



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2016 – 11:56 PM EDT

PDB ID : 5HCR  
Title : Crystal structure of antimicrobial peptide Oncocin 10wt 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

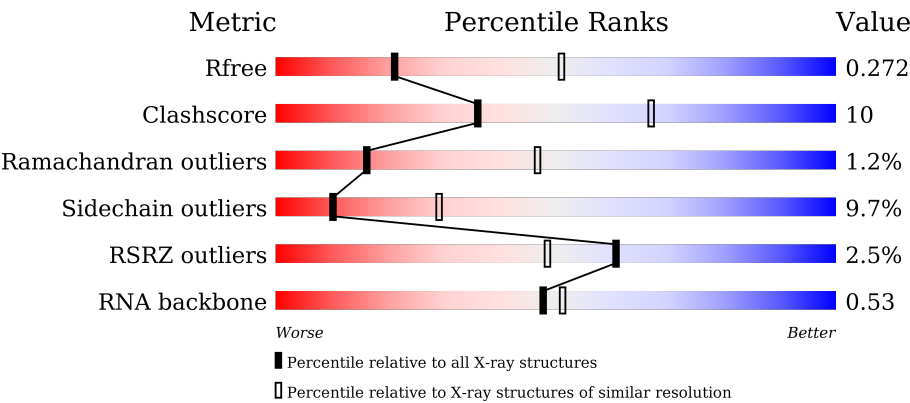
# 1 Overall quality at a glance i

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.
















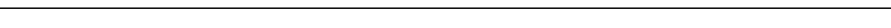











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	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>%</div><div>61%28%5%6%</div></div>
1	2A	2915	<div><div>%</div><div>52%36%7%. </div></div>
2	1B	121	<div><div></div><div>73%26%..</div></div>
2	2B	121	<div><div>%</div><div>38%49%12%. </div></div>


























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Mol	Chain	Length	Quality of chain
3	1D	276	 72%22%5%
3	2D	276	 72%25%. .
4	1E	206	 75%19%. .
4	2E	206	 70%25%. .
5	1F	210	 73%21%. .
5	2F	210	 63%30%. .
6	1G	182	 2%66%28%5%.
6	2G	182	 10%56%37%7%.
7	1H	180	 %71%21%5%.
7	2H	180	 12%62%29%5%.
8	1I	148	 %66%25%7%.
8	2I	148	 4%66%27%5%.
9	1N	140	 81%16%.
9	2N	140	 76%19%.
10	1O	122	 81%16%.
10	2O	122	 76%22%.
11	1P	150	 71%21%7%.
11	2P	150	 4%65%25%9%.
12	1Q	141	 %75%21%.
12	2Q	141	 %70%28%.
13	1R	118	 74%20%6%
13	2R	118	 75%22%.
14	1S	112	 67%27%. .
14	2S	112	 8%57%37%. .
15	1T	146	 68%19%. 10%




















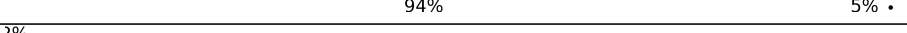
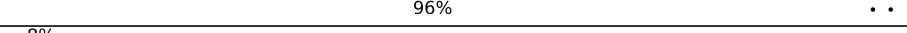




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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	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	19	
55	2z	19	

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	10	101	-	-	-	X
56	MG	11	101	-	-	-	X
56	MG	17	101	-	-	-	X
56	MG	1A	3001	-	-	-	X
56	MG	1A	3003	-	-	-	X
56	MG	1A	3007	-	-	-	X
56	MG	1A	3035	-	-	-	X
56	MG	1A	3054	-	-	-	X
56	MG	1A	3059	-	-	-	X
56	MG	1A	3078	-	-	-	X
56	MG	1A	3079	-	-	-	X
56	MG	1A	3110	-	-	-	X
56	MG	1A	3125	-	-	-	X
56	MG	1A	3127	-	-	-	X
56	MG	1A	3128	-	-	-	X
56	MG	1A	3130	-	-	-	X
56	MG	1A	3136	-	-	-	X
56	MG	1A	3138	-	-	-	X
56	MG	1A	3139	-	-	-	X
56	MG	1A	3140	-	-	-	X
56	MG	1A	3144	-	-	-	X
56	MG	1A	3148	-	-	-	X
56	MG	1A	3151	-	-	-	X
56	MG	1A	3152	-	-	-	X
56	MG	1A	3154	-	-	-	X
56	MG	1A	3155	-	-	-	X
56	MG	1A	3161	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3166	-	-	-	X
56	MG	1A	3178	-	-	-	X
56	MG	1A	3185	-	-	-	X
56	MG	1A	3186	-	-	-	X
56	MG	1A	3199	-	-	-	X
56	MG	1A	3200	-	-	-	X
56	MG	1A	3202	-	-	-	X
56	MG	1A	3205	-	-	-	X
56	MG	1A	3218	-	-	-	X
56	MG	1A	3219	-	-	-	X
56	MG	1A	3222	-	-	-	X
56	MG	1A	3241	-	-	-	X
56	MG	1A	3245	-	-	-	X
56	MG	1A	3253	-	-	-	X
56	MG	1A	3262	-	-	-	X
56	MG	1A	3270	-	-	-	X
56	MG	1A	3282	-	-	-	X
56	MG	1A	3293	-	-	-	X
56	MG	1A	3299	-	-	-	X
56	MG	1A	3302	-	-	-	X
56	MG	1A	3303	-	-	-	X
56	MG	1A	3305	-	-	-	X
56	MG	1A	3360	-	-	-	X
56	MG	1A	3375	-	-	-	X
56	MG	1A	3405	-	-	-	X
56	MG	1A	3432	-	-	-	X
56	MG	1A	3442	-	-	-	X
56	MG	1A	3443	-	-	-	X
56	MG	1A	3460	-	-	-	X
56	MG	1A	3473	-	-	-	X
56	MG	1A	3475	-	-	-	X
56	MG	1A	3485	-	-	-	X
56	MG	1A	3498	-	-	-	X
56	MG	1A	3509	-	-	-	X
56	MG	1A	3510	-	-	-	X
56	MG	1A	3511	-	-	-	X
56	MG	1A	3512	-	-	-	X
56	MG	1A	3571	-	-	-	X
56	MG	1A	3578	-	-	-	X
56	MG	1A	3582	-	-	-	X
56	MG	1A	3583	-	-	-	X
56	MG	1A	3584	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3590	-	-	-	X
56	MG	1A	3597	-	-	-	X
56	MG	1A	3610	-	-	-	X
56	MG	1A	3611	-	-	-	X
56	MG	1A	3646	-	-	-	X
56	MG	1A	3655	-	-	-	X
56	MG	1A	3660	-	-	-	X
56	MG	1A	3667	-	-	-	X
56	MG	1A	3668	-	-	-	X
56	MG	1A	3690	-	-	-	X
56	MG	1A	3703	-	-	-	X
56	MG	1A	3730	-	-	-	X
56	MG	1A	3731	-	-	-	X
56	MG	1A	3751	-	-	-	X
56	MG	1A	3770	-	-	-	X
56	MG	1A	3771	-	-	-	X
56	MG	1A	3789	-	-	-	X
56	MG	1A	3790	-	-	-	X
56	MG	1A	3803	-	-	-	X
56	MG	1A	3820	-	-	-	X
56	MG	1A	3839	-	-	-	X
56	MG	1A	3847	-	-	-	X
56	MG	1A	3863	-	-	-	X
56	MG	1A	3910	-	-	-	X
56	MG	1A	3918	-	-	-	X
56	MG	1A	3941	-	-	-	X
56	MG	1A	3945	-	-	-	X
56	MG	1A	3948	-	-	-	X
56	MG	1A	3949	-	-	-	X
56	MG	1A	3956	-	-	-	X
56	MG	1A	3959	-	-	-	X
56	MG	1A	3993	-	-	-	X
56	MG	1A	3996	-	-	-	X
56	MG	1A	4028	-	-	-	X
56	MG	1A	4041	-	-	-	X
56	MG	1A	4042	-	-	-	X
56	MG	1A	4045	-	-	-	X
56	MG	1A	4046	-	-	-	X
56	MG	1A	4048	-	-	-	X
56	MG	1A	4055	-	-	-	X
56	MG	1A	4056	-	-	-	X
56	MG	1A	4057	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	4061	-	-	-	X
56	MG	1A	4067	-	-	-	X
56	MG	1A	4073	-	-	-	X
56	MG	1A	4074	-	-	-	X
56	MG	1A	4080	-	-	-	X
56	MG	1A	4084	-	-	-	X
56	MG	1A	4088	-	-	-	X
56	MG	1A	4089	-	-	-	X
56	MG	1A	4090	-	-	-	X
56	MG	1A	4092	-	-	-	X
56	MG	1A	4093	-	-	-	X
56	MG	1A	4094	-	-	-	X
56	MG	1B	212	-	-	-	X
56	MG	1D	307	-	-	-	X
56	MG	1D	308	-	-	-	X
56	MG	1D	310	-	-	-	X
56	MG	1D	311	-	-	-	X
56	MG	1E	308	-	-	-	X
56	MG	1F	304	-	-	-	X
56	MG	1H	203	-	-	-	X
56	MG	1N	202	-	-	-	X
56	MG	1P	204	-	-	-	X
56	MG	1P	206	-	-	-	X
56	MG	1Q	3002	-	-	-	X
56	MG	1Q	3004	-	-	-	X
56	MG	1Q	3006	-	-	-	X
56	MG	1R	201	-	-	-	X
56	MG	1R	205	-	-	-	X
56	MG	1U	202	-	-	-	X
56	MG	1U	204	-	-	-	X
56	MG	1U	205	-	-	-	X
56	MG	1U	206	-	-	-	X
56	MG	1V	201	-	-	-	X
56	MG	1W	3005	-	-	-	X
56	MG	1X	3001	-	-	-	X
56	MG	1a	1604	-	-	-	X
56	MG	1a	1632	-	-	-	X
56	MG	1a	1662	-	-	-	X
56	MG	1a	1663	-	-	-	X
56	MG	1a	1671	-	-	-	X
56	MG	1a	1702	-	-	-	X
56	MG	1a	1708	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	1711	-	-	-	X
56	MG	1a	1720	-	-	-	X
56	MG	1a	1723	-	-	-	X
56	MG	1a	1729	-	-	-	X
56	MG	1a	1732	-	-	-	X
56	MG	1a	1753	-	-	-	X
56	MG	1a	1756	-	-	-	X
56	MG	1a	1770	-	-	-	X
56	MG	1a	1793	-	-	-	X
56	MG	1a	1827	-	-	-	X
56	MG	1a	1829	-	-	-	X
56	MG	1a	1836	-	-	-	X
56	MG	1a	1844	-	-	-	X
56	MG	1a	1858	-	-	-	X
56	MG	1a	1900	-	-	-	X
56	MG	1h	3003	-	-	-	X
56	MG	1q	3301	-	-	-	X
56	MG	1q	3302	-	-	-	X
56	MG	1t	3001	-	-	-	X
56	MG	2A	3020	-	-	-	X
56	MG	2A	3021	-	-	-	X
56	MG	2A	3025	-	-	-	X
56	MG	2A	3043	-	-	-	X
56	MG	2A	3046	-	-	-	X
56	MG	2A	3048	-	-	-	X
56	MG	2A	3052	-	-	-	X
56	MG	2A	3062	-	-	-	X
56	MG	2A	3064	-	-	-	X
56	MG	2A	3090	-	-	-	X
56	MG	2A	3100	-	-	-	X
56	MG	2A	3105	-	-	-	X
56	MG	2A	3120	-	-	-	X
56	MG	2A	3123	-	-	-	X
56	MG	2A	3138	-	-	-	X
56	MG	2A	3140	-	-	-	X
56	MG	2A	3145	-	-	-	X
56	MG	2A	3146	-	-	-	X
56	MG	2A	3156	-	-	-	X
56	MG	2A	3173	-	-	-	X
56	MG	2A	3174	-	-	-	X
56	MG	2A	3176	-	-	-	X
56	MG	2A	3179	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3180	-	-	-	X
56	MG	2A	3184	-	-	-	X
56	MG	2A	3186	-	-	-	X
56	MG	2A	3187	-	-	-	X
56	MG	2A	3189	-	-	-	X
56	MG	2A	3190	-	-	-	X
56	MG	2A	3196	-	-	-	X
56	MG	2A	3197	-	-	-	X
56	MG	2A	3199	-	-	-	X
56	MG	2A	3203	-	-	-	X
56	MG	2A	3216	-	-	-	X
56	MG	2A	3217	-	-	-	X
56	MG	2A	3221	-	-	-	X
56	MG	2A	3222	-	-	-	X
56	MG	2A	3229	-	-	-	X
56	MG	2A	3248	-	-	-	X
56	MG	2A	3249	-	-	-	X
56	MG	2A	3256	-	-	-	X
56	MG	2A	3257	-	-	-	X
56	MG	2A	3260	-	-	-	X
56	MG	2A	3270	-	-	-	X
56	MG	2A	3277	-	-	-	X
56	MG	2A	3281	-	-	-	X
56	MG	2A	3285	-	-	-	X
56	MG	2A	3286	-	-	-	X
56	MG	2A	3289	-	-	-	X
56	MG	2A	3290	-	-	-	X
56	MG	2A	3292	-	-	-	X
56	MG	2A	3296	-	-	-	X
56	MG	2A	3298	-	-	-	X
56	MG	2A	3299	-	-	-	X
56	MG	2A	3311	-	-	-	X
56	MG	2A	3314	-	-	-	X
56	MG	2A	3315	-	-	-	X
56	MG	2A	3320	-	-	-	X
56	MG	2A	3322	-	-	-	X
56	MG	2A	3323	-	-	-	X
56	MG	2A	3324	-	-	-	X
56	MG	2A	3330	-	-	-	X
56	MG	2A	3347	-	-	-	X
56	MG	2A	3353	-	-	-	X
56	MG	2A	3356	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3358	-	-	-	X
56	MG	2A	3362	-	-	-	X
56	MG	2A	3365	-	-	-	X
56	MG	2A	3378	-	-	-	X
56	MG	2A	3379	-	-	-	X
56	MG	2A	3386	-	-	-	X
56	MG	2A	3387	-	-	-	X
56	MG	2A	3388	-	-	-	X
56	MG	2A	3390	-	-	-	X
56	MG	2A	3391	-	-	-	X
56	MG	2A	3395	-	-	-	X
56	MG	2A	3408	-	-	-	X
56	MG	2A	3419	-	-	-	X
56	MG	2A	3421	-	-	-	X
56	MG	2A	3422	-	-	-	X
56	MG	2A	3451	-	-	-	X
56	MG	2A	3459	-	-	-	X
56	MG	2A	3470	-	-	-	X
56	MG	2A	3485	-	-	-	X
56	MG	2A	3486	-	-	-	X
56	MG	2A	3491	-	-	-	X
56	MG	2A	3493	-	-	-	X
56	MG	2A	3503	-	-	-	X
56	MG	2A	3525	-	-	-	X
56	MG	2A	3529	-	-	-	X
56	MG	2A	3532	-	-	-	X
56	MG	2A	3533	-	-	-	X
56	MG	2A	3540	-	-	-	X
56	MG	2A	3551	-	-	-	X
56	MG	2A	3553	-	-	-	X
56	MG	2A	3555	-	-	-	X
56	MG	2A	3556	-	-	-	X
56	MG	2B	3005	-	-	-	X
56	MG	2D	303	-	-	-	X
56	MG	2D	305	-	-	-	X
56	MG	2E	302	-	-	-	X
56	MG	2F	303	-	-	-	X
56	MG	2U	202	-	-	-	X
56	MG	2a	1604	-	-	-	X
56	MG	2a	1618	-	-	-	X
56	MG	2a	1620	-	-	-	X
56	MG	2a	1631	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2a	1682	-	-	-	X
56	MG	2a	1684	-	-	-	X
56	MG	2a	1701	-	-	-	X
56	MG	2a	1704	-	-	-	X
56	MG	2a	1712	-	-	-	X
56	MG	2a	1715	-	-	-	X
56	MG	2a	1732	-	-	-	X
56	MG	2a	1752	-	-	-	X
56	MG	2a	1760	-	-	-	X
56	MG	2a	1771	-	-	-	X
56	MG	2a	1786	-	-	-	X
56	MG	2a	1788	-	-	-	X
56	MG	2a	1799	-	-	-	X
56	MG	2a	1806	-	-	-	X
56	MG	2a	1812	-	-	-	X
56	MG	2a	1816	-	-	-	X
56	MG	2a	1817	-	-	-	X
56	MG	2e	202	-	-	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 288674 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	1		
15	2T	131	Total	C	N	O	0	0	0
			1083	675	224	183	1		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			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 10wt.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	13	Total	C	N	O	0	0	0
			108	72	20	16			
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	4	Total	Mg	0	0
			4	4		
56	17	6	Total	Mg	0	0
			6	6		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	6	Total	Mg	0	0
			6	6		
56	1N	8	Total	Mg	0	0
			8	8		
56	1u	1	Total	Mg	0	0
			1	1		
56	18	4	Total	Mg	0	0
			4	4		
56	1o	2	Total	Mg	0	0
			2	2		
56	2W	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	1	Total 1	Mg 1	0	0
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1P	6	Total 6	Mg 6	0	0
56	2B	10	Total 10	Mg 10	0	0
56	1q	4	Total 4	Mg 4	0	0
56	2a	217	Total 217	Mg 217	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1E	8	Total 8	Mg 8	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	4	Total 4	Mg 4	0	0
56	2F	3	Total 3	Mg 3	0	0
56	16	3	Total 3	Mg 3	0	0
56	28	1	Total 1	Mg 1	0	0
56	2e	3	Total 3	Mg 3	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1A	1096	Total 1096	Mg 1096	0	0
56	1t	1	Total 1	Mg 1	0	0
56	2p	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	1X	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	20	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	1D	13	Total 13	Mg 13	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	3	Total 3	Mg 3	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	1	Total 1	Mg 1	0	0
56	1a	307	Total 307	Mg 307	0	0
56	2Q	5	Total 5	Mg 5	0	0
56	15	3	Total 3	Mg 3	0	0
56	1x	10	Total 10	Mg 10	0	0
56	1R	6	Total 6	Mg 6	0	0
56	1m	2	Total 2	Mg 2	0	0
56	2U	2	Total 2	Mg 2	0	0
56	1G	3	Total 3	Mg 3	0	0
56	2O	2	Total 2	Mg 2	0	0
56	11	4	Total 4	Mg 4	0	0
56	1d	2	Total 2	Mg 2	0	0
56	2n	1	Total 1	Mg 1	0	0
56	1H	3	Total 3	Mg 3	0	0

