01	123.41	119.90
1	2A	820	A	O5'-P-OP2	-5.00	101.20	105.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	1X	93	GLU	Peptide
20	1Y	54	LYS	Peptide
5	2F	20	LEU	Peptide
19	2X	93	GLU	Peptide
34	2c	186	PHE	Peptide



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	59154	0	29828	546	0
1	2A	60091	0	30300	842	0
2	1B	2572	0	1306	29	0
2	2B	2573	0	1306	58	0
3	1D	2136	0	2218	55	0
3	2D	2142	0	2229	58	0
4	1E	1559	0	1618	35	0
4	2E	1559	0	1618	53	0
5	1F	1584	0	1625	33	0
5	2F	1580	0	1619	49	0
6	1G	1425	0	1443	34	0
6	2G	1424	0	1434	67	0
7	1H	1330	0	1407	25	0
7	2H	1330	0	1407	37	0
8	1I	1085	0	1114	25	0
8	2I	1061	0	1080	28	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	20	0
10	1O	933	0	996	16	0
10	2O	933	0	996	21	0
11	1P	1139	0	1223	31	0
11	2P	1135	0	1212	40	0
12	1Q	1122	0	1179	18	0
12	2Q	1122	0	1179	27	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	21	0
14	1S	877	0	938	33	0
14	2S	870	0	923	32	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	19	0
16	1U	959	0	1019	11	0
16	2U	959	0	1018	24	0
17	1V	771	0	830	9	0
17	2V	771	0	830	18	0
18	1W	886	0	940	8	0
18	2W	886	0	940	19	0
19	1X	750	0	814	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	15	0
20	1Y	806	0	881	25	0
20	2Y	806	0	881	28	0
21	1Z	1470	0	1478	24	0
21	2Z	1454	0	1452	48	0
22	10	598	0	614	11	0
22	20	598	0	614	11	0
23	11	755	0	826	12	0
23	21	755	0	826	12	0
24	12	588	0	643	7	0
24	22	588	0	643	15	0
25	13	469	0	518	7	0
25	23	464	0	514	18	0
26	14	558	0	544	31	0
26	24	532	0	503	21	0
27	15	455	0	465	7	0
27	25	455	0	465	13	0
28	16	453	0	472	7	0
28	26	449	0	469	6	0
29	17	418	0	467	8	0
29	27	418	0	467	11	0
30	18	517	0	582	18	0
30	28	517	0	582	28	0
31	19	307	0	335	7	0
31	29	307	0	335	8	0
32	1a	31750	0	16028	0	0
32	2a	31877	0	16090	0	0
33	1b	1786	0	1744	0	0
33	2b	1697	0	1574	0	0
34	1c	1480	0	1400	0	0
34	2c	1412	0	1246	0	0
35	1d	1618	0	1579	0	0
35	2d	1630	0	1633	0	0
36	1e	1129	0	1184	0	0
36	2e	1095	0	1124	0	0
37	1f	806	0	793	0	0
37	2f	817	0	808	0	0
38	1g	1183	0	1165	0	0
38	2g	1167	0	1119	0	0
39	1h	1088	0	1126	0	0
39	2h	1074	0	1100	0	0
40	1i	976	0	973	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	932	0	891	0	0
41	1j	682	0	598	0	0
41	2j	678	0	612	0	0
42	1k	826	0	829	0	0
42	2k	829	0	825	0	0
43	1l	920	0	958	0	0
43	2l	918	0	947	0	0
44	1m	923	0	962	0	0
44	2m	903	0	923	0	0
45	1n	482	0	507	0	0
45	2n	459	0	467	0	0
46	1o	715	0	729	0	0
46	2o	728	0	760	0	0
47	1p	671	0	679	0	0
47	2p	677	0	686	0	0
48	1q	811	0	858	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	642	0	629	0	0
50	2s	646	0	644	0	0
51	1t	712	0	759	0	0
51	2t	731	0	807	0	0
52	1u	187	0	186	0	0
52	2u	199	0	208	0	0
53	1v	109	0	55	0	0
53	2v	109	0	55	0	0
54	1x	1625	0	829	0	0
54	2x	1625	0	829	0	0
55	1z	101	0	109	0	0
55	2z	101	0	109	0	0
56	10	7	0	0	0	0
56	11	1	0	0	0	0
56	13	2	0	0	0	0
56	14	1	0	0	0	0
56	15	4	0	0	0	0
56	16	2	0	0	0	0
56	17	4	0	0	0	0
56	18	5	0	0	0	0
56	19	3	0	0	0	0
56	1A	1051	0	0	0	0
56	1B	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1D	17	0	0	0	0
56	1E	10	0	0	0	0
56	1F	7	0	0	0	0
56	1G	3	0	0	0	0
56	1H	4	0	0	0	0
56	1N	8	0	0	0	0
56	1O	2	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	6	0	0	0	0
56	1T	5	0	0	0	0
56	1U	5	0	0	0	0
56	1V	1	0	0	0	0
56	1W	6	0	0	0	0
56	1X	2	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	306	0	0	0	0
56	1b	2	0	0	0	0
56	1c	1	0	0	0	0
56	1d	2	0	0	0	0
56	1e	4	0	0	0	0
56	1f	1	0	0	0	0
56	1h	3	0	0	0	0
56	1k	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	1q	4	0	0	0	0
56	1r	3	0	0	0	0
56	1t	1	0	0	0	0
56	1x	11	0	0	0	0
56	20	1	0	0	0	0
56	25	1	0	0	0	0
56	26	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	583	0	0	0	0
56	2B	10	0	0	0	0
56	2D	4	0	0	0	0
56	2E	7	0	0	0	0
56	2F	2	0	0	0	0
56	2G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2N	1	0	0	0	0
56	2O	3	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	5	0	0	0	0
56	2R	1	0	0	0	0
56	2U	2	0	0	0	0
56	2V	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2a	244	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2k	2	0	0	0	0
56	2l	3	0	0	0	0
56	2n	2	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	6	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	10	8	0	0	0	0
59	11	7	0	0	0	0
59	12	2	0	0	0	0
59	13	4	0	0	0	0
59	15	7	0	0	1	0
59	16	5	0	0	1	0
59	17	8	0	0	0	0
59	18	9	0	0	0	0
59	19	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1A	2110	0	0	87	0
59	1B	42	0	0	4	0
59	1D	24	0	0	0	0
59	1E	30	0	0	4	0
59	1F	16	0	0	1	0
59	1G	6	0	0	0	0
59	1H	3	0	0	1	0
59	1I	1	0	0	0	0
59	1N	7	0	0	0	0
59	1O	4	0	0	0	0
59	1P	21	0	0	1	0
59	1Q	11	0	0	0	0
59	1R	16	0	0	4	0
59	1S	2	0	0	0	0
59	1T	7	0	0	1	0
59	1U	14	0	0	0	0
59	1V	4	0	0	1	0
59	1W	5	0	0	0	0
59	1X	4	0	0	0	0
59	1Y	1	0	0	0	0
59	1Z	4	0	0	0	0
59	1a	393	0	0	0	0
59	1b	1	0	0	0	0
59	1c	1	0	0	0	0
59	1d	5	0	0	0	0
59	1e	3	0	0	0	0
59	1f	1	0	0	0	0
59	1h	3	0	0	0	0
59	1i	1	0	0	0	0
59	1j	1	0	0	0	0
59	1k	1	0	0	0	0
59	1l	3	0	0	0	0
59	1m	1	0	0	0	0
59	1o	1	0	0	0	0
59	1p	1	0	0	0	0
59	1q	1	0	0	0	0
59	1s	1	0	0	0	0
59	1v	1	0	0	0	0
59	1x	8	0	0	0	0
59	1z	1	0	0	0	0
59	20	3	0	0	0	0
59	21	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	23	2	0	0	0	0
59	26	1	0	0	0	0
59	27	2	0	0	0	0
59	28	2	0	0	0	0
59	2A	813	0	0	62	0
59	2B	10	0	0	0	0
59	2D	16	0	0	1	0
59	2E	9	0	0	2	0
59	2F	5	0	0	0	0
59	2N	1	0	0	0	0
59	2O	3	0	0	0	0
59	2P	9	0	0	0	0
59	2Q	2	0	0	0	0
59	2R	3	0	0	0	0
59	2T	1	0	0	0	0
59	2U	3	0	0	0	0
59	2W	1	0	0	0	0
59	2X	2	0	0	0	0
59	2Y	1	0	0	1	0
59	2Z	4	0	0	2	0
59	2a	321	0	0	0	0
59	2d	1	0	0	0	0
59	2e	1	0	0	0	0
59	2i	2	0	0	0	0
59	2j	1	0	0	0	0
59	2l	1	0	0	0	0
59	2m	3	0	0	0	0
59	2p	1	0	0	0	0
59	2q	1	0	0	0	0
59	2t	4	0	0	0	0
59	2x	7	0	0	0	0
59	2z	1	0	0	0	0
All	All	288518	0	189963	2459	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 10.

All (2459) 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)
1:2A:1828:U:H5'	3:2D:259:THR:HG22	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:54:LYS:HA	20:1Y:56:PRO:HD3	1.49	0.94
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.33	0.93
1:2A:1098:C:H42	1:2A:1151:G:H1	1.12	0.92
1:1A:1064:U:HO2'	1:1A:1066:A:H2	1.05	0.92
1:1A:353:A:H2	1:1A:1254:A:HO2'	0.94	0.90
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.36	0.90
1:1A:1735:A:H62	1:1A:1744:A:H2	1.15	0.90
1:1A:1828:U:H5'	3:1D:259:THR:HG22	1.52	0.90
1:1A:786:U:OP2	59:1A:4101:HOH:O	1.90	0.89
1:2A:2226:G:H3'	1:2A:2227:G:C8	2.07	0.89
1:2A:1248:A:H2	1:2A:1286:A:H62	1.20	0.89
1:1A:2465:G:OP1	59:1A:4102:HOH:O	1.91	0.89
1:1A:1000:G:OP2	12:1Q:14:ARG:NH2	2.06	0.88
1:1A:1355:G:OP2	29:17:9:ARG:NH1	2.07	0.88
1:1A:1316:G:OP2	59:1A:4103:HOH:O	1.92	0.87
1:2A:1735:A:H62	1:2A:1744:A:H2	1.23	0.87
29:17:24:THR:HG22	29:17:27:GLY:H	1.40	0.87
15:1T:16:ARG:NH2	15:1T:83:ILE:O	2.06	0.86
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.57	0.86
26:14:53:GLU:HB3	26:14:54:GLY:HA2	1.57	0.86
1:1A:2502:U:OP2	59:1A:4104:HOH:O	1.93	0.86
7:1H:3:ARG:HG2	7:1H:6:ARG:HG2	1.58	0.85
1:2A:655:A:OP1	11:2P:65:ARG:NH1	2.09	0.85
15:1T:54:ARG:HA	15:1T:59:THR:HB	1.60	0.84
1:1A:536:G:N7	59:1A:4108:HOH:O	2.08	0.84
1:1A:2100:U:OP1	23:11:21:ARG:NH2	2.11	0.84
23:11:21:ARG:HH11	23:11:21:ARG:HG2	1.42	0.83
1:1A:2330:G:N7	59:1A:4123:HOH:O	2.10	0.83
1:2A:2816:G:N1	1:2A:2901:G:O6	2.10	0.83
6:2G:80:PHE:O	6:2G:82:LEU:N	2.11	0.82
3:1D:71:ASP:HB3	3:1D:103:ARG:HH22	1.41	0.82
1:2A:1067:G:H22	1:2A:1187:A:H2	1.27	0.82
1:1A:1303:C:OP1	59:1A:4105:HOH:O	1.97	0.82
15:2T:54:ARG:HA	15:2T:59:THR:HB	1.62	0.81
1:2A:1355:G:OP2	29:27:9:ARG:NH1	2.14	0.81
3:2D:276:LYS:HD3	3:2D:276:LYS:H	1.44	0.81
1:1A:550:A:OP1	59:1A:4106:HOH:O	1.98	0.81
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.43	0.81
1:2A:2226:G:H3'	1:2A:2227:G:H8	1.40	0.81
1:1A:534:C:OP1	59:1A:4108:HOH:O	1.98	0.80
18:1W:14:PRO:HG2	18:1W:78:GLU:HG2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2815:G:H2'	1:2A:2816:G:H8	1.46	0.80
1:1A:475:G:O6	59:1A:4107:HOH:O	1.98	0.80
1:2A:1188:A:OP1	9:2N:25:ARG:NH2	2.15	0.80
1:2A:141:G:H4'	19:2X:35:THR:HG21	1.61	0.80
1:2A:786:U:OP2	59:2A:3602:HOH:O	1.99	0.80
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.64	0.80
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.64	0.80
14:2S:99:LYS:NZ	14:2S:103:GLU:OE2	2.14	0.80
6:1G:49:ASP:O	6:1G:51:ARG:N	2.15	0.79
1:1A:1000:G:O6	59:1A:4109:HOH:O	1.99	0.79
26:14:57:GLU:HB3	26:14:58:ARG:HG2	1.63	0.79
2:2B:4:C:H42	2:2B:117:G:H1	1.28	0.79
1:1A:1693:G:OP1	59:1A:4103:HOH:O	2.00	0.79
1:2A:673:G:H4'	30:28:46:ARG:HH22	1.48	0.79
1:2A:1316:G:OP2	59:2A:3601:HOH:O	1.98	0.79
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.28	0.79
1:2A:1404:A:N6	1:2A:1417:U:O4	2.16	0.78
1:1A:1813:A:OP1	59:1A:4101:HOH:O	2.01	0.78
4:1E:54:GLN:HE21	4:1E:55:ASN:H	1.30	0.78
1:1A:2221:C:OP1	59:1A:4110:HOH:O	2.02	0.78
1:2A:1310:A:OP2	59:2A:3603:HOH:O	2.01	0.78
2:2B:22:U:H3	2:2B:61:G:H1	1.31	0.78
1:1A:1694:C:OP1	59:1A:4103:HOH:O	2.02	0.78
6:2G:41:GLN:HE22	6:2G:153:ARG:HB3	1.48	0.78
1:2A:1813:A:OP1	59:2A:3602:HOH:O	2.01	0.78
1:2A:8:U:H3	1:2A:2640:A:H2	1.28	0.78
6:2G:13:GLU:O	6:2G:15:VAL:N	2.17	0.78
1:2A:1649:C:OP2	59:2A:3605:HOH:O	2.02	0.78
1:2A:2588:A:H5'	27:25:3:LYS:HD2	1.67	0.77
1:2A:2441:A:OP2	59:2A:3604:HOH:O	2.02	0.77
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.66	0.77
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.47	0.77
8:2I:65:ALA:HB1	8:2I:136:VAL:HG11	1.66	0.77
1:1A:2466:G:OP2	59:1A:4111:HOH:O	2.03	0.77
1:1A:1248:A:H2	1:1A:1286:A:H62	1.31	0.77
1:2A:1064:U:H3	1:2A:1187:A:H62	1.32	0.77
1:2A:2310:G:H2'	1:2A:2311:G:H8	1.50	0.77
1:1A:2456:G:OP1	5:1F:74:ARG:NH2	2.18	0.76
1:2A:117:U:OP2	59:2A:3607:HOH:O	2.03	0.76
1:1A:893:U:O4	1:1A:977:A:N6	2.19	0.76
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.65	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:58:A:OP2	59:1B:301:HOH:O	2.03	0.75
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.68	0.75
1:1A:2795:G:N7	59:1A:4142:HOH:O	2.18	0.75
5:2F:20:LEU:HD13	5:2F:21:ALA:H	1.52	0.75
1:2A:2815:G:H2'	1:2A:2816:G:C8	2.21	0.75
1:2A:957:C:OP1	12:2Q:8:LYS:NZ	2.20	0.75
1:1A:2768:U:O4	1:1A:2770:A:N6	2.20	0.74
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.20	0.74
1:1A:2586:C:OP2	59:1A:4112:HOH:O	2.04	0.74
11:2P:65:ARG:HG3	30:28:25:MET:HG3	1.69	0.74
1:2A:1377:G:OP1	59:2A:3606:HOH:O	2.03	0.74
31:19:20:HIS:O	59:19:5001:HOH:O	2.05	0.74
1:2A:1039:C:OP1	16:2U:53:ARG:NH2	2.20	0.74
1:2A:1694:C:OP1	59:2A:3601:HOH:O	2.06	0.74
1:1A:1218:A:HO2'	1:1A:1219:U:H6	1.35	0.74
1:2A:900:G:H2'	1:2A:901:G:H8	1.53	0.74
22:10:11:ARG:O	22:10:14:ARG:NH2	2.21	0.73
1:1A:2458:G:OP2	59:1A:4114:HOH:O	2.05	0.73
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.71	0.73
1:1A:2753:A:OP1	31:19:22:ARG:NH2	2.20	0.73
1:2A:777:C:OP1	59:2A:3609:HOH:O	2.06	0.73
1:2A:10:G:H2'	1:2A:11:U:H5''	1.70	0.73
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.70	0.73
14:2S:10:ARG:NH2	14:2S:91:PRO:O	2.20	0.73
1:1A:1479:A:H61	1:1A:1604:A:H62	1.34	0.73
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.71	0.73
1:2A:183:A:N7	59:2A:3636:HOH:O	2.19	0.73
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.22	0.73
1:1A:1552:A:HO2'	1:1A:1553:A:H8	1.37	0.73
1:2A:2600:A:OP1	59:2A:3608:HOH:O	2.06	0.73
16:2U:92:ARG:HA	16:2U:95:LEU:HB2	1.71	0.73
1:1A:1188:A:OP1	9:1N:25:ARG:NH2	2.22	0.72
22:20:11:ARG:O	22:20:14:ARG:NH2	2.23	0.72
1:1A:1038:G:OP1	16:1U:50:ARG:NH2	2.20	0.72
16:2U:49:HIS:HA	16:2U:52:ARG:HG2	1.70	0.72
1:1A:1514:C:OP1	59:1A:4116:HOH:O	2.08	0.72
7:2H:9:ILE:HB	7:2H:50:VAL:HB	1.69	0.72
1:2A:2067:G:H5'	27:25:19:ARG:HA	1.69	0.72
7:2H:3:ARG:HH11	7:2H:3:ARG:HB3	1.55	0.72
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.71	0.72
26:24:46:GLN:O	26:24:48:ARG:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.55	0.72
1:2A:1512:G:HO2'	1:2A:1592:C:HO2'	1.34	0.72
1:2A:1104:G:H3'	1:2A:1105:U:H6	1.55	0.72
1:2A:1360:C:OP2	59:2A:3606:HOH:O	2.08	0.72
1:2A:2328:C:H2'	1:2A:2329:G:H8	1.55	0.71
1:2A:2800:C:OP1	4:2E:61:ARG:NH2	2.23	0.71
1:2A:680:C:N4	1:2A:697:G:O6	2.17	0.71
1:2A:1185:U:OP2	9:2N:63:THR:OG1	2.08	0.71
1:2A:2694:C:OP1	15:2T:53:ARG:NH2	2.22	0.71
1:1A:2561:G:OP1	59:1A:4117:HOH:O	2.08	0.71
1:2A:552:A:O2'	1:2A:553:A:H5'	1.91	0.71
18:2W:14:PRO:HG2	18:2W:78:GLU:HG2	1.71	0.71
1:2A:1035:A:OP2	59:2A:3610:HOH:O	2.09	0.71
1:2A:1154:C:H3'	1:2A:1155:G:C8	2.26	0.71
1:1A:2824:C:H5'	27:15:29:THR:HG21	1.73	0.71
1:1A:725:C:OP1	59:1A:4115:HOH:O	2.08	0.71
1:1A:894:G:OP1	59:1A:4119:HOH:O	2.08	0.71
1:1A:655:A:OP1	11:1P:65:ARG:NH1	2.21	0.71
1:2A:2053:G:N7	59:2A:3654:HOH:O	2.24	0.70
4:2E:132:HIS:NE2	59:2E:402:HOH:O	2.23	0.70
1:1A:1015:C:OP2	59:1A:4121:HOH:O	2.09	0.70
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.73	0.70
2:1B:23:G:O6	59:1B:302:HOH:O	2.07	0.70
59:1E:402:HOH:O	13:1R:3:HIS:NE2	2.24	0.70
2:2B:11:C:OP2	2:2B:12:C:N4	2.17	0.70
1:1A:138:A:H8	1:1A:1453:C:HO2'	1.40	0.70
1:1A:869:G:OP1	59:1A:4120:HOH:O	2.08	0.70
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.10	0.70
2:2B:75:G:H22	21:2Z:73:GLN:NE2	1.88	0.70
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.73	0.70
6:2G:33:ARG:NH1	6:2G:33:ARG:HB2	2.07	0.70
1:2A:1116:G:H1	1:2A:1124:C:H42	15.34	0.70
1:2A:2517:U:OP1	4:2E:144:ARG:NH2	2.25	0.70
1:1A:1218:A:H4'	1:1A:1219:U:OP1	1.92	0.70
1:1A:893:U:OP2	59:1A:4122:HOH:O	2.09	0.70
1:1A:2024:G:OP2	59:1A:4124:HOH:O	2.10	0.70
4:1E:127:ASP:OD2	59:1E:401:HOH:O	2.10	0.70
1:1A:1354:G:H4'	29:17:7:PRO:HB2	1.72	0.70
1:1A:553:A:N1	59:1A:4190:HOH:O	2.25	0.70
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.73	0.70
1:1A:1021:C:OP1	59:1A:4118:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1070:G:O2'	59:2A:3612:HOH:O	2.10	0.70
1:1A:271:U:OP1	8:1I:50:ARG:NH2	2.25	0.69
14:2S:35:ILE:HD13	14:2S:97:ARG:HH21	1.57	0.69
6:2G:43:LEU:HD12	6:2G:45:GLU:HG3	1.73	0.69
8:2I:129:THR:HG22	8:2I:139:GLN:HE22	1.56	0.69
1:1A:2298:A:H62	1:1A:2355:U:H3	1.38	0.69
1:2A:267:G:HO2'	1:2A:268:G:H8	1.38	0.69
1:1A:2816:G:N1	1:1A:2901:G:O6	2.18	0.69
5:1F:89:VAL:O	59:1F:401:HOH:O	2.11	0.69
26:24:59:PHE:HA	26:24:61:ARG:N	2.07	0.69
1:1A:426:G:N7	59:1A:4181:HOH:O	2.24	0.69
1:1A:929:G:O6	1:1A:938:C:N4	2.25	0.69
4:1E:110:GLY:O	59:1E:402:HOH:O	2.11	0.69
1:2A:1066:A:H62	1:2A:1185:U:H3	1.38	0.69
17:2V:6:LYS:HB2	17:2V:38:LEU:HD21	1.74	0.69
1:2A:2456:G:OP1	5:2F:74:ARG:NH2	2.24	0.69
1:2A:816:G:OP2	59:2A:3614:HOH:O	2.11	0.69
1:1A:2007:A:OP1	59:1A:4125:HOH:O	2.11	0.68
1:1A:258:A:H2'	1:1A:259:A:C8	3.09	0.68
1:2A:2595:U:O4	59:2A:3613:HOH:O	2.11	0.68
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.11	0.68
2:2B:8:U:H3	2:2B:113:G:H1	1.41	0.68
12:1Q:59:ARG:HA	12:1Q:60:ARG:NH2	2.07	0.68
1:2A:163:G:O6	59:2A:3611:HOH:O	2.09	0.68
1:2A:829:A:OP2	59:2A:3608:HOH:O	2.10	0.68
24:22:35:LEU:HD11	24:22:49:LYS:HB3	1.75	0.68
1:2A:2405:C:OP2	30:28:30:ARG:NH1	2.25	0.68
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.75	0.68
1:1A:2395:G:OP2	22:10:55:ARG:NH1	2.27	0.68
21:2Z:94:GLU:OE2	59:2Z:5001:HOH:O	2.11	0.68
6:1G:50:ALA:O	6:1G:52:ILE:N	2.26	0.68
1:2A:1092:G:H1'	1:2A:1155:G:H22	1.59	0.68
1:1A:1229:C:OP2	59:1A:4126:HOH:O	2.11	0.68
6:2G:108:ASN:HA	26:24:37:SER:HB2	1.76	0.68
1:2A:2058:G:O6	59:2A:3615:HOH:O	2.12	0.68
21:2Z:90:VAL:O	59:2Z:5002:HOH:O	2.11	0.68
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.23	0.67
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.77	0.67
2:2B:43:C:O2	6:2G:95:ARG:NH1	2.25	0.67
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.26	0.67
1:1A:8:U:N3	1:1A:2640:A:H2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:175:LYS:O	59:1H:301:HOH:O	2.11	0.67
1:2A:1494:G:O2'	1:2A:1574:A:N1	2.26	0.67
1:2A:330:G:H21	1:2A:353:A:H62	1.41	0.67
26:14:44:THR:O	26:14:46:GLN:N	2.27	0.67
1:1A:481:C:H4'	59:1A:4893:HOH:O	1.93	0.67
26:14:46:GLN:O	26:14:48:ARG:N	2.27	0.67
1:1A:8:U:H3	1:1A:2640:A:H2	1.43	0.67
2:1B:102:A:N7	59:1B:305:HOH:O	2.27	0.67
8:1I:48:GLU:HG2	8:1I:52:ARG:HH22	1.59	0.67
14:1S:59:LYS:HD2	14:1S:60:GLY:N	2.09	0.67
1:2A:721:A:OP1	5:2F:63:LYS:NZ	2.26	0.67
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.76	0.67
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.75	0.67
1:2A:894:G:H2'	1:2A:895:A:C8	2.30	0.67
15:2T:65:LYS:HE2	15:2T:67:SER:HB2	1.75	0.67
28:16:13:CYS:SG	28:16:47:THR:HG21	2.35	0.66
1:1A:1989:G:OP1	59:1A:4130:HOH:O	2.13	0.66
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.76	0.66
4:1E:29:GLY:HA3	59:1E:410:HOH:O	1.94	0.66
19:2X:31:HIS:HD2	19:2X:33:LYS:H	1.42	0.66
2:1B:76:G:O6	59:1B:303:HOH:O	2.12	0.66
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.76	0.66
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.60	0.66
1:2A:2284:A:H2'	1:2A:2285:A:C8	2.31	0.66
1:2A:929:G:N2	1:2A:948:C:O2	27.41	0.66
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.78	0.66
1:1A:638:G:OP1	59:1A:4129:HOH:O	2.13	0.66
12:1Q:32:TYR:CE1	12:1Q:133:ARG:HG3	2.30	0.66
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.59	0.66
15:2T:55:ASN:H	15:2T:59:THR:HG22	1.60	0.66
1:1A:1543:C:OP1	59:1A:4131:HOH:O	2.14	0.66
1:1A:2364:G:N7	59:1A:4209:HOH:O	2.27	0.66
1:1A:141:G:N2	1:1A:172:C:N3	54.86	0.66
1:2A:2626:U:OP1	59:2A:3603:HOH:O	2.12	0.66
1:2A:57:U:H2'	1:2A:58:G:H8	5.33	0.66
20:2Y:94:LYS:NZ	59:2Y:601:HOH:O	2.28	0.66
1:1A:1312:U:OP1	59:1A:4128:HOH:O	2.12	0.66
1:1A:932:C:H2'	1:1A:933:A:H5''	1.78	0.66
17:1V:69:LYS:NZ	59:1V:301:HOH:O	2.29	0.65
1:2A:1198:C:OP1	16:2U:92:ARG:NH1	2.29	0.65
3:2D:242:ARG:N	3:2D:242:ARG:HD3	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1377:G:OP1	59:1A:4132:HOH:O	2.14	0.65
1:2A:1421:C:OP2	59:2A:3616:HOH:O	2.13	0.65
4:2E:9:VAL:HG13	4:2E:25:VAL:O	1.96	0.65
7:2H:144:VAL:O	7:2H:148:ILE:HG12	1.97	0.65
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.31	0.65
21:2Z:70:LEU:HG	21:2Z:91:LEU:HD21	1.77	0.65
1:1A:2649:G:P	4:1E:82:ARG:HH22	2.19	0.65
24:22:32:LEU:HD11	24:22:54:LYS:HG3	1.79	0.65
1:1A:1089:G:OP2	59:1A:4133:HOH:O	2.14	0.65
1:1A:2493:G:OP1	59:1A:4134:HOH:O	2.14	0.65
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.61	0.65
1:2A:1042:G:OP1	16:2U:92:ARG:HG2	1.97	0.65
23:21:21:ARG:HD3	23:21:35:THR:HG21	1.78	0.65
1:2A:353:A:H2	1:2A:1254:A:HO2'	1.44	0.65
12:2Q:32:TYR:CE1	12:2Q:133:ARG:HG3	2.32	0.65
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.78	0.65
1:2A:2125:G:H22	1:2A:2207:G:H1'	1.62	0.65
1:1A:2253:G:OP1	59:1A:4115:HOH:O	2.14	0.65
1:2A:1154:C:H2'	1:2A:1155:G:C8	3.05	0.65
2:2B:6:C:H42	2:2B:115:G:H1	1.43	0.65
26:14:46:GLN:HB2	26:14:48:ARG:HE	1.61	0.65
1:2A:181:U:OP2	59:2A:3621:HOH:O	2.15	0.65
1:2A:1828:U:OP2	3:2D:274:ARG:NH2	2.29	0.65
1:2A:2726:G:OP2	59:2A:3619:HOH:O	2.14	0.65
4:2E:111:ARG:HG3	4:2E:160:TYR:CD2	2.31	0.65
1:2A:1280:G:OP1	59:2A:3617:HOH:O	2.13	0.64
1:2A:1111:U:N3	1:2A:1114:A:OP2	2.25	0.64
1:2A:241:C:OP2	30:28:5:LYS:NZ	2.24	0.64
1:2A:2622:U:C4	27:25:3:LYS:HG2	2.32	0.64
1:2A:533:C:OP1	59:2A:3618:HOH:O	2.14	0.64
7:2H:11:VAL:HG13	7:2H:15:VAL:HG22	1.80	0.64
21:2Z:134:PRO:HG3	21:2Z:161:VAL:HG21	1.78	0.64
1:1A:1379:G:N7	59:1A:4221:HOH:O	2.30	0.64
1:1A:1698:A:N6	59:1R:301:HOH:O	2.31	0.64
1:2A:1455:G:H2'	1:2A:1456:C:C6	2.32	0.64
1:1A:288:G:N3	59:1A:4136:HOH:O	2.30	0.64
1:2A:2043:U:OP1	59:2A:3620:HOH:O	2.15	0.64
4:1E:181:LEU:HD21	15:1T:6:LEU:HD12	1.79	0.64
11:2P:95:VAL:HG12	11:2P:123:LEU:HD22	1.78	0.64
6:2G:115:ARG:HG2	6:2G:115:ARG:HH11	1.63	0.64
1:1A:1360:C:OP2	59:1A:4132:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.80	0.64
31:19:19:ARG:NH2	59:19:5002:HOH:O	2.08	0.64
1:2A:1638:G:H2'	1:2A:1639:G:C8	2.33	0.64
1:2A:57:U:H2'	1:2A:58:G:C8	5.40	0.64
7:2H:103:LEU:HB3	7:2H:115:VAL:HG13	1.78	0.64
1:2A:2368:U:OP1	22:20:20:ARG:NH1	2.29	0.64
3:2D:238:GLY:O	3:2D:239:ARG:HB2	1.96	0.64
1:2A:1450:U:H2'	1:2A:1451:U:C6	2.32	0.64
1:1A:2210:U:H2'	1:1A:2211:G:H8	1.62	0.63
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	1.81	0.63
21:2Z:157:LEU:HD11	21:2Z:163:LEU:HD13	1.80	0.63
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.80	0.63
1:1A:2206:C:H2'	1:1A:2207:G:C8	2.34	0.63
6:2G:107:LEU:HA	6:2G:111:LEU:HD22	1.80	0.63
6:2G:151:ALA:HB3	6:2G:153:ARG:HH11	1.62	0.63
1:2A:935:C:O2'	1:2A:936:A:O5'	2.16	0.63
11:2P:95:VAL:HA	11:2P:99:LEU:HD21	1.79	0.63
21:2Z:134:PRO:O	21:2Z:136:PHE:N	2.31	0.63
1:1A:2330:G:N2	14:1S:3:ARG:HA	2.12	0.63
26:24:14:ILE:HG22	26:24:22:ILE:HD13	1.81	0.63
1:1A:2123:U:O2	1:1A:2208:G:O6	2.17	0.63
1:1A:1846:G:O6	3:1D:35:LYS:NZ	2.31	0.63
1:2A:663:U:H2'	1:2A:664:C:C6	2.34	0.63
1:1A:267:G:OP2	59:1A:4135:HOH:O	2.16	0.63
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.31	0.63
25:13:3:ARG:NH1	25:13:60:GLU:OE1	2.28	0.62
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.79	0.62
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.81	0.62
1:2A:1361:U:H2'	1:2A:1362:A:H8	1.64	0.62
1:2A:2022:A:H2'	1:2A:2023:G:C8	2.34	0.62
1:2A:2643:A:O2'	1:2A:2820:G:O2'	2.14	0.62
1:1A:2122:G:H2'	1:1A:2123:U:O4'	1.99	0.62
3:1D:108:PRO:HD2	3:1D:111:LEU:HG	1.82	0.62
14:1S:15:ARG:O	14:1S:19:LYS:HG2	1.98	0.62
1:2A:2226:G:H5''	1:2A:2227:G:N7	2.14	0.62
1:2A:267:G:O2'	1:2A:268:G:H8	1.82	0.62
21:2Z:53:ILE:HD11	21:2Z:99:TYR:HB2	1.80	0.62
1:1A:1739:U:O2'	3:1D:14:ARG:NH2	2.33	0.62
17:1V:98:GLU:OE2	17:1V:100:ARG:NH1	2.33	0.62
1:2A:842:C:H2'	1:2A:843:C:C6	2.35	0.62
7:2H:44:VAL:HB	7:2H:51:ARG:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:14:ASP:N	8:2I:17:GLN:OE1	2.30	0.62
1:2A:508:A:O2'	20:2Y:49:VAL:O	2.16	0.62
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.81	0.62
1:1A:1826:U:H2'	1:1A:1827:C:C6	2.34	0.62
6:2G:48:GLU:HA	6:2G:51:ARG:HE	1.65	0.62
26:14:63:TYR:N	26:14:64:GLY:HA2	2.14	0.62
1:1A:846:A:OP1	1:1A:846:A:H8	1.82	0.62
12:1Q:58:PHE:O	12:1Q:60:ARG:NH2	2.33	0.62
1:2A:1064:U:OP1	1:2A:1080:U:O2'	2.15	0.62
16:2U:104:GLN:OE1	16:2U:105:VAL:N	2.27	0.62
1:1A:214:G:H21	1:1A:216:A:H62	1.48	0.62
23:21:22:GLY:O	23:21:32:LYS:NZ	2.32	0.62
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	1.82	0.62
4:1E:1:MET:HE3	4:1E:199:ARG:HB3	1.80	0.62
1:2A:629:U:OP1	5:2F:102:PRO:HA	1.99	0.62
3:1D:146:GLU:HB2	3:1D:189:CYS:HB3	1.80	0.61
1:2A:172:C:H2'	1:2A:173:U:C6	2.35	0.61
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.82	0.61
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.32	0.61
1:1A:2121:G:H1	1:1A:2210:U:H3	1.48	0.61
20:1Y:68:HIS:ND1	20:1Y:70:SER:HB3	2.16	0.61
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.34	0.61
15:1T:51:ARG:NH1	59:1T:3101:HOH:O	2.20	0.61
10:2O:1:MET:HE3	10:2O:67:LYS:HG2	1.82	0.61
25:13:8:LEU:HD13	25:13:31:LEU:HD23	1.82	0.61
1:1A:2657:C:OP2	1:1A:2744:G:O2'	2.16	0.61
1:2A:1845:A:OP2	3:2D:54:ARG:NH2	2.33	0.61
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.32	0.61
15:1T:118:ARG:HH11	15:1T:118:ARG:HG3	1.66	0.61
1:2A:98:G:O2'	24:22:7:ARG:NH2	2.33	0.61
2:2B:90:A:C5	2:2B:91:C:H1'	2.35	0.61
1:1A:69:A:N7	19:1X:31:HIS:HE1	1.98	0.61
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.83	0.61
1:2A:1823:C:OP1	59:2A:3623:HOH:O	2.16	0.61
1:2A:1311:G:O5'	18:2W:15:ARG:NH2	2.33	0.61
1:1A:1465:U:O2'	1:1A:1466:G:OP1	2.19	0.61
1:1A:1091:A:H3'	1:1A:1092:G:H5'	1.81	0.61
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.81	0.61
14:1S:3:ARG:HD3	14:1S:4:LEU:N	2.16	0.61
1:1A:916:A:OP1	12:1Q:6:ARG:NH1	2.34	0.60
1:2A:1354:G:H4'	29:27:7:PRO:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:554:G:N1	59:2A:3625:HOH:O	2.26	0.60
16:1U:76:TYR:OH	16:1U:92:ARG:NH1	2.32	0.60
1:2A:2325:C:H2'	1:2A:2326:G:C8	2.36	0.60
1:1A:1221:A:O2'	1:1A:1222:C:O4'	2.16	0.60
1:2A:585:G:OP2	59:2A:3624:HOH:O	2.16	0.60
7:2H:3:ARG:HB3	7:2H:3:ARG:NH1	2.16	0.60
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.82	0.60
18:2W:4:LYS:HB2	18:2W:106:ILE:HG12	1.82	0.60
1:1A:629:U:OP1	5:1F:102:PRO:HA	2.01	0.60
1:2A:2375:C:OP1	22:20:55:ARG:NH1	2.33	0.60
29:27:34:ARG:NH1	29:27:41:ARG:O	2.35	0.60
2:2B:40:U:N3	2:2B:43:C:OP2	2.34	0.60
14:2S:49:VAL:HG12	14:2S:80:LEU:HD22	1.82	0.60
1:1A:2901:G:N2	59:1A:4151:HOH:O	2.19	0.60
2:1B:66:A:H61	2:1B:108:U:H2'	1.66	0.60
1:2A:1826:U:H2'	1:2A:1827:C:C6	2.36	0.60
1:2A:2100:U:OP1	23:21:21:ARG:NH2	2.34	0.60
1:2A:1416:G:HO2'	1:2A:1417:U:H5	1.50	0.60
1:2A:2298:A:H62	1:2A:2355:U:H3	1.48	0.60
11:2P:38:GLN:HG2	11:2P:45:LEU:H	1.67	0.60
1:1A:137:G:H2'	1:1A:138:A:H8	10.02	0.60
1:1A:324:G:OP2	20:1Y:84:ARG:NH2	2.34	0.60
1:1A:330:G:H21	1:1A:353:A:H62	1.50	0.60
30:28:14:VAL:HG23	30:28:24:ALA:HB2	1.83	0.60
1:2A:1337:U:H2'	1:2A:1338:C:C6	2.37	0.60
1:2A:2733:A:OP1	59:2A:3622:HOH:O	2.16	0.60
1:1A:996:G:OP1	12:1Q:16:ARG:NH2	2.34	0.60
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.34	0.60
4:2E:199:ARG:HH12	4:2E:202:LYS:HE3	1.67	0.60
1:1A:2230:G:N7	59:1A:4224:HOH:O	2.30	0.59
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.84	0.59
4:1E:54:GLN:HE21	4:1E:55:ASN:N	1.97	0.59
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.83	0.59
25:23:8:LEU:HD13	25:23:31:LEU:HD23	1.85	0.59
1:2A:1104:G:H3'	1:2A:1105:U:C6	2.36	0.59
15:2T:64:ARG:HB2	15:2T:73:GLU:HG2	1.82	0.59
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.01	0.59
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.85	0.59
14:1S:59:LYS:HD2	14:1S:60:GLY:H	1.66	0.59
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.17	0.59
21:1Z:70:LEU:HG	21:1Z:91:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2803:C:H2'	1:1A:2804:G:H8	1.65	0.59
1:2A:1041:A:H2'	1:2A:1042:G:H8	1.66	0.59
1:2A:2879:C:H2'	1:2A:2880:C:O4'	2.02	0.59
1:2A:873:U:OP1	59:2A:3604:HOH:O	2.17	0.59
1:1A:2366:C:H1'	22:10:39:ARG:HH21	1.67	0.59
1:2A:1833:A:H4'	3:2D:259:THR:HG23	1.83	0.59
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.84	0.59
1:1A:1847:G:OP1	3:1D:88:ARG:NH2	2.35	0.59
1:2A:1101:G:H5''	1:2A:1102:A:H5'	1.84	0.59
4:2E:199:ARG:NH1	4:2E:202:LYS:HE3	2.17	0.59
7:2H:3:ARG:HH12	7:2H:5:GLY:N	2.00	0.59
11:2P:121:LYS:O	11:2P:123:LEU:N	2.36	0.59
1:2A:2302:U:H2'	1:2A:2303:C:C6	2.37	0.59
11:1P:62:LEU:O	30:18:13:ARG:HD3	2.02	0.59
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.34	0.59
1:2A:1064:U:HO2'	1:2A:1066:A:H2	1.48	0.59
1:1A:1565:U:H2'	1:1A:1566:G:O4'	2.03	0.59
6:1G:109:VAL:HG13	26:14:33:VAL:HG11	1.85	0.59
1:2A:2338:A:H2'	1:2A:2339:A:C8	2.37	0.59
1:2A:524:G:N1	1:2A:527:A:OP2	2.35	0.59
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.03	0.59
1:1A:478:C:OP1	59:1A:4107:HOH:O	2.17	0.58
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.18	0.58
1:2A:1084:G:H1	1:2A:1161:C:H42	1.51	0.58
1:2A:2858:U:OP2	15:2T:95:ARG:NH1	2.32	0.58
1:1A:2226:G:OP2	1:1A:2226:G:H4'	2.02	0.58
1:2A:1361:U:H2'	1:2A:1362:A:C8	2.38	0.58
6:2G:41:GLN:NE2	6:2G:154:GLY:O	2.34	0.58
1:2A:661:A:H2'	11:2P:117:GLU:OE2	2.03	0.58
13:2R:78:LYS:HG3	13:2R:82:GLU:HG3	1.85	0.58
1:1A:1153:U:O2'	1:1A:1154:C:H6	1.86	0.58
1:1A:2298:A:OP1	59:1A:4138:HOH:O	2.17	0.58
1:1A:2044:G:H5'	1:1A:2628:C:H4'	1.86	0.58
3:1D:126:GLN:NE2	3:1D:127:VAL:H	2.02	0.58
1:2A:2858:U:O4	15:2T:23:ARG:NH2	2.33	0.58
1:2A:310:C:H2'	1:2A:311:C:H6	1.68	0.58
6:2G:115:ARG:HG2	6:2G:136:ARG:HH21	1.67	0.58
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.85	0.58
19:2X:36:LYS:HA	19:2X:39:ILE:HD12	1.84	0.58
1:1A:1430:G:O2'	1:1A:1441:U:O2	2.16	0.58
1:1A:541:C:OP1	27:15:16:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1240:C:H2'	1:2A:1241:G:H8	1.67	0.58
14:2S:34:HIS:ND1	14:2S:53:SER:OG	2.34	0.58
21:2Z:130:PRO:HB2	21:2Z:131:ARG:HH21	1.67	0.58
1:1A:595:G:OP2	17:1V:78:LYS:NZ	2.32	0.58
25:23:30:ARG:H	25:23:33:GLN:NE2	2.02	0.58
1:2A:2328:C:H2'	1:2A:2329:G:C8	2.37	0.58
4:2E:1:MET:HE3	4:2E:199:ARG:HD2	1.86	0.58
30:28:32:LEU:O	30:28:36:LYS:HE3	2.04	0.58
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.67	0.58
1:1A:2800:C:OP1	4:1E:61:ARG:NH2	2.37	0.58
18:1W:12:ILE:HD13	18:1W:17:VAL:HG13	1.85	0.58
22:20:27:GLU:HG3	22:20:68:GLU:HA	1.86	0.58
1:2A:1423:A:OP1	29:27:10:ARG:NH2	2.37	0.58
1:2A:2568:G:H2'	1:2A:2569:C:C6	2.39	0.58
1:2A:897:U:H5'	25:23:49:LYS:HD2	1.85	0.58
13:1R:63:ARG:NH2	59:1R:303:HOH:O	2.37	0.58
1:2A:475:G:N7	59:2A:3685:HOH:O	2.32	0.58
8:2I:126:TYR:HB2	8:2I:142:VAL:HG23	1.86	0.58
12:1Q:60:ARG:CZ	12:1Q:60:ARG:H	2.16	0.58
24:22:17:SER:N	24:22:20:GLU:OE2	2.37	0.58
1:1A:1220:G:H21	1:1A:1221:A:H4'	1.69	0.57
1:1A:1245:C:H2'	1:1A:1246:C:C6	2.77	0.57
8:1I:4:ILE:HD11	8:1I:44:LEU:HD12	1.86	0.57
1:2A:1828:U:H5'	3:2D:259:THR:CG2	2.29	0.57
1:2A:2314:G:O2'	6:2G:132:ASN:HB2	2.04	0.57
1:1A:1784:C:OP1	15:1T:96:ARG:NH1	2.36	0.57
1:1A:2323:U:H5'	6:1G:88:ILE:HD11	1.85	0.57
1:2A:1232:U:H4'	17:2V:79:VAL:HG22	1.86	0.57
1:2A:1808:U:H2'	1:2A:1814:A:N6	2.19	0.57
1:2A:2465:G:H1'	59:2A:3654:HOH:O	2.03	0.57
1:2A:645:A:OP2	59:2A:3626:HOH:O	2.17	0.57
2:2B:15:A:OP2	2:2B:69:G:N2	2.34	0.57
2:2B:29:A:O2'	2:2B:58:A:N1	2.37	0.57
1:2A:1475:C:H2'	1:2A:1476:U:C6	2.40	0.57
1:2A:2278:A:H5''	1:2A:2279:A:H5'	1.85	0.57
5:2F:155:LEU:HD11	5:2F:176:LEU:HD12	1.85	0.57
6:2G:35:GLU:HG2	6:2G:36:LYS:HE2	1.86	0.57
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.86	0.57
1:1A:154:C:H42	1:1A:159:G:H1	1.52	0.57
1:2A:1451:U:H2'	1:2A:1452:C:C6	2.39	0.57
1:2A:2043:U:OP1	59:2A:3625:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2896:U:H2'	1:2A:2897:C:H6	1.69	0.57
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.04	0.57
17:2V:1:MET:HA	17:2V:42:GLY:HA3	1.86	0.57
26:14:26:SER:OG	26:14:27:THR:N	2.38	0.57
1:1A:2771:G:N7	59:1A:4240:HOH:O	2.33	0.57
1:2A:531:A:H4'	1:2A:532:G:O5'	4.01	0.57
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.85	0.57
10:2O:4:PRO:O	10:2O:5:GLN:HB2	2.05	0.57
1:1A:1397:U:OP2	59:1A:4140:HOH:O	2.18	0.57
1:2A:703:U:H2'	1:2A:704:C:C6	2.40	0.57
1:2A:706:G:H5'	5:2F:99:TYR:CE2	2.39	0.57
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.85	0.57
8:2I:50:ARG:HB3	8:2I:54:GLN:HE22	1.70	0.57
1:1A:309:C:H2'	1:1A:310:C:H6	1.69	0.57
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.20	0.57
1:2A:2896:U:H2'	1:2A:2897:C:C6	2.40	0.57
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.86	0.57
1:1A:159:G:O2'	1:1A:160:C:H5'	2.03	0.57
12:1Q:109:VAL:HG13	12:1Q:113:GLN:HB2	1.87	0.57
2:2B:28:C:H5''	14:2S:31:SER:OG	2.05	0.57
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.04	0.57
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	1.87	0.57
13:1R:55:ALA:HB2	13:1R:79:LEU:HD13	1.86	0.56
18:1W:18:ARG:NH1	18:1W:76:VAL:O	2.38	0.56
1:2A:69:A:N7	19:2X:31:HIS:HE1	2.03	0.56
1:2A:2761:A:H1'	7:2H:63:SER:HB3	1.86	0.56
1:1A:1219:U:OP1	1:1A:1221:A:N6	2.36	0.56
1:1A:1222:C:H2'	1:1A:1223:C:C6	2.40	0.56
15:2T:24:PRO:HA	15:2T:49:VAL:HG22	1.87	0.56
8:1I:37:VAL:HG13	8:1I:38:LEU:HD12	1.88	0.56
1:2A:865:A:C4	1:2A:1233:A:C2	2.93	0.56
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.87	0.56
21:2Z:11:GLU:O	21:2Z:36:LYS:NZ	2.36	0.56
28:16:10:LEU:HG	28:16:54:ILE:HG13	1.87	0.56
1:1A:2376:G:O6	30:18:39:LYS:HE3	2.06	0.56
1:1A:1070:G:C4	1:1A:1179:C:H1'	2.40	0.56
1:2A:1101:G:H4'	1:2A:1131:A:H8	1.70	0.56
1:2A:2310:G:H2'	1:2A:2311:G:C8	2.36	0.56
1:2A:272:G:H4'	1:2A:273:U:OP1	2.05	0.56
20:2Y:23:ARG:HG2	20:2Y:42:VAL:HG22	1.86	0.56
1:1A:552:A:C2	1:1A:2064:C:H4'	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2441:A:H2'	1:1A:2441:A:N3	2.21	0.56
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.71	0.56
23:21:56:GLN:HA	23:21:56:GLN:HE21	1.69	0.56
17:2V:31:ALA:O	17:2V:61:VAL:HG12	2.06	0.56
1:1A:666:G:H21	1:1A:670:A:H2	1.54	0.56
8:1I:14:ASP:N	8:1I:17:GLN:OE1	2.33	0.56
20:1Y:92:ASN:CB	20:1Y:94:LYS:H	2.14	0.56
1:1A:1450:U:H2'	1:1A:1451:U:C6	2.41	0.56
1:1A:2583:A:N7	4:1E:144:ARG:HD2	2.20	0.56
1:2A:1992:A:OP1	59:2A:3627:HOH:O	2.18	0.56
1:2A:2763:G:C4	7:2H:2:SER:HA	2.41	0.56
1:2A:2785:C:OP1	4:2E:166:THR:OG1	2.21	0.56
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.88	0.56
8:2I:102:SER:OG	8:2I:103:ARG:N	2.39	0.56
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HG2	1.87	0.56
1:1A:2859:A:OP2	1:1A:2875:U:H5	1.88	0.56
1:1A:555:C:H4'	1:1A:556:A:H5''	1.87	0.56
28:26:14:THR:OG1	28:26:48:VAL:O	2.19	0.56
1:2A:2384:G:H2'	1:2A:2385:C:C6	2.41	0.56
1:1A:1231:G:H5''	17:1V:81:TYR:CE1	2.40	0.56
1:1A:1245:C:H2'	1:1A:1246:C:H6	2.05	0.56
1:1A:1474:G:H2'	1:1A:1475:C:C6	2.40	0.56
13:1R:21:TYR:OH	13:1R:43:GLU:HG2	2.06	0.56
15:1T:108:ARG:HH22	15:1T:112:ARG:HH11	1.53	0.56
1:1A:1039:C:OP1	16:1U:53:ARG:NH2	2.39	0.56
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.39	0.56
4:2E:24:THR:HG23	4:2E:184:VAL:HG12	1.88	0.56
21:1Z:157:LEU:HD11	21:1Z:163:LEU:HD13	1.87	0.56
1:2A:1244:C:H2'	1:2A:1245:C:H6	2.36	0.56
1:2A:1992:A:OP2	3:2D:242:ARG:NH2	2.39	0.56
7:2H:9:ILE:N	7:2H:50:VAL:O	2.39	0.56
1:1A:2588:A:H5'	27:15:3:LYS:HD2	1.86	0.56
1:2A:2389:A:H4'	14:2S:23:ARG:HH11	1.70	0.56
1:2A:624:G:O2'	1:2A:701:A:N6	2.39	0.56
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.87	0.56
5:2F:117:ARG:HH12	11:2P:1:MET:N	2.04	0.56
1:1A:1833:A:O2'	3:1D:259:THR:HG21	2.06	0.55
7:1H:144:VAL:O	7:1H:148:ILE:HG12	2.06	0.55
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.38	0.55
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.88	0.55
17:2V:25:LEU:H	17:2V:92:THR:HG1	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1S:64:GLU:HB3	26:14:59:PHE:CD1	86.20	0.55
1:1A:1153:U:HO2'	1:1A:1154:C:P	2.29	0.55
1:1A:1064:U:H3	1:1A:1187:A:H62	1.54	0.55
1:1A:238:G:OP2	30:18:13:ARG:NH2	2.39	0.55
1:1A:57:U:H2'	1:1A:58:G:C8	5.61	0.55
1:2A:2347:A:H61	22:20:43:THR:HG22	1.71	0.55
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.87	0.55
1:1A:2494:C:N3	12:1Q:124:LYS:NZ	2.53	0.55
1:2A:1010:G:OP1	59:2A:3631:HOH:O	2.18	0.55
1:2A:1292:A:OP1	5:2F:95:ARG:NH2	2.40	0.55
1:2A:1638:G:H2'	1:2A:1639:G:H8	1.71	0.55
1:2A:927:G:H1	1:2A:940:U:H3	1.54	0.55
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.88	0.55
1:1A:1066:A:H62	1:1A:1185:U:H3	1.52	0.55
5:1F:14:PRO:HD2	5:1F:127:GLU:OE1	2.07	0.55
1:2A:1465:U:O2'	1:2A:1466:G:OP1	2.21	0.55
1:1A:2347:A:H61	22:10:43:THR:CG2	2.19	0.55
1:2A:2122:G:O6	1:2A:2209:C:N4	2.38	0.55
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.87	0.55
20:2Y:1:MET:HG2	20:2Y:2:ARG:H	1.70	0.55
1:1A:2208:G:H2'	1:1A:2209:C:C6	2.40	0.55
1:2A:1494:G:H1'	1:2A:1573:A:N1	2.22	0.55
1:2A:200:G:H2'	1:2A:201:A:O4'	2.07	0.55
15:1T:65:LYS:HE2	15:1T:67:SER:HB2	1.89	0.55
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.89	0.55
14:2S:26:LEU:HD22	14:2S:87:PHE:CD1	2.41	0.55
1:2A:2330:G:N1	14:2S:3:ARG:HA	2.21	0.55
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.41	0.55
1:2A:1041:A:H4'	16:2U:91:ASP:OD2	2.07	0.55
1:1A:1076:G:H21	31:19:36:GLN:HE22	1.54	0.55
1:1A:2227:G:O2'	1:1A:2228:A:OP1	2.25	0.55
28:26:13:CYS:SG	28:26:47:THR:HG21	2.47	0.55
1:2A:1409:G:P	23:21:3:LYS:HG3	2.47	0.55
1:1A:2332:G:H5''	1:1A:2333:A:OP2	2.07	0.55
1:2A:1753:G:H2'	1:2A:1754:C:C6	2.42	0.55
1:2A:2124:C:O2	1:2A:2207:G:N2	2.40	0.55
1:2A:412:G:OP1	59:2A:3629:HOH:O	2.18	0.55
3:2D:68:LYS:HD2	3:2D:70:TRP:CZ2	2.42	0.55
1:1A:2803:C:H2'	1:1A:2804:G:C8	2.42	0.54
1:1A:610:U:H2'	1:1A:611:C:C6	2.42	0.54
6:1G:49:ASP:C	6:1G:51:ARG:H	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1070:G:C4	1:2A:1179:C:H1'	2.43	0.54
2:2B:3:C:H2'	2:2B:4:C:C6	2.43	0.54
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.22	0.54
29:17:5:TRP:NE1	29:17:7:PRO:HG3	2.22	0.54
1:1A:1093:A:OP2	1:1A:1154:C:N4	2.36	0.54
30:28:63:PRO:HG2	30:28:64:TYR:CD2	2.42	0.54
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.89	0.54
1:1A:1845:A:OP2	3:1D:54:ARG:NH2	2.38	0.54
1:1A:2208:G:H4'	1:1A:2209:C:OP1	2.07	0.54
1:1A:2600:A:OP2	59:1A:4143:HOH:O	2.18	0.54
1:2A:118:G:H4'	1:2A:148:A:H5'	1.90	0.54
1:2A:2297:A:H4'	1:2A:2298:A:O4'	2.06	0.54
1:2A:2327:C:H2'	1:2A:2328:C:C6	2.42	0.54
1:2A:945:A:H2'	1:2A:946:A:O4'	2.07	0.54
1:1A:2648:U:H5''	4:1E:82:ARG:HH21	1.72	0.54
11:1P:121:LYS:O	11:1P:123:LEU:N	2.40	0.54
1:1A:1200:A:OP1	16:1U:55:ARG:HD3	2.07	0.54
1:2A:1734:U:O2	1:2A:1746:A:H5'	2.08	0.54
4:2E:54:GLN:HE21	4:2E:58:ARG:HB2	1.72	0.54
16:2U:86:ALA:HB2	16:2U:116:ALA:HB2	1.89	0.54
25:13:7:LYS:HG3	25:13:34:GLU:HG2	1.88	0.54
1:1A:598:U:H2'	1:1A:599:G:C8	2.43	0.54
14:1S:15:ARG:NE	14:1S:88:ASP:OD2	2.39	0.54
1:2A:1833:A:O2'	3:2D:259:THR:HG21	2.08	0.54
19:2X:35:THR:HG22	19:2X:37:THR:H	1.72	0.54
1:2A:1812:C:H1'	1:2A:2620:U:H5''	1.90	0.54
1:1A:172:C:H2'	1:1A:173:U:C6	2.43	0.54
1:1A:1735:A:N6	1:1A:1744:A:H2	1.96	0.54
3:1D:10:THR:OG1	3:1D:13:ARG:HB2	2.08	0.54
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.08	0.54
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.89	0.54
1:2A:425:G:OP2	59:2A:3630:HOH:O	2.18	0.54
1:2A:907:A:C2	1:2A:962:A:C4	2.96	0.54
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.08	0.54
4:2E:12:THR:HG22	15:2T:58:ASN:OD1	2.07	0.54
1:1A:1100:G:N2	1:1A:1149:C:O2	2.23	0.54
1:1A:2339:A:H2'	1:1A:2340:G:C8	2.43	0.54
1:1A:439:C:O2	1:1A:475:G:N2	74.55	0.54
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.35	0.54
1:2A:321:G:H5''	1:2A:322:A:OP1	2.08	0.54
1:2A:988:G:O3'	59:2A:3628:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:170:LEU:HB3	4:2E:184:VAL:HG22	1.90	0.54
5:2F:197:ASP:O	5:2F:200:GLU:HB2	2.08	0.54
14:2S:41:ASP:OD2	14:2S:44:LYS:NZ	2.40	0.54
1:1A:1540:A:H2'	1:1A:1541:A:C8	2.42	0.54
1:1A:309:C:H2'	1:1A:310:C:C6	2.43	0.54
1:2A:810:A:H5'	3:2D:210:GLY:HA2	1.90	0.54
1:1A:552:A:N1	1:1A:2063:A:H2'	2.23	0.54
1:1A:2315:G:H22	1:1A:2323:U:H3	1.56	0.54
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.07	0.54
20:1Y:5:MET:HE1	20:1Y:32:PRO:HA	1.90	0.54
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.40	0.54
1:2A:235:G:H4'	1:2A:412:G:C5	2.44	0.54
1:2A:2548:U:H2'	1:2A:2549:C:C6	2.43	0.54
1:2A:601:G:H2'	1:2A:602:C:C6	2.43	0.54
1:2A:82:A:N1	1:2A:96:G:O2'	2.37	0.54
6:2G:33:ARG:NH1	6:2G:162:THR:OG1	2.40	0.54
7:2H:117:PRO:HG3	7:2H:123:PHE:CD2	2.43	0.54
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.90	0.54
1:1A:554:G:N3	1:1A:554:G:O4'	2.39	0.53
15:1T:118:ARG:HG3	15:1T:118:ARG:NH1	2.23	0.53
1:2A:909:A:H2'	1:2A:910:G:C8	2.43	0.53
1:1A:1378:C:OP1	59:1A:4145:HOH:O	2.19	0.53
1:2A:863:C:O2'	1:2A:885:U:H5''	2.09	0.53
21:2Z:152:ALA:O	21:2Z:155:LEU:HB2	2.09	0.53
1:1A:2517:U:OP1	4:1E:144:ARG:NH2	2.41	0.53
1:2A:2227:G:H3'	1:2A:2228:A:H5''	1.88	0.53
1:2A:2323:U:C5	1:2A:2324:C:H5	2.27	0.53
1:2A:82:A:H5''	20:2Y:8:LYS:HE3	1.90	0.53
8:2I:14:ASP:O	8:2I:17:GLN:HB3	2.08	0.53
12:2Q:109:VAL:HG13	12:2Q:113:GLN:HB2	1.90	0.53
1:1A:1153:U:H6	1:1A:1154:C:C6	2.27	0.53
3:1D:9:TYR:CZ	3:1D:13:ARG:HG2	2.44	0.53
1:1A:956:A:H2'	12:1Q:9:TYR:OH	2.08	0.53
1:2A:346:G:O2'	1:2A:1249:U:N3	2.40	0.53
1:2A:2382:G:O2'	28:26:46:HIS:ND1	2.40	0.53
1:1A:1158:U:H2'	1:1A:1159:G:C8	2.44	0.53
1:1A:2249:G:N3	1:1A:2249:G:H2'	2.23	0.53
1:1A:266:C:OP2	59:1A:4141:HOH:O	2.18	0.53
1:1A:369:A:H2'	1:1A:370:A:H8	3.23	0.53
1:1A:717:C:N4	59:1A:4304:HOH:O	2.40	0.53
1:1A:1844:G:H4'	3:1D:51:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1105:U:H4'	1:2A:1106:U:H5'	1.90	0.53
1:2A:1233:A:OP2	59:2A:3633:HOH:O	2.19	0.53
3:2D:108:PRO:HD2	3:2D:111:LEU:HG	1.90	0.53
28:16:35:GLU:OE2	28:16:50:ARG:NH1	2.41	0.53
1:1A:1210:U:H2'	1:1A:1211:C:C6	2.42	0.53
14:1S:34:HIS:ND1	14:1S:53:SER:OG	2.38	0.53
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.44	0.53
1:1A:2347:A:H61	22:10:43:THR:HG22	1.73	0.53
1:1A:552:A:O2'	1:1A:553:A:H5'	2.08	0.53
2:1B:89:G:H2'	2:1B:90:A:C8	2.43	0.53
8:1I:106:GLY:HA2	8:1I:107:VAL:HB	1.90	0.53
1:2A:1194:G:H2'	1:2A:1195:C:C6	2.43	0.53
1:2A:22:G:O3'	59:2A:3632:HOH:O	2.18	0.53
1:2A:2308:C:H5	1:2A:2329:G:H21	1.57	0.53
3:2D:276:LYS:CD	3:2D:276:LYS:H	2.19	0.53
11:2P:39:LYS:HA	11:2P:45:LEU:HG	1.91	0.53
1:1A:138:A:H8	1:1A:1453:C:O2'	1.92	0.53
1:2A:1457:A:H2'	1:2A:1458:G:C8	2.43	0.53
6:2G:33:ARG:HH11	6:2G:33:ARG:HB2	1.74	0.53
1:2A:2760:A:O2'	7:2H:63:SER:O	2.17	0.53
1:1A:1697:G:OP1	13:1R:40:LYS:NZ	2.41	0.53
6:2G:32:PRO:HB3	6:2G:172:LEU:HD22	1.91	0.53
1:2A:2061:C:OP2	9:2N:109:LYS:NZ	2.42	0.53
26:14:47:GLN:O	26:14:49:PHE:N	2.41	0.53
1:1A:1149:C:H2'	1:1A:1150:U:H5	1.74	0.53
1:1A:1465:U:HO2'	1:1A:1466:G:P	2.32	0.53
1:1A:274:C:H2'	1:1A:275:C:C6	2.44	0.53
1:1A:558:U:H2'	1:1A:559:C:C6	2.44	0.53
1:2A:2668:A:O3'	7:2H:160:LYS:NZ	2.42	0.53
1:2A:2713:U:H4'	1:2A:2714:C:OP1	2.08	0.53
1:2A:542:G:H2'	1:2A:543:U:C6	2.44	0.53
2:2B:19:G:H2'	2:2B:20:C:O4'	2.08	0.53
3:2D:71:ASP:CB	3:2D:103:ARG:HH22	2.22	0.53
1:2A:1002:U:OP2	12:2Q:14:ARG:NH1	2.42	0.53
13:2R:37:THR:HA	13:2R:111:LEU:HD12	1.91	0.53
3:1D:71:ASP:HB3	3:1D:103:ARG:NH2	2.20	0.52
4:1E:170:LEU:HB3	4:1E:184:VAL:HG22	1.91	0.52
1:1A:62:A:O3'	19:1X:71:GLY:HA3	2.09	0.52
1:2A:2483:G:H2'	1:2A:2486:C:H42	1.74	0.52
1:2A:353:A:HO2'	1:2A:354:A:H8	1.54	0.52
1:2A:898:G:H2'	1:2A:899:G:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:40:ASP:OD1	21:2Z:42:VAL:HG13	2.09	0.52
26:14:53:GLU:HB3	26:14:54:GLY:CA	2.34	0.52
4:1E:120:TRP:CE3	4:1E:155:LYS:HD3	2.44	0.52
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.90	0.52
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.91	0.52
1:2A:1094:C:H1'	1:2A:1158:U:O2'	2.09	0.52
3:2D:145:VAL:HG12	3:2D:146:GLU:O	2.09	0.52
1:1A:1184:C:O3'	9:1N:25:ARG:NH1	2.41	0.52
1:1A:224:C:H2'	1:1A:225:C:C6	2.44	0.52
1:1A:2052:A:C6	1:1A:2509:C:H1'	2.45	0.52
1:1A:354:A:N1	59:1A:4247:HOH:O	2.34	0.52
1:1A:922:C:H2'	1:1A:923:U:O4'	2.10	0.52
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.91	0.52
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.90	0.52
25:23:5:LYS:HE2	25:23:34:GLU:OE2	2.09	0.52
1:2A:1342:C:H2'	1:2A:1343:C:H6	1.74	0.52
1:2A:1524:G:HO2'	1:2A:1604:A:H2	1.53	0.52
1:2A:2568:G:H2'	1:2A:2569:C:H6	1.74	0.52
1:2A:821:G:N3	59:2A:3694:HOH:O	2.33	0.52
1:1A:1920:G:N3	1:1A:1920:G:H2'	2.24	0.52
1:2A:1873:C:H5'	3:2D:253:GLN:NE2	2.24	0.52
6:2G:73:ALA:HB3	6:2G:85:GLY:H	1.75	0.52
13:2R:21:TYR:OH	13:2R:43:GLU:HG2	2.10	0.52
1:1A:1155:G:H21	1:1A:1156:A:H2	1.57	0.52
6:1G:115:ARG:HG3	6:1G:136:ARG:HH22	1.74	0.52
1:2A:10:G:N7	59:2A:3696:HOH:O	2.34	0.52
1:2A:1924:G:OP1	3:2D:241:PRO:HB2	2.08	0.52
1:2A:732:G:N2	1:2A:834:A:H61	2.07	0.52
26:14:15:ILE:HD12	26:14:21:VAL:HG22	1.91	0.52
1:1A:1726:U:OP2	59:1A:4147:HOH:O	2.19	0.52
1:2A:1189:G:H2'	1:2A:1190:C:H6	3.27	0.52
3:2D:71:ASP:HB3	3:2D:103:ARG:HH22	1.75	0.52
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.45	0.52
11:1P:95:VAL:HG22	11:1P:125:VAL:HB	1.92	0.52
1:2A:1455:G:H2'	1:2A:1456:C:H6	1.74	0.52
1:2A:104:C:H2'	1:2A:105:U:H6	1.75	0.52
1:2A:1116:G:H1	1:2A:1124:C:N4	15.42	0.52
1:2A:1282:A:OP1	59:2A:3635:HOH:O	2.19	0.52
1:2A:228:G:H1'	1:2A:258:A:N1	40.03	0.52
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.42	0.52
1:1A:2297:A:H4'	1:1A:2298:A:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.26	0.52
14:1S:3:ARG:C	14:1S:3:ARG:HD3	2.29	0.52
1:2A:1047:G:H2'	1:2A:1048:G:O4'	2.10	0.52
1:2A:2704:A:H2'	1:2A:2705:G:H8	1.74	0.52
1:1A:1232:U:H4'	17:1V:79:VAL:HG22	1.92	0.52
1:1A:1323:A:OP1	13:1R:36:THR:HG23	2.10	0.52
1:1A:1409:G:N7	23:11:3:LYS:HE2	2.25	0.52
1:1A:2622:U:C4	27:15:3:LYS:HG2	2.45	0.52
1:1A:2723:U:O2'	1:1A:2725:A:H5'	2.10	0.52
1:1A:286:G:N7	1:1A:447:U:H2'	2.25	0.52
1:2A:1625:A:H2'	1:2A:1626:A:C8	2.44	0.52
1:2A:2489:A:OP2	31:29:2:LYS:NZ	2.24	0.52
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.90	0.52
19:2X:35:THR:HG22	19:2X:37:THR:N	2.25	0.52
23:11:21:ARG:NH1	23:11:21:ARG:HG2	2.16	0.51
29:17:34:ARG:NH1	29:17:41:ARG:O	2.42	0.51
1:1A:183:A:OP1	11:1P:46:LYS:NZ	2.43	0.51
1:1A:2043:U:O2'	1:1A:2628:C:H5'	2.10	0.51
1:1A:924:A:H2'	1:1A:925:G:C8	4.73	0.51
1:2A:1518:A:N6	1:2A:1566:G:O2'	2.43	0.51
1:2A:324:G:N2	1:2A:339:C:O2	2.31	0.51
1:1A:125:C:O3'	59:1A:4149:HOH:O	2.19	0.51
1:1A:2307:U:OP2	14:1S:9:ARG:NH2	2.43	0.51
4:1E:179:GLU:HB3	4:1E:181:LEU:HD22	1.92	0.51
8:1I:68:LEU:HD11	8:1I:109:ILE:HD11	1.92	0.51
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.10	0.51
25:23:39:ASP:OD1	25:23:44:ARG:HD2	2.10	0.51
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.93	0.51
1:2A:173:U:H4'	1:2A:206:A:H4'	1.92	0.51
1:2A:2017:C:H4'	1:2A:2018:G:OP1	2.09	0.51
1:2A:609:C:OP2	11:2P:21:ARG:NH2	2.43	0.51
1:2A:945:A:H2'	1:2A:946:A:H8	1.74	0.51
3:2D:137:PRO:O	3:2D:140:THR:HG23	2.11	0.51
3:2D:71:ASP:OD2	3:2D:103:ARG:NH2	2.42	0.51
5:2F:117:ARG:HH12	11:2P:1:MET:H2	1.56	0.51
1:1A:468:A:H1'	1:1A:1245:C:O4'	2.10	0.51
1:1A:1451:U:H2'	1:1A:1452:C:C6	2.46	0.51
1:1A:2207:G:H2'	1:1A:2208:G:H8	1.76	0.51
1:1A:355:A:OP1	59:1A:4148:HOH:O	2.19	0.51
5:1F:18:ARG:HG2	5:1F:19:GLU:H	1.75	0.51
12:1Q:60:ARG:CZ	12:1Q:60:ARG:N	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.92	0.51
2:2B:119:G:H2'	2:2B:120:A:O4'	2.10	0.51
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.92	0.51
12:2Q:110:THR:HG23	12:2Q:113:GLN:OE1	2.10	0.51
1:1A:1066:A:H3'	1:1A:1066:A:C8	2.45	0.51
1:1A:1873:C:H5'	3:1D:253:GLN:NE2	2.25	0.51
1:1A:2429:A:H2'	1:1A:2430:U:C6	2.45	0.51
1:1A:2640:A:O2'	1:1A:2641:G:OP2	2.25	0.51
1:1A:859:U:H2'	1:1A:860:C:C6	2.45	0.51
1:1A:942:C:H2'	1:1A:943:C:C6	2.45	0.51
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.26	0.51
1:2A:1020:G:C2	1:2A:1035:A:C8	2.98	0.51
1:2A:1092:G:H1'	1:2A:1155:G:N2	2.24	0.51
1:2A:1887:G:O2'	1:2A:1906:A:N6	2.43	0.51
1:2A:480:C:N3	1:2A:497:A:H2'	2.26	0.51
2:2B:44:G:OP1	6:2G:98:ARG:NH2	2.28	0.51
27:15:16:ARG:HH11	27:15:16:ARG:HG2	1.76	0.51
1:1A:1552:A:O2'	1:1A:1553:A:H8	1.91	0.51
1:1A:216:A:H3'	1:1A:217:A:C5'	2.41	0.51
1:1A:504:A:N3	1:1A:506:G:H5''	2.25	0.51
2:1B:7:G:H5'	14:1S:29:PHE:CE2	2.46	0.51
19:1X:57:LEU:CD1	19:1X:78:LYS:HB2	2.41	0.51
1:2A:2037:U:H2'	1:2A:2038:U:C6	2.45	0.51
1:2A:2419:U:H2'	1:2A:2420:G:C8	2.46	0.51
1:2A:356:G:H5''	1:2A:357:C:OP2	2.11	0.51
3:2D:134:ARG:HD3	3:2D:135:PHE:CE1	2.45	0.51
16:2U:97:ASP:OD1	16:2U:101:ARG:HD2	2.11	0.51
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.90	0.51
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.92	0.51
59:1A:5442:HOH:O	23:11:33:LYS:HE3	2.10	0.51
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.92	0.51
1:1A:2575:A:C2	1:1A:2658:U:H4'	2.46	0.51
2:1B:90:A:N7	2:1B:91:C:H1'	2.25	0.51
3:1D:126:GLN:HE21	3:1D:127:VAL:H	1.58	0.51
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.91	0.51
1:2A:172:C:H2'	1:2A:173:U:H6	1.76	0.51
1:2A:2650:A:N7	1:2A:2787:A:H2	2.09	0.51
1:2A:2659:C:H2'	1:2A:2660:U:C6	2.46	0.51
1:2A:2830:A:H2'	1:2A:2831:G:C8	2.46	0.51
3:2D:77:ALA:HB2	3:2D:97:TYR:CD2	2.46	0.51
6:2G:15:VAL:HG13	6:2G:175:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1070:G:O2'	59:1A:4127:HOH:O	2.12	0.51
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.25	0.51
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.93	0.51
9:1N:8:GLN:HA	9:1N:8:GLN:HE21	1.76	0.51
15:1T:127:ALA:O	15:1T:128:GLU:HB3	2.10	0.51
1:2A:358:C:H4'	20:2Y:73:ARG:HD2	1.93	0.51
1:2A:913:C:H2'	1:2A:914:U:H6	1.75	0.51
1:2A:968:C:H2'	1:2A:969:C:H6	1.76	0.51
3:2D:145:VAL:HB	3:2D:155:LEU:HB2	1.92	0.51
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.92	0.51
1:1A:1086:C:H42	1:1A:1159:G:H1	1.57	0.51
1:1A:931:C:H3'	1:1A:932:C:H5''	1.92	0.51
1:1A:955:A:H2'	1:1A:956:A:H5''	4.48	0.51
1:1A:775:G:C6	3:1D:208:LYS:HB2	2.45	0.51
1:2A:1104:G:H5''	1:2A:1105:U:H2'	1.92	0.51
1:2A:117:U:OP1	59:2A:3638:HOH:O	2.19	0.51
1:2A:1210:U:H2'	1:2A:1211:C:C6	2.46	0.51
1:2A:1320:A:N3	1:2A:1321:A:H1'	2.26	0.51
1:2A:2050:G:H2'	1:2A:2052:A:OP1	2.11	0.51
1:2A:2376:G:O6	30:28:39:LYS:HE3	2.11	0.51
7:2H:46:GLU:HB2	7:2H:49:VAL:HG12	1.91	0.51
16:2U:112:ARG:NH2	17:2V:47:VAL:HB	2.25	0.51
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.35	0.51
12:1Q:21:THR:HG21	12:1Q:101:ARG:HB2	1.93	0.51
1:2A:1096:G:H2'	1:2A:1097:C:C6	2.46	0.51
1:2A:1565:U:H2'	1:2A:1566:G:O4'	2.11	0.51
1:2A:33:C:O2'	1:2A:34:G:OP1	2.28	0.51
1:2A:982:G:OP1	30:28:52:LYS:HD2	2.11	0.51
2:2B:54:G:N2	2:2B:55:U:O2	2.44	0.51
7:2H:106:THR:HG22	7:2H:112:PRO:HB3	1.93	0.51
1:2A:468:A:H1'	1:2A:1245:C:O4'	2.10	0.51
1:2A:858:C:H2'	1:2A:859:U:H6	1.77	0.51
1:2A:910:G:C6	1:2A:911:C:N4	2.79	0.51
14:2S:23:ARG:NH2	14:2S:84:GLN:HB3	2.25	0.51
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.11	0.50
14:1S:48:LEU:HD23	14:1S:82:ILE:HD11	1.91	0.50
1:2A:1090:A:H5''	1:2A:1092:G:O4'	2.11	0.50
1:2A:1096:G:H2'	1:2A:1097:C:H6	1.76	0.50
1:2A:1150:U:H2'	1:2A:1151:G:H8	1.76	0.50
1:2A:237:C:O2	30:28:12:LYS:NZ	2.31	0.50
1:2A:647:G:H2'	1:2A:648:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:237:C:O2	1:1A:281:G:N2	64.67	0.50
5:1F:28:ILE:HA	5:1F:112:MET:HG2	1.92	0.50
8:1I:14:ASP:O	8:1I:17:GLN:HB3	2.11	0.50
9:1N:68:GLU:HG2	9:1N:88:GLU:OE2	2.12	0.50
1:2A:1015:C:OP2	59:2A:3634:HOH:O	2.19	0.50
1:2A:1073:A:N6	1:2A:1170:G:H2'	2.27	0.50
1:2A:1682:C:H2'	1:2A:1683:A:C8	2.45	0.50
1:2A:1814:A:OP2	59:2A:3602:HOH:O	2.19	0.50
1:2A:2095:U:H2'	1:2A:2096:U:C6	2.46	0.50
2:2B:50:G:OP1	14:2S:63:THR:N	2.45	0.50
1:2A:720:G:O2'	5:2F:74:ARG:HD3	2.12	0.50
1:1A:1054:A:OP2	9:1N:37:LYS:NZ	2.37	0.50
1:1A:201:A:H2'	1:1A:202:G:O4'	2.11	0.50
3:1D:175:LEU:HD12	3:1D:185:VAL:HG21	1.92	0.50
4:1E:111:ARG:HG3	4:1E:160:TYR:CD2	2.46	0.50
7:1H:56:SER:OG	7:1H:61:HIS:ND1	2.37	0.50
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.46	0.50
1:2A:1457:A:H2'	1:2A:1458:G:H8	1.76	0.50
7:2H:95:ARG:HG2	7:2H:106:THR:OG1	2.10	0.50
20:2Y:44:ILE:HD13	20:2Y:44:ILE:H	1.75	0.50
1:1A:2254:U:H2'	1:1A:2255:U:C6	2.47	0.50
1:1A:924:A:H2'	1:1A:925:G:H5'	1.94	0.50
4:1E:34:VAL:HG13	4:1E:48:GLN:HG2	1.93	0.50
1:2A:2685:G:H2'	1:2A:2686:A:C8	2.46	0.50
1:2A:2845:U:H2'	1:2A:2846:G:C8	2.46	0.50
1:2A:363:A:H2'	1:2A:364:G:O4'	2.12	0.50
1:2A:867:A:H2'	1:2A:990:G:H5''	1.93	0.50
1:2A:2428:C:OP1	11:2P:65:ARG:NH2	2.45	0.50
1:2A:1426:G:O2'	15:2T:122:ASP:OD2	93.50	0.50
26:14:63:TYR:CD1	26:14:63:TYR:N	2.79	0.50
5:1F:18:ARG:NH2	5:1F:127:GLU:OE2	2.45	0.50
12:1Q:2:LEU:HD12	12:1Q:2:LEU:H	1.76	0.50
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG13	1.93	0.50
23:21:77:ALA:HA	23:21:80:LEU:HD13	1.94	0.50
1:2A:12:A:N1	1:2A:549:U:H2'	2.27	0.50
6:2G:12:TYR:HA	6:2G:16:ARG:HG3	1.94	0.50
6:2G:48:GLU:HA	6:2G:51:ARG:NE	2.26	0.50
1:2A:1067:G:N7	9:2N:66:LYS:HE2	2.27	0.50
1:2A:2539:U:O2'	1:2A:2540:G:H3'	2.12	0.50
1:2A:900:G:N3	1:2A:1381:A:H2	127.07	0.50
1:1A:206:A:C2	1:1A:223:U:H4'	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2694:C:O2	10:1O:70:LYS:NZ	2.34	0.50
1:1A:353:A:HO2'	1:1A:354:A:H8	1.54	0.50
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.94	0.50
21:1Z:110:GLY:HA3	21:1Z:174:VAL:HG11	1.93	0.50
1:2A:2272:C:O2'	1:2A:2273:U:H5'	2.12	0.50
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.93	0.50
21:2Z:183:LEU:HD12	21:2Z:186:GLU:OE1	2.11	0.50
1:1A:1067:G:N2	1:1A:1068:U:O4	2.43	0.50
1:1A:1198:C:OP1	16:1U:92:ARG:NH1	2.44	0.50
1:1A:1475:C:H2'	1:1A:1476:U:C6	2.46	0.50
1:2A:1211:C:H2'	1:2A:1212:U:C6	2.46	0.50
1:2A:1240:C:H2'	1:2A:1241:G:C8	2.45	0.50
1:2A:2331:A:H2'	1:2A:2331:A:N3	2.27	0.50
1:2A:885:U:H2'	1:2A:886:C:C6	2.46	0.50
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	1.93	0.50
8:2I:129:THR:HG22	8:2I:139:GLN:NE2	2.24	0.50
16:2U:83:LEU:O	16:2U:87:GLY:N	2.45	0.50
20:2Y:37:VAL:HG21	20:2Y:72:VAL:HG21	1.93	0.50
1:1A:1223:C:H2'	1:1A:1224:C:H6	1.75	0.50
1:1A:2858:U:H4'	1:1A:2877:A:C2	2.47	0.50
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.47	0.50
10:1O:98:VAL:HG13	10:1O:117:LEU:HB3	1.94	0.50
1:2A:924:A:H2'	1:2A:925:G:C8	4.71	0.50
9:2N:30:ILE:HG22	9:2N:34:LEU:HD22	1.93	0.50
17:2V:21:ARG:HG2	17:2V:91:TYR:CD2	2.47	0.50
1:1A:842:C:H2'	1:1A:843:C:C6	2.47	0.49
29:27:24:THR:O	29:27:28:ARG:HG3	2.11	0.49
1:2A:396:G:OP2	59:2A:3639:HOH:O	2.20	0.49
1:1A:137:G:H2'	1:1A:138:A:C8	9.19	0.49
1:1A:551:C:C5	1:1A:2791:U:H2'	2.47	0.49
1:1A:637:U:H5''	59:1A:5743:HOH:O	2.11	0.49
1:1A:830:A:H5'	1:1A:831:G:OP1	2.12	0.49
6:1G:170:ARG:HD3	6:1G:174:GLU:HG3	1.93	0.49
1:2A:2088:G:O2'	1:2A:2090:G:H5''	2.12	0.49
1:2A:324:G:OP2	20:2Y:84:ARG:NH2	2.45	0.49
4:2E:119:ARG:HD2	4:2E:120:TRP:NE1	2.27	0.49
17:2V:14:VAL:HA	17:2V:18:LEU:HD12	1.94	0.49
1:1A:1158:U:H2'	1:1A:1159:G:H8	1.76	0.49
3:1D:68:LYS:HD2	3:1D:70:TRP:CZ2	2.48	0.49
19:1X:57:LEU:HD12	19:1X:78:LYS:HB2	1.94	0.49
1:2A:614:G:HO2'	30:28:64:TYR:HH	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:104:C:H2'	1:2A:105:U:C6	2.46	0.49
1:2A:1231:G:H5'	17:2V:81:TYR:CE1	2.48	0.49
6:1G:118:ARG:O	6:1G:181:ARG:HB3	2.11	0.49
12:1Q:52:VAL:O	12:1Q:56:ARG:HG3	2.12	0.49
1:2A:1556:A:H2'	1:2A:1557:G:C8	2.47	0.49
1:2A:320:C:H2'	1:2A:321:G:O4'	2.12	0.49
1:1A:277:G:O6	59:1A:4139:HOH:O	2.18	0.49
1:1A:1830:C:OP2	3:1D:183:ARG:NH2	2.46	0.49
4:1E:48:GLN:OE1	4:1E:66:HIS:NE2	2.39	0.49
1:2A:1201:A:O4'	16:2U:51:LYS:NZ	2.45	0.49
1:2A:69:A:H5''	1:2A:71:A:C8	2.47	0.49
1:2A:919:G:N2	1:2A:950:U:C2	2.81	0.49
1:2A:2318:G:N1	6:2G:43:LEU:O	2.39	0.49
28:16:21:TYR:CE2	28:16:38:LYS:HG2	2.48	0.49
1:1A:964:G:N2	1:1A:2280:A:OP2	2.45	0.49
1:1A:714:G:H5'	1:1A:715:G:OP2	2.12	0.49
2:1B:45:A:O4'	6:1G:95:ARG:NH1	2.46	0.49
5:1F:129:PHE:CD1	5:1F:163:VAL:HG21	2.47	0.49
1:1A:2651:G:OP1	9:1N:97:ARG:NH2	2.46	0.49
25:23:7:LYS:NZ	25:23:32:GLN:O	2.46	0.49
1:2A:1246:C:H2'	1:2A:1247:G:H8	3.25	0.49
1:2A:1820:C:H5''	1:2A:1821:A:OP1	2.12	0.49
1:2A:1920:G:N3	1:2A:1920:G:H2'	2.28	0.49
1:2A:894:G:H2'	1:2A:895:A:H8	1.78	0.49
1:2A:6:G:H4'	9:2N:13:TRP:CH2	2.47	0.49
1:1A:1311:G:O4'	18:1W:15:ARG:NH2	2.43	0.49
1:1A:1652:C:H4'	1:1A:1653:A:O5'	2.13	0.49
1:1A:2107:U:H2'	1:1A:2108:G:C8	2.47	0.49
1:1A:1002:U:OP2	12:1Q:14:ARG:HD3	2.13	0.49
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.31	0.49
1:2A:1156:A:N3	1:2A:1157:G:H1'	2.28	0.49
1:2A:2691:C:OP2	4:2E:111:ARG:NH2	2.45	0.49
1:2A:353:A:H2	1:2A:1254:A:O2'	1.96	0.49
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.48	0.49
26:14:16:CYS:SG	26:14:17:GLY:N	2.86	0.49
3:1D:167:GLY:H	3:1D:168:ARG:CZ	7.90	0.49
1:2A:895:A:H2	25:23:24:LYS:HB3	1.78	0.49
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.34	0.49
15:2T:23:ARG:HG3	15:2T:120:ARG:NH1	2.27	0.49
21:2Z:100:VAL:HG21	21:2Z:134:PRO:HG2	1.95	0.49
12:1Q:34:LEU:HD11	12:1Q:129:THR:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.95	0.49
21:1Z:145:GLU:O	21:1Z:148:ASP:N	2.35	0.49
1:2A:1072:A:C2	1:2A:2499:A:H5'	2.48	0.49
1:2A:1336:C:H2'	1:2A:1337:U:C6	2.48	0.49
1:2A:183:A:OP1	11:2P:46:LYS:NZ	2.45	0.49
1:2A:1953:A:H2'	1:2A:1954:G:O4'	2.13	0.49
1:2A:1967:U:H2'	1:2A:1968:C:C6	2.48	0.49
1:2A:670:A:H2'	1:2A:671:G:O4'	2.12	0.49
1:2A:810:A:H5'	3:2D:210:GLY:CA	2.42	0.49
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.46	0.49
6:2G:41:GLN:HG3	6:2G:60:LEU:HD21	1.95	0.49
14:2S:58:LEU:H	14:2S:58:LEU:HD23	1.77	0.49
14:2S:67:ARG:O	14:2S:71:ARG:HG3	2.13	0.49
20:2Y:49:VAL:HG21	20:2Y:61:ILE:HG23	1.95	0.49
1:1A:1067:G:C5	1:1A:1068:U:C4	6.57	0.49
1:1A:171:C:H2'	1:1A:172:C:C6	3.51	0.49
1:1A:1826:U:H2'	1:1A:1827:C:H6	1.78	0.49
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.95	0.49
14:1S:64:GLU:HB3	26:14:59:PHE:HD1	86.71	0.49
1:2A:1403:G:O2'	1:2A:1404:A:H5'	2.12	0.49
1:2A:1313:A:C2	1:2A:2034:A:C4	3.01	0.49
1:2A:2086:C:H2'	1:2A:2087:C:C6	2.48	0.49
1:2A:2760:A:H3'	1:2A:2761:A:H8	1.78	0.49
1:2A:2765:A:N3	31:29:15:LYS:NZ	2.55	0.49
1:2A:550:A:OP1	59:2A:3637:HOH:O	2.19	0.49
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.43	0.49
4:2E:72:VAL:HG12	4:2E:73:GLU:O	2.13	0.49
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.95	0.49
18:2W:24:ILE:HA	18:2W:27:LYS:HG3	1.94	0.49
1:1A:2207:G:H2'	1:1A:2208:G:C8	2.47	0.48
11:1P:126:VAL:HG12	11:1P:148:LEU:HD13	1.95	0.48
21:1Z:52:SER:OG	21:1Z:53:ILE:N	2.44	0.48
1:2A:2205:G:H2'	1:2A:2206:C:O4'	2.13	0.48
1:2A:2302:U:O2'	1:2A:2385:C:O2	2.29	0.48
1:2A:2386:G:O2'	1:2A:2388:A:N7	2.40	0.48
1:2A:359:C:H5''	20:2Y:6:HIS:ND1	2.28	0.48
1:2A:644:G:N3	1:2A:644:G:H5'	2.28	0.48
1:2A:663:U:H2'	1:2A:664:C:H6	1.77	0.48
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.95	0.48
26:14:14:ILE:HD11	26:14:24:THR:HG21	1.94	0.48
1:1A:1091:A:H5'	1:1A:1092:G:C8	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1099:A:H2'	1:1A:1100:G:O4'	2.13	0.48
1:1A:1716:C:OP1	59:1A:4154:HOH:O	2.20	0.48
1:2A:614:G:O2'	30:28:4:MET:HG3	2.14	0.48
1:2A:1513:C:C5	1:2A:1592:C:H2'	2.47	0.48
1:2A:634:C:H2'	1:2A:635:G:O4'	2.13	0.48
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.48	0.48
7:2H:71:LEU:HA	7:2H:71:LEU:HD12	1.74	0.48
29:17:24:THR:O	29:17:28:ARG:HG3	2.13	0.48
1:1A:670:A:H2'	1:1A:671:G:O4'	2.13	0.48
1:1A:703:U:H2'	1:1A:704:C:C6	2.48	0.48
1:2A:1076:G:H21	31:29:36:GLN:HE22	1.60	0.48
1:2A:1239:G:N2	1:2A:1240:C:C2	2.82	0.48
1:2A:822:G:H4'	1:2A:823:A:O5'	2.13	0.48
1:2A:2800:C:P	4:2E:61:ARG:HH21	2.35	0.48
5:2F:101:LEU:O	5:2F:106:ARG:HD3	2.13	0.48
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.95	0.48
1:1A:1073:A:N6	1:1A:1170:G:H2'	2.28	0.48
1:1A:120:G:OP2	59:1A:4150:HOH:O	2.19	0.48
8:1I:110:ASP:HA	8:1I:111:PRO:HD2	1.67	0.48
1:2A:1685:U:H2'	1:2A:1686:C:H5''	1.94	0.48
1:2A:1826:U:H2'	1:2A:1827:C:H6	1.77	0.48
1:2A:2037:U:H2'	1:2A:2038:U:H6	1.79	0.48
1:2A:2239:G:C5	1:2A:2240:C:C4	3.01	0.48
1:2A:2563:U:H2'	1:2A:2565:U:H5''	1.95	0.48
1:2A:898:G:H2'	1:2A:899:G:H8	1.77	0.48
20:2Y:49:VAL:HG11	20:2Y:55:TYR:CD2	2.48	0.48
1:1A:2117:U:H3	1:1A:2214:G:H1	1.62	0.48
1:1A:2338:A:H2'	1:1A:2339:A:C8	2.48	0.48
1:1A:800:C:H2'	1:1A:801:C:C6	2.48	0.48
1:2A:1726:U:O2	1:2A:1793:G:H3'	2.12	0.48
6:2G:111:LEU:HB3	6:2G:117:PHE:CE2	2.49	0.48
21:2Z:7:ALA:HB3	21:2Z:61:LEU:HD12	1.94	0.48
1:1A:2845:U:H2'	1:1A:2846:G:C8	2.48	0.48
1:2A:724:C:H2'	1:2A:725:C:C6	2.49	0.48
18:2W:33:ARG:NH2	18:2W:52:GLU:OE1	2.43	0.48
1:1A:2095:U:H2'	1:1A:2096:U:C6	2.48	0.48
1:1A:2212:G:H5'	1:1A:2213:G:OP2	2.14	0.48
12:1Q:12:GLN:HG3	12:1Q:73:PRO:HD2	1.95	0.48
21:1Z:45:ASP:O	21:1Z:49:ARG:HG3	2.13	0.48
25:23:46:ASN:O	25:23:50:VAL:HG22	2.13	0.48
1:2A:105:U:H2'	1:2A:106:G:H8	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1373:G:H2'	1:2A:1375:C:C5	2.48	0.48
1:2A:1474:G:H2'	1:2A:1475:C:C6	2.48	0.48
1:2A:1980:G:N7	59:2A:3700:HOH:O	2.35	0.48
1:2A:964:G:N2	1:2A:2280:A:OP2	2.42	0.48
1:2A:623:C:O2	1:2A:627:C:H4'	2.14	0.48
4:2E:97:LYS:N	4:2E:100:GLU:OE1	2.33	0.48
9:2N:96:GLU:H	9:2N:96:GLU:CD	2.16	0.48
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.14	0.48
1:1A:1337:U:H2'	1:1A:1338:C:C6	2.49	0.48
1:1A:1889:A:N6	1:1A:1904:G:O2'	2.46	0.48
1:2A:1103:G:H2'	1:2A:1104:G:C8	2.49	0.48
1:2A:555:C:H4'	1:2A:556:A:H5''	1.95	0.48
2:2B:1:U:H2'	2:2B:2:C:C5	2.49	0.48
6:2G:41:GLN:NE2	6:2G:153:ARG:HB3	2.24	0.48
15:2T:53:ARG:HH11	15:2T:53:ARG:HB3	1.78	0.48
21:2Z:54:HIS:ND1	21:2Z:101:PRO:HG3	2.28	0.48
22:10:43:THR:HG23	22:10:43:THR:O	2.14	0.48
1:1A:2123:U:H2'	1:1A:2124:C:C6	2.49	0.48
1:1A:258:A:C6	1:1A:259:A:C6	3.96	0.48
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.79	0.48
10:1O:17:ARG:HG3	10:1O:17:ARG:HH11	3.66	0.48
1:2A:94:G:H4'	24:22:48:HIS:NE2	2.29	0.48
1:2A:138:A:C8	1:2A:1453:C:O2'	2.66	0.48
1:2A:1406:G:H2'	1:2A:1407:C:C6	3.12	0.48
1:2A:2207:G:N1	1:2A:2208:G:O6	2.47	0.48
1:2A:516:A:H2'	1:2A:517:G:O4'	2.13	0.48
1:2A:830:A:C8	1:2A:838:G:C5	3.02	0.48
4:2E:14:ILE:HD11	4:2E:173:VAL:HG11	1.94	0.48
15:2T:84:GLN:HG2	15:2T:85:LYS:HD3	1.95	0.48
20:2Y:5:MET:HE1	20:2Y:32:PRO:HA	1.96	0.48
1:1A:326:U:O4	59:1A:4153:HOH:O	2.20	0.48
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.14	0.48
1:1A:359:C:HO2'	20:1Y:35:TYR:HH	1.62	0.48
1:2A:1060:G:O2'	1:2A:1061:G:H5'	2.14	0.48
1:2A:209:A:C8	1:2A:254:G:C6	3.02	0.48
1:2A:484:U:H5''	29:27:40:TRP:CD2	2.49	0.48
1:2A:646:G:H2'	1:2A:647:G:H8	1.79	0.48
2:2B:73:A:C4	2:2B:105:A:C2	3.02	0.48
4:2E:127:ASP:OD2	59:2E:401:HOH:O	2.20	0.48
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.44	0.48
6:2G:98:ARG:H	6:2G:98:ARG:HG2	1.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:75:THR:HG21	12:2Q:87:LYS:NZ	2.29	0.48
14:2S:15:ARG:HB3	14:2S:19:LYS:NZ	2.28	0.48
1:1A:2659:C:H2'	1:1A:2660:U:C6	2.49	0.47
8:1I:72:LEU:C	8:1I:74:ASN:H	2.18	0.47
14:1S:43:GLU:OE2	26:14:67:TYR:HE2	109.53	0.47
1:2A:903:C:H4'	22:20:23:VAL:HG21	1.96	0.47
1:2A:113:C:H2'	1:2A:114:G:O4'	2.13	0.47
1:2A:1620:C:H2'	1:2A:1621:C:C6	2.49	0.47
1:2A:94:G:H4'	24:22:48:HIS:CD2	2.49	0.47
6:2G:29:TRP:HE3	6:2G:33:ARG:HE	1.61	0.47
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.53	0.47
10:2O:63:VAL:HG12	10:2O:106:LEU:HD11	1.96	0.47
23:11:51:VAL:HG21	23:11:74:VAL:HG21	1.96	0.47
1:1A:1520:C:H2'	1:1A:1521:G:H8	1.79	0.47
1:1A:1888:G:N2	1:1A:1904:G:H2'	2.30	0.47
1:1A:2122:G:C2	1:1A:2123:U:H1'	2.48	0.47
9:1N:15:LEU:HD12	9:1N:16:ILE:H	1.79	0.47
1:2A:1095:A:H2'	1:2A:1096:G:C8	2.49	0.47
4:2E:163:GLU:HG2	4:2E:164:ARG:N	2.28	0.47
5:2F:109:GLY:O	5:2F:113:ALA:N	2.43	0.47
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HG12	1.96	0.47
26:14:63:TYR:HD1	26:14:63:TYR:N	2.11	0.47
1:1A:288:G:C5	1:1A:289:G:H1'	5.65	0.47
2:1B:9:G:P	14:1S:25:ARG:HH22	2.36	0.47
1:2A:1090:A:N3	1:2A:1092:G:C8	2.82	0.47
1:2A:1104:G:C8	1:2A:1105:U:H2'	2.49	0.47
1:2A:346:G:HO2'	1:2A:1249:U:H3	1.63	0.47
1:2A:1333:U:O4	13:2R:106:GLY:HA3	2.14	0.47
1:2A:1381:A:H2'	1:2A:1382:G:C8	2.49	0.47
1:2A:1404:A:H2'	1:2A:1405:A:H5'	1.97	0.47
1:2A:1693:G:OP1	59:2A:3601:HOH:O	2.20	0.47
1:2A:2832:A:OP1	4:2E:159:HIS:NE2	2.45	0.47
2:2B:98:G:H2'	2:2B:99:G:O4'	2.13	0.47
7:2H:54:ARG:HB3	7:2H:65:HIS:CG	2.49	0.47
20:2Y:90:LEU:HD13	20:2Y:92:ASN:HD21	1.79	0.47
26:14:55:ARG:HD3	26:14:55:ARG:HA	1.57	0.47
27:15:35:GLU:HG2	59:15:206:HOH:O	2.13	0.47
1:1A:1425:G:O2'	1:1A:1426:G:OP1	4.80	0.47
1:1A:785:G:OP1	59:1A:4155:HOH:O	2.20	0.47
1:2A:2303:C:O2'	1:2A:2304:C:H5'	2.14	0.47
1:2A:2735:C:OP2	4:2E:109:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:138:LEU:HD23	11:2P:145:PRO:HG3	1.97	0.47
19:2X:88:LYS:HG2	19:2X:93:GLU:HG3	1.96	0.47
2:1B:28:C:H2'	2:1B:29:A:O4'	2.15	0.47
1:1A:1176:G:H21	9:1N:73:THR:HG21	1.79	0.47
1:1A:2416:G:H5''	11:1P:75:ILE:HD12	1.96	0.47
26:24:24:THR:OG1	26:24:25:TYR:N	2.47	0.47
27:25:16:ARG:HG3	27:25:17:ASP:N	2.30	0.47
1:2A:29:G:H2'	1:2A:30:C:C6	2.49	0.47
1:2A:345:A:OP2	5:2F:169:ASN:HB2	2.15	0.47
1:2A:504:A:N3	1:2A:506:G:H5''	2.29	0.47
1:2A:558:U:H2'	1:2A:559:C:C6	2.50	0.47
3:2D:175:LEU:HD12	3:2D:185:VAL:HG21	1.97	0.47
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.50	0.47
1:1A:982:G:N2	1:1A:1021:C:N3	38.18	0.47
1:1A:1778:G:H8	1:1A:1778:G:H5''	1.80	0.47
1:1A:329:U:H2'	1:1A:330:G:O4'	2.14	0.47
1:1A:401:C:H2'	1:1A:402:C:C6	2.49	0.47
5:1F:195:ASP:HB3	5:1F:198:ALA:H	1.79	0.47
18:1W:14:PRO:HG2	18:1W:78:GLU:CG	2.39	0.47
1:2A:1170:G:H5'	31:29:37:GLY:HA2	1.95	0.47
1:2A:2227:G:C3'	1:2A:2228:A:H5''	2.44	0.47
1:2A:593:A:N6	1:2A:2510:C:O3'	2.47	0.47
1:2A:54:A:H2'	1:2A:55:C:O4'	2.15	0.47
1:2A:610:U:H2'	1:2A:611:C:C6	2.49	0.47
1:2A:590:U:H5'	1:2A:989:A:N1	2.30	0.47
5:2F:29:ASN:H	5:2F:112:MET:CE	2.26	0.47
13:2R:38:VAL:HB	13:2R:39:PRO:HD3	1.97	0.47
1:1A:1404:A:N1	1:1A:1417:U:O4	2.48	0.47
1:1A:2650:A:OP2	59:1A:4157:HOH:O	2.21	0.47
2:1B:33:G:C2	2:1B:50:G:C2	3.02	0.47
4:1E:82:ARG:HG2	4:1E:83:ASP:N	2.29	0.47
7:1H:11:VAL:HG13	7:1H:15:VAL:HG22	1.96	0.47
15:1T:56:GLY:O	15:1T:59:THR:HG23	2.14	0.47
6:2G:62:LEU:HA	26:24:27:THR:HG21	1.96	0.47
1:2A:186:C:OP2	59:2A:3636:HOH:O	2.20	0.47
1:2A:250:A:N3	1:2A:456:G:O2'	2.39	0.47
3:2D:3:VAL:HG13	3:2D:17:THR:HB	1.97	0.47
4:2E:50:GLY:HA3	4:2E:75:VAL:HG11	1.96	0.47
14:2S:95:HIS:CG	14:2S:96:GLY:N	2.82	0.47
31:19:17:ILE:HA	31:19:17:ILE:HD12	1.66	0.47
1:1A:302:C:N3	1:1A:384:G:N2	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:38:ILE:HD11	20:1Y:66:PRO:HG3	1.95	0.47
24:22:9:GLN:OE1	24:22:56:GLN:HG2	2.15	0.47
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.97	0.47
1:2A:1166:C:H2'	1:2A:1167:G:O4'	2.15	0.47
1:2A:2012:U:H2'	1:2A:2013:G:H5''	1.95	0.47
1:2A:955:A:N1	1:2A:2288:G:H1'	2.30	0.47
1:2A:2044:G:H5'	1:2A:2628:C:H4'	1.96	0.47
1:2A:264:U:H2'	1:2A:265:C:C6	2.50	0.47
1:2A:2657:C:OP2	1:2A:2744:G:O2'	2.31	0.47
1:2A:592:G:H2'	1:2A:2051:A:C5	2.49	0.47
1:2A:989:A:OP2	59:2A:3640:HOH:O	2.20	0.47
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.50	0.47
1:1A:1899:G:H2'	1:1A:1900:C:C6	2.49	0.47
1:1A:239:A:C5	1:1A:240:G:H1'	2.49	0.47
1:1A:2699:U:O4	59:1A:4152:HOH:O	2.20	0.47
1:1A:2020:C:H4'	1:1A:2735:C:O2	2.14	0.47
14:1S:15:ARG:HE	14:1S:88:ASP:CG	2.18	0.47
20:1Y:11:ASP:OD2	20:1Y:97:ARG:NH2	2.47	0.47
1:2A:1176:G:C2	1:2A:1177:A:C4	3.02	0.47
1:2A:1244:C:H2'	1:2A:1245:C:C6	2.99	0.47
1:2A:1333:U:C2	1:2A:1372:C:O2	2.68	0.47
1:2A:1381:A:H2'	1:2A:1382:G:H8	1.79	0.47
1:2A:1523:A:H2'	1:2A:1524:G:O4'	2.15	0.47