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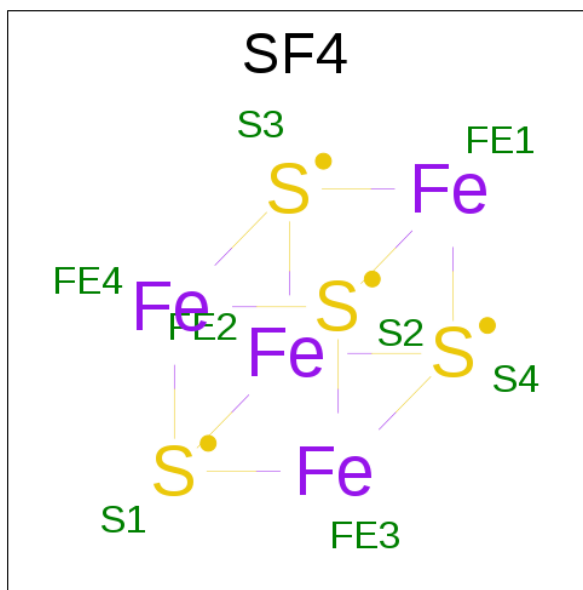
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2Y	2	Total Mg 2 2	0	0
56	2x	5	Total Mg 5 5	0	0
56	1Z	2	Total Mg 2 2	0	0
56	2D	6	Total Mg 6 6	0	0
56	2q	2	Total Mg 2 2	0	0
56	2k	1	Total Mg 1 1	0	0
56	1U	6	Total Mg 6 6	0	0
56	1O	3	Total Mg 3 3	0	0
56	1r	3	Total Mg 3 3	0	0
56	19	3	Total Mg 3 3	0	0
56	1l	1	Total Mg 1 1	0	0
56	1F	7	Total Mg 7 7	0	0
56	10	6	Total Mg 6 6	0	0
56	2t	1	Total Mg 1 1	0	0
56	1Q	7	Total Mg 7 7	0	0
56	2A	559	Total Mg 559 559	0	0
56	1h	3	Total Mg 3 3	0	0
56	2Z	1	Total Mg 1 1	0	0
56	1B	27	Total Mg 27 27	0	0
56	1c	1	Total Mg 1 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 1 1	0	0
57	14	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	29	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	2n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	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	2345	Total	O	0	0
			2345	2345		
59	1B	45	Total	O	0	0
			45	45		
59	1D	20	Total	O	0	0
			20	20		
59	1E	29	Total	O	0	0
			29	29		
59	1F	18	Total	O	0	0
			18	18		
59	1G	4	Total	O	0	0
			4	4		
59	1H	4	Total	O	0	0
			4	4		
59	1I	1	Total	O	0	0
			1	1		
59	1N	12	Total	O	0	0
			12	12		
59	1O	6	Total	O	0	0
			6	6		
59	1P	16	Total	O	0	0
			16	16		
59	1Q	12	Total	O	0	0
			12	12		
59	1R	10	Total	O	0	0
			10	10		
59	1S	1	Total	O	0	0
			1	1		
59	1T	14	Total	O	0	0
			14	14		
59	1U	11	Total	O	0	0
			11	11		
59	1V	5	Total	O	0	0
			5	5		
59	1W	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	6	Total 6	O 6	0	0
59	1Y	1	Total 1	O 1	0	0
59	1Z	6	Total 6	O 6	0	0
59	10	7	Total 7	O 7	0	0
59	11	9	Total 9	O 9	0	0
59	12	1	Total 1	O 1	0	0
59	13	5	Total 5	O 5	0	0
59	14	1	Total 1	O 1	0	0
59	15	9	Total 9	O 9	0	0
59	16	6	Total 6	O 6	0	0
59	17	3	Total 3	O 3	0	0
59	18	15	Total 15	O 15	0	0
59	19	4	Total 4	O 4	0	0
59	1a	395	Total 395	O 395	0	0
59	1b	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	4	Total 4	O 4	0	0
59	1i	1	Total 1	O 1	0	0
59	1j	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1k	2	Total 2	O 2	0	0
59	1l	3	Total 3	O 3	0	0
59	1o	3	Total 3	O 3	0	0
59	1s	1	Total 1	O 1	0	0
59	1v	2	Total 2	O 2	0	0
59	1x	11	Total 11	O 11	0	0
59	1z	1	Total 1	O 1	0	0
59	2A	810	Total 810	O 810	0	0
59	2B	10	Total 10	O 10	0	0
59	2D	15	Total 15	O 15	0	0
59	2E	9	Total 9	O 9	0	0
59	2F	4	Total 4	O 4	0	0
59	2O	2	Total 2	O 2	0	0
59	2P	6	Total 6	O 6	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	2	Total 2	O 2	0	0
59	2T	2	Total 2	O 2	0	0
59	2U	4	Total 4	O 4	0	0
59	2V	1	Total 1	O 1	0	0
59	2W	1	Total 1	O 1	0	0
59	2X	2	Total 2	O 2	0	0

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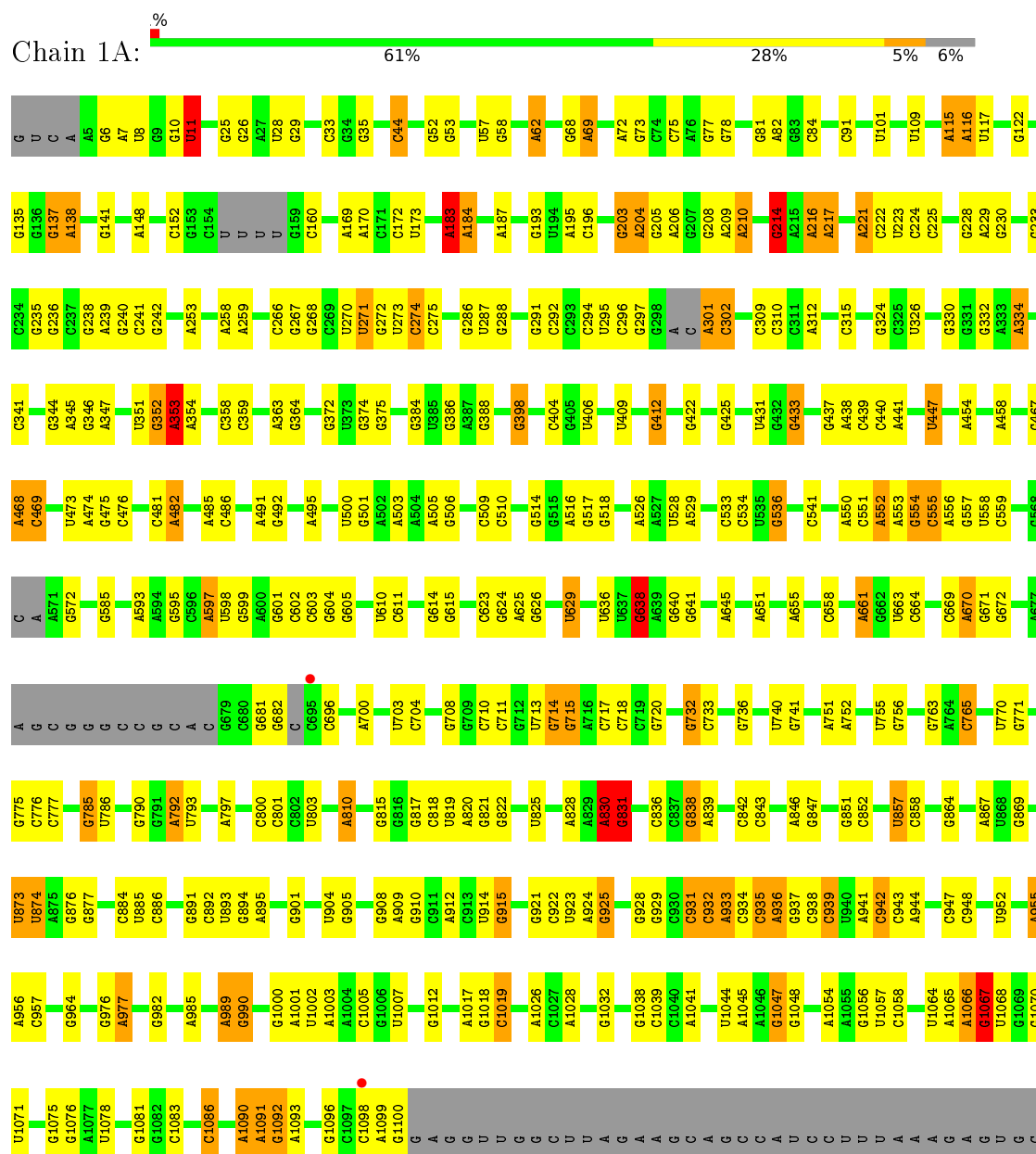
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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59	2Z	4	Total 4	O 4	0	0
59	20	3	Total 3	O 3	0	0
59	21	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	28	4	Total 4	O 4	0	0
59	2a	235	Total 235	O 235	0	0
59	2d	2	Total 2	O 2	0	0
59	2e	3	Total 3	O 3	0	0
59	2i	1	Total 1	O 1	0	0
59	2m	1	Total 1	O 1	0	0
59	2n	1	Total 1	O 1	0	0
59	2p	1	Total 1	O 1	0	0
59	2t	4	Total 4	O 4	0	0
59	2x	5	Total 5	O 5	0	0
59	2z	1	Total 1	O 1	0	0