1:2A:1948:A:H2'	1:2A:1949:A:C8	2.49	0.47
1:2A:2830:A:C2	1:2A:2831:G:C4	3.03	0.47
1:2A:900:G:H2'	1:2A:901:G:C8	2.41	0.47
4:2E:119:ARG:HD2	4:2E:120:TRP:CD1	2.49	0.47
8:2I:62:LYS:O	8:2I:66:GLU:HG2	2.15	0.47
12:2Q:48:GLU:OE1	12:2Q:51:ARG:NH2	2.42	0.47
1:1A:1626:A:H8	1:1A:1626:A:OP2	1.97	0.47
1:1A:222:C:H2'	1:1A:223:U:H6	1.80	0.47
1:1A:1829:G:O2'	3:1D:181:GLU:OE2	2.22	0.47
1:2A:1036:C:OP2	59:2A:3610:HOH:O	2.21	0.47
1:2A:925:G:H2'	1:2A:926:G:O4'	2.15	0.47
3:2D:142:VAL:HG23	3:2D:193:VAL:HA	1.96	0.47
9:2N:34:LEU:HD12	9:2N:34:LEU:HA	1.75	0.47
30:18:32:LEU:O	30:18:36:LYS:HE3	2.14	0.47
1:1A:1520:C:H2'	1:1A:1521:G:C8	2.50	0.47
1:1A:271:U:H4'	8:1I:50:ARG:HH12	1.79	0.47
1:1A:341:C:H2'	1:1A:341:C:O2	2.86	0.47
8:1I:108:THR:O	8:1I:109:ILE:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:104:ARG:HH22	15:1T:43:GLN:HE22	1.61	0.47
27:25:16:ARG:O	27:25:20:ARG:HG3	2.15	0.47
1:2A:947:C:H2'	1:2A:948:C:C6	2.50	0.47
1:2A:981:U:H2'	1:2A:982:G:O4'	2.14	0.47
6:2G:148:MET:HG3	6:2G:148:MET:H	1.43	0.47
1:1A:1820:C:H5''	1:1A:1821:A:OP1	2.15	0.46
2:1B:66:A:N6	2:1B:108:U:H2'	2.29	0.46
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.71	0.46
18:1W:79:GLY:HA3	18:1W:100:THR:HG22	1.98	0.46
1:2A:1013:U:H4'	25:23:14:GLY:O	2.15	0.46
1:2A:1064:U:H3	1:2A:1187:A:N6	2.06	0.46
1:2A:2537:G:H5'	1:2A:2754:C:O2'	2.15	0.46
1:2A:323:A:P	20:2Y:86:ARG:HH21	2.37	0.46
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.48	0.46
6:2G:49:ASP:O	6:2G:51:ARG:N	2.48	0.46
8:2I:77:LEU:HB3	8:2I:142:VAL:HG12	1.96	0.46
9:2N:99:LEU:HD22	9:2N:103:VAL:HG23	1.96	0.46
30:18:61:LEU:O	30:18:63:PRO:HD3	2.15	0.46
31:19:27:CYS:SG	31:19:28:GLU:N	2.88	0.46
1:1A:1391:G:OP2	59:1A:4156:HOH:O	2.20	0.46
2:1B:32:C:C2	2:1B:51:G:N2	2.83	0.46
1:2A:1515:A:H2'	1:2A:1516:G:O4'	2.15	0.46
1:2A:2218:U:H1'	1:2A:2219:A:C8	2.50	0.46
1:2A:904:U:O2	1:2A:2279:A:H2'	2.16	0.46
1:2A:806:G:H2'	1:2A:807:A:O4'	2.15	0.46
3:2D:274:ARG:HG2	3:2D:275:LYS:N	2.29	0.46
3:2D:33:LEU:HD11	3:2D:103:ARG:HA	1.97	0.46
20:2Y:38:ILE:HD13	20:2Y:66:PRO:HA	1.97	0.46
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.42	0.46
1:1A:1248:A:H2	1:1A:1286:A:N6	2.07	0.46
1:1A:825:U:H6	1:1A:825:U:OP2	3.59	0.46
1:1A:2330:G:N2	14:1S:3:ARG:HG2	2.30	0.46
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.97	0.46
25:23:30:ARG:H	25:23:33:GLN:HE21	1.64	0.46
1:2A:2314:G:C2	1:2A:2325:C:N3	2.83	0.46
1:2A:364:G:H2'	1:2A:365:G:O4'	2.15	0.46
1:2A:668:A:C2	1:2A:2380:A:H1'	2.51	0.46
1:2A:678:A:H61	1:2A:701:A:H1'	1.80	0.46
1:2A:956:A:H2'	12:2Q:9:TYR:OH	2.15	0.46
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.47	0.46
1:1A:10:G:H2'	1:1A:11:U:H5''	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:501:G:H4'	1:1A:526:A:N1	2.30	0.46
1:1A:663:U:H2'	1:1A:664:C:C6	2.50	0.46
1:1A:671:G:H8	1:1A:671:G:O5'	1.97	0.46
1:2A:1132:G:H2'	1:2A:1134:G:H5'	1.96	0.46
1:2A:1632:A:H2'	1:2A:1633:C:C6	2.51	0.46
1:2A:183:A:H61	1:2A:186:C:H3'	1.80	0.46
1:2A:2554:G:H2'	1:2A:2555:G:C8	2.51	0.46
1:2A:1684:C:H5''	1:2A:2721:C:O2'	2.15	0.46
1:2A:982:G:OP2	30:28:52:LYS:NZ	2.38	0.46
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.63	0.46
4:2E:31:CYS:HA	4:2E:32:PRO:HD2	1.81	0.46
2:2B:75:G:O3'	21:2Z:10:ARG:NH2	2.49	0.46
26:14:33:VAL:HG12	26:14:34:GLU:H	1.81	0.46
1:1A:1002:U:O2	2:1B:90:A:O2'	2.27	0.46
1:1A:2356:G:OP2	28:16:38:LYS:NZ	2.46	0.46
2:1B:50:G:H5''	14:1S:61:ASN:ND2	2.30	0.46
13:1R:57:ARG:HB3	13:1R:59:ASP:OD1	2.16	0.46
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.98	0.46
26:24:16:CYS:SG	26:24:17:GLY:N	2.89	0.46
1:2A:105:U:H2'	1:2A:106:G:C8	2.51	0.46
1:2A:1266:C:C2	1:2A:1274:G:C2	3.04	0.46
1:2A:206:A:C2	1:2A:223:U:H4'	2.50	0.46
1:2A:2284:A:H2'	1:2A:2285:A:H8	1.80	0.46
1:2A:2375:C:H2'	1:2A:2376:G:O4'	2.15	0.46
1:2A:2672:G:H2'	1:2A:2673:A:C8	2.51	0.46
1:2A:332:G:N3	1:2A:352:G:O2'	2.46	0.46
1:2A:612:A:OP1	5:2F:95:ARG:NH1	2.49	0.46
16:2U:66:ASN:O	16:2U:70:ARG:HG3	2.16	0.46
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.98	0.46
18:2W:79:GLY:HA3	18:2W:100:THR:HG22	1.98	0.46
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.36	0.46
20:2Y:94:LYS:HA	20:2Y:94:LYS:HD3	1.74	0.46
1:1A:2333:A:H2'	1:1A:2334:G:O4'	2.16	0.46
1:1A:806:G:H2'	1:1A:807:A:O4'	2.16	0.46
1:2A:1835:U:O2	3:2D:50:THR:HB	2.16	0.46
1:2A:338:G:H2'	1:2A:339:C:C6	2.50	0.46
1:2A:554:G:O4'	1:2A:554:G:N3	2.48	0.46
4:2E:181:LEU:HA	4:2E:181:LEU:HD12	1.74	0.46
4:2E:24:THR:HG22	4:2E:186:GLY:O	2.15	0.46
24:12:22:GLU:HG2	24:12:64:LEU:HD11	1.97	0.46
1:1A:1603:C:OP2	1:1A:1604:A:O2'	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1953:A:H2'	1:1A:1954:G:O4'	2.15	0.46
1:1A:680:C:H2'	1:1A:681:G:O4'	2.16	0.46
2:1B:2:C:H2'	2:1B:3:C:C6	2.51	0.46
1:2A:1703:C:H2'	1:2A:1704:C:C6	2.51	0.46
1:2A:2566:U:H5''	1:2A:2567:C:OP2	2.15	0.46
1:2A:1874:C:OP1	3:2D:257:LEU:HD23	2.14	0.46
1:2A:2829:A:OP1	13:2R:2:ARG:NH2	2.48	0.46
21:2Z:5:LEU:HD13	21:2Z:47:VAL:HG21	1.98	0.46
1:1A:899:G:H1	1:1A:969:C:H42	1.64	0.46
2:1B:24:G:N7	2:1B:56:G:H2'	2.30	0.46
3:1D:184:LYS:HE3	3:1D:184:LYS:HB3	4.48	0.46
4:1E:9:VAL:HG13	4:1E:25:VAL:O	2.16	0.46
26:24:44:THR:O	26:24:46:GLN:N	2.49	0.46
1:2A:488:G:O6	59:2A:3641:HOH:O	2.21	0.46
1:2A:948:C:H2'	1:2A:949:C:C6	2.50	0.46
3:2D:67:PHE:CD1	3:2D:153:ALA:HB3	2.51	0.46
6:2G:47:LYS:HB3	6:2G:48:GLU:H	1.39	0.46
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.96	0.46
1:2A:2889:C:O3'	13:2R:90:ARG:NH1	2.49	0.46
1:1A:1500:U:O2'	1:1A:1501:G:N7	2.45	0.46
1:1A:440:C:H2'	1:1A:441:A:C8	2.51	0.46
26:24:26:SER:OG	26:24:27:THR:N	2.49	0.46
26:24:62:ARG:C	26:24:64:GLY:H	2.19	0.46
1:2A:1064:U:O2'	1:2A:1066:A:H2	1.97	0.46
1:2A:1409:G:OP2	23:21:3:LYS:HG3	2.16	0.46
3:2D:146:GLU:HB2	3:2D:189:CYS:HB3	1.97	0.46
5:2F:29:ASN:H	5:2F:112:MET:HE1	1.81	0.46
6:2G:64:THR:HB	6:2G:94:LEU:HD11	1.98	0.46
9:2N:37:LYS:HG3	9:2N:42:TRP:NE1	2.31	0.46
1:2A:998:G:H5''	12:2Q:13:GLN:HB3	1.98	0.46
21:2Z:19:ARG:NH1	21:2Z:84:GLU:HB2	2.31	0.46
3:1D:127:VAL:HA	3:1D:193:VAL:HG22	1.98	0.46
7:1H:101:ARG:HA	7:1H:101:ARG:HD2	1.72	0.46
1:1A:1176:G:H21	9:1N:73:THR:CG2	2.29	0.46
10:1O:103:ALA:HB1	10:1O:105:GLU:HG2	1.98	0.46
1:2A:1856:G:H4'	3:2D:242:ARG:CZ	2.46	0.46
1:2A:552:A:C2	1:2A:2064:C:H4'	2.51	0.46
1:2A:2347:A:H61	22:20:43:THR:CG2	2.29	0.46
1:2A:791:G:H2'	1:2A:792:A:H5'	1.97	0.46
11:2P:2:LYS:NZ	11:2P:4:SER:OG	2.37	0.46
12:2Q:59:ARG:O	12:2Q:60:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1475:C:H2'	1:1A:1476:U:H6	1.81	0.45
1:1A:2578:G:H2'	1:1A:2579:C:C6	2.50	0.45
1:1A:624:G:O2'	1:1A:701:A:N6	2.48	0.45
6:1G:97:ASP:O	6:1G:101:ILE:HG13	2.16	0.45
1:2A:1256:G:N2	1:2A:1257:A:N7	5.33	0.45
1:2A:1302:C:H2'	1:2A:1303:C:O4'	2.71	0.45
1:2A:665:C:O2'	1:2A:2361:C:OP1	2.16	0.45
1:2A:309:C:H2'	1:2A:310:C:C6	2.50	0.45
1:2A:945:A:H2'	1:2A:946:A:C8	2.51	0.45
12:2Q:12:GLN:HG2	12:2Q:73:PRO:HD2	1.98	0.45
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.52	0.45
21:2Z:89:PHE:HE2	21:2Z:96:VAL:HG21	1.81	0.45
1:1A:1086:C:H2'	1:1A:1087:G:O4'	3.28	0.45
1:1A:1404:A:N3	1:1A:1404:A:H5'	2.32	0.45
1:1A:1868:C:O2'	59:1A:4144:HOH:O	2.18	0.45
1:1A:2290:G:N7	22:10:14:ARG:NH1	2.64	0.45
1:1A:591:U:C4	1:1A:592:G:C6	3.04	0.45
1:1A:867:A:H2'	1:1A:990:G:H5''	1.98	0.45
3:1D:71:ASP:CB	3:1D:103:ARG:HH22	2.19	0.45
1:2A:1548:U:H2'	1:2A:1549:C:C6	2.51	0.45
1:2A:358:C:H2'	1:2A:359:C:H6	1.80	0.45
1:2A:704:C:H2'	1:2A:705:C:C6	2.50	0.45
1:2A:885:U:H1'	1:2A:1235:G:H1'	1.98	0.45
2:2B:11:C:H3'	2:2B:12:C:C6	2.51	0.45
18:2W:38:TYR:O	27:25:28:PRO:HB3	2.15	0.45
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.80	0.45
26:14:20:ASN:OD1	26:14:21:VAL:N	2.50	0.45
1:1A:1500:U:OP1	13:1R:77:ARG:NH1	2.44	0.45
1:1A:1531:A:H2'	1:1A:1532:G:C8	2.51	0.45
1:1A:1633:C:H2'	1:1A:1634:C:C6	2.50	0.45
1:1A:2282:G:OP1	22:10:18:ALA:HB1	2.16	0.45
1:1A:253:A:C8	1:1A:254:G:H1'	2.51	0.45
3:1D:108:PRO:HG3	3:1D:143:HIS:CE1	2.51	0.45
21:1Z:155:LEU:HD12	21:1Z:155:LEU:HA	1.75	0.45
1:2A:1100:G:N2	1:2A:1149:C:O2	2.45	0.45
1:2A:1150:U:H2'	1:2A:1151:G:C8	2.52	0.45
1:2A:1627:G:H2'	1:2A:1628:C:O4'	2.16	0.45
1:2A:2573:U:H1'	10:2O:23:ARG:HH11	1.81	0.45
1:2A:2698:U:H2'	1:2A:2699:U:O4'	2.17	0.45
17:2V:20:LEU:HD12	17:2V:20:LEU:HA	1.77	0.45
1:1A:2302:U:H2'	1:1A:2303:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2563:U:C2	1:1A:2565:U:H5'	2.52	0.45
8:1I:6:LEU:HG	8:1I:36:ALA:HA	1.99	0.45
13:1R:11:ASN:OD1	59:1R:301:HOH:O	2.21	0.45
13:1R:26:LYS:HE2	13:1R:70:LEU:O	2.17	0.45
21:1Z:180:VAL:O	21:1Z:183:LEU:HB2	2.16	0.45
1:2A:1098:C:H2'	1:2A:1099:A:H5'	1.98	0.45
1:2A:1424:A:H4'	1:2A:1425:G:OP2	2.17	0.45
1:2A:1702:C:O2'	1:2A:1703:C:H5'	2.16	0.45
1:2A:2254:U:H2'	1:2A:2255:U:C6	2.51	0.45
1:2A:530:G:O3'	1:2A:531:A:H8	1.99	0.45
1:2A:1830:C:OP2	3:2D:183:ARG:NH2	2.48	0.45
3:2D:5:LYS:HB3	3:2D:5:LYS:HE3	1.67	0.45
6:2G:115:ARG:CG	6:2G:115:ARG:HH11	2.29	0.45
1:2A:2756:G:N2	7:2H:143:GLN:OE1	2.49	0.45
9:2N:20:GLY:HA2	9:2N:61:ARG:NE	2.30	0.45
12:2Q:16:ARG:O	12:2Q:17:LEU:HD23	2.17	0.45
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.98	0.45
21:2Z:1:MET:HA	21:2Z:55:HIS:HB3	1.97	0.45
1:1A:1359:C:OP1	59:1A:4132:HOH:O	2.21	0.45
1:1A:2644:G:H5'	1:1A:2820:G:O2'	2.16	0.45
4:1E:55:ASN:HB3	4:1E:58:ARG:HG3	1.97	0.45
2:1B:50:G:H5''	14:1S:61:ASN:HD21	1.82	0.45
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.16	0.45
1:2A:1044:U:O2'	1:2A:1045:A:H5'	2.17	0.45
1:2A:1050:C:C2	1:2A:1188:A:C5	3.04	0.45
1:2A:126:C:H2'	1:2A:127:C:C6	2.97	0.45
1:2A:1404:A:H2'	1:2A:1405:A:C5'	2.47	0.45
1:2A:2330:G:C2	14:2S:3:ARG:HA	2.51	0.45
6:2G:97:ASP:O	6:2G:101:ILE:HG13	2.16	0.45
9:2N:36:GLY:HA2	9:2N:38:HIS:CE1	2.51	0.45
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.57	0.45
1:1A:141:G:C2	1:1A:172:C:N3	54.52	0.45
1:1A:2035:A:H2'	1:1A:2036:A:C8	2.52	0.45
1:1A:222:C:H2'	1:1A:223:U:C6	2.52	0.45
1:1A:2300:G:OP1	59:1A:4158:HOH:O	2.21	0.45
1:1A:671:G:H2'	1:1A:672:G:O4'	2.16	0.45
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.73	0.45
20:1Y:92:ASN:HD22	20:1Y:92:ASN:N	2.14	0.45
21:1Z:152:ALA:O	21:1Z:155:LEU:HB2	2.17	0.45
24:22:3:LEU:HD23	24:22:3:LEU:HA	1.82	0.45
1:2A:141:G:H2'	1:2A:142:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:825:U:H6	1:2A:825:U:OP1	4.81	0.45
7:2H:3:ARG:NE	7:2H:54:ARG:HH12	2.14	0.45
8:2I:72:LEU:HA	8:2I:75:LEU:HD22	1.97	0.45
11:2P:86:LYS:HB3	11:2P:118:GLY:HA3	1.99	0.45
25:13:38:GLU:HB3	25:13:40:THR:HG23	1.98	0.45
7:1H:71:LEU:HD12	7:1H:71:LEU:HA	1.77	0.45
1:1A:609:C:OP2	11:1P:21:ARG:NH2	2.50	0.45
11:1P:76:LYS:HE2	11:1P:76:LYS:HB3	1.84	0.45
14:1S:63:THR:OG1	14:1S:64:GLU:N	4.42	0.45
59:1A:4195:HOH:O	15:1T:119:LYS:NZ	2.50	0.45
1:2A:1305:G:C6	1:2A:1306:C:C4	3.04	0.45
1:2A:182:G:H2'	1:2A:183:A:O4'	2.17	0.45
1:2A:2326:G:H2'	1:2A:2327:C:C6	2.51	0.45
1:2A:232:A:C2	1:2A:243:A:C4	3.05	0.45
4:2E:182:LEU:HA	4:2E:182:LEU:HD12	1.65	0.45
10:2O:6:THR:HG22	10:2O:8:LEU:HD22	1.99	0.45
10:2O:64:ARG:NH1	10:2O:81:ASP:OD1	2.48	0.45
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.51	0.45
18:2W:45:TYR:CZ	18:2W:49:LYS:HE3	2.52	0.45
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	1.99	0.45
1:2A:325:C:OP2	20:2Y:73:ARG:NH1	2.50	0.45
1:1A:1067:G:H22	1:1A:1187:A:H2	1.60	0.45
1:1A:2358:C:H2'	1:1A:2359:U:C6	2.52	0.45
1:1A:2878:G:H2'	1:1A:2879:C:O4'	2.17	0.45
1:1A:433:G:OP2	59:1A:4160:HOH:O	2.21	0.45
1:1A:509:C:H2'	1:1A:510:C:C6	2.52	0.45
1:1A:645:A:OP2	11:1P:108:LYS:NZ	2.48	0.45
22:20:43:THR:O	22:20:43:THR:HG23	2.17	0.45
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.52	0.45
1:2A:1104:G:H5'	1:2A:1105:U:H5''	1.99	0.45
1:2A:1735:A:N6	1:2A:1744:A:H2	2.04	0.45
1:2A:1906:A:H2'	1:2A:1907:C:O4'	2.16	0.45
1:2A:2709:U:H2'	1:2A:2710:C:C6	2.51	0.45
1:2A:2818:A:H62	1:2A:2899:G:H2'	1.81	0.45
2:2B:66:A:H61	2:2B:108:U:H2'	1.81	0.45
4:2E:116:VAL:HG21	4:2E:138:PRO:HB3	1.98	0.45
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.17	0.45
8:2I:44:LEU:HD12	8:2I:44:LEU:HA	1.82	0.45
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.98	0.45
1:1A:942:C:H2'	1:1A:943:C:H6	1.82	0.45
1:1A:2696:G:H5'	10:1O:68:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1S:43:GLU:OE1	14:1S:43:GLU:N	5.90	0.45
1:2A:242:G:N7	30:28:5:LYS:HE2	2.32	0.45
1:2A:1051:C:C2	1:2A:1182:G:N2	2.84	0.45
1:2A:1369:G:C2	1:2A:1370:G:C8	13.44	0.45
26:14:62:ARG:HD3	26:14:62:ARG:HA	1.68	0.45
1:1A:1614:G:H5'	3:1D:60:ARG:HA	1.99	0.45
1:1A:1835:U:O2	3:1D:50:THR:HB	2.16	0.45
1:1A:235:G:H4'	1:1A:412:G:C5	2.52	0.45
1:1A:301:A:H2'	1:1A:302:C:C6	2.52	0.45
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.98	0.45
25:23:23:LEU:HD13	25:23:50:VAL:HG11	1.99	0.45
31:29:17:ILE:HG22	31:29:24:TYR:HB2	1.99	0.45
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.17	0.45
1:2A:1404:A:C6	1:2A:1417:U:O4	2.70	0.45
1:2A:2124:C:H1'	1:2A:2208:G:N1	2.32	0.45
1:2A:2494:C:H2'	1:2A:2495:G:O4'	2.17	0.45
1:2A:563:G:H2'	1:2A:564:C:C6	2.52	0.45
1:2A:598:U:H2'	1:2A:599:G:C8	2.52	0.45
1:2A:929:G:O6	1:2A:938:C:N4	2.49	0.45
1:2A:942:C:H2'	1:2A:943:C:H6	1.82	0.45
2:2B:6:C:N4	2:2B:115:G:H1	2.12	0.45
5:2F:106:ARG:HG2	5:2F:106:ARG:H	1.50	0.45
6:2G:41:GLN:O	6:2G:43:LEU:HB2	2.17	0.45
10:2O:23:ARG:HG3	10:2O:24:VAL:N	2.32	0.45
21:2Z:179:ASP:O	21:2Z:182:LYS:HB2	2.17	0.45
1:1A:1187:A:C4	1:1A:1189:G:C8	3.05	0.44
1:1A:1792:A:H2'	59:1A:5466:HOH:O	2.16	0.44
1:1A:2205:G:H5'	1:1A:2206:C:OP2	2.17	0.44
1:1A:2554:G:H2'	1:1A:2555:G:C8	2.51	0.44
1:1A:2744:G:H3'	1:1A:2745:A:O4'	2.17	0.44
1:1A:720:G:O2'	5:1F:74:ARG:HD3	2.16	0.44
6:1G:181:ARG:HG3	6:1G:182:LYS:H	1.82	0.44
11:1P:46:LYS:HB3	11:1P:46:LYS:HE3	1.75	0.44
1:2A:1042:G:H2'	1:2A:1042:G:N3	2.32	0.44
1:2A:1061:G:H2'	1:2A:1062:G:H8	1.83	0.44
1:2A:1189:G:H2'	1:2A:1190:C:C6	3.40	0.44
1:2A:1567:G:H2'	1:2A:1568:U:O4'	2.18	0.44
2:2B:12:C:H2'	22:20:73:GLY:HA3	1.99	0.44
1:2A:1854:G:OP1	3:2D:52:ARG:NH1	2.50	0.44
5:2F:9:ILE:HG21	5:2F:125:LEU:HD13	1.99	0.44
11:2P:126:VAL:HG12	11:2P:148:LEU:CD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:57:ILE:HD12	21:2Z:71:VAL:HG23	1.99	0.44
1:1A:387:A:H2'	1:1A:388:G:C8	2.52	0.44
6:1G:41:GLN:NE2	6:1G:154:GLY:O	2.43	0.44
28:26:35:GLU:HG3	28:26:50:ARG:HG3	1.99	0.44
1:2A:1443:C:H2'	1:2A:1444:C:O4'	2.87	0.44
1:2A:1426:G:H1'	1:2A:1617:A:N1	2.32	0.44
1:2A:2494:C:N3	12:2Q:124:LYS:NZ	2.61	0.44
1:2A:47:A:H4'	1:2A:48:U:H5''	1.99	0.44
1:2A:791:G:C2'	1:2A:792:A:H5'	2.47	0.44
6:2G:43:LEU:HB3	6:2G:44:GLY:H	1.59	0.44
8:2I:90:GLY:O	8:2I:121:LYS:HE3	2.17	0.44
11:2P:125:VAL:HG13	11:2P:138:LEU:HD21	1.98	0.44
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.98	0.44
25:13:23:LEU:HD13	25:13:50:VAL:HG11	1.99	0.44
1:1A:170:A:H2'	1:1A:171:C:O4'	2.17	0.44
1:1A:1868:C:N4	1:1A:1919:U:H2'	2.32	0.44
1:1A:482:A:H5''	59:1A:4893:HOH:O	2.18	0.44
1:1A:517:G:H2'	1:1A:518:G:O4'	2.17	0.44
1:1A:1924:G:OP1	3:1D:241:PRO:HB2	2.17	0.44
6:1G:139:LEU:HD12	6:1G:139:LEU:H	1.83	0.44
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.54	0.44
1:1A:2428:C:OP1	11:1P:65:ARG:NH2	2.50	0.44
14:1S:36:TYR:CD1	14:1S:36:TYR:N	2.85	0.44
26:24:61:ARG:HD2	26:24:61:ARG:HA	1.67	0.44
1:2A:1113:G:O2'	1:2A:1141:A:O2'	2.32	0.44
1:2A:2020:C:H4'	1:2A:2735:C:O2	2.18	0.44
1:2A:2763:G:C6	7:2H:2:SER:HB2	2.53	0.44
1:2A:448:A:H2'	1:2A:449:A:C8	2.53	0.44
1:2A:898:G:N2	1:2A:971:A:H1'	2.32	0.44
1:2A:2760:A:H5'	7:2H:4:ILE:HD12	1.98	0.44
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.90	0.44
26:14:35:VAL:HG22	26:14:36:CYS:H	1.82	0.44
31:19:15:LYS:HE2	31:19:17:ILE:HD13	2.00	0.44
1:1A:2210:U:H2'	1:1A:2211:G:C8	2.47	0.44
1:1A:2899:G:OP2	59:1A:4159:HOH:O	2.21	0.44
1:1A:751:A:H2'	1:1A:752:A:O4'	2.38	0.44
7:1H:113:VAL:HG11	7:1H:151:ILE:HD13	1.99	0.44
14:1S:67:ARG:O	14:1S:71:ARG:HG3	2.17	0.44
1:1A:1426:G:C8	15:1T:118:ARG:HG2	88.54	0.44
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.90	0.44
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:41:PRO:HG3	26:24:49:PHE:CE2	2.52	0.44
1:2A:2824:C:C5'	27:25:29:THR:HG21	2.47	0.44
1:2A:1101:G:H21	1:2A:1148:A:H62	1.65	0.44
1:2A:1268:G:C2	1:2A:1272:G:C5	3.05	0.44
1:2A:592:G:OP2	59:2A:3642:HOH:O	2.21	0.44
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.62	0.44
6:2G:114:ILE:HB	6:2G:117:PHE:HB2	2.00	0.44
18:2W:41:LYS:HE3	27:25:25:LEU:HD11	1.99	0.44
1:1A:1573:A:OP2	59:1A:4162:HOH:O	2.21	0.44
1:1A:1734:U:O2	1:1A:1746:A:H5'	2.17	0.44
1:1A:1845:A:H8	1:1A:1845:A:OP1	2.00	0.44
1:1A:2316:A:H5''	6:1G:134:GLY:HA3	1.98	0.44
1:1A:25:G:C6	1:1A:26:G:N1	2.86	0.44
1:1A:2648:U:H5''	4:1E:82:ARG:NH2	2.32	0.44
1:1A:2855:G:H2'	1:1A:2856:U:O4'	2.18	0.44
1:1A:2896:U:H2'	1:1A:2897:C:C6	2.53	0.44
1:1A:775:G:C5	3:1D:208:LYS:HB2	2.53	0.44
1:1A:810:A:H2	3:1D:219:PRO:HG3	1.82	0.44
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.81	0.44
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	2.00	0.44
23:21:18:ILE:HG12	23:21:37:ILE:HG23	1.99	0.44
26:24:59:PHE:HA	26:24:61:ARG:H	1.81	0.44
1:2A:483:G:C8	29:27:37:LYS:HG2	2.53	0.44
1:2A:53:G:O2'	1:2A:124:A:N1	2.47	0.44
1:2A:1561:U:H2'	1:2A:1562:G:H8	1.83	0.44
1:2A:239:A:C5	1:2A:240:G:H1'	2.53	0.44
1:2A:335:G:H5''	1:2A:336:C:OP2	2.18	0.44
1:2A:945:A:C4	1:2A:946:A:C8	3.06	0.44
5:2F:33:LEU:HD13	5:2F:112:MET:HE2	1.99	0.44
1:2A:706:G:H5'	5:2F:99:TYR:CD2	2.52	0.44
7:2H:139:GLN:O	7:2H:143:GLN:N	2.47	0.44
11:2P:65:ARG:HG3	30:28:25:MET:CG	2.45	0.44
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.50	0.44
16:2U:104:GLN:OE1	16:2U:105:VAL:HG23	2.18	0.44
1:1A:288:G:N7	1:1A:289:G:H1'	6.67	0.44
20:1Y:92:ASN:HB2	20:1Y:94:LYS:N	2.15	0.44
1:2A:2100:U:O3'	23:21:35:THR:OG1	2.27	0.44
1:2A:2043:U:O2'	1:2A:2628:C:H5'	2.18	0.44
1:2A:503:A:C6	1:2A:505:A:C6	3.05	0.44
1:2A:636:U:H4'	1:2A:639:A:N6	2.33	0.44
1:2A:875:A:N7	1:2A:2259:C:H5'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:95:C:H2'	2:2B:96:U:C6	2.52	0.44
1:2A:610:U:H1'	5:2F:90:PHE:CG	2.53	0.44
6:2G:13:GLU:O	6:2G:17:PRO:HD2	2.17	0.44
10:2O:35:VAL:HG13	10:2O:65:THR:HG23	1.99	0.44
1:1A:1939:A:O2'	1:1A:1941:C:N4	2.50	0.44
6:1G:79:ASN:N	6:1G:79:ASN:OD1	2.50	0.44
10:1O:23:ARG:HG3	10:1O:24:VAL:N	2.33	0.44
15:1T:127:ALA:C	15:1T:129:ARG:H	2.21	0.44
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.53	0.44
21:1Z:138:GLU:HB2	21:1Z:156:LYS:HE2	2.00	0.44
23:21:76:ARG:HB2	23:21:97:LEU:HD13	1.98	0.44
1:2A:1000:G:H2'	1:2A:1001:A:H2'	1.99	0.44
1:2A:1549:C:H2'	1:2A:1550:C:H6	1.83	0.44
1:2A:1886:G:C2'	1:2A:1887:G:H5'	2.48	0.44
1:2A:2113:U:H4'	1:2A:2114:G:O5'	2.18	0.44
1:2A:2363:A:H2'	1:2A:2364:G:H5'	2.00	0.44
1:2A:2484:U:H2'	1:2A:2484:U:O2	2.16	0.44
1:2A:2700:U:P	1:2A:2731:G:H22	2.40	0.44
1:2A:2715:C:H2'	1:2A:2716:A:O4'	2.18	0.44
1:2A:972:G:H2'	1:2A:973:G:O4'	2.18	0.44
4:2E:175:VAL:O	4:2E:177:PRO:HD3	2.17	0.44
1:2A:1714:A:OP1	10:2O:5:GLN:HG3	2.17	0.44
12:2Q:12:GLN:HE21	12:2Q:72:LYS:NZ	2.14	0.44
20:2Y:38:ILE:HD11	20:2Y:66:PRO:HG3	2.00	0.44
26:14:9:LEU:HA	26:14:9:LEU:HD23	1.81	0.44
1:1A:1332:A:C5	1:1A:1333:U:C4	3.23	0.44
1:1A:1840:A:H2'	1:1A:1841:G:O4'	2.18	0.44
1:1A:2244:U:H2'	1:1A:2245:G:C8	2.53	0.44
1:1A:77:G:H1'	1:1A:78:G:H8	4.54	0.44
1:1A:933:A:H1'	1:1A:935:C:OP2	2.18	0.44
5:1F:132:VAL:HG22	5:1F:163:VAL:HG22	2.00	0.44
5:1F:53:THR:HB	5:1F:56:GLU:OE2	2.18	0.44
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	2.00	0.44
20:1Y:6:HIS:H	20:1Y:6:HIS:HD2	1.64	0.44
25:23:48:GLU:HA	25:23:51:ALA:HB2	2.00	0.44
30:28:34:TRP:CE2	30:28:35:GLN:HB2	2.53	0.44
1:2A:1047:G:H22	1:2A:1199:G:H1'	1.83	0.44
1:2A:1887:G:C6	1:2A:1888:G:N1	2.86	0.44
1:2A:2076:C:H5'	1:2A:2077:G:O5'	2.18	0.44
1:2A:2115:G:N2	1:2A:2217:C:H1'	2.33	0.44
1:2A:241:C:O2'	59:2A:3643:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:786:U:H2'	1:2A:787:G:C8	2.53	0.44
3:2D:206:LEU:HA	3:2D:206:LEU:HD23	1.70	0.44
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.18	0.44
1:1A:1423:A:OP1	29:17:10:ARG:NH2	2.50	0.44
1:1A:2596:U:H4'	1:1A:2597:C:OP1	2.17	0.44
1:1A:644:G:H5'	1:1A:644:G:N3	2.32	0.44
14:1S:32:LEU:HA	14:1S:32:LEU:HD23	1.75	0.44
25:23:26:LEU:HD21	25:23:46:ASN:HB2	1.99	0.44
1:2A:1059:U:H2'	1:2A:1060:G:H8	1.83	0.44
1:2A:1245:C:H2'	1:2A:1246:C:C6	2.96	0.44
1:2A:1309:G:H2'	1:2A:2035:A:N6	2.32	0.44
1:2A:151:G:H2'	1:2A:152:C:C6	2.53	0.44
1:2A:1553:A:H4'	1:2A:1555:A:C5	2.53	0.44
1:2A:2091:G:C2	1:2A:2453:C:C2	3.06	0.44
1:2A:2307:U:OP2	14:2S:9:ARG:NH2	2.46	0.44
1:2A:2314:G:C2'	1:2A:2315:G:H5'	2.48	0.44
1:2A:2370:C:H2'	1:2A:2371:A:O4'	2.17	0.44
1:2A:250:A:H2'	1:2A:251:C:O4'	2.18	0.44
1:2A:2623:C:OP2	27:25:2:ALA:N	2.51	0.44
1:2A:263:G:C2	1:2A:264:U:C2	3.06	0.44
1:2A:2788:A:H4'	1:2A:2789:G:H5''	1.99	0.44
1:2A:416:A:H4'	1:2A:417:G:H5'	2.00	0.44
4:2E:144:ARG:HB3	4:2E:145:LYS:H	1.46	0.44
6:2G:102:PHE:CE1	6:2G:141:PHE:CE1	3.05	0.44
6:2G:11:TYR:OH	6:2G:16:ARG:NE	2.51	0.44
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.17	0.44
15:2T:56:GLY:O	15:2T:59:THR:HG23	2.18	0.44
1:1A:682:G:O5'	1:1A:682:G:H8	2.01	0.43
1:1A:699:A:H2'	1:1A:700:A:C8	3.71	0.43
1:1A:863:C:O2'	1:1A:885:U:H5''	2.18	0.43
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	1.99	0.43
1:1A:1288:G:O2'	11:1P:7:ARG:NH2	2.51	0.43
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.53	0.43
24:22:32:LEU:HA	24:22:35:LEU:HB2	1.99	0.43
24:22:4:SER:HA	24:22:7:ARG:NH1	2.33	0.43
1:2A:139:A:HO2'	1:2A:1452:C:HO2'	1.61	0.43
1:2A:1480:G:H2'	1:2A:1481:G:O4'	2.18	0.43
1:2A:330:G:H21	1:2A:353:A:N6	2.12	0.43
11:2P:47:ASP:HA	11:2P:48:PRO:HD3	1.80	0.43
12:2Q:12:GLN:HG3	12:2Q:72:LYS:HZ2	1.83	0.43
1:2A:605:G:OP2	16:2U:10:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2W:14:PRO:HG2	18:2W:78:GLU:CG	2.43	0.43
1:1A:2398:U:OP1	22:10:55:ARG:NH2	2.51	0.43
30:18:28:GLY:O	30:18:36:LYS:NZ	2.41	0.43
1:1A:1073:A:H61	1:1A:1170:G:H2'	1.83	0.43
1:1A:2759:G:O6	1:1A:2767:C:H5''	2.18	0.43
2:1B:90:A:C5	2:1B:91:C:H1'	2.53	0.43
3:1D:16:MET:HE1	3:1D:208:LYS:HD3	2.00	0.43
14:1S:26:LEU:HD22	14:1S:87:PHE:CE1	2.53	0.43
1:2A:1133:A:H2'	1:2A:1133:A:N3	2.33	0.43
1:2A:2125:G:N2	1:2A:2207:G:H1'	2.30	0.43
1:2A:235:G:H4'	1:2A:412:G:C6	2.53	0.43
1:2A:596:C:N3	4:2E:145:LYS:NZ	2.60	0.43
2:2B:78:A:H2'	2:2B:79:C:O4'	2.19	0.43
4:2E:101:ARG:O	4:2E:201:THR:HG22	2.19	0.43
1:2A:2798:U:O2'	4:2E:65:GLY:HA3	2.18	0.43
5:2F:53:THR:HG22	5:2F:56:GLU:HG3	2.00	0.43
7:2H:7:LEU:O	7:2H:69:ARG:HD3	2.19	0.43
1:2A:1185:U:H2'	9:2N:63:THR:HG21	1.99	0.43
1:1A:2083:A:C2	1:1A:2514:A:N6	2.86	0.43
1:1A:885:U:H2'	1:1A:886:C:C6	2.53	0.43
5:1F:140:LEU:HD13	5:1F:140:LEU:HA	1.82	0.43
5:1F:164:ARG:O	5:1F:168:ARG:HG3	2.18	0.43
6:1G:41:GLN:HE22	6:1G:153:ARG:HB3	1.83	0.43
13:1R:111:LEU:O	59:1R:302:HOH:O	2.21	0.43
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.33	0.43
1:2A:1406:G:OP1	10:2O:49:ARG:NH1	111.75	0.43
1:2A:552:A:N1	1:2A:2063:A:H2'	2.34	0.43
1:2A:224:C:H2'	1:2A:225:C:C6	2.54	0.43
1:2A:25:G:C6	1:2A:26:G:N1	2.87	0.43
1:2A:2858:U:H4'	1:2A:2877:A:C2	2.53	0.43
1:2A:560:A:H2'	1:2A:561:C:C6	2.52	0.43
1:2A:922:C:H2'	1:2A:923:U:O4'	2.19	0.43
1:2A:931:C:H2'	1:2A:932:C:H4'	1.99	0.43
6:2G:114:ILE:HA	6:2G:136:ARG:HH22	1.84	0.43
1:2A:508:A:O4'	20:2Y:48:ALA:HB1	2.18	0.43
21:2Z:48:PHE:HE1	21:2Z:71:VAL:HG11	1.83	0.43
30:18:23:VAL:HG11	30:18:47:LYS:HD3	2.00	0.43
1:1A:838:G:O6	59:1A:4146:HOH:O	2.19	0.43
1:1A:2224:U:O4'	3:1D:151:LYS:HE2	2.18	0.43
7:1H:125:VAL:HG12	7:1H:127:GLU:O	2.18	0.43
7:1H:7:LEU:HA	7:1H:8:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	1.99	0.43
8:1I:31:LEU:HD21	8:1I:38:LEU:HG	2.00	0.43
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.68	0.43
1:2A:1142:U:H2'	1:2A:1143:A:O4'	2.19	0.43
1:2A:1561:U:H2'	1:2A:1562:G:C8	2.54	0.43
1:2A:26:G:O2'	1:2A:27:A:OP2	2.34	0.43
1:2A:818:C:H2'	1:2A:819:U:C6	3.02	0.43
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	2.00	0.43
7:2H:69:ARG:HG3	7:2H:70:THR:N	2.33	0.43
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.18	0.43
8:2I:4:ILE:HD11	8:2I:44:LEU:CD1	2.47	0.43
11:2P:84:ASN:OD1	11:2P:117:GLU:HB2	2.18	0.43
22:10:82:ARG:HA	22:10:83:PRO:HD3	1.73	0.43
1:1A:2331:A:N3	1:1A:2331:A:H2'	2.33	0.43
1:1A:2734:G:H2'	1:1A:2735:C:C6	2.54	0.43
1:1A:387:A:H2'	1:1A:388:G:H8	1.83	0.43
2:1B:80:U:H2'	2:1B:81:G:C8	2.54	0.43
3:1D:242:ARG:N	3:1D:242:ARG:HD3	2.33	0.43
4:1E:31:CYS:HA	4:1E:32:PRO:HD2	1.79	0.43
1:2A:1003:A:C6	1:2A:1004:A:C6	3.07	0.43
1:2A:1024:G:H3'	1:2A:1025:A:H5''	2.00	0.43
1:2A:2387:A:H5''	1:2A:2388:A:OP2	2.18	0.43
1:2A:310:C:H2'	1:2A:311:C:C6	2.51	0.43
1:2A:703:U:H2'	1:2A:704:C:H6	1.81	0.43
3:2D:232:PRO:O	59:2D:401:HOH:O	2.21	0.43
3:2D:71:ASP:HB3	3:2D:72:LYS:HG3	1.99	0.43
8:2I:62:LYS:HE2	8:2I:133:HIS:HE1	1.82	0.43
13:2R:13:HIS:CE1	13:2R:16:HIS:HB2	2.53	0.43
1:1A:1247:G:H5'	11:1P:3:LEU:HD23	2.00	0.43
16:1U:34:LYS:HE2	16:1U:34:LYS:HA	2.01	0.43
1:2A:1000:G:OP2	12:2Q:14:ARG:NH2	2.52	0.43
1:2A:1887:G:O6	1:2A:1888:G:N1	2.52	0.43
1:2A:2249:G:N7	59:2A:3701:HOH:O	2.35	0.43
1:2A:2298:A:C4	1:2A:2300:G:C8	3.07	0.43
1:2A:2327:C:O2'	1:2A:2328:C:H5'	2.19	0.43
1:2A:2548:U:N3	1:2A:2549:C:C4	2.87	0.43
2:2B:11:C:H3'	2:2B:12:C:C5	2.54	0.43
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.99	0.43
14:2S:111:GLU:H	14:2S:111:GLU:HG2	1.70	0.43
17:2V:43:GLU:OE2	17:2V:43:GLU:N	2.51	0.43
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.51	0.43
30:18:31:HIS:CE1	30:18:32:LEU:HD22	2.53	0.43
1:1A:1216:G:H2'	1:1A:1217:G:H5'	2.00	0.43
1:1A:1524:G:O2'	1:1A:1604:A:C2	2.72	0.43
1:1A:1633:C:H2'	1:1A:1634:C:H6	1.83	0.43
1:1A:2485:C:H5''	1:1A:2486:C:OP2	2.18	0.43
1:1A:2704:A:H2'	1:1A:2705:G:H8	1.84	0.43
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.84	0.43
7:1H:103:LEU:HD23	7:1H:148:ILE:HD12	2.00	0.43
7:1H:5:GLY:HA2	7:1H:69:ARG:HB3	2.00	0.43
11:1P:42:SER:O	59:1P:301:HOH:O	2.22	0.43
1:2A:1041:A:C6	1:2A:1205:G:N1	2.87	0.43
1:2A:1404:A:N1	1:2A:1417:U:O4	2.52	0.43
1:2A:2784:C:H2'	1:2A:2785:C:C6	2.53	0.43
1:2A:537:A:C2	1:2A:538:A:C4	3.07	0.43
1:2A:588:U:H2'	1:2A:589:A:O4'	2.19	0.43
1:2A:818:C:H2'	1:2A:819:U:H6	2.44	0.43
1:2A:955:A:C6	1:2A:956:A:C6	3.07	0.43
2:2B:59:A:H3'	2:2B:60:C:C6	2.53	0.43
2:2B:90:A:N7	2:2B:91:C:H1'	2.33	0.43
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.99	0.43
3:2D:33:LEU:HA	3:2D:33:LEU:HD23	1.75	0.43
5:2F:33:LEU:HB3	11:2P:6:LEU:HD21	2.01	0.43
6:2G:16:ARG:NH2	6:2G:31:VAL:HG13	2.33	0.43
9:2N:96:GLU:HB2	9:2N:122:VAL:HG12	2.01	0.43
11:2P:82:GLY:HA3	11:2P:115:LEU:HD11	2.00	0.43
26:14:14:ILE:HG23	26:14:31:ILE:HB	2.00	0.43
1:1A:124:A:H5''	1:1A:125:C:C6	2.54	0.43
1:1A:2514:A:P	59:1A:4236:HOH:O	2.76	0.43
1:1A:628:U:H4'	1:1A:704:C:H4'	2.00	0.43
2:1B:48:A:H4'	14:1S:95:HIS:CD2	2.51	0.43
6:1G:138:GLN:HE21	6:1G:153:ARG:HH21	1.67	0.43
7:1H:4:ILE:O	7:1H:69:ARG:HG2	2.19	0.43
10:1O:21:CYS:HB2	10:1O:39:ILE:HD12	2.01	0.43
1:1A:878:G:H5'	11:1P:45:LEU:HD21	2.01	0.43
21:1Z:31:ARG:H	21:1Z:31:ARG:HG3	1.63	0.43
1:2A:298:G:N3	1:2A:540:C:H4'	110.69	0.43
2:2B:80:U:O2'	2:2B:81:G:H8	2.02	0.43
4:2E:77:ILE:HD13	4:2E:195:LEU:HD22	2.00	0.43
5:2F:196:LEU:HA	5:2F:196:LEU:HD13	1.83	0.43
12:2Q:2:LEU:H	12:2Q:2:LEU:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2225:C:O2	1:1A:2231:G:C2	2.71	0.43
1:1A:439:C:N3	1:1A:475:G:N1	72.80	0.43
1:1A:475:G:OP2	59:1A:4161:HOH:O	2.21	0.43
1:1A:1614:G:H4'	3:1D:59:LYS:HG2	2.01	0.43
4:1E:78:LEU:O	4:1E:79:ARG:HD3	2.19	0.43
1:2A:1132:G:C6	1:2A:1134:G:C4	3.07	0.43
1:2A:795:C:O2	1:2A:1663:A:H2'	2.19	0.43
1:2A:1915:C:H2'	1:2A:1916:C:H6	1.84	0.43
1:2A:38:C:H2'	1:2A:39:C:C6	2.54	0.43
2:2B:32:C:H42	2:2B:50:G:H1	1.67	0.43
8:2I:140:LEU:HA	8:2I:140:LEU:HD23	1.83	0.43
11:2P:101:VAL:HA	11:2P:106:LEU:O	2.18	0.43
25:13:18:ASP:OD1	25:13:18:ASP:N	2.52	0.43
1:1A:1065:A:N1	1:1A:1185:U:O2'	2.47	0.43
1:1A:2203:G:N2	1:1A:2204:C:N3	2.66	0.43
1:1A:2283:U:H5''	1:1A:2284:A:OP1	2.19	0.43
1:1A:894:G:N9	1:1A:977:A:H8	2.17	0.43
3:1D:164:GLN:NE2	3:1D:166:GLN:OE1	2.52	0.43
16:1U:112:ARG:NH2	17:1V:47:VAL:HB	2.34	0.43
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.54	0.43
30:28:26:LYS:HG2	30:28:48:PHE:CD1	2.54	0.43
1:2A:1039:C:O2'	1:2A:1041:A:OP1	2.29	0.43
1:2A:1072:A:N6	1:2A:1171:A:C4	2.86	0.43
1:2A:1332:A:H5''	1:2A:1333:U:OP2	2.19	0.43
1:2A:2898:C:H2'	1:2A:2899:G:O4'	2.19	0.43
1:2A:323:A:H5''	1:2A:324:G:OP2	2.18	0.43
6:2G:126:ASP:CG	6:2G:130:ASN:HD22	2.21	0.43
19:2X:52:VAL:HG12	19:2X:82:GLN:O	2.19	0.43
20:2Y:20:TYR:CZ	20:2Y:43:ASN:HA	2.54	0.43
23:11:21:ARG:HD3	23:11:35:THR:HG21	2.01	0.42
1:1A:11:U:H2'	1:1A:11:U:O2	2.18	0.42
1:1A:1209:G:H2'	1:1A:1210:U:C6	2.54	0.42
1:1A:1992:A:OP2	3:1D:242:ARG:NH2	2.52	0.42
1:1A:503:A:N1	1:1A:524:G:H4'	2.33	0.42
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	2.01	0.42
7:1H:86:GLU:OE1	7:1H:132:ARG:NH2	2.52	0.42
1:1A:921:G:O2'	21:1Z:151:HIS:HE1	2.02	0.42
28:26:10:LEU:HG	28:26:54:ILE:HG13	2.01	0.42
1:2A:1262:C:H42	1:2A:1276:G:H1	1.65	0.42
1:2A:1897:A:H2'	1:2A:1898:A:C8	2.54	0.42
1:2A:2537:G:H2'	1:2A:2538:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:338:G:H2'	1:2A:339:C:O4'	2.18	0.42
1:2A:903:C:OP2	22:20:77:ARG:NH2	2.52	0.42
2:2B:51:G:H2'	2:2B:52:A:C8	2.54	0.42
6:2G:36:LYS:HG2	6:2G:160:VAL:HB	2.01	0.42
8:2I:48:GLU:HG3	8:2I:52:ARG:NH1	2.34	0.42
1:1A:159:G:C2'	1:1A:160:C:H5'	2.49	0.42
6:1G:102:PHE:CE1	6:1G:141:PHE:HE2	2.37	0.42
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.54	0.42
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.54	0.42
1:2A:1109:C:O2	1:2A:1109:C:H2'	2.19	0.42
1:2A:1116:G:H1'	1:2A:1134:G:C8	2.55	0.42
1:2A:1258:A:H61	1:2A:1280:G:H1'	1.84	0.42
1:2A:1869:G:C8	1:2A:1948:A:H1'	2.54	0.42
1:2A:754:C:H42	1:2A:769:G:H1	1.67	0.42
1:2A:794:G:C8	18:2W:89:ALA:HB1	2.54	0.42
1:2A:820:A:H2'	1:2A:820:A:N3	2.33	0.42
1:2A:732:G:H21	1:2A:834:A:H61	1.66	0.42
1:2A:846:A:OP1	1:2A:846:A:H8	2.01	0.42
1:2A:921:G:O2'	21:2Z:151:HIS:HE1	2.02	0.42
2:2B:78:A:C2	2:2B:100:A:C4	3.08	0.42
2:2B:42:C:H2'	2:2B:43:C:H6	1.84	0.42
5:2F:157:VAL:HG21	5:2F:181:LEU:HD13	2.00	0.42
8:2I:75:LEU:HD11	8:2I:105:HIS:CG	2.54	0.42
13:2R:52:ILE:O	13:2R:55:ALA:N	2.52	0.42
2:2B:50:G:OP2	14:2S:62:LYS:HE3	2.19	0.42
21:2Z:127:LYS:O	21:2Z:128:VAL:HG12	2.19	0.42
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.19	0.42
24:12:28:LYS:HG3	24:12:53:LEU:HD21	2.00	0.42
26:14:14:ILE:H	26:14:14:ILE:HG12	1.57	0.42
1:1A:1090:A:H4'	1:1A:1091:A:H5''	2.02	0.42
1:1A:2022:A:H2'	1:1A:2023:G:C8	2.55	0.42
1:1A:209:A:N1	1:1A:253:A:O2'	2.46	0.42
1:1A:271:U:H4'	8:1I:50:ARG:NH1	2.34	0.42
1:1A:601:G:H2'	1:1A:602:C:C6	2.54	0.42
1:1A:870:A:H2'	1:1A:871:C:C6	2.79	0.42
5:1F:32:LEU:HB3	5:1F:112:MET:HE1	2.01	0.42
25:23:4:LEU:O	25:23:36:VAL:HA	2.19	0.42
1:2A:1386:U:H3'	1:2A:1442:U:O2	2.20	0.42
1:2A:2207:G:H8	1:2A:2207:G:OP2	2.03	0.42
1:2A:2278:A:H5''	1:2A:2279:A:C5'	2.48	0.42
1:2A:2303:C:C2'	1:2A:2304:C:H5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2657:C:H2'	1:2A:2658:U:O4'	2.20	0.42
1:2A:2890:C:H2'	1:2A:2891:A:O4'	2.20	0.42
1:2A:31:C:O2'	1:2A:32:U:H5'	2.19	0.42
1:2A:646:G:H2'	1:2A:647:G:C8	2.54	0.42
1:2A:772:G:OP2	1:2A:772:G:H8	2.02	0.42
5:2F:112:MET:HE3	5:2F:112:MET:HB3	1.76	0.42
5:2F:160:ASN:HB3	5:2F:163:VAL:HB	2.01	0.42
12:2Q:32:TYR:OH	12:2Q:111:GLU:HB2	2.19	0.42
13:2R:54:LEU:HA	13:2R:54:LEU:HD12	1.84	0.42
1:1A:1066:A:H8	1:1A:1066:A:H3'	1.84	0.42
1:1A:1072:A:C2	1:1A:2499:A:H5'	2.54	0.42
1:1A:1151:G:N3	1:1A:1151:G:H2'	2.34	0.42
1:1A:122:G:N2	59:1A:4291:HOH:O	2.47	0.42
1:1A:1272:G:C4	1:1A:1273:G:C8	3.61	0.42
1:1A:216:A:H8	1:1A:217:A:H5'	1.84	0.42
1:1A:241:C:OP2	30:18:5:LYS:NZ	2.41	0.42
1:1A:2657:C:H2'	1:1A:2658:U:O4'	2.19	0.42
1:1A:2670:G:O2'	7:1H:175:LYS:NZ	2.48	0.42
1:1A:989:A:C4	1:1A:2459:A:C2	3.07	0.42
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.54	0.42
6:1G:47:LYS:HG2	6:1G:47:LYS:H	1.67	0.42
7:1H:157:TYR:CE1	7:1H:172:LYS:HG3	2.55	0.42
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	2.01	0.42
1:1A:141:G:O2'	19:1X:35:THR:HG21	2.19	0.42
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	2.00	0.42
21:1Z:5:LEU:O	21:1Z:59:LEU:HA	2.19	0.42
21:1Z:92:SER:O	21:1Z:94:GLU:N	2.53	0.42
2:2B:83:G:H4'	25:23:52:HIS:CG	2.54	0.42
1:2A:1024:G:H3'	1:2A:1025:A:C5'	2.49	0.42
1:2A:1058:C:O2'	1:2A:1059:U:H5'	2.19	0.42
1:2A:1098:C:N4	1:2A:1151:G:H1	1.95	0.42
1:2A:2059:G:H2'	1:2A:2060:C:O4'	2.19	0.42
1:2A:2325:C:H2'	1:2A:2326:G:H8	1.81	0.42
1:2A:2358:C:H2'	1:2A:2359:U:C6	2.53	0.42
1:2A:238:G:C6	1:2A:239:A:C6	3.08	0.42
1:2A:827:A:H2	1:2A:1806:G:N3	2.17	0.42
1:2A:870:A:H2'	1:2A:871:C:C6	2.89	0.42
1:2A:996:G:C6	1:2A:997:A:N7	2.88	0.42
2:2B:54:G:C2	2:2B:55:U:O2	2.72	0.42
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	2.02	0.42
14:2S:68:GLN:HE21	14:2S:71:ARG:HH11	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:80:ASP:OD1	15:2T:64:ARG:NH2	2.52	0.42
20:2Y:76:CYS:SG	20:2Y:78:ALA:HB3	2.60	0.42
21:2Z:155:LEU:HD12	21:2Z:155:LEU:HA	1.92	0.42
1:1A:2346:A:C8	1:1A:2348:G:C5	3.07	0.42
1:1A:930:C:H2'	1:1A:931:C:C1'	2.50	0.42
3:1D:8:PRO:HB3	3:1D:14:ARG:HB2	2.01	0.42
1:1A:346:G:C8	5:1F:171:PRO:HG3	2.55	0.42
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	2.00	0.42
10:1O:104:ARG:HH22	15:1T:43:GLN:NE2	2.18	0.42
30:28:31:HIS:CE1	30:28:32:LEU:HD13	2.55	0.42
1:2A:1280:G:C2	1:2A:1281:G:N2	2.87	0.42
1:2A:1557:G:H2'	1:2A:1558:C:O4'	2.19	0.42
1:2A:1643:C:H2'	1:2A:1644:C:C6	2.55	0.42
1:2A:2302:U:H2'	1:2A:2303:C:H6	1.81	0.42
1:2A:243:A:C6	1:2A:244:A:C5	3.08	0.42
1:2A:2706:C:H2'	1:2A:2707:U:H6	1.85	0.42
1:2A:323:A:H1'	1:2A:342:C:H1'	2.02	0.42
1:2A:751:A:H2'	1:2A:752:A:O4'	2.37	0.42
2:2B:16:G:H1	2:2B:68:C:H42	1.66	0.42
4:2E:37:ARG:HA	4:2E:42:ASP:OD2	2.19	0.42
6:2G:128:ARG:HE	6:2G:128:ARG:HB2	1.69	0.42
1:2A:2219:A:OP1	8:2I:33:ARG:NH2	2.53	0.42
1:2A:184:A:H62	11:2P:38:GLN:HE22	1.66	0.42
1:2A:2848:G:H5'	13:2R:46:GLY:HA2	2.02	0.42
13:2R:67:LEU:HD23	13:2R:76:VAL:HG21	2.01	0.42
1:1A:1153:U:C6	1:1A:1154:C:C6	3.07	0.42
1:1A:115:A:C8	1:1A:116:A:C8	3.07	0.42
1:1A:1402:U:H2'	1:1A:1403:G:O4'	2.19	0.42
1:1A:214:G:N2	1:1A:216:A:H62	2.13	0.42
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.84	0.42
11:1P:77:ARG:HB2	11:1P:78:PRO:HD2	2.01	0.42
1:2A:1104:G:H5'	1:2A:1105:U:P	2.59	0.42
1:2A:2107:U:H2'	1:2A:2108:G:C8	2.54	0.42
1:2A:2286:C:H6	1:2A:2286:C:H5'	1.85	0.42
1:2A:2828:G:H2'	1:2A:2830:A:N7	2.35	0.42
1:2A:330:G:H2'	1:2A:332:G:OP2	2.19	0.42
1:2A:651:A:C6	1:2A:661:A:C8	3.08	0.42
2:2B:55:U:H1'	6:2G:29:TRP:HE1	1.84	0.42
10:2O:98:VAL:HG13	10:2O:117:LEU:HB3	2.02	0.42
23:11:97:LEU:HD23	23:11:97:LEU:HA	1.92	0.42
1:1A:1404:A:C6	1:1A:1417:U:O4	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1553:A:H4'	1:1A:1555:A:C4	2.55	0.42
1:1A:2544:A:H2'	1:1A:2545:A:O4'	2.20	0.42
3:1D:102:LYS:C	3:1D:103:ARG:HG2	2.38	0.42
11:1P:91:PHE:CE1	11:1P:99:LEU:HD11	2.55	0.42
26:24:58:ARG:HB3	26:24:59:PHE:CD1	2.55	0.42
29:27:30:VAL:O	29:27:34:ARG:HG3	2.19	0.42
1:2A:80:G:N1	1:2A:100:A:OP2	2.46	0.42
1:2A:1898:A:H3'	1:2A:1899:G:O4'	2.20	0.42
1:2A:604:G:H2'	1:2A:605:G:C8	2.54	0.42
1:2A:769:G:H2'	1:2A:770:U:O4'	2.20	0.42
1:2A:966:G:C6	1:2A:967:U:C4	3.08	0.42
1:2A:967:U:H2'	1:2A:968:C:C6	2.55	0.42
3:2D:16:MET:HG3	3:2D:206:LEU:O	2.20	0.42
10:2O:70:LYS:HE2	10:2O:70:LYS:HB3	1.93	0.42
1:2A:2305:C:P	14:2S:89:ARG:HH22	2.42	0.42
16:2U:17:ILE:HA	16:2U:17:ILE:HD13	1.89	0.42
21:2Z:75:ASN:HB2	21:2Z:85:HIS:HB3	2.01	0.42
1:1A:1409:G:OP2	23:11:3:LYS:HD2	2.20	0.42
1:1A:1399:A:H2'	1:1A:1400:G:O4'	2.20	0.42
1:1A:2107:U:H2'	1:1A:2108:G:H8	1.84	0.42
1:1A:2429:A:H2'	1:1A:2430:U:H6	1.85	0.42
5:1F:11:VAL:HB	5:1F:18:ARG:HB3	2.00	0.42
7:1H:76:VAL:O	7:1H:80:SER:OG	2.38	0.42
15:1T:118:ARG:HH11	15:1T:118:ARG:CG	2.32	0.42
1:2A:1348:G:H2'	1:2A:1349:C:O4'	2.74	0.42
1:2A:1765:G:H8	1:2A:1769:A:H62	1.66	0.42
1:2A:2567:C:H2'	1:2A:2568:G:O4'	2.19	0.42
1:2A:2690:A:H4'	4:2E:165:VAL:HG11	2.02	0.42
1:2A:2854:G:H2'	1:2A:2855:G:C8	2.55	0.42
1:2A:647:G:C2	1:2A:648:C:C2	3.08	0.42
1:2A:680:C:H2'	1:2A:681:G:O4'	2.19	0.42
1:2A:825:U:H6	1:2A:825:U:P	3.51	0.42
1:2A:850:A:H5''	1:2A:851:G:OP1	2.20	0.42
1:2A:866:A:H2'	1:2A:867:A:O4'	2.20	0.42
1:2A:991:G:N2	1:2A:1015:C:C2	2.88	0.42
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.40	0.42
10:2O:68:GLU:CB	10:2O:78:ARG:HB2	2.49	0.42
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.51	0.42
15:2T:116:ALA:HB1	15:2T:121:ILE:HD11	2.02	0.42
1:1A:1732:C:H2'	1:1A:1733:G:O4'	2.20	0.42
8:1I:109:ILE:HG23	8:1I:110:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1067:G:C5	1:2A:1184:C:C4	3.08	0.42
1:2A:126:C:H2'	1:2A:127:C:H6	2.19	0.42
1:2A:1546:C:O4'	3:2D:100:GLY:HA2	2.20	0.42
1:2A:2224:U:H2'	1:2A:2225:C:C6	2.54	0.42
6:2G:142:PRO:HG2	6:2G:143:GLU:OE2	2.19	0.42
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	2.02	0.42
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.54	0.42
11:2P:95:VAL:HG13	11:2P:125:VAL:HB	2.02	0.42
20:2Y:5:MET:HB2	20:2Y:5:MET:HE2	1.85	0.42
23:11:82:LEU:HA	23:11:85:LEU:HD12	2.02	0.42
26:14:68:ARG:NH2	26:14:68:ARG:HB3	2.35	0.42
1:1A:1313:A:C2	1:1A:2034:A:C4	3.08	0.42
1:1A:1531:A:H2'	1:1A:1532:G:H8	1.84	0.42
1:1A:2224:U:O2'	1:1A:2225:C:H5'	2.20	0.42
1:1A:485:A:H2'	1:1A:486:C:O4'	2.19	0.42
1:1A:908:G:H2'	1:1A:909:A:O4'	2.20	0.42
6:1G:43:LEU:HD12	6:1G:43:LEU:HA	1.85	0.42
1:1A:2330:G:H22	14:1S:3:ARG:NE	2.18	0.42
20:1Y:55:TYR:N	20:1Y:55:TYR:CD1	2.87	0.42
25:23:29:ARG:H	25:23:33:GLN:NE2	2.18	0.42
1:2A:115:A:H3'	1:2A:116:A:H5''	2.02	0.42
1:2A:1047:G:N2	1:2A:1199:G:H1'	2.35	0.42
1:2A:1198:C:H2'	1:2A:1199:G:O4'	2.20	0.42
1:2A:1334:C:H2'	1:2A:1335:C:C6	2.55	0.42
1:2A:1878:A:C4	1:2A:1879:G:C8	3.07	0.42
1:2A:2588:A:O4'	27:25:3:LYS:HB2	2.20	0.42
1:2A:946:A:C5	1:2A:947:C:C4	3.08	0.42
2:2B:2:C:P	2:2B:2:C:H3'	2.60	0.42
9:2N:131:GLN:H	9:2N:131:GLN:HG2	1.58	0.42
9:2N:73:THR:HB	9:2N:82:LEU:HD11	2.00	0.42
12:2Q:77:LYS:HE3	12:2Q:84:GLY:O	2.20	0.42
14:2S:63:THR:OG1	14:2S:64:GLU:N	3.25	0.42
21:2Z:128:VAL:HG23	21:2Z:160:GLY:O	2.20	0.42
23:11:4:VAL:HG22	23:11:11:ARG:HB3	2.01	0.41
1:1A:1149:C:H2'	1:1A:1150:U:C5	2.53	0.41
1:1A:2284:A:H2'	1:1A:2285:A:C8	2.54	0.41
1:1A:761:G:H2'	1:1A:762:A:O4'	2.20	0.41
4:1E:101:ARG:HB2	4:1E:201:THR:HG21	2.01	0.41
5:1F:37:VAL:HG21	11:1P:6:LEU:HD11	2.00	0.41
2:1B:57:A:H1'	6:1G:29:TRP:HB2	2.01	0.41
20:1Y:7:VAL:HG21	20:1Y:72:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2438:C:H5''	1:2A:2439:G:OP1	2.19	0.41
1:2A:2700:U:O2	1:2A:2700:U:H5'	2.19	0.41
1:2A:2881:G:C2	1:2A:2882:A:N6	2.87	0.41
1:2A:772:G:C8	1:2A:772:G:OP2	2.73	0.41
5:2F:192:LEU:HD13	5:2F:194:MET:HE2	2.00	0.41
8:2I:104:GLN:HG3	8:2I:105:HIS:CD2	2.55	0.41
19:2X:65:ARG:HD3	19:2X:70:LEU:HG	2.01	0.41
3:1D:134:ARG:NH1	3:1D:188:GLU:OE2	2.53	0.41
5:1F:106:ARG:H	5:1F:106:ARG:HG2	1.49	0.41
1:2A:75:C:OP1	24:22:59:ARG:HD3	2.19	0.41
1:2A:1439:U:C4	1:2A:1440:A:C5	3.08	0.41
1:2A:16:G:H2'	1:2A:17:C:C6	2.55	0.41
1:2A:1840:A:H8	1:2A:1840:A:O5'	2.03	0.41
1:2A:1890:G:OP2	1:2A:1890:G:H8	2.03	0.41
1:2A:2249:G:N3	1:2A:2249:G:H2'	2.35	0.41
1:2A:2796:C:H2'	1:2A:2797:C:H6	1.84	0.41
1:2A:345:A:H5'	1:2A:363:A:H1'	2.01	0.41
1:2A:539:A:H1'	1:2A:603:C:H1'	2.03	0.41
1:2A:622:G:N2	1:2A:627:C:O3'	2.53	0.41
1:2A:909:A:H2'	1:2A:910:G:H8	1.85	0.41
2:2B:111:G:H2'	2:2B:112:U:O4'	2.19	0.41
1:2A:1739:U:O2'	3:2D:14:ARG:NH2	2.53	0.41
12:2Q:72:LYS:HB3	12:2Q:94:VAL:HG23	2.03	0.41
30:18:23:VAL:CG1	30:18:47:LYS:HD3	2.50	0.41
1:1A:182:G:OP2	59:1A:4163:HOH:O	2.21	0.41
1:1A:2115:G:P	8:1I:22:LYS:HD2	2.60	0.41
1:1A:2783:C:H2'	1:1A:2784:C:C6	2.55	0.41
1:1A:1614:G:H5''	3:1D:61:LEU:HD22	2.01	0.41
8:1I:132:PRO:HD2	8:1I:136:VAL:O	2.20	0.41
21:1Z:67:LEU:HA	21:1Z:68:PRO:HD3	1.94	0.41
1:2A:1095:A:H2'	1:2A:1096:G:H8	1.85	0.41
1:2A:1096:G:C4	1:2A:1097:C:C5	3.08	0.41
1:2A:554:G:C5	1:2A:2043:U:H5''	2.55	0.41
1:2A:2596:U:H4'	1:2A:2597:C:OP1	2.19	0.41
1:2A:2602:C:H2'	1:2A:2603:G:C8	2.56	0.41
1:2A:534:C:H2'	1:2A:535:U:O4'	2.21	0.41
3:2D:43:ARG:HA	3:2D:48:ARG:O	2.21	0.41
4:2E:101:ARG:NH2	4:2E:171:GLU:HB2	2.36	0.41
1:2A:719:C:H5''	5:2F:81:PRO:HD2	2.02	0.41
6:2G:44:GLY:N	6:2G:88:ILE:O	2.54	0.41
7:2H:95:ARG:HA	7:2H:128:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:6:LEU:HD13	15:2T:6:LEU:HA	1.78	0.41
16:2U:44:ASN:N	16:2U:44:ASN:HD22	2.18	0.41
1:1A:1055:A:N3	1:1A:1198:C:H1'	2.36	0.41
1:1A:1248:A:N6	1:1A:1285:U:H2'	2.35	0.41
1:1A:1477:C:H2'	1:1A:1478:U:O4'	2.20	0.41
1:1A:1763:G:C6	1:1A:1764:U:C4	3.08	0.41
1:1A:553:A:C2	59:1A:4190:HOH:O	2.73	0.41
3:1D:68:LYS:O	3:1D:69:ARG:HB2	2.21	0.41
6:1G:131:TYR:HB3	6:1G:159:VAL:CG1	2.50	0.41
7:1H:7:LEU:HG	7:1H:69:ARG:NH1	2.34	0.41
10:1O:87:ILE:HD12	10:1O:91:LEU:HA	2.02	0.41
14:1S:41:ASP:OD2	14:1S:44:LYS:HG3	2.20	0.41
16:1U:8:VAL:HG22	16:1U:11:ARG:HH21	1.85	0.41
18:1W:18:ARG:HG3	18:1W:76:VAL:HB	2.01	0.41
19:1X:31:HIS:HD2	19:1X:33:LYS:N	2.07	0.41
1:2A:1056:G:C6	1:2A:1058:C:C4	3.09	0.41
1:2A:1080:U:H2'	1:2A:1081:G:C8	2.56	0.41
1:2A:1307:A:H2	27:25:10:LYS:HD2	1.85	0.41
1:2A:1308:U:C4	1:2A:1309:G:C6	3.08	0.41
1:2A:1330:G:N2	1:2A:1373:G:H5''	2.35	0.41
1:2A:2080:A:O2'	5:2F:69:HIS:HD2	2.03	0.41
1:2A:2495:G:C2	1:2A:2496:G:C8	3.08	0.41
1:2A:348:G:H2'	1:2A:349:G:O4'	2.21	0.41
2:2B:102:A:H8	2:2B:102:A:O5'	2.04	0.41
4:2E:115:GLY:O	4:2E:119:ARG:HB2	2.21	0.41
5:2F:33:LEU:HA	5:2F:33:LEU:HD12	1.83	0.41
6:2G:33:ARG:HH12	6:2G:162:THR:CB	2.33	0.41
6:2G:27:ASN:HB3	6:2G:30:GLU:HG3	2.02	0.41
1:2A:909:A:OP1	12:2Q:22:LYS:HG3	2.21	0.41
28:16:2:ALA:N	59:16:201:HOH:O	2.54	0.41
1:1A:1424:A:H4'	1:1A:1425:G:OP2	2.19	0.41
1:1A:1451:U:H2'	1:1A:1452:C:H6	1.84	0.41
1:1A:1474:G:H2'	1:1A:1475:C:H6	1.83	0.41
1:1A:149:C:C5	1:1A:150:C:H5	3.67	0.41
1:1A:2388:A:H2'	1:1A:2389:A:C8	2.55	0.41
1:1A:2400:G:H5''	1:1A:2401:U:O4'	2.21	0.41
1:1A:488:G:OP2	59:1A:4164:HOH:O	2.22	0.41
1:1A:638:G:C5	1:1A:639:A:C8	12.99	0.41
1:1A:830:A:O4'	3:1D:227:ASN:ND2	2.53	0.41
2:1B:78:A:C2	2:1B:100:A:C4	3.08	0.41
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:345:A:H3'	5:1F:169:ASN:HD21	1.85	0.41
7:1H:3:ARG:HG3	7:1H:4:ILE:N	2.35	0.41
17:1V:49:THR:HG22	17:1V:49:THR:O	2.20	0.41
21:1Z:24:LEU:HB2	21:1Z:41:LEU:HD23	2.00	0.41
1:2A:2405:C:P	30:28:30:ARG:NH1	2.93	0.41
1:2A:1059:U:H2'	1:2A:1060:G:C8	2.55	0.41
1:2A:1109:C:H42	1:2A:1119:G:H1	1.69	0.41
1:2A:1155:G:H8	1:2A:1155:G:O5'	2.03	0.41
1:2A:1697:G:H2'	1:2A:1698:A:O4'	2.21	0.41
1:2A:2371:A:H2'	1:2A:2372:A:O4'	2.20	0.41
1:2A:2421:G:C2	1:2A:2422:A:H1'	2.55	0.41
1:2A:1683:A:H4'	1:2A:2722:A:O2'	2.20	0.41
1:2A:623:C:OP1	5:2F:108:LYS:NZ	2.35	0.41
1:2A:945:A:HO2'	1:2A:946:A:P	2.43	0.41
2:2B:4:C:C2	2:2B:118:G:N2	2.89	0.41
2:2B:53:A:H2'	2:2B:54:G:O4'	2.21	0.41
6:2G:76:SER:CB	6:2G:84:LYS:H	2.34	0.41
8:2I:29:TYR:CD2	8:2I:30:LEU:HD23	2.55	0.41
11:2P:59:LEU:HD23	11:2P:59:LEU:HA	1.87	0.41
14:2S:62:LYS:HB3	14:2S:97:ARG:NE	2.36	0.41
16:2U:110:VAL:O	16:2U:113:ALA:HB3	2.21	0.41
24:12:51:ARG:HD3	24:12:55:ARG:NH1	2.35	0.41
24:12:61:LEU:HD23	24:12:61:LEU:HA	1.93	0.41
1:1A:1185:U:OP1	9:1N:25:ARG:NH1	2.52	0.41
1:1A:885:U:H1'	1:1A:1235:G:H1'	2.03	0.41
1:1A:2659:C:H2'	1:1A:2660:U:H6	1.85	0.41
1:1A:2797:C:H2'	1:1A:2798:U:O4'	2.21	0.41
1:1A:612:A:OP1	5:1F:95:ARG:NH1	2.54	0.41
1:1A:614:G:H2'	1:1A:615:G:C8	3.80	0.41
1:1A:830:A:C5	3:1D:229:VAL:HG21	2.56	0.41
4:1E:85:ASN:HA	4:1E:86:PRO:HD2	1.94	0.41
20:1Y:38:ILE:HD13	20:1Y:66:PRO:HA	2.03	0.41
21:1Z:40:ASP:OD2	21:1Z:42:VAL:HG13	2.20	0.41
1:2A:1038:G:OP1	16:2U:50:ARG:NH2	2.50	0.41
1:2A:183:A:H5''	1:2A:184:A:O5'	2.21	0.41
1:2A:2333:A:H2'	1:2A:2334:G:O4'	2.20	0.41
1:2A:2704:A:H2'	1:2A:2705:G:C8	2.54	0.41
1:2A:2706:C:H2'	1:2A:2707:U:C6	2.56	0.41
1:2A:745:A:H2'	1:2A:746:G:O4'	2.20	0.41
3:2D:147:LEU:HA	3:2D:147:LEU:HD12	1.88	0.41
5:2F:183:VAL:O	5:2F:187:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:135:LEU:HA	11:2P:135:LEU:HD23	1.92	0.41
16:2U:16:LYS:HB3	16:2U:16:LYS:HE2	1.88	0.41
26:14:46:GLN:O	26:14:48:ARG:HG2	2.21	0.41
1:1A:1777:G:H2'	1:1A:1778:G:H5''	2.02	0.41
1:1A:210:A:H5''	1:1A:447:U:OP1	2.20	0.41
3:1D:38:LYS:HA	3:1D:38:LYS:HD2	1.83	0.41
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.34	0.41
8:1I:129:THR:HG22	8:1I:139:GLN:NE2	2.19	0.41
1:1A:1311:G:O5'	18:1W:15:ARG:NH2	2.53	0.41
19:1X:57:LEU:HD11	19:1X:78:LYS:CE	2.51	0.41
26:24:59:PHE:HA	26:24:60:GLN:C	2.41	0.41
1:2A:1313:A:H2'	1:2A:1314:A:O4'	2.21	0.41
1:2A:1585:G:H2'	1:2A:1586:U:C6	2.55	0.41
1:2A:1643:C:H2'	1:2A:1644:C:H6	1.85	0.41
1:2A:1684:C:H4'	1:2A:2721:C:O2	2.21	0.41
1:2A:1840:A:H2'	1:2A:1841:G:O4'	2.20	0.41
1:2A:253:A:C8	1:2A:254:G:H1'	2.56	0.41
1:2A:2753:A:H2'	1:2A:2754:C:O4'	2.19	0.41
2:2B:10:C:C4	2:2B:11:C:C5	3.08	0.41
3:2D:10:THR:OG1	3:2D:13:ARG:HG2	2.20	0.41
4:2E:89:ASP:OD2	4:2E:89:ASP:N	2.53	0.41
6:2G:173:LEU:HB3	6:2G:178:PHE:CG	2.55	0.41
7:2H:44:VAL:HG21	7:2H:51:ARG:HB2	2.01	0.41
15:2T:64:ARG:NH1	15:2T:103:ARG:HA	2.35	0.41
21:2Z:132:ASN:O	21:2Z:134:PRO:HD3	2.20	0.41
27:15:11:THR:HG23	27:15:15:ARG:HB3	2.03	0.41
6:1G:138:GLN:HE21	6:1G:153:ARG:NH2	2.19	0.41
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.36	0.41
1:2A:1248:A:C8	1:2A:1250:G:C6	3.08	0.41
1:2A:1593:C:H2'	1:2A:1594:C:C6	2.55	0.41
1:2A:793:U:O2	1:2A:2035:A:H1'	2.21	0.41
1:2A:20:A:O2'	1:2A:21:C:H5'	2.21	0.41
1:2A:2114:G:C6	1:2A:2236:A:C8	3.08	0.41
1:2A:2662:C:H2'	1:2A:2663:C:H6	1.86	0.41
1:2A:376:G:H2'	1:2A:377:G:C8	2.55	0.41
1:2A:666:G:H21	1:2A:670:A:H2	1.69	0.41
1:2A:6:G:H4'	9:2N:13:TRP:HH2	1.85	0.41
1:2A:184:A:C4	1:2A:851:G:C6	3.09	0.41
1:2A:989:A:C4	1:2A:2459:A:C2	3.09	0.41
2:2B:25:A:H2'	2:2B:26:A:O4'	2.20	0.41
3:2D:68:LYS:O	3:2D:69:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2691:C:H5'	4:2E:189:PRO:HA	2.01	0.41
6:2G:28:VAL:O	6:2G:31:VAL:HG12	2.21	0.41
13:2R:97:VAL:CG2	13:2R:114:VAL:HG13	2.51	0.41
1:2A:2305:C:H5'	14:2S:10:ARG:HD2	2.02	0.41
14:2S:62:LYS:O	14:2S:65:VAL:HB	2.21	0.41
17:2V:48:GLY:HA3	17:2V:52:VAL:HG12	2.02	0.41
21:2Z:30:ASN:ND2	21:2Z:90:VAL:HB	2.36	0.41
26:14:48:ARG:O	26:14:50:VAL:N	2.53	0.41
1:1A:238:G:P	30:18:13:ARG:HH22	2.43	0.41
1:1A:1091:A:OP1	1:1A:1091:A:H8	2.03	0.41
1:1A:1540:A:C6	1:1A:1541:A:C6	3.08	0.41
1:1A:554:G:C5	1:1A:2043:U:H5''	2.56	0.41
3:1D:167:GLY:H	3:1D:168:ARG:NH2	8.24	0.41
7:1H:23:ARG:HD2	7:1H:34:GLU:OE1	2.20	0.41
11:1P:81:GLN:NE2	11:1P:105:LEU:O	2.54	0.41
20:1Y:5:MET:HE2	20:1Y:5:MET:HB2	1.88	0.41
31:29:14:CYS:HA	31:29:27:CYS:HB2	2.02	0.41
1:2A:1037:C:H4'	1:2A:1037:C:OP2	5.78	0.41
1:2A:1146:U:C2	1:2A:1147:C:C5	3.09	0.41
1:2A:2622:U:H5'	1:2A:2622:U:H6	1.85	0.41
2:2B:33:G:C6	2:2B:34:U:C4	3.08	0.41
2:2B:33:G:C2	2:2B:50:G:C2	3.09	0.41
3:2D:204:ILE:H	3:2D:204:ILE:HG12	2.41	0.41
7:2H:127:GLU:C	7:2H:129:THR:H	2.24	0.41
14:2S:39:ILE:HB	14:2S:49:VAL:HG22	2.02	0.41
15:2T:122:ASP:O	15:2T:126:ALA:N	2.53	0.41
24:12:3:LEU:O	24:12:7:ARG:HG3	2.21	0.41
30:18:4:MET:HE3	30:18:63:PRO:CG	2.50	0.41
1:1A:1066:A:H8	1:1A:1067:G:H5''	1.85	0.41
1:1A:1220:G:H1'	1:1A:1221:A:O5'	2.21	0.41
1:1A:2416:G:H8	1:1A:2416:G:OP2	2.04	0.41
1:1A:610:U:O4	1:1A:716:A:H1'	2.21	0.41
2:1B:88:C:H2'	2:1B:89:G:O4'	2.21	0.41
6:1G:128:ARG:HB2	6:1G:128:ARG:HE	1.64	0.41
20:1Y:28:LYS:HD2	20:1Y:40:GLU:HG3	2.03	0.41
1:2A:138:A:H8	1:2A:1453:C:O2'	2.02	0.41
1:2A:153:G:O6	1:2A:160:C:N4	2.42	0.41
1:2A:2086:C:H2'	1:2A:2087:C:H6	1.86	0.41
1:2A:2207:G:C2	1:2A:2208:G:C6	3.08	0.41
1:2A:223:U:O2	1:2A:456:G:C2	2.74	0.41
1:2A:2311:G:C2	1:2A:2328:C:N3	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2390:G:H2'	1:2A:2391:C:C6	2.55	0.41
1:2A:514:G:N7	18:2W:49:LYS:NZ	2.67	0.41
1:2A:671:G:H8	1:2A:671:G:O5'	2.04	0.41
2:2B:61:G:C6	2:2B:62:C:C4	3.09	0.41
2:2B:87:G:HO2'	2:2B:88:C:H5	1.68	0.41
4:2E:52:LEU:HB2	4:2E:76:ARG:HB3	2.03	0.41
10:2O:1:MET:CE	10:2O:67:LYS:HG2	2.50	0.41
17:2V:89:GLN:HA	17:2V:90:PRO:HD3	1.94	0.41
21:2Z:92:SER:O	21:2Z:94:GLU:N	2.54	0.41
11:1P:63:PRO:HG2	30:18:25:MET:HB2	2.03	0.41
1:1A:1215:G:N2	1:1A:1224:C:C2	2.89	0.41
1:1A:1616:A:H2'	1:1A:1617:A:C8	2.56	0.41
1:1A:173:U:H4'	1:1A:206:A:H4'	2.03	0.41
1:1A:2225:C:C2	1:1A:2231:G:C2	3.09	0.41
1:1A:904:U:O2	1:1A:2279:A:H2'	2.21	0.41
1:1A:2719:G:H1'	13:1R:71:GLN:HE22	1.86	0.41
9:1N:39:ARG:HA	9:1N:40:PRO:HD3	1.98	0.41
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.50	0.41
15:1T:26:ASP:OD1	15:1T:120:ARG:NH2	2.40	0.41
1:2A:2622:U:O4	27:25:3:LYS:HG2	2.21	0.41
30:28:8:LYS:HB3	30:28:12:LYS:HE3	2.03	0.41
1:2A:107:G:C2	1:2A:108:A:C8	3.09	0.41
1:2A:1067:G:C6	1:2A:1184:C:C4	3.09	0.41
1:2A:1342:C:OP1	1:2A:2721:C:H4'	2.21	0.41
1:2A:1633:C:H2'	1:2A:1634:C:H6	1.86	0.41
1:2A:2040:A:OP2	27:25:9:LYS:NZ	2.52	0.41
1:2A:2124:C:H1'	1:2A:2208:G:H1	1.86	0.41
1:2A:2419:U:H2'	1:2A:2420:G:H8	1.84	0.41
1:2A:2845:U:C4	1:2A:2892:A:N6	2.89	0.41
1:2A:6:G:H2'	1:2A:7:A:C8	2.55	0.41
1:2A:716:A:H4'	1:2A:717:C:O5'	2.21	0.41
1:2A:784:G:C6	1:2A:785:G:C2	3.09	0.41
1:2A:894:G:C4	1:2A:977:A:H8	2.38	0.41
9:2N:37:LYS:HA	9:2N:42:TRP:CD1	2.55	0.41
12:2Q:12:GLN:HE21	12:2Q:72:LYS:HZ2	1.69	0.41
13:2R:60:LEU:HA	13:2R:60:LEU:HD23	1.86	0.41
14:2S:62:LYS:HB2	14:2S:62:LYS:HE3	1.96	0.41
21:2Z:67:LEU:HA	21:2Z:68:PRO:HD3	1.95	0.41
25:13:7:LYS:NZ	25:13:32:GLN:O	2.54	0.40
1:1A:1714:A:H4'	1:1A:1715:A:O5'	2.20	0.40
1:1A:2086:C:H2'	1:1A:2087:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2415:C:O3'	11:1P:77:ARG:NH2	2.54	0.40
1:1A:2811:A:N3	1:1A:2903:U:H1'	2.35	0.40
1:1A:307:U:H2'	1:1A:308:C:C6	2.56	0.40
1:1A:286:G:O2'	1:1A:447:U:OP2	2.32	0.40
5:1F:101:LEU:O	5:1F:106:ARG:HD3	2.21	0.40
19:1X:31:HIS:HA	19:1X:32:PRO:HD3	1.93	0.40
25:23:18:ASP:OD1	25:23:18:ASP:N	2.53	0.40
30:28:22:VAL:CG2	30:28:59:LYS:HG3	2.51	0.40
30:28:33:ASN:HA	30:28:36:LYS:HD2	2.02	0.40
1:2A:1043:C:C2	1:2A:1180:G:C2	27.87	0.40
1:2A:1682:C:H2'	1:2A:1683:A:H8	1.87	0.40
1:2A:195:A:H2'	1:2A:196:C:O4'	2.21	0.40
1:2A:2282:G:H2'	1:2A:2283:U:C6	2.55	0.40
1:2A:1813:A:C2	1:2A:2598:A:C5	3.09	0.40
1:2A:630:A:C6	1:2A:631:A:C6	3.08	0.40
1:2A:673:G:C5	1:2A:674:C:C4	3.09	0.40
1:2A:830:A:H3'	59:2A:3891:HOH:O	2.20	0.40
1:2A:982:G:N3	1:2A:982:G:H2'	2.91	0.40
3:2D:13:ARG:HA	3:2D:13:ARG:HD2	1.73	0.40
10:2O:9:GLU:O	10:2O:83:ALA:HA	2.22	0.40
13:2R:92:GLY:HA2	13:2R:94:TYR:CZ	2.56	0.40
16:2U:83:LEU:HD12	16:2U:88:ILE:HD12	2.04	0.40
21:2Z:19:ARG:HH11	21:2Z:19:ARG:HD3	1.75	0.40
1:1A:1474:G:O2'	1:1A:1475:C:H5'	2.21	0.40
1:1A:2802:A:H2'	1:1A:2802:A:N3	2.36	0.40
1:1A:454:A:H8	1:1A:454:A:OP2	2.05	0.40
1:1A:1536:G:O2'	3:1D:101:GLU:HB2	2.21	0.40
3:1D:123:ALA:HA	3:1D:124:PRO:HD3	1.92	0.40
7:1H:56:SER:OG	7:1H:58:GLU:HG2	2.22	0.40
1:1A:878:G:H5'	11:1P:45:LEU:CD2	2.51	0.40
22:20:82:ARG:HA	22:20:83:PRO:HD3	1.64	0.40
24:22:51:ARG:HH11	24:22:51:ARG:HG3	1.86	0.40
1:2A:1018:G:OP1	1:2A:1231:G:O2'	2.25	0.40
1:2A:1104:G:H5'	1:2A:1105:U:OP2	2.22	0.40
1:2A:1675:G:H2'	1:2A:1676:C:C6	2.56	0.40
1:2A:288:G:N7	1:2A:289:G:H1'	7.10	0.40
1:2A:332:G:C5	1:2A:353:A:C6	3.10	0.40
1:2A:466:U:H2'	1:2A:467:G:C8	2.57	0.40
1:2A:591:U:C4	1:2A:592:G:C6	3.09	0.40
4:2E:188:VAL:HA	4:2E:189:PRO:HD3	1.98	0.40
7:2H:109:PHE:HB2	7:2H:111:HIS:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:120:ALA:HB1	11:2P:138:LEU:HA	2.04	0.40
12:2Q:38:GLU:OE2	12:2Q:128:LYS:N	2.35	0.40
12:2Q:84:GLY:O	12:2Q:85:LYS:HB2	2.22	0.40
18:2W:51:LEU:HD23	18:2W:105:VAL:HG11	2.03	0.40
18:2W:83:LYS:O	18:2W:84:ARG:HD3	2.21	0.40
1:1A:75:C:OP1	24:12:59:ARG:HD3	2.21	0.40
29:17:3:ARG:HD3	29:17:3:ARG:HA	1.91	0.40
1:1A:982:G:N2	1:1A:1021:C:C4	37.59	0.40
1:1A:1897:A:H2'	1:1A:1898:A:C8	2.56	0.40
1:1A:2206:C:O2'	1:1A:2207:G:H5'	2.22	0.40
1:1A:955:A:N1	1:1A:2288:G:H1'	2.36	0.40
4:1E:175:VAL:HB	4:1E:182:LEU:HD12	2.03	0.40
11:1P:83:VAL:HG23	11:1P:87:ASP:HB2	2.03	0.40
20:1Y:90:LEU:HD12	20:1Y:90:LEU:HA	1.88	0.40
24:22:16:LEU:HB3	24:22:20:GLU:HB2	2.03	0.40
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	2.02	0.40
1:2A:1100:G:H3'	1:2A:1101:G:H8	1.86	0.40
1:2A:1596:C:H2'	1:2A:1597:C:C6	2.56	0.40
1:2A:1715:A:H5''	1:2A:2561:G:OP1	2.22	0.40
1:2A:792:A:H2'	1:2A:2623:C:H5''	2.02	0.40
1:2A:2700:U:OP2	1:2A:2731:G:N2	2.53	0.40
1:2A:2854:G:H2'	1:2A:2855:G:H8	1.86	0.40
1:2A:29:G:C6	1:2A:30:C:C4	3.08	0.40
1:2A:384:G:O2'	1:2A:385:U:H5'	2.21	0.40
1:2A:298:G:O2'	1:2A:540:C:H5''	110.43	0.40
1:2A:996:G:C6	1:2A:1010:G:C6	3.10	0.40
3:2D:245:PRO:HA	3:2D:246:PRO:HD3	1.92	0.40
4:2E:33:VAL:HG13	4:2E:89:ASP:C	2.41	0.40
5:2F:102:PRO:O	5:2F:106:ARG:HG2	2.22	0.40
5:2F:129:PHE:O	5:2F:132:VAL:HG13	2.19	0.40
7:2H:123:PHE:CE1	7:2H:133:VAL:HG22	2.56	0.40
10:2O:29:ASN:OD1	10:2O:29:ASN:N	2.51	0.40
18:2W:4:LYS:CB	18:2W:106:ILE:HG12	2.47	0.40
18:2W:54:ALA:HB1	18:2W:107:LEU:HD22	2.02	0.40
26:14:35:VAL:HG22	26:14:36:CYS:N	2.36	0.40
1:1A:2341:G:H2'	1:1A:2342:G:O4'	2.22	0.40
1:1A:2898:C:H2'	1:1A:2899:G:O4'	2.20	0.40
3:1D:25:THR:HG21	3:1D:113:VAL:HG11	2.04	0.40
3:1D:38:LYS:HE3	3:1D:39:LYS:O	2.21	0.40
3:1D:72:LYS:HE3	3:1D:75:ILE:HD12	2.04	0.40
4:1E:82:ARG:HG2	4:1E:83:ASP:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.56	0.40
5:1F:183:VAL:O	5:1F:187:VAL:HG23	2.21	0.40
6:1G:111:LEU:HB2	6:1G:112:PRO:HD3	2.03	0.40
10:1O:80:ASP:OD1	15:1T:64:ARG:NH2	2.54	0.40
11:1P:59:LEU:HD21	30:18:10:ALA:HA	2.04	0.40
1:2A:1054:A:O5'	1:2A:1054:A:H8	2.05	0.40
1:2A:1041:A:N6	1:2A:1205:G:C6	2.89	0.40
1:2A:1228:G:OP1	25:23:30:ARG:NH1	2.49	0.40
1:2A:919:G:C2	1:2A:1325:G:C2	138.02	0.40
1:2A:1399:A:H2'	1:2A:1400:G:O4'	2.21	0.40
1:2A:2288:G:H2'	1:2A:2289:A:H5''	2.04	0.40
1:2A:2343:U:H5'	1:2A:2347:A:N6	2.36	0.40
1:2A:798:A:P	29:27:3:ARG:HH22	2.44	0.40
5:2F:23:ASP:O	5:2F:24:LEU:HD13	2.21	0.40
6:2G:96:ARG:O	6:2G:99:MET:HB3	2.21	0.40
13:2R:28:LEU:HD23	13:2R:28:LEU:HA	1.90	0.40
14:2S:3:ARG:HG2	14:2S:3:ARG:HH11	1.86	0.40
16:2U:76:TYR:CE2	16:2U:80:ILE:HD11	2.56	0.40
1:1A:1223:C:O2'	1:1A:1224:C:H5'	2.20	0.40
1:1A:814:G:O2'	1:1A:1424:A:N1	2.48	0.40
1:1A:1591:A:H2'	1:1A:1592:C:O4'	2.22	0.40
1:1A:173:U:H2'	1:1A:174:G:H8	1.86	0.40
6:1G:15:VAL:HG13	6:1G:175:LEU:HB3	2.04	0.40
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.46	0.40
13:1R:38:VAL:HB	13:1R:39:PRO:HD3	2.03	0.40
21:1Z:102:LEU:HD13	21:1Z:123:ASP:HA	2.04	0.40
1:2A:1048:G:N2	1:2A:1198:C:C2	2.89	0.40
1:2A:1834:C:O5'	1:2A:1834:C:H6	2.05	0.40
1:2A:673:G:C6	1:2A:674:C:C4	3.09	0.40
1:2A:901:G:H2'	1:2A:902:C:C6	2.56	0.40
4:2E:55:ASN:HA	4:2E:56:PRO:HD3	1.95	0.40
6:2G:108:ASN:O	26:24:37:SER:N	2.51	0.40
10:2O:108:GLU:HG3	10:2O:108:GLU:H	1.60	0.40
11:2P:85:LEU:HG	11:2P:115:LEU:O	2.22	0.40
1:2A:437:G:C5	11:2P:72:PRO:HB3	2.56	0.40
1:2A:1699:G:C6	13:2R:9:LYS:HB2	2.56	0.40
14:2S:29:PHE:HD1	14:2S:92:TYR:HH	1.69	0.40
19:2X:47:PHE:O	19:2X:49:VAL:HG13	2.21	0.40
21:2Z:97:GLU:HA	21:2Z:126:VAL:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	250 (92%)	21 (8%)	2 (1%)	26	62
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	34	69
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	34	69
5	1F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	34	69
5	2F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	34	69
6	1G	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	8	28
6	2G	179/182 (98%)	152 (85%)	22 (12%)	5 (3%)	6	21
7	1H	172/180 (96%)	158 (92%)	13 (8%)	1 (1%)	30	65
7	2H	172/180 (96%)	157 (91%)	13 (8%)	2 (1%)	16	47
8	1I	144/148 (97%)	119 (83%)	24 (17%)	1 (1%)	26	62
8	2I	144/148 (97%)	117 (81%)	26 (18%)	1 (1%)	26	62
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	26	62
10	1O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	24	58
10	2O	120/122 (98%)	116 (97%)	3 (2%)	1 (1%)	24	58
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	26	62
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	14	42
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	127 (91%)	10 (7%)	2 (1%)	14	42
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	21	55
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	24	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	19	52
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	19	52
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	17	50
20	1Y	105/110 (96%)	91 (87%)	12 (11%)	2 (2%)	10	32
20	2Y	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	19	52
21	1Z	184/206 (89%)	170 (92%)	13 (7%)	1 (0%)	34	69
21	2Z	184/206 (89%)	166 (90%)	14 (8%)	4 (2%)	8	28
22	10	73/85 (86%)	69 (94%)	3 (4%)	1 (1%)	14	42
22	20	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	49 (73%)	9 (13%)	9 (13%)	0	1
26	24	67/71 (94%)	49 (73%)	12 (18%)	6 (9%)	1	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	8	28
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	178 (78%)	42 (18%)	9 (4%)	4	12
33	2b	229/256 (90%)	183 (80%)	41 (18%)	5 (2%)	8	28
34	1c	204/239 (85%)	169 (83%)	33 (16%)	2 (1%)	19	52
34	2c	204/239 (85%)	167 (82%)	34 (17%)	3 (2%)	13	40
35	1d	206/209 (99%)	179 (87%)	25 (12%)	2 (1%)	19	52
35	2d	206/209 (99%)	182 (88%)	18 (9%)	6 (3%)	6	19
36	1e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	9	29
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	14	42
37	1f	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	19	52
37	2f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	19	52
38	1g	153/156 (98%)	136 (89%)	17 (11%)	0	100	100
38	2g	153/156 (98%)	134 (88%)	19 (12%)	0	100	100
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	105 (84%)	15 (12%)	5 (4%)	4	12
40	2i	125/128 (98%)	104 (83%)	14 (11%)	7 (6%)	2	6
41	1j	95/105 (90%)	77 (81%)	12 (13%)	6 (6%)	2	4
41	2j	94/105 (90%)	81 (86%)	11 (12%)	2 (2%)	9	29
42	1k	112/129 (87%)	97 (87%)	13 (12%)	2 (2%)	11	34
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	21	55
43	1l	120/132 (91%)	112 (93%)	8 (7%)	0	100	100
43	2l	120/132 (91%)	111 (92%)	9 (8%)	0	100	100
44	1m	116/126 (92%)	100 (86%)	13 (11%)	3 (3%)	7	22
44	2m	114/126 (90%)	96 (84%)	15 (13%)	3 (3%)	7	22
45	1n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	11	36
45	2n	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
46	1o	86/89 (97%)	75 (87%)	10 (12%)	1 (1%)	16	47
46	2o	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	8	26
47	1p	80/88 (91%)	67 (84%)	11 (14%)	2 (2%)	7	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	68 (85%)	12 (15%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	19	52
48	2q	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
49	1r	66/88 (75%)	58 (88%)	6 (9%)	2 (3%)	5	18
49	2r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	13	40
50	1s	82/93 (88%)	70 (85%)	12 (15%)	0	100	100
50	2s	81/93 (87%)	67 (83%)	14 (17%)	0	100	100
51	1t	94/106 (89%)	81 (86%)	11 (12%)	2 (2%)	9	29
51	2t	94/106 (89%)	81 (86%)	10 (11%)	3 (3%)	5	17
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	3	9
52	2u	21/27 (78%)	17 (81%)	3 (14%)	1 (5%)	3	9
55	1z	10/14 (71%)	6 (60%)	1 (10%)	3 (30%)	0	0
55	2z	10/14 (71%)	8 (80%)	1 (10%)	1 (10%)	1	1
All	All	11430/12156 (94%)	10379 (91%)	909 (8%)	142 (1%)	16	47