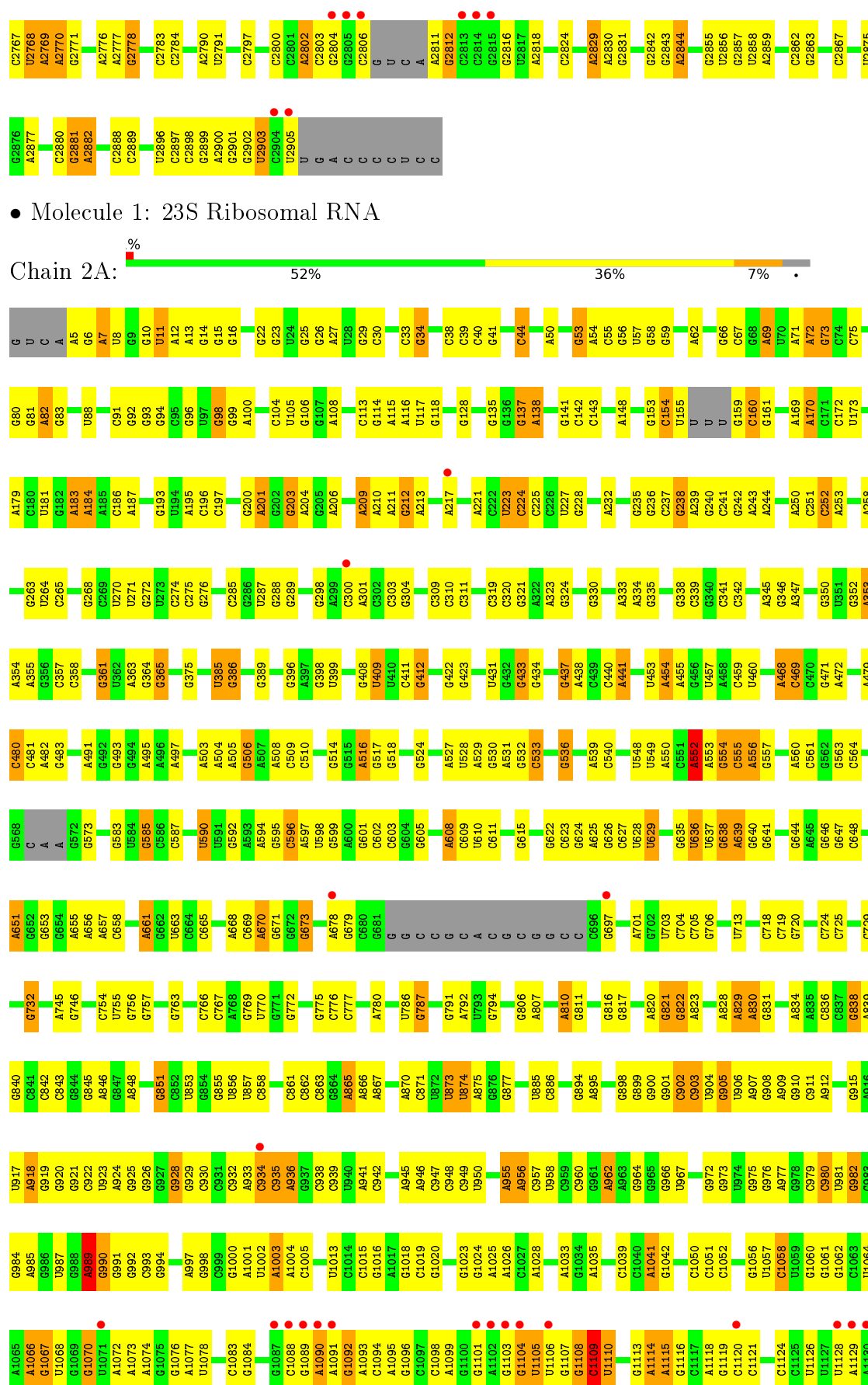
### 3 Residue-property plots

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

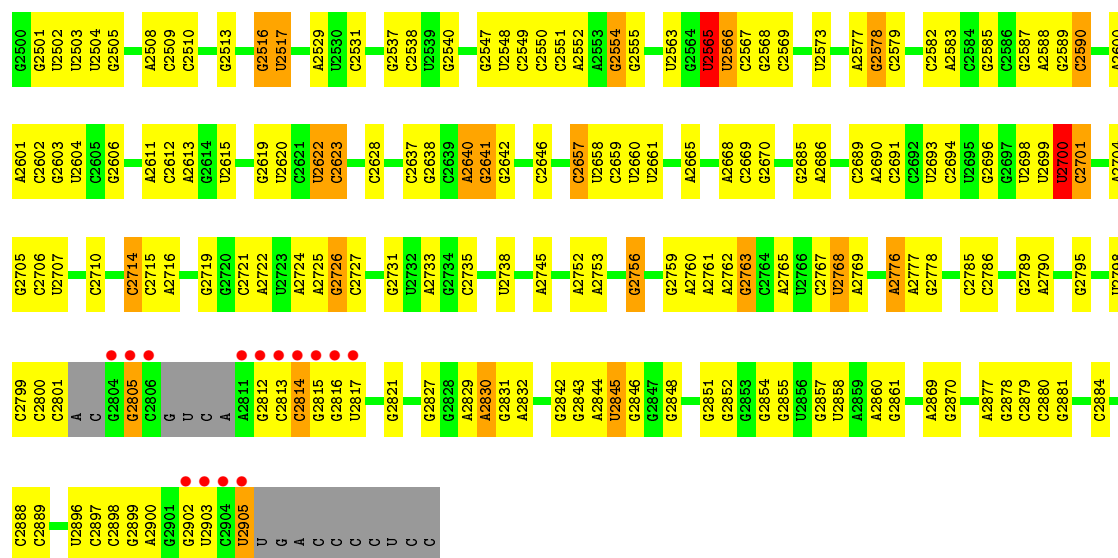
#### • Molecule 1: 23S Ribosomal RNA



G2641	C2503	G2429	G2315	C2206	G	U1938	A1803	G1886	U1559	G1461	U1345	C1229	G
G2642	G2504	U2430	A2316	G2207	A	A1939	G1806	A1887	C1560	C1462	A1346	G1230	U
A2650	A2509	A2433	G2319	G2208	C	A1940	G1807	G1888	U1565	A1463	A1347	G1231	A
G2667	G2535	U2434	A2320	U2210	G	C1941	U1807	C1691	G1566	G1464	G1348	U1232	A
U2668	G2536	U2436	A2321	G2211	U	U1947	U1808	G1692	G1570	U1465	C1349	C1245	U
A2665	G2540	A2437	A2322	G2212	C	A1948	A1810	G1693	G1578	G1466	C1350	G1246	A
G2670	C2550	G2438	C2324	G2213	U	A1949	A1813	C1694	C1578	A1468	G1354	A1248	C
C2678	C2561	U2440	G2326	G2214	G	G1950	G1813	G1697	G	A1254	G1355	A1249	U
A2690	G2562	C2441	C2327	G2215	A	G1951	C1820	U1697	U	A1257	G1356	A1254	C
C2694	U2563	U2442	C2328	G2216	C	U1952	C1821	A1700	A	A1258	G1357	A1255	U
U2698	G2564	U2443	C2329	G2217	C	A1953	A1821	C1704	C	G1470	U1358	A1257	G
U2699	C2565	A2444	G2330	U2218	C	G1954	G1822	G1705	G1583	G1471	C1359	C1262	A
C2701	U2566	A2445	A2331	G2219	C	C1955	G1823	C1706	G1588	U1476	C1360	G1263	U
C2702	U2567	U2446	G2332	G2220	C	U1956	U1826	G1713	A1588	A1477	G1369	G1264	U
C2703	G2568	A2447	C2333	A2228	C	A1957	C1827	A1714	C1589	A1478	G1370	C1265	U
A2704	C2569	U2448	G2334	U2229	G	U1958	U1828	A1715	C1590	A1479	G1371	C1266	U
G2705	U2570	A2449	A2335	G2230	C	A1959	G1829	G1720	A1604	C1482	G1372	C1267	U
C2708	C2571	U2450	G2336	A2236	U	U1976	C1830	G1721	G1605	A1490	G1373	C1275	U
U2709	U2572	G2451	U2340	U2237	C	U1984	G1831	U1726	A1606	C1491	G1374	G1276	U
C2710	G2573	U2452	G2345	G2238	C	G1985	A1832	U1727	A1612	G1496	A1381	U1279	U
C2711	A2574	U2453	U2346	U2239	C	U1986	A1833	G1728	G1613	G1497	G1382	G1280	U
C2712	G2575	A2454	A2347	G2240	G	G1987	G1841	C1731	A1615	U1500	G1383	G1281	U
C2713	U2576	U2455	G2348	U2241	U	G1988	G1842	C1732	A1616	G1501	A1173	G1282	U
U2714	C2577	U2456	C2349	U2242	G	G1989	A1844	G1733	A1617	C1502	A1174	G1283	U
C2715	G2578	A2457	U2350	G2243	C	A1990	A1845	U1734	G1628	U1285	G1175	G1284	U
C2716	U2579	U2458	G2351	U2244	C	A1991	A1846	A1735	A1629	A1287	G1176	G1285	U
U2717	C2580	U2459	U2352	G2245	G	A1992	G1847	U1736	U1624	G1288	G1177	G1286	U
C2718	G2581	G2460	C2353	U2246	U	A1993	G1853	A1744	A1625	C1301	U1397	G1287	U
C2719	U2582	U2461	U2354	U2247	C	C2004	G1854	G1745	A1626	A1405	A1406	A1298	U
C2720	G2583	U2462	G2355	U2248	G	U2012	A1859	A1746	G1627	G1521	G1409	G1302	U
C2721	U2584	U2463	U2356	U2249	C	U2013	C1868	C1756	A1632	G1522	A1410	C1303	U
U2722	G2585	A2464	C2357	G2250	C	U2014	G1869	C1757	C1630	G1523	U1312	G1304	U
C2723	U2586	U2465	G2358	U2251	G	C2017	C1873	G1760	C1634	G1524	A1418	A1313	U
C2724	C2587	U2466	U2359	U2252	U	G2018	A1877	G1761	G1635	G1525	A1419	A1314	U
C2725	U2588	U2467	G2360	U2253	C	C	G1899	G1762	G1640	U1527	U1313	A1315	U
C2726	G2589	A2468	C2361	U2254	G	G	G1902	U1763	C1644	G1528	A1424	G1316	U
U2727	C2590	U2469	U2362	U2255	C	U2022	C1903	C1774	A1648	G1532	G1425	G1317	U
C2728	U2591	U2470	G2363	U2256	U	C	A1910	G1775	C1649	A1535	U1429	U1318	U
C2729	G2592	U2471	C2364	U2257	C	U2023	G1917	G1776	G1652	G1536	G1430	A1319	U
C2730	U2593	U2472	U2365	U2258	G	C	G1924	G1783	A1653	U1537	A1438	A1323	U
U2731	C2594	U2473	U2366	U2259	C	A	G1925	C1784	A1654	C1538	U1441	A1332	U
C2732	U2595	U2474	G2367	U2260	C	U2043	A1921	A1789	A1655	A1540	U1442	U1337	U
C2733	G2596	U2475	C2368	U2261	C	G	G1924	A1792	U1674	A1552	U1450	C1338	U
C2734	U2597	U2476	U2369	U2262	C	U2044	G1925	G1793	G1675	A1553	U1451	C1339	U
C2735	G2598	U2477	G2370	U2263	C	A	A2052	G1794	C1676	C1554	C1452	C1342	U
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C2738	A2613	U2480	C2373	U2266	C	C	G						
C2617	C2617	U2481	G2374	U2267	C	C	G						
U2620	U2620	U2482	U2375	U2268	C	C	G						
C2621	C2621	U2483	G2376	U2269	C	C	G						
U2622	U2622	U2484	U2377	U2270	C	C	G						
C2623	C2623	U2485	G2378	U2271	C	C	G						
U2624	U2624	U2486	U2379	U2272	C	C	G						
C2625	C2625	U2487	G2380	U2273	C	C	G						
U2626	U2626	U2488	U2381	U2274	C	C	G						
C2627	C2627	U2489	G2382	U2275	C	C	G						
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C2640	C2640	U2502	C2397	U2288	C	C	G						
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C2642	C2642	U2504	A2405	U2290	C	C	G						
U2643	U2643	U2505	U2406	U2291	C	C	G						
C2644	C2644	U2506	G2407	U2292	C	C	G						
U2645	U2645	U2507	U2408	U2293	C	C	G						
C2646	C2646	U2508	A2409	U2294	C	C	G						
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C2648	C2648	U2510	G2411	U2296	C	C	G						
U2649	U2649	U2511	A2412	U2297	C	C	G						
C2650	C2650	U2512	U2413	U2298	C	C	G						
U2651	U2651	U2513	G2414	U2299	C	C	G						
C2652	C2652	U2514	A2415	U2300	C	C	G						
U2653	U2653	U2515	U2416	U2301	C	C	G						
C2654	C2654	U2516	G2417	U2302	C	C	G						
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C2656	C2656	U2518	G2419	U2304	C	C	G						
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C2664	C2664	U2526	A2427	U2312	C	C	G						
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C2666	C2666	U2528	G2429	U2314	C	C	G						
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C2668	C2668	U2530	U2431	U2316	C	C	G						
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C2670	C2670	U2532	A2433	U2318	C	C	G						
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U2679	U2679	U2541	U2442	U2327	C	C	G						
C2680	C2680	U2542	G2443	U2328	C	C	G						
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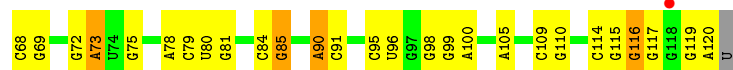
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U2412	A2331	G	G	U2097	G1994	A1889	G1793	U1885	C1588	G1486	A1404	G1297	G1216	A1133
G2413	G2332	G2251	G	U2100	G2012	G1890	G1794	A1886	C1593	G1487	A1405	A1298	A	U1134
G2414	A2333	G2252	G	U2101	G2013	G1891	G1795	A1887	C1592	G1488	G1406	G1301	U	U1135
G2415	G2334	A2252	G	U2107	U2014	U1894	U1796	G1893	C1594	G1489	C1407	C1302	G	G1136
G2416	G2335	G	G	G2108	G	G	C1797	C1694	A1604	A1490	G1408	G1301	A	A1141
U2417	G2336	G	G	G2115	C2017	A1897	A1803	A1698	G1605	G1494	A1409	U1308	G	U1142
G2418	C2337	G	A	G2116	G2018	A1898	G1804	A1699	G1605	G1495	A1410	G1309	C1222	U1146
G2419	A2338	U2272	G	G2120	A2022	G1906	U1805	G1702	A1612	G1496	A1411	A1310	C1223	G
G2420	A2339	U2273	G	G2121	G2023	C1907	G1806	C1703	G1615	G1501	A1412	A1311	C1224	U1146
G2421	G2340	G2274	G	G2122	C2027	G	U1807	G1703	G1619	G1502	G1413	G1312	C1225	G
A2422	G	G2275	C	G2123	G	A1910	U1808	C1703	G1619	G1507	G1414	U1312	G	C1149
G2428	U2343	G	G	G2124	A2035	A1911	A1810	G1713	U1624	G1508	C1415	A1313	G1230	U1150
A2429	A2344	A2278	C	G2125	A2036	G1920	G1812	A1715	A1625	G1509	G1416	A1314	U1231	G1151
U2430	A2345	A2279	G	C	U2037	A1921	G1813	G1716	A1626	G1512	A1417	G1315	U1232	G1152
G	A2346	A2280	G	G	U2038	A1922	A1814	U1717	A1627	G1513	A1418	G1316	U1233	U1153
G	A2347	G2281	G	C	G2039	A1923	A1815	G1718	A1628	C1513	A1419	A1317	G1234	C1154
A2433	C2353	G2282	U	C	A2040	G1924	A1816	U1719	A1629	A1517	G1425	U1318	G1235	G1155
A2436	C2354	A2283	G	U	A2041	G	G	U1720	C1630	A1331	G1426	G1322	G1236	A1156
G2439	U2355	A2284	A	C	G	G	G	G	C1631	A1332	G1427	G1330	G1237	A1157
G2440	C2358	G2285	A	C	C2042	G1927	A1819	U1726	A1631	G1524	A1429	A1331	G1238	U1158
G2441	G2359	G2286	U	G	U2043	G	C1820	G	A1632	G1528	G1430	A1332	G1239	G1159
G2446	C2360	G2287	A	U	G2044	A1934	A1821	C1732	A1633	G1528	C1431	U1333	G1241	C1160
A2450	G2361	A2289	C	G	U2049	C1935	G1822	G1733	C1634	G1528	C1431	U1333	G1242	C1161
C2451	A2362	G2290	C	G	G2050	U1936	C1823	G1734	U1635	U1534	A1439	U1345	G1243	G1166
G2452	A2363	C2294	C	A	A2051	A1937	U1826	A1735	U1638	A1535	A1440	A1347	G1247	G1167
G2457	C2367	A2297	C	U	G2052	U1938	C1827	U1739	G1639	G1536	U1441	G1348	A1248	G1170
U2456	U2368	A2298	U	G	A2054	A1948	C1828	G1740	G1639	G1537	U1442	C1349	U1249	A1171
G2459	G2370	G2300	G	U	G	A1949	G1829	G1741	C1644	G1538	C1443	C1350	G	G
G2465	A2371	G2301	G	G	C2057	U1950	G1831	A1744	C1644	U1542	G1444	G1354	G1252	A1174
G2468	C2375	U2302	G	G	G2058	G1951	G1832	G1745	C1649	C1549	G1445	G1355	G1253	U1175
G2476	G2376	C2303	C	G	G2059	U1952	A1833	A1746	C1652	C1550	G1446	G1356	G1256	G1176
A2480	U2377	C2304	A	G	C2061	C1955	U1834	G	C1652	G1557	C1447	U1357	A1257	C1179
G2481	A2380	G2305	C	U	C2064	A1958	A1845	C1756	A1653	A1553	C1448	U1358	A1264	G1180
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G2483	G2382	G2311	U	G	U2072	U1960	G1846	U1759	A1655	A1555	U1450	C1360	C1266	G1182
U2484	G2383	C2312	G	G	A2073	U1961	G1854	G1760	C1656	G1557	C1453	A1362	C1266	G1183
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C2485	A2386	G2315	C	C	A2078	G1969	G1858	U1767	A1663	G1566	G1461	G1372	G1276	A1187
C2486	G2387	A2316	C	C	U2079	A1973	A1859	G1768	G1667	G1570	C1462	G1373	G1277	G1189
A2487	A2388	G2317	C	C	A2080	G1973	A1859	G1768	G1667	G1570	U1465	U1374	C1278	C1190
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A2489	A2394	G2319	C	U	G2082	U1984	G1869	G1777	G1672	A1574	G1466	G1377	G1281	C1195
G2494	G2395	A2322	C	G	A2083	G1985	G1869	G1778	G1673	C1575	G1470	A1381	G1281	G1198
G2495	C2396	U2323	C	G	G2088	G1985	C1873	G1782	U1674	C1576	A1472	A1381	G1284	C1198
G2496	C2397	G2327	U	C	U2089	C1988	C1874	G1783	C1675	G1579	A1473	A1387	U1285	G1199
G2497	U2398	A2325	C	C	G2090	G1989	C1874	G1783	A1677	U	G1474	A1387	A1286	A1200
G2498	G2399	G2326	C	C	G2091	A1877	A1877	G1786	G1681	A	C1475	A1399	A1291	U1210
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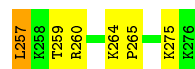
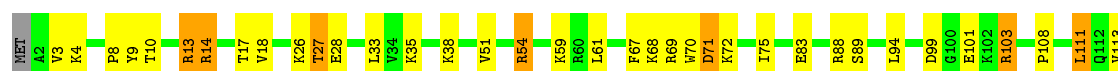
- Molecule 2: 5S Ribosomal RNA