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
6	1G	50	ALA
6	1G	51	ARG
6	1G	126	ASP
7	1H	126	PRO
17	1V	79	VAL
26	14	45	GLY
26	14	46	GLN
26	14	47	GLN
26	14	48	ARG
26	14	50	VAL
26	14	53	GLU
26	14	62	ARG
26	14	68	ARG
33	1b	16	HIS
33	1b	17	PHE
33	1b	121	LEU
33	1b	125	PRO
40	1i	54	ASP

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Mol	Chain	Res	Type
41	1j	55	LYS
41	1j	56	HIS
41	1j	82	ILE
44	1m	4	ILE
45	1n	3	ARG
46	1o	19	PRO
47	1p	76	GLN
48	1q	68	ARG
55	1z	10	PRO
55	1z	11	ARG
3	2D	239	ARG
6	2G	14	GLU
6	2G	47	LYS
6	2G	50	ALA
6	2G	81	LYS
6	2G	126	ASP
7	2H	55	PRO
7	2H	126	PRO
8	2I	10	GLU
21	2Z	128	VAL
21	2Z	135	GLU
26	24	47	GLN
26	24	50	VAL
26	24	68	ARG
29	27	46	VAL
33	2b	17	PHE
33	2b	230	VAL
35	2d	47	ARG
41	2j	78	ASN
42	2k	49	GLY
55	2z	11	ARG
5	1F	130	ALA
10	1O	5	GLN
21	1Z	93	ASP
33	1b	22	LYS
33	1b	23	ARG
33	1b	231	GLU
34	1c	205	GLY
36	1e	98	THR
40	1i	44	VAL
40	1i	56	LEU
41	1j	31	GLY

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Mol	Chain	Res	Type
42	1k	49	GLY
49	1r	32	ARG
51	1t	47	GLY
3	2D	3	VAL
5	2F	130	ALA
10	2O	5	GLN
12	2Q	60	ARG
14	2S	57	LYS
17	2V	79	VAL
20	2Y	54	LYS
21	2Z	93	ASP
26	24	45	GLY
26	24	54	GLY
33	2b	93	VAL
33	2b	97	TRP
33	2b	125	PRO
35	2d	20	TYR
36	2e	37	ARG
44	2m	21	TYR
44	2m	106	ASN
49	2r	25	THR
51	2t	47	GLY
51	2t	99	LEU
52	2u	3	LYS
4	1E	52	LEU
20	1Y	53	PRO
20	1Y	54	LYS
26	14	49	PHE
33	1b	52	GLU
36	1e	85	GLY
41	1j	78	ASN
44	1m	21	TYR
47	1p	77	ALA
49	1r	25	THR
52	1u	3	LYS
4	2E	52	LEU
26	24	62	ARG
34	2c	66	VAL
35	2d	46	LYS
35	2d	129	ASN
40	2i	56	LEU
46	2o	19	PRO

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Mol	Chain	Res	Type
11	1P	122	PRO
37	1f	40	VAL
55	1z	9	ARG
9	2N	2	LYS
11	2P	45	LEU
12	2Q	59	ARG
40	2i	54	ASP
41	2j	82	ILE
51	2t	10	LEU
8	1I	107	VAL
34	1c	66	VAL
51	1t	100	ILE
11	2P	122	PRO
36	2e	69	VAL
40	2i	96	LEU
46	2o	88	ARG
33	1b	128	GLU
36	1e	69	VAL
40	1i	11	LYS
40	1i	96	LEU
44	1m	67	GLU
21	2Z	127	LYS
34	2c	91	LEU
35	2d	45	GLN
37	2f	40	VAL
40	2i	11	LYS
19	2X	94	GLY
35	2d	136	PRO
40	2i	44	VAL
44	2m	4	ILE
15	1T	37	GLY
35	1d	8	VAL
35	1d	136	PRO
42	1k	105	VAL
40	2i	39	GLY
40	2i	41	VAL
22	10	13	GLY
41	1j	77	PRO
34	2c	108	ASN

### 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	215/218 (99%)	186 (86%)	29 (14%)	5	14
3	2D	216/218 (99%)	192 (89%)	24 (11%)	8	23
4	1E	164/166 (99%)	145 (88%)	19 (12%)	7	20
4	2E	164/166 (99%)	143 (87%)	21 (13%)	5	16
5	1F	160/166 (96%)	143 (89%)	17 (11%)	8	24
5	2F	159/166 (96%)	143 (90%)	16 (10%)	9	27
6	1G	143/156 (92%)	126 (88%)	17 (12%)	6	19
6	2G	142/156 (91%)	121 (85%)	21 (15%)	4	11
7	1H	144/148 (97%)	135 (94%)	9 (6%)	22	53
7	2H	144/148 (97%)	128 (89%)	16 (11%)	8	23
8	1I	110/124 (89%)	89 (81%)	21 (19%)	2	5
8	2I	104/124 (84%)	94 (90%)	10 (10%)	10	29
9	1N	118/119 (99%)	104 (88%)	14 (12%)	6	19
9	2N	118/119 (99%)	106 (90%)	12 (10%)	9	26
10	1O	100/100 (100%)	95 (95%)	5 (5%)	30	64
10	2O	100/100 (100%)	92 (92%)	8 (8%)	15	40
11	1P	116/116 (100%)	103 (89%)	13 (11%)	7	22
11	2P	115/116 (99%)	101 (88%)	14 (12%)	6	18
12	1Q	111/111 (100%)	99 (89%)	12 (11%)	8	23
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	15	39
13	1R	101/101 (100%)	82 (81%)	19 (19%)	2	6
13	2R	101/101 (100%)	83 (82%)	18 (18%)	2	6
14	1S	87/88 (99%)	80 (92%)	7 (8%)	15	40
14	2S	85/88 (97%)	71 (84%)	14 (16%)	3	8
15	1T	115/127 (91%)	102 (89%)	13 (11%)	7	22
15	2T	113/127 (89%)	100 (88%)	13 (12%)	7	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	84 (90%)	9 (10%)	10	29
16	2U	93/94 (99%)	83 (89%)	10 (11%)	8	23
17	1V	80/82 (98%)	68 (85%)	12 (15%)	3	11
17	2V	80/82 (98%)	72 (90%)	8 (10%)	9	27
18	1W	90/92 (98%)	83 (92%)	7 (8%)	16	41
18	2W	90/92 (98%)	81 (90%)	9 (10%)	9	27
19	1X	77/78 (99%)	74 (96%)	3 (4%)	39	74
19	2X	77/78 (99%)	75 (97%)	2 (3%)	54	86
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	24	57
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	14	38
21	1Z	159/179 (89%)	144 (91%)	15 (9%)	11	31
21	2Z	156/179 (87%)	142 (91%)	14 (9%)	12	34
22	10	60/67 (90%)	55 (92%)	5 (8%)	14	38
22	20	60/67 (90%)	56 (93%)	4 (7%)	20	50
23	11	80/83 (96%)	73 (91%)	7 (9%)	12	35
23	21	80/83 (96%)	72 (90%)	8 (10%)	9	27
24	12	65/67 (97%)	59 (91%)	6 (9%)	11	32
24	22	65/67 (97%)	58 (89%)	7 (11%)	8	23
25	13	51/52 (98%)	46 (90%)	5 (10%)	10	28
25	23	50/52 (96%)	46 (92%)	4 (8%)	15	40
26	14	60/63 (95%)	51 (85%)	9 (15%)	3	11
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	10
27	15	50/52 (96%)	47 (94%)	3 (6%)	24	56
27	25	50/52 (96%)	46 (92%)	4 (8%)	15	40
28	16	51/52 (98%)	48 (94%)	3 (6%)	24	57
28	26	50/52 (96%)	43 (86%)	7 (14%)	4	13
29	17	41/42 (98%)	37 (90%)	4 (10%)	10	28
29	27	41/42 (98%)	39 (95%)	2 (5%)	31	65
30	18	54/55 (98%)	49 (91%)	5 (9%)	11	32
30	28	54/55 (98%)	50 (93%)	4 (7%)	17	43
31	19	34/34 (100%)	33 (97%)	1 (3%)	50	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	33 (97%)	1 (3%)	50	83
33	1b	177/220 (80%)	146 (82%)	31 (18%)	2	7
33	2b	158/220 (72%)	129 (82%)	29 (18%)	2	6
34	1c	127/188 (68%)	116 (91%)	11 (9%)	13	35
34	2c	108/188 (57%)	94 (87%)	14 (13%)	5	15
35	1d	161/181 (89%)	145 (90%)	16 (10%)	10	28
35	2d	164/181 (91%)	142 (87%)	22 (13%)	5	14
36	1e	113/123 (92%)	98 (87%)	15 (13%)	5	14
36	2e	106/123 (86%)	90 (85%)	16 (15%)	3	10
37	1f	83/90 (92%)	78 (94%)	5 (6%)	24	56
37	2f	86/90 (96%)	79 (92%)	7 (8%)	15	39
38	1g	111/127 (87%)	98 (88%)	13 (12%)	7	20
38	2g	107/127 (84%)	95 (89%)	12 (11%)	7	22
39	1h	114/119 (96%)	98 (86%)	16 (14%)	4	13
39	2h	111/119 (93%)	99 (89%)	12 (11%)	8	23
40	1i	89/99 (90%)	72 (81%)	17 (19%)	2	5
40	2i	80/99 (81%)	68 (85%)	12 (15%)	3	11
41	1j	60/92 (65%)	49 (82%)	11 (18%)	2	6
41	2j	62/92 (67%)	51 (82%)	11 (18%)	2	7
42	1k	82/99 (83%)	76 (93%)	6 (7%)	17	44
42	2k	82/99 (83%)	74 (90%)	8 (10%)	10	28
43	1l	95/109 (87%)	89 (94%)	6 (6%)	22	53
43	2l	94/109 (86%)	90 (96%)	4 (4%)	35	70
44	1m	90/101 (89%)	80 (89%)	10 (11%)	8	23
44	2m	87/101 (86%)	80 (92%)	7 (8%)	15	40
45	1n	47/50 (94%)	42 (89%)	5 (11%)	8	24
45	2n	43/50 (86%)	34 (79%)	9 (21%)	1	4
46	1o	75/80 (94%)	68 (91%)	7 (9%)	11	32
46	2o	78/80 (98%)	69 (88%)	9 (12%)	7	21
47	1p	67/74 (90%)	59 (88%)	8 (12%)	6	19
47	2p	68/74 (92%)	60 (88%)	8 (12%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	91/97 (94%)	88 (97%)	3 (3%)	45	79
48	2q	94/97 (97%)	90 (96%)	4 (4%)	35	70
49	1r	59/77 (77%)	50 (85%)	9 (15%)	3	10
49	2r	59/77 (77%)	49 (83%)	10 (17%)	2	7
50	1s	65/80 (81%)	60 (92%)	5 (8%)	16	41
50	2s	67/80 (84%)	57 (85%)	10 (15%)	4	11
51	1t	66/82 (80%)	57 (86%)	9 (14%)	5	14
51	2t	71/82 (87%)	68 (96%)	3 (4%)	36	71
52	1u	16/22 (73%)	16 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	26	59
55	1z	12/14 (86%)	11 (92%)	1 (8%)	14	38
55	2z	12/14 (86%)	10 (83%)	2 (17%)	3	8
All	All	9159/10094 (91%)	8156 (89%)	1003 (11%)	8	23

All (1003) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	13	ARG
3	1D	34	VAL
3	1D	37	LEU
3	1D	61	LEU
3	1D	69	ARG
3	1D	71	ASP
3	1D	88	ARG
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	111	LEU
3	1D	113	VAL
3	1D	138	VAL
3	1D	142	VAL
3	1D	150	LYS
3	1D	155	LEU
3	1D	162	SER
3	1D	164	GLN
3	1D	193	VAL
3	1D	200	ASP

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Mol	Chain	Res	Type
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
3	1D	259	THR
3	1D	260	ARG
3	1D	275	LYS
4	1E	7	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	34	VAL
4	1E	40	GLU
4	1E	49	LEU
4	1E	54	GLN
4	1E	73	GLU
4	1E	75	VAL
4	1E	79	ARG
4	1E	82	ARG
4	1E	97	LYS
4	1E	111	ARG
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	175	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	12	LEU
5	1F	17	ARG
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	108	LYS
5	1F	110	LEU
5	1F	112	MET
5	1F	125	LEU
5	1F	140	LEU
5	1F	162	LEU
5	1F	191	ARG

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Mol	Chain	Res	Type
5	1F	192	LEU
5	1F	195	ASP
6	1G	3	LEU
6	1G	7	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	45	GLU
6	1G	79	ASN
6	1G	82	LEU
6	1G	128	ARG
6	1G	133	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	143	GLU
6	1G	148	MET
6	1G	153	ARG
6	1G	165	THR
6	1G	170	ARG
6	1G	175	LEU
7	1H	13	LYS
7	1H	25	LYS
7	1H	43	VAL
7	1H	45	VAL
7	1H	69	ARG
7	1H	80	SER
7	1H	84	SER
7	1H	98	LEU
7	1H	129	THR
8	1I	9	LEU
8	1I	10	GLU
8	1I	20	ASP
8	1I	38	LEU
8	1I	43	ASN
8	1I	57	ARG
8	1I	61	ARG
8	1I	64	GLU
8	1I	66	GLU
8	1I	68	LEU
8	1I	75	LEU
8	1I	76	THR
8	1I	77	LEU
8	1I	78	THR

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Mol	Chain	Res	Type
8	1I	92	VAL
8	1I	101	LEU
8	1I	108	THR
8	1I	109	ILE
8	1I	116	LEU
8	1I	127	VAL
8	1I	140	LEU
9	1N	8	GLN
9	1N	12	ARG
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	67	LEU
9	1N	73	THR
9	1N	87	LEU
9	1N	97	ARG
9	1N	99	LEU
9	1N	120	LEU
10	1O	8	LEU
10	1O	10	VAL
10	1O	23	ARG
10	1O	24	VAL
10	1O	105	GLU
11	1P	55	ARG
11	1P	59	LEU
11	1P	70	GLN
11	1P	83	VAL
11	1P	95	VAL
11	1P	98	GLU
11	1P	99	LEU
11	1P	106	LEU
11	1P	112	LEU
11	1P	121	LYS
11	1P	125	VAL
11	1P	148	LEU
11	1P	149	GLU
12	1Q	1	MET
12	1Q	5	ARG
12	1Q	7	MET

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Mol	Chain	Res	Type
12	1Q	8	LYS
12	1Q	16	ARG
12	1Q	35	VAL
12	1Q	45	GLN
12	1Q	55	VAL
12	1Q	60	ARG
12	1Q	63	LYS
12	1Q	75	THR
12	1Q	110	THR
13	1R	1	MET
13	1R	6	SER
13	1R	18	LEU
13	1R	28	LEU
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	60	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	75	LEU
13	1R	79	LEU
13	1R	91	GLN
13	1R	100	LEU
13	1R	102	GLU
13	1R	111	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	20	ARG
14	1S	36	TYR
14	1S	50	SER
14	1S	59	LYS
14	1S	69	VAL
14	1S	110	LEU
15	1T	16	ARG
15	1T	17	THR
15	1T	39	ARG
15	1T	49	VAL
15	1T	59	THR
15	1T	64	ARG
15	1T	67	SER

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Mol	Chain	Res	Type
15	1T	78	LEU
15	1T	85	LYS
15	1T	96	ARG
15	1T	107	ASP
15	1T	108	ARG
15	1T	118	ARG
16	1U	5	LYS
16	1U	8	VAL
16	1U	36	ARG
16	1U	60	LEU
16	1U	74	LEU
16	1U	83	LEU
16	1U	95	LEU
16	1U	104	GLN
16	1U	108	GLU
17	1V	18	LEU
17	1V	21	ARG
17	1V	28	GLU
17	1V	43	GLU
17	1V	46	VAL
17	1V	51	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	95	LEU
17	1V	100	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	51	LEU
18	1W	78	GLU
18	1W	107	LEU
19	1X	35	THR
19	1X	57	LEU
19	1X	88	LYS
20	1Y	1	MET
20	1Y	23	ARG
20	1Y	43	ASN
20	1Y	67	LEU
20	1Y	90	LEU

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Mol	Chain	Res	Type
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	46	LYS
21	1Z	58	VAL
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	107	THR
21	1Z	126	VAL
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	170	THR
22	10	10	THR
22	10	20	ARG
22	10	49	LYS
22	10	55	ARG
22	10	82	ARG
23	11	21	ARG
23	11	23	LYS
23	11	30	VAL
23	11	40	ARG
23	11	50	ARG
23	11	59	THR
23	11	95	LEU
24	12	19	VAL
24	12	30	ARG
24	12	32	LEU
24	12	49	LYS
24	12	53	LEU
24	12	70	GLN
25	13	8	LEU
25	13	17	LYS
25	13	23	LEU
25	13	56	VAL
25	13	60	GLU
26	14	14	ILE
26	14	33	VAL
26	14	34	GLU
26	14	49	PHE

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Mol	Chain	Res	Type
26	14	56	VAL
26	14	58	ARG
26	14	60	GLN
26	14	63	TYR
26	14	68	ARG
27	15	16	ARG
27	15	29	THR
27	15	40	LYS
28	16	33	LYS
28	16	38	LYS
28	16	48	VAL
29	17	1	MET
29	17	9	ARG
29	17	24	THR
29	17	43	THR
30	18	14	VAL
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
30	18	46	ARG
31	19	17	ILE
33	1b	8	LYS
33	1b	10	LEU
33	1b	11	LEU
33	1b	17	PHE
33	1b	21	ARG
33	1b	24	TRP
33	1b	47	THR
33	1b	67	THR
33	1b	76	GLN
33	1b	78	GLN
33	1b	80	ILE
33	1b	82	ARG
33	1b	86	GLU
33	1b	93	VAL
33	1b	112	VAL
33	1b	116	GLU
33	1b	127	ILE
33	1b	128	GLU
33	1b	143	GLU
33	1b	144	ARG
33	1b	145	LEU

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Mol	Chain	Res	Type
33	1b	170	GLU
33	1b	185	ILE
33	1b	187	LEU
33	1b	190	THR
33	1b	198	ASP
33	1b	208	ILE
33	1b	217	ARG
33	1b	221	LEU
33	1b	226	ARG
33	1b	233	SER
34	1c	3	ASN
34	1c	15	THR
34	1c	17	ASP
34	1c	47	LEU
34	1c	70	VAL
34	1c	82	GLU
34	1c	115	LEU
34	1c	131	ARG
34	1c	150	LYS
34	1c	151	VAL
34	1c	188	LEU
35	1d	3	ARG
35	1d	5	ILE
35	1d	31	CYS
35	1d	45	GLN
35	1d	49	ARG
35	1d	58	LEU
35	1d	70	ILE
35	1d	73	ARG
35	1d	101	LEU
35	1d	107	ARG
35	1d	162	LEU
35	1d	168	ARG
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
35	1d	200	GLU
36	1e	12	LEU
36	1e	18	ARG
36	1e	24	ARG
36	1e	31	LEU
36	1e	40	ARG

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Mol	Chain	Res	Type
36	1e	41	VAL
36	1e	47	LYS
36	1e	67	VAL
36	1e	73	ASN
36	1e	75	THR
36	1e	78	HIS
36	1e	79	GLU
36	1e	81	GLU
36	1e	91	LEU
36	1e	147	ASP
37	1f	43	LEU
37	1f	46	ARG
37	1f	65	VAL
37	1f	74	ASP
37	1f	75	LEU
38	1g	8	GLU
38	1g	12	LEU
38	1g	13	GLN
38	1g	15	ASP
38	1g	16	LEU
38	1g	21	VAL
38	1g	50	ILE
38	1g	51	GLN
38	1g	56	GLN
38	1g	104	LEU
38	1g	113	GLU
38	1g	114	ARG
38	1g	131	LYS
39	1h	2	LEU
39	1h	19	VAL
39	1h	26	VAL
39	1h	50	ARG
39	1h	52	ASP
39	1h	54	ASP
39	1h	63	LEU
39	1h	75	ARG
39	1h	78	GLN
39	1h	91	ARG
39	1h	99	GLU
39	1h	109	ILE
39	1h	112	LEU
39	1h	120	THR

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Mol	Chain	Res	Type
39	1h	122	ARG
39	1h	127	LEU
40	1i	16	ARG
40	1i	23	ASN
40	1i	27	THR
40	1i	42	ARG
40	1i	50	LEU
40	1i	54	ASP
40	1i	75	ASP
40	1i	81	ILE
40	1i	83	ARG
40	1i	86	VAL
40	1i	92	TYR
40	1i	102	LEU
40	1i	104	ARG
40	1i	107	ARG
40	1i	108	VAL
40	1i	113	LYS
40	1i	128	ARG
41	1j	9	ARG
41	1j	30	SER
41	1j	46	ARG
41	1j	48	THR
41	1j	84	GLN
41	1j	85	LEU
41	1j	92	THR
41	1j	95	GLU
41	1j	96	ILE
41	1j	97	GLU
41	1j	98	ILE
42	1k	25	TYR
42	1k	31	THR
42	1k	48	ILE
42	1k	84	VAL
42	1k	106	LYS
42	1k	109	VAL
43	1l	27	LEU
43	1l	33	ARG
43	1l	41	ARG
43	1l	52	LEU
43	1l	67	THR
43	1l	97	ARG

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Mol	Chain	Res	Type
44	1m	3	ARG
44	1m	4	ILE
44	1m	11	ARG
44	1m	19	LEU
44	1m	56	LEU
44	1m	65	LYS
44	1m	70	LEU
44	1m	102	ARG
44	1m	110	ARG
44	1m	114	ARG
45	1n	6	LEU
45	1n	13	THR
45	1n	18	VAL
45	1n	22	THR
45	1n	46	GLU
46	1o	3	ILE
46	1o	26	GLU
46	1o	38	ARG
46	1o	39	LEU
46	1o	41	GLU
46	1o	83	GLU
46	1o	84	LYS
47	1p	1	MET
47	1p	2	VAL
47	1p	5	ARG
47	1p	11	SER
47	1p	19	ILE
47	1p	20	VAL
47	1p	47	ASP
47	1p	69	THR
48	1q	82	MET
48	1q	89	LEU
48	1q	98	LEU
49	1r	26	LEU
49	1r	31	LEU
49	1r	37	VAL
49	1r	38	GLU
49	1r	54	ARG
49	1r	55	ARG
49	1r	68	LYS
49	1r	76	LEU
49	1r	82	THR

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Mol	Chain	Res	Type
50	1s	3	ARG
50	1s	28	LYS
50	1s	37	ARG
50	1s	63	THR
50	1s	65	ASN
51	1t	9	ASN
51	1t	10	LEU
51	1t	24	LEU
51	1t	30	LYS
51	1t	45	GLN
51	1t	60	GLU
51	1t	62	LEU
51	1t	84	LEU
51	1t	93	GLU
55	1z	1	VAL
3	2D	3	VAL
3	2D	13	ARG
3	2D	61	LEU
3	2D	71	ASP
3	2D	87	ASN
3	2D	94	LEU
3	2D	99	ASP
3	2D	103	ARG
3	2D	106	ILE
3	2D	134	ARG
3	2D	138	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	183	ARG
3	2D	193	VAL
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	257	LEU
3	2D	259	THR
3	2D	260	ARG
3	2D	262	ARG
3	2D	276	LYS
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL

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Mol	Chain	Res	Type
4	2E	24	THR
4	2E	34	VAL
4	2E	49	LEU
4	2E	52	LEU
4	2E	75	VAL
4	2E	76	ARG
4	2E	77	ILE
4	2E	79	ARG
4	2E	82	ARG
4	2E	111	ARG
4	2E	116	VAL
4	2E	119	ARG
4	2E	144	ARG
4	2E	163	GLU
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
4	2E	202	LYS
5	2F	12	LEU
5	2F	20	LEU
5	2F	33	LEU
5	2F	53	THR
5	2F	57	VAL
5	2F	74	ARG
5	2F	88	VAL
5	2F	106	ARG
5	2F	112	MET
5	2F	135	LYS
5	2F	140	LEU
5	2F	169	ASN
5	2F	188	ARG
5	2F	192	LEU
5	2F	196	LEU
5	2F	197	ASP
6	2G	3	LEU
6	2G	13	GLU
6	2G	14	GLU
6	2G	16	ARG
6	2G	28	VAL
6	2G	33	ARG
6	2G	91	ARG
6	2G	98	ARG

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Mol	Chain	Res	Type
6	2G	111	LEU
6	2G	113	ARG
6	2G	115	ARG
6	2G	133	LEU
6	2G	136	ARG
6	2G	140	ILE
6	2G	143	GLU
6	2G	145	THR
6	2G	148	MET
6	2G	149	VAL
6	2G	162	THR
6	2G	165	THR
6	2G	170	ARG
7	2H	3	ARG
7	2H	23	ARG
7	2H	32	GLU
7	2H	33	LEU
7	2H	41	MET
7	2H	42	ARG
7	2H	45	VAL
7	2H	49	VAL
7	2H	59	ARG
7	2H	63	SER
7	2H	69	ARG
7	2H	71	LEU
7	2H	98	LEU
7	2H	115	VAL
7	2H	139	GLN
7	2H	175	LYS
8	2I	43	ASN
8	2I	61	ARG
8	2I	75	LEU
8	2I	77	LEU
8	2I	101	LEU
8	2I	108	THR
8	2I	116	LEU
8	2I	121	LYS
8	2I	127	VAL
8	2I	140	LEU
9	2N	33	LEU
9	2N	34	LEU
9	2N	46	VAL

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Mol	Chain	Res	Type
9	2N	48	MET
9	2N	61	ARG
9	2N	63	THR
9	2N	87	LEU
9	2N	97	ARG
9	2N	99	LEU
9	2N	120	LEU
9	2N	131	GLN
9	2N	137	LYS
10	2O	8	LEU
10	2O	10	VAL
10	2O	20	MET
10	2O	21	CYS
10	2O	24	VAL
10	2O	53	LYS
10	2O	69	ILE
10	2O	113	LYS
11	2P	3	LEU
11	2P	15	ARG
11	2P	21	ARG
11	2P	55	ARG
11	2P	59	LEU
11	2P	65	ARG
11	2P	70	GLN
11	2P	83	VAL
11	2P	96	THR
11	2P	112	LEU
11	2P	121	LYS
11	2P	123	LEU
11	2P	125	VAL
11	2P	148	LEU
12	2Q	7	MET
12	2Q	16	ARG
12	2Q	35	VAL
12	2Q	45	GLN
12	2Q	48	GLU
12	2Q	64	ILE
12	2Q	81	VAL
12	2Q	109	VAL
12	2Q	110	THR
13	2R	1	MET
13	2R	6	SER

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Mol	Chain	Res	Type
13	2R	18	LEU
13	2R	24	GLN
13	2R	28	LEU
13	2R	29	LEU
13	2R	44	LEU
13	2R	54	LEU
13	2R	60	LEU
13	2R	65	LEU
13	2R	75	LEU
13	2R	79	LEU
13	2R	82	GLU
13	2R	91	GLN
13	2R	100	LEU
13	2R	102	GLU
13	2R	111	LEU
13	2R	114	VAL
14	2S	4	LEU
14	2S	13	ARG
14	2S	19	LYS
14	2S	20	ARG
14	2S	35	ILE
14	2S	36	TYR
14	2S	44	LYS
14	2S	49	VAL
14	2S	50	SER
14	2S	58	LEU
14	2S	67	ARG
14	2S	75	GLU
14	2S	83	LYS
14	2S	111	GLU
15	2T	8	LYS
15	2T	28	VAL
15	2T	34	VAL
15	2T	53	ARG
15	2T	59	THR
15	2T	64	ARG
15	2T	67	SER
15	2T	78	LEU
15	2T	85	LYS
15	2T	96	ARG
15	2T	98	LYS
15	2T	107	ASP

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Mol	Chain	Res	Type
15	2T	118	ARG
16	2U	36	ARG
16	2U	44	ASN
16	2U	52	ARG
16	2U	59	ARG
16	2U	60	LEU
16	2U	74	LEU
16	2U	83	LEU
16	2U	92	ARG
16	2U	104	GLN
16	2U	108	GLU
17	2V	15	GLU
17	2V	18	LEU
17	2V	21	ARG
17	2V	35	LEU
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
17	2V	95	LEU
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	51	LEU
18	2W	60	ASN
18	2W	92	ARG
18	2W	100	THR
18	2W	107	LEU
19	2X	57	LEU
19	2X	92	LEU
20	2Y	6	HIS
20	2Y	8	LYS
20	2Y	21	LYS
20	2Y	23	ARG
20	2Y	43	ASN
20	2Y	44	ILE
20	2Y	67	LEU
21	2Z	31	ARG
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	86	VAL
21	2Z	91	LEU

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Mol	Chain	Res	Type
21	2Z	107	THR
21	2Z	126	VAL
21	2Z	131	ARG
21	2Z	135	GLU
21	2Z	136	PHE
21	2Z	150	LEU
21	2Z	155	LEU
21	2Z	170	THR
21	2Z	185	GLU
22	20	10	THR
22	20	20	ARG
22	20	55	ARG
22	20	82	ARG
23	21	21	ARG
23	21	30	VAL
23	21	35	THR
23	21	40	ARG
23	21	56	GLN
23	21	59	THR
23	21	69	LYS
23	21	95	LEU
24	22	2	LYS
24	22	30	ARG
24	22	32	LEU
24	22	35	LEU
24	22	53	LEU
24	22	64	LEU
24	22	70	GLN
25	23	3	ARG
25	23	8	LEU
25	23	31	LEU
25	23	54	VAL
26	24	14	ILE
26	24	33	VAL
26	24	56	VAL
26	24	58	ARG
26	24	61	ARG
26	24	63	TYR
26	24	68	ARG
26	24	69	LYS
27	25	16	ARG
27	25	40	LYS

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Mol	Chain	Res	Type
27	25	55	ARG
27	25	60	VAL
28	26	6	ARG
28	26	14	THR
28	26	28	ARG
28	26	33	LYS
28	26	38	LYS
28	26	40	CYS
28	26	48	VAL
29	27	9	ARG
29	27	43	THR
30	28	14	VAL
30	28	26	LYS
30	28	31	HIS
30	28	34	TRP
31	29	17	ILE
33	2b	8	LYS
33	2b	17	PHE
33	2b	19	HIS
33	2b	24	TRP
33	2b	32	ILE
33	2b	47	THR
33	2b	51	LEU
33	2b	63	MET
33	2b	67	THR
33	2b	80	ILE
33	2b	81	VAL
33	2b	83	MET
33	2b	90	MET
33	2b	93	VAL
33	2b	108	ILE
33	2b	114	ARG
33	2b	117	GLU
33	2b	128	GLU
33	2b	153	ARG
33	2b	154	LEU
33	2b	160	ASP
33	2b	165	VAL
33	2b	175	ARG
33	2b	179	LYS
33	2b	187	LEU
33	2b	198	ASP

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Mol	Chain	Res	Type
33	2b	222	ILE
33	2b	223	ILE
33	2b	224	GLN
34	2c	3	ASN
34	2c	5	ILE
34	2c	14	ILE
34	2c	16	ARG
34	2c	47	LEU
34	2c	52	LEU
34	2c	54	ARG
34	2c	70	VAL
34	2c	125	GLU
34	2c	131	ARG
34	2c	143	GLU
34	2c	162	GLN
34	2c	178	LEU
34	2c	182	ILE
35	2d	3	ARG
35	2d	5	ILE
35	2d	25	ARG
35	2d	26	CYS
35	2d	31	CYS
35	2d	34	GLU
35	2d	38	TYR
35	2d	47	ARG
35	2d	49	ARG
35	2d	58	LEU
35	2d	61	LYS
35	2d	73	ARG
35	2d	86	LYS
35	2d	96	LEU
35	2d	122	ARG
35	2d	132	ARG
35	2d	135	LEU
35	2d	157	LEU
35	2d	170	VAL
35	2d	181	MET
35	2d	187	ARG
35	2d	194	LEU
36	2e	27	ARG
36	2e	31	LEU
36	2e	34	VAL

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Mol	Chain	Res	Type
36	2e	40	ARG
36	2e	41	VAL
36	2e	47	LYS
36	2e	50	GLU
36	2e	51	VAL
36	2e	68	GLU
36	2e	71	LEU
36	2e	78	HIS
36	2e	91	LEU
36	2e	115	VAL
36	2e	116	THR
36	2e	121	LYS
36	2e	152	ARG
37	2f	23	LYS
37	2f	28	ARG
37	2f	43	LEU
37	2f	46	ARG
37	2f	65	VAL
37	2f	72	VAL
37	2f	75	LEU
38	2g	12	LEU
38	2g	15	ASP
38	2g	16	LEU
38	2g	21	VAL
38	2g	38	LEU
38	2g	42	ILE
38	2g	45	ASP
38	2g	72	ARG
38	2g	104	LEU
38	2g	110	GLN
38	2g	114	ARG
38	2g	120	ILE
39	2h	50	ARG
39	2h	51	VAL
39	2h	52	ASP
39	2h	54	ASP
39	2h	63	LEU
39	2h	78	GLN
39	2h	84	ARG
39	2h	99	GLU
39	2h	111	ILE
39	2h	112	LEU

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Mol	Chain	Res	Type
39	2h	120	THR
39	2h	122	ARG
40	2i	3	GLN
40	2i	38	GLN
40	2i	50	LEU
40	2i	54	ASP
40	2i	64	THR
40	2i	75	ASP
40	2i	81	ILE
40	2i	89	ASN
40	2i	102	LEU
40	2i	107	ARG
40	2i	124	GLN
40	2i	128	ARG
41	2j	6	ILE
41	2j	8	LEU
41	2j	13	HIS
41	2j	16	LEU
41	2j	21	GLN
41	2j	25	GLU
41	2j	48	THR
41	2j	68	HIS
41	2j	95	GLU
41	2j	96	ILE
41	2j	98	ILE
42	2k	18	ARG
42	2k	48	ILE
42	2k	75	TYR
42	2k	77	MET
42	2k	78	GLN
42	2k	109	VAL
42	2k	114	VAL
42	2k	126	ARG
43	2l	23	LYS
43	2l	28	LYS
43	2l	55	VAL
43	2l	97	ARG
44	2m	3	ARG
44	2m	35	GLU
44	2m	55	ARG
44	2m	82	MET
44	2m	83	ASP

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Mol	Chain	Res	Type
44	2m	106	ASN
44	2m	110	ARG
45	2n	11	LYS
45	2n	17	LYS
45	2n	18	VAL
45	2n	22	THR
45	2n	29	ARG
45	2n	33	VAL
45	2n	46	GLU
45	2n	50	LYS
45	2n	53	LEU
46	2o	3	ILE
46	2o	5	LYS
46	2o	22	THR
46	2o	26	GLU
46	2o	38	ARG
46	2o	39	LEU
46	2o	41	GLU
46	2o	71	GLN
46	2o	84	LYS
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG
47	2p	11	SER
47	2p	21	VAL
47	2p	27	LYS
47	2p	28	ARG
47	2p	69	THR
48	2q	6	LEU
48	2q	24	GLU
48	2q	74	LEU
48	2q	77	VAL
49	2r	26	LEU
49	2r	29	PHE
49	2r	31	LEU
49	2r	35	ARG
49	2r	37	VAL
49	2r	38	GLU
49	2r	41	LYS
49	2r	42	ARG
49	2r	54	ARG
49	2r	76	LEU

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Mol	Chain	Res	Type
50	2s	3	ARG
50	2s	18	LYS
50	2s	22	LEU
50	2s	28	LYS
50	2s	37	ARG
50	2s	41	VAL
50	2s	63	THR
50	2s	65	ASN
50	2s	77	THR
50	2s	78	ARG
51	2t	24	LEU
51	2t	62	LEU
51	2t	71	THR
52	2u	10	ARG
55	2z	2	ASP
55	2z	7	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	126	GLN
3	1D	143	HIS
3	1D	164	GLN
3	1D	253	GLN
4	1E	54	GLN
5	1F	69	HIS
5	1F	169	ASN
5	1F	203	GLN
5	1F	204	ASN
6	1G	130	ASN
8	1I	43	ASN
8	1I	139	GLN
9	1N	8	GLN
11	1P	38	GLN
11	1P	70	GLN
13	1R	71	GLN
13	1R	91	GLN
14	1S	95	HIS
15	1T	38	ASN
15	1T	43	GLN
15	1T	123	GLN

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Mol	Chain	Res	Type
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	92	ASN
21	1Z	73	GLN
21	1Z	151	HIS
24	12	38	GLN
24	12	70	GLN
31	19	36	GLN
33	1b	146	GLN
34	1c	6	HIS
34	1c	102	ASN
34	1c	123	GLN
34	1c	170	GLN
35	1d	45	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	160	GLN
36	1e	20	GLN
36	1e	141	GLN
37	1f	32	ASN
37	1f	100	ASN
38	1g	56	GLN
38	1g	86	GLN
38	1g	110	GLN
38	1g	148	ASN
40	1i	23	ASN
40	1i	38	GLN
40	1i	58	HIS
40	1i	73	GLN
40	1i	89	ASN
40	1i	117	HIS
40	1i	124	GLN
41	1j	56	HIS
42	1k	93	GLN
43	1l	78	GLN
43	1l	99	HIS
44	1m	92	HIS
46	1o	28	GLN
48	1q	26	GLN
50	1s	47	HIS
50	1s	56	GLN
50	1s	65	ASN

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Mol	Chain	Res	Type
50	1s	69	HIS
51	1t	9	ASN
51	1t	16	HIS
51	1t	26	ASN
51	1t	45	GLN
3	2D	253	GLN
4	2E	85	ASN
5	2F	69	HIS
5	2F	203	GLN
6	2G	40	ASN
6	2G	41	GLN
6	2G	108	ASN
6	2G	130	ASN
8	2I	43	ASN
8	2I	54	GLN
8	2I	133	HIS
8	2I	139	GLN
11	2P	38	GLN
12	2Q	12	GLN
14	2S	68	GLN
15	2T	123	GLN
16	2U	44	ASN
17	2V	64	HIS
19	2X	31	HIS
19	2X	82	GLN
20	2Y	43	ASN
20	2Y	92	ASN
21	2Z	73	GLN
23	21	56	GLN
25	23	33	GLN
28	26	32	ASN
30	28	35	GLN
31	29	36	GLN
33	2b	45	GLN
33	2b	78	GLN
33	2b	95	GLN
33	2b	110	GLN
34	2c	3	ASN
34	2c	6	HIS
34	2c	102	ASN
34	2c	123	GLN
34	2c	136	GLN

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Mol	Chain	Res	Type
35	2d	123	HIS
35	2d	125	HIS
35	2d	160	GLN
35	2d	201	GLN
36	2e	141	GLN
37	2f	73	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	97	GLN
38	2g	110	GLN
38	2g	122	HIS
38	2g	148	ASN
40	2i	3	GLN
40	2i	89	ASN
41	2j	21	GLN
41	2j	56	HIS
41	2j	84	GLN
42	2k	22	HIS
42	2k	93	GLN
43	2l	75	HIS
43	2l	78	GLN
44	2m	77	ASN
46	2o	28	GLN
46	2o	71	GLN
50	2s	69	HIS
51	2t	18	GLN
51	2t	75	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	392 (14%)	28 (1%)
1	2A	2781/2915 (95%)	470 (16%)	26 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	34 (28%)	2 (1%)
32	1a	1472/1521 (96%)	270 (18%)	0
32	2a	1479/1521 (97%)	281 (18%)	0
53	1v	4/24 (16%)	1 (25%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	12 (16%)	0
54	2x	75/77 (97%)	15 (20%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	8865/9316 (95%)	1485 (16%)	56 (0%)

All (1485) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	32	U
1	1A	33	C
1	1A	35	G
1	1A	44	C
1	1A	69	A
1	1A	72	A
1	1A	73	G
1	1A	82	A
1	1A	91	C
1	1A	115	A
1	1A	116	A
1	1A	117	U
1	1A	137	G
1	1A	148	A
1	1A	154	C
1	1A	160	C
1	1A	184	A
1	1A	187	A
1	1A	188	U
1	1A	189	C
1	1A	193	G
1	1A	202	G
1	1A	203	G
1	1A	204	A
1	1A	209	A
1	1A	210	A
1	1A	212	G
1	1A	216	A
1	1A	217	A
1	1A	221	A
1	1A	236	G
1	1A	238	G
1	1A	249	G
1	1A	268	G
1	1A	270	U
1	1A	271	U

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Mol	Chain	Res	Type
1	1A	272	G
1	1A	273	U
1	1A	288	G
1	1A	295	U
1	1A	298	G
1	1A	302	C
1	1A	334	A
1	1A	347	A
1	1A	352	G
1	1A	353	A
1	1A	368	A
1	1A	375	G
1	1A	377	G
1	1A	380	A
1	1A	386	G
1	1A	406	U
1	1A	412	G
1	1A	422	G
1	1A	431	U
1	1A	432	G
1	1A	433	G
1	1A	437	G
1	1A	447	U
1	1A	454	A
1	1A	467	G
1	1A	469	C
1	1A	473	U
1	1A	476	C
1	1A	481	C
1	1A	482	A
1	1A	495	A
1	1A	506	G
1	1A	528	U
1	1A	529	A
1	1A	533	C
1	1A	554	G
1	1A	555	C
1	1A	556	A
1	1A	557	G
1	1A	572	G
1	1A	585	G
1	1A	595	G

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Mol	Chain	Res	Type
1	1A	597	A
1	1A	608	A
1	1A	614	G
1	1A	615	G
1	1A	625	A
1	1A	626	G
1	1A	629	U
1	1A	638	G
1	1A	640	G
1	1A	661	A
1	1A	670	A
1	1A	671	G
1	1A	682	G
1	1A	696	C
1	1A	715	G
1	1A	732	G
1	1A	763	G
1	1A	776	C
1	1A	810	A
1	1A	820	A
1	1A	821	G
1	1A	822	G
1	1A	828	A
1	1A	830	A
1	1A	831	G
1	1A	836	C
1	1A	838	G
1	1A	848	A
1	1A	851	G
1	1A	858	C
1	1A	873	U
1	1A	874	U
1	1A	876	G
1	1A	878	G
1	1A	883	C
1	1A	905	G
1	1A	912	A
1	1A	915	G
1	1A	925	G
1	1A	931	C
1	1A	932	C
1	1A	933	A

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Mol	Chain	Res	Type
1	1A	934	C
1	1A	935	C
1	1A	936	A
1	1A	938	C
1	1A	941	A
1	1A	942	C
1	1A	955	A
1	1A	976	G
1	1A	985	A
1	1A	989	A
1	1A	990	G
1	1A	1002	U
1	1A	1003	A
1	1A	1005	C
1	1A	1018	G
1	1A	1019	C
1	1A	1028	A
1	1A	1041	A
1	1A	1050	C
1	1A	1057	U
1	1A	1058	C
1	1A	1067	G
1	1A	1071	U
1	1A	1078	U
1	1A	1083	C
1	1A	1086	C
1	1A	1091	A
1	1A	1092	G
1	1A	1096	G
1	1A	1150	U
1	1A	1151	G
1	1A	1152	G
1	1A	1154	C
1	1A	1157	G
1	1A	1173	A
1	1A	1174	A
1	1A	1175	U
1	1A	1179	C
1	1A	1180	G
1	1A	1183	G
1	1A	1186	U
1	1A	1200	A

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Mol	Chain	Res	Type
1	1A	1215	G
1	1A	1217	G
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1221	A
1	1A	1262	C
1	1A	1264	A
1	1A	1285	U
1	1A	1286	A
1	1A	1289	G
1	1A	1298	A
1	1A	1301	G
1	1A	1316	G
1	1A	1317	A
1	1A	1318	U
1	1A	1345	U
1	1A	1346	A
1	1A	1348	G
1	1A	1366	A
1	1A	1397	U
1	1A	1404	A
1	1A	1405	A
1	1A	1410	A
1	1A	1415	C
1	1A	1418	A
1	1A	1429	A
1	1A	1430	G
1	1A	1440	A
1	1A	1461	G
1	1A	1462	C
1	1A	1466	G
1	1A	1467	G
1	1A	1473	C
1	1A	1482	C
1	1A	1490	A
1	1A	1496	G
1	1A	1507	G
1	1A	1513	C
1	1A	1517	A
1	1A	1524	G
1	1A	1528	G

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Mol	Chain	Res	Type
1	1A	1538	C
1	1A	1539	A
1	1A	1541	A
1	1A	1553	A
1	1A	1554	C
1	1A	1555	A
1	1A	1570	G
1	1A	1578	C
1	1A	1588	A
1	1A	1589	C
1	1A	1604	A
1	1A	1612	A
1	1A	1615	A
1	1A	1624	U
1	1A	1627	G
1	1A	1630	C
1	1A	1631	A
1	1A	1632	A
1	1A	1653	A
1	1A	1654	A
1	1A	1655	A
1	1A	1693	G
1	1A	1694	C
1	1A	1720	G
1	1A	1746	A
1	1A	1747	A
1	1A	1766	A
1	1A	1767	U
1	1A	1768	G
1	1A	1778	G
1	1A	1786	G
1	1A	1793	G
1	1A	1794	G
1	1A	1803	A
1	1A	1810	A
1	1A	1812	C
1	1A	1821	A
1	1A	1830	C
1	1A	1831	G
1	1A	1832	A
1	1A	1846	G
1	1A	1858	G

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Mol	Chain	Res	Type
1	1A	1859	A
1	1A	1869	G
1	1A	1877	A
1	1A	1899	G
1	1A	1910	A
1	1A	1921	A
1	1A	1927	G
1	1A	1934	A
1	1A	1936	U
1	1A	1940	A
1	1A	1948	A
1	1A	1950	G
1	1A	1951	G
1	1A	1952	U
1	1A	1953	A
1	1A	1958	A
1	1A	1959	A
1	1A	1973	A
1	1A	1976	U
1	1A	1984	U
1	1A	1986	C
1	1A	1988	C
1	1A	1991	A
1	1A	1992	A
1	1A	1993	A
1	1A	2013	G
1	1A	2014	U
1	1A	2018	G
1	1A	2044	G
1	1A	2052	A
1	1A	2053	G
1	1A	2054	A
1	1A	2060	C
1	1A	2064	C
1	1A	2076	C
1	1A	2077	G
1	1A	2081	A
1	1A	2082	G
1	1A	2083	A
1	1A	2090	G
1	1A	2091	G
1	1A	2101	G

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Mol	Chain	Res	Type
1	1A	2204	C
1	1A	2205	G
1	1A	2206	C
1	1A	2207	G
1	1A	2209	C
1	1A	2212	G
1	1A	2213	G
1	1A	2216	C
1	1A	2219	A
1	1A	2226	G
1	1A	2227	G
1	1A	2228	A
1	1A	2229	U
1	1A	2236	A
1	1A	2249	G
1	1A	2250	G
1	1A	2251	C
1	1A	2279	A
1	1A	2280	A
1	1A	2284	A
1	1A	2286	C
1	1A	2294	C
1	1A	2298	A
1	1A	2316	A
1	1A	2331	A
1	1A	2332	G
1	1A	2336	G
1	1A	2338	A
1	1A	2347	A
1	1A	2354	C
1	1A	2358	C
1	1A	2361	C
1	1A	2390	G
1	1A	2394	G
1	1A	2396	C
1	1A	2416	G
1	1A	2417	U
1	1A	2421	G
1	1A	2433	A
1	1A	2434	U
1	1A	2436	A
1	1A	2440	G

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Mol	Chain	Res	Type
1	1A	2441	A
1	1A	2442	U
1	1A	2443	A
1	1A	2446	A
1	1A	2450	A
1	1A	2456	G
1	1A	2459	A
1	1A	2479	G
1	1A	2485	C
1	1A	2487	A
1	1A	2489	A
1	1A	2513	G
1	1A	2516	G
1	1A	2517	U
1	1A	2529	A
1	1A	2536	G
1	1A	2540	G
1	1A	2560	G
1	1A	2565	U
1	1A	2566	U
1	1A	2577	A
1	1A	2578	G
1	1A	2584	C
1	1A	2593	G
1	1A	2613	A
1	1A	2620	U
1	1A	2621	C
1	1A	2622	U
1	1A	2623	C
1	1A	2640	A
1	1A	2641	G
1	1A	2665	A
1	1A	2700	U
1	1A	2701	C
1	1A	2702	C
1	1A	2713	U
1	1A	2714	C
1	1A	2724	A
1	1A	2725	A
1	1A	2726	G
1	1A	2738	U
1	1A	2745	A

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Mol	Chain	Res	Type
1	1A	2770	A
1	1A	2773	G
1	1A	2776	A
1	1A	2777	A
1	1A	2778	G
1	1A	2790	A
1	1A	2792	G
1	1A	2802	A
1	1A	2803	C
1	1A	2806	C
1	1A	2812	G
1	1A	2829	A
1	1A	2830	A
1	1A	2842	G
1	1A	2844	A
1	1A	2881	G
1	1A	2889	C
1	1A	2902	G
1	1A	2903	U
2	1B	13	A
2	1B	15	A
2	1B	25	A
2	1B	56	G
2	1B	65	C
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	10	G
32	1a	23	G
32	1a	33	A
32	1a	40	G
32	1a	45	G
32	1a	49	C
32	1a	52	A
32	1a	62	G
32	1a	65	G
32	1a	66	U
32	1a	74	G
32	1a	75	C
32	1a	76	G
32	1a	77	G

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Mol	Chain	Res	Type
32	1a	78	G
32	1a	88	C
32	1a	91	G
32	1a	95	A
32	1a	110	A
32	1a	115	C
32	1a	126	C
32	1a	133	G
32	1a	136	A
32	1a	139	G
32	1a	155	A
32	1a	159	U
32	1a	161	G
32	1a	162	G
32	1a	163	G
32	1a	168	U
32	1a	169	C
32	1a	178	G
32	1a	190	U
32	1a	202	A
32	1a	203	A
32	1a	204	A
32	1a	206	G
32	1a	208	C
32	1a	209	U
32	1a	210	U
32	1a	211	U
32	1a	212	G
32	1a	218	U
32	1a	243	G
32	1a	247	G
32	1a	254	G
32	1a	258	A
32	1a	262	G
32	1a	263	C
32	1a	276	C
32	1a	277	G
32	1a	285	G
32	1a	317	A
32	1a	324	C
32	1a	325	A
32	1a	326	C

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Mol	Chain	Res	Type
32	1a	339	U
32	1a	342	G
32	1a	343	G
32	1a	344	G
32	1a	348	C
32	1a	349	A
32	1a	350	G
32	1a	352	A
32	1a	363	U
32	1a	368	C
32	1a	369	A
32	1a	380	G
32	1a	393	A
32	1a	394	C
32	1a	402	G
32	1a	408	A
32	1a	409	G
32	1a	419	G
32	1a	420	G
32	1a	425	U
32	1a	435	A
32	1a	441	G
32	1a	443	A
32	1a	447	A
32	1a	449	C
32	1a	455	A
32	1a	456	C
32	1a	457	G
32	1a	467	A
32	1a	469	G
32	1a	470	G
32	1a	477	G
32	1a	481	A
32	1a	482	U
32	1a	489	G
32	1a	493	A
32	1a	494	A
32	1a	495	C
32	1a	496	U
32	1a	497	C
32	1a	502	C
32	1a	503	C

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Mol	Chain	Res	Type
32	1a	505	G
32	1a	510	C
32	1a	511	G
32	1a	515	U
32	1a	516	A
32	1a	517	A
32	1a	531	A
32	1a	543	A
32	1a	545	U
32	1a	547	A
32	1a	556	A
32	1a	557	A
32	1a	560	G
32	1a	561	G
32	1a	576	G
32	1a	580	C
32	1a	602	C
32	1a	614	G
32	1a	637	A
32	1a	649	A
32	1a	671	A
32	1a	672	G
32	1a	677	G
32	1a	678	A
32	1a	707	U
32	1a	708	G
32	1a	715	G
32	1a	731	C
32	1a	733	C
32	1a	736	G
32	1a	739	G
32	1a	743	A
32	1a	761	A
32	1a	776	A
32	1a	777	U
32	1a	778	A
32	1a	799	A
32	1a	800	A
32	1a	801	C
32	1a	805	G
32	1a	812	A
32	1a	813	G

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Mol	Chain	Res	Type
32	1a	820	G
32	1a	824	C
32	1a	825	U
32	1a	826	C
32	1a	829	G
32	1a	838	A
32	1a	850	A
32	1a	880	G
32	1a	892	A
32	1a	893	A
32	1a	894	G
32	1a	904	G
32	1a	905	G
32	1a	912	C
32	1a	938	U
32	1a	939	U
32	1a	946	A
32	1a	947	A
32	1a	949	G
32	1a	950	C
32	1a	952	A
32	1a	953	A
32	1a	954	G
32	1a	955	A
32	1a	959	U
32	1a	961	A
32	1a	970	U
32	1a	971	G
32	1a	972	A
32	1a	977	C
32	1a	980	G
32	1a	982	G
32	1a	983	A
32	1a	984	A
32	1a	988	G
32	1a	990	G
32	1a	992	G
32	1a	995	A
32	1a	999	U
32	1a	1025	G
32	1a	1027	A
32	1a	1029	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1036	G
32	1a	1037	C
32	1a	1039	U
32	1a	1048	U
32	1a	1049	C
32	1a	1077	G
32	1a	1078	U
32	1a	1084	A
32	1a	1091	G
32	1a	1103	G
32	1a	1107	G
32	1a	1115	C
32	1a	1116	G
32	1a	1117	G
32	1a	1119	U
32	1a	1120	C
32	1a	1121	G
32	1a	1122	G
32	1a	1128	C
32	1a	1134	A
32	1a	1135	A
32	1a	1139	G
32	1a	1142	U
32	1a	1143	G
32	1a	1149	G
32	1a	1158	A
32	1a	1165	A
32	1a	1166	G
32	1a	1171	C
32	1a	1175	G
32	1a	1178	U
32	1a	1179	G
32	1a	1183	A
32	1a	1184	G
32	1a	1195	A
32	1a	1196	C
32	1a	1200	C
32	1a	1209	A
32	1a	1220	A
32	1a	1222	U
32	1a	1235	G
32	1a	1238	A

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Mol	Chain	Res	Type
32	1a	1239	U
32	1a	1240	G
32	1a	1242	C
32	1a	1245	C
32	1a	1248	G
32	1a	1252	C
32	1a	1260	U
32	1a	1261	A
32	1a	1262	A
32	1a	1268	A
32	1a	1269	A
32	1a	1281	A
32	1a	1282	G
32	1a	1284	U
32	1a	1294	G
32	1a	1301	A
32	1a	1304	C
32	1a	1320	G
32	1a	1322	A
32	1a	1328	A
32	1a	1329	G
32	1a	1335	G
32	1a	1342	A
32	1a	1345	C
32	1a	1348	G
32	1a	1353	G
32	1a	1360	A
32	1a	1379	A
32	1a	1380	C
32	1a	1381	A
32	1a	1402	G
32	1a	1425	G
32	1a	1426	G
32	1a	1432	A
32	1a	1433	C
32	1a	1434	G
32	1a	1465	G
32	1a	1475	G
32	1a	1480	A
32	1a	1481	A
32	1a	1482	G
32	1a	1484	U