- Molecule 2: 5S Ribosomal RNA

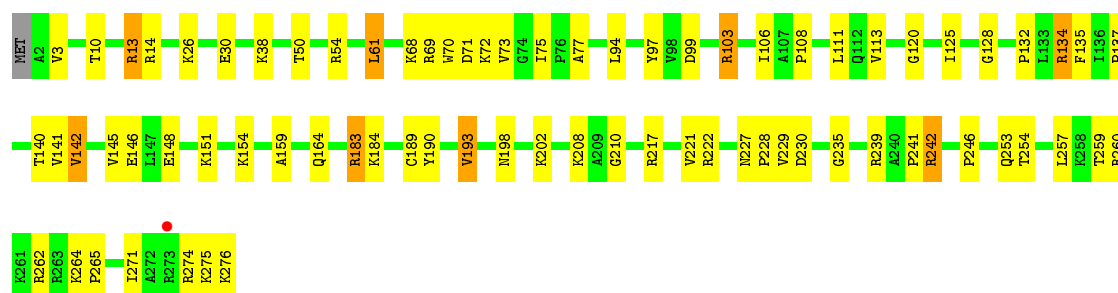


- Molecule 3: 50S ribosomal protein L2



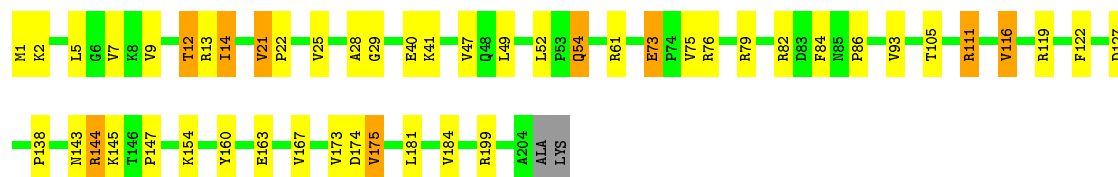
- Molecule 3: 50S ribosomal protein L2





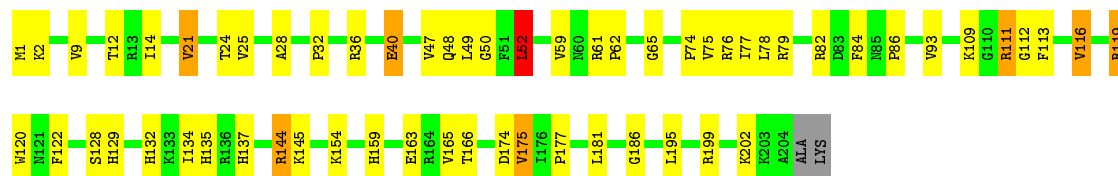
- Molecule 4: 50S ribosomal protein L3

Chain 1E: 75% 19% . .



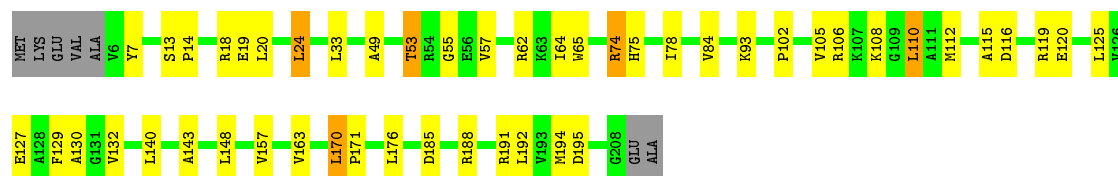
- Molecule 4: 50S ribosomal protein L3

Chain 2E: 70% 25% . .



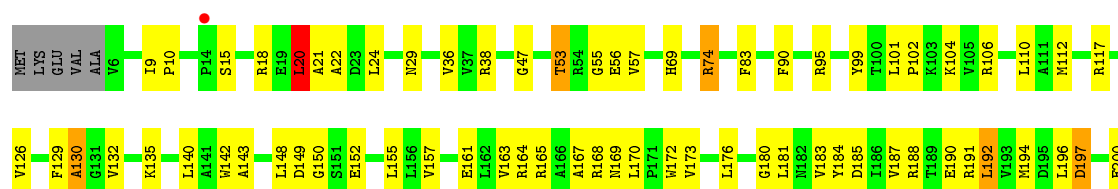
- Molecule 5: 50S ribosomal protein L4

Chain 1F: 73% 21% . .



- Molecule 5: 50S ribosomal protein L4

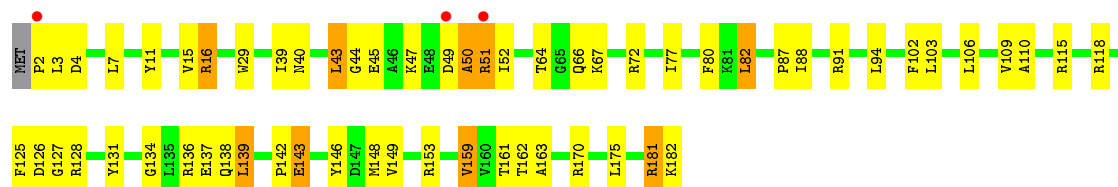
Chain 2F: 63% 30% . .





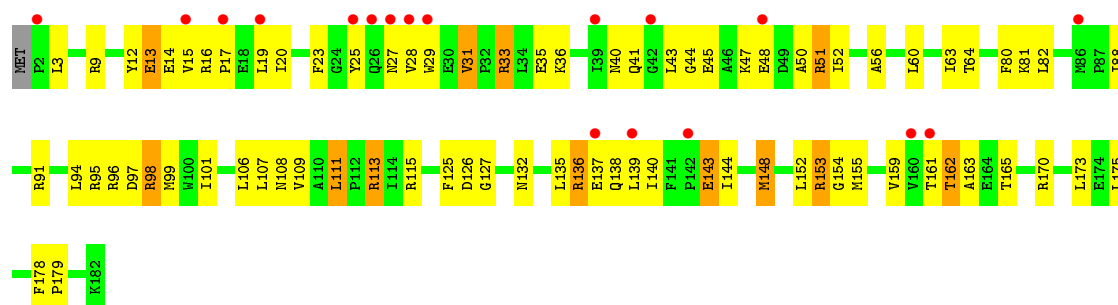
- Molecule 6: 50S ribosomal protein L5

Chain 1G: 2% 66% 28% 5% .



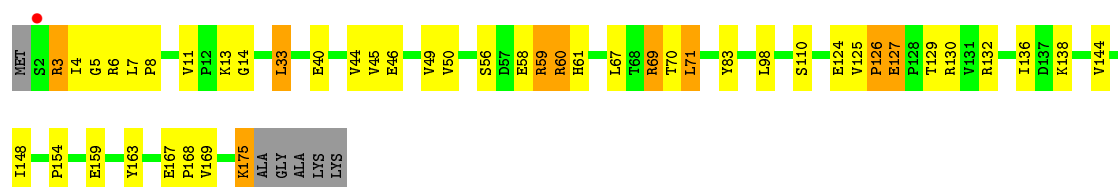
- Molecule 6: 50S ribosomal protein L5

Chain 2G: 10% 56% 37% 7% .



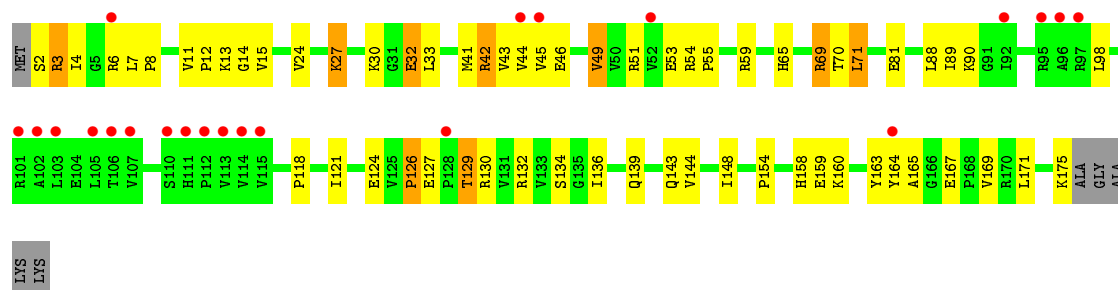
- Molecule 7: 50S ribosomal protein L6

Chain 1H: % 71% 21% 5% .



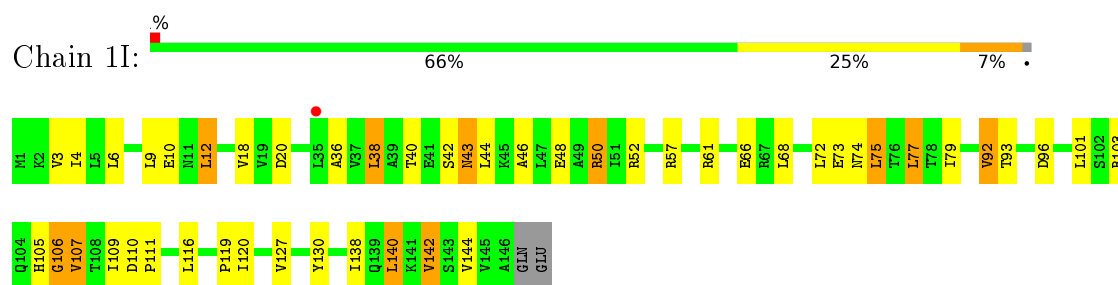
- Molecule 7: 50S ribosomal protein L6

Chain 2H: 12% 62% 29% 5% .

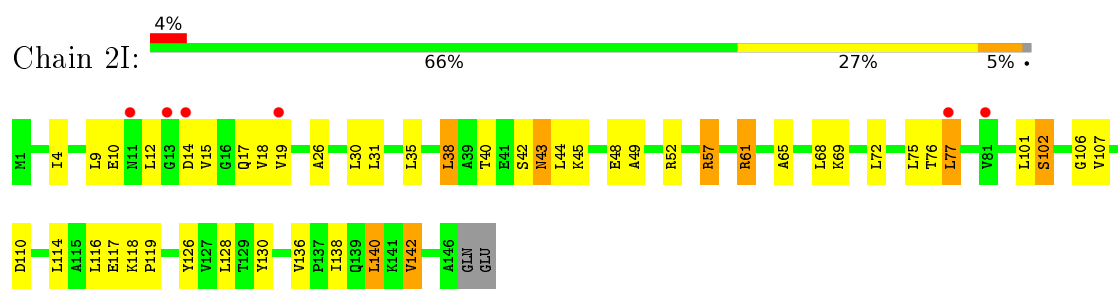


- Molecule 8: 50S ribosomal protein L9

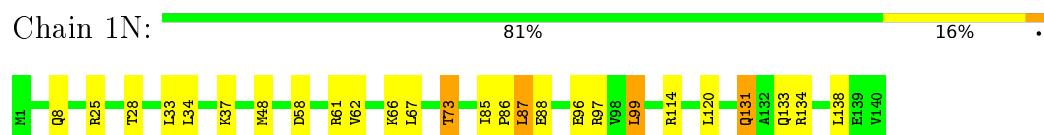




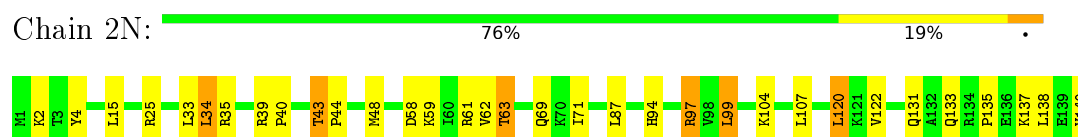
- Molecule 8: 50S ribosomal protein L9



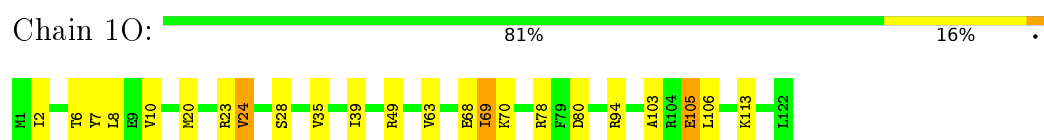
- Molecule 9: 50S ribosomal protein L13



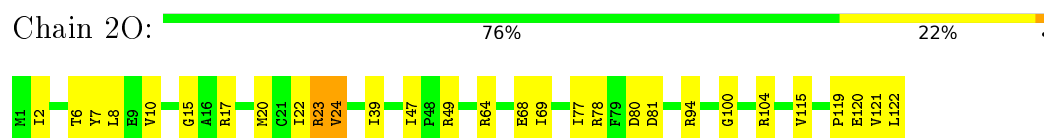
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

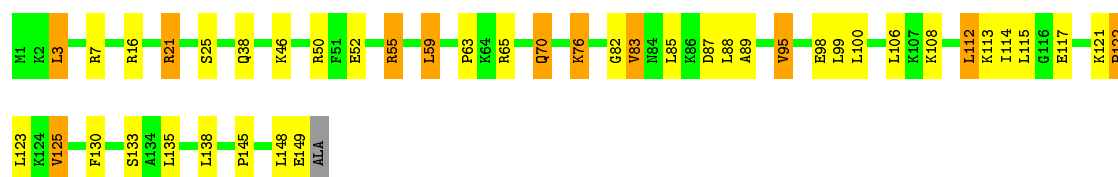


- Molecule 10: 50S ribosomal protein L14

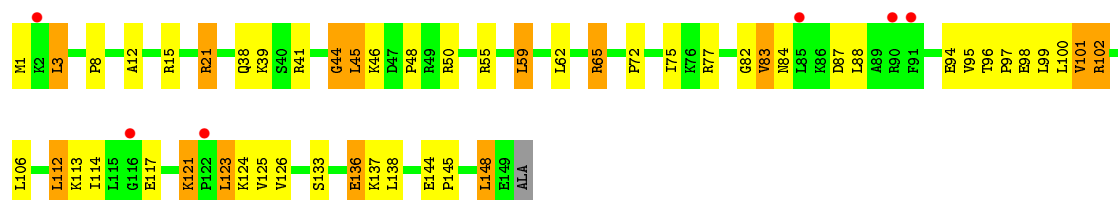


- Molecule 11: 50S ribosomal protein L15

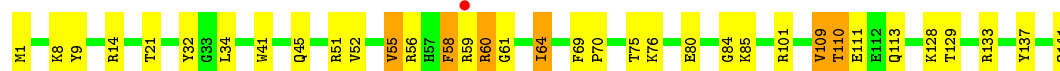
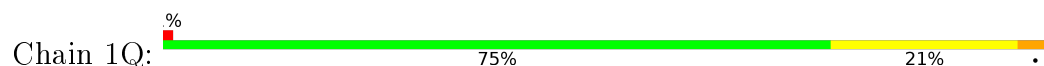