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Mol	Chain	Res	Type
32	1a	1495	G
32	1a	1497	A
32	1a	1507	G
32	1a	1508	G
53	1v	15	A
54	1x	9	G
54	1x	13	C
54	1x	17(A)	U
54	1x	18	G
54	1x	19	G
54	1x	20	U
54	1x	21	A
54	1x	34	C
54	1x	44	A
54	1x	47	U
54	1x	51	C
54	1x	76	A
1	2A	7	A
1	2A	9	G
1	2A	11	U
1	2A	13	A
1	2A	14	G
1	2A	33	C
1	2A	34	G
1	2A	44	C
1	2A	48	U
1	2A	49	G
1	2A	56	G
1	2A	59	G
1	2A	69	A
1	2A	72	A
1	2A	73	G
1	2A	82	A
1	2A	88	U
1	2A	91	C
1	2A	93	G
1	2A	98	G
1	2A	99	G
1	2A	115	A
1	2A	116	A
1	2A	117	U
1	2A	122	G

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Mol	Chain	Res	Type
1	2A	125	C
1	2A	137	G
1	2A	138	A
1	2A	154	C
1	2A	155	U
1	2A	161	G
1	2A	169	A
1	2A	170	A
1	2A	184	A
1	2A	187	A
1	2A	193	G
1	2A	203	G
1	2A	204	A
1	2A	209	A
1	2A	210	A
1	2A	212	G
1	2A	216	A
1	2A	217	A
1	2A	218	U
1	2A	221	A
1	2A	236	G
1	2A	238	G
1	2A	268	G
1	2A	270	U
1	2A	271	U
1	2A	272	G
1	2A	273	U
1	2A	274	C
1	2A	287	U
1	2A	288	G
1	2A	300	C
1	2A	301	A
1	2A	327	G
1	2A	334	A
1	2A	335	G
1	2A	347	A
1	2A	350	G
1	2A	352	G
1	2A	353	A
1	2A	356	G
1	2A	361	G
1	2A	365	G

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Mol	Chain	Res	Type
1	2A	375	G
1	2A	385	U
1	2A	386	G
1	2A	412	G
1	2A	431	U
1	2A	437	G
1	2A	438	A
1	2A	441	A
1	2A	453	U
1	2A	454	A
1	2A	461	C
1	2A	468	A
1	2A	469	C
1	2A	479	A
1	2A	480	C
1	2A	482	A
1	2A	495	A
1	2A	506	G
1	2A	528	U
1	2A	529	A
1	2A	533	C
1	2A	552	A
1	2A	554	G
1	2A	555	C
1	2A	556	A
1	2A	557	G
1	2A	568	G
1	2A	573	G
1	2A	585	G
1	2A	590	U
1	2A	595	G
1	2A	596	C
1	2A	597	A
1	2A	608	A
1	2A	625	A
1	2A	626	G
1	2A	629	U
1	2A	640	G
1	2A	651	A
1	2A	658	C
1	2A	661	A
1	2A	669	C

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Mol	Chain	Res	Type
1	2A	670	A
1	2A	678	A
1	2A	681	G
1	2A	697	G
1	2A	732	G
1	2A	763	G
1	2A	772	G
1	2A	776	C
1	2A	784	G
1	2A	810	A
1	2A	811	G
1	2A	821	G
1	2A	822	G
1	2A	828	A
1	2A	829	A
1	2A	830	A
1	2A	831	G
1	2A	836	C
1	2A	838	G
1	2A	851	G
1	2A	858	C
1	2A	865	A
1	2A	873	U
1	2A	874	U
1	2A	894	G
1	2A	903	C
1	2A	905	G
1	2A	912	A
1	2A	913	C
1	2A	925	G
1	2A	928	G
1	2A	930	C
1	2A	931	C
1	2A	932	C
1	2A	933	A
1	2A	934	C
1	2A	935	C
1	2A	936	A
1	2A	938	C
1	2A	941	A
1	2A	942	C
1	2A	944	A

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Mol	Chain	Res	Type
1	2A	945	A
1	2A	946	A
1	2A	947	C
1	2A	951	G
1	2A	955	A
1	2A	956	A
1	2A	962	A
1	2A	964	G
1	2A	976	G
1	2A	982	G
1	2A	985	A
1	2A	989	A
1	2A	990	G
1	2A	997	A
1	2A	1003	A
1	2A	1005	C
1	2A	1018	G
1	2A	1019	C
1	2A	1028	A
1	2A	1041	A
1	2A	1042	G
1	2A	1043	C
1	2A	1050	C
1	2A	1057	U
1	2A	1058	C
1	2A	1065	A
1	2A	1067	G
1	2A	1070	G
1	2A	1071	U
1	2A	1078	U
1	2A	1081	G
1	2A	1083	C
1	2A	1088	C
1	2A	1090	A
1	2A	1091	A
1	2A	1092	G
1	2A	1093	A
1	2A	1098	C
1	2A	1103	G
1	2A	1104	G
1	2A	1105	U
1	2A	1106	U

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Mol	Chain	Res	Type
1	2A	1107	G
1	2A	1108	G
1	2A	1109	C
1	2A	1110	U
1	2A	1115	A
1	2A	1118	A
1	2A	1120	C
1	2A	1121	C
1	2A	1128	U
1	2A	1133	A
1	2A	1136	G
1	2A	1142	U
1	2A	1143	A
1	2A	1146	U
1	2A	1154	C
1	2A	1156	A
1	2A	1157	G
1	2A	1158	U
1	2A	1159	G
1	2A	1161	C
1	2A	1163	C
1	2A	1175	U
1	2A	1178	U
1	2A	1179	C
1	2A	1180	G
1	2A	1183	G
1	2A	1200	A
1	2A	1216	G
1	2A	1256	G
1	2A	1263	G
1	2A	1264	A
1	2A	1274	G
1	2A	1281	G
1	2A	1285	U
1	2A	1289	G
1	2A	1295	G
1	2A	1298	A
1	2A	1301	G
1	2A	1316	G
1	2A	1317	A
1	2A	1318	U
1	2A	1329	A

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Mol	Chain	Res	Type
1	2A	1332	A
1	2A	1345	U
1	2A	1346	A
1	2A	1348	G
1	2A	1359	C
1	2A	1366	A
1	2A	1374	U
1	2A	1387	A
1	2A	1390	C
1	2A	1399	A
1	2A	1404	A
1	2A	1405	A
1	2A	1410	A
1	2A	1413	G
1	2A	1415	C
1	2A	1429	A
1	2A	1430	G
1	2A	1431	C
1	2A	1461	G
1	2A	1462	C
1	2A	1465	U
1	2A	1466	G
1	2A	1473	C
1	2A	1490	A
1	2A	1495	A
1	2A	1496	G
1	2A	1501	G
1	2A	1505	G
1	2A	1508	C
1	2A	1513	C
1	2A	1517	A
1	2A	1528	G
1	2A	1534	U
1	2A	1535	A
1	2A	1538	C
1	2A	1542	U
1	2A	1554	C
1	2A	1555	A
1	2A	1570	G
1	2A	1577	C
1	2A	1579	G
1	2A	1589	C

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Mol	Chain	Res	Type
1	2A	1593	C
1	2A	1604	A
1	2A	1605	G
1	2A	1612	A
1	2A	1615	A
1	2A	1624	U
1	2A	1630	C
1	2A	1631	A
1	2A	1640	G
1	2A	1653	A
1	2A	1654	A
1	2A	1655	A
1	2A	1658	G
1	2A	1686	C
1	2A	1694	C
1	2A	1720	G
1	2A	1746	A
1	2A	1766	A
1	2A	1771	C
1	2A	1786	G
1	2A	1788	G
1	2A	1792	A
1	2A	1793	G
1	2A	1794	G
1	2A	1799	G
1	2A	1803	A
1	2A	1810	A
1	2A	1812	C
1	2A	1821	A
1	2A	1830	C
1	2A	1831	G
1	2A	1846	G
1	2A	1858	G
1	2A	1859	A
1	2A	1869	G
1	2A	1877	A
1	2A	1880	G
1	2A	1887	G
1	2A	1889	A
1	2A	1891	G
1	2A	1898	A
1	2A	1899	G

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Mol	Chain	Res	Type
1	2A	1905	A
1	2A	1910	A
1	2A	1921	A
1	2A	1927	G
1	2A	1934	A
1	2A	1935	C
1	2A	1950	G
1	2A	1951	G
1	2A	1952	U
1	2A	1955	C
1	2A	1959	A
1	2A	1976	U
1	2A	1984	U
1	2A	1988	C
1	2A	1991	A
1	2A	1992	A
1	2A	1993	A
1	2A	2005	G
1	2A	2014	U
1	2A	2018	G
1	2A	2026	A
1	2A	2041	A
1	2A	2044	G
1	2A	2052	A
1	2A	2054	A
1	2A	2060	C
1	2A	2064	C
1	2A	2067	G
1	2A	2073	G
1	2A	2076	C
1	2A	2077	G
1	2A	2081	A
1	2A	2082	G
1	2A	2083	A
1	2A	2090	G
1	2A	2103	A
1	2A	2120	U
1	2A	2123	U
1	2A	2207	G
1	2A	2209	C
1	2A	2210	U
1	2A	2213	G

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Mol	Chain	Res	Type
1	2A	2219	A
1	2A	2226	G
1	2A	2227	G
1	2A	2228	A
1	2A	2229	U
1	2A	2236	A
1	2A	2246	G
1	2A	2249	G
1	2A	2250	G
1	2A	2251	C
1	2A	2268	U
1	2A	2279	A
1	2A	2280	A
1	2A	2286	C
1	2A	2289	A
1	2A	2294	C
1	2A	2298	A
1	2A	2304	C
1	2A	2308	C
1	2A	2316	A
1	2A	2318	G
1	2A	2319	G
1	2A	2323	U
1	2A	2328	C
1	2A	2329	G
1	2A	2330	G
1	2A	2331	A
1	2A	2336	G
1	2A	2345	G
1	2A	2346	A
1	2A	2347	A
1	2A	2354	C
1	2A	2358	C
1	2A	2361	C
1	2A	2387	A
1	2A	2394	G
1	2A	2396	C
1	2A	2407	G
1	2A	2411	G
1	2A	2413	C
1	2A	2417	U
1	2A	2421	G

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Mol	Chain	Res	Type
1	2A	2433	A
1	2A	2434	U
1	2A	2436	A
1	2A	2439	G
1	2A	2440	G
1	2A	2441	A
1	2A	2442	U
1	2A	2445	A
1	2A	2446	A
1	2A	2450	A
1	2A	2456	G
1	2A	2459	A
1	2A	2476	C
1	2A	2487	A
1	2A	2497	G
1	2A	2501	G
1	2A	2508	A
1	2A	2513	G
1	2A	2516	G
1	2A	2517	U
1	2A	2529	A
1	2A	2531	C
1	2A	2540	G
1	2A	2565	U
1	2A	2566	U
1	2A	2577	A
1	2A	2578	G
1	2A	2584	C
1	2A	2585	G
1	2A	2613	A
1	2A	2620	U
1	2A	2622	U
1	2A	2623	C
1	2A	2626	U
1	2A	2641	G
1	2A	2665	A
1	2A	2674	G
1	2A	2700	U
1	2A	2701	C
1	2A	2702	C
1	2A	2713	U
1	2A	2724	A

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Mol	Chain	Res	Type
1	2A	2725	A
1	2A	2726	G
1	2A	2738	U
1	2A	2745	A
1	2A	2776	A
1	2A	2777	A
1	2A	2778	G
1	2A	2790	A
1	2A	2805	G
1	2A	2812	G
1	2A	2817	U
1	2A	2819	A
1	2A	2827	G
1	2A	2829	A
1	2A	2830	A
1	2A	2842	G
1	2A	2844	A
1	2A	2881	G
1	2A	2884	C
1	2A	2888	C
1	2A	2889	C
1	2A	2900	A
1	2A	2902	G
1	2A	2903	U
1	2A	2904	C
2	2B	2	C
2	2B	4	C
2	2B	7	G
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	22	U
2	2B	23	G
2	2B	28	C
2	2B	30	C
2	2B	31	C
2	2B	34	U
2	2B	35	U
2	2B	37	C
2	2B	42	C
2	2B	43	C
2	2B	45	A

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Mol	Chain	Res	Type
2	2B	46	A
2	2B	50	G
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	59	A
2	2B	65	C
2	2B	67	G
2	2B	73	A
2	2B	85	G
2	2B	90	A
2	2B	110	G
2	2B	111	G
2	2B	116	G
2	2B	117	G
2	2B	120	A
32	2a	6	U
32	2a	10	G
32	2a	15	U
32	2a	23	G
32	2a	33	A
32	2a	40	G
32	2a	48	C
32	2a	49	C
32	2a	51	A
32	2a	52	A
32	2a	53	G
32	2a	60	A
32	2a	66	U
32	2a	67	G
32	2a	75	C
32	2a	79	G
32	2a	84	A
32	2a	85	C
32	2a	95	A
32	2a	99	G
32	2a	109	G
32	2a	110	A
32	2a	114	A
32	2a	115	C
32	2a	126	C

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Mol	Chain	Res	Type
32	2a	138	A
32	2a	146	A
32	2a	158	C
32	2a	168	U
32	2a	169	C
32	2a	177	U
32	2a	189	U
32	2a	190	U
32	2a	202	A
32	2a	204	A
32	2a	210	U
32	2a	211	U
32	2a	212	G
32	2a	213	C
32	2a	239	A
32	2a	243	G
32	2a	247	G
32	2a	262	G
32	2a	263	C
32	2a	275	A
32	2a	277	G
32	2a	285	G
32	2a	294	A
32	2a	297	G
32	2a	302	G
32	2a	317	A
32	2a	324	C
32	2a	328	G
32	2a	340	A
32	2a	346	G
32	2a	347	G
32	2a	348	C
32	2a	349	A
32	2a	350	G
32	2a	361	U
32	2a	363	U
32	2a	365	C
32	2a	368	C
32	2a	380	G
32	2a	394	C
32	2a	400	U
32	2a	402	G

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Mol	Chain	Res	Type
32	2a	408	A
32	2a	410	A
32	2a	419	G
32	2a	425	U
32	2a	426	A
32	2a	435	A
32	2a	437	C
32	2a	446	A
32	2a	447	A
32	2a	455	A
32	2a	456	C
32	2a	469	G
32	2a	470	G
32	2a	481	A
32	2a	482	U
32	2a	489	G
32	2a	493	A
32	2a	494	A
32	2a	495	C
32	2a	502	C
32	2a	505	G
32	2a	511	G
32	2a	515	U
32	2a	516	A
32	2a	517	A
32	2a	531	A
32	2a	543	A
32	2a	544	U
32	2a	545	U
32	2a	546	C
32	2a	548	C
32	2a	550	G
32	2a	552	G
32	2a	556	A
32	2a	557	A
32	2a	560	G
32	2a	576	G
32	2a	580	C
32	2a	614	G
32	2a	615	G
32	2a	636	U
32	2a	637	A

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Mol	Chain	Res	Type
32	2a	645	G
32	2a	649	A
32	2a	658	G
32	2a	671	A
32	2a	672	G
32	2a	677	G
32	2a	679	A
32	2a	704	C
32	2a	705	G
32	2a	707	U
32	2a	708	G
32	2a	715	G
32	2a	726	G
32	2a	733	C
32	2a	739	G
32	2a	758	G
32	2a	761	A
32	2a	772	U
32	2a	776	A
32	2a	777	U
32	2a	778	A
32	2a	800	A
32	2a	801	C
32	2a	803	A
32	2a	805	G
32	2a	811	U
32	2a	812	A
32	2a	813	G
32	2a	820	G
32	2a	824	C
32	2a	825	U
32	2a	826	C
32	2a	829	G
32	2a	837	A
32	2a	852	G
32	2a	862	U
32	2a	863	G
32	2a	880	G
32	2a	892	A
32	2a	893	A
32	2a	904	G
32	2a	905	G

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Mol	Chain	Res	Type
32	2a	909	C
32	2a	911	G
32	2a	912	C
32	2a	913	A
32	2a	920	G
32	2a	938	U
32	2a	939	U
32	2a	946	A
32	2a	947	A
32	2a	949	G
32	2a	952	A
32	2a	953	A
32	2a	954	G
32	2a	955	A
32	2a	956	A
32	2a	967	C
32	2a	970	U
32	2a	971	G
32	2a	977	C
32	2a	979	A
32	2a	981	G
32	2a	982	G
32	2a	984	A
32	2a	995	A
32	2a	1000	G
32	2a	1001	G
32	2a	1028	C
32	2a	1033	G
32	2a	1036	G
32	2a	1037	C
32	2a	1038	A
32	2a	1039	U
32	2a	1048	U
32	2a	1049	C
32	2a	1064	G
32	2a	1077	G
32	2a	1078	U
32	2a	1084	A
32	2a	1096	C
32	2a	1100	G
32	2a	1101	C
32	2a	1105	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1108	U
32	2a	1109	U
32	2a	1112	C
32	2a	1113	A
32	2a	1117	G
32	2a	1118	U
32	2a	1119	U
32	2a	1120	C
32	2a	1121	G
32	2a	1122	G
32	2a	1129	A
32	2a	1140	A
32	2a	1142	U
32	2a	1149	G
32	2a	1165	A
32	2a	1168	G
32	2a	1171	C
32	2a	1172	G
32	2a	1173	A
32	2a	1178	U
32	2a	1179	G
32	2a	1184	G
32	2a	1191	C
32	2a	1193	U
32	2a	1194	U
32	2a	1195	A
32	2a	1196	C
32	2a	1220	A
32	2a	1222	U
32	2a	1223	G
32	2a	1228	C
32	2a	1238	A
32	2a	1239	U
32	2a	1240	G
32	2a	1242	C
32	2a	1244	C
32	2a	1255	G
32	2a	1260	U
32	2a	1262	A
32	2a	1263	U
32	2a	1264	C
32	2a	1268	A

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Mol	Chain	Res	Type
32	2a	1269	A
32	2a	1279	C
32	2a	1281	A
32	2a	1284	U
32	2a	1285	C
32	2a	1287	G
32	2a	1293	G
32	2a	1302	C
32	2a	1304	C
32	2a	1305	G
32	2a	1307	C
32	2a	1308	C
32	2a	1320	G
32	2a	1328	A
32	2a	1329	G
32	2a	1339	A
32	2a	1341	C
32	2a	1342	A
32	2a	1345	C
32	2a	1347	U
32	2a	1351	G
32	2a	1353	G
32	2a	1361	C
32	2a	1380	C
32	2a	1381	A
32	2a	1388	G
32	2a	1402	G
32	2a	1407	C
32	2a	1425	G
32	2a	1426	G
32	2a	1431	U
32	2a	1433	C
32	2a	1434	G
32	2a	1477	A
32	2a	1480	A
32	2a	1481	A
32	2a	1482	G
32	2a	1483	G
32	2a	1484	U
32	2a	1495	G
32	2a	1497	A
32	2a	1498	G

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Mol	Chain	Res	Type
32	2a	1507	G
32	2a	1508	G
32	2a	1509	A
32	2a	1510	U
53	2v	15	A
54	2x	9	G
54	2x	13	C
54	2x	16	C
54	2x	17	C
54	2x	17(A)	U
54	2x	20	U
54	2x	21	A
54	2x	31	G
54	2x	42	G
54	2x	47	U
54	2x	51	C
54	2x	55	PSU
54	2x	56	C
54	2x	65	C
54	2x	76	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	183	A
1	1A	184	A
1	1A	187	A
1	1A	237	C
1	1A	301	A
1	1A	516	A
1	1A	715	G
1	1A	792	A
1	1A	810	A
1	1A	820	A
1	1A	822	G
1	1A	873	U
1	1A	1002	U
1	1A	1018	G
1	1A	1153	U
1	1A	1218	A
1	1A	1220	G
1	1A	1285	U

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Mol	Chain	Res	Type
1	1A	1425	G
1	1A	1465	U
1	1A	1653	A
1	1A	2013	G
1	1A	2208	G
1	1A	2417	U
1	1A	2433	A
1	1A	2441	A
1	1A	2450	A
1	1A	2700	U
1	2A	184	A
1	2A	237	C
1	2A	270	U
1	2A	272	G
1	2A	300	C
1	2A	333	A
1	2A	516	A
1	2A	669	C
1	2A	820	A
1	2A	902	C
1	2A	945	A
1	2A	1047	G
1	2A	1090	A
1	2A	1102	A
1	2A	1114	A
1	2A	1238	A
1	2A	1425	G
1	2A	1465	U
1	2A	1604	A
1	2A	1653	A
1	2A	1934	A
1	2A	2013	G
1	2A	2328	C
1	2A	2417	U
1	2A	2450	A
1	2A	2700	U
2	2B	42	C
2	2B	45	A

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

8 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$
54	5MC	1x	32	54	14,22,23	1.21	1 (7%)	17,32,35	1.25	2 (11%)
54	5MU	1x	54	54	13,22,23	0.61	0	16,32,35	2.71	2 (12%)
54	PSU	1x	55	54	15,21,22	1.34	1 (6%)	16,30,33	2.15	4 (25%)
54	4SU	1x	8	54	12,21,22	1.06	1 (8%)	15,30,33	1.74	1 (6%)
54	5MC	2x	32	54	14,22,23	1.28	1 (7%)	17,32,35	1.25	2 (11%)
54	5MU	2x	54	54	13,22,23	0.56	0	16,32,35	2.91	2 (12%)
54	PSU	2x	55	54	15,21,22	1.30	1 (6%)	16,30,33	2.16	3 (18%)
54	4SU	2x	8	54	12,21,22	0.92	1 (8%)	15,30,33	1.76	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
54	5MC	1x	32	54	-	0/3/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/3/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/3/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/3/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	55	PSU	C5-C1'	-4.25	1.48	1.52
54	2x	55	PSU	C5-C1'	-3.62	1.49	1.52
54	1x	8	4SU	C2-N3	-3.43	1.31	1.38
54	2x	8	4SU	C2-N3	-2.73	1.32	1.38
54	1x	32	5MC	C5-C4	4.23	1.48	1.41
54	2x	32	5MC	C5-C4	4.39	1.48	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	54	5MU	C5-C4-N3	-8.34	118.35	125.35
54	1x	54	5MU	C5-C4-N3	-7.08	119.40	125.35
54	2x	8	4SU	C5-C4-N3	-6.38	116.80	123.56
54	1x	8	4SU	C5-C4-N3	-6.27	116.92	123.56
54	1x	55	PSU	C5-C6-N1	-3.84	119.03	124.38
54	2x	55	PSU	C5-C6-N1	-3.09	120.06	124.38
54	2x	32	5MC	CM5-C5-C4	-3.01	118.28	121.47
54	1x	55	PSU	C5-C1'-C2'	-2.78	110.71	115.44
54	1x	32	5MC	CM5-C5-C4	-2.33	119.00	121.47
54	2x	32	5MC	N4-C4-N3	2.15	120.08	116.92
54	2x	55	PSU	O4'-C1'-C2'	2.29	107.16	104.69
54	1x	55	PSU	O4'-C1'-C2'	2.43	107.32	104.69
54	1x	32	5MC	N4-C4-N3	3.44	121.96	116.92
54	1x	55	PSU	C4-N3-C2	6.16	120.30	115.16
54	2x	55	PSU	C4-N3-C2	7.13	121.11	115.16
54	1x	54	5MU	C4-N3-C2	7.64	121.53	115.16
54	2x	54	5MU	C4-N3-C2	7.80	121.66	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2444 ligands modelled in this entry, 2442 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	SF4	1d	301	35	0,12,12	0.00	-	0,24,24	0.00	-
58	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	SF4	1d	301	35	-	0/0/48/48	0/6/5/5
58	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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2746/2915 (94%)	-0.04	25 (0%) 85 79	23, 42, 86, 108	0
1	2A	2790/2915 (95%)	-0.34	57 (2%) 68 58	27, 47, 93, 110	0
2	1B	120/121 (99%)	-0.19	0 100 100	36, 64, 82, 95	0
2	2B	120/121 (99%)	0.06	2 (1%) 73 63	43, 70, 85, 96	0
3	1D	275/276 (99%)	-0.38	0 100 100	21, 41, 57, 80	0
3	2D	275/276 (99%)	-0.50	1 (0%) 93 90	24, 43, 60, 80	0
4	1E	204/206 (99%)	-0.28	0 100 100	20, 44, 67, 83	0
4	2E	204/206 (99%)	-0.31	1 (0%) 91 88	24, 48, 69, 84	0
5	1F	203/210 (96%)	-0.20	1 (0%) 91 88	23, 51, 77, 93	0
5	2F	203/210 (96%)	-0.35	2 (0%) 84 77	27, 55, 79, 94	0
6	1G	181/182 (99%)	-0.25	4 (2%) 65 54	52, 70, 83, 96	0
6	2G	181/182 (99%)	0.51	16 (8%) 12 6	58, 74, 85, 96	0
7	1H	174/180 (96%)	-0.12	1 (0%) 90 86	49, 65, 77, 89	0
7	2H	174/180 (96%)	0.97	31 (17%) 2 1	55, 70, 81, 91	0
8	1I	146/148 (98%)	0.01	0 100 100	48, 75, 85, 89	0
8	2I	146/148 (98%)	0.42	9 (6%) 24 15	51, 76, 86, 91	0
9	1N	140/140 (100%)	-0.23	0 100 100	33, 47, 69, 82	0
9	2N	140/140 (100%)	-0.15	0 100 100	36, 53, 71, 84	0
10	1O	122/122 (100%)	-0.32	0 100 100	32, 44, 63, 71	0
10	2O	122/122 (100%)	-0.45	0 100 100	35, 47, 64, 72	0
11	1P	149/150 (99%)	-0.20	0 100 100	24, 54, 76, 85	0
11	2P	149/150 (99%)	0.15	6 (4%) 42 30	27, 58, 78, 89	0
12	1Q	141/141 (100%)	-0.13	1 (0%) 89 84	33, 50, 66, 88	0
12	2Q	141/141 (100%)	-0.43	1 (0%) 89 84	37, 54, 69, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.18	0 100 100	31, 40, 55, 66	0
13	2R	118/118 (100%)	-0.38	0 100 100	34, 44, 56, 69	0
14	1S	110/112 (98%)	-0.21	0 100 100	46, 63, 73, 77	0
14	2S	110/112 (98%)	0.61	8 (7%) 18 10	52, 67, 77, 80	0
15	1T	131/146 (89%)	-0.26	1 (0%) 87 81	37, 50, 75, 86	0
15	2T	131/146 (89%)	-0.41	0 100 100	39, 53, 76, 85	0
16	1U	116/118 (98%)	-0.16	0 100 100	28, 40, 56, 75	0
16	2U	116/118 (98%)	-0.36	2 (1%) 73 63	32, 45, 62, 76	0
17	1V	101/101 (100%)	-0.27	0 100 100	29, 49, 68, 80	0
17	2V	101/101 (100%)	0.01	0 100 100	32, 56, 73, 80	0
18	1W	112/113 (99%)	-0.29	2 (1%) 71 61	27, 37, 57, 91	0
18	2W	112/113 (99%)	-0.42	0 100 100	31, 40, 61, 91	0
19	1X	95/96 (98%)	-0.19	0 100 100	28, 47, 69, 80	0
19	2X	95/96 (98%)	-0.13	3 (3%) 51 39	33, 51, 70, 81	0
20	1Y	107/110 (97%)	-0.00	1 (0%) 85 79	45, 59, 78, 87	0
20	2Y	107/110 (97%)	0.59	12 (11%) 7 3	51, 63, 81, 90	0
21	1Z	186/206 (90%)	-0.39	0 100 100	52, 69, 83, 93	0
21	2Z	186/206 (90%)	0.39	7 (3%) 44 32	55, 72, 85, 94	0
22	10	75/85 (88%)	-0.54	0 100 100	16, 36, 52, 67	0
22	20	75/85 (88%)	0.24	6 (8%) 15 7	40, 64, 77, 80	0
23	11	97/98 (98%)	-0.17	1 (1%) 84 77	30, 48, 75, 79	0
23	21	97/98 (98%)	-0.13	2 (2%) 67 56	34, 51, 76, 81	0
24	12	70/72 (97%)	-0.10	0 100 100	42, 59, 73, 82	0
24	22	70/72 (97%)	0.17	3 (4%) 39 27	47, 63, 76, 80	0
25	13	59/60 (98%)	-0.14	0 100 100	32, 46, 67, 78	0
25	23	59/60 (98%)	0.40	3 (5%) 32 21	37, 51, 71, 82	0
26	14	69/71 (97%)	0.13	5 (7%) 18 10	63, 82, 95, 99	0
26	24	69/71 (97%)	0.86	15 (21%) 1 1	69, 85, 96, 100	0
27	15	59/60 (98%)	-0.38	0 100 100	22, 38, 57, 73	0
27	25	59/60 (98%)	-0.43	0 100 100	27, 42, 61, 74	0
28	16	53/54 (98%)	-0.37	0 100 100	37, 48, 66, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	-0.39	0 100 100	40, 52, 63, 69	0
29	17	48/49 (97%)	-0.18	1 (2%) 67 56	26, 31, 65, 78	0
29	27	48/49 (97%)	-0.12	3 (6%) 23 14	29, 34, 65, 80	0
30	18	64/65 (98%)	-0.12	0 100 100	34, 41, 53, 61	0
30	28	64/65 (98%)	-0.11	0 100 100	37, 45, 57, 64	0
31	19	37/37 (100%)	0.10	0 100 100	40, 49, 69, 74	0
31	29	37/37 (100%)	0.22	2 (5%) 29 19	44, 54, 70, 76	0
32	1a	1477/1521 (97%)	-0.09	37 (2%) 61 48	35, 71, 97, 112	0
32	2a	1483/1521 (97%)	-0.04	38 (2%) 59 47	45, 79, 100, 110	0
33	1b	231/256 (90%)	0.42	17 (7%) 17 9	66, 83, 94, 100	0
33	2b	231/256 (90%)	0.70	26 (11%) 7 3	72, 89, 96, 104	0
34	1c	206/239 (86%)	0.21	13 (6%) 23 14	68, 83, 91, 96	0
34	2c	206/239 (86%)	0.61	23 (11%) 7 3	70, 85, 92, 95	0
35	1d	208/209 (99%)	0.10	5 (2%) 62 50	54, 76, 88, 96	0
35	2d	208/209 (99%)	-0.03	4 (1%) 70 59	62, 75, 86, 92	0
36	1e	148/162 (91%)	-0.28	0 100 100	46, 66, 78, 89	0
36	2e	148/162 (91%)	-0.20	0 100 100	60, 75, 84, 92	0
37	1f	100/101 (99%)	-0.25	0 100 100	58, 74, 83, 90	0
37	2f	100/101 (99%)	-0.31	1 (1%) 84 77	60, 74, 84, 88	0
38	1g	155/156 (99%)	0.26	10 (6%) 22 13	61, 79, 93, 97	0
38	2g	155/156 (99%)	0.78	19 (12%) 5 3	69, 80, 92, 97	0
39	1h	137/138 (99%)	-0.19	0 100 100	54, 69, 79, 87	0
39	2h	137/138 (99%)	0.20	6 (4%) 38 26	65, 77, 86, 91	0
40	1i	127/128 (99%)	0.47	9 (7%) 19 10	64, 86, 93, 96	0
40	2i	127/128 (99%)	1.32	32 (25%) 1 0	64, 88, 95, 96	0
41	1j	97/105 (92%)	0.68	11 (11%) 7 3	63, 86, 95, 98	0
41	2j	96/105 (91%)	1.16	18 (18%) 2 1	76, 91, 99, 101	0
42	1k	114/129 (88%)	-0.21	1 (0%) 85 79	40, 69, 83, 92	0
42	2k	114/129 (88%)	0.10	3 (2%) 59 47	53, 76, 86, 93	0
43	1l	122/132 (92%)	-0.22	1 (0%) 87 81	46, 62, 73, 79	0
43	2l	122/132 (92%)	-0.16	3 (2%) 61 48	56, 69, 78, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	118/126 (93%)	-0.01	0 100 100	65, 80, 87, 92	0
44	2m	116/126 (92%)	0.42	8 (6%) 20 11	70, 83, 89, 93	0
45	1n	60/61 (98%)	0.37	3 (5%) 32 21	63, 75, 88, 89	0
45	2n	60/61 (98%)	1.34	15 (25%) 1 0	76, 87, 92, 96	0
46	1o	88/89 (98%)	-0.01	2 (2%) 64 52	51, 67, 82, 90	0
46	2o	88/89 (98%)	0.02	0 100 100	59, 73, 83, 89	0
47	1p	82/88 (93%)	0.40	3 (3%) 45 33	60, 78, 87, 93	0
47	2p	82/88 (93%)	0.24	2 (2%) 62 50	62, 71, 82, 91	0
48	1q	99/105 (94%)	-0.02	0 100 100	51, 69, 80, 84	0
48	2q	99/105 (94%)	0.10	2 (2%) 68 58	59, 73, 83, 90	0
49	1r	68/88 (77%)	0.33	4 (5%) 26 16	58, 70, 84, 87	0
49	2r	68/88 (77%)	0.56	8 (11%) 6 3	63, 73, 85, 90	0
50	1s	84/93 (90%)	0.43	1 (1%) 81 73	68, 81, 90, 95	0
50	2s	83/93 (89%)	1.68	24 (28%) 1 0	82, 91, 99, 104	0
51	1t	96/106 (90%)	0.21	2 (2%) 67 56	61, 75, 84, 93	0
51	2t	96/106 (90%)	0.11	0 100 100	55, 73, 84, 88	0
52	1u	23/27 (85%)	0.45	1 (4%) 39 27	71, 78, 80, 84	0
52	2u	23/27 (85%)	1.68	9 (39%) 0 0	73, 80, 85, 86	0
53	1v	5/24 (20%)	0.67	1 (20%) 1 1	61, 64, 90, 97	0
53	2v	5/24 (20%)	1.25	1 (20%) 1 1	65, 68, 91, 97	0
54	1x	72/77 (93%)	-0.21	0 100 100	28, 58, 83, 92	0
54	2x	72/77 (93%)	0.10	1 (1%) 78 69	41, 79, 91, 102	0
55	1z	12/14 (85%)	0.29	0 100 100	23, 39, 59, 84	0
55	2z	12/14 (85%)	-0.04	1 (8%) 14 7	26, 42, 64, 85	0
All	All	20520/21472 (95%)	-0.03	600 (2%) 55 43	16, 62, 92, 112	0

All (600) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	1a	980	G	8.3
32	2a	980	G	7.8
32	1a	981	G	7.5
1	2A	2812	G	7.0
32	1a	979	A	6.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
38	2g	156	TRP	6.8
38	1g	80	VAL	6.3
32	2a	979	A	6.2
32	2a	981	G	6.1
38	2g	78	ARG	6.0
45	2n	25	VAL	5.6
38	2g	80	VAL	5.5
20	1Y	1	MET	5.5
26	24	68	ARG	5.5
40	2i	15	ALA	5.5
50	2s	40	ILE	5.4
38	2g	82	GLY	5.3
7	2H	112	PRO	5.2
20	2Y	1	MET	5.2
32	1a	982	G	5.1
7	2H	115	VAL	5.1
26	24	45	GLY	5.1
40	2i	7	THR	5.0
7	2H	111	HIS	5.0
50	2s	71	LEU	4.9
1	2A	2811	A	4.9
34	2c	186	PHE	4.9
1	2A	2815	G	4.9
40	2i	9	ARG	4.8
1	2A	1091	A	4.8
35	1d	23	GLY	4.8
38	1g	81	GLY	4.8
41	2j	63	PHE	4.8
32	2a	1025	G	4.7
12	1Q	59	ARG	4.7
26	24	49	PHE	4.7
40	2i	8	GLY	4.7
38	2g	154	TYR	4.7
6	2G	48	GLU	4.6
52	2u	16	GLY	4.6
32	2a	1268	A	4.6
52	2u	14	TRP	4.5
1	1A	1554	C	4.4
32	1a	211	U	4.4
50	2s	49	ILE	4.4
7	2H	113	VAL	4.4
32	1a	978	U	4.4

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Mol	Chain	Res	Type	RSRZ
29	17	48	LYS	4.4
45	2n	38	GLY	4.4
7	2H	128	PRO	4.3
45	2n	39	LEU	4.3
1	1A	2815	G	4.3
33	1b	227	GLY	4.3
50	2s	31	ILE	4.3
40	2i	36	TYR	4.2
32	2a	1510	U	4.2
38	2g	83	ALA	4.1
32	2a	982	G	4.1
41	2j	6	ILE	4.1
1	2A	2813	C	4.1
7	2H	103	LEU	4.1
41	2j	40	LEU	4.1
41	1j	10	GLY	4.0
40	2i	21	PRO	4.0
38	2g	84	ASN	4.0
7	2H	114	VAL	4.0
38	1g	78	ARG	4.0
38	1g	79	ARG	3.9
32	1a	209	U	3.9
40	2i	27	THR	3.9
1	2A	2904	C	3.9
45	2n	49	HIS	3.9
38	1g	82	GLY	3.9
33	2b	132	LYS	3.9
32	2a	1024	A	3.8
34	2c	124	ILE	3.8
33	2b	133	LYS	3.8
34	2c	189	ALA	3.8
32	2a	1239	U	3.8
33	1b	228	GLY	3.8
50	2s	16	LEU	3.8
1	2A	1128	U	3.8
1	2A	2805	G	3.8
38	2g	86	GLN	3.8
52	2u	17	THR	3.8
32	2a	1000	G	3.8
33	2b	131	PRO	3.8
8	2I	14	ASP	3.8
14	2S	58	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
41	2j	20	ALA	3.8
8	2I	11	ASN	3.7
32	2a	1509	A	3.7
33	2b	101	MET	3.7
39	2h	96	GLY	3.7
1	2A	2816	G	3.7
19	2X	92	LEU	3.7
7	2H	105	LEU	3.7
1	1A	2813	C	3.6
39	2h	122	ARG	3.6
23	2l	2	SER	3.6
29	27	48	LYS	3.6
38	1g	84	ASN	3.6
34	2c	57	ILE	3.6
1	2A	1129	A	3.5
32	1a	1024	A	3.5
7	2H	95	ARG	3.5
7	2H	97	ARG	3.5
1	2A	2902	G	3.5
44	2m	92	HIS	3.5
1	2A	1132	G	3.5
7	2H	107	VAL	3.5
32	2a	211	U	3.5
45	2n	34	TYR	3.5
50	2s	8	GLY	3.4
6	2G	86	MET	3.4
33	1b	214	ILE	3.4
33	2b	187	LEU	3.4
1	1A	2814	C	3.4
1	2A	2814	C	3.4
6	2G	19	LEU	3.4
48	2q	98	LEU	3.4
26	24	46	GLN	3.4
49	2r	23	LYS	3.4
1	2A	678	A	3.4
7	2H	94	TYR	3.4
1	2A	1089	G	3.4
1	2A	1130	A	3.3
32	2a	978	U	3.3
40	1i	19	LEU	3.3
7	2H	166	GLY	3.3
41	1j	98	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
26	14	53	GLU	3.3
32	1a	1120	C	3.3
38	1g	156	TRP	3.3
38	2g	79	ARG	3.3
1	2A	1554	C	3.3
40	2i	62	TYR	3.3
11	2P	91	PHE	3.3
1	1A	1220	G	3.3
1	2A	697	G	3.3
50	2s	80	TYR	3.3
33	2b	197	VAL	3.3
32	1a	1002	G	3.3
34	2c	6	HIS	3.3
34	1c	193	TYR	3.3
1	2A	217	A	3.2
50	2s	29	ARG	3.2
31	29	37	GLY	3.2
22	20	69	PHE	3.2
7	2H	102	ALA	3.2
26	14	55	ARG	3.2
1	1A	2205	G	3.2
7	2H	106	THR	3.2
50	2s	47	HIS	3.2
33	1b	135	GLN	3.2
33	1b	28	PHE	3.2
26	24	67	TYR	3.2
1	1A	1149	C	3.2
7	2H	48	GLY	3.1
32	1a	1025	G	3.1
32	2a	1265	G	3.1
6	2G	35	GLU	3.1
26	24	51	ASP	3.1
32	1a	1023	U	3.1
8	2I	72	LEU	3.1
26	14	52	THR	3.1
43	1l	64	TYR	3.1
53	2v	14	A	3.1
32	2a	1021	C	3.1
39	2h	128	GLY	3.1
50	2s	64	GLU	3.1
1	2A	2806	C	3.1
32	1a	72	C	3.1

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Mol	Chain	Res	Type	RSRZ
33	2b	31	TYR	3.1
33	2b	70	PHE	3.1
32	1a	1268	A	3.1
6	2G	25	TYR	3.1
20	2Y	5	MET	3.1
41	2j	89	ASP	3.1
34	1c	78	GLY	3.1
41	2j	38	ILE	3.1
1	1A	2905	U	3.0
40	2i	20	ARG	3.0
7	2H	82	GLY	3.0
1	2A	2804	G	3.0
44	2m	95	GLY	3.0
14	2S	20	ARG	3.0
33	2b	227	GLY	3.0
5	2F	14	PRO	3.0
7	2H	99	VAL	3.0
41	2j	85	LEU	3.0
1	1A	2812	G	3.0
50	2s	6	LYS	3.0
33	1b	122	PHE	3.0
1	1A	2206	C	3.0
49	1r	25	THR	3.0
1	1A	2811	A	3.0
33	2b	152	PHE	2.9
33	2b	150	SER	2.9
7	2H	101	ARG	2.9
11	2P	92	GLU	2.9
6	2G	26	GLN	2.9
40	2i	5	TYR	2.9
40	2i	87	GLN	2.9
1	2A	1149	C	2.9
40	2i	37	PHE	2.9
21	2Z	5	LEU	2.9
18	1W	111	HIS	2.9
45	2n	11	LYS	2.9
32	2a	986	C	2.9
32	1a	825	U	2.9
26	24	59	PHE	2.9
34	1c	160	ALA	2.9
1	1A	2806	C	2.9
1	2A	669	C	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	2b	232	PRO	2.9
41	2j	72	VAL	2.9
2	2B	118	G	2.9
40	2i	61	ALA	2.9
5	2F	15	SER	2.8
1	1A	934	C	2.8
32	1a	1026	C	2.8
6	1G	51	ARG	2.8
34	2c	159	GLY	2.8
40	1i	33	PHE	2.8
6	1G	49	ASP	2.8
40	2i	66	ARG	2.8
22	20	45	PHE	2.8
22	20	75	LEU	2.8
38	1g	77	SER	2.8
1	1A	1098	C	2.8
34	2c	197	GLY	2.8
50	2s	38	SER	2.8
33	1b	33	TYR	2.8
34	1c	201	TYR	2.8
32	1a	1239	U	2.8
7	2H	110	SER	2.8
34	2c	158	GLY	2.8
32	2a	985	C	2.8
8	2I	12	LEU	2.8
19	2X	68	ARG	2.8
40	1i	15	ALA	2.8
41	1j	97	GLU	2.8
50	2s	43	GLU	2.8
1	2A	1101	G	2.8
1	2A	1127	U	2.8
38	2g	81	GLY	2.8
50	2s	12	ASP	2.8
20	2Y	90	LEU	2.8
32	1a	985	C	2.8
1	2A	2121	G	2.8
45	1n	2	ALA	2.8
6	2G	27	ASN	2.7
32	2a	1023	U	2.7
40	1i	8	GLY	2.7
45	2n	8	GLU	2.7
45	2n	16	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	1104	G	2.7
12	2Q	60	ARG	2.7
22	20	76	GLY	2.7
32	2a	983	A	2.7
32	2a	999	U	2.7
52	2u	6	ARG	2.7
21	2Z	96	VAL	2.7
26	24	40	HIS	2.7
20	2Y	58	GLY	2.7
7	2H	96	ALA	2.7
26	24	44	THR	2.7
47	2p	19	ILE	2.7
34	2c	143	GLU	2.7
38	2g	6	ARG	2.7
23	11	2	SER	2.7
40	2i	6	GLY	2.7
50	2s	23	ASN	2.7
54	2x	47	U	2.7
39	2h	127	LEU	2.7
8	2l	85	GLU	2.7
26	14	57	GLU	2.7
40	2i	10	ARG	2.7
41	2j	74	ILE	2.7
33	1b	136	VAL	2.7
40	2i	53	VAL	2.7
51	1t	55	ILE	2.6
41	1j	90	LEU	2.6
20	2Y	42	VAL	2.6
40	2i	30	GLY	2.6
1	2A	1088	C	2.6
32	1a	977	C	2.6
49	2r	46	GLU	2.6
32	1a	1509	A	2.6
34	2c	77	ILE	2.6
2	2B	119	G	2.6
41	1j	71	LEU	2.6
1	2A	2900	A	2.6
18	1W	112	GLY	2.6
37	2f	97	PHE	2.6
41	2j	65	LEU	2.6
40	2i	72	GLY	2.6
41	1j	72	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
32	2a	1243	A	2.6
41	2j	67	THR	2.6
34	1c	39	ILE	2.6
42	2k	13	GLN	2.6
52	2u	22	ARG	2.6
40	1i	26	VAL	2.6
47	2p	59	TRP	2.6
33	2b	81	VAL	2.6
33	1b	188	ALA	2.6
50	2s	48	THR	2.6
1	1A	2805	G	2.6
32	2a	1022	C	2.6
32	2a	1026	C	2.6
33	2b	37	ASN	2.6
34	1c	63	ASN	2.6
8	2I	13	GLY	2.6
1	2A	1134	G	2.6
14	2S	34	HIS	2.6
32	1a	1121	G	2.6
32	2a	977	C	2.6
43	2l	64	TYR	2.6
38	1g	83	ALA	2.6
41	2j	98	ILE	2.5
35	1d	176	LEU	2.5
35	2d	183	GLY	2.5
1	2A	1131	A	2.5
32	1a	1022	C	2.5
40	2i	28	VAL	2.5
1	1A	2804	G	2.5
20	2Y	55	TYR	2.5
47	1p	19	ILE	2.5
26	24	52	THR	2.5
44	2m	60	VAL	2.5
1	2A	1103	G	2.5
7	2H	35	VAL	2.5
33	2b	122	PHE	2.5
50	2s	24	ALA	2.5
33	2b	78	GLN	2.5
48	2q	100	LYS	2.5
32	1a	77	G	2.5
38	2g	155	ARG	2.5
32	1a	999	U	2.5

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Mol	Chain	Res	Type	RSRZ
34	1c	64	VAL	2.5
6	2G	181	ARG	2.5
42	1k	13	GLN	2.5
32	2a	707	U	2.5
38	1g	153	HIS	2.5
52	2u	23	PRO	2.5
33	2b	118	LEU	2.5
33	2b	165	VAL	2.5
38	2g	75	VAL	2.5
40	2i	67	GLY	2.5
1	1A	695	C	2.5
1	2A	1120	C	2.5
32	1a	208	C	2.5
41	1j	4	ILE	2.5
41	1j	40	LEU	2.5
41	1j	85	LEU	2.5
43	2l	62	SER	2.5
8	2I	107	VAL	2.5
11	2P	90	ARG	2.5
34	1c	65	ALA	2.5
34	2c	146	ALA	2.5
1	1A	2904	C	2.5
6	2G	152	LEU	2.5
22	20	72	ARG	2.5
40	2i	17	VAL	2.5
44	2m	102	ARG	2.5
33	2b	188	ALA	2.5
42	2k	90	GLY	2.5
46	1o	20	GLY	2.5
41	2j	75	ILE	2.5
7	2H	116	GLU	2.4
32	1a	707	U	2.4
6	2G	137	GLU	2.4
1	2A	2901	G	2.4
49	2r	43	PHE	2.4
41	2j	27	ALA	2.4
35	2d	146	ILE	2.4
50	2s	20	LEU	2.4
1	2A	2817	U	2.4
32	1a	986	C	2.4
34	2c	205	GLY	2.4
40	2i	45	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	2c	185	GLY	2.4
1	1A	682	G	2.4
40	2i	68	GLY	2.4
14	2S	84	GLN	2.4
32	2a	1159	G	2.4
34	1c	87	LEU	2.4
44	2m	75	ALA	2.4
33	2b	214	ILE	2.4
45	2n	53	LEU	2.4
34	1c	184	TYR	2.4
34	2c	180	ALA	2.4
1	1A	33	C	2.4
33	1b	222	ILE	2.4
20	2Y	45	VAL	2.4
20	2Y	59	GLY	2.4
33	2b	134	GLU	2.4
40	2i	92	TYR	2.4
1	2A	2905	U	2.4
24	22	1	MET	2.4
1	2A	1135	U	2.3
32	1a	212	G	2.3
32	1a	984	A	2.3
50	1s	40	ILE	2.3
1	2A	2206	C	2.3
32	1a	87	C	2.3
21	2Z	56	VAL	2.3
25	23	59	VAL	2.3
19	2X	69	TYR	2.3
38	2g	18	TYR	2.3
39	2h	101	PRO	2.3
21	2Z	93	ASP	2.3
40	2i	4	TYR	2.3
41	2j	8	LEU	2.3
50	2s	65	ASN	2.3
51	1t	9	ASN	2.3
33	2b	33	TYR	2.3
6	1G	48	GLU	2.3
26	24	57	GLU	2.3
41	1j	96	ILE	2.3
26	14	49	PHE	2.3
32	2a	79	G	2.3
32	2a	976	G	2.3