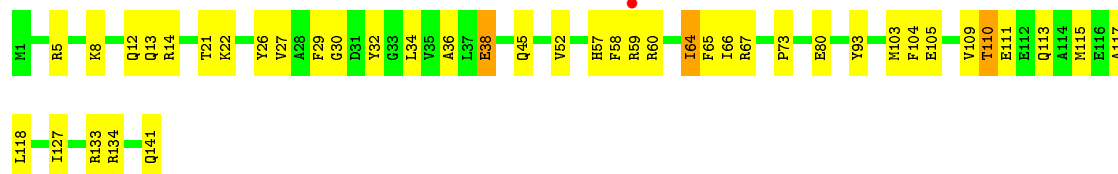
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



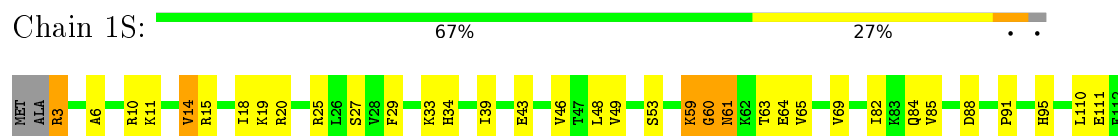
- Molecule 13: 50S ribosomal protein L17



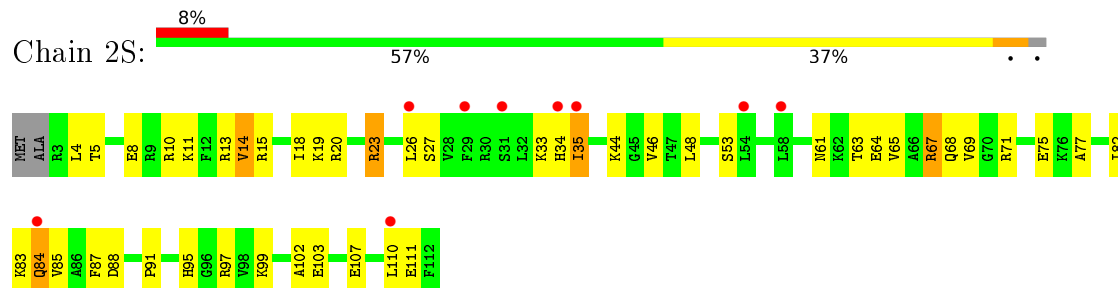
- Molecule 13: 50S ribosomal protein L17



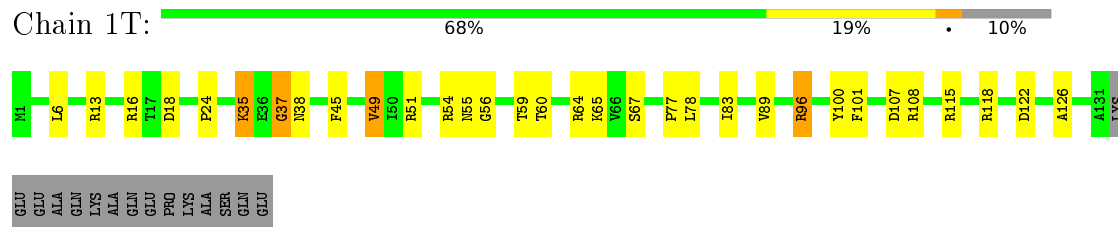
- Molecule 14: 50S ribosomal protein L18



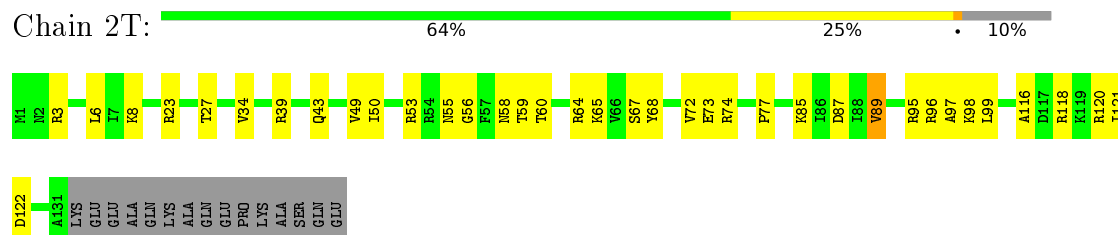
- Molecule 14: 50S ribosomal protein L18



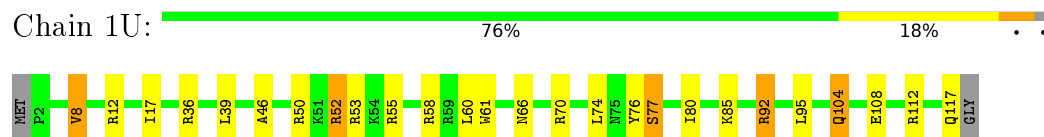
- Molecule 15: 50S ribosomal protein L19



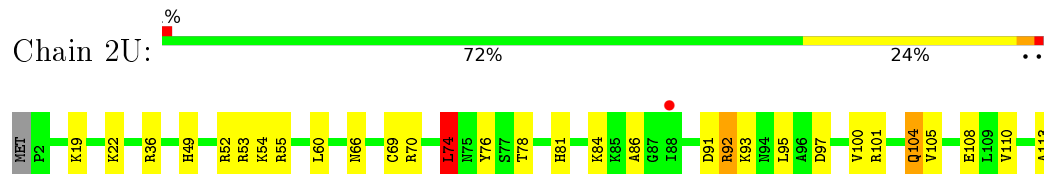
- Molecule 15: 50S ribosomal protein L19




- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



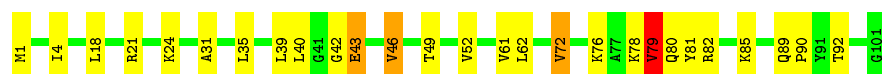
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  77% 20% ..




- Molecule 17: 50S ribosomal protein L21

Chain 2V:  73% 23% ..




- Molecule 18: 50S ribosomal protein L22

Chain 1W:  80% 17% ..




- Molecule 18: 50S ribosomal protein L22

Chain 2W:  74% 22% ..




- Molecule 19: 50S ribosomal protein L23

Chain 1X:  76% 22% ..



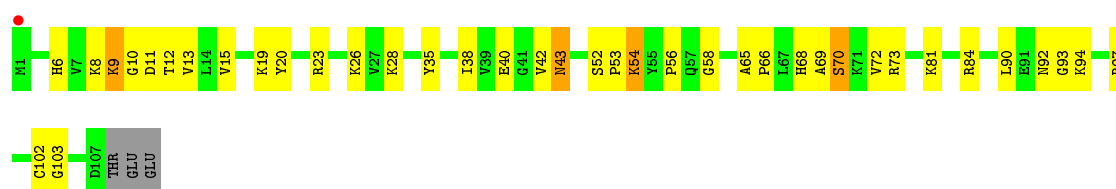
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  3% 73% 24% ..

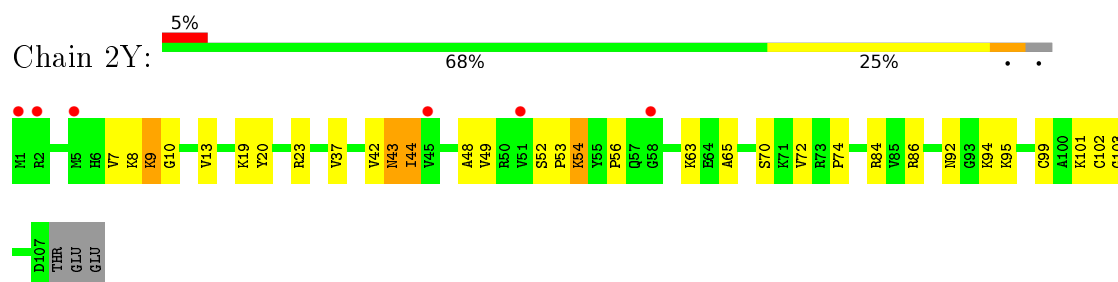


- Molecule 20: 50S ribosomal protein L24

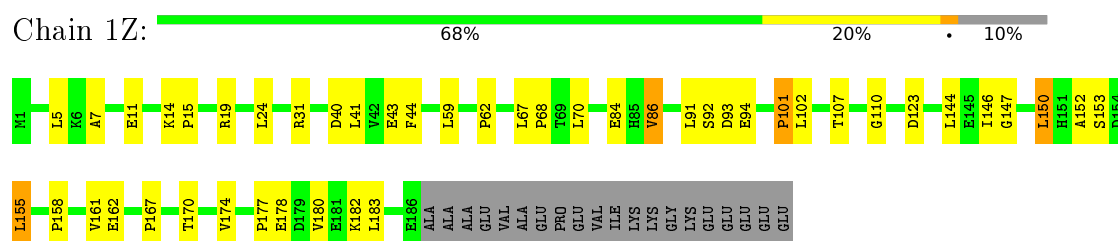
Chain 1Y:  62% 32% ..



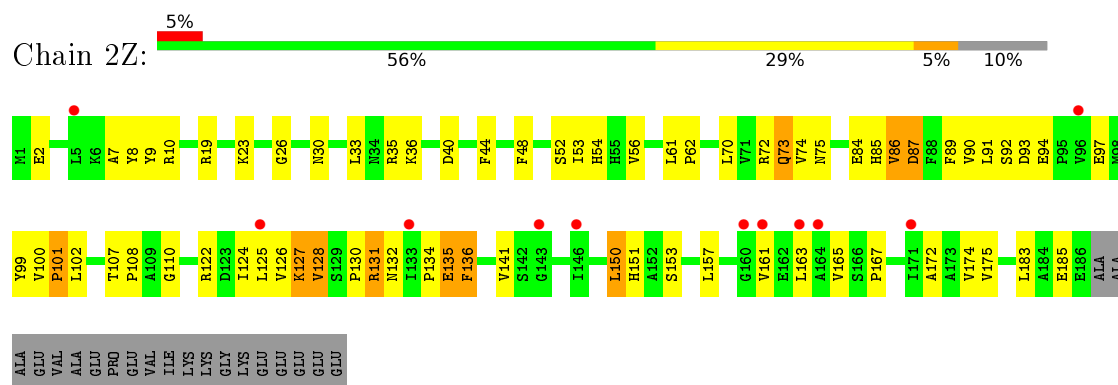
- Molecule 20: 50S ribosomal protein L24



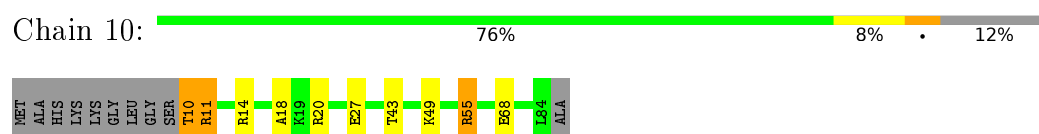
- Molecule 21: 50S ribosomal protein L25



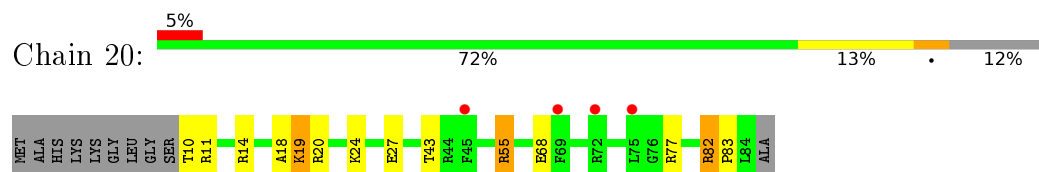
- Molecule 21: 50S ribosomal protein L25



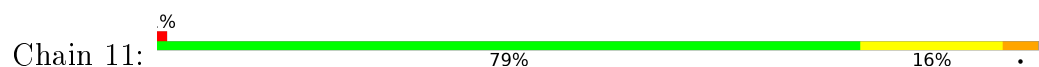
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27

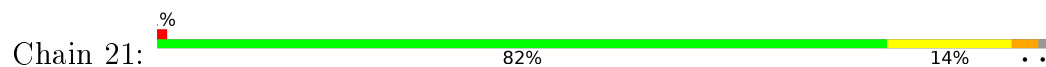


- Molecule 23: 50S ribosomal protein L28

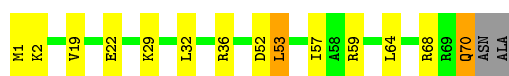
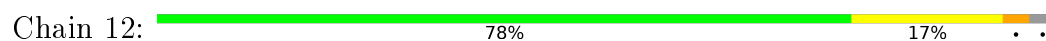




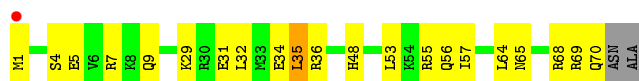
- Molecule 23: 50S ribosomal protein L28



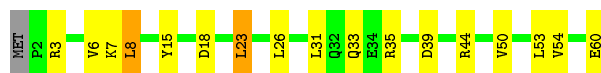
- Molecule 24: 50S ribosomal protein L29



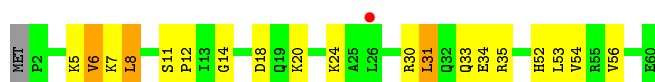
- Molecule 24: 50S ribosomal protein L29



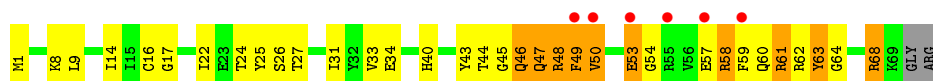
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30

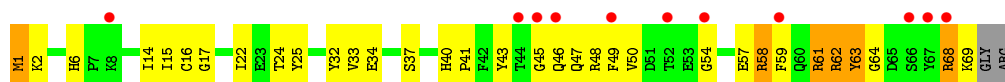


- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31





- Molecule 27: 50S ribosomal protein L32

Chain 15: 82% 13% ..



- Molecule 27: 50S ribosomal protein L32

Chain 25: 78% 18% ..



- Molecule 28: 50S ribosomal protein L33

Chain 16: 67% 28% ..



- Molecule 28: 50S ribosomal protein L33

Chain 26: 85% 9% ..



- Molecule 29: 50S ribosomal protein L34

Chain 17: 2% 59% 37% ..



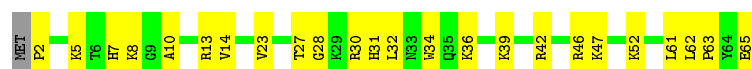
- Molecule 29: 50S ribosomal protein L34

Chain 27: 6% 78% 20% .



- Molecule 30: 50S ribosomal protein L35

Chain 18: 62% 37% .



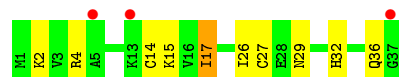
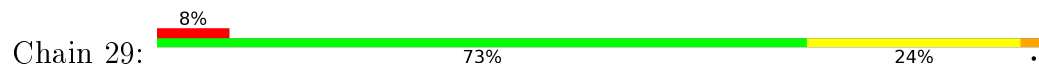
- Molecule 30: 50S ribosomal protein L35



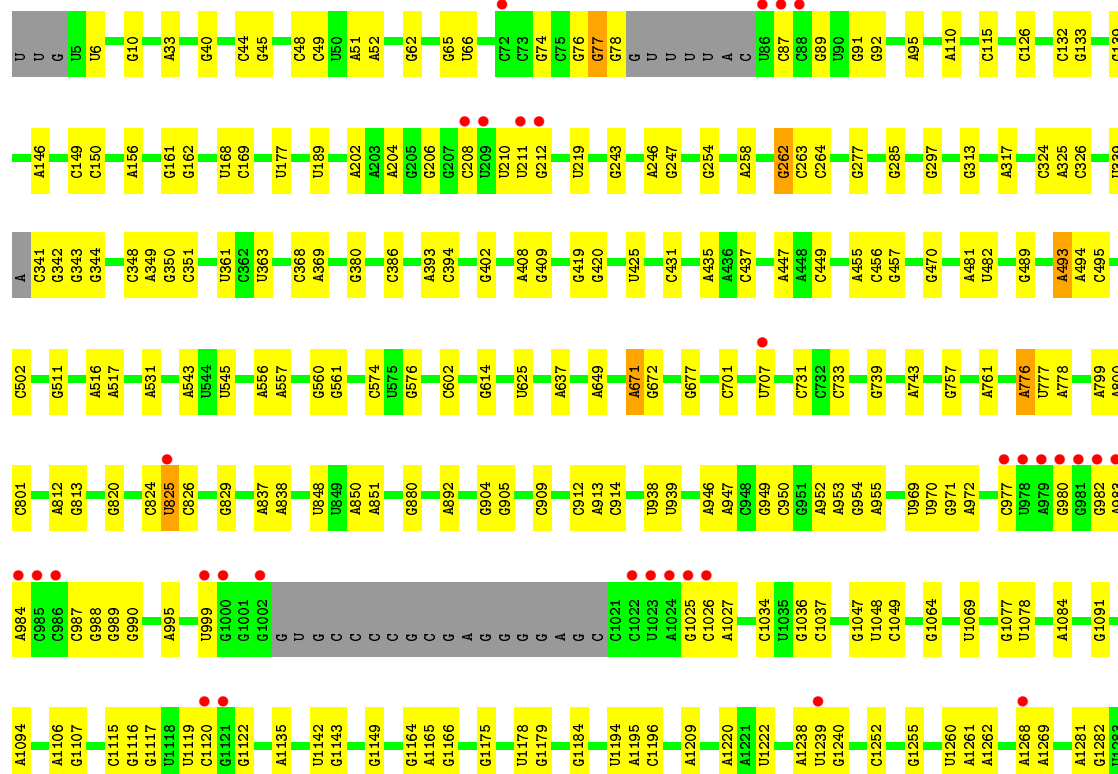
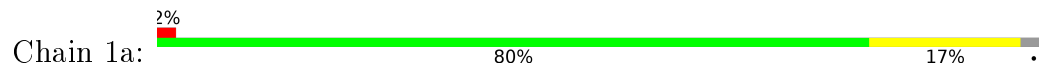
- Molecule 31: 50S ribosomal protein L36



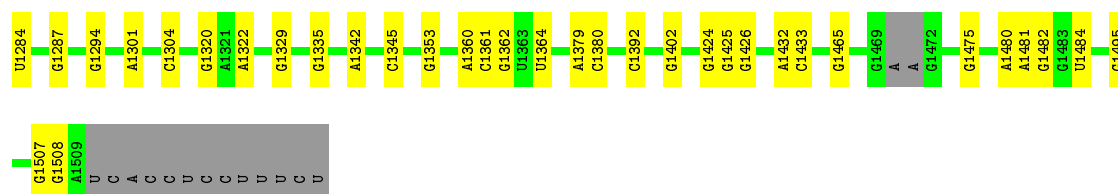
- Molecule 31: 50S ribosomal protein L36



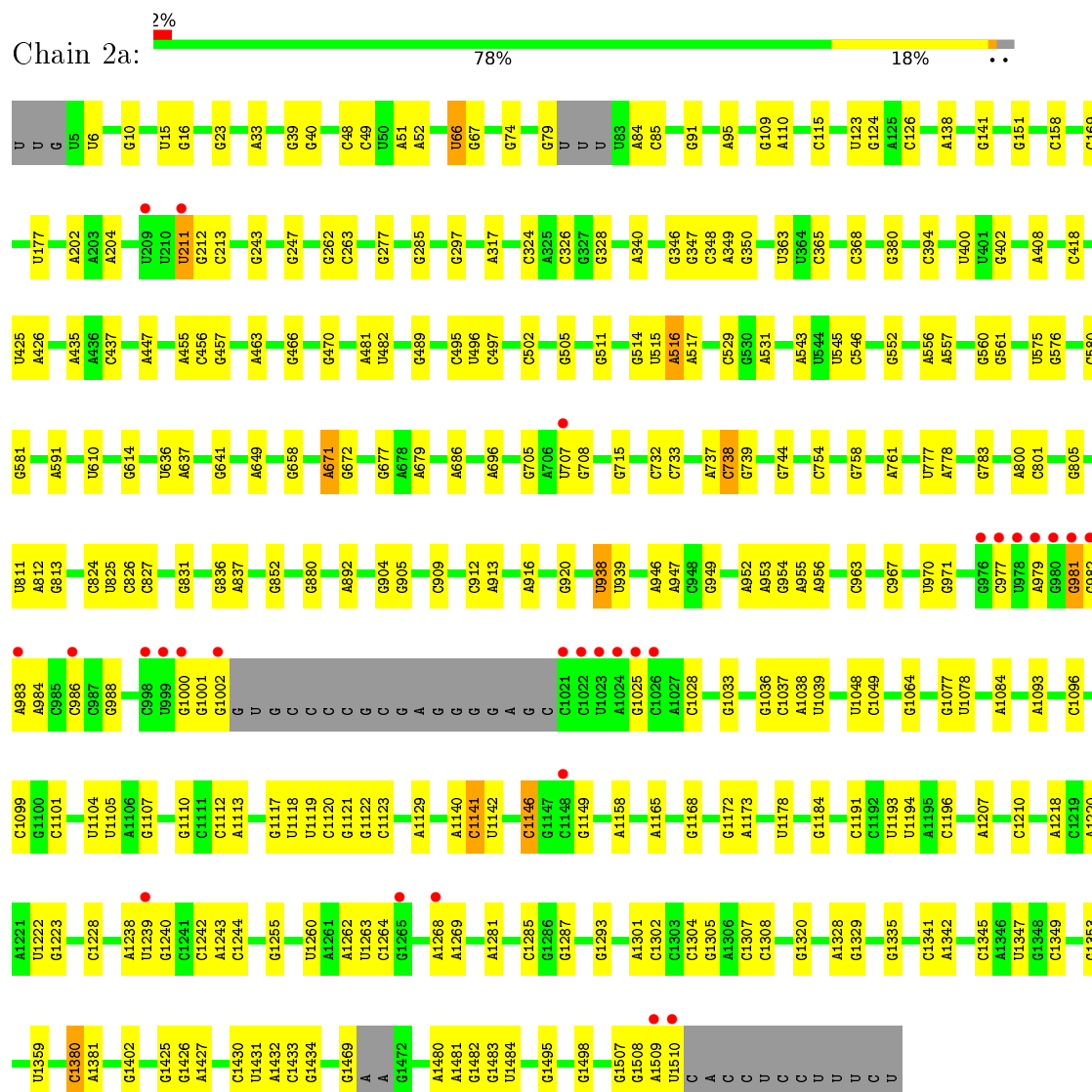
- Molecule 32: 16S Ribosomal RNA



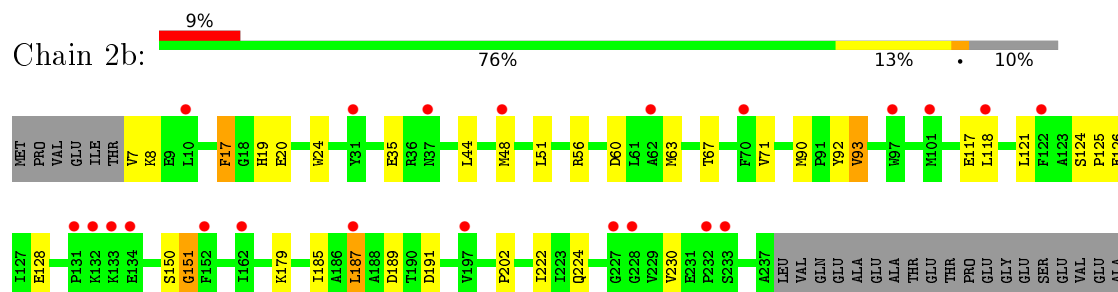




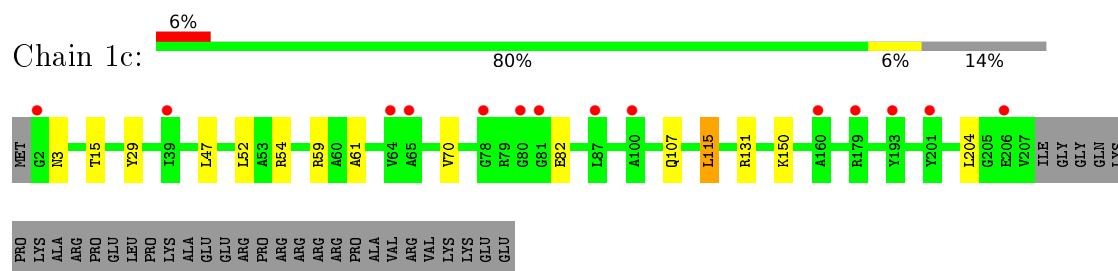
• Molecule 32: 16S Ribosomal RNA



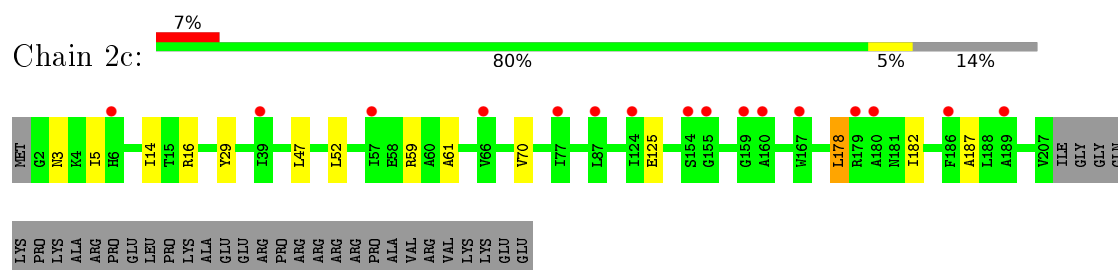
- Molecule 33: 30S ribosomal protein S2



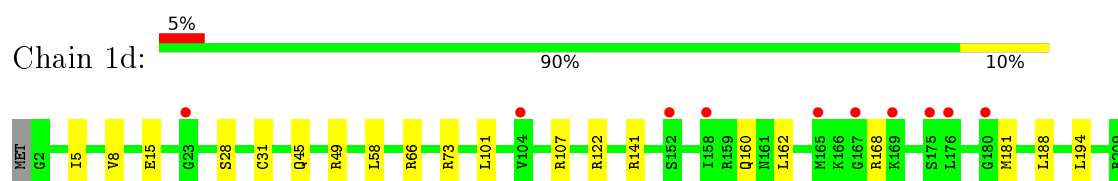
- Molecule 34: 30S ribosomal protein S3



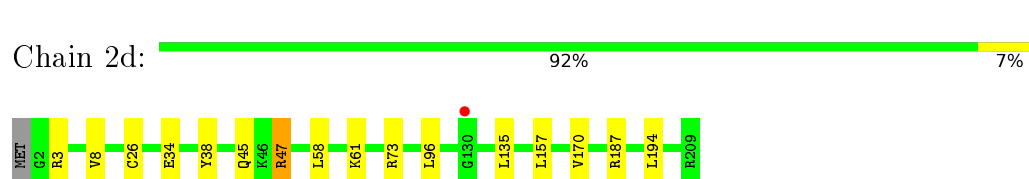
- Molecule 34: 30S ribosomal protein S3



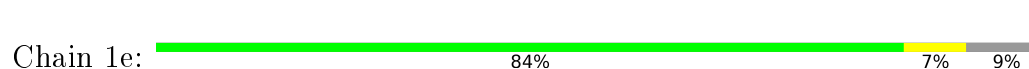
- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5





- Molecule 36: 30S ribosomal protein S5

Chain 2e: 83% 9% 9%



- Molecule 37: 30S ribosomal protein S6

Chain 1f: 94% 5%



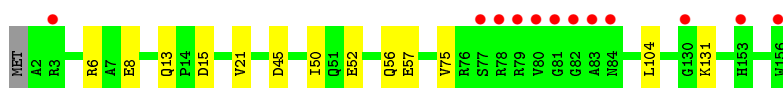
- Molecule 37: 30S ribosomal protein S6

Chain 2f: 96% 2% 2%



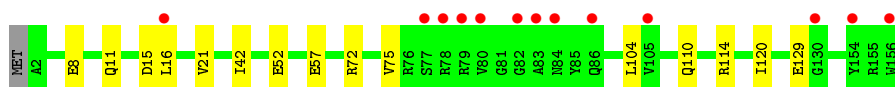
- Molecule 38: 30S ribosomal protein S7

Chain 1g: 91% 8% 8%



- Molecule 38: 30S ribosomal protein S7

Chain 2g: 90% 8% 10%



- Molecule 39: 30S ribosomal protein S8

Chain 1h: 92% 7%

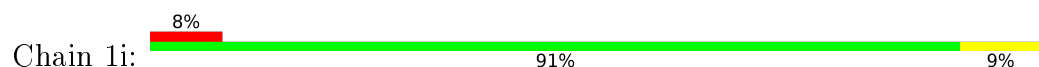


- Molecule 39: 30S ribosomal protein S8

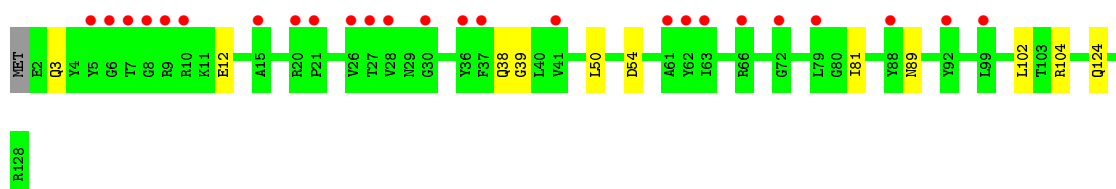
Chain 2h: 90% 9% 1%



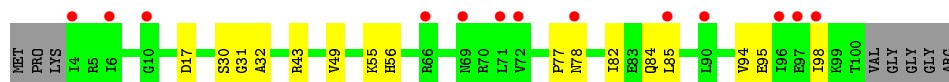
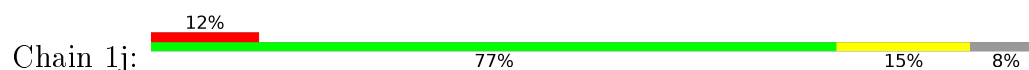
- Molecule 40: 30S ribosomal protein S9



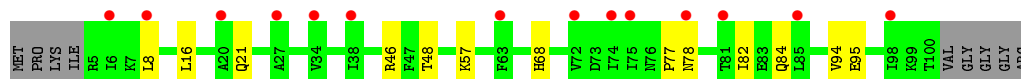
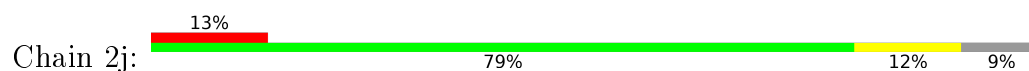
- Molecule 40: 30S ribosomal protein S9



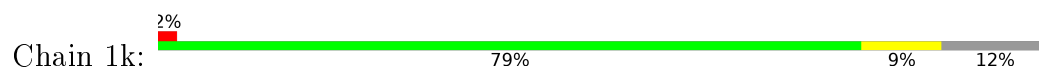
- Molecule 41: 30S ribosomal protein S10



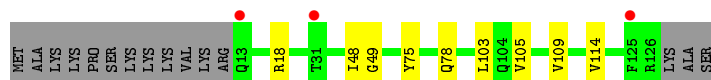
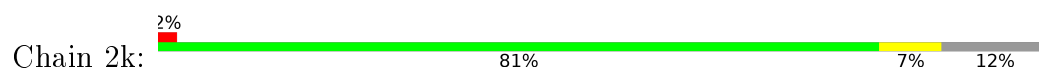
- Molecule 41: 30S ribosomal protein S10