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Mol	Chain	Res	Type	RSRZ
35	2d	184	LYS	2.3
8	2I	19	VAL	2.3
34	2c	153	VAL	2.3
38	2g	16	LEU	2.3
1	2A	2207	G	2.3
11	2P	85	LEU	2.3
33	1b	225	ALA	2.3
40	2i	99	LEU	2.3
45	2n	36	PHE	2.3
7	2H	43	VAL	2.3
1	1A	2204	C	2.3
1	2A	2125	G	2.3
32	2a	984	A	2.3
7	2H	87	LEU	2.3
33	1b	123	ALA	2.3
35	1d	120	LEU	2.3
38	2g	85	TYR	2.3
49	2r	58	LEU	2.3
29	27	46	VAL	2.3
6	2G	2	PRO	2.3
1	2A	5	A	2.3
1	2A	1553	A	2.3
32	2a	1432	A	2.3
34	2c	87	LEU	2.3
7	2H	44	VAL	2.3
25	23	60	GLU	2.3
1	2A	2903	U	2.3
29	27	47	ARG	2.3
25	23	26	LEU	2.3
34	2c	155	GLY	2.3
32	2a	1257	A	2.3
1	2A	2208	G	2.3
45	1n	8	GLU	2.3
6	2G	17	PRO	2.2
24	22	8	LYS	2.2
34	1c	206	GLU	2.2
8	2I	81	VAL	2.2
50	2s	45	VAL	2.2
32	2a	1001	G	2.2
33	2b	228	GLY	2.2
49	2r	66	LEU	2.2
14	2S	40	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	1A	2209	C	2.2
6	2G	28	VAL	2.2
6	2G	160	VAL	2.2
40	1i	28	VAL	2.2
20	2Y	81	LYS	2.2
45	1n	17	LYS	2.2
44	2m	63	THR	2.2
1	2A	1087	G	2.2
40	2i	128	ARG	2.2
1	2A	1124	C	2.2
40	2i	26	VAL	2.2
32	1a	86	U	2.2
5	1F	14	PRO	2.2
6	1G	50	ALA	2.2
33	1b	131	PRO	2.2
35	2d	49	ARG	2.2
1	2A	698	C	2.2
32	2a	998	C	2.2
26	24	54	GLY	2.2
34	1c	80	GLY	2.2
32	1a	1027	A	2.2
40	2i	63	ILE	2.2
49	1r	29	PHE	2.2
52	2u	8	THR	2.2
1	2A	1092	G	2.2
52	1u	18	TYR	2.2
6	2G	49	ASP	2.2
34	2c	204	LEU	2.2
38	2g	115	ARG	2.2
46	1o	88	ARG	2.2
33	2b	123	ALA	2.2
40	1i	81	ILE	2.2
44	2m	76	ALA	2.2
50	2s	76	PRO	2.2
55	2z	12	PRO	2.2
7	2H	108	GLY	2.2
32	2a	1184	G	2.2
49	2r	57	GLY	2.2
1	2A	1106	U	2.2
53	1v	14	A	2.2
35	1d	133	VAL	2.2
49	1r	21	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
14	2S	22	GLY	2.2
32	1a	1000	G	2.2
47	1p	68	ASP	2.2
38	2g	88	PRO	2.2
7	2H	52	VAL	2.2
33	1b	114	ARG	2.2
44	2m	94	ARG	2.2
11	2P	88	LEU	2.1
1	2A	1126	U	2.1
31	29	5	ALA	2.1
40	2i	82	ALA	2.1
49	2r	24	ALA	2.1
26	24	66	SER	2.1
14	2S	45	GLY	2.1
23	21	28	GLY	2.1
24	22	63	VAL	2.1
32	2a	209	U	2.1
50	2s	28	LYS	2.1
15	1T	38	ASN	2.1
33	1b	232	PRO	2.1
7	2H	56	SER	2.1
32	2a	78	G	2.1
20	2Y	46	LYS	2.1
1	2A	1090	A	2.1
32	1a	139	G	2.1
33	1b	190	THR	2.1
26	24	25	TYR	2.1
4	2E	1	MET	2.1
22	20	73	GLY	2.1
39	2h	131	GLY	2.1
34	2c	42	LEU	2.1
42	2k	125	PHE	2.1
47	1p	39	TYR	2.1
32	1a	71	G	2.1
34	2c	8	ILE	2.1
41	2j	26	ALA	2.1
45	2n	42	ILE	2.1
38	2g	130	GLY	2.1
32	1a	88	C	2.1
45	2n	37	PHE	2.1
1	2A	1071	U	2.1
14	2S	35	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
33	2b	201	ILE	2.1
1	1A	679	G	2.1
34	2c	179	ARG	2.1
40	2i	127	LYS	2.1
20	2Y	65	ALA	2.1
34	1c	100	ALA	2.1
45	2n	2	ALA	2.1
40	1i	65	VAL	2.1
40	1i	90	PRO	2.1
16	2U	116	ALA	2.1
41	2j	34	VAL	2.1
45	2n	56	VAL	2.1
49	2r	21	LYS	2.1
1	2A	934	C	2.0
1	2A	1102	A	2.0
33	2b	97	TRP	2.0
21	2Z	4	ARG	2.0
26	24	62	ARG	2.0
33	1b	29	ALA	2.0
49	1r	31	LEU	2.0
3	2D	273	ARG	2.0
1	1A	1150	U	2.0
7	2H	164	TYR	2.0
34	2c	167	TRP	2.0
34	2c	184	TYR	2.0
50	2s	52	TYR	2.0
11	2P	122	PRO	2.0
41	2j	23	ILE	2.0
43	2l	28	LYS	2.0
1	2A	9	G	2.0
32	2a	1002	G	2.0
32	2a	1266	C	2.0
35	1d	165	MET	2.0
6	2G	136	ARG	2.0
16	2U	117	GLN	2.0
21	2Z	65	GLN	2.0
41	1j	78	ASN	2.0
21	2Z	133	ILE	2.0
52	2u	13	ILE	2.0
7	1H	2	SER	2.0
32	1a	210	U	2.0
1	1A	2203	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	2A	10	G	2.0
1	2A	2122	G	2.0
7	2H	131	VAL	2.0
20	2Y	2	ARG	2.0
52	2u	15	ARG	2.0
45	2n	47	LEU	2.0
50	2s	59	PRO	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	PSU	2x	55	20/21	0.85	0.14	-	67,79,90,98	0
54	5MU	2x	54	21/22	0.93	0.18	-	66,79,92,102	0
54	PSU	1x	55	20/21	0.95	0.15	-	49,60,75,77	0
54	5MC	2x	32	21/22	0.93	0.20	-	72,77,87,99	0
54	4SU	1x	8	20/21	0.96	0.13	-	51,58,69,71	0
54	5MU	1x	54	21/22	0.96	0.13	-	48,57,75,82	0
54	5MC	1x	32	21/22	0.96	0.16	-	50,57,66,75	0
54	4SU	2x	8	20/21	0.92	0.11	-	68,80,91,95	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1q	201	1/1	0.97	0.67	65.88	68,68,68,68	0
56	MG	2A	3099	1/1	0.94	0.51	61.45	45,45,45,45	0
56	MG	2a	3026	1/1	0.90	0.80	57.46	72,72,72,72	0
56	MG	1A	3108	1/1	0.95	0.49	56.24	49,49,49,49	0
56	MG	1A	3942	1/1	0.98	0.40	51.24	34,34,34,34	0
56	MG	2A	3564	1/1	0.96	0.46	51.16	34,34,34,34	0
56	MG	2E	304	1/1	0.93	0.68	51.15	74,74,74,74	0
56	MG	1A	3463	1/1	0.81	0.47	48.41	53,53,53,53	0
56	MG	1A	3214	1/1	0.96	0.37	45.61	34,34,34,34	0
56	MG	1A	4026	1/1	0.93	0.63	43.51	41,41,41,41	0
56	MG	1A	3867	1/1	0.94	0.56	40.82	40,40,40,40	0
56	MG	1A	3033	1/1	0.96	0.45	40.45	47,47,47,47	0
56	MG	1E	303	1/1	0.90	0.55	39.65	51,51,51,51	0
56	MG	1A	3166	1/1	0.94	0.41	38.10	47,47,47,47	0
56	MG	1A	3988	1/1	0.89	0.62	37.05	38,38,38,38	0
56	MG	1A	3442	1/1	0.86	0.84	35.68	57,57,57,57	0
56	MG	1A	3465	1/1	0.98	0.33	35.53	36,36,36,36	0
56	MG	2a	3205	1/1	0.85	0.68	35.39	78,78,78,78	0
56	MG	1A	3858	1/1	0.81	0.36	34.66	52,52,52,52	0
56	MG	2a	3119	1/1	0.73	0.57	32.76	62,62,62,62	0
56	MG	2a	3116	1/1	0.96	0.42	31.44	51,51,51,51	0
56	MG	2A	3441	1/1	0.84	0.29	29.40	51,51,51,51	0
56	MG	2A	3419	1/1	0.95	0.37	28.58	51,51,51,51	0
56	MG	2A	3413	1/1	0.95	0.29	27.28	44,44,44,44	0
56	MG	1A	3277	1/1	0.41	0.53	26.92	68,68,68,68	0
56	MG	2A	3106	1/1	0.96	0.38	26.80	33,33,33,33	0
56	MG	1A	3123	1/1	0.93	0.27	26.38	25,25,25,25	0
56	MG	1A	3004	1/1	0.90	0.44	26.30	44,44,44,44	0
56	MG	1U	203	1/1	0.92	0.72	26.16	40,40,40,40	0
56	MG	1a	1820	1/1	0.86	0.43	25.41	82,82,82,82	0
56	MG	1A	4032	1/1	0.93	0.62	25.25	47,47,47,47	0
56	MG	1N	202	1/1	0.86	0.68	25.09	49,49,49,49	0
56	MG	2A	3055	1/1	0.97	0.61	24.04	46,46,46,46	0
56	MG	1A	3532	1/1	0.91	0.31	23.94	43,43,43,43	0
56	MG	1A	3352	1/1	0.96	0.40	23.80	49,49,49,49	0
56	MG	2A	3042	1/1	0.96	0.30	23.45	50,50,50,50	0
56	MG	1A	3796	1/1	0.98	0.56	23.13	42,42,42,42	0
56	MG	2A	3141	1/1	0.99	0.34	22.91	35,35,35,35	0
56	MG	2A	3159	1/1	0.97	0.28	22.67	31,31,31,31	0
56	MG	2A	3091	1/1	0.95	0.36	22.56	37,37,37,37	0
56	MG	1A	4044	1/1	0.95	0.61	22.43	39,39,39,39	0
56	MG	1A	3115	1/1	0.88	0.39	22.40	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3881	1/1	0.85	0.26	22.22	63,63,63,63	0
56	MG	1A	3528	1/1	0.93	0.45	21.27	54,54,54,54	0
56	MG	1A	3263	1/1	0.94	0.38	21.22	56,56,56,56	0
56	MG	1A	3498	1/1	0.95	0.55	21.12	50,50,50,50	0
56	MG	1A	4010	1/1	0.90	0.38	20.69	58,58,58,58	0
56	MG	2A	3340	1/1	0.97	0.34	20.67	51,51,51,51	0
56	MG	1A	3303	1/1	0.81	0.48	20.53	48,48,48,48	0
56	MG	2A	3062	1/1	0.88	0.25	20.51	33,33,33,33	0
56	MG	2P	201	1/1	0.92	0.26	20.38	33,33,33,33	0
56	MG	2A	3238	1/1	0.97	0.40	20.35	48,48,48,48	0
56	MG	2A	3207	1/1	0.94	0.28	20.19	23,23,23,23	0
56	MG	2A	3146	1/1	0.91	0.30	20.05	41,41,41,41	0
56	MG	1A	3147	1/1	0.87	0.27	19.64	49,49,49,49	0
56	MG	2A	3232	1/1	0.98	0.26	19.41	38,38,38,38	0
56	MG	1a	1882	1/1	0.90	0.31	19.34	55,55,55,55	0
56	MG	1A	3107	1/1	0.99	0.48	19.33	50,50,50,50	0
56	MG	2A	3342	1/1	0.98	0.31	19.30	46,46,46,46	0
56	MG	2A	3394	1/1	0.88	0.33	19.14	61,61,61,61	0
56	MG	2A	3309	1/1	0.93	0.29	19.05	44,44,44,44	0
56	MG	2A	3552	1/1	0.95	0.34	18.68	50,50,50,50	0
56	MG	1A	3240	1/1	0.84	0.43	18.37	48,48,48,48	0
56	MG	1F	305	1/1	0.95	0.45	18.26	28,28,28,28	0
56	MG	1D	316	1/1	0.94	0.49	18.18	76,76,76,76	0
56	MG	2A	3430	1/1	0.90	0.24	17.92	57,57,57,57	0
56	MG	1A	4031	1/1	0.83	0.63	17.89	54,54,54,54	0
56	MG	2a	3225	1/1	0.93	0.49	17.88	67,67,67,67	0
56	MG	2A	3053	1/1	0.91	0.40	17.83	49,49,49,49	0
56	MG	2A	3254	1/1	0.99	0.34	17.56	60,60,60,60	0
56	MG	2A	3222	1/1	0.97	0.30	17.52	45,45,45,45	0
56	MG	1A	3030	1/1	0.98	0.44	17.34	52,52,52,52	0
56	MG	2A	3572	1/1	0.82	0.37	16.99	61,61,61,61	0
56	MG	1A	4036	1/1	0.87	0.50	16.98	44,44,44,44	0
56	MG	2E	303	1/1	0.84	0.37	16.83	53,53,53,53	0
56	MG	1a	1670	1/1	0.84	0.41	16.75	60,60,60,60	0
56	MG	1A	3121	1/1	0.93	0.42	16.74	42,42,42,42	0
56	MG	2A	3233	1/1	0.94	0.27	16.63	62,62,62,62	0
56	MG	2A	3200	1/1	0.87	0.25	16.62	41,41,41,41	0
56	MG	2A	3550	1/1	0.92	0.45	16.41	37,37,37,37	0
56	MG	1A	4029	1/1	0.96	0.59	16.38	40,40,40,40	0
56	MG	1A	3189	1/1	0.97	0.41	16.24	28,28,28,28	0
56	MG	2A	3009	1/1	0.91	0.58	15.96	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3789	1/1	0.94	0.34	15.72	31,31,31,31	0
56	MG	1A	4011	1/1	0.94	0.37	15.67	48,48,48,48	0
56	MG	1h	3003	1/1	0.83	0.34	15.61	79,79,79,79	0
56	MG	1A	3152	1/1	0.94	0.34	15.55	50,50,50,50	0
56	MG	1A	3211	1/1	0.96	0.43	15.47	46,46,46,46	0
56	MG	1F	302	1/1	0.89	0.29	15.39	56,56,56,56	0
56	MG	2A	3102	1/1	0.95	0.29	15.17	41,41,41,41	0
56	MG	2V	201	1/1	0.96	0.66	15.11	51,51,51,51	0
56	MG	2A	3185	1/1	0.96	0.47	15.03	43,43,43,43	0
56	MG	2A	3093	1/1	0.79	0.30	14.97	64,64,64,64	0
56	MG	2A	3522	1/1	0.92	0.24	14.92	39,39,39,39	0
56	MG	1A	3016	1/1	0.94	0.32	14.83	49,49,49,49	0
56	MG	1P	204	1/1	0.99	0.38	14.68	31,31,31,31	0
56	MG	1A	3434	1/1	0.97	0.41	14.64	41,41,41,41	0
56	MG	2A	3272	1/1	0.96	0.25	14.28	61,61,61,61	0
56	MG	1a	1730	1/1	0.96	0.31	13.96	49,49,49,49	0
56	MG	1P	205	1/1	0.97	0.44	13.88	49,49,49,49	0
56	MG	1A	3418	1/1	0.94	0.39	13.68	43,43,43,43	0
56	MG	1A	4003	1/1	0.95	0.29	13.59	24,24,24,24	0
56	MG	1N	207	1/1	0.98	0.48	13.48	45,45,45,45	0
56	MG	2A	3221	1/1	0.91	0.32	13.31	35,35,35,35	0
56	MG	1a	1831	1/1	0.97	0.23	13.30	63,63,63,63	0
56	MG	1A	3170	1/1	0.91	0.28	13.21	32,32,32,32	0
56	MG	1A	3053	1/1	0.90	0.44	13.03	38,38,38,38	0
56	MG	1A	3267	1/1	0.93	0.35	13.02	57,57,57,57	0
56	MG	2A	3305	1/1	0.89	0.29	13.01	38,38,38,38	0
56	MG	1A	3346	1/1	0.91	0.36	12.91	33,33,33,33	0
56	MG	1U	204	1/1	0.96	0.48	12.86	44,44,44,44	0
56	MG	2A	3060	1/1	0.93	0.25	12.81	42,42,42,42	0
56	MG	2a	3022	1/1	0.70	0.23	12.77	70,70,70,70	0
56	MG	2A	3194	1/1	0.96	0.30	12.58	45,45,45,45	0
56	MG	1A	3534	1/1	0.97	0.31	12.56	65,65,65,65	0
56	MG	2A	3184	1/1	0.94	0.26	12.49	59,59,59,59	0
56	MG	2A	3046	1/1	0.89	0.34	12.43	62,62,62,62	0
56	MG	1A	3419	1/1	0.88	0.30	12.37	52,52,52,52	0
56	MG	1A	3737	1/1	0.94	0.23	12.35	29,29,29,29	0
56	MG	1A	3128	1/1	0.95	0.37	12.33	49,49,49,49	0
56	MG	1A	3896	1/1	0.94	0.29	12.21	32,32,32,32	0
56	MG	1A	3103	1/1	0.94	0.42	12.09	41,41,41,41	0
56	MG	2A	3219	1/1	0.90	0.36	11.86	38,38,38,38	0
56	MG	1a	1671	1/1	0.87	0.29	11.78	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3344	1/1	0.96	0.25	11.78	32,32,32,32	0
56	MG	2a	3089	1/1	0.82	0.37	11.74	75,75,75,75	0
56	MG	1A	4001	1/1	0.85	0.34	11.72	52,52,52,52	0
56	MG	1A	3452	1/1	0.94	0.25	11.70	42,42,42,42	0
56	MG	1D	304	1/1	0.96	0.46	11.54	50,50,50,50	0
56	MG	2A	3121	1/1	0.88	0.25	11.52	42,42,42,42	0
56	MG	2a	3234	1/1	0.90	0.57	11.39	79,79,79,79	0
56	MG	2A	3576	1/1	0.93	0.49	11.36	50,50,50,50	0
56	MG	1A	3106	1/1	0.99	0.24	11.34	26,26,26,26	0
56	MG	2A	3379	1/1	0.97	0.25	11.33	42,42,42,42	0
56	MG	2A	3142	1/1	0.98	0.28	11.32	39,39,39,39	0
56	MG	2A	3225	1/1	0.91	0.28	11.14	42,42,42,42	0
56	MG	1A	3943	1/1	0.83	0.31	11.08	35,35,35,35	0
56	MG	2A	3181	1/1	0.98	0.30	11.04	43,43,43,43	0
56	MG	2A	3139	1/1	0.89	0.31	11.02	47,47,47,47	0
56	MG	2A	3520	1/1	0.96	0.27	10.76	75,75,75,75	0
56	MG	1A	3102	1/1	0.97	0.28	10.74	37,37,37,37	0
56	MG	2a	3178	1/1	0.77	0.31	10.69	75,75,75,75	0
56	MG	1a	1722	1/1	0.92	0.31	10.67	60,60,60,60	0
56	MG	1Q	3002	1/1	0.96	0.33	10.57	38,38,38,38	0
56	MG	2A	3191	1/1	0.98	0.20	10.57	45,45,45,45	0
56	MG	1a	1707	1/1	0.96	0.28	10.51	46,46,46,46	0
56	MG	2A	3038	1/1	0.97	0.27	10.47	50,50,50,50	0
56	MG	1A	3221	1/1	0.91	0.27	10.32	56,56,56,56	0
56	MG	1a	1727	1/1	0.96	0.26	10.26	39,39,39,39	0
56	MG	2A	3300	1/1	0.94	0.23	10.24	42,42,42,42	0
56	MG	1A	3511	1/1	0.92	0.32	10.23	51,51,51,51	0
56	MG	2A	3390	1/1	0.89	0.26	10.20	63,63,63,63	0
56	MG	1A	3995	1/1	0.96	0.26	10.19	10,10,10,10	0
56	MG	2A	3420	1/1	0.94	0.29	10.19	59,59,59,59	0
56	MG	2A	3411	1/1	0.96	0.25	10.18	39,39,39,39	0
56	MG	1A	3809	1/1	0.97	0.25	10.01	40,40,40,40	0
56	MG	2A	3547	1/1	0.94	0.34	10.01	37,37,37,37	0
56	MG	1U	205	1/1	0.97	0.42	10.00	43,43,43,43	0
56	MG	2a	3233	1/1	0.70	0.36	9.95	66,66,66,66	0
56	MG	1A	3560	1/1	0.97	0.27	9.93	24,24,24,24	0
56	MG	2a	3117	1/1	0.95	0.39	9.66	68,68,68,68	0
56	MG	1A	3098	1/1	0.74	0.23	9.45	71,71,71,71	0
56	MG	2a	3212	1/1	0.94	0.34	9.45	56,56,56,56	0
56	MG	1A	3582	1/1	0.95	0.23	9.41	44,44,44,44	0
56	MG	1A	3231	1/1	0.92	0.40	9.39	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1880	1/1	0.97	0.21	9.31	50,50,50,50	0
56	MG	1W	3006	1/1	0.92	0.40	9.31	42,42,42,42	0
56	MG	2a	3099	1/1	0.82	0.46	9.30	63,63,63,63	0
56	MG	1A	4013	1/1	0.96	0.34	8.82	47,47,47,47	0
56	MG	1D	313	1/1	0.97	0.38	8.74	44,44,44,44	0
56	MG	2A	3402	1/1	0.97	0.23	8.62	55,55,55,55	0
56	MG	2A	3148	1/1	0.84	0.26	8.57	41,41,41,41	0
56	MG	2A	3014	1/1	0.85	0.20	8.56	44,44,44,44	0
56	MG	2a	3005	1/1	0.97	0.43	8.46	51,51,51,51	0
56	MG	2A	3450	1/1	0.95	0.33	8.41	52,52,52,52	0
56	MG	1A	3062	1/1	0.84	0.32	8.37	57,57,57,57	0
56	MG	1A	3092	1/1	0.97	0.24	8.20	40,40,40,40	0
56	MG	1A	3521	1/1	0.96	0.23	8.16	46,46,46,46	0
56	MG	1a	1604	1/1	0.84	0.27	8.13	70,70,70,70	0
56	MG	2A	3049	1/1	0.97	0.21	8.10	33,33,33,33	0
56	MG	1a	1643	1/1	0.86	0.20	8.03	52,52,52,52	0
56	MG	1A	3118	1/1	0.97	0.27	8.02	20,20,20,20	0
56	MG	2A	3267	1/1	0.89	0.22	7.99	63,63,63,63	0
56	MG	2A	3308	1/1	0.99	0.25	7.86	41,41,41,41	0
56	MG	2B	3005	1/1	0.97	0.24	7.85	51,51,51,51	0
56	MG	1A	3769	1/1	0.97	0.22	7.83	37,37,37,37	0
56	MG	1A	3987	1/1	0.95	0.22	7.79	35,35,35,35	0
56	MG	1A	3210	1/1	0.90	0.27	7.77	46,46,46,46	0
56	MG	2a	3097	1/1	0.98	0.31	7.72	47,47,47,47	0
56	MG	1A	3464	1/1	0.95	0.24	7.69	43,43,43,43	0
56	MG	1A	3617	1/1	0.97	0.20	7.65	28,28,28,28	0
56	MG	2A	3410	1/1	0.91	0.24	7.64	40,40,40,40	0
56	MG	2A	3163	1/1	0.96	0.24	7.63	64,64,64,64	0
56	MG	1A	3094	1/1	0.98	0.25	7.56	24,24,24,24	0
56	MG	2A	3317	1/1	0.92	0.25	7.54	40,40,40,40	0
56	MG	1R	205	1/1	0.91	0.39	7.46	52,52,52,52	0
56	MG	1F	301	1/1	0.96	0.24	7.36	39,39,39,39	0
56	MG	2A	3386	1/1	0.88	0.26	7.26	57,57,57,57	0
56	MG	1A	3945	1/1	0.96	0.31	7.23	30,30,30,30	0
56	MG	2A	3567	1/1	0.96	0.20	7.22	54,54,54,54	0
56	MG	1a	1833	1/1	0.93	0.24	7.21	47,47,47,47	0
56	MG	1a	1860	1/1	0.93	0.40	7.15	61,61,61,61	0
56	MG	2n	502	1/1	0.94	0.61	7.14	73,73,73,73	0
56	MG	1A	3998	1/1	0.94	0.33	7.06	51,51,51,51	0
56	MG	1a	1903	1/1	0.99	0.31	7.06	56,56,56,56	0
56	MG	1A	3175	1/1	0.98	0.23	7.05	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3239	1/1	0.93	0.43	7.02	60,60,60,60	0
56	MG	1A	3651	1/1	0.93	0.23	7.02	25,25,25,25	0
56	MG	2A	3376	1/1	0.97	0.26	6.95	29,29,29,29	0
56	MG	1A	3611	1/1	0.95	0.24	6.86	28,28,28,28	0
56	MG	1A	3900	1/1	0.86	0.39	6.85	42,42,42,42	0
56	MG	1a	1847	1/1	0.83	0.25	6.85	54,54,54,54	0
56	MG	1A	4022	1/1	0.98	0.43	6.82	66,66,66,66	0
56	MG	1A	3638	1/1	0.91	0.24	6.81	22,22,22,22	0
56	MG	1a	1701	1/1	0.91	0.24	6.74	50,50,50,50	0
56	MG	17	101	1/1	0.97	0.36	6.67	34,34,34,34	0
56	MG	1E	306	1/1	0.95	0.22	6.64	74,74,74,74	0
56	MG	1A	3001	1/1	0.86	0.22	6.62	45,45,45,45	0
56	MG	1A	3561	1/1	0.94	0.27	6.58	34,34,34,34	0
56	MG	1A	3209	1/1	0.90	0.30	6.55	41,41,41,41	0
56	MG	1A	3685	1/1	0.98	0.20	6.53	47,47,47,47	0
56	MG	1B	211	1/1	0.91	0.31	6.46	54,54,54,54	0
56	MG	1A	3193	1/1	0.97	0.22	6.43	20,20,20,20	0
56	MG	2D	304	1/1	0.98	0.40	6.43	34,34,34,34	0
56	MG	2A	3311	1/1	0.92	0.20	6.41	44,44,44,44	0
56	MG	1A	4037	1/1	0.91	0.26	6.37	62,62,62,62	0
56	MG	2A	3513	1/1	0.95	0.19	6.34	38,38,38,38	0
56	MG	2A	3231	1/1	0.91	0.17	6.28	53,53,53,53	0
56	MG	2A	3256	1/1	0.76	0.17	6.22	79,79,79,79	0
56	MG	1A	3119	1/1	0.98	0.24	6.15	35,35,35,35	0
56	MG	1U	202	1/1	0.95	0.32	6.11	43,43,43,43	0
56	MG	1A	3026	1/1	0.97	0.35	6.08	36,36,36,36	0
56	MG	2A	3400	1/1	0.95	0.18	6.08	31,31,31,31	0
56	MG	1A	3767	1/1	0.98	0.24	6.07	21,21,21,21	0
56	MG	2A	3011	1/1	0.99	0.35	6.01	42,42,42,42	0
56	MG	1A	3190	1/1	0.94	0.25	5.99	59,59,59,59	0
56	MG	1A	3570	1/1	0.98	0.21	5.89	18,18,18,18	0
56	MG	1A	3172	1/1	0.97	0.29	5.85	32,32,32,32	0
56	MG	1A	3766	1/1	0.95	0.23	5.84	49,49,49,49	0
56	MG	2A	3331	1/1	0.89	0.20	5.79	36,36,36,36	0
56	MG	2A	3500	1/1	0.78	0.21	5.75	57,57,57,57	0
56	MG	1Q	3004	1/1	0.92	0.43	5.73	46,46,46,46	0
56	MG	1A	3150	1/1	0.95	0.25	5.72	40,40,40,40	0
56	MG	1a	1719	1/1	0.94	0.21	5.62	47,47,47,47	0
56	MG	2A	3114	1/1	0.94	0.17	5.57	34,34,34,34	0
56	MG	1A	3095	1/1	0.92	0.22	5.54	41,41,41,41	0
56	MG	2A	3201	1/1	0.92	0.20	5.44	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3297	1/1	0.90	0.19	5.42	49,49,49,49	0
56	MG	2A	3092	1/1	0.95	0.23	5.42	55,55,55,55	0
56	MG	1A	3457	1/1	0.90	0.29	5.37	48,48,48,48	0
56	MG	1A	3583	1/1	0.96	0.20	5.37	33,33,33,33	0
56	MG	1A	3146	1/1	0.86	0.27	5.37	43,43,43,43	0
56	MG	1A	4040	1/1	0.95	0.34	5.31	35,35,35,35	0
56	MG	1a	1839	1/1	0.96	0.23	5.20	62,62,62,62	0
56	MG	1A	3075	1/1	0.81	0.33	5.16	60,60,60,60	0
56	MG	1a	1751	1/1	0.93	0.24	5.14	63,63,63,63	0
56	MG	2A	3147	1/1	0.98	0.19	5.12	33,33,33,33	0
56	MG	1a	1662	1/1	0.96	0.28	5.11	73,73,73,73	0
56	MG	1A	3610	1/1	0.95	0.21	5.07	33,33,33,33	0
56	MG	1A	4041	1/1	0.87	0.28	5.07	39,39,39,39	0
56	MG	1a	1811	1/1	0.91	0.30	5.06	71,71,71,71	0
56	MG	2a	3125	1/1	0.83	0.22	5.06	66,66,66,66	0
56	MG	1A	4017	1/1	0.92	0.28	5.04	41,41,41,41	0
56	MG	1E	309	1/1	0.96	0.27	4.96	32,32,32,32	0
56	MG	2a	3129	1/1	0.78	0.21	4.91	73,73,73,73	0
56	MG	2a	3090	1/1	0.92	0.22	4.91	60,60,60,60	0
56	MG	1A	3373	1/1	0.98	0.23	4.89	49,49,49,49	0
56	MG	1Q	3006	1/1	0.96	0.30	4.87	48,48,48,48	0
56	MG	1a	1822	1/1	0.93	0.17	4.81	74,74,74,74	0
56	MG	1a	1694	1/1	0.88	0.18	4.80	41,41,41,41	0
56	MG	2A	3111	1/1	0.94	0.48	4.78	62,62,62,62	0
56	MG	2A	3574	1/1	0.89	0.29	4.74	53,53,53,53	0
56	MG	1A	3700	1/1	0.88	0.26	4.74	37,37,37,37	0
56	MG	1A	3302	1/1	0.99	0.21	4.73	33,33,33,33	0
56	MG	1A	3905	1/1	0.95	0.20	4.73	39,39,39,39	0
56	MG	1a	1886	1/1	0.96	0.22	4.72	53,53,53,53	0
56	MG	1A	3891	1/1	0.95	0.23	4.67	51,51,51,51	0
56	MG	28	8001	1/1	0.90	0.39	4.67	56,56,56,56	0
56	MG	1A	3076	1/1	0.97	0.22	4.66	42,42,42,42	0
56	MG	1A	3991	1/1	0.91	0.25	4.62	53,53,53,53	0
56	MG	1A	3169	1/1	0.99	0.26	4.49	41,41,41,41	0
56	MG	2A	3264	1/1	0.98	0.22	4.48	65,65,65,65	0
56	MG	1A	3002	1/1	0.88	0.23	4.43	43,43,43,43	0
56	MG	1B	206	1/1	0.88	0.21	4.40	38,38,38,38	0
56	MG	2A	3176	1/1	0.98	0.28	4.39	44,44,44,44	0
56	MG	2A	3304	1/1	0.90	0.18	4.33	40,40,40,40	0
56	MG	2A	3203	1/1	0.93	0.21	4.33	58,58,58,58	0
56	MG	1A	3540	1/1	0.96	0.21	4.32	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3123	1/1	0.91	0.18	4.28	57,57,57,57	0
56	MG	1A	3215	1/1	0.94	0.21	4.22	26,26,26,26	0
56	MG	2A	3368	1/1	0.97	0.23	4.21	63,63,63,63	0
56	MG	2A	3274	1/1	0.95	0.21	4.06	47,47,47,47	0
56	MG	2A	3160	1/1	0.96	0.17	4.04	42,42,42,42	0
56	MG	2A	3089	1/1	0.89	0.20	4.01	45,45,45,45	0
56	MG	2A	3334	1/1	0.92	0.16	3.99	44,44,44,44	0
56	MG	1D	303	1/1	0.92	0.24	3.94	47,47,47,47	0
56	MG	1e	203	1/1	0.98	0.33	3.93	76,76,76,76	0
56	MG	2A	3377	1/1	0.90	0.18	3.89	21,21,21,21	0
56	MG	1A	3601	1/1	0.92	0.23	3.87	28,28,28,28	0
56	MG	2a	3177	1/1	0.99	0.22	3.84	52,52,52,52	0
56	MG	2A	3409	1/1	0.95	0.20	3.81	59,59,59,59	0
56	MG	2A	3036	1/1	0.91	0.23	3.81	35,35,35,35	0
56	MG	1a	1607	1/1	0.88	0.29	3.78	66,66,66,66	0
56	MG	2A	3568	1/1	0.96	0.34	3.78	43,43,43,43	0
56	MG	1t	3001	1/1	0.87	0.40	3.77	64,64,64,64	0
56	MG	1A	4000	1/1	0.93	0.26	3.75	54,54,54,54	0
56	MG	1D	310	1/1	0.96	0.27	3.74	33,33,33,33	0
56	MG	2A	3553	1/1	0.98	0.26	3.73	35,35,35,35	0
56	MG	1a	1661	1/1	0.90	0.23	3.72	57,57,57,57	0
56	MG	2A	3315	1/1	0.97	0.20	3.69	40,40,40,40	0
56	MG	2A	3296	1/1	0.93	0.21	3.65	39,39,39,39	0
56	MG	2A	3173	1/1	0.92	0.22	3.62	49,49,49,49	0
56	MG	2A	3482	1/1	0.91	0.21	3.61	63,63,63,63	0
56	MG	1A	3718	1/1	0.98	0.23	3.58	18,18,18,18	0
56	MG	2a	3130	1/1	0.96	0.30	3.51	58,58,58,58	0
56	MG	2A	3266	1/1	0.95	0.19	3.48	54,54,54,54	0
56	MG	2A	3182	1/1	0.96	0.20	3.43	37,37,37,37	0
56	MG	2A	3443	1/1	0.90	0.16	3.39	52,52,52,52	0
56	MG	1A	3279	1/1	0.80	0.25	3.38	46,46,46,46	0
56	MG	2A	3387	1/1	0.92	0.15	3.29	51,51,51,51	0
56	MG	1a	1602	1/1	0.92	0.24	3.24	51,51,51,51	0
56	MG	1A	3605	1/1	0.92	0.23	3.18	35,35,35,35	0
56	MG	1A	3738	1/1	0.93	0.22	3.15	18,18,18,18	0
56	MG	1a	1672	1/1	0.91	0.21	3.15	61,61,61,61	0
56	MG	1A	3569	1/1	0.88	0.25	3.15	25,25,25,25	0
56	MG	1A	3596	1/1	0.94	0.19	3.14	53,53,53,53	0
56	MG	2A	3189	1/1	0.86	0.23	3.12	61,61,61,61	0
56	MG	1A	4049	1/1	0.89	0.26	3.12	57,57,57,57	0
56	MG	1r	3001	1/1	0.85	0.22	3.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3573	1/1	0.85	0.21	3.08	42,42,42,42	0
56	MG	2A	3582	1/1	0.87	0.17	3.07	50,50,50,50	0
56	MG	1A	3719	1/1	0.98	0.21	3.03	7,7,7,7	0
56	MG	1D	308	1/1	0.97	0.20	3.02	13,13,13,13	0
56	MG	2a	3013	1/1	0.86	0.22	3.01	73,73,73,73	0
56	MG	1A	3813	1/1	0.95	0.22	2.95	55,55,55,55	0
56	MG	1q	203	1/1	0.89	0.25	2.93	64,64,64,64	0
56	MG	1X	3001	1/1	0.89	0.24	2.93	44,44,44,44	0
56	MG	2a	3138	1/1	0.90	0.18	2.85	73,73,73,73	0
56	MG	1A	4047	1/1	0.96	0.25	2.84	36,36,36,36	0
56	MG	1A	3041	1/1	0.92	0.21	2.83	56,56,56,56	0
56	MG	1a	1709	1/1	0.90	0.19	2.80	54,54,54,54	0
56	MG	1D	301	1/1	0.90	0.22	2.69	58,58,58,58	0
56	MG	2U	201	1/1	0.91	0.19	2.66	40,40,40,40	0
56	MG	2A	3179	1/1	0.94	0.15	2.66	43,43,43,43	0
56	MG	2A	3214	1/1	0.89	0.27	2.65	49,49,49,49	0
56	MG	1A	3236	1/1	0.93	0.26	2.59	49,49,49,49	0
56	MG	2A	3562	1/1	0.94	0.24	2.58	37,37,37,37	0
56	MG	1A	3918	1/1	0.99	0.21	2.58	25,25,25,25	0
56	MG	1A	3894	1/1	0.97	0.24	2.56	58,58,58,58	0
56	MG	1A	3416	1/1	0.88	0.21	2.54	70,70,70,70	0
56	MG	1A	3723	1/1	0.89	0.21	2.54	49,49,49,49	0
56	MG	1A	4030	1/1	0.96	0.24	2.51	41,41,41,41	0
56	MG	15	105	1/1	0.85	0.20	2.50	57,57,57,57	0
56	MG	1A	3606	1/1	0.97	0.20	2.49	43,43,43,43	0
56	MG	1a	1714	1/1	0.86	0.22	2.48	58,58,58,58	0
56	MG	2A	3577	1/1	0.89	0.19	2.45	54,54,54,54	0
56	MG	1W	3003	1/1	0.97	0.23	2.42	37,37,37,37	0
56	MG	2A	3444	1/1	0.96	0.17	2.40	39,39,39,39	0
56	MG	1A	3658	1/1	0.91	0.21	2.32	21,21,21,21	0
56	MG	1A	3627	1/1	0.93	0.20	2.29	20,20,20,20	0
56	MG	1A	3636	1/1	0.96	0.20	2.28	19,19,19,19	0
56	MG	1A	3613	1/1	0.95	0.20	2.27	30,30,30,30	0
56	MG	1a	1835	1/1	0.98	0.19	2.27	34,34,34,34	0
56	MG	1A	3356	1/1	0.94	0.18	2.27	49,49,49,49	0
56	MG	1A	3774	1/1	0.99	0.22	2.27	21,21,21,21	0
56	MG	2A	3350	1/1	0.95	0.15	2.25	46,46,46,46	0
56	MG	1A	3143	1/1	0.93	0.15	2.24	55,55,55,55	0
56	MG	1D	305	1/1	0.91	0.25	2.22	58,58,58,58	0
56	MG	2A	3349	1/1	0.95	0.14	2.21	49,49,49,49	0
56	MG	2A	3069	1/1	0.95	0.18	2.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3750	1/1	0.96	0.19	2.11	18,18,18,18	0
56	MG	1A	3111	1/1	0.96	0.22	2.10	39,39,39,39	0
56	MG	1A	3112	1/1	0.96	0.20	2.09	35,35,35,35	0
56	MG	1A	3120	1/1	0.98	0.18	2.03	37,37,37,37	0
56	MG	2a	3102	1/1	0.88	0.17	2.03	72,72,72,72	0
56	MG	1A	3449	1/1	0.93	0.22	2.02	77,77,77,77	0
56	MG	1A	3699	1/1	0.86	0.21	2.01	17,17,17,17	0
56	MG	1A	3158	1/1	0.91	0.19	1.97	37,37,37,37	0
56	MG	1A	4042	1/1	0.88	0.22	1.93	51,51,51,51	0
56	MG	1A	3865	1/1	0.97	0.19	1.92	32,32,32,32	0
56	MG	1A	3727	1/1	0.95	0.22	1.84	25,25,25,25	0
56	MG	1A	3195	1/1	0.86	0.19	1.75	45,45,45,45	0
56	MG	2A	3208	1/1	0.96	0.18	1.72	49,49,49,49	0
56	MG	2A	3265	1/1	0.94	0.17	1.71	59,59,59,59	0
56	MG	2A	3554	1/1	0.98	0.15	1.70	44,44,44,44	0
56	MG	2A	3583	1/1	0.97	0.29	1.66	42,42,42,42	0
56	MG	1A	3678	1/1	0.88	0.18	1.62	67,67,67,67	0
56	MG	1D	312	1/1	0.93	0.18	1.60	47,47,47,47	0
56	MG	1a	1762	1/1	0.63	0.18	1.59	80,80,80,80	0
56	MG	15	103	1/1	0.93	0.21	1.58	45,45,45,45	0
56	MG	1A	3533	1/1	0.95	0.18	1.55	37,37,37,37	0
56	MG	2t	201	1/1	0.87	0.27	1.55	62,62,62,62	0
56	MG	2a	3055	1/1	0.91	0.22	1.54	70,70,70,70	0
56	MG	1a	1869	1/1	0.94	0.13	1.53	63,63,63,63	0
56	MG	2A	3580	1/1	0.90	0.23	1.52	51,51,51,51	0
56	MG	2a	3058	1/1	0.80	0.18	1.49	66,66,66,66	0
56	MG	2A	3130	1/1	0.90	0.15	1.49	50,50,50,50	0
56	MG	1A	3506	1/1	0.94	0.18	1.48	57,57,57,57	0
56	MG	1A	3624	1/1	0.93	0.19	1.47	35,35,35,35	0
56	MG	1A	3671	1/1	0.90	0.17	1.47	47,47,47,47	0
56	MG	1a	1849	1/1	0.96	0.19	1.42	54,54,54,54	0
56	MG	1a	1900	1/1	0.90	0.24	1.35	62,62,62,62	0
56	MG	2a	3243	1/1	0.94	0.17	1.32	58,58,58,58	0
56	MG	1a	1738	1/1	0.89	0.17	1.29	59,59,59,59	0
56	MG	1A	3612	1/1	0.94	0.22	1.29	24,24,24,24	0
56	MG	2A	3329	1/1	0.96	0.15	1.25	39,39,39,39	0
56	MG	1A	3129	1/1	0.97	0.15	1.21	35,35,35,35	0
56	MG	2D	303	1/1	0.81	0.17	1.16	60,60,60,60	0
56	MG	1A	3538	1/1	0.94	0.21	1.14	14,14,14,14	0
56	MG	2A	3008	1/1	0.84	0.16	1.10	59,59,59,59	0
56	MG	2a	3009	1/1	0.90	0.15	1.10	81,81,81,81	0
56	MG	1b	3001	1/1	0.73	0.24	1.08	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3097	1/1	0.87	0.22	1.08	40,40,40,40	0
56	MG	2a	3167	1/1	0.97	0.20	1.07	40,40,40,40	0
56	MG	2x	3003	1/1	0.97	0.18	1.05	51,51,51,51	0
56	MG	1A	3530	1/1	0.97	0.17	1.01	29,29,29,29	0
56	MG	1a	1840	1/1	0.96	0.13	1.00	67,67,67,67	0
56	MG	1A	3134	1/1	0.92	0.15	0.99	31,31,31,31	0
56	MG	1a	1691	1/1	0.92	0.15	0.95	50,50,50,50	0
56	MG	2A	3249	1/1	0.93	0.15	0.95	57,57,57,57	0
56	MG	2A	3356	1/1	0.98	0.15	0.90	37,37,37,37	0
56	MG	1a	1641	1/1	0.90	0.25	0.86	70,70,70,70	0
56	MG	1a	1807	1/1	0.91	0.19	0.82	71,71,71,71	0
56	MG	2A	3383	1/1	0.92	0.15	0.81	64,64,64,64	0
56	MG	1A	3973	1/1	0.97	0.18	0.79	49,49,49,49	0
56	MG	1D	302	1/1	0.94	0.18	0.77	33,33,33,33	0
56	MG	1A	3202	1/1	0.95	0.17	0.71	50,50,50,50	0
56	MG	1A	3731	1/1	0.92	0.19	0.63	29,29,29,29	0
56	MG	1A	3019	1/1	0.94	0.19	0.60	61,61,61,61	0
56	MG	2A	3156	1/1	0.91	0.15	0.55	53,53,53,53	0
56	MG	1a	1633	1/1	0.98	0.14	0.51	52,52,52,52	0
56	MG	1A	3730	1/1	0.93	0.17	0.49	33,33,33,33	0
56	MG	2A	3495	1/1	0.87	0.14	0.47	75,75,75,75	0
56	MG	2A	3210	1/1	0.91	0.18	0.47	49,49,49,49	0
56	MG	1A	3740	1/1	0.97	0.17	0.45	13,13,13,13	0
56	MG	1A	3563	1/1	0.94	0.19	0.43	50,50,50,50	0
56	MG	2a	3020	1/1	0.83	0.17	0.40	72,72,72,72	0
56	MG	1A	3250	1/1	0.90	0.19	0.39	42,42,42,42	0
56	MG	1A	3608	1/1	0.95	0.16	0.38	39,39,39,39	0
56	MG	1a	1716	1/1	0.96	0.15	0.34	68,68,68,68	0
56	MG	2A	3581	1/1	0.96	0.14	0.28	51,51,51,51	0
56	MG	2a	3019	1/1	0.92	0.17	0.26	67,67,67,67	0
56	MG	1A	4046	1/1	0.91	0.17	0.25	56,56,56,56	0
56	MG	1a	1817	1/1	0.98	0.13	0.23	49,49,49,49	0
56	MG	2A	3570	1/1	0.97	0.12	0.23	50,50,50,50	0
56	MG	1A	3773	1/1	0.98	0.19	0.21	22,22,22,22	0
56	MG	2a	3214	1/1	0.97	0.16	0.20	75,75,75,75	0
56	MG	1A	3545	1/1	0.96	0.17	0.14	31,31,31,31	0
56	MG	1a	1768	1/1	0.86	0.20	0.12	90,90,90,90	0
56	MG	1A	3607	1/1	0.88	0.16	0.10	50,50,50,50	0
56	MG	2a	3192	1/1	0.95	0.16	0.10	56,56,56,56	0
56	MG	2A	3306	1/1	0.98	0.16	0.08	26,26,26,26	0
56	MG	1A	3726	1/1	0.97	0.19	0.08	29,29,29,29	0
56	MG	1A	4016	1/1	0.90	0.19	0.07	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3474	1/1	0.81	0.14	0.07	58,58,58,58	0
56	MG	1a	1765	1/1	0.89	0.13	0.05	65,65,65,65	0
56	MG	2O	202	1/1	0.99	0.16	0.05	53,53,53,53	0
56	MG	1A	3224	1/1	0.92	0.16	0.03	36,36,36,36	0
56	MG	2A	3302	1/1	0.93	0.13	0.03	64,64,64,64	0
56	MG	1A	3923	1/1	0.95	0.18	0.03	37,37,37,37	0
56	MG	2q	201	1/1	0.81	0.21	0.01	71,71,71,71	0
56	MG	2a	3021	1/1	0.98	0.16	-0.01	78,78,78,78	0
56	MG	1T	201	1/1	0.94	0.16	-0.04	59,59,59,59	0
56	MG	1E	301	1/1	0.96	0.18	-0.08	58,58,58,58	0
56	MG	1a	1757	1/1	0.90	0.16	-0.08	64,64,64,64	0
56	MG	2A	3516	1/1	0.94	0.14	-0.11	38,38,38,38	0
56	MG	1D	314	1/1	0.92	0.14	-0.14	48,48,48,48	0
56	MG	2a	3083	1/1	0.90	0.14	-0.15	43,43,43,43	0
56	MG	2A	3162	1/1	0.94	0.14	-0.16	47,47,47,47	0
56	MG	2U	202	1/1	0.98	0.17	-0.16	45,45,45,45	0
56	MG	2A	3322	1/1	0.93	0.15	-0.16	29,29,29,29	0
56	MG	1A	3410	1/1	0.91	0.17	-0.18	51,51,51,51	0
56	MG	1A	3717	1/1	0.97	0.17	-0.18	44,44,44,44	0
56	MG	2A	3460	1/1	0.72	0.14	-0.20	53,53,53,53	0
56	MG	1a	1627	1/1	0.81	0.12	-0.20	68,68,68,68	0
56	MG	1B	220	1/1	0.96	0.14	-0.22	27,27,27,27	0
56	MG	2a	3163	1/1	0.97	0.15	-0.24	55,55,55,55	0
56	MG	2A	3325	1/1	0.95	0.14	-0.25	32,32,32,32	0
56	MG	2A	3395	1/1	0.84	0.12	-0.26	78,78,78,78	0
56	MG	1A	3644	1/1	0.97	0.15	-0.26	38,38,38,38	0
56	MG	2A	3059	1/1	0.91	0.14	-0.31	50,50,50,50	0
56	MG	2a	3242	1/1	0.92	0.13	-0.33	57,57,57,57	0
56	MG	2A	3155	1/1	0.98	0.14	-0.34	33,33,33,33	0
57	ZN	26	102	1/1	0.94	0.12	-0.35	68,68,68,68	0
56	MG	2A	3301	1/1	0.95	0.12	-0.37	48,48,48,48	0
57	ZN	16	102	1/1	0.99	0.13	-0.38	45,45,45,45	0
56	MG	2A	3323	1/1	0.93	0.14	-0.39	54,54,54,54	0
56	MG	2A	3579	1/1	0.86	0.14	-0.42	42,42,42,42	0
56	MG	15	104	1/1	0.95	0.19	-0.43	49,49,49,49	0
56	MG	1A	3440	1/1	0.89	0.16	-0.47	51,51,51,51	0
56	MG	2a	3073	1/1	0.96	0.15	-0.49	68,68,68,68	0
56	MG	1A	3689	1/1	0.99	0.19	-0.51	14,14,14,14	0
56	MG	1A	3819	1/1	0.89	0.16	-0.52	89,89,89,89	0
56	MG	1a	1809	1/1	0.91	0.17	-0.52	67,67,67,67	0
56	MG	2B	3003	1/1	0.98	0.21	-0.52	64,64,64,64	0
56	MG	2A	3120	1/1	0.94	0.13	-0.53	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2Q	203	1/1	0.91	0.12	-0.53	52,52,52,52	0
56	MG	2A	3074	1/1	0.87	0.13	-0.53	47,47,47,47	0
56	MG	2A	3084	1/1	0.86	0.12	-0.59	51,51,51,51	0
56	MG	2A	3104	1/1	0.86	0.12	-0.61	42,42,42,42	0
57	ZN	1n	501	1/1	0.94	0.14	-0.63	86,86,86,86	0
56	MG	2A	3382	1/1	0.90	0.14	-0.66	71,71,71,71	0
56	MG	1a	1744	1/1	0.99	0.15	-0.67	80,80,80,80	0
56	MG	1D	307	1/1	0.94	0.15	-0.69	39,39,39,39	0
57	ZN	15	102	1/1	0.99	0.13	-0.70	43,43,43,43	0
56	MG	2a	3232	1/1	0.95	0.14	-0.73	62,62,62,62	0
56	MG	1A	3616	1/1	0.90	0.17	-0.77	28,28,28,28	0
56	MG	1a	1685	1/1	0.94	0.15	-0.78	23,23,23,23	0
56	MG	2A	3514	1/1	0.98	0.09	-0.79	58,58,58,58	0
56	MG	2D	301	1/1	0.96	0.14	-0.79	54,54,54,54	0
56	MG	2A	3569	1/1	0.91	0.13	-0.81	41,41,41,41	0
56	MG	1A	3756	1/1	0.99	0.17	-0.82	46,46,46,46	0
56	MG	2A	3543	1/1	0.91	0.10	-0.82	66,66,66,66	0
56	MG	1B	204	1/1	0.93	0.13	-0.83	53,53,53,53	0
56	MG	1a	1678	1/1	0.95	0.15	-0.84	60,60,60,60	0
57	ZN	25	501	1/1	0.99	0.10	-0.84	49,49,49,49	0
56	MG	1D	309	1/1	0.91	0.12	-0.87	37,37,37,37	0
56	MG	1A	3424	1/1	0.96	0.15	-0.88	62,62,62,62	0
56	MG	2A	3019	1/1	0.96	0.12	-0.93	47,47,47,47	0
56	MG	1A	4024	1/1	0.97	0.16	-0.95	29,29,29,29	0
56	MG	2a	3038	1/1	0.90	0.14	-0.95	85,85,85,85	0
56	MG	2G	3001	1/1	0.41	0.19	-0.96	60,60,60,60	0
56	MG	1a	1708	1/1	0.97	0.14	-0.97	61,61,61,61	0
56	MG	2A	3416	1/1	0.65	0.12	-0.97	56,56,56,56	0
56	MG	1A	3749	1/1	0.96	0.16	-0.99	27,27,27,27	0
56	MG	1A	3826	1/1	0.91	0.14	-1.01	35,35,35,35	0
56	MG	2d	503	1/1	0.89	0.12	-1.01	72,72,72,72	0
57	ZN	19	501	1/1	0.99	0.12	-1.05	44,44,44,44	0
56	MG	1a	1655	1/1	0.94	0.14	-1.05	60,60,60,60	0
56	MG	2A	3407	1/1	0.94	0.13	-1.06	31,31,31,31	0
56	MG	1A	4051	1/1	1.00	0.15	-1.07	44,44,44,44	0
56	MG	1a	1896	1/1	0.96	0.12	-1.08	45,45,45,45	0
56	MG	1A	3441	1/1	0.94	0.17	-1.09	50,50,50,50	0
57	ZN	29	501	1/1	0.95	0.09	-1.10	65,65,65,65	0
56	MG	1N	205	1/1	0.91	0.17	-1.11	53,53,53,53	0
58	SF4	1d	301	8/8	0.99	0.13	-1.15	64,69,73,86	0
56	MG	2a	3196	1/1	0.95	0.13	-1.17	54,54,54,54	0
56	MG	1A	3117	1/1	0.96	0.15	-1.18	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	17	102	1/1	0.99	0.15	-1.18	33,33,33,33	0
56	MG	1a	1657	1/1	0.95	0.11	-1.20	72,72,72,72	0
56	MG	1d	302	1/1	0.93	0.09	-1.22	70,70,70,70	0
56	MG	2A	3307	1/1	0.98	0.12	-1.26	32,32,32,32	0
56	MG	1A	3907	1/1	0.91	0.17	-1.30	13,13,13,13	0
56	MG	1A	3104	1/1	0.95	0.14	-1.32	38,38,38,38	0
56	MG	1B	215	1/1	0.82	0.15	-1.35	68,68,68,68	0
56	MG	1A	3783	1/1	0.91	0.16	-1.38	22,22,22,22	0
56	MG	1A	4038	1/1	0.95	0.16	-1.42	66,66,66,66	0
58	SF4	2d	501	8/8	0.99	0.11	-1.44	58,77,81,90	0
56	MG	1a	1906	1/1	0.94	0.14	-1.45	83,83,83,83	0
56	MG	1A	3729	1/1	0.98	0.16	-1.47	22,22,22,22	0
56	MG	1A	3014	1/1	0.92	0.11	-1.47	58,58,58,58	0
56	MG	2A	3277	1/1	0.95	0.11	-1.51	36,36,36,36	0
56	MG	2A	3507	1/1	0.91	0.12	-1.54	48,48,48,48	0
56	MG	2A	3041	1/1	0.96	0.10	-1.56	49,49,49,49	0
56	MG	1A	3761	1/1	0.87	0.12	-1.57	52,52,52,52	0
56	MG	1a	1904	1/1	0.94	0.10	-1.58	53,53,53,53	0
56	MG	1A	3141	1/1	0.81	0.10	-1.59	56,56,56,56	0
57	ZN	2Y	501	1/1	0.94	0.04	-1.60	88,88,88,88	0
56	MG	1a	1703	1/1	0.98	0.12	-1.69	48,48,48,48	0
56	MG	1A	3575	1/1	0.92	0.11	-1.71	39,39,39,39	0
56	MG	2A	3389	1/1	0.96	0.11	-1.72	36,36,36,36	0
56	MG	1D	311	1/1	0.96	0.11	-1.73	49,49,49,49	0
56	MG	1A	3619	1/1	0.98	0.15	-1.73	16,16,16,16	0
56	MG	1A	3309	1/1	0.88	0.11	-1.74	65,65,65,65	0
56	MG	1A	4033	1/1	0.86	0.14	-1.74	50,50,50,50	0
56	MG	2A	3565	1/1	0.91	0.09	-1.76	62,62,62,62	0
56	MG	1a	1658	1/1	0.97	0.09	-1.76	68,68,68,68	0
56	MG	1A	3633	1/1	0.92	0.15	-1.78	29,29,29,29	0
56	MG	2A	3050	1/1	0.93	0.09	-1.82	44,44,44,44	0
56	MG	1A	3790	1/1	0.98	0.14	-1.86	21,21,21,21	0
56	MG	1A	3542	1/1	0.96	0.11	-1.86	29,29,29,29	0
56	MG	1a	1870	1/1	0.96	0.09	-1.86	56,56,56,56	0
56	MG	1A	3544	1/1	0.97	0.14	-1.90	30,30,30,30	0
56	MG	2A	3044	1/1	0.96	0.11	-1.92	46,46,46,46	0
56	MG	1A	3664	1/1	0.93	0.10	-1.93	57,57,57,57	0
56	MG	1A	3736	1/1	0.97	0.16	-1.94	30,30,30,30	0
56	MG	1a	1905	1/1	0.98	0.10	-1.95	83,83,83,83	0
56	MG	1R	204	1/1	0.88	0.18	-2.02	48,48,48,48	0
56	MG	1a	1666	1/1	0.91	0.14	-2.02	55,55,55,55	0
56	MG	2n	503	1/1	0.90	0.08	-2.04	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	ZN	24	501	1/1	0.50	0.05	-2.06	126,126,126,126	0
57	ZN	14	501	1/1	0.94	0.09	-2.10	102,102,102,102	0
56	MG	2E	301	1/1	0.98	0.12	-2.11	24,24,24,24	0
56	MG	1A	3752	1/1	0.97	0.14	-2.15	55,55,55,55	0
56	MG	1A	3825	1/1	0.96	0.12	-2.17	33,33,33,33	0
56	MG	1A	3086	1/1	0.99	0.14	-2.18	31,31,31,31	0
56	MG	1a	1640	1/1	0.95	0.13	-2.18	77,77,77,77	0
57	ZN	2n	501	1/1	0.85	0.07	-2.21	105,105,105,105	0
56	MG	2A	3533	1/1	0.98	0.08	-2.23	47,47,47,47	0
56	MG	1A	3131	1/1	0.94	0.12	-2.29	32,32,32,32	0
56	MG	1G	3001	1/1	0.90	0.08	-2.31	47,47,47,47	0
56	MG	2A	3164	1/1	0.96	0.07	-2.33	42,42,42,42	0
56	MG	1a	1616	1/1	0.96	0.10	-2.33	76,76,76,76	0
56	MG	1A	4014	1/1	0.98	0.12	-2.34	51,51,51,51	0
56	MG	1a	1702	1/1	0.94	0.08	-2.34	67,67,67,67	0
56	MG	1A	3082	1/1	0.98	0.14	-2.38	28,28,28,28	0
56	MG	1A	3757	1/1	0.94	0.12	-2.40	41,41,41,41	0
57	ZN	1Y	501	1/1	0.99	0.09	-2.41	63,63,63,63	0
56	MG	1A	3960	1/1	0.97	0.13	-2.41	41,41,41,41	0
56	MG	1a	1605	1/1	0.93	0.11	-2.46	84,84,84,84	0
56	MG	2A	3268	1/1	0.85	0.10	-2.47	63,63,63,63	0
56	MG	1a	1802	1/1	0.96	0.10	-2.53	77,77,77,77	0
56	MG	1G	3003	1/1	0.96	0.05	-2.54	59,59,59,59	0
56	MG	1A	3997	1/1	0.92	0.11	-2.60	18,18,18,18	0
56	MG	2a	3104	1/1	0.94	0.11	-2.62	40,40,40,40	0
56	MG	1A	3472	1/1	0.88	0.08	-2.66	66,66,66,66	0
56	MG	1A	3781	1/1	0.98	0.14	-2.66	28,28,28,28	0
56	MG	2A	3479	1/1	0.98	0.11	-2.69	31,31,31,31	0
56	MG	1x	104	1/1	0.95	0.07	-2.73	47,47,47,47	0
56	MG	1A	3084	1/1	0.95	0.08	-2.73	25,25,25,25	0
56	MG	2A	3464	1/1	0.97	0.11	-2.76	53,53,53,53	0
56	MG	1A	3824	1/1	0.96	0.14	-2.78	31,31,31,31	0
56	MG	1n	502	1/1	0.97	0.09	-2.80	47,47,47,47	0
56	MG	1a	1630	1/1	0.98	0.14	-2.90	38,38,38,38	0
56	MG	1A	3701	1/1	0.93	0.14	-2.96	22,22,22,22	0
56	MG	1B	222	1/1	0.96	0.11	-2.97	58,58,58,58	0
56	MG	1A	3387	1/1	0.93	0.05	-2.99	64,64,64,64	0
56	MG	1A	3572	1/1	0.97	0.09	-3.02	51,51,51,51	0
56	MG	1a	1711	1/1	0.95	0.10	-3.05	54,54,54,54	0
56	MG	2x	3005	1/1	0.86	0.08	-3.21	70,70,70,70	0
56	MG	1A	3780	1/1	0.93	0.10	-3.22	48,48,48,48	0
56	MG	1A	3803	1/1	0.97	0.14	-3.22	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	210	1/1	0.95	0.10	-3.25	45,45,45,45	0
56	MG	2a	3168	1/1	0.62	0.09	-3.28	83,83,83,83	0
56	MG	2A	3098	1/1	0.92	0.08	-3.31	53,53,53,53	0
56	MG	2A	3470	1/1	0.97	0.06	-3.33	42,42,42,42	0
56	MG	1W	3005	1/1	0.92	0.12	-3.39	41,41,41,41	0
56	MG	1A	3909	1/1	0.97	0.14	-3.39	25,25,25,25	0
56	MG	1A	3792	1/1	0.94	0.11	-3.46	47,47,47,47	0
56	MG	1a	1608	1/1	0.94	0.12	-3.49	68,68,68,68	0
56	MG	1a	1639	1/1	0.92	0.08	-3.50	70,70,70,70	0
56	MG	1A	3946	1/1	0.94	0.12	-3.54	51,51,51,51	0
56	MG	1A	3064	1/1	0.99	0.14	-3.57	41,41,41,41	0
56	MG	2A	3054	1/1	0.93	0.09	-3.60	41,41,41,41	0
56	MG	1A	3113	1/1	0.97	0.14	-3.61	42,42,42,42	0
56	MG	1A	3822	1/1	0.88	0.10	-3.67	34,34,34,34	0
56	MG	2A	3298	1/1	0.96	0.07	-3.67	45,45,45,45	0
56	MG	1A	3972	1/1	0.91	0.13	-3.77	22,22,22,22	0
56	MG	1A	3676	1/1	0.99	0.13	-3.82	23,23,23,23	0
56	MG	1A	3626	1/1	0.91	0.10	-4.03	24,24,24,24	0
56	MG	1a	1668	1/1	0.93	0.06	-4.04	71,71,71,71	0
56	MG	1A	3204	1/1	0.90	0.07	-4.06	38,38,38,38	0
56	MG	2A	3081	1/1	0.95	0.06	-4.08	37,37,37,37	0
56	MG	2A	3124	1/1	0.91	0.06	-4.09	62,62,62,62	0
56	MG	2D	302	1/1	0.92	0.10	-4.13	57,57,57,57	0
56	MG	1A	3547	1/1	0.99	0.14	-4.19	38,38,38,38	0
56	MG	2a	3072	1/1	0.79	0.10	-4.40	64,64,64,64	0
56	MG	2a	3078	1/1	0.89	0.07	-4.41	49,49,49,49	0
56	MG	1A	3922	1/1	0.97	0.09	-4.42	75,75,75,75	0
56	MG	2A	3282	1/1	0.96	0.10	-4.63	31,31,31,31	0
56	MG	1A	3185	1/1	0.92	0.09	-4.76	44,44,44,44	0
56	MG	2A	3499	1/1	0.93	0.10	-4.92	31,31,31,31	0
56	MG	1A	3621	1/1	0.98	0.11	-5.06	24,24,24,24	0
56	MG	1A	3948	1/1	0.99	0.11	-5.15	18,18,18,18	0
56	MG	1A	3753	1/1	0.96	0.10	-5.38	67,67,67,67	0
56	MG	2A	3485	1/1	0.96	0.08	-5.56	35,35,35,35	0
56	MG	1A	3603	1/1	0.97	0.13	-5.64	26,26,26,26	0
56	MG	1A	3711	1/1	0.97	0.12	-5.73	45,45,45,45	0
56	MG	1A	3996	1/1	0.98	0.12	-6.00	29,29,29,29	0
56	MG	1A	3083	1/1	0.96	0.15	-6.32	29,29,29,29	0
56	MG	1A	3879	1/1	0.98	0.09	-6.32	24,24,24,24	0
56	MG	1A	3598	1/1	0.98	0.08	-6.41	21,21,21,21	0
56	MG	2a	3187	1/1	0.82	0.10	-6.56	56,56,56,56	0
56	MG	1A	3653	1/1	0.99	0.12	-6.64	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3484	1/1	0.99	0.05	-6.75	37,37,37,37	0
56	MG	1A	3920	1/1	0.94	0.13	-6.92	23,23,23,23	0
56	MG	1A	3930	1/1	0.94	0.08	-6.95	23,23,23,23	0
56	MG	2a	3095	1/1	0.96	0.05	-7.00	58,58,58,58	0
56	MG	2a	3197	1/1	0.94	0.08	-7.26	74,74,74,74	0
56	MG	1A	3184	1/1	0.91	0.05	-7.67	61,61,61,61	0
56	MG	1A	3553	1/1	0.98	0.10	-7.99	38,38,38,38	0
56	MG	2A	3434	1/1	0.95	0.07	-8.02	55,55,55,55	0
56	MG	2A	3456	1/1	0.94	0.06	-8.03	41,41,41,41	0
56	MG	1A	3864	1/1	0.99	0.08	-8.58	15,15,15,15	0
56	MG	1A	3821	1/1	0.97	0.11	-8.83	26,26,26,26	0
56	MG	1A	3666	1/1	0.99	0.09	-8.98	9,9,9,9	0
56	MG	1A	3935	1/1	0.99	0.10	-9.05	20,20,20,20	0
56	MG	1A	3919	1/1	0.96	0.12	-9.14	47,47,47,47	0
56	MG	1a	1681	1/1	0.89	0.08	-9.55	44,44,44,44	0
56	MG	1a	1740	1/1	0.97	0.10	-9.70	57,57,57,57	0
56	MG	1A	3706	1/1	0.96	0.09	-10.66	38,38,38,38	0
56	MG	2A	3501	1/1	0.97	0.06	-11.96	43,43,43,43	0
56	MG	2A	3421	1/1	0.98	0.04	-12.63	50,50,50,50	0
56	MG	1a	1656	1/1	0.94	0.10	-14.64	25,25,25,25	0
56	MG	2a	3228	1/1	0.94	0.07	-	67,67,67,67	0
56	MG	1A	3275	1/1	0.86	0.29	-	53,53,53,53	0
56	MG	2A	3555	1/1	0.96	0.08	-	43,43,43,43	0
56	MG	1A	3811	1/1	0.92	0.17	-	50,50,50,50	0
56	MG	1A	3733	1/1	0.96	0.13	-	37,37,37,37	0
56	MG	2A	3175	1/1	0.95	0.09	-	40,40,40,40	0
56	MG	1A	3469	1/1	0.98	0.15	-	47,47,47,47	0
56	MG	1A	3963	1/1	0.95	0.31	-	54,54,54,54	0
56	MG	1A	3042	1/1	0.89	0.41	-	47,47,47,47	0
56	MG	2a	3176	1/1	0.93	0.38	-	87,87,87,87	0
56	MG	1A	3316	1/1	0.89	0.18	-	81,81,81,81	0
56	MG	2a	3007	1/1	0.93	0.09	-	91,91,91,91	0
56	MG	1B	209	1/1	0.75	0.28	-	61,61,61,61	0
56	MG	2A	3364	1/1	0.82	0.24	-	55,55,55,55	0
56	MG	1A	3662	1/1	0.87	0.14	-	55,55,55,55	0
56	MG	2a	3074	1/1	0.93	0.12	-	63,63,63,63	0
56	MG	2a	3077	1/1	0.85	0.11	-	95,95,95,95	0
56	MG	2A	3273	1/1	0.92	0.15	-	36,36,36,36	0
56	MG	2A	3393	1/1	0.94	0.18	-	71,71,71,71	0
56	MG	1A	3382	1/1	0.96	0.24	-	29,29,29,29	0
56	MG	2A	3281	1/1	0.96	0.34	-	50,50,50,50	0
56	MG	1A	3683	1/1	0.99	0.15	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3531	1/1	0.95	0.12	-	58,58,58,58	0
56	MG	2a	3158	1/1	0.95	0.26	-	72,72,72,72	0
56	MG	1A	3341	1/1	0.85	0.11	-	58,58,58,58	0
56	MG	2A	3051	1/1	0.96	0.17	-	49,49,49,49	0
56	MG	2A	3242	1/1	0.76	0.17	-	55,55,55,55	0
56	MG	2A	3209	1/1	0.95	0.73	-	49,49,49,49	0
56	MG	2A	3169	1/1	0.94	0.45	-	54,54,54,54	0
56	MG	1a	1769	1/1	0.80	0.10	-	74,74,74,74	0
56	MG	2A	3202	1/1	0.78	0.19	-	50,50,50,50	0
56	MG	2a	3147	1/1	0.88	0.07	-	74,74,74,74	0
56	MG	2A	3143	1/1	0.98	0.34	-	51,51,51,51	0
56	MG	1A	3471	1/1	0.97	0.11	-	66,66,66,66	0
56	MG	2A	3110	1/1	0.91	0.31	-	49,49,49,49	0
56	MG	2A	3481	1/1	0.95	0.12	-	41,41,41,41	0
56	MG	1A	3060	1/1	0.97	0.14	-	51,51,51,51	0
56	MG	2A	3029	1/1	0.85	0.27	-	59,59,59,59	0
56	MG	16	101	1/1	0.95	0.18	-	51,51,51,51	0
56	MG	1a	1791	1/1	0.06	0.74	-	89,89,89,89	0