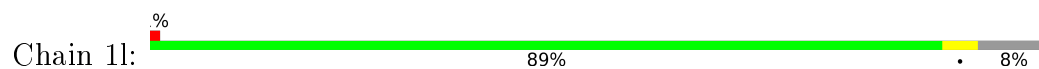
- Molecule 42: 30S ribosomal protein S11



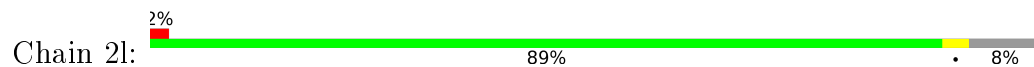
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



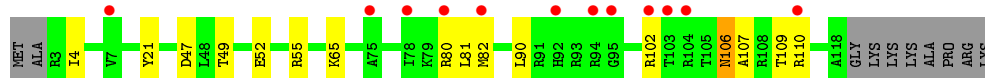
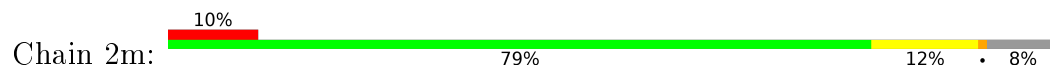
- Molecule 43: 30S ribosomal protein S12



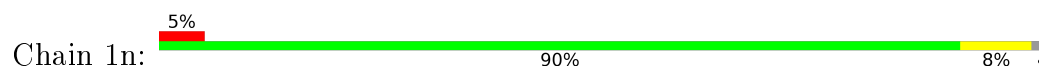
- Molecule 44: 30S ribosomal protein S13



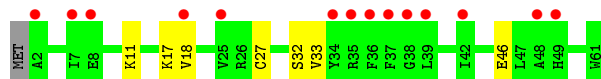
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



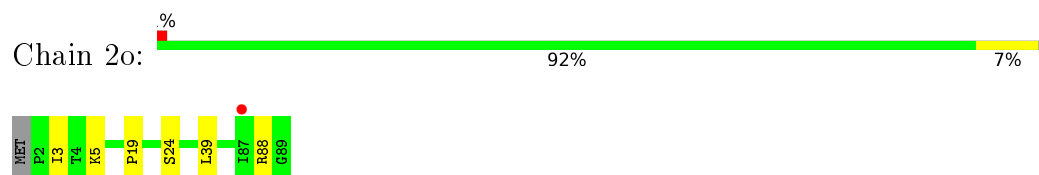
- Molecule 45: 30S ribosomal protein S14 type Z



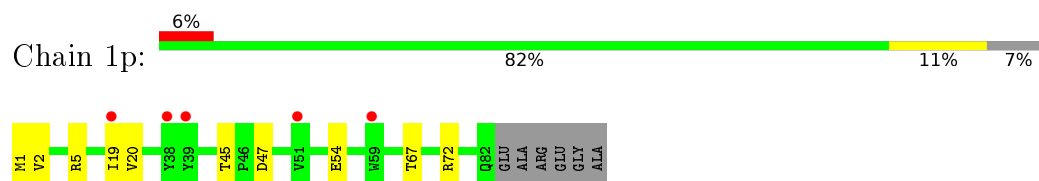
- Molecule 46: 30S ribosomal protein S15



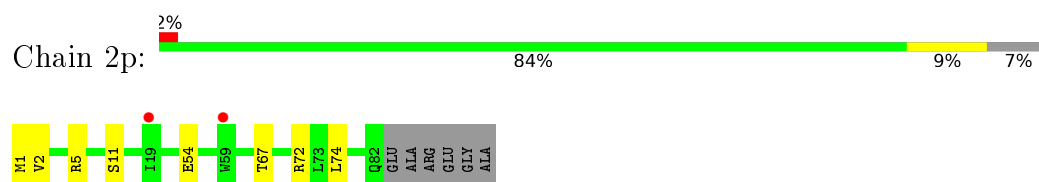
- Molecule 46: 30S ribosomal protein S15



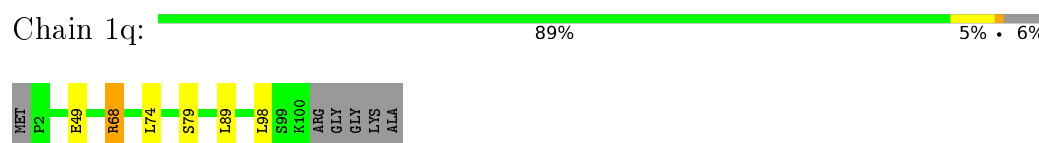
- Molecule 47: 30S ribosomal protein S16



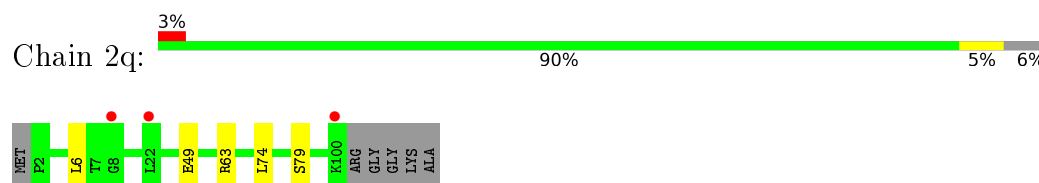
- Molecule 47: 30S ribosomal protein S16



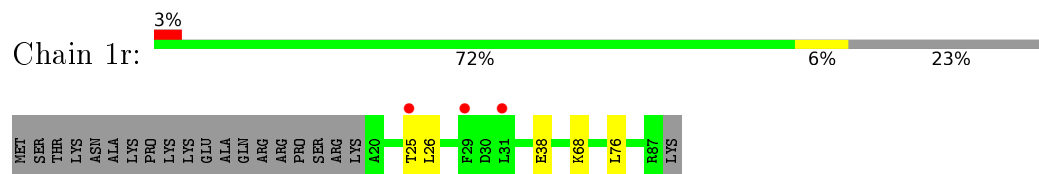
- Molecule 48: 30S ribosomal protein S17



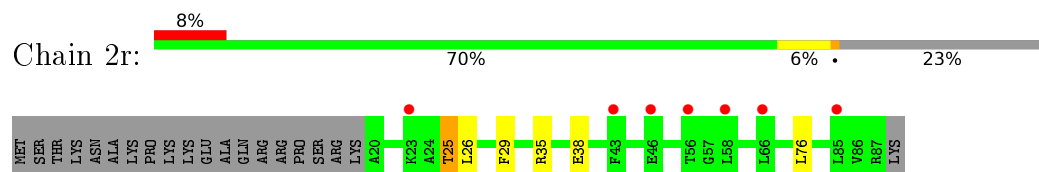
- Molecule 48: 30S ribosomal protein S17



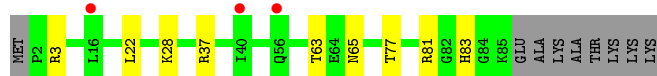
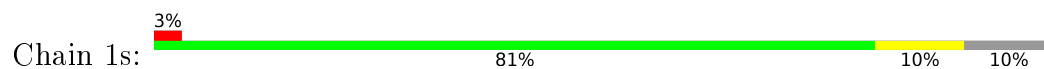
- Molecule 49: 30S ribosomal protein S18



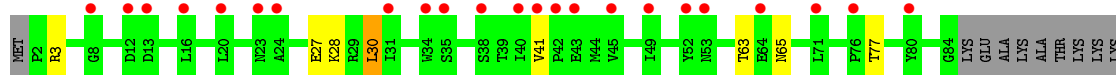
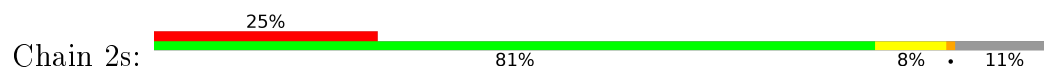
- Molecule 49: 30S ribosomal protein S18



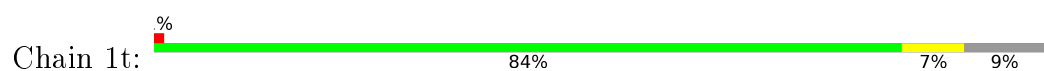
- Molecule 50: 30S ribosomal protein S19



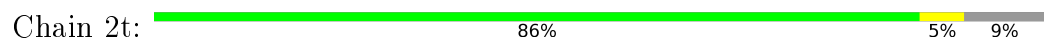
- Molecule 50: 30S ribosomal protein S19



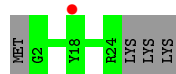
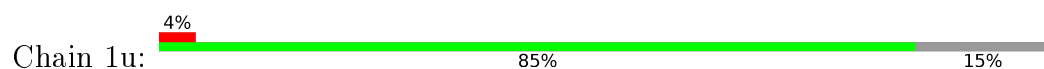
- Molecule 51: 30S ribosomal protein S20



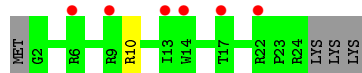
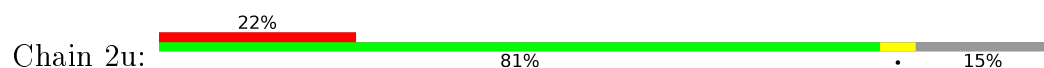
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



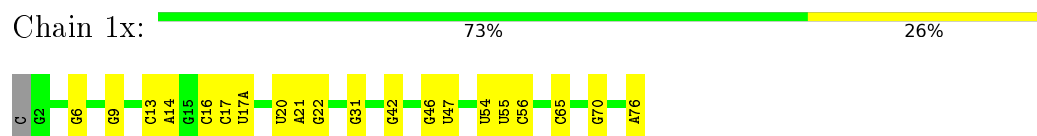
- Molecule 53: mRNA



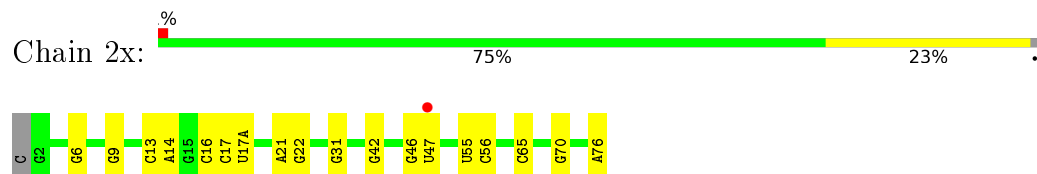
- Molecule 53: mRNA



- Molecule 54: P-site tRNA



- Molecule 54: P-site tRNA



- Molecule 55: Oncocin 10wt



- Molecule 55: Oncocin 10wt





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.83Å 450.81Å 622.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 2.80 49.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.62-2.80) 99.0 (49.62-2.80)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.215 , 0.268 0.221 , 0.272	Depositor DCC
$R_{free}$ test set	71167 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.225	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>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 1417435 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	288674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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	0.58	6/66249 (0.0%)	0.96	66/103407 (0.1%)
1	2A	0.46	2/67298 (0.0%)	0.94	47/105044 (0.0%)
2	1B	0.46	0/2877	0.86	0/4488
2	2B	0.52	0/2878	0.95	1/4490 (0.0%)
3	1D	0.41	0/2186	0.56	0/2944
3	2D	0.36	0/2192	0.56	0/2951
4	1E	0.41	0/1592	0.55	0/2149
4	2E	0.36	0/1592	0.56	0/2149
5	1F	0.39	0/1619	0.56	0/2193
5	2F	0.35	0/1615	0.57	0/2188
6	1G	0.31	0/1450	0.57	1/1959 (0.1%)
6	2G	0.35	0/1449	0.58	0/1958
7	1H	0.35	0/1356	0.56	1/1834 (0.1%)
7	2H	0.34	0/1356	0.55	0/1834
8	1I	0.32	0/1100	0.57	0/1501
8	2I	0.30	0/1076	0.54	0/1471
9	1N	0.38	0/1144	0.53	0/1543
9	2N	0.34	0/1144	0.55	0/1543
10	1O	0.40	0/943	0.57	1/1269 (0.1%)
10	2O	0.36	0/943	0.60	1/1269 (0.1%)
11	1P	0.38	0/1156	0.60	0/1537
11	2P	0.36	0/1152	0.59	1/1533 (0.1%)
12	1Q	0.40	0/1143	0.56	0/1527
12	2Q	0.36	0/1143	0.56	0/1527
13	1R	0.39	0/982	0.63	1/1312 (0.1%)
13	2R	0.33	0/982	0.56	0/1312
14	1S	0.36	0/887	0.56	0/1180
14	2S	0.35	0/880	0.56	0/1172
15	1T	0.36	0/1105	0.54	0/1477
15	2T	0.34	0/1097	0.53	0/1468
16	1U	0.45	0/977	0.54	0/1301
16	2U	0.38	0/977	0.54	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1V	0.39	0/782	0.57	0/1049
17	2V	0.37	0/782	0.52	0/1049
18	1W	0.42	0/897	0.56	0/1205
18	2W	0.36	0/897	0.56	0/1205
19	1X	0.40	0/764	0.53	0/1025
19	2X	0.37	0/764	0.59	1/1025 (0.1%)
20	1Y	0.40	0/819	0.57	0/1095
20	2Y	0.35	0/819	0.57	0/1095
21	1Z	0.32	0/1502	0.52	0/2041
21	2Z	0.35	0/1486	0.53	0/2022
22	10	0.42	0/606	0.59	0/808
22	20	0.33	0/606	0.54	0/808
23	11	0.37	0/762	0.54	0/1014
23	21	0.34	0/762	0.52	0/1014
24	12	0.35	0/590	0.53	0/781
24	22	0.33	0/590	0.50	0/781
25	13	0.38	0/474	0.56	0/635
25	23	0.30	0/469	0.52	0/630
26	14	0.37	0/571	0.65	0/768
26	24	0.35	0/545	0.68	0/737
27	15	0.40	0/469	0.65	0/635
27	25	0.32	0/469	0.55	0/635
28	16	0.38	0/460	0.55	0/613
28	26	0.35	0/456	0.50	0/608
29	17	0.43	0/426	0.55	0/561
29	27	0.37	0/426	0.54	0/561
30	18	0.41	0/525	0.59	0/691
30	28	0.35	0/525	0.54	0/691
31	19	0.40	0/310	0.51	0/407
31	29	0.38	0/310	0.61	0/407
32	1a	0.40	0/35537	0.89	16/55456 (0.0%)
32	2a	0.38	0/35680	0.89	31/55681 (0.1%)
33	1b	0.32	0/1820	0.56	1/2468 (0.0%)
33	2b	2.73	8/1728 (0.5%)	0.72	4/2352 (0.2%)
34	1c	0.29	0/1504	0.52	1/2047 (0.0%)
34	2c	0.32	0/1435	0.54	1/1960 (0.1%)
35	1d	0.31	0/1648	0.52	0/2222
35	2d	0.31	0/1659	0.54	0/2230
36	1e	0.30	0/1145	0.54	0/1543
36	2e	0.30	0/1111	0.56	0/1504
37	1f	0.32	0/819	0.53	0/1111
37	2f	0.30	0/830	0.51	0/1125
38	1g	0.30	0/1198	0.47	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	2g	0.30	0/1185	0.47	0/1602
39	1h	0.29	0/1108	0.51	0/1494
39	2h	0.29	0/1094	0.52	0/1478
40	1i	0.31	0/995	0.54	0/1339
40	2i	0.33	0/949	0.56	0/1284
41	1j	0.31	0/695	0.56	0/950
41	2j	0.31	0/690	0.58	0/943
42	1k	0.29	0/840	0.52	0/1138
42	2k	0.30	0/844	0.52	0/1145
43	1l	0.31	0/936	0.52	0/1263
43	2l	0.32	0/934	0.59	1/1262 (0.1%)
44	1m	0.28	0/933	0.55	0/1254
44	2m	0.32	0/913	0.55	0/1230
45	1n	0.33	0/491	0.56	0/653
45	2n	0.31	0/467	0.47	0/624
46	1o	0.31	0/726	0.51	0/970
46	2o	0.30	0/739	0.51	0/985
47	1p	0.27	0/686	0.53	0/926
47	2p	0.31	0/693	0.54	0/935
48	1q	0.32	0/824	0.53	0/1105
48	2q	0.32	0/836	0.51	0/1117
49	1r	0.31	0/560	0.55	0/746
49	2r	0.32	0/560	0.54	0/746
50	1s	0.29	0/657	0.59	0/890
50	2s	0.33	0/661	0.61	0/893
51	1t	0.29	0/714	0.60	0/948
51	2t	0.29	0/733	0.49	0/969
52	1u	0.28	0/191	0.50	0/252
52	2u	0.33	0/203	0.56	0/266
53	1v	0.58	0/122	1.23	0/188
53	2v	0.54	0/122	1.09	0/188
54	1x	0.57	2/1725 (0.1%)	1.16	17/2689 (0.6%)
54	2x	0.56	0/1725	1.17	13/2689 (0.5%)
55	1z	0.46	0/114	0.77	0/158
55	2z	0.39	0/106	0.51	0/146
All	All	0.49	18/306288 (0.0%)	0.85	207/458204 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	59.29	2.28	1.39
33	2b	92	TYR	CD2-CE2	53.39	2.19	1.39
33	2b	92	TYR	CE2-CZ	41.90	1.93	1.38
33	2b	92	TYR	CE1-CZ	41.71	1.92	1.38
33	2b	92	TYR	CG-CD1	33.77	1.83	1.39
33	2b	92	TYR	CG-CD2	32.09	1.80	1.39
33	2b	151	GLY	N-CA	22.68	1.80	1.46
33	2b	150	SER	C-N	10.43	1.51	1.33
1	1A	1187	A	N9-C4	-7.08	1.33	1.37
1	1A	552	A	N9-C4	-6.81	1.33	1.37
54	1x	22	G	N7-C5	6.37	1.43	1.39
1	2A	552	A	N9-C4	-6.03	1.34	1.37
54	1x	14	A	N7-C5	-5.89	1.35	1.39
1	1A	2298	A	N9-C4	-5.80	1.34	1.37
1	1A	1066	A	N9-C4	-5.34	1.34	1.37
1	1A	1934	A	N9-C4	5.24	1.41	1.37
1	1A	353	A	N9-C4	-5.15	1.34	1.37
1	2A	1187	A	N9-C4	-5.02	1.34	1.37