56	MG	1a	1888	1/1	0.92	0.20	-	75,75,75,75	0
56	MG	1a	1890	1/1	0.96	0.48	-	58,58,58,58	0
56	MG	1A	3884	1/1	0.96	0.07	-	63,63,63,63	0
56	MG	1a	1856	1/1	0.97	0.12	-	70,70,70,70	0
56	MG	1A	3003	1/1	0.99	0.09	-	58,58,58,58	0
56	MG	1a	1814	1/1	0.97	0.22	-	63,63,63,63	0
56	MG	1A	3226	1/1	0.94	0.12	-	53,53,53,53	0
56	MG	2a	3200	1/1	0.90	0.17	-	56,56,56,56	0
56	MG	1A	4007	1/1	0.92	0.31	-	58,58,58,58	0
56	MG	13	101	1/1	0.93	0.21	-	52,52,52,52	0
56	MG	1A	3280	1/1	0.96	0.08	-	70,70,70,70	0
56	MG	1a	1885	1/1	0.92	0.20	-	66,66,66,66	0
56	MG	1A	3604	1/1	0.91	0.19	-	26,26,26,26	0
56	MG	1A	3902	1/1	0.89	0.14	-	41,41,41,41	0
56	MG	1A	3491	1/1	0.84	0.09	-	83,83,83,83	0
56	MG	1a	1828	1/1	0.98	0.26	-	67,67,67,67	0
56	MG	1A	3124	1/1	0.90	0.31	-	54,54,54,54	0
56	MG	1A	3289	1/1	0.89	0.38	-	49,49,49,49	0
56	MG	1a	1836	1/1	0.97	0.28	-	59,59,59,59	0
56	MG	1A	3191	1/1	0.95	0.13	-	40,40,40,40	0
56	MG	1A	4043	1/1	0.95	0.11	-	45,45,45,45	0
56	MG	2A	3486	1/1	0.89	0.10	-	51,51,51,51	0
56	MG	2A	3440	1/1	0.92	0.16	-	62,62,62,62	0
56	MG	1A	3893	1/1	0.35	0.28	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3115	1/1	0.94	0.25	-	52,52,52,52	0
56	MG	2A	3064	1/1	0.82	0.31	-	56,56,56,56	0
56	MG	1o	3001	1/1	0.91	0.06	-	77,77,77,77	0
56	MG	1A	3319	1/1	0.86	0.11	-	55,55,55,55	0
56	MG	2A	3244	1/1	0.88	0.30	-	73,73,73,73	0
56	MG	1A	3688	1/1	0.98	0.19	-	23,23,23,23	0
56	MG	1A	3292	1/1	0.93	0.10	-	44,44,44,44	0
56	MG	2A	3133	1/1	0.94	0.09	-	40,40,40,40	0
56	MG	1A	3763	1/1	0.98	0.18	-	46,46,46,46	0
56	MG	1A	3877	1/1	0.94	0.21	-	61,61,61,61	0
56	MG	2A	3116	1/1	0.94	0.23	-	55,55,55,55	0
56	MG	1A	3982	1/1	0.87	0.24	-	74,74,74,74	0
56	MG	2A	3215	1/1	0.71	0.15	-	63,63,63,63	0
56	MG	2A	3369	1/1	0.93	0.12	-	65,65,65,65	0
56	MG	1A	3969	1/1	0.96	0.12	-	39,39,39,39	0
56	MG	1A	3071	1/1	0.87	0.17	-	52,52,52,52	0
56	MG	2a	3059	1/1	0.98	0.13	-	58,58,58,58	0
56	MG	2A	3127	1/1	0.91	0.17	-	54,54,54,54	0
56	MG	10	104	1/1	0.94	0.19	-	46,46,46,46	0
56	MG	2A	3405	1/1	0.97	0.30	-	45,45,45,45	0
56	MG	1A	3407	1/1	0.96	0.07	-	71,71,71,71	0
56	MG	1F	306	1/1	0.80	0.35	-	64,64,64,64	0
56	MG	1A	3584	1/1	0.92	0.11	-	52,52,52,52	0
56	MG	1A	3105	1/1	0.96	0.16	-	39,39,39,39	0
56	MG	1A	3505	1/1	0.87	0.29	-	66,66,66,66	0
56	MG	2A	3168	1/1	0.93	0.46	-	51,51,51,51	0
56	MG	2A	3431	1/1	0.95	0.24	-	68,68,68,68	0
56	MG	1A	3703	1/1	0.95	0.05	-	58,58,58,58	0
56	MG	2A	3471	1/1	0.93	0.26	-	54,54,54,54	0
56	MG	1A	3765	1/1	0.93	0.14	-	56,56,56,56	0
56	MG	11	101	1/1	0.83	0.28	-	83,83,83,83	0
56	MG	1A	3956	1/1	0.93	0.09	-	69,69,69,69	0
56	MG	1a	1725	1/1	0.96	0.27	-	59,59,59,59	0
56	MG	1A	3771	1/1	0.86	0.07	-	54,54,54,54	0
56	MG	1B	212	1/1	0.93	0.14	-	47,47,47,47	0
56	MG	1o	3002	1/1	0.97	0.18	-	55,55,55,55	0
56	MG	1A	3875	1/1	0.93	0.17	-	50,50,50,50	0
56	MG	1A	3078	1/1	0.99	0.15	-	21,21,21,21	0
56	MG	1G	3002	1/1	0.83	0.16	-	69,69,69,69	0
56	MG	1a	1747	1/1	0.94	0.28	-	59,59,59,59	0
56	MG	2A	3468	1/1	0.93	0.13	-	64,64,64,64	0
56	MG	1A	3012	1/1	0.86	0.31	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3588	1/1	0.94	0.12	-	69,69,69,69	0
56	MG	2a	3140	1/1	0.92	0.19	-	83,83,83,83	0
56	MG	1A	3656	1/1	0.96	0.12	-	56,56,56,56	0
56	MG	1A	3235	1/1	0.97	0.07	-	42,42,42,42	0
56	MG	1A	3018	1/1	0.95	0.50	-	58,58,58,58	0
56	MG	2A	3335	1/1	0.94	0.25	-	52,52,52,52	0
56	MG	2A	3227	1/1	0.94	0.41	-	49,49,49,49	0
56	MG	1R	203	1/1	0.93	0.23	-	56,56,56,56	0
56	MG	2A	3078	1/1	0.96	0.12	-	53,53,53,53	0
56	MG	1A	3198	1/1	0.93	0.42	-	41,41,41,41	0
56	MG	2A	3535	1/1	0.93	0.14	-	69,69,69,69	0
56	MG	2a	3159	1/1	0.87	0.29	-	76,76,76,76	0
56	MG	1A	3100	1/1	0.96	0.17	-	31,31,31,31	0
56	MG	1A	3354	1/1	0.95	0.20	-	54,54,54,54	0
56	MG	2a	3076	1/1	0.92	0.39	-	68,68,68,68	0
56	MG	1A	3535	1/1	0.94	0.19	-	24,24,24,24	0
56	MG	1Q	3003	1/1	0.92	0.21	-	54,54,54,54	0
56	MG	2a	3211	1/1	0.98	0.21	-	60,60,60,60	0
56	MG	1A	3777	1/1	0.95	0.22	-	43,43,43,43	0
56	MG	10	101	1/1	0.86	0.34	-	68,68,68,68	0
56	MG	2a	3018	1/1	0.86	0.28	-	66,66,66,66	0
56	MG	2A	3239	1/1	0.84	0.26	-	49,49,49,49	0
56	MG	1A	3850	1/1	0.84	0.21	-	80,80,80,80	0
56	MG	2A	3251	1/1	0.95	0.36	-	55,55,55,55	0
56	MG	2A	3418	1/1	0.95	0.19	-	62,62,62,62	0
56	MG	1A	3842	1/1	0.92	0.31	-	55,55,55,55	0
56	MG	1A	3439	1/1	0.88	0.33	-	50,50,50,50	0
56	MG	1A	3490	1/1	0.89	0.09	-	66,66,66,66	0
56	MG	1A	3831	1/1	0.98	0.08	-	54,54,54,54	0
56	MG	1A	3768	1/1	0.95	0.15	-	82,82,82,82	0
56	MG	1A	3820	1/1	0.94	0.17	-	50,50,50,50	0
56	MG	2a	3065	1/1	0.91	0.10	-	84,84,84,84	0
56	MG	1A	3744	1/1	0.95	0.16	-	63,63,63,63	0
56	MG	2A	3566	1/1	0.89	0.66	-	58,58,58,58	0
56	MG	2A	3412	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	1A	3951	1/1	0.98	0.16	-	31,31,31,31	0
56	MG	2A	3052	1/1	0.88	0.40	-	66,66,66,66	0
56	MG	2a	3053	1/1	0.95	0.12	-	83,83,83,83	0
56	MG	2A	3370	1/1	0.98	0.05	-	62,62,62,62	0
56	MG	2A	3310	1/1	0.96	0.08	-	46,46,46,46	0
56	MG	1A	3485	1/1	0.93	0.11	-	67,67,67,67	0
56	MG	1A	3673	1/1	0.95	0.20	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3022	1/1	0.87	0.44	-	66,66,66,66	0
56	MG	2A	3259	1/1	0.90	0.19	-	40,40,40,40	0
56	MG	2A	3517	1/1	0.98	0.07	-	47,47,47,47	0
56	MG	1A	3047	1/1	0.95	0.46	-	46,46,46,46	0
56	MG	2A	3006	1/1	0.91	0.13	-	71,71,71,71	0
56	MG	2a	3051	1/1	0.93	0.22	-	76,76,76,76	0
56	MG	1A	3149	1/1	0.95	0.19	-	34,34,34,34	0
56	MG	2A	3228	1/1	0.94	0.34	-	44,44,44,44	0
56	MG	1A	3721	1/1	0.98	0.13	-	45,45,45,45	0
56	MG	2A	3045	1/1	0.95	0.15	-	45,45,45,45	0
56	MG	2a	3139	1/1	0.92	0.20	-	94,94,94,94	0
56	MG	1A	3901	1/1	0.53	0.65	-	68,68,68,68	0
56	MG	1a	1879	1/1	0.92	0.20	-	51,51,51,51	0
56	MG	1A	3400	1/1	0.97	0.15	-	48,48,48,48	0
56	MG	2a	3121	1/1	0.97	0.38	-	57,57,57,57	0
56	MG	2Q	204	1/1	0.93	0.23	-	46,46,46,46	0
56	MG	1A	3254	1/1	0.91	0.21	-	32,32,32,32	0
56	MG	1A	3258	1/1	0.94	0.18	-	45,45,45,45	0
56	MG	1A	3713	1/1	0.95	0.06	-	38,38,38,38	0
56	MG	1a	1867	1/1	0.93	0.10	-	51,51,51,51	0
56	MG	2A	3288	1/1	0.72	0.36	-	70,70,70,70	0
56	MG	1A	3913	1/1	0.97	0.08	-	41,41,41,41	0
56	MG	2a	3047	1/1	0.69	0.24	-	89,89,89,89	0
56	MG	2A	3260	1/1	0.98	0.18	-	54,54,54,54	0
56	MG	2A	3337	1/1	0.92	0.12	-	41,41,41,41	0
56	MG	2a	3161	1/1	0.96	0.14	-	62,62,62,62	0
56	MG	1A	3090	1/1	0.80	0.32	-	53,53,53,53	0
56	MG	2A	3048	1/1	0.94	0.38	-	57,57,57,57	0
56	MG	1A	3941	1/1	0.85	0.24	-	73,73,73,73	0
56	MG	1A	3445	1/1	0.93	0.13	-	58,58,58,58	0
56	MG	1a	1855	1/1	0.95	0.29	-	75,75,75,75	0
56	MG	1A	3324	1/1	0.95	0.10	-	66,66,66,66	0
56	MG	2A	3021	1/1	0.95	0.33	-	60,60,60,60	0
56	MG	1a	1843	1/1	0.83	0.40	-	71,71,71,71	0
56	MG	1A	3046	1/1	0.95	0.07	-	60,60,60,60	0
56	MG	1A	3021	1/1	0.90	0.24	-	48,48,48,48	0
56	MG	1A	3594	1/1	0.95	0.20	-	62,62,62,62	0
56	MG	2A	3013	1/1	0.72	0.25	-	67,67,67,67	0
56	MG	1A	4023	1/1	0.95	0.24	-	40,40,40,40	0
56	MG	1A	3429	1/1	0.97	0.29	-	53,53,53,53	0
56	MG	1a	1611	1/1	0.92	0.16	-	85,85,85,85	0
56	MG	2a	3108	1/1	0.81	0.07	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3010	1/1	0.92	0.43	-	51,51,51,51	0
56	MG	2A	3361	1/1	0.91	0.05	-	72,72,72,72	0
56	MG	1A	3629	1/1	0.98	0.27	-	58,58,58,58	0
56	MG	2a	3079	1/1	0.94	0.48	-	55,55,55,55	0
56	MG	2A	3279	1/1	0.94	0.34	-	71,71,71,71	0
56	MG	1A	3939	1/1	0.94	0.24	-	57,57,57,57	0
56	MG	2A	3094	1/1	0.92	0.24	-	48,48,48,48	0
56	MG	1A	3989	1/1	0.94	0.07	-	70,70,70,70	0
56	MG	1A	3667	1/1	0.94	0.16	-	42,42,42,42	0
56	MG	1A	3144	1/1	0.98	0.17	-	22,22,22,22	0
56	MG	2A	3312	1/1	0.95	0.23	-	39,39,39,39	0
56	MG	1A	3861	1/1	0.81	0.10	-	68,68,68,68	0
56	MG	1A	3574	1/1	0.84	0.16	-	57,57,57,57	0
56	MG	2A	3336	1/1	0.97	0.24	-	49,49,49,49	0
56	MG	1A	3477	1/1	0.90	0.24	-	67,67,67,67	0
56	MG	2A	3071	1/1	0.95	0.53	-	56,56,56,56	0
56	MG	2F	302	1/1	0.94	0.09	-	44,44,44,44	0
56	MG	1A	3008	1/1	0.95	0.23	-	51,51,51,51	0
56	MG	1A	3993	1/1	0.91	0.13	-	73,73,73,73	0
56	MG	1a	1837	1/1	0.97	0.34	-	50,50,50,50	0
56	MG	19	504	1/1	0.95	0.11	-	56,56,56,56	0
56	MG	1a	1720	1/1	0.98	0.33	-	43,43,43,43	0
56	MG	1A	3164	1/1	0.97	0.41	-	51,51,51,51	0
56	MG	1A	3631	1/1	0.91	0.15	-	55,55,55,55	0
56	MG	1a	1615	1/1	0.95	0.30	-	83,83,83,83	0
56	MG	1A	3253	1/1	0.86	0.09	-	81,81,81,81	0
56	MG	2A	3034	1/1	0.97	0.12	-	61,61,61,61	0
56	MG	1A	3468	1/1	0.93	0.15	-	59,59,59,59	0
56	MG	1a	1812	1/1	0.88	0.27	-	78,78,78,78	0
56	MG	2A	3496	1/1	0.96	0.14	-	59,59,59,59	0
56	MG	2A	3433	1/1	0.96	0.12	-	62,62,62,62	0
56	MG	2E	305	1/1	0.83	0.19	-	68,68,68,68	0
56	MG	1A	3273	1/1	0.96	0.54	-	45,45,45,45	0
56	MG	1A	3249	1/1	0.91	0.28	-	53,53,53,53	0
56	MG	2A	3462	1/1	0.92	0.41	-	74,74,74,74	0
56	MG	1A	3760	1/1	0.97	0.17	-	42,42,42,42	0
56	MG	1A	3073	1/1	0.70	0.19	-	74,74,74,74	0
56	MG	1A	3061	1/1	0.93	0.51	-	51,51,51,51	0
56	MG	1a	1767	1/1	0.86	0.08	-	84,84,84,84	0
56	MG	2a	3193	1/1	0.94	0.24	-	76,76,76,76	0
56	MG	1A	3840	1/1	0.95	0.25	-	67,67,67,67	0
56	MG	2A	3129	1/1	0.97	0.07	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1884	1/1	0.89	0.29	-	56,56,56,56	0
56	MG	1a	1783	1/1	0.86	0.20	-	75,75,75,75	0
56	MG	1A	3966	1/1	0.89	0.09	-	52,52,52,52	0
56	MG	1A	3848	1/1	0.82	0.17	-	57,57,57,57	0
56	MG	1a	1706	1/1	0.96	0.12	-	52,52,52,52	0
56	MG	1A	3928	1/1	0.99	0.21	-	51,51,51,51	0
56	MG	1A	3411	1/1	0.92	0.18	-	51,51,51,51	0
56	MG	1Q	3005	1/1	0.89	0.16	-	53,53,53,53	0
56	MG	1B	225	1/1	0.87	0.16	-	77,77,77,77	0
56	MG	1A	3816	1/1	0.92	0.10	-	67,67,67,67	0
56	MG	2a	3135	1/1	0.93	0.11	-	61,61,61,61	0
56	MG	1A	3890	1/1	0.96	0.11	-	62,62,62,62	0
56	MG	1A	3908	1/1	0.97	0.15	-	20,20,20,20	0
56	MG	1A	3523	1/1	0.91	0.16	-	59,59,59,59	0
56	MG	1a	1647	1/1	0.94	0.11	-	58,58,58,58	0
56	MG	2A	3211	1/1	0.92	0.15	-	52,52,52,52	0
56	MG	1a	1808	1/1	0.93	0.41	-	85,85,85,85	0
56	MG	2A	3339	1/1	0.90	0.14	-	55,55,55,55	0
56	MG	1a	1894	1/1	0.91	0.45	-	56,56,56,56	0
56	MG	2a	3132	1/1	0.92	0.13	-	71,71,71,71	0
56	MG	1A	3609	1/1	0.89	0.24	-	28,28,28,28	0
56	MG	1A	3453	1/1	0.95	0.23	-	49,49,49,49	0
56	MG	2a	3162	1/1	0.83	0.15	-	47,47,47,47	0
56	MG	1a	1842	1/1	0.98	0.18	-	61,61,61,61	0
56	MG	2A	3140	1/1	0.95	0.32	-	62,62,62,62	0
56	MG	1A	3455	1/1	0.97	0.32	-	52,52,52,52	0
56	MG	1a	1680	1/1	0.93	0.18	-	57,57,57,57	0
56	MG	2A	3112	1/1	0.94	0.21	-	36,36,36,36	0
56	MG	1A	3593	1/1	0.92	0.23	-	30,30,30,30	0
56	MG	1x	106	1/1	0.81	0.30	-	54,54,54,54	0
56	MG	2a	3149	1/1	0.37	0.77	-	100,100,100,100	0
56	MG	1A	3657	1/1	0.97	0.12	-	19,19,19,19	0
56	MG	1W	3001	1/1	0.94	0.28	-	52,52,52,52	0
56	MG	1A	3428	1/1	0.93	0.10	-	55,55,55,55	0
56	MG	2A	3170	1/1	0.94	0.17	-	35,35,35,35	0
56	MG	1A	3255	1/1	0.90	0.25	-	44,44,44,44	0
56	MG	1A	3712	1/1	0.95	0.08	-	58,58,58,58	0
56	MG	2A	3023	1/1	0.67	0.15	-	55,55,55,55	0
56	MG	1k	3001	1/1	0.87	0.29	-	65,65,65,65	0
56	MG	2a	3219	1/1	0.96	0.09	-	58,58,58,58	0
56	MG	1A	3501	1/1	0.79	0.31	-	83,83,83,83	0
56	MG	1A	3085	1/1	0.96	0.19	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3252	1/1	0.86	0.37	-	53,53,53,53	0
56	MG	1A	3099	1/1	0.94	0.30	-	42,42,42,42	0
56	MG	1A	3580	1/1	0.82	0.24	-	68,68,68,68	0
56	MG	1A	3322	1/1	0.83	0.26	-	63,63,63,63	0
56	MG	2A	3348	1/1	0.98	0.12	-	72,72,72,72	0
56	MG	1a	1851	1/1	0.96	0.17	-	49,49,49,49	0
56	MG	1A	4020	1/1	0.62	0.50	-	67,67,67,67	0
56	MG	10	103	1/1	0.90	0.12	-	69,69,69,69	0
56	MG	1A	3219	1/1	0.80	0.20	-	63,63,63,63	0
56	MG	1A	3067	1/1	0.71	0.14	-	64,64,64,64	0
56	MG	1A	3674	1/1	0.94	0.11	-	30,30,30,30	0
56	MG	1A	3089	1/1	0.95	0.32	-	44,44,44,44	0
56	MG	2a	3120	1/1	0.88	0.23	-	66,66,66,66	0
56	MG	1a	1631	1/1	0.93	0.24	-	44,44,44,44	0
56	MG	2a	3143	1/1	0.90	0.13	-	90,90,90,90	0
56	MG	2A	3167	1/1	0.69	0.23	-	58,58,58,58	0
56	MG	1A	3833	1/1	0.95	0.15	-	56,56,56,56	0
56	MG	1A	3492	1/1	0.77	0.15	-	81,81,81,81	0
56	MG	1A	3845	1/1	0.96	0.20	-	57,57,57,57	0
56	MG	1A	3808	1/1	0.90	0.39	-	57,57,57,57	0
56	MG	2A	3136	1/1	0.93	0.16	-	45,45,45,45	0
56	MG	2a	3189	1/1	0.94	0.23	-	57,57,57,57	0
56	MG	2A	3427	1/1	0.95	0.23	-	68,68,68,68	0
56	MG	2A	3493	1/1	0.96	0.14	-	41,41,41,41	0
56	MG	2a	3052	1/1	0.95	0.13	-	73,73,73,73	0
56	MG	1A	3459	1/1	0.75	0.34	-	57,57,57,57	0
56	MG	2A	3031	1/1	0.97	0.23	-	55,55,55,55	0
56	MG	1A	3088	1/1	0.93	0.17	-	52,52,52,52	0
56	MG	1A	3591	1/1	0.97	0.13	-	45,45,45,45	0
56	MG	1a	1692	1/1	0.96	0.09	-	50,50,50,50	0
56	MG	1a	1868	1/1	0.98	0.18	-	49,49,49,49	0
56	MG	2A	3469	1/1	0.56	0.47	-	67,67,67,67	0
56	MG	2a	3202	1/1	0.98	0.12	-	70,70,70,70	0
56	MG	2A	3131	1/1	0.90	0.17	-	48,48,48,48	0
56	MG	1B	213	1/1	0.93	0.41	-	65,65,65,65	0
56	MG	1a	1761	1/1	0.92	0.23	-	66,66,66,66	0
56	MG	1A	3798	1/1	0.83	0.14	-	59,59,59,59	0
56	MG	1A	3898	1/1	0.97	0.18	-	36,36,36,36	0
56	MG	1A	3710	1/1	0.85	0.08	-	48,48,48,48	0
56	MG	1A	3870	1/1	0.88	0.06	-	41,41,41,41	0
56	MG	2A	3381	1/1	0.96	0.32	-	45,45,45,45	0
56	MG	1H	201	1/1	0.88	0.52	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3229	1/1	0.96	0.14	-	55,55,55,55	0
56	MG	1A	3270	1/1	0.78	0.34	-	63,63,63,63	0
56	MG	1O	202	1/1	0.98	0.12	-	51,51,51,51	0
56	MG	1A	3747	1/1	0.98	0.18	-	28,28,28,28	0
56	MG	1A	3571	1/1	0.90	0.10	-	66,66,66,66	0
56	MG	1A	3328	1/1	0.93	0.12	-	56,56,56,56	0
56	MG	1a	1697	1/1	0.71	0.30	-	70,70,70,70	0
56	MG	2A	3347	1/1	0.95	0.12	-	55,55,55,55	0
56	MG	2O	203	1/1	0.92	0.20	-	57,57,57,57	0
56	MG	1a	1750	1/1	0.79	0.22	-	72,72,72,72	0
56	MG	2a	3070	1/1	0.96	0.30	-	57,57,57,57	0
56	MG	2A	3197	1/1	0.95	0.09	-	47,47,47,47	0
56	MG	1A	3815	1/1	0.81	0.23	-	52,52,52,52	0
56	MG	1A	3020	1/1	0.93	0.26	-	56,56,56,56	0
56	MG	1A	3070	1/1	0.89	0.17	-	65,65,65,65	0
56	MG	1a	1756	1/1	0.83	0.40	-	93,93,93,93	0
56	MG	2a	3086	1/1	0.91	0.48	-	65,65,65,65	0
56	MG	1A	3775	1/1	0.98	0.22	-	22,22,22,22	0
56	MG	1A	3579	1/1	0.97	0.19	-	49,49,49,49	0
56	MG	1a	1759	1/1	0.93	0.10	-	82,82,82,82	0
56	MG	2A	3177	1/1	0.98	0.37	-	40,40,40,40	0
56	MG	1a	1784	1/1	0.90	0.11	-	73,73,73,73	0
56	MG	1A	3433	1/1	0.91	0.18	-	50,50,50,50	0
56	MG	2A	3017	1/1	0.96	0.22	-	52,52,52,52	0
56	MG	1A	3181	1/1	0.98	0.39	-	46,46,46,46	0
56	MG	1A	3906	1/1	0.90	0.09	-	42,42,42,42	0
56	MG	2a	3101	1/1	0.87	0.32	-	64,64,64,64	0
56	MG	1a	1636	1/1	0.95	0.22	-	68,68,68,68	0
56	MG	1A	3899	1/1	0.90	0.25	-	53,53,53,53	0
56	MG	1A	3080	1/1	0.90	0.15	-	52,52,52,52	0
56	MG	2A	3088	1/1	0.78	0.20	-	46,46,46,46	0
56	MG	2A	3503	1/1	0.88	0.18	-	61,61,61,61	0
56	MG	1a	1818	1/1	0.94	0.20	-	78,78,78,78	0
56	MG	1A	3315	1/1	0.90	0.10	-	51,51,51,51	0
56	MG	1A	3462	1/1	0.89	0.25	-	45,45,45,45	0
56	MG	2A	3103	1/1	0.97	0.12	-	50,50,50,50	0
56	MG	1A	3600	1/1	0.87	0.23	-	31,31,31,31	0
56	MG	2a	3067	1/1	0.99	0.17	-	56,56,56,56	0
56	MG	1A	3260	1/1	0.93	0.18	-	49,49,49,49	0
56	MG	2A	3158	1/1	0.97	0.21	-	52,52,52,52	0
56	MG	1A	3602	1/1	0.97	0.21	-	41,41,41,41	0
56	MG	1A	3338	1/1	0.92	0.09	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3396	1/1	0.92	0.15	-	44,44,44,44	0
56	MG	1a	1634	1/1	0.95	0.39	-	66,66,66,66	0
56	MG	1A	3512	1/1	0.85	0.12	-	53,53,53,53	0
56	MG	2A	3404	1/1	0.77	0.17	-	69,69,69,69	0
56	MG	2A	3247	1/1	0.95	0.26	-	63,63,63,63	0
56	MG	1A	3355	1/1	0.95	0.09	-	51,51,51,51	0
56	MG	1A	3555	1/1	0.99	0.12	-	39,39,39,39	0
56	MG	1H	204	1/1	0.90	0.31	-	62,62,62,62	0
56	MG	2B	3004	1/1	0.89	0.25	-	59,59,59,59	0
56	MG	1R	206	1/1	0.95	0.18	-	34,34,34,34	0
56	MG	2a	3226	1/1	0.95	0.41	-	75,75,75,75	0
56	MG	1A	3868	1/1	0.89	0.17	-	65,65,65,65	0
56	MG	2a	3204	1/1	0.93	0.20	-	62,62,62,62	0
56	MG	1A	3427	1/1	0.95	0.32	-	41,41,41,41	0
56	MG	1a	1838	1/1	0.98	0.22	-	62,62,62,62	0
56	MG	1A	3649	1/1	0.95	0.07	-	28,28,28,28	0
56	MG	2a	3137	1/1	0.37	0.23	-	97,97,97,97	0
56	MG	1A	3663	1/1	0.95	0.28	-	55,55,55,55	0
56	MG	2A	3425	1/1	0.94	0.45	-	72,72,72,72	0
56	MG	2A	3258	1/1	0.97	0.20	-	32,32,32,32	0
56	MG	1A	3059	1/1	0.97	0.06	-	46,46,46,46	0
56	MG	1A	3734	1/1	0.95	0.17	-	27,27,27,27	0
56	MG	2A	3033	1/1	0.97	0.23	-	55,55,55,55	0
56	MG	1A	3376	1/1	0.88	0.16	-	60,60,60,60	0
56	MG	2A	3072	1/1	0.94	0.24	-	55,55,55,55	0
56	MG	1A	3036	1/1	0.92	0.24	-	52,52,52,52	0
56	MG	1a	1872	1/1	0.90	0.19	-	67,67,67,67	0
56	MG	1A	3423	1/1	0.97	0.14	-	62,62,62,62	0
56	MG	1A	3323	1/1	0.86	0.11	-	46,46,46,46	0
56	MG	2a	3062	1/1	0.98	0.11	-	66,66,66,66	0
56	MG	20	8001	1/1	0.91	0.17	-	72,72,72,72	0
56	MG	2a	3145	1/1	0.94	0.12	-	91,91,91,91	0
56	MG	1A	3785	1/1	0.97	0.09	-	57,57,57,57	0
56	MG	1A	3218	1/1	0.95	0.19	-	52,52,52,52	0
56	MG	1A	3527	1/1	0.86	0.20	-	32,32,32,32	0
56	MG	1l	201	1/1	0.93	0.10	-	62,62,62,62	0
56	MG	2a	3061	1/1	0.94	0.15	-	72,72,72,72	0
56	MG	2A	3284	1/1	0.98	0.22	-	65,65,65,65	0
56	MG	1A	4006	1/1	0.88	0.23	-	77,77,77,77	0
56	MG	2a	3008	1/1	0.96	0.22	-	60,60,60,60	0
56	MG	1A	3880	1/1	0.96	0.10	-	42,42,42,42	0
56	MG	2A	3510	1/1	0.95	0.25	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3028	1/1	0.91	0.09	-	58,58,58,58	0
56	MG	1A	3632	1/1	0.96	0.24	-	45,45,45,45	0
56	MG	2A	3016	1/1	0.94	0.26	-	59,59,59,59	0
56	MG	2a	3191	1/1	0.83	0.26	-	66,66,66,66	0
56	MG	1A	3947	1/1	0.99	0.06	-	37,37,37,37	0
56	MG	1Y	502	1/1	0.89	0.33	-	59,59,59,59	0
56	MG	1A	4045	1/1	0.94	0.70	-	50,50,50,50	0
56	MG	1A	3742	1/1	0.97	0.39	-	60,60,60,60	0
56	MG	2a	3033	1/1	0.92	0.13	-	76,76,76,76	0
56	MG	1A	3321	1/1	0.95	0.44	-	52,52,52,52	0
56	MG	2a	3213	1/1	0.66	0.14	-	87,87,87,87	0
56	MG	1A	3213	1/1	0.97	0.12	-	23,23,23,23	0
56	MG	1q	204	1/1	0.95	0.10	-	58,58,58,58	0
56	MG	1A	3971	1/1	0.92	0.23	-	61,61,61,61	0
56	MG	1A	3187	1/1	0.96	0.10	-	54,54,54,54	0
56	MG	19	502	1/1	0.95	0.22	-	46,46,46,46	0
56	MG	1a	1834	1/1	0.89	0.17	-	72,72,72,72	0
56	MG	1E	302	1/1	0.98	0.19	-	19,19,19,19	0
56	MG	1A	3467	1/1	0.95	0.21	-	44,44,44,44	0
56	MG	1c	3001	1/1	0.90	0.21	-	68,68,68,68	0
56	MG	1A	3293	1/1	0.95	0.17	-	36,36,36,36	0
56	MG	2A	3180	1/1	0.87	0.71	-	52,52,52,52	0
56	MG	2A	3280	1/1	0.91	0.15	-	46,46,46,46	0
56	MG	2a	3006	1/1	0.90	0.10	-	66,66,66,66	0
56	MG	2A	3061	1/1	0.94	0.29	-	44,44,44,44	0
56	MG	1A	3772	1/1	0.97	0.09	-	61,61,61,61	0
56	MG	2a	3014	1/1	0.73	0.23	-	74,74,74,74	0
56	MG	1A	3314	1/1	0.90	0.24	-	57,57,57,57	0
56	MG	2A	3115	1/1	0.95	0.34	-	54,54,54,54	0
56	MG	2A	3275	1/1	0.92	0.21	-	34,34,34,34	0
56	MG	1a	1897	1/1	0.88	0.11	-	50,50,50,50	0
56	MG	2A	3067	1/1	0.97	0.17	-	57,57,57,57	0
56	MG	1A	3068	1/1	0.79	0.10	-	67,67,67,67	0
56	MG	1A	3114	1/1	0.94	0.35	-	48,48,48,48	0
56	MG	1A	3915	1/1	0.94	0.17	-	38,38,38,38	0
56	MG	2a	3035	1/1	0.86	0.06	-	76,76,76,76	0
56	MG	2A	3415	1/1	0.95	0.27	-	43,43,43,43	0
56	MG	2A	3367	1/1	0.85	0.10	-	52,52,52,52	0
56	MG	1A	3347	1/1	0.97	0.16	-	41,41,41,41	0
56	MG	2a	3171	1/1	0.78	0.13	-	77,77,77,77	0
56	MG	1a	1771	1/1	0.87	0.20	-	75,75,75,75	0
56	MG	1A	3618	1/1	0.98	0.17	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3118	1/1	0.96	0.30	-	56,56,56,56	0
56	MG	2A	3134	1/1	0.92	0.15	-	35,35,35,35	0
56	MG	1A	3622	1/1	0.98	0.14	-	21,21,21,21	0
56	MG	1A	3450	1/1	0.76	0.22	-	64,64,64,64	0
56	MG	1A	3802	1/1	0.98	0.16	-	64,64,64,64	0
56	MG	1A	3646	1/1	0.95	0.14	-	21,21,21,21	0
56	MG	1A	3379	1/1	0.91	0.19	-	47,47,47,47	0
56	MG	1A	3639	1/1	0.98	0.14	-	11,11,11,11	0
56	MG	2R	8001	1/1	0.95	0.17	-	50,50,50,50	0
56	MG	1a	1628	1/1	0.80	0.24	-	57,57,57,57	0
56	MG	1A	3990	1/1	0.87	0.13	-	64,64,64,64	0
56	MG	1A	3335	1/1	0.95	0.12	-	43,43,43,43	0
56	MG	2a	3118	1/1	0.98	0.26	-	68,68,68,68	0
56	MG	2A	3190	1/1	0.79	0.39	-	61,61,61,61	0
56	MG	1A	3856	1/1	0.96	0.20	-	52,52,52,52	0
56	MG	1A	3834	1/1	0.90	0.17	-	58,58,58,58	0
56	MG	1A	4025	1/1	0.90	0.19	-	51,51,51,51	0
56	MG	26	101	1/1	0.89	0.15	-	46,46,46,46	0
56	MG	1A	3138	1/1	0.96	0.11	-	55,55,55,55	0
56	MG	2A	3452	1/1	0.96	0.13	-	59,59,59,59	0
56	MG	1A	3650	1/1	0.93	0.30	-	46,46,46,46	0
56	MG	1A	3885	1/1	0.96	0.11	-	56,56,56,56	0
56	MG	2a	3114	1/1	0.94	0.14	-	70,70,70,70	0
56	MG	1A	3914	1/1	0.97	0.23	-	22,22,22,22	0
56	MG	1A	3967	1/1	0.95	0.14	-	53,53,53,53	0
56	MG	1a	1823	1/1	0.84	0.22	-	69,69,69,69	0
56	MG	2A	3289	1/1	0.97	0.37	-	44,44,44,44	0
56	MG	2A	3518	1/1	0.91	0.17	-	67,67,67,67	0
56	MG	1A	3804	1/1	0.96	0.10	-	50,50,50,50	0
56	MG	2a	3066	1/1	0.98	0.10	-	50,50,50,50	0
56	MG	2a	3237	1/1	0.96	0.25	-	69,69,69,69	0
56	MG	1A	3332	1/1	0.95	0.23	-	61,61,61,61	0
56	MG	1A	3558	1/1	0.95	0.22	-	27,27,27,27	0
56	MG	1a	1625	1/1	0.83	0.09	-	78,78,78,78	0
56	MG	1A	3091	1/1	0.82	0.17	-	61,61,61,61	0
56	MG	2A	3508	1/1	0.96	0.07	-	61,61,61,61	0
56	MG	2A	3538	1/1	0.93	0.19	-	52,52,52,52	0
56	MG	1A	3283	1/1	0.91	0.18	-	60,60,60,60	0
56	MG	2A	3090	1/1	0.95	0.10	-	51,51,51,51	0
56	MG	2A	3152	1/1	0.96	0.16	-	48,48,48,48	0
56	MG	1A	3970	1/1	0.88	0.37	-	53,53,53,53	0
56	MG	1A	3936	1/1	0.82	0.20	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1609	1/1	0.79	0.28	-	60,60,60,60	0
56	MG	1A	3268	1/1	0.72	0.36	-	50,50,50,50	0
56	MG	1A	3436	1/1	0.87	0.19	-	68,68,68,68	0
56	MG	1a	1780	1/1	0.39	0.25	-	93,93,93,93	0
56	MG	1A	3550	1/1	0.83	0.18	-	58,58,58,58	0
56	MG	2a	3218	1/1	0.99	0.23	-	55,55,55,55	0
56	MG	2A	3257	1/1	0.86	0.14	-	62,62,62,62	0
56	MG	1A	3051	1/1	0.92	0.16	-	57,57,57,57	0
56	MG	2a	3082	1/1	0.80	0.42	-	61,61,61,61	0
56	MG	1A	4028	1/1	0.98	0.12	-	68,68,68,68	0
56	MG	1A	3431	1/1	0.95	0.14	-	14,14,14,14	0
56	MG	2A	3286	1/1	0.91	0.19	-	47,47,47,47	0
56	MG	1E	305	1/1	0.92	0.24	-	58,58,58,58	0
56	MG	14	502	1/1	0.86	0.13	-	79,79,79,79	0
56	MG	2A	3058	1/1	0.83	0.14	-	56,56,56,56	0
56	MG	1A	3295	1/1	0.97	0.12	-	63,63,63,63	0
56	MG	2a	3064	1/1	0.98	0.45	-	51,51,51,51	0
56	MG	2A	3532	1/1	0.97	0.16	-	56,56,56,56	0
56	MG	2A	3234	1/1	0.94	0.49	-	52,52,52,52	0
56	MG	1F	307	1/1	0.97	0.39	-	49,49,49,49	0
56	MG	2A	3476	1/1	0.98	0.10	-	45,45,45,45	0
56	MG	1A	3200	1/1	0.90	0.16	-	54,54,54,54	0
56	MG	1A	3318	1/1	0.92	0.12	-	46,46,46,46	0
56	MG	1E	307	1/1	0.78	0.40	-	74,74,74,74	0
56	MG	2A	3095	1/1	0.82	0.19	-	48,48,48,48	0
56	MG	1A	3810	1/1	0.97	0.20	-	63,63,63,63	0
56	MG	2A	3012	1/1	0.97	0.10	-	52,52,52,52	0
56	MG	1a	1795	1/1	0.90	0.22	-	64,64,64,64	0
56	MG	1A	3394	1/1	0.93	0.10	-	58,58,58,58	0
56	MG	2Q	205	1/1	0.91	0.26	-	57,57,57,57	0
56	MG	1A	3161	1/1	0.93	0.17	-	61,61,61,61	0
56	MG	2a	3185	1/1	0.92	0.21	-	79,79,79,79	0
56	MG	1a	1832	1/1	0.96	0.27	-	54,54,54,54	0
56	MG	2a	3229	1/1	0.97	0.29	-	66,66,66,66	0
56	MG	1A	3291	1/1	0.88	0.22	-	55,55,55,55	0
56	MG	1A	3066	1/1	0.82	0.43	-	63,63,63,63	0
56	MG	2A	3128	1/1	0.95	0.38	-	61,61,61,61	0
56	MG	1A	3296	1/1	0.90	0.08	-	47,47,47,47	0
56	MG	2a	3071	1/1	0.87	0.19	-	58,58,58,58	0
56	MG	1A	3483	1/1	0.92	0.26	-	65,65,65,65	0
56	MG	1A	3032	1/1	0.96	0.11	-	65,65,65,65	0
56	MG	1A	3369	1/1	0.93	0.22	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3854	1/1	0.90	0.07	-	76,76,76,76	0
56	MG	2a	3084	1/1	0.89	0.20	-	75,75,75,75	0
56	MG	1A	3682	1/1	0.98	0.05	-	59,59,59,59	0
56	MG	1A	3481	1/1	0.63	0.29	-	76,76,76,76	0
56	MG	1a	1648	1/1	0.91	0.23	-	64,64,64,64	0
56	MG	2A	3365	1/1	0.99	0.15	-	44,44,44,44	0
56	MG	1A	3495	1/1	0.85	0.43	-	51,51,51,51	0
56	MG	18	103	1/1	0.91	0.12	-	49,49,49,49	0
56	MG	2A	3453	1/1	0.99	0.19	-	83,83,83,83	0
56	MG	1A	3487	1/1	0.87	0.37	-	64,64,64,64	0
56	MG	2A	3151	1/1	0.90	0.17	-	45,45,45,45	0
56	MG	2A	3216	1/1	0.96	0.34	-	44,44,44,44	0
56	MG	1A	3739	1/1	0.92	0.18	-	22,22,22,22	0
56	MG	1A	3461	1/1	0.84	0.49	-	46,46,46,46	0
56	MG	1A	3514	1/1	0.77	0.12	-	72,72,72,72	0
56	MG	2a	3109	1/1	0.82	0.41	-	73,73,73,73	0
56	MG	1A	3330	1/1	0.92	0.27	-	62,62,62,62	0
56	MG	1A	3344	1/1	0.89	0.13	-	54,54,54,54	0
56	MG	1a	1632	1/1	0.96	0.25	-	53,53,53,53	0
56	MG	1A	3343	1/1	0.93	0.28	-	31,31,31,31	0
56	MG	1A	3940	1/1	0.71	0.42	-	78,78,78,78	0
56	MG	1A	3910	1/1	0.98	0.25	-	34,34,34,34	0
56	MG	2A	3263	1/1	0.95	0.23	-	24,24,24,24	0
56	MG	1A	3397	1/1	0.88	0.12	-	47,47,47,47	0
56	MG	2A	3509	1/1	0.72	0.14	-	80,80,80,80	0
56	MG	1O	201	1/1	0.85	0.41	-	54,54,54,54	0
56	MG	2A	3338	1/1	0.89	0.21	-	54,54,54,54	0
56	MG	2A	3491	1/1	0.91	0.11	-	39,39,39,39	0
56	MG	2A	3165	1/1	0.94	0.12	-	54,54,54,54	0
56	MG	1A	3486	1/1	0.84	0.20	-	65,65,65,65	0
56	MG	1A	3746	1/1	0.98	0.15	-	15,15,15,15	0
56	MG	1a	1624	1/1	0.96	0.30	-	65,65,65,65	0
56	MG	1r	3002	1/1	0.59	0.22	-	85,85,85,85	0
56	MG	1A	3852	1/1	0.85	0.21	-	72,72,72,72	0
56	MG	1a	1745	1/1	0.86	0.19	-	62,62,62,62	0
56	MG	1A	3976	1/1	0.88	0.23	-	49,49,49,49	0
56	MG	2A	3380	1/1	0.90	0.17	-	45,45,45,45	0
56	MG	1A	3414	1/1	0.87	0.10	-	79,79,79,79	0
56	MG	1A	3565	1/1	0.99	0.18	-	17,17,17,17	0
56	MG	1A	3058	1/1	0.87	0.06	-	49,49,49,49	0
56	MG	1a	1728	1/1	0.89	0.30	-	55,55,55,55	0
56	MG	1A	3307	1/1	0.94	0.10	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3835	1/1	0.95	0.24	-	49,49,49,49	0
56	MG	1A	3284	1/1	0.85	0.37	-	52,52,52,52	0
56	MG	1A	3557	1/1	0.94	0.12	-	44,44,44,44	0
56	MG	2a	3088	1/1	0.88	0.20	-	73,73,73,73	0
56	MG	1A	3251	1/1	0.78	0.23	-	60,60,60,60	0
56	MG	1a	1805	1/1	0.80	0.10	-	70,70,70,70	0
56	MG	2a	3179	1/1	0.95	0.06	-	47,47,47,47	0
56	MG	2A	3537	1/1	0.94	0.29	-	59,59,59,59	0
56	MG	1A	3261	1/1	0.85	0.26	-	68,68,68,68	0
56	MG	1A	3208	1/1	0.92	0.08	-	57,57,57,57	0
56	MG	1A	3216	1/1	0.97	0.17	-	66,66,66,66	0
56	MG	2a	3186	1/1	0.74	0.14	-	80,80,80,80	0
56	MG	1A	3408	1/1	0.90	0.05	-	66,66,66,66	0
56	MG	2d	502	1/1	0.94	0.56	-	61,61,61,61	0
56	MG	2a	3032	1/1	0.96	0.07	-	65,65,65,65	0
56	MG	2A	3489	1/1	0.93	0.32	-	43,43,43,43	0
56	MG	2a	3004	1/1	0.39	0.68	-	87,87,87,87	0
56	MG	2a	3136	1/1	0.97	0.25	-	72,72,72,72	0
56	MG	2a	3166	1/1	0.96	0.24	-	63,63,63,63	0
56	MG	1A	3480	1/1	0.92	0.18	-	75,75,75,75	0
56	MG	1A	3072	1/1	0.87	0.18	-	53,53,53,53	0
56	MG	1A	3953	1/1	0.95	0.18	-	61,61,61,61	0
56	MG	1A	3799	1/1	0.91	0.34	-	54,54,54,54	0
56	MG	1A	3043	1/1	0.89	0.16	-	49,49,49,49	0
56	MG	2A	3529	1/1	0.80	0.13	-	62,62,62,62	0
56	MG	2A	3068	1/1	0.78	0.22	-	68,68,68,68	0
56	MG	2a	3024	1/1	0.90	0.26	-	58,58,58,58	0
56	MG	2a	3081	1/1	0.89	0.22	-	69,69,69,69	0
56	MG	1a	1786	1/1	0.93	0.08	-	83,83,83,83	0
56	MG	1A	3484	1/1	0.91	0.12	-	70,70,70,70	0
56	MG	1A	3035	1/1	0.96	0.07	-	58,58,58,58	0
56	MG	1x	101	1/1	0.86	0.26	-	69,69,69,69	0
56	MG	1A	3513	1/1	0.85	0.09	-	72,72,72,72	0
56	MG	1a	1846	1/1	0.70	0.08	-	71,71,71,71	0
56	MG	1A	3679	1/1	0.87	0.23	-	51,51,51,51	0
56	MG	1A	3887	1/1	0.80	0.10	-	29,29,29,29	0
56	MG	2A	3414	1/1	0.98	0.20	-	39,39,39,39	0
56	MG	1A	3979	1/1	0.87	0.16	-	59,59,59,59	0
56	MG	2a	3141	1/1	0.92	0.18	-	57,57,57,57	0
56	MG	1A	3983	1/1	0.91	0.17	-	62,62,62,62	0
56	MG	1A	3395	1/1	0.81	0.17	-	59,59,59,59	0
56	MG	2A	3047	1/1	0.94	0.22	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3791	1/1	0.95	0.11	-	60,60,60,60	0
56	MG	2A	3526	1/1	0.93	0.22	-	54,54,54,54	0
56	MG	2a	3235	1/1	0.97	0.38	-	64,64,64,64	0
56	MG	1A	3836	1/1	0.94	0.11	-	36,36,36,36	0
56	MG	1A	3807	1/1	0.92	0.16	-	58,58,58,58	0
56	MG	1A	3055	1/1	0.92	0.19	-	55,55,55,55	0
56	MG	1F	303	1/1	0.93	0.16	-	40,40,40,40	0
56	MG	1x	102	1/1	0.88	0.07	-	69,69,69,69	0
56	MG	2a	3023	1/1	0.87	0.45	-	74,74,74,74	0
56	MG	1A	3787	1/1	0.87	0.11	-	45,45,45,45	0
56	MG	2A	3020	1/1	0.83	0.27	-	60,60,60,60	0
56	MG	1A	3640	1/1	0.91	0.09	-	70,70,70,70	0
56	MG	1A	3177	1/1	0.97	0.14	-	56,56,56,56	0
56	MG	1A	3526	1/1	0.94	0.14	-	50,50,50,50	0
56	MG	1A	3348	1/1	0.86	0.22	-	63,63,63,63	0
56	MG	2A	3026	1/1	0.94	0.10	-	56,56,56,56	0
56	MG	1A	3554	1/1	0.96	0.17	-	38,38,38,38	0
56	MG	1a	1642	1/1	0.80	0.82	-	68,68,68,68	0
56	MG	2A	3237	1/1	0.85	0.26	-	48,48,48,48	0
56	MG	2A	3461	1/1	0.86	0.15	-	78,78,78,78	0
56	MG	1A	3585	1/1	0.86	0.12	-	68,68,68,68	0
56	MG	2A	3523	1/1	0.92	0.19	-	57,57,57,57	0
56	MG	2A	3392	1/1	0.91	0.36	-	43,43,43,43	0
56	MG	2a	3098	1/1	0.99	0.16	-	49,49,49,49	0
56	MG	1A	3832	1/1	0.99	0.22	-	68,68,68,68	0
56	MG	1A	3288	1/1	0.81	0.17	-	70,70,70,70	0
56	MG	2A	3065	1/1	0.85	0.42	-	58,58,58,58	0
56	MG	2A	3187	1/1	0.90	0.19	-	53,53,53,53	0
56	MG	2a	3174	1/1	0.95	0.13	-	56,56,56,56	0
56	MG	2a	3041	1/1	0.82	0.25	-	79,79,79,79	0
56	MG	1A	3186	1/1	0.94	0.15	-	47,47,47,47	0
56	MG	1a	1679	1/1	0.97	0.15	-	52,52,52,52	0
56	MG	2a	3043	1/1	0.86	0.12	-	85,85,85,85	0
56	MG	1a	1796	1/1	0.96	0.17	-	50,50,50,50	0
56	MG	1a	1741	1/1	0.86	0.54	-	68,68,68,68	0
56	MG	1a	1764	1/1	0.96	0.13	-	67,67,67,67	0
56	MG	1A	3860	1/1	0.83	0.15	-	72,72,72,72	0
56	MG	2a	3127	1/1	0.92	0.28	-	51,51,51,51	0
56	MG	1A	3375	1/1	0.95	0.21	-	59,59,59,59	0
56	MG	2A	3206	1/1	0.80	0.09	-	64,64,64,64	0
56	MG	1A	3233	1/1	0.96	0.60	-	54,54,54,54	0
56	MG	1A	3917	1/1	0.94	0.25	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3144	1/1	0.96	0.22	-	53,53,53,53	0
56	MG	2a	3002	1/1	0.91	0.44	-	68,68,68,68	0
56	MG	1H	203	1/1	0.94	0.20	-	60,60,60,60	0
56	MG	2a	3201	1/1	0.88	0.13	-	83,83,83,83	0
56	MG	2A	3352	1/1	0.95	0.29	-	66,66,66,66	0
56	MG	2a	3110	1/1	0.83	0.16	-	53,53,53,53	0
56	MG	1A	3770	1/1	0.85	0.30	-	68,68,68,68	0
56	MG	2Q	202	1/1	0.95	0.16	-	51,51,51,51	0
56	MG	1A	3805	1/1	0.79	0.12	-	47,47,47,47	0
56	MG	1A	3451	1/1	0.79	0.42	-	81,81,81,81	0
56	MG	1A	3496	1/1	0.89	0.19	-	68,68,68,68	0
56	MG	1A	3857	1/1	0.95	0.14	-	51,51,51,51	0
56	MG	1A	3725	1/1	0.94	0.13	-	39,39,39,39	0
56	MG	2a	3028	1/1	0.88	0.49	-	61,61,61,61	0
56	MG	2A	3432	1/1	0.93	0.21	-	64,64,64,64	0
56	MG	2A	3073	1/1	0.91	0.30	-	37,37,37,37	0
56	MG	1a	1732	1/1	0.86	0.26	-	53,53,53,53	0
56	MG	1a	1623	1/1	0.96	0.23	-	79,79,79,79	0
56	MG	2A	3294	1/1	0.92	0.28	-	58,58,58,58	0
56	MG	2a	3180	1/1	0.93	0.09	-	79,79,79,79	0
56	MG	1A	3964	1/1	0.83	0.56	-	76,76,76,76	0
56	MG	2a	3092	1/1	0.95	0.46	-	65,65,65,65	0
56	MG	1a	1864	1/1	0.94	0.07	-	68,68,68,68	0
56	MG	1A	3814	1/1	0.95	0.17	-	58,58,58,58	0
56	MG	2a	3039	1/1	0.91	0.41	-	75,75,75,75	0
56	MG	1B	214	1/1	0.57	0.11	-	80,80,80,80	0
56	MG	1A	4005	1/1	0.94	0.17	-	31,31,31,31	0
56	MG	2a	3173	1/1	0.99	0.19	-	57,57,57,57	0
56	MG	1A	3180	1/1	0.99	0.12	-	50,50,50,50	0
56	MG	1A	3415	1/1	0.89	0.09	-	73,73,73,73	0
56	MG	1a	1652	1/1	0.87	0.21	-	65,65,65,65	0
56	MG	2B	3007	1/1	0.96	0.13	-	55,55,55,55	0
56	MG	1A	3537	1/1	0.95	0.14	-	37,37,37,37	0
56	MG	1A	3694	1/1	0.97	0.12	-	43,43,43,43	0
56	MG	1a	1638	1/1	0.75	0.23	-	57,57,57,57	0
56	MG	2A	3132	1/1	0.86	0.12	-	62,62,62,62	0
56	MG	1B	203	1/1	0.86	0.20	-	66,66,66,66	0
56	MG	1A	3312	1/1	0.94	0.17	-	60,60,60,60	0
56	MG	2A	3085	1/1	0.90	0.25	-	34,34,34,34	0
56	MG	2A	3199	1/1	0.95	0.35	-	47,47,47,47	0
56	MG	2A	3080	1/1	0.85	0.09	-	37,37,37,37	0
56	MG	1A	3156	1/1	0.96	0.40	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1x	103	1/1	0.94	0.11	-	70,70,70,70	0
56	MG	1A	3846	1/1	0.94	0.13	-	43,43,43,43	0
56	MG	1a	1803	1/1	0.83	0.21	-	80,80,80,80	0
56	MG	2a	3244	1/1	0.86	0.10	-	76,76,76,76	0
56	MG	1A	3716	1/1	0.86	0.22	-	53,53,53,53	0
56	MG	1A	3034	1/1	0.94	0.35	-	42,42,42,42	0
56	MG	1A	3069	1/1	0.78	0.17	-	65,65,65,65	0
56	MG	2a	3069	1/1	0.96	0.17	-	65,65,65,65	0
56	MG	1A	3242	1/1	0.97	0.32	-	48,48,48,48	0
56	MG	1a	1726	1/1	0.92	0.26	-	66,66,66,66	0
56	MG	2A	3399	1/1	0.94	0.16	-	49,49,49,49	0
56	MG	2A	3316	1/1	0.97	0.35	-	43,43,43,43	0
56	MG	2A	3229	1/1	0.85	0.26	-	46,46,46,46	0
56	MG	1a	1674	1/1	0.98	0.10	-	57,57,57,57	0
56	MG	1a	1733	1/1	0.99	0.51	-	53,53,53,53	0
56	MG	1A	3406	1/1	0.83	0.22	-	56,56,56,56	0
56	MG	1A	3944	1/1	0.94	0.27	-	19,19,19,19	0
56	MG	1A	4012	1/1	0.96	0.20	-	81,81,81,81	0
56	MG	10	102	1/1	0.88	0.07	-	56,56,56,56	0
56	MG	1A	3655	1/1	0.96	0.20	-	56,56,56,56	0
56	MG	1a	1682	1/1	0.87	0.11	-	70,70,70,70	0
56	MG	1a	1752	1/1	0.92	0.20	-	72,72,72,72	0
56	MG	1A	3797	1/1	0.98	0.13	-	73,73,73,73	0
56	MG	1A	3806	1/1	0.89	0.19	-	56,56,56,56	0
56	MG	2A	3230	1/1	0.91	0.49	-	51,51,51,51	0
56	MG	2A	3548	1/1	0.96	0.16	-	42,42,42,42	0
56	MG	2A	3248	1/1	0.98	0.18	-	56,56,56,56	0
56	MG	2A	3027	1/1	0.87	0.14	-	64,64,64,64	0
56	MG	2A	3082	1/1	0.91	0.16	-	56,56,56,56	0
56	MG	1A	3539	1/1	0.99	0.13	-	26,26,26,26	0
56	MG	1A	3932	1/1	0.96	0.27	-	46,46,46,46	0
56	MG	1A	3888	1/1	0.96	0.43	-	37,37,37,37	0
56	MG	1a	1853	1/1	0.92	0.06	-	56,56,56,56	0
56	MG	2a	3165	1/1	0.95	0.32	-	50,50,50,50	0
56	MG	1A	3851	1/1	0.93	0.25	-	42,42,42,42	0
56	MG	1a	1700	1/1	0.89	0.20	-	80,80,80,80	0
56	MG	2l	203	1/1	0.88	0.10	-	67,67,67,67	0
56	MG	2a	3134	1/1	0.88	0.48	-	79,79,79,79	0
56	MG	2A	3561	1/1	0.96	0.11	-	41,41,41,41	0
56	MG	1a	1861	1/1	0.92	0.25	-	68,68,68,68	0
56	MG	1A	3110	1/1	0.90	0.13	-	39,39,39,39	0
56	MG	1A	3157	1/1	0.97	0.29	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1758	1/1	0.89	0.08	-	64,64,64,64	0
56	MG	1A	3390	1/1	0.91	0.09	-	54,54,54,54	0
56	MG	2A	3192	1/1	0.87	0.14	-	45,45,45,45	0
56	MG	1T	205	1/1	0.77	0.16	-	66,66,66,66	0
56	MG	1A	3999	1/1	0.82	0.27	-	71,71,71,71	0
56	MG	2A	3417	1/1	0.89	0.19	-	62,62,62,62	0
56	MG	1a	1742	1/1	0.84	0.34	-	61,61,61,61	0
56	MG	2A	3454	1/1	0.96	0.21	-	58,58,58,58	0
56	MG	1A	3203	1/1	0.96	0.82	-	47,47,47,47	0
56	MG	1B	223	1/1	0.86	0.14	-	74,74,74,74	0
56	MG	2A	3556	1/1	0.98	0.20	-	41,41,41,41	0
56	MG	2A	3324	1/1	0.91	0.27	-	64,64,64,64	0
56	MG	1B	219	1/1	0.97	0.15	-	53,53,53,53	0
56	MG	1a	1878	1/1	0.92	0.08	-	78,78,78,78	0
56	MG	2a	3155	1/1	0.91	0.36	-	91,91,91,91	0
56	MG	1P	203	1/1	0.91	0.23	-	67,67,67,67	0
56	MG	2A	3388	1/1	0.84	0.20	-	46,46,46,46	0
56	MG	2A	3391	1/1	0.94	0.31	-	61,61,61,61	0
56	MG	2a	3183	1/1	0.94	0.34	-	54,54,54,54	0
56	MG	2a	3112	1/1	0.93	0.11	-	67,67,67,67	0
56	MG	1A	3388	1/1	0.93	0.29	-	42,42,42,42	0
56	MG	1a	1827	1/1	0.94	0.30	-	63,63,63,63	0
56	MG	1A	3474	1/1	0.89	0.34	-	59,59,59,59	0
56	MG	1A	3426	1/1	0.92	0.48	-	67,67,67,67	0
56	MG	1A	3722	1/1	0.96	0.22	-	56,56,56,56	0
56	MG	1A	3984	1/1	0.82	0.18	-	77,77,77,77	0
56	MG	2E	306	1/1	0.97	0.41	-	43,43,43,43	0
56	MG	1a	1735	1/1	0.78	0.10	-	72,72,72,72	0
56	MG	2A	3545	1/1	0.98	0.09	-	50,50,50,50	0
56	MG	1A	3817	1/1	0.93	0.28	-	61,61,61,61	0
56	MG	1A	3155	1/1	0.93	0.27	-	51,51,51,51	0
56	MG	1A	3227	1/1	0.87	0.10	-	65,65,65,65	0
56	MG	1r	3003	1/1	0.92	0.07	-	58,58,58,58	0
56	MG	1A	3220	1/1	0.93	0.22	-	43,43,43,43	0
56	MG	2A	3076	1/1	0.91	0.47	-	61,61,61,61	0
56	MG	2A	3250	1/1	0.96	0.12	-	61,61,61,61	0
56	MG	1A	3869	1/1	0.91	0.22	-	85,85,85,85	0
56	MG	2A	3463	1/1	0.97	0.12	-	58,58,58,58	0
56	MG	2A	3371	1/1	0.94	0.12	-	49,49,49,49	0
56	MG	1a	1622	1/1	0.77	0.28	-	74,74,74,74	0
56	MG	2x	3002	1/1	0.92	0.06	-	58,58,58,58	0
56	MG	1a	1743	1/1	0.92	0.98	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3079	1/1	0.98	0.25	-	51,51,51,51	0
56	MG	2A	3534	1/1	0.85	0.11	-	52,52,52,52	0
56	MG	2A	3318	1/1	0.96	0.48	-	64,64,64,64	0
56	MG	2A	3498	1/1	0.96	0.09	-	69,69,69,69	0
56	MG	2A	3113	1/1	0.90	0.08	-	54,54,54,54	0
56	MG	1R	202	1/1	0.95	0.25	-	68,68,68,68	0
56	MG	1A	3707	1/1	0.97	0.18	-	40,40,40,40	0
56	MG	1A	3206	1/1	0.97	0.11	-	51,51,51,51	0
56	MG	2A	3384	1/1	0.98	0.28	-	47,47,47,47	0
56	MG	1A	3281	1/1	0.97	0.19	-	59,59,59,59	0
56	MG	2a	3220	1/1	0.85	0.34	-	87,87,87,87	0
56	MG	1A	3478	1/1	0.96	0.45	-	51,51,51,51	0
56	MG	2A	3477	1/1	0.90	0.07	-	61,61,61,61	0
56	MG	1A	3503	1/1	0.74	0.29	-	82,82,82,82	0
56	MG	2A	3357	1/1	0.89	0.20	-	75,75,75,75	0
56	MG	2A	3320	1/1	0.88	0.19	-	67,67,67,67	0
56	MG	1A	3389	1/1	0.84	0.16	-	50,50,50,50	0
56	MG	2A	3236	1/1	0.92	0.29	-	41,41,41,41	0
56	MG	1A	3677	1/1	0.95	0.24	-	50,50,50,50	0
56	MG	1A	3362	1/1	0.96	0.45	-	42,42,42,42	0
56	MG	1A	3698	1/1	0.88	0.24	-	46,46,46,46	0
56	MG	1A	3691	1/1	0.93	0.27	-	59,59,59,59	0
56	MG	2A	3458	1/1	0.96	0.20	-	31,31,31,31	0
56	MG	18	101	1/1	0.89	0.19	-	66,66,66,66	0
56	MG	1a	1875	1/1	0.97	0.36	-	65,65,65,65	0
56	MG	2A	3497	1/1	0.91	0.24	-	49,49,49,49	0
56	MG	1A	3050	1/1	0.90	0.23	-	63,63,63,63	0
56	MG	2A	3270	1/1	0.94	0.29	-	61,61,61,61	0
56	MG	2A	3137	1/1	0.74	0.11	-	55,55,55,55	0
56	MG	2A	3512	1/1	0.90	0.09	-	40,40,40,40	0
56	MG	1a	1877	1/1	0.94	0.29	-	56,56,56,56	0
56	MG	2a	3040	1/1	0.79	0.36	-	83,83,83,83	0
56	MG	1A	3368	1/1	0.84	0.28	-	50,50,50,50	0
56	MG	1a	1824	1/1	0.79	0.50	-	52,52,52,52	0
56	MG	1A	3590	1/1	0.93	0.16	-	56,56,56,56	0
56	MG	1A	3160	1/1	0.89	0.13	-	42,42,42,42	0
56	MG	1A	3381	1/1	0.91	0.16	-	61,61,61,61	0
56	MG	1A	3048	1/1	0.85	0.24	-	41,41,41,41	0
56	MG	1B	221	1/1	0.84	0.16	-	63,63,63,63	0
56	MG	1A	3623	1/1	0.93	0.35	-	40,40,40,40	0
56	MG	2A	3117	1/1	0.90	0.37	-	51,51,51,51	0
56	MG	1A	3245	1/1	0.90	0.22	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1863	1/1	0.97	0.23	-	47,47,47,47	0
56	MG	1A	3244	1/1	0.70	0.31	-	55,55,55,55	0
56	MG	2A	3438	1/1	0.90	0.20	-	70,70,70,70	0
56	MG	1A	3886	1/1	0.97	0.17	-	42,42,42,42	0
56	MG	2a	3198	1/1	0.95	0.23	-	76,76,76,76	0
56	MG	1A	3383	1/1	0.88	0.17	-	51,51,51,51	0
56	MG	1a	1779	1/1	0.90	0.12	-	73,73,73,73	0
56	MG	1A	3929	1/1	0.98	0.16	-	27,27,27,27	0
56	MG	2A	3007	1/1	0.86	0.14	-	50,50,50,50	0
56	MG	2A	3422	1/1	0.87	0.24	-	52,52,52,52	0
56	MG	2A	3157	1/1	0.96	0.27	-	47,47,47,47	0
56	MG	1A	4002	1/1	0.81	0.21	-	71,71,71,71	0
56	MG	2A	3447	1/1	0.91	0.15	-	77,77,77,77	0
56	MG	2a	3037	1/1	0.85	0.19	-	72,72,72,72	0
56	MG	1A	3933	1/1	0.98	0.24	-	54,54,54,54	0
56	MG	2A	3551	1/1	0.97	0.57	-	55,55,55,55	0
56	MG	1h	3001	1/1	0.78	0.13	-	74,74,74,74	0
56	MG	2a	3131	1/1	0.90	0.06	-	63,63,63,63	0
56	MG	2A	3319	1/1	0.96	0.20	-	57,57,57,57	0
56	MG	1a	1797	1/1	0.96	0.19	-	42,42,42,42	0
56	MG	2A	3451	1/1	0.86	0.12	-	63,63,63,63	0
56	MG	1A	3374	1/1	0.94	0.12	-	59,59,59,59	0
56	MG	2A	3122	1/1	0.94	0.20	-	43,43,43,43	0
56	MG	2A	3436	1/1	0.95	0.37	-	68,68,68,68	0
56	MG	1A	3294	1/1	0.94	0.18	-	60,60,60,60	0
56	MG	2A	3406	1/1	0.98	0.23	-	49,49,49,49	0
56	MG	2A	3558	1/1	0.93	0.12	-	37,37,37,37	0
56	MG	1A	3889	1/1	0.96	0.08	-	53,53,53,53	0
56	MG	1D	317	1/1	0.93	0.22	-	69,69,69,69	0
56	MG	2A	3525	1/1	0.58	0.30	-	53,53,53,53	0
56	MG	1A	3641	1/1	0.95	0.14	-	22,22,22,22	0
56	MG	1a	1693	1/1	0.96	0.16	-	65,65,65,65	0
56	MG	1A	3476	1/1	0.70	0.22	-	66,66,66,66	0
56	MG	1A	3325	1/1	0.90	0.10	-	75,75,75,75	0
56	MG	1a	1845	1/1	0.96	0.26	-	52,52,52,52	0
56	MG	2A	3119	1/1	0.94	0.20	-	46,46,46,46	0
56	MG	1N	206	1/1	0.97	0.06	-	34,34,34,34	0
56	MG	1A	4019	1/1	0.89	0.50	-	93,93,93,93	0
56	MG	2A	3571	1/1	0.98	0.35	-	43,43,43,43	0
56	MG	2A	3546	1/1	0.97	0.13	-	42,42,42,42	0
56	MG	18	105	1/1	0.96	0.24	-	43,43,43,43	0
56	MG	1A	3637	1/1	0.96	0.22	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3353	1/1	0.94	0.20	-	57,57,57,57	0
56	MG	1a	1819	1/1	0.90	0.25	-	58,58,58,58	0
56	MG	1A	3735	1/1	0.98	0.16	-	27,27,27,27	0
56	MG	1a	1789	1/1	0.67	0.22	-	78,78,78,78	0
56	MG	2a	3106	1/1	0.94	0.18	-	59,59,59,59	0
56	MG	1A	3855	1/1	0.97	0.23	-	15,15,15,15	0
56	MG	2a	3215	1/1	0.99	0.34	-	80,80,80,80	0
56	MG	1a	1646	1/1	0.87	0.22	-	68,68,68,68	0
56	MG	1a	1871	1/1	0.97	0.18	-	58,58,58,58	0
56	MG	1A	3109	1/1	0.94	0.15	-	69,69,69,69	0
56	MG	1A	3926	1/1	0.94	0.16	-	66,66,66,66	0
56	MG	1A	3182	1/1	0.94	0.07	-	59,59,59,59	0
56	MG	2a	3015	1/1	0.94	0.28	-	79,79,79,79	0
56	MG	1A	3625	1/1	0.98	0.24	-	30,30,30,30	0
56	MG	2a	3217	1/1	0.95	0.24	-	59,59,59,59	0
56	MG	19	503	1/1	0.91	0.27	-	61,61,61,61	0
56	MG	1A	3531	1/1	0.94	0.18	-	56,56,56,56	0
56	MG	1a	1865	1/1	0.91	0.18	-	65,65,65,65	0
56	MG	1A	3980	1/1	0.95	0.48	-	63,63,63,63	0
56	MG	1a	1610	1/1	0.97	0.06	-	52,52,52,52	0
56	MG	1E	308	1/1	0.92	0.21	-	70,70,70,70	0
56	MG	1A	3837	1/1	0.94	0.30	-	74,74,74,74	0
56	MG	1B	202	1/1	0.92	0.20	-	59,59,59,59	0
56	MG	2A	3332	1/1	0.97	0.17	-	50,50,50,50	0
56	MG	2A	3096	1/1	0.75	0.29	-	40,40,40,40	0
56	MG	1A	3345	1/1	0.95	0.26	-	64,64,64,64	0
56	MG	2A	3372	1/1	0.93	0.18	-	62,62,62,62	0
56	MG	1A	3589	1/1	0.97	0.15	-	65,65,65,65	0
56	MG	1A	4048	1/1	0.96	0.09	-	32,32,32,32	0
56	MG	1a	1677	1/1	0.95	0.47	-	61,61,61,61	0
56	MG	1a	1892	1/1	0.96	0.41	-	67,67,67,67	0
56	MG	2A	3341	1/1	0.92	0.13	-	39,39,39,39	0
56	MG	2O	201	1/1	0.96	0.14	-	54,54,54,54	0
56	MG	2A	3101	1/1	0.97	0.06	-	60,60,60,60	0
56	MG	1A	3317	1/1	0.93	0.24	-	67,67,67,67	0
56	MG	2a	3012	1/1	0.87	0.47	-	69,69,69,69	0
56	MG	1A	3728	1/1	0.89	0.18	-	23,23,23,23	0
56	MG	1A	3201	1/1	0.95	0.26	-	39,39,39,39	0
56	MG	1A	3748	1/1	0.97	0.10	-	36,36,36,36	0
56	MG	1A	3696	1/1	0.94	0.10	-	62,62,62,62	0
56	MG	1A	3524	1/1	0.99	0.22	-	24,24,24,24	0
56	MG	1A	3176	1/1	0.84	0.25	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3005	1/1	0.76	0.11	-	70,70,70,70	0
56	MG	1a	1792	1/1	0.94	0.18	-	59,59,59,59	0
56	MG	1a	1790	1/1	0.93	0.20	-	33,33,33,33	0
56	MG	1B	224	1/1	0.90	0.18	-	69,69,69,69	0
56	MG	10	105	1/1	0.86	0.20	-	57,57,57,57	0
56	MG	2a	3207	1/1	0.93	0.14	-	58,58,58,58	0
56	MG	1A	3305	1/1	0.87	0.18	-	83,83,83,83	0
56	MG	2A	3240	1/1	0.87	0.40	-	57,57,57,57	0
56	MG	1E	310	1/1	0.96	0.12	-	45,45,45,45	0
56	MG	1B	207	1/1	0.87	0.30	-	70,70,70,70	0
56	MG	2A	3070	1/1	0.95	0.46	-	58,58,58,58	0
56	MG	1a	1601	1/1	0.87	0.16	-	66,66,66,66	0
56	MG	1A	4039	1/1	0.91	0.27	-	56,56,56,56	0
56	MG	2A	3403	1/1	0.94	0.12	-	34,34,34,34	0
56	MG	2a	3085	1/1	0.85	0.46	-	61,61,61,61	0
56	MG	2a	3057	1/1	0.93	0.36	-	75,75,75,75	0
56	MG	1A	3934	1/1	0.95	0.13	-	62,62,62,62	0
56	MG	1A	3564	1/1	0.94	0.11	-	42,42,42,42	0
56	MG	1A	3981	1/1	0.89	0.31	-	63,63,63,63	0
56	MG	2a	3105	1/1	0.91	0.29	-	58,58,58,58	0
56	MG	1A	3331	1/1	0.88	0.15	-	53,53,53,53	0
56	MG	1a	1739	1/1	0.84	0.18	-	72,72,72,72	0
56	MG	1A	3873	1/1	0.90	0.20	-	25,25,25,25	0
56	MG	1A	3039	1/1	0.85	0.12	-	54,54,54,54	0
56	MG	1A	3829	1/1	0.83	0.08	-	56,56,56,56	0
56	MG	1A	3549	1/1	0.95	0.11	-	68,68,68,68	0
56	MG	1a	1766	1/1	0.58	0.31	-	79,79,79,79	0
56	MG	1a	1664	1/1	0.84	0.14	-	57,57,57,57	0
56	MG	1a	1645	1/1	0.92	0.11	-	71,71,71,71	0
56	MG	1A	3784	1/1	0.97	0.22	-	31,31,31,31	0
56	MG	2A	3109	1/1	0.72	0.11	-	66,66,66,66	0
56	MG	2A	3183	1/1	0.87	0.07	-	58,58,58,58	0
56	MG	2A	3511	1/1	0.94	0.06	-	50,50,50,50	0
56	MG	1N	208	1/1	0.95	0.08	-	60,60,60,60	0
56	MG	2A	3397	1/1	0.97	0.25	-	64,64,64,64	0
56	MG	2A	3465	1/1	0.86	0.11	-	46,46,46,46	0
56	MG	2a	3240	1/1	0.85	0.29	-	65,65,65,65	0
56	MG	1A	3614	1/1	0.98	0.07	-	26,26,26,26	0
56	MG	2A	3328	1/1	0.89	0.13	-	45,45,45,45	0
56	MG	2a	3227	1/1	0.98	0.32	-	81,81,81,81	0
56	MG	1A	4015	1/1	0.57	0.53	-	61,61,61,61	0
56	MG	1A	3165	1/1	0.91	0.34	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1704	1/1	0.98	0.20	-	40,40,40,40	0
56	MG	1d	303	1/1	0.97	0.23	-	62,62,62,62	0
56	MG	1a	1850	1/1	0.95	0.29	-	46,46,46,46	0
56	MG	1A	3361	1/1	0.93	0.31	-	59,59,59,59	0
56	MG	2e	3001	1/1	0.92	0.06	-	68,68,68,68	0
56	MG	2A	3536	1/1	0.94	0.11	-	67,67,67,67	0
56	MG	1A	3009	1/1	0.79	0.31	-	50,50,50,50	0
56	MG	1a	1806	1/1	0.98	0.31	-	67,67,67,67	0
56	MG	2A	3213	1/1	0.89	0.09	-	67,67,67,67	0
56	MG	2a	3010	1/1	0.87	0.10	-	83,83,83,83	0
56	MG	1a	1669	1/1	0.98	0.30	-	62,62,62,62	0
56	MG	2A	3401	1/1	0.96	0.20	-	39,39,39,39	0
56	MG	1A	3882	1/1	0.96	0.10	-	36,36,36,36	0
56	MG	2a	3003	1/1	0.90	0.53	-	60,60,60,60	0
56	MG	1a	1731	1/1	0.98	0.10	-	55,55,55,55	0
56	MG	1B	205	1/1	0.97	0.12	-	49,49,49,49	0
56	MG	1A	3985	1/1	0.90	0.21	-	73,73,73,73	0
56	MG	1a	1801	1/1	0.93	0.19	-	70,70,70,70	0
56	MG	2E	302	1/1	0.89	0.49	-	63,63,63,63	0
56	MG	1A	3897	1/1	0.96	0.29	-	33,33,33,33	0
56	MG	2a	3017	1/1	0.91	0.91	-	68,68,68,68	0
56	MG	2a	3060	1/1	0.96	0.37	-	63,63,63,63	0
56	MG	1A	3246	1/1	0.85	0.31	-	65,65,65,65	0
56	MG	1A	3704	1/1	0.88	0.21	-	34,34,34,34	0
56	MG	1A	3950	1/1	0.85	0.10	-	55,55,55,55	0
56	MG	1A	3404	1/1	0.88	0.22	-	82,82,82,82	0
56	MG	1a	1637	1/1	0.91	0.17	-	64,64,64,64	0
56	MG	1A	3709	1/1	0.97	0.19	-	54,54,54,54	0
56	MG	2A	3563	1/1	0.89	0.21	-	58,58,58,58	0
56	MG	1A	3475	1/1	0.85	0.07	-	61,61,61,61	0
56	MG	1a	1781	1/1	0.83	0.17	-	87,87,87,87	0
56	MG	2A	3166	1/1	0.88	0.25	-	51,51,51,51	0
56	MG	2a	3050	1/1	0.97	0.29	-	71,71,71,71	0
56	MG	1A	3225	1/1	0.91	0.22	-	40,40,40,40	0
56	MG	1a	1734	1/1	0.85	0.25	-	66,66,66,66	0
56	MG	2A	3204	1/1	0.91	0.11	-	53,53,53,53	0
56	MG	1a	1621	1/1	0.89	0.36	-	83,83,83,83	0
56	MG	1A	3101	1/1	0.94	0.34	-	35,35,35,35	0
56	MG	1A	3986	1/1	0.91	0.20	-	44,44,44,44	0
56	MG	1A	3458	1/1	0.93	0.14	-	72,72,72,72	0
56	MG	1A	3162	1/1	0.92	0.39	-	38,38,38,38	0
56	MG	1B	226	1/1	0.96	0.07	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3029	1/1	0.82	0.21	-	57,57,57,57	0
56	MG	2A	3269	1/1	0.94	0.22	-	43,43,43,43	0
56	MG	2A	3446	1/1	0.83	0.12	-	47,47,47,47	0
56	MG	2A	3519	1/1	0.87	0.28	-	53,53,53,53	0
56	MG	2A	3153	1/1	0.95	0.25	-	42,42,42,42	0
56	MG	2A	3255	1/1	0.95	0.13	-	42,42,42,42	0
56	MG	2A	3224	1/1	0.92	0.15	-	33,33,33,33	0
56	MG	1A	3380	1/1	0.94	0.19	-	39,39,39,39	0
56	MG	1A	3340	1/1	0.83	0.17	-	56,56,56,56	0
56	MG	2A	3424	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	1N	203	1/1	0.98	0.28	-	46,46,46,46	0
56	MG	1A	3135	1/1	0.94	0.27	-	44,44,44,44	0
56	MG	1A	3871	1/1	0.90	0.16	-	67,67,67,67	0
56	MG	1a	1710	1/1	0.97	0.23	-	54,54,54,54	0
56	MG	2A	3217	1/1	0.95	0.40	-	45,45,45,45	0
56	MG	1a	1777	1/1	0.96	0.23	-	73,73,73,73	0
56	MG	1A	3298	1/1	0.95	0.07	-	52,52,52,52	0
56	MG	1A	3628	1/1	0.96	0.29	-	63,63,63,63	0
56	MG	1B	218	1/1	0.98	0.17	-	60,60,60,60	0
56	MG	2A	3149	1/1	0.87	0.41	-	59,59,59,59	0
56	MG	2Y	502	1/1	0.97	0.12	-	57,57,57,57	0
56	MG	1A	3017	1/1	0.96	0.23	-	47,47,47,47	0
56	MG	2Q	201	1/1	0.87	0.54	-	55,55,55,55	0
56	MG	1A	3264	1/1	0.87	0.21	-	66,66,66,66	0
56	MG	1a	1712	1/1	0.94	0.26	-	65,65,65,65	0
56	MG	1a	1754	1/1	0.90	0.20	-	53,53,53,53	0
56	MG	1A	3912	1/1	0.95	0.16	-	49,49,49,49	0
56	MG	2A	3351	1/1	0.95	0.32	-	62,62,62,62	0
56	MG	1A	3921	1/1	0.90	0.12	-	80,80,80,80	0
56	MG	1A	3243	1/1	0.94	0.34	-	43,43,43,43	0
56	MG	1a	1613	1/1	0.62	0.24	-	76,76,76,76	0
56	MG	1A	4035	1/1	0.93	0.10	-	81,81,81,81	0
56	MG	1A	3937	1/1	0.98	0.54	-	51,51,51,51	0
56	MG	2a	3029	1/1	0.95	0.24	-	59,59,59,59	0
56	MG	1a	1660	1/1	0.95	0.38	-	54,54,54,54	0
56	MG	1A	4018	1/1	0.84	0.38	-	62,62,62,62	0
56	MG	2A	3145	1/1	0.96	0.09	-	50,50,50,50	0
56	MG	1A	3448	1/1	0.86	0.31	-	58,58,58,58	0
56	MG	1A	3843	1/1	0.95	0.13	-	37,37,37,37	0
56	MG	1A	3183	1/1	0.85	0.09	-	59,59,59,59	0
56	MG	1A	3764	1/1	0.91	0.14	-	54,54,54,54	0
56	MG	1A	3754	1/1	0.97	0.18	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4004	1/1	0.95	0.44	-	31,31,31,31	0
56	MG	2a	3160	1/1	0.94	0.34	-	59,59,59,59	0
56	MG	1A	3384	1/1	0.86	0.14	-	66,66,66,66	0
56	MG	1a	1895	1/1	0.97	0.12	-	56,56,56,56	0
56	MG	1A	3779	1/1	0.95	0.12	-	45,45,45,45	0
56	MG	1A	3052	1/1	0.95	0.27	-	48,48,48,48	0
56	MG	1A	3256	1/1	0.89	0.15	-	51,51,51,51	0
56	MG	1A	3228	1/1	0.90	0.22	-	51,51,51,51	0
56	MG	1A	3794	1/1	0.96	0.22	-	62,62,62,62	0
56	MG	1a	1696	1/1	0.85	0.13	-	67,67,67,67	0
56	MG	1a	1799	1/1	0.94	0.27	-	76,76,76,76	0
56	MG	1a	1650	1/1	0.94	0.34	-	72,72,72,72	0
56	MG	1A	3081	1/1	0.91	0.34	-	62,62,62,62	0
56	MG	1A	3136	1/1	0.92	0.39	-	47,47,47,47	0
56	MG	1A	3399	1/1	0.95	0.36	-	68,68,68,68	0
56	MG	1a	1617	1/1	0.82	0.54	-	74,74,74,74	0
56	MG	1A	3222	1/1	0.90	0.32	-	38,38,38,38	0
56	MG	1A	3265	1/1	0.87	0.24	-	55,55,55,55	0
56	MG	1a	1816	1/1	0.92	0.21	-	88,88,88,88	0
56	MG	1A	3552	1/1	0.92	0.29	-	58,58,58,58	0
56	MG	1A	3823	1/1	0.86	0.19	-	39,39,39,39	0
56	MG	1A	3828	1/1	0.90	0.16	-	55,55,55,55	0
56	MG	1A	3931	1/1	0.94	0.30	-	49,49,49,49	0
56	MG	2a	3182	1/1	0.79	0.15	-	64,64,64,64	0
56	MG	1A	3049	1/1	0.95	0.16	-	49,49,49,49	0
56	MG	2A	3314	1/1	0.97	0.19	-	28,28,28,28	0
56	MG	1x	110	1/1	0.84	0.08	-	78,78,78,78	0
56	MG	16	103	1/1	0.95	0.14	-	57,57,57,57	0
56	MG	2A	3241	1/1	0.97	0.24	-	56,56,56,56	0
56	MG	1a	1902	1/1	0.86	0.31	-	59,59,59,59	0
56	MG	2a	3194	1/1	0.91	0.43	-	75,75,75,75	0
56	MG	1f	3001	1/1	0.87	0.20	-	66,66,66,66	0
56	MG	2A	3056	1/1	0.94	0.18	-	57,57,57,57	0
56	MG	1P	201	1/1	0.77	0.34	-	55,55,55,55	0
56	MG	2A	3278	1/1	0.86	0.28	-	65,65,65,65	0
56	MG	1A	3126	1/1	0.86	0.31	-	55,55,55,55	0
56	MG	1A	3148	1/1	0.96	0.39	-	42,42,42,42	0
56	MG	1A	3037	1/1	0.89	0.07	-	65,65,65,65	0
56	MG	1A	3010	1/1	0.93	0.39	-	53,53,53,53	0
56	MG	1A	3412	1/1	0.76	0.76	-	77,77,77,77	0
56	MG	2l	201	1/1	0.88	0.13	-	64,64,64,64	0
56	MG	1A	3643	1/1	0.97	0.20	-	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	202	1/1	0.90	0.18	-	59,59,59,59	0
56	MG	1A	3847	1/1	0.57	0.14	-	81,81,81,81	0
56	MG	2a	3094	1/1	0.96	0.18	-	51,51,51,51	0
56	MG	2A	3198	1/1	0.88	0.35	-	53,53,53,53	0
56	MG	10	107	1/1	0.96	0.09	-	58,58,58,58	0
56	MG	1a	1620	1/1	0.97	0.10	-	79,79,79,79	0
56	MG	1A	3525	1/1	0.98	0.07	-	60,60,60,60	0
56	MG	1A	3788	1/1	0.89	0.13	-	25,25,25,25	0
56	MG	1A	3259	1/1	0.79	0.24	-	66,66,66,66	0
56	MG	1A	3668	1/1	0.97	0.27	-	84,84,84,84	0
56	MG	2B	3002	1/1	0.44	0.17	-	70,70,70,70	0
56	MG	1X	3002	1/1	0.96	0.16	-	37,37,37,37	0
56	MG	1A	3377	1/1	0.96	0.42	-	67,67,67,67	0
56	MG	1a	1760	1/1	0.68	0.39	-	78,78,78,78	0
56	MG	1A	3687	1/1	0.97	0.20	-	21,21,21,21	0
56	MG	1a	1653	1/1	0.88	0.09	-	70,70,70,70	0
56	MG	1A	3239	1/1	0.94	0.16	-	41,41,41,41	0
56	MG	1A	3974	1/1	0.94	0.20	-	48,48,48,48	0
56	MG	2a	3151	1/1	0.91	0.09	-	64,64,64,64	0
56	MG	1A	3370	1/1	0.94	0.35	-	53,53,53,53	0
56	MG	1a	1891	1/1	0.77	0.26	-	82,82,82,82	0
56	MG	1A	3872	1/1	0.95	0.14	-	46,46,46,46	0
56	MG	2A	3327	1/1	0.92	0.10	-	68,68,68,68	0
56	MG	2A	3066	1/1	0.89	0.15	-	54,54,54,54	0
56	MG	1A	3695	1/1	0.94	0.15	-	63,63,63,63	0
56	MG	1a	1612	1/1	0.98	0.05	-	63,63,63,63	0
56	MG	1A	3140	1/1	0.78	0.09	-	50,50,50,50	0
56	MG	2a	3188	1/1	0.90	0.44	-	74,74,74,74	0
56	MG	1A	3551	1/1	0.95	0.20	-	32,32,32,32	0
56	MG	2A	3502	1/1	0.88	0.24	-	75,75,75,75	0
56	MG	2A	3475	1/1	0.89	0.33	-	67,67,67,67	0
56	MG	2A	3345	1/1	0.94	0.17	-	68,68,68,68	0
56	MG	1A	3927	1/1	0.90	0.44	-	59,59,59,59	0
56	MG	1A	3116	1/1	0.94	0.17	-	47,47,47,47	0
56	MG	1A	3741	1/1	0.98	0.21	-	32,32,32,32	0
56	MG	2a	3208	1/1	0.93	0.12	-	68,68,68,68	0
56	MG	2A	3108	1/1	0.88	0.22	-	47,47,47,47	0
56	MG	1A	3830	1/1	0.94	0.17	-	54,54,54,54	0
56	MG	2A	3515	1/1	0.86	0.12	-	63,63,63,63	0
56	MG	1A	3518	1/1	0.91	0.36	-	52,52,52,52	0
56	MG	2A	3035	1/1	0.96	0.10	-	59,59,59,59	0
56	MG	1A	3515	1/1	0.73	0.23	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3024	1/1	0.93	0.13	-	67,67,67,67	0
56	MG	2a	3153	1/1	0.89	0.74	-	99,99,99,99	0
56	MG	2a	3124	1/1	0.87	0.35	-	76,76,76,76	0
56	MG	2A	3527	1/1	0.91	0.17	-	68,68,68,68	0
56	MG	2A	3030	1/1	0.91	0.08	-	57,57,57,57	0
56	MG	1A	3892	1/1	0.95	0.33	-	46,46,46,46	0
56	MG	2a	3016	1/1	0.99	0.14	-	58,58,58,58	0
56	MG	1A	3079	1/1	0.97	0.17	-	31,31,31,31	0
56	MG	1a	1874	1/1	0.96	0.15	-	64,64,64,64	0
56	MG	1A	3568	1/1	0.98	0.13	-	51,51,51,51	0
56	MG	2A	3287	1/1	0.97	0.10	-	46,46,46,46	0
56	MG	1a	1770	1/1	0.93	0.15	-	87,87,87,87	0
56	MG	2A	3205	1/1	0.97	0.05	-	62,62,62,62	0
56	MG	1a	1665	1/1	0.92	0.18	-	47,47,47,47	0
56	MG	1A	3473	1/1	0.95	0.06	-	63,63,63,63	0
56	MG	1A	3548	1/1	0.97	0.15	-	65,65,65,65	0
56	MG	1A	3417	1/1	0.89	0.19	-	60,60,60,60	0
56	MG	1A	3199	1/1	0.91	0.30	-	48,48,48,48	0
56	MG	2A	3193	1/1	0.84	0.31	-	63,63,63,63	0
56	MG	2A	3243	1/1	0.91	0.19	-	62,62,62,62	0
56	MG	1A	3015	1/1	0.98	0.26	-	40,40,40,40	0
56	MG	2A	3494	1/1	0.96	0.12	-	69,69,69,69	0
56	MG	2A	3223	1/1	0.98	0.27	-	39,39,39,39	0
56	MG	1A	3866	1/1	0.95	0.28	-	65,65,65,65	0
56	MG	1A	3949	1/1	0.93	0.30	-	59,59,59,59	0
56	MG	1A	3675	1/1	0.95	0.17	-	39,39,39,39	0
56	MG	2A	3083	1/1	0.82	0.28	-	66,66,66,66	0
56	MG	1A	3271	1/1	0.86	0.10	-	66,66,66,66	0
56	MG	1A	3435	1/1	0.82	0.14	-	62,62,62,62	0
56	MG	1Z	301	1/1	0.91	0.07	-	74,74,74,74	0
56	MG	1a	1729	1/1	0.97	0.57	-	57,57,57,57	0
56	MG	1A	3874	1/1	0.95	0.13	-	45,45,45,45	0
56	MG	1A	3145	1/1	0.97	0.14	-	37,37,37,37	0
56	MG	2a	3210	1/1	0.94	0.22	-	69,69,69,69	0
56	MG	1A	3359	1/1	0.90	0.52	-	51,51,51,51	0
56	MG	2A	3188	1/1	0.91	0.25	-	49,49,49,49	0
56	MG	2a	3209	1/1	0.96	0.06	-	76,76,76,76	0
56	MG	1A	3559	1/1	0.95	0.22	-	36,36,36,36	0
56	MG	2A	3015	1/1	0.94	0.43	-	72,72,72,72	0
56	MG	1A	3776	1/1	0.98	0.22	-	44,44,44,44	0
56	MG	2B	3001	1/1	0.96	0.28	-	65,65,65,65	0
56	MG	1A	3543	1/1	0.97	0.19	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3446	1/1	0.90	0.13	-	52,52,52,52	0
56	MG	1A	3841	1/1	0.97	0.24	-	41,41,41,41	0
56	MG	2A	3293	1/1	0.87	0.18	-	57,57,57,57	0
56	MG	1A	3541	1/1	0.94	0.16	-	56,56,56,56	0
56	MG	1A	3494	1/1	0.97	0.47	-	58,58,58,58	0
56	MG	1A	3327	1/1	0.92	0.07	-	64,64,64,64	0
56	MG	1b	3002	1/1	0.85	0.33	-	87,87,87,87	0
56	MG	2a	3056	1/1	0.83	1.00	-	79,79,79,79	0
56	MG	1A	3661	1/1	0.97	0.07	-	51,51,51,51	0
56	MG	2a	3144	1/1	0.95	0.20	-	75,75,75,75	0
56	MG	1a	1825	1/1	0.94	0.35	-	61,61,61,61	0
56	MG	2A	3105	1/1	0.81	0.20	-	55,55,55,55	0
56	MG	1A	3057	1/1	0.88	0.33	-	56,56,56,56	0
56	MG	1A	3402	1/1	0.80	0.24	-	73,73,73,73	0
56	MG	2A	3252	1/1	0.97	0.51	-	56,56,56,56	0
56	MG	1A	3372	1/1	0.95	0.12	-	56,56,56,56	0
56	MG	1A	3862	1/1	0.79	0.18	-	25,25,25,25	0
56	MG	2a	3156	1/1	0.96	0.33	-	70,70,70,70	0
56	MG	1A	3024	1/1	0.90	0.17	-	52,52,52,52	0
56	MG	2A	3220	1/1	0.97	0.49	-	50,50,50,50	0
56	MG	1N	204	1/1	0.78	0.40	-	59,59,59,59	0
56	MG	1A	3684	1/1	0.95	0.23	-	41,41,41,41	0
56	MG	1A	3337	1/1	0.86	0.27	-	48,48,48,48	0
56	MG	1a	1862	1/1	0.94	0.08	-	53,53,53,53	0
56	MG	1P	202	1/1	0.95	0.28	-	46,46,46,46	0
56	MG	1A	3648	1/1	0.96	0.15	-	51,51,51,51	0
56	MG	1A	3758	1/1	0.80	0.12	-	66,66,66,66	0
56	MG	2x	3006	1/1	0.92	0.08	-	78,78,78,78	0
56	MG	2A	3226	1/1	0.94	0.64	-	52,52,52,52	0
56	MG	1A	3093	1/1	0.96	0.23	-	46,46,46,46	0
56	MG	1A	3329	1/1	0.96	0.10	-	50,50,50,50	0
56	MG	1A	3454	1/1	0.91	0.43	-	50,50,50,50	0
56	MG	2A	3448	1/1	0.94	0.11	-	65,65,65,65	0
56	MG	2A	3439	1/1	0.86	0.15	-	54,54,54,54	0
56	MG	1a	1737	1/1	0.87	0.28	-	66,66,66,66	0
56	MG	1A	3955	1/1	0.97	0.20	-	47,47,47,47	0
56	MG	1A	3262	1/1	0.82	0.21	-	58,58,58,58	0
56	MG	1A	3681	1/1	0.87	0.12	-	39,39,39,39	0
56	MG	1a	1899	1/1	0.98	0.08	-	50,50,50,50	0
56	MG	2a	3103	1/1	0.92	0.18	-	59,59,59,59	0
56	MG	1A	3437	1/1	0.93	0.49	-	56,56,56,56	0
56	MG	1x	109	1/1	0.85	0.55	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3295	1/1	0.91	0.09	-	50,50,50,50	0
56	MG	2A	3075	1/1	0.62	0.39	-	75,75,75,75	0
56	MG	1A	3686	1/1	0.92	0.24	-	58,58,58,58	0
56	MG	2A	3373	1/1	0.84	0.10	-	47,47,47,47	0
56	MG	1a	1635	1/1	0.88	0.26	-	64,64,64,64	0
56	MG	1A	3497	1/1	0.94	0.26	-	56,56,56,56	0
56	MG	2A	3524	1/1	0.88	0.12	-	33,33,33,33	0
56	MG	1a	1619	1/1	0.94	0.26	-	71,71,71,71	0
56	MG	1A	3447	1/1	0.81	0.38	-	75,75,75,75	0
56	MG	1E	304	1/1	0.94	0.21	-	64,64,64,64	0
56	MG	2A	3560	1/1	0.97	0.14	-	41,41,41,41	0
56	MG	1A	3031	1/1	0.95	0.18	-	51,51,51,51	0
56	MG	1a	1614	1/1	0.91	0.16	-	57,57,57,57	0
56	MG	1a	1746	1/1	0.82	0.26	-	60,60,60,60	0
56	MG	2a	3036	1/1	0.83	0.10	-	73,73,73,73	0
56	MG	2A	3246	1/1	0.79	0.18	-	67,67,67,67	0
56	MG	2A	3445	1/1	0.96	0.07	-	74,74,74,74	0
56	MG	1A	3045	1/1	0.90	0.15	-	53,53,53,53	0
56	MG	2A	3271	1/1	0.88	0.29	-	36,36,36,36	0
56	MG	1A	3371	1/1	0.91	0.19	-	39,39,39,39	0
56	MG	2A	3097	1/1	0.77	0.20	-	54,54,54,54	0
56	MG	2A	3037	1/1	0.89	0.29	-	62,62,62,62	0
56	MG	2A	3442	1/1	0.93	0.17	-	66,66,66,66	0
56	MG	1a	1800	1/1	0.82	0.26	-	84,84,84,84	0
56	MG	1a	1821	1/1	0.91	0.14	-	77,77,77,77	0
56	MG	1a	1826	1/1	0.85	0.12	-	80,80,80,80	0
56	MG	1a	1763	1/1	0.84	0.11	-	76,76,76,76	0
56	MG	1A	3234	1/1	0.97	0.32	-	54,54,54,54	0
56	MG	1A	3174	1/1	0.99	0.24	-	40,40,40,40	0
56	MG	1a	1866	1/1	0.89	0.25	-	72,72,72,72	0
56	MG	1A	3466	1/1	0.94	0.24	-	48,48,48,48	0
56	MG	1A	3876	1/1	0.91	0.22	-	68,68,68,68	0
56	MG	1a	1775	1/1	0.95	0.36	-	65,65,65,65	0
56	MG	1a	1683	1/1	0.93	0.68	-	56,56,56,56	0
56	MG	2a	3049	1/1	0.95	0.07	-	91,91,91,91	0
56	MG	1A	3958	1/1	0.93	0.15	-	46,46,46,46	0
56	MG	1a	1793	1/1	0.94	0.59	-	68,68,68,68	0
56	MG	1A	3396	1/1	0.86	0.13	-	58,58,58,58	0
56	MG	1Q	3001	1/1	0.94	0.41	-	47,47,47,47	0
56	MG	2A	3366	1/1	0.95	0.21	-	58,58,58,58	0
56	MG	2A	3313	1/1	0.90	0.21	-	49,49,49,49	0
56	MG	2A	3575	1/1	0.82	0.71	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1651	1/1	0.93	0.13	-	61,61,61,61	0
56	MG	1A	3567	1/1	0.93	0.25	-	51,51,51,51	0
56	MG	1A	3838	1/1	0.93	0.14	-	45,45,45,45	0
56	MG	1A	3320	1/1	0.96	0.26	-	49,49,49,49	0
56	MG	1A	3310	1/1	0.96	0.06	-	65,65,65,65	0
56	MG	2a	3087	1/1	0.93	0.45	-	60,60,60,60	0
56	MG	2A	3398	1/1	0.96	0.07	-	57,57,57,57	0
56	MG	1A	3745	1/1	0.82	0.32	-	54,54,54,54	0
56	MG	1A	3961	1/1	0.85	0.33	-	47,47,47,47	0
56	MG	2A	3150	1/1	0.90	0.08	-	56,56,56,56	0
56	MG	2A	3358	1/1	0.85	0.26	-	53,53,53,53	0
56	MG	1A	3357	1/1	0.94	0.14	-	50,50,50,50	0
56	MG	18	104	1/1	0.78	0.32	-	59,59,59,59	0
56	MG	2A	3018	1/1	0.88	0.23	-	57,57,57,57	0
56	MG	2A	3528	1/1	0.92	0.08	-	56,56,56,56	0
56	MG	1A	3670	1/1	0.93	0.10	-	56,56,56,56	0
56	MG	2A	3212	1/1	0.96	0.43	-	58,58,58,58	0
56	MG	2A	3505	1/1	0.94	0.12	-	48,48,48,48	0
56	MG	2A	3002	1/1	0.89	0.23	-	59,59,59,59	0
56	MG	1a	1687	1/1	0.97	0.18	-	54,54,54,54	0
56	MG	1A	3297	1/1	0.88	0.27	-	59,59,59,59	0
56	MG	1A	3578	1/1	0.96	0.09	-	39,39,39,39	0
56	MG	1A	3173	1/1	0.90	0.29	-	24,24,24,24	0
56	MG	1a	1829	1/1	0.93	0.18	-	73,73,73,73	0
56	MG	1A	3516	1/1	0.76	0.19	-	75,75,75,75	0
56	MG	1A	4050	1/1	0.94	0.24	-	53,53,53,53	0
56	MG	2A	3346	1/1	0.84	0.27	-	65,65,65,65	0
56	MG	1A	3300	1/1	0.86	0.19	-	51,51,51,51	0
56	MG	1A	3413	1/1	0.82	0.17	-	60,60,60,60	0
56	MG	1A	3358	1/1	0.86	0.33	-	54,54,54,54	0
56	MG	2A	3480	1/1	0.88	0.11	-	74,74,74,74	0
56	MG	1a	1893	1/1	0.96	0.28	-	59,59,59,59	0
56	MG	1A	3786	1/1	0.84	0.30	-	67,67,67,67	0
56	MG	1A	3168	1/1	0.86	0.20	-	41,41,41,41	0
56	MG	1A	3493	1/1	0.90	0.20	-	63,63,63,63	0
56	MG	1A	3054	1/1	0.87	0.33	-	56,56,56,56	0
56	MG	1A	3378	1/1	0.85	0.16	-	53,53,53,53	0
56	MG	1A	3336	1/1	0.84	0.29	-	61,61,61,61	0
56	MG	1x	108	1/1	0.99	0.21	-	57,57,57,57	0
56	MG	1A	3197	1/1	0.89	0.21	-	30,30,30,30	0
56	MG	1A	3192	1/1	0.98	0.18	-	50,50,50,50	0
56	MG	2N	8001	1/1	0.86	0.07	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3672	1/1	0.98	0.10	-	50,50,50,50	0
56	MG	1A	3529	1/1	0.96	0.05	-	62,62,62,62	0
56	MG	1A	3365	1/1	0.85	0.53	-	44,44,44,44	0
56	MG	1a	1798	1/1	0.95	0.29	-	64,64,64,64	0
56	MG	1a	1772	1/1	0.88	0.28	-	66,66,66,66	0
56	MG	1A	3755	1/1	0.94	0.05	-	65,65,65,65	0
56	MG	1A	3654	1/1	0.94	0.24	-	60,60,60,60	0
56	MG	2a	3154	1/1	0.91	0.20	-	84,84,84,84	0
56	MG	1A	3599	1/1	0.91	0.16	-	51,51,51,51	0
56	MG	1A	3403	1/1	0.98	0.20	-	49,49,49,49	0
56	MG	2a	3238	1/1	0.92	0.53	-	61,61,61,61	0
56	MG	1A	3573	1/1	0.93	0.10	-	74,74,74,74	0
56	MG	1A	3520	1/1	0.81	0.15	-	41,41,41,41	0
56	MG	1A	3732	1/1	0.93	0.12	-	32,32,32,32	0
56	MG	1A	3839	1/1	0.93	0.28	-	54,54,54,54	0
56	MG	1W	3002	1/1	0.92	0.21	-	47,47,47,47	0
56	MG	2A	3195	1/1	0.90	0.41	-	58,58,58,58	0
56	MG	2a	3146	1/1	0.91	0.16	-	66,66,66,66	0
56	MG	1a	1721	1/1	0.97	0.16	-	65,65,65,65	0
56	MG	1A	3311	1/1	0.94	0.14	-	57,57,57,57	0
56	MG	1A	3290	1/1	0.93	0.27	-	47,47,47,47	0
56	MG	2a	3128	1/1	0.92	0.43	-	63,63,63,63	0
56	MG	2A	3374	1/1	0.97	0.22	-	57,57,57,57	0
56	MG	13	102	1/1	0.88	0.27	-	63,63,63,63	0
56	MG	2A	3126	1/1	0.93	0.36	-	54,54,54,54	0
56	MG	2a	3231	1/1	0.91	0.29	-	79,79,79,79	0
56	MG	1a	1898	1/1	0.90	0.53	-	65,65,65,65	0
56	MG	2A	3086	1/1	0.96	0.15	-	30,30,30,30	0
56	MG	1A	3432	1/1	0.97	0.41	-	44,44,44,44	0
56	MG	2F	301	1/1	0.92	0.21	-	63,63,63,63	0
56	MG	1F	304	1/1	0.88	0.15	-	40,40,40,40	0
56	MG	1A	3178	1/1	0.99	0.27	-	50,50,50,50	0
56	MG	1A	3844	1/1	0.96	0.13	-	63,63,63,63	0
56	MG	1a	1830	1/1	0.96	0.26	-	55,55,55,55	0
56	MG	2a	3111	1/1	0.97	0.21	-	46,46,46,46	0
56	MG	1A	3595	1/1	0.98	0.33	-	47,47,47,47	0
56	MG	1A	3421	1/1	0.79	0.13	-	65,65,65,65	0
56	MG	1a	1859	1/1	0.97	0.28	-	72,72,72,72	0
56	MG	1A	4008	1/1	0.94	0.12	-	47,47,47,47	0
56	MG	1A	3188	1/1	0.94	0.23	-	54,54,54,54	0
56	MG	1A	3556	1/1	0.91	0.12	-	70,70,70,70	0
56	MG	1A	3087	1/1	0.94	0.27	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3362	1/1	0.94	0.17	-	54,54,54,54	0
56	MG	2A	3504	1/1	0.89	0.12	-	45,45,45,45	0
56	MG	2A	3003	1/1	0.97	0.09	-	58,58,58,58	0
56	MG	2A	3578	1/1	0.88	0.19	-	58,58,58,58	0
56	MG	2k	3001	1/1	0.88	0.38	-	70,70,70,70	0
56	MG	2A	3539	1/1	0.93	0.24	-	48,48,48,48	0
56	MG	2x	3004	1/1	0.98	0.06	-	74,74,74,74	0
56	MG	1B	201	1/1	0.93	0.14	-	44,44,44,44	0
56	MG	2A	3466	1/1	0.94	0.08	-	56,56,56,56	0
56	MG	1a	1675	1/1	0.94	0.15	-	62,62,62,62	0
56	MG	1a	1773	1/1	0.95	0.20	-	57,57,57,57	0
56	MG	1q	202	1/1	0.91	0.31	-	62,62,62,62	0
56	MG	1A	3171	1/1	0.95	0.20	-	47,47,47,47	0
56	MG	2a	3027	1/1	0.74	0.17	-	88,88,88,88	0
56	MG	1A	3592	1/1	0.87	0.22	-	42,42,42,42	0
56	MG	1A	3391	1/1	0.93	0.26	-	56,56,56,56	0
56	MG	1a	1724	1/1	0.87	0.27	-	70,70,70,70	0
56	MG	17	103	1/1	0.98	0.07	-	53,53,53,53	0
56	MG	2A	3542	1/1	0.90	0.21	-	50,50,50,50	0
56	MG	1A	3074	1/1	0.89	0.28	-	61,61,61,61	0
56	MG	18	102	1/1	0.96	0.20	-	66,66,66,66	0
56	MG	1A	3393	1/1	0.90	0.26	-	46,46,46,46	0
56	MG	1a	1736	1/1	0.86	0.33	-	63,63,63,63	0
56	MG	1A	3212	1/1	0.85	0.31	-	49,49,49,49	0
56	MG	2a	3181	1/1	0.91	0.15	-	71,71,71,71	0
56	MG	1A	3665	1/1	0.94	0.07	-	64,64,64,64	0
56	MG	2A	3171	1/1	0.91	0.15	-	52,52,52,52	0
56	MG	2a	3100	1/1	0.88	0.39	-	57,57,57,57	0
56	MG	1A	3027	1/1	0.98	0.19	-	60,60,60,60	0
56	MG	1A	3800	1/1	0.96	0.10	-	55,55,55,55	0
56	MG	1A	3313	1/1	0.78	0.28	-	71,71,71,71	0
56	MG	2a	3063	1/1	0.92	0.13	-	66,66,66,66	0
56	MG	1A	3743	1/1	0.97	0.09	-	60,60,60,60	0
56	MG	1a	1603	1/1	0.96	0.19	-	59,59,59,59	0
56	MG	1A	3669	1/1	0.97	0.12	-	55,55,55,55	0
56	MG	1a	1848	1/1	0.88	0.08	-	85,85,85,85	0
56	MG	2a	3031	1/1	0.94	0.37	-	48,48,48,48	0
56	MG	1A	3659	1/1	0.95	0.36	-	73,73,73,73	0
56	MG	1A	3883	1/1	0.92	0.09	-	66,66,66,66	0
56	MG	1A	3938	1/1	0.92	0.17	-	47,47,47,47	0
56	MG	1A	3500	1/1	0.98	0.13	-	51,51,51,51	0
56	MG	1A	3693	1/1	0.94	0.14	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1D	315	1/1	0.92	0.33	-	56,56,56,56	0
56	MG	2A	3186	1/1	0.95	0.26	-	43,43,43,43	0
56	MG	1a	1715	1/1	0.81	0.11	-	76,76,76,76	0
56	MG	2a	3107	1/1	0.97	0.11	-	63,63,63,63	0
56	MG	1A	3818	1/1	0.96	0.19	-	62,62,62,62	0
56	MG	2a	3241	1/1	0.92	0.22	-	67,67,67,67	0
56	MG	2A	3488	1/1	0.95	0.20	-	31,31,31,31	0
56	MG	2A	3359	1/1	0.88	0.15	-	75,75,75,75	0
56	MG	1A	3207	1/1	0.99	0.23	-	40,40,40,40	0
56	MG	1A	3248	1/1	0.92	0.27	-	60,60,60,60	0
56	MG	2A	3299	1/1	0.96	0.17	-	44,44,44,44	0
56	MG	2A	3333	1/1	0.92	0.08	-	61,61,61,61	0
56	MG	1a	1626	1/1	0.92	0.46	-	69,69,69,69	0
56	MG	1A	3952	1/1	0.94	0.24	-	57,57,57,57	0
56	MG	1A	3205	1/1	0.84	0.11	-	55,55,55,55	0
56	MG	2A	3087	1/1	0.90	0.13	-	36,36,36,36	0
56	MG	2A	3541	1/1	0.96	0.09	-	67,67,67,67	0
56	MG	2A	3490	1/1	0.95	0.13	-	30,30,30,30	0
56	MG	2A	3291	1/1	0.92	0.46	-	56,56,56,56	0
56	MG	1A	3142	1/1	0.95	0.20	-	43,43,43,43	0
56	MG	2A	3355	1/1	0.93	0.14	-	42,42,42,42	0
56	MG	1A	3285	1/1	0.57	1.20	-	79,79,79,79	0
56	MG	2a	3199	1/1	0.94	0.34	-	59,59,59,59	0
56	MG	1A	3342	1/1	0.89	0.13	-	40,40,40,40	0
56	MG	1A	3125	1/1	0.95	0.17	-	49,49,49,49	0
56	MG	1a	1748	1/1	0.90	0.10	-	61,61,61,61	0
56	MG	2a	3030	1/1	0.87	0.17	-	59,59,59,59	0
56	MG	2A	3521	1/1	0.89	0.18	-	59,59,59,59	0
56	MG	1A	3581	1/1	0.94	0.13	-	51,51,51,51	0
56	MG	2a	3044	1/1	0.98	0.23	-	95,95,95,95	0
56	MG	2A	3385	1/1	0.94	0.19	-	43,43,43,43	0
56	MG	1A	4027	1/1	0.79	0.31	-	72,72,72,72	0
56	MG	1A	3587	1/1	0.97	0.36	-	42,42,42,42	0
56	MG	1A	3482	1/1	0.91	0.17	-	61,61,61,61	0
56	MG	1a	1844	1/1	0.96	0.07	-	38,38,38,38	0
56	MG	2a	3223	1/1	0.98	0.21	-	57,57,57,57	0
56	MG	2A	3426	1/1	0.94	0.24	-	67,67,67,67	0
56	MG	1a	1689	1/1	0.98	0.07	-	60,60,60,60	0
56	MG	1A	3708	1/1	0.97	0.18	-	45,45,45,45	0
56	MG	1A	3634	1/1	0.95	0.18	-	19,19,19,19	0
56	MG	1A	3536	1/1	0.96	0.20	-	62,62,62,62	0
56	MG	1T	203	1/1	0.82	0.20	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3522	1/1	0.96	0.18	-	62,62,62,62	0
56	MG	1A	3425	1/1	0.91	0.15	-	57,57,57,57	0
56	MG	1A	3597	1/1	0.91	0.13	-	49,49,49,49	0
56	MG	1a	1753	1/1	0.54	0.32	-	83,83,83,83	0
56	MG	1A	3392	1/1	0.95	0.08	-	55,55,55,55	0
56	MG	1A	3957	1/1	0.98	0.18	-	44,44,44,44	0
56	MG	2A	3100	1/1	0.94	0.35	-	62,62,62,62	0
56	MG	1A	3276	1/1	0.93	0.22	-	74,74,74,74	0
56	MG	2A	3290	1/1	0.79	0.17	-	57,57,57,57	0
56	MG	1A	3167	1/1	0.83	0.19	-	59,59,59,59	0
56	MG	2a	3126	1/1	0.80	0.36	-	66,66,66,66	0
56	MG	1A	3269	1/1	0.81	0.32	-	56,56,56,56	0
56	MG	2A	3040	1/1	0.97	0.11	-	43,43,43,43	0
56	MG	1A	3978	1/1	0.88	0.18	-	59,59,59,59	0
56	MG	1a	1713	1/1	0.84	0.43	-	65,65,65,65	0
56	MG	1A	3007	1/1	0.96	0.23	-	53,53,53,53	0
56	MG	2a	3170	1/1	0.93	0.21	-	53,53,53,53	0
56	MG	1A	3430	1/1	0.89	0.41	-	41,41,41,41	0
56	MG	2A	3135	1/1	0.91	0.16	-	48,48,48,48	0
56	MG	2a	3048	1/1	0.76	0.12	-	91,91,91,91	0
56	MG	1x	105	1/1	0.85	0.12	-	57,57,57,57	0
56	MG	1A	3965	1/1	0.96	0.17	-	35,35,35,35	0
56	MG	1A	4034	1/1	0.92	0.23	-	44,44,44,44	0
56	MG	1A	3217	1/1	0.94	0.29	-	48,48,48,48	0
56	MG	1A	3962	1/1	0.97	0.10	-	34,34,34,34	0
56	MG	2A	3178	1/1	0.85	0.31	-	59,59,59,59	0
56	MG	1a	1654	1/1	0.89	0.17	-	67,67,67,67	0
56	MG	1A	3130	1/1	0.97	0.67	-	48,48,48,48	0
56	MG	2p	101	1/1	0.98	0.30	-	68,68,68,68	0
56	MG	1A	3286	1/1	0.95	0.08	-	45,45,45,45	0
56	MG	1a	1659	1/1	0.97	0.16	-	60,60,60,60	0
56	MG	1A	3163	1/1	0.94	0.31	-	43,43,43,43	0
56	MG	1A	3132	1/1	0.99	0.39	-	17,17,17,17	0
56	MG	1A	3849	1/1	0.98	0.09	-	55,55,55,55	0
56	MG	1A	3241	1/1	0.91	0.22	-	49,49,49,49	0
56	MG	1A	3895	1/1	0.98	0.31	-	38,38,38,38	0
56	MG	1a	1663	1/1	0.83	0.22	-	67,67,67,67	0
56	MG	1A	3507	1/1	0.88	0.38	-	93,93,93,93	0
56	MG	2A	3449	1/1	0.95	0.14	-	62,62,62,62	0
56	MG	2A	3138	1/1	0.57	0.20	-	62,62,62,62	0
56	MG	1A	3562	1/1	0.94	0.20	-	50,50,50,50	0
56	MG	1T	202	1/1	0.91	0.08	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3137	1/1	0.96	0.30	-	49,49,49,49	0
56	MG	1A	3456	1/1	0.90	0.13	-	58,58,58,58	0
56	MG	2A	3235	1/1	0.98	0.72	-	55,55,55,55	0
56	MG	1U	201	1/1	0.97	0.15	-	38,38,38,38	0
56	MG	2A	3057	1/1	0.89	0.29	-	50,50,50,50	0
56	MG	1A	3444	1/1	0.89	0.23	-	65,65,65,65	0
56	MG	1A	3975	1/1	0.83	0.14	-	63,63,63,63	0
56	MG	1A	3642	1/1	0.83	0.15	-	67,67,67,67	0
56	MG	1A	3238	1/1	0.95	0.38	-	53,53,53,53	0
56	MG	2a	3175	1/1	0.83	0.17	-	53,53,53,53	0
56	MG	2a	3091	1/1	0.97	0.24	-	63,63,63,63	0
56	MG	1A	3489	1/1	0.91	0.33	-	55,55,55,55	0
56	MG	2A	3492	1/1	0.95	0.24	-	45,45,45,45	0
56	MG	1A	3122	1/1	0.90	0.55	-	60,60,60,60	0
56	MG	1A	3339	1/1	0.83	0.27	-	78,78,78,78	0
56	MG	1A	3517	1/1	0.96	0.49	-	56,56,56,56	0
56	MG	2A	3161	1/1	0.93	0.31	-	46,46,46,46	0
56	MG	1A	3363	1/1	0.96	0.14	-	42,42,42,42	0
56	MG	1a	1667	1/1	0.67	0.87	-	68,68,68,68	0
56	MG	1a	1629	1/1	0.90	0.24	-	54,54,54,54	0
56	MG	2A	3483	1/1	0.94	0.16	-	47,47,47,47	0
56	MG	1A	3916	1/1	0.89	0.19	-	60,60,60,60	0
56	MG	1e	201	1/1	0.94	0.13	-	59,59,59,59	0
56	MG	2E	307	1/1	0.96	0.09	-	70,70,70,70	0
56	MG	1A	3349	1/1	0.92	0.28	-	51,51,51,51	0
56	MG	1A	3903	1/1	0.93	0.11	-	66,66,66,66	0
56	MG	2a	3046	1/1	0.58	0.11	-	77,77,77,77	0
56	MG	2A	3004	1/1	0.85	0.12	-	55,55,55,55	0
56	MG	1A	3630	1/1	0.94	0.20	-	50,50,50,50	0
56	MG	1T	204	1/1	0.91	0.13	-	72,72,72,72	0
56	MG	2B	3009	1/1	0.88	0.39	-	57,57,57,57	0
56	MG	1A	3576	1/1	0.95	0.30	-	48,48,48,48	0
56	MG	2A	3077	1/1	0.89	0.39	-	63,63,63,63	0
56	MG	1A	3405	1/1	0.91	0.08	-	59,59,59,59	0
56	MG	1A	3724	1/1	0.93	0.34	-	55,55,55,55	0
56	MG	1A	3005	1/1	0.91	0.27	-	60,60,60,60	0
56	MG	2l	202	1/1	0.97	0.31	-	57,57,57,57	0
56	MG	2A	3408	1/1	0.94	0.16	-	47,47,47,47	0
56	MG	1A	3351	1/1	0.72	0.39	-	59,59,59,59	0
56	MG	1A	3586	1/1	0.96	0.18	-	32,32,32,32	0
56	MG	1A	3499	1/1	0.76	0.16	-	81,81,81,81	0
56	MG	1a	1852	1/1	0.95	0.15	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1857	1/1	0.97	0.16	-	47,47,47,47	0
56	MG	2A	3472	1/1	0.97	0.13	-	54,54,54,54	0
56	MG	1a	1705	1/1	0.99	0.10	-	64,64,64,64	0
56	MG	2B	3006	1/1	0.83	0.17	-	50,50,50,50	0
56	MG	2a	3184	1/1	0.96	0.21	-	56,56,56,56	0
56	MG	1A	3159	1/1	0.87	0.26	-	42,42,42,42	0
56	MG	2a	3122	1/1	0.91	0.18	-	69,69,69,69	0
56	MG	2a	3042	1/1	0.84	0.10	-	78,78,78,78	0
56	MG	2A	3487	1/1	0.93	0.46	-	60,60,60,60	0
56	MG	1A	3488	1/1	0.93	0.15	-	53,53,53,53	0
56	MG	1A	3793	1/1	0.93	0.09	-	72,72,72,72	0
56	MG	2a	3195	1/1	0.92	0.11	-	53,53,53,53	0
56	MG	2a	3169	1/1	0.60	0.17	-	75,75,75,75	0
56	MG	2A	3375	1/1	0.94	0.18	-	50,50,50,50	0
56	MG	2A	3043	1/1	0.96	0.23	-	58,58,58,58	0
56	MG	2A	3001	1/1	0.73	0.38	-	55,55,55,55	0
56	MG	1A	3153	1/1	0.98	0.13	-	43,43,43,43	0
56	MG	1A	3566	1/1	0.99	0.19	-	42,42,42,42	0
56	MG	15	101	1/1	0.95	0.24	-	43,43,43,43	0
56	MG	1a	1695	1/1	0.86	0.09	-	77,77,77,77	0
56	MG	1A	3044	1/1	0.96	0.20	-	50,50,50,50	0
56	MG	1a	1782	1/1	0.88	0.15	-	67,67,67,67	0
56	MG	2A	3025	1/1	0.68	0.25	-	61,61,61,61	0
56	MG	1A	4009	1/1	0.96	0.46	-	48,48,48,48	0
56	MG	2B	3008	1/1	0.91	0.15	-	73,73,73,73	0
56	MG	1A	3510	1/1	0.96	0.21	-	39,39,39,39	0
56	MG	1A	3360	1/1	0.84	0.19	-	61,61,61,61	0
56	MG	1A	3968	1/1	0.83	0.28	-	65,65,65,65	0
56	MG	2A	3506	1/1	0.96	0.02	-	34,34,34,34	0
56	MG	1A	3056	1/1	0.95	0.41	-	49,49,49,49	0
56	MG	1A	3266	1/1	0.96	0.17	-	78,78,78,78	0
56	MG	1A	3443	1/1	0.96	0.17	-	47,47,47,47	0
56	MG	1a	1788	1/1	0.81	0.22	-	81,81,81,81	0
56	MG	2a	3148	1/1	0.97	0.05	-	77,77,77,77	0
56	MG	2A	3028	1/1	0.83	0.14	-	48,48,48,48	0
56	MG	1N	201	1/1	0.83	0.30	-	70,70,70,70	0
56	MG	2A	3218	1/1	0.87	0.11	-	64,64,64,64	0
56	MG	1A	3652	1/1	0.96	0.12	-	24,24,24,24	0
56	MG	1A	3282	1/1	0.96	0.46	-	47,47,47,47	0
56	MG	1A	3577	1/1	0.92	0.10	-	38,38,38,38	0
56	MG	1A	3878	1/1	0.93	0.23	-	60,60,60,60	0
56	MG	1B	216	1/1	0.96	0.09	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1901	1/1	0.94	0.14	-	46,46,46,46	0
56	MG	2a	3096	1/1	0.95	0.10	-	72,72,72,72	0
56	MG	1A	3364	1/1	0.62	0.49	-	57,57,57,57	0
56	MG	1a	1723	1/1	0.84	0.07	-	60,60,60,60	0
56	MG	1A	3460	1/1	0.93	0.17	-	51,51,51,51	0
56	MG	1a	1794	1/1	0.90	0.30	-	63,63,63,63	0
56	MG	1A	3762	1/1	0.97	0.12	-	51,51,51,51	0
56	MG	2a	3142	1/1	0.90	0.13	-	83,83,83,83	0
56	MG	2a	3206	1/1	0.99	0.42	-	62,62,62,62	0
56	MG	2A	3261	1/1	0.90	0.17	-	34,34,34,34	0
56	MG	1e	204	1/1	0.92	0.10	-	64,64,64,64	0
56	MG	1A	3977	1/1	0.93	0.30	-	50,50,50,50	0
56	MG	1A	3422	1/1	0.83	0.15	-	72,72,72,72	0
56	MG	1a	1699	1/1	0.89	0.25	-	71,71,71,71	0
56	MG	1a	1717	1/1	0.96	0.08	-	69,69,69,69	0
56	MG	2A	3253	1/1	0.83	0.33	-	68,68,68,68	0
56	MG	2a	3221	1/1	0.97	0.19	-	57,57,57,57	0
56	MG	1A	3438	1/1	0.90	0.26	-	62,62,62,62	0
56	MG	1e	202	1/1	0.96	0.10	-	66,66,66,66	0
56	MG	1A	3179	1/1	0.94	0.15	-	47,47,47,47	0
56	MG	1A	3096	1/1	0.93	0.14	-	40,40,40,40	0
56	MG	1Z	303	1/1	0.87	0.14	-	64,64,64,64	0
56	MG	1A	3904	1/1	0.95	0.22	-	44,44,44,44	0
56	MG	2A	3172	1/1	0.95	0.18	-	47,47,47,47	0
56	MG	1A	3470	1/1	0.98	0.07	-	57,57,57,57	0
56	MG	2A	3125	1/1	0.97	0.18	-	43,43,43,43	0
56	MG	1a	1690	1/1	0.88	0.22	-	82,82,82,82	0
56	MG	2A	3063	1/1	0.80	0.26	-	56,56,56,56	0
56	MG	2A	3354	1/1	0.96	0.17	-	75,75,75,75	0
56	MG	1A	3647	1/1	0.86	0.25	-	55,55,55,55	0
56	MG	2a	3190	1/1	0.97	0.11	-	67,67,67,67	0
56	MG	1A	3077	1/1	0.92	0.21	-	53,53,53,53	0
56	MG	1A	3223	1/1	0.98	0.16	-	55,55,55,55	0
56	MG	2a	3034	1/1	0.79	0.49	-	72,72,72,72	0
56	MG	2a	3203	1/1	0.93	0.11	-	53,53,53,53	0
56	MG	1A	3151	1/1	0.82	0.26	-	49,49,49,49	0
56	MG	1A	3635	1/1	0.82	0.24	-	56,56,56,56	0
56	MG	2A	3276	1/1	0.81	0.23	-	58,58,58,58	0
56	MG	1a	1749	1/1	0.85	0.24	-	66,66,66,66	0
56	MG	1A	3546	1/1	0.92	0.17	-	41,41,41,41	0
56	MG	1A	3247	1/1	0.84	0.32	-	72,72,72,72	0
56	MG	2A	3549	1/1	0.97	0.23	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3366	1/1	0.87	0.31	-	46,46,46,46	0
56	MG	1A	3720	1/1	0.92	0.31	-	64,64,64,64	0
56	MG	1A	3232	1/1	0.93	0.17	-	57,57,57,57	0
56	MG	1a	1776	1/1	0.94	0.38	-	76,76,76,76	0
56	MG	2A	3360	1/1	0.95	0.06	-	73,73,73,73	0
56	MG	2a	3133	1/1	0.86	0.31	-	93,93,93,93	0
56	MG	1A	3237	1/1	0.92	0.20	-	52,52,52,52	0
56	MG	1A	3127	1/1	0.96	0.17	-	50,50,50,50	0
56	MG	2A	3423	1/1	0.96	0.41	-	71,71,71,71	0
56	MG	1a	1774	1/1	0.90	0.46	-	63,63,63,63	0
56	MG	1a	1854	1/1	0.96	0.22	-	51,51,51,51	0
56	MG	2A	3437	1/1	0.89	0.19	-	83,83,83,83	0
56	MG	1a	1673	1/1	0.84	0.10	-	46,46,46,46	0
56	MG	2A	3478	1/1	0.97	0.07	-	47,47,47,47	0
56	MG	1A	3801	1/1	0.93	0.14	-	52,52,52,52	0
56	MG	1D	306	1/1	0.89	0.20	-	43,43,43,43	0
56	MG	1A	3925	1/1	0.92	0.17	-	54,54,54,54	0
56	MG	2a	3045	1/1	0.92	0.16	-	81,81,81,81	0
56	MG	1A	3040	1/1	0.92	0.24	-	58,58,58,58	0
56	MG	1A	3715	1/1	0.98	0.14	-	49,49,49,49	0
56	MG	2A	3321	1/1	0.97	0.17	-	53,53,53,53	0
56	MG	2A	3330	1/1	0.98	0.13	-	58,58,58,58	0
56	MG	1W	3004	1/1	0.92	0.24	-	43,43,43,43	0
56	MG	2a	3075	1/1	0.95	0.10	-	60,60,60,60	0
56	MG	1A	3853	1/1	0.89	0.22	-	49,49,49,49	0
56	MG	1a	1618	1/1	0.86	0.27	-	65,65,65,65	0
56	MG	2A	3363	1/1	0.95	0.25	-	53,53,53,53	0
56	MG	2A	3557	1/1	0.96	0.27	-	45,45,45,45	0
56	MG	1A	3615	1/1	0.98	0.18	-	57,57,57,57	0
56	MG	2a	3150	1/1	0.87	0.23	-	63,63,63,63	0
56	MG	1A	3301	1/1	0.94	0.23	-	33,33,33,33	0
56	MG	1a	1684	1/1	0.89	0.18	-	58,58,58,58	0
56	MG	1a	1887	1/1	0.95	0.25	-	66,66,66,66	0
56	MG	1a	1649	1/1	0.97	0.26	-	56,56,56,56	0
56	MG	1A	3038	1/1	0.91	0.10	-	52,52,52,52	0
56	MG	1A	3065	1/1	0.96	0.27	-	60,60,60,60	0
56	MG	1A	3795	1/1	0.96	0.14	-	24,24,24,24	0
56	MG	1A	3645	1/1	0.98	0.07	-	32,32,32,32	0
56	MG	2a	3113	1/1	0.94	0.27	-	51,51,51,51	0
56	MG	1A	3680	1/1	0.93	0.07	-	71,71,71,71	0
56	MG	1A	3013	1/1	0.90	0.26	-	64,64,64,64	0
56	MG	1A	3697	1/1	0.99	0.05	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3194	1/1	0.96	0.17	-	41,41,41,41	0
56	MG	2x	3001	1/1	0.91	0.06	-	79,79,79,79	0
56	MG	2A	3544	1/1	0.88	0.24	-	61,61,61,61	0
56	MG	1a	1873	1/1	0.91	0.10	-	56,56,56,56	0
56	MG	1A	4021	1/1	0.91	0.23	-	33,33,33,33	0
56	MG	1A	3620	1/1	0.94	0.16	-	19,19,19,19	0
56	MG	1A	3705	1/1	0.97	0.32	-	35,35,35,35	0
56	MG	1a	1810	1/1	0.85	0.06	-	86,86,86,86	0
56	MG	2A	3459	1/1	0.66	0.26	-	70,70,70,70	0
56	MG	1A	3778	1/1	0.92	0.17	-	20,20,20,20	0
56	MG	1A	3333	1/1	0.97	0.07	-	51,51,51,51	0
56	MG	25	502	1/1	0.92	0.57	-	56,56,56,56	0
56	MG	1A	3401	1/1	0.89	0.17	-	67,67,67,67	0
56	MG	1a	1606	1/1	0.91	0.12	-	73,73,73,73	0
56	MG	2A	3343	1/1	0.97	0.25	-	60,60,60,60	0
56	MG	2a	3011	1/1	0.90	0.71	-	68,68,68,68	0
56	MG	1B	208	1/1	0.86	0.16	-	61,61,61,61	0
56	MG	1A	3420	1/1	0.91	0.15	-	50,50,50,50	0
56	MG	10	106	1/1	0.95	0.32	-	62,62,62,62	0
56	MG	2A	3262	1/1	0.98	0.17	-	55,55,55,55	0
56	MG	1a	1787	1/1	0.89	0.35	-	70,70,70,70	0
56	MG	2A	3245	1/1	0.88	0.07	-	78,78,78,78	0
56	MG	1A	3287	1/1	0.86	0.25	-	57,57,57,57	0
56	MG	1A	3063	1/1	0.96	0.42	-	52,52,52,52	0
56	MG	1A	3334	1/1	0.89	0.18	-	55,55,55,55	0
56	MG	2A	3283	1/1	0.91	0.13	-	51,51,51,51	0
56	MG	1A	3508	1/1	0.80	0.25	-	64,64,64,64	0
56	MG	2a	3230	1/1	0.98	0.10	-	70,70,70,70	0
56	MG	1A	3992	1/1	0.90	0.18	-	50,50,50,50	0
56	MG	2A	3154	1/1	0.93	0.34	-	55,55,55,55	0
56	MG	2A	3530	1/1	0.93	0.20	-	48,48,48,48	0
56	MG	1a	1686	1/1	0.92	0.17	-	53,53,53,53	0
56	MG	2a	3068	1/1	0.95	0.11	-	43,43,43,43	0
56	MG	1A	3812	1/1	0.97	0.15	-	54,54,54,54	0
56	MG	1A	3326	1/1	0.87	0.08	-	63,63,63,63	0
56	MG	1A	3299	1/1	0.94	0.36	-	30,30,30,30	0
56	MG	1V	201	1/1	0.98	0.36	-	45,45,45,45	0
56	MG	1a	1755	1/1	0.92	0.34	-	60,60,60,60	0
56	MG	2A	3022	1/1	0.90	0.30	-	63,63,63,63	0
56	MG	1A	3863	1/1	0.98	0.23	-	49,49,49,49	0
56	MG	2a	3001	1/1	0.84	0.54	-	54,54,54,54	0
56	MG	2A	3559	1/1	0.98	0.04	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3502	1/1	0.95	0.19	-	77,77,77,77	0
56	MG	1a	1883	1/1	0.96	0.23	-	58,58,58,58	0
56	MG	1a	1698	1/1	0.90	0.27	-	75,75,75,75	0
56	MG	2A	3303	1/1	0.91	0.12	-	42,42,42,42	0
56	MG	2A	3107	1/1	0.91	0.13	-	50,50,50,50	0
56	MG	1A	3751	1/1	0.92	0.19	-	40,40,40,40	0
56	MG	1a	1785	1/1	0.84	0.14	-	66,66,66,66	0
56	MG	1a	1718	1/1	0.94	0.14	-	64,64,64,64	0
56	MG	2A	3378	1/1	0.94	0.15	-	53,53,53,53	0
56	MG	1B	217	1/1	0.97	0.14	-	36,36,36,36	0
56	MG	1A	3519	1/1	0.83	0.25	-	33,33,33,33	0
56	MG	2A	3123	1/1	0.99	0.13	-	51,51,51,51	0
56	MG	2A	3457	1/1	0.86	0.33	-	55,55,55,55	0
56	MG	1A	3994	1/1	0.63	0.35	-	51,51,51,51	0
56	MG	1A	3759	1/1	0.96	0.07	-	54,54,54,54	0
56	MG	1A	3859	1/1	0.75	0.10	-	59,59,59,59	0
56	MG	1a	1804	1/1	0.94	0.12	-	88,88,88,88	0
56	MG	1a	1778	1/1	0.94	0.18	-	78,78,78,78	0
56	MG	2a	3164	1/1	0.83	0.25	-	65,65,65,65	0
56	MG	1A	3827	1/1	0.97	0.10	-	27,27,27,27	0
56	MG	1R	201	1/1	0.91	0.25	-	38,38,38,38	0
56	MG	1A	3702	1/1	0.93	0.10	-	73,73,73,73	0
56	MG	2A	3174	1/1	0.93	0.42	-	48,48,48,48	0
56	MG	2a	3222	1/1	0.91	0.17	-	67,67,67,67	0
56	MG	1a	1644	1/1	0.90	0.11	-	68,68,68,68	0
56	MG	2a	3157	1/1	0.96	0.45	-	66,66,66,66	0
56	MG	1A	3479	1/1	0.90	0.20	-	78,78,78,78	0
56	MG	2A	3429	1/1	0.90	0.24	-	64,64,64,64	0
56	MG	2a	3093	1/1	0.96	0.18	-	62,62,62,62	0
56	MG	1A	3133	1/1	0.95	0.08	-	32,32,32,32	0
56	MG	1A	3504	1/1	0.97	0.22	-	52,52,52,52	0
56	MG	17	104	1/1	0.93	0.32	-	57,57,57,57	0
56	MG	2a	3025	1/1	0.97	0.10	-	58,58,58,58	0
56	MG	1A	3367	1/1	0.93	0.32	-	51,51,51,51	0
56	MG	1A	3274	1/1	0.94	0.10	-	69,69,69,69	0
56	MG	1A	3308	1/1	0.93	0.15	-	64,64,64,64	0
56	MG	1A	3911	1/1	0.96	0.20	-	66,66,66,66	0
56	MG	1A	3690	1/1	0.93	0.36	-	41,41,41,41	0
56	MG	1a	1676	1/1	0.82	0.53	-	51,51,51,51	0
56	MG	1A	3011	1/1	0.93	0.66	-	65,65,65,65	0
56	MG	1A	3257	1/1	0.90	0.39	-	68,68,68,68	0
56	MG	2k	3002	1/1	0.90	0.14	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3924	1/1	0.92	0.11	-	67,67,67,67	0
56	MG	2A	3467	1/1	0.96	0.12	-	58,58,58,58	0
56	MG	1A	3154	1/1	0.93	0.40	-	44,44,44,44	0
56	MG	2a	3152	1/1	0.82	0.19	-	89,89,89,89	0
56	MG	1A	3139	1/1	0.95	0.24	-	28,28,28,28	0
56	MG	1a	1815	1/1	0.93	0.09	-	70,70,70,70	0
56	MG	1A	3386	1/1	0.85	0.18	-	51,51,51,51	0
56	MG	1A	3385	1/1	0.95	0.16	-	51,51,51,51	0
56	MG	2A	3428	1/1	0.96	0.09	-	64,64,64,64	0
56	MG	1a	1813	1/1	0.77	0.12	-	99,99,99,99	0
56	MG	2A	3326	1/1	0.94	0.19	-	34,34,34,34	0
56	MG	1A	3350	1/1	0.94	0.06	-	65,65,65,65	0
56	MG	1A	3230	1/1	0.94	0.11	-	61,61,61,61	0
56	MG	2a	3172	1/1	0.94	0.14	-	78,78,78,78	0
56	MG	2f	3001	1/1	0.95	0.10	-	58,58,58,58	0
56	MG	2B	3010	1/1	0.93	0.26	-	66,66,66,66	0
56	MG	2a	3080	1/1	0.97	0.52	-	61,61,61,61	0
56	MG	1A	3660	1/1	0.94	0.28	-	38,38,38,38	0
56	MG	1A	3304	1/1	0.87	0.28	-	74,74,74,74	0
56	MG	2a	3216	1/1	0.88	0.20	-	57,57,57,57	0
56	MG	1a	1881	1/1	0.91	0.18	-	84,84,84,84	0
56	MG	2a	3224	1/1	0.91	0.12	-	75,75,75,75	0
56	MG	1a	1876	1/1	0.85	0.20	-	61,61,61,61	0
56	MG	1A	3409	1/1	0.88	0.65	-	81,81,81,81	0
56	MG	1A	3714	1/1	0.96	0.17	-	32,32,32,32	0
56	MG	1A	3782	1/1	0.94	0.12	-	43,43,43,43	0
56	MG	1x	111	1/1	0.85	0.10	-	80,80,80,80	0
56	MG	1A	3398	1/1	0.96	0.09	-	47,47,47,47	0
56	MG	1a	1889	1/1	0.86	0.27	-	64,64,64,64	0
56	MG	2A	3473	1/1	0.89	0.13	-	40,40,40,40	0
56	MG	2A	3455	1/1	0.95	0.10	-	67,67,67,67	0
56	MG	2A	3285	1/1	0.93	0.28	-	58,58,58,58	0
56	MG	1A	3196	1/1	0.91	0.15	-	45,45,45,45	0
56	MG	1A	3278	1/1	0.76	0.35	-	72,72,72,72	0
56	MG	2A	3353	1/1	0.93	0.21	-	54,54,54,54	0
56	MG	1A	3954	1/1	0.91	0.19	-	83,83,83,83	0
56	MG	2A	3540	1/1	0.92	0.31	-	39,39,39,39	0
56	MG	2a	3236	1/1	0.91	0.22	-	67,67,67,67	0
56	MG	2A	3039	1/1	0.72	0.26	-	65,65,65,65	0
56	MG	1A	3692	1/1	0.92	0.18	-	57,57,57,57	0
56	MG	1a	1688	1/1	0.93	0.26	-	76,76,76,76	0
56	MG	1x	107	1/1	0.92	0.06	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1858	1/1	0.91	0.20	-	69,69,69,69	0
56	MG	1A	3006	1/1	0.91	0.37	-	61,61,61,61	0
56	MG	2A	3292	1/1	0.90	0.14	-	60,60,60,60	0
56	MG	2a	3054	1/1	0.93	0.13	-	83,83,83,83	0
56	MG	1A	3023	1/1	0.96	0.39	-	57,57,57,57	0
56	MG	2A	3435	1/1	0.98	0.12	-	53,53,53,53	0
56	MG	1A	3025	1/1	0.93	0.11	-	60,60,60,60	0
56	MG	1A	3959	1/1	0.88	0.19	-	57,57,57,57	0
56	MG	1A	3272	1/1	0.97	0.11	-	70,70,70,70	0
56	MG	1Z	302	1/1	0.70	0.59	-	73,73,73,73	0
56	MG	1h	3002	1/1	0.92	0.22	-	64,64,64,64	0
56	MG	1A	3306	1/1	0.92	0.26	-	62,62,62,62	0
56	MG	1a	1841	1/1	0.96	0.15	-	40,40,40,40	0
56	MG	2A	3196	1/1	0.93	0.06	-	37,37,37,37	0
56	MG	1A	3509	1/1	0.96	0.24	-	60,60,60,60	0
56	MG	2A	3032	1/1	0.81	0.62	-	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.