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	C-N-CA	16.53	157.01	122.30
54	1x	46	G	C6-N1-C2	-10.98	118.51	125.10
1	1A	552	A	C2-N3-C4	-10.97	105.11	110.60
54	2x	14	A	C4-C5-C6	9.84	121.92	117.00
1	1A	847	G	O5'-P-OP2	-9.71	96.96	105.70
54	2x	46	G	C6-N1-C2	-9.65	119.31	125.10
54	1x	14	A	C4-C5-C6	9.54	121.77	117.00
54	1x	14	A	C5-N7-C8	8.92	108.36	103.90
33	2b	151	GLY	N-CA-C	8.87	135.27	113.10
1	1A	1066	A	C2-N3-C4	-8.84	106.18	110.60
32	2a	1141	C	C2-N1-C1'	8.74	128.41	118.80
1	2A	552	A	C2-N3-C4	-8.66	106.27	110.60
32	2a	1141	C	N1-C2-O2	8.61	124.07	118.90
1	2A	1109	C	C2-N1-C1'	8.53	128.18	118.80
54	2x	14	A	C5-N7-C8	8.42	108.11	103.90
1	1A	552	A	N3-C4-N9	-8.40	120.68	127.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1380	C	N1-C2-O2	8.28	123.87	118.90
1	1A	353	A	C2-N3-C4	-8.23	106.48	110.60
1	1A	552	A	N3-C4-C5	8.21	132.55	126.80
1	2A	2324	C	N1-C2-O2	8.15	123.79	118.90
1	1A	2027	C	O5'-P-OP1	-8.12	98.39	105.70
32	2a	1380	C	C2-N1-C1'	8.12	127.73	118.80
54	1x	22	G	C5-N7-C8	-8.05	100.27	104.30
54	2x	22	G	C5-N7-C8	-7.96	100.32	104.30
1	1A	536	G	O4'-C1'-N9	7.89	114.51	108.20
1	1A	1187	A	C2-N3-C4	-7.81	106.69	110.60
1	1A	11	U	C2-N1-C1'	7.68	126.92	117.70
54	1x	46	G	C5-C6-N1	7.67	115.33	111.50
1	1A	1806	G	O5'-P-OP2	-7.66	98.81	105.70
1	1A	138	A	N7-C8-N9	7.50	117.55	113.80
1	2A	2324	C	N3-C2-O2	-7.42	116.71	121.90
1	1A	214	G	O4'-C1'-N9	7.33	114.06	108.20
1	2A	300	C	C2-N1-C1'	7.29	126.82	118.80
1	1A	989	A	C5-N7-C8	-7.28	100.26	103.90
54	1x	22	G	C4-C5-C6	-7.26	114.44	118.80
1	1A	597	A	O5'-P-OP1	-7.18	99.23	105.70
1	2A	300	C	N1-C2-O2	7.17	123.20	118.90
54	2x	14	A	C5-C6-N1	-7.11	114.14	117.70
19	2X	57	LEU	CA-CB-CG	7.11	131.65	115.30
1	1A	2083	A	O4'-C1'-N9	7.08	113.87	108.20
1	1A	2298	A	C2-N3-C4	-7.07	107.07	110.60
1	2A	2324	C	C2-N1-C1'	6.99	126.49	118.80
32	1a	341	C	N1-C2-O2	6.93	123.06	118.90
54	1x	22	G	N3-C4-N9	-6.90	121.86	126.00
54	1x	22	G	N1-C6-O6	-6.86	115.78	119.90
32	2a	1380	C	N3-C2-O2	-6.83	117.12	121.90
32	1a	341	C	C6-N1-C2	-6.79	117.58	120.30
1	1A	138	A	C8-N9-C4	-6.77	103.09	105.80
1	2A	2484	U	C2-N1-C1'	6.77	125.82	117.70
1	2A	552	A	N3-C4-C5	6.73	131.51	126.80
1	2A	536	G	O4'-C1'-N9	6.73	113.58	108.20
32	1a	341	C	C2-N1-C1'	6.71	126.19	118.80
1	1A	1187	A	N3-C4-C5	6.68	131.48	126.80
32	1a	87	C	N1-C2-O2	6.67	122.90	118.90
32	2a	1380	C	C6-N1-C2	-6.62	117.65	120.30
1	2A	2484	U	N1-C2-O2	6.56	127.39	122.80
54	1x	14	A	C5-C6-N1	-6.53	114.44	117.70
1	2A	2565	U	O5'-P-OP1	-6.52	99.83	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1141	C	N3-C2-O2	-6.50	117.35	121.90
32	2a	982	G	N3-C4-C5	-6.42	125.39	128.60
1	2A	787	G	O5'-P-OP1	-6.41	99.94	105.70
43	2l	29	GLY	N-CA-C	-6.37	97.18	113.10
1	2A	552	A	N3-C4-N9	-6.35	122.32	127.40
54	2x	46	G	C5-C6-N1	6.34	114.67	111.50
1	1A	2083	A	C2-N3-C4	-6.33	107.44	110.60
54	2x	46	G	N3-C2-N2	-6.33	115.47	119.90
54	1x	46	G	C5-C6-O6	-6.32	124.81	128.60
1	1A	1187	A	N3-C4-N9	-6.31	122.35	127.40
1	1A	1248	A	O4'-C1'-N9	6.30	113.24	108.20
32	1a	825	U	C5-C6-N1	6.26	125.83	122.70
1	2A	1358	U	C2-N1-C1'	6.24	125.19	117.70
1	1A	138	A	C5-N7-C8	-6.23	100.78	103.90
32	2a	66	U	P-O3'-C3'	6.23	127.17	119.70
32	2a	738	C	C2-N1-C1'	6.22	125.64	118.80
1	1A	1066	A	C5-N7-C8	-6.21	100.80	103.90
1	1A	1066	A	N7-C8-N9	6.17	116.89	113.80
1	2A	1109	C	C5-C6-N1	6.16	124.08	121.00
1	1A	2014	U	O5'-P-OP1	-6.16	100.16	105.70
1	2A	1187	A	C2-N3-C4	-6.14	107.53	110.60
1	1A	353	A	N1-C2-N3	6.09	132.35	129.30
32	2a	1141	C	C6-N1-C2	-6.08	117.87	120.30
32	1a	87	C	C2-N3-C4	6.08	122.94	119.90
1	1A	830	A	P-O3'-C3'	6.03	126.94	119.70
1	2A	1109	C	N1-C2-O2	6.02	122.51	118.90
1	2A	2814	C	C6-N1-C2	-6.00	117.90	120.30
1	1A	1067	G	N3-C4-N9	-5.97	122.42	126.00
54	2x	22	G	C4-C5-C6	-5.97	115.22	118.80
1	1A	1957	A	O4'-C1'-N9	5.94	112.95	108.20
32	2a	1207	A	C5-C6-N6	5.94	128.45	123.70
1	2A	2013	G	P-O3'-C3'	5.93	126.82	119.70
1	2A	1109	C	C6-N1-C1'	-5.91	113.71	120.80
32	2a	1141	C	C6-N1-C1'	-5.91	113.71	120.80
1	1A	977	A	C5-N7-C8	-5.90	100.95	103.90
32	2a	938	U	C2-N1-C1'	5.88	124.76	117.70
1	1A	1067	G	N3-C2-N2	-5.88	115.79	119.90
1	2A	409	U	O4'-C1'-N1	5.85	112.88	108.20
1	1A	1538	C	C2-N1-C1'	5.85	125.23	118.80
54	2x	14	A	C4-N9-C1'	5.84	136.81	126.30
1	1A	1744	A	C2-N3-C4	-5.83	107.69	110.60
54	1x	22	G	C8-N9-C1'	5.82	134.56	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2700	U	N3-C2-O2	-5.75	118.17	122.20
1	2A	2484	U	N3-C2-O2	-5.74	118.18	122.20
1	1A	1066	A	N1-C2-N3	5.72	132.16	129.30
1	1A	2013	G	P-O3'-C3'	5.69	126.53	119.70
32	1a	341	C	N3-C2-O2	-5.69	117.92	121.90
54	1x	22	G	N7-C8-N9	5.68	115.94	113.10
10	1O	8	LEU	CA-CB-CG	5.68	128.36	115.30
32	1a	361	U	C2-N1-C1'	-5.68	110.89	117.70
1	2A	1109	C	C6-N1-C2	-5.64	118.04	120.30
1	2A	989	A	N1-C6-N6	5.62	121.97	118.60
1	1A	1218	A	P-O3'-C3'	5.62	126.44	119.70
32	2a	738	C	N1-C2-O2	5.62	122.27	118.90
32	2a	1146	C	N1-C2-O2	5.59	122.25	118.90
32	2a	982	G	C4-N9-C1'	5.59	133.77	126.50
1	1A	138	A	O4'-C1'-N9	5.59	112.67	108.20
32	1a	341	C	C5-C6-N1	5.58	123.79	121.00
1	1A	409	U	C2-N1-C1'	-5.56	111.03	117.70
54	2x	14	A	C8-N9-C1'	-5.55	117.71	127.70
34	1c	115	LEU	CA-CB-CG	5.54	128.03	115.30
54	1x	22	G	C6-C5-N7	5.53	133.72	130.40
32	2a	1207	A	N1-C6-N6	-5.53	115.28	118.60
32	1a	262	G	P-O3'-C3'	5.52	126.32	119.70
33	1b	187	LEU	CA-CB-CG	5.52	127.99	115.30
1	2A	636	U	N3-C2-O2	-5.51	118.34	122.20
32	1a	77	G	C5-C6-O6	5.50	131.90	128.60
1	1A	2449	U	OP2-P-O3'	5.46	117.22	105.20
32	2a	514	G	C4-N9-C1'	5.46	133.60	126.50
33	2b	118	LEU	CA-CB-CG	5.46	127.86	115.30
32	2a	1349	C	N1-C2-O2	5.45	122.17	118.90
1	1A	790	G	O5'-P-OP2	-5.45	100.80	105.70
1	1A	1044	U	O5'-P-OP2	-5.43	100.81	105.70
32	2a	516	A	OP1-P-O3'	5.41	117.10	105.20
1	1A	398	G	O4'-C1'-N9	5.39	112.51	108.20
1	2A	2905	U	N1-C2-O2	5.39	126.58	122.80
1	1A	831	G	O5'-P-OP2	-5.37	100.87	105.70
1	1A	1404	A	C2-N3-C4	5.37	113.29	110.60
34	2c	178	LEU	CA-CB-CG	5.37	127.65	115.30
32	1a	776	A	O4'-C1'-N9	5.35	112.48	108.20
1	1A	2265	C	N1-C2-O2	-5.35	115.69	118.90
32	2a	1146	C	C2-N1-C1'	5.35	124.68	118.80
1	2A	2286	C	OP1-P-O3'	5.35	116.96	105.20
1	1A	989	A	C4-C5-N7	5.34	113.37	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	981	G	N1-C6-O6	-5.34	116.69	119.90
1	2A	1358	U	C5-C6-N1	5.34	125.37	122.70
32	1a	77	G	N1-C6-O6	-5.33	116.70	119.90
1	2A	2905	U	C2-N1-C1'	5.33	124.09	117.70
32	2a	671	A	P-O3'-C3'	5.33	126.09	119.70
1	2A	1314	A	N1-C6-N6	5.31	121.79	118.60
1	2A	1359	C	C2-N1-C1'	5.30	124.63	118.80
1	1A	989	A	C2-N3-C4	-5.29	107.95	110.60
6	1G	82	LEU	CA-CB-CG	5.29	127.47	115.30
1	2A	1311	G	C8-N9-C4	5.29	108.52	106.40
32	2a	1380	C	C6-N1-C1'	-5.27	114.47	120.80
1	1A	989	A	N1-C6-N6	5.27	121.76	118.60
1	2A	1693	G	O4'-C1'-N9	-5.25	104.00	108.20
1	1A	891	G	O4'-C1'-N9	5.25	112.40	108.20
1	1A	2857	G	O4'-C1'-N9	5.24	112.39	108.20
1	2A	1248	A	O4'-C1'-N9	5.24	112.39	108.20
1	1A	138	A	C6-C5-N7	-5.24	128.63	132.30
1	1A	2346	A	O4'-C1'-N9	5.24	112.39	108.20
54	2x	22	G	C8-N9-C1'	5.23	133.81	127.00
2	2B	42	C	P-O3'-C3'	5.23	125.98	119.70
1	1A	183	A	P-O3'-C3'	5.23	125.98	119.70
32	1a	493	A	C8-N9-C4	-5.23	103.71	105.80
32	2a	732	C	P-O3'-C3'	5.22	125.96	119.70
1	1A	830	A	O4'-C1'-N9	5.21	112.37	108.20
32	2a	1025	G	C4-N9-C1'	-5.20	119.73	126.50
54	2x	22	G	C5-C6-N1	5.20	114.10	111.50
1	1A	638	G	O4'-C1'-N9	5.20	112.36	108.20
11	2P	44	GLY	C-N-CA	5.19	134.67	121.70
32	1a	969	U	P-O3'-C3'	5.18	125.91	119.70
1	2A	2083	A	N1-C6-N6	5.17	121.70	118.60
1	1A	1744	A	N1-C6-N6	5.17	121.70	118.60
1	1A	1294	U	O5'-P-OP1	-5.16	101.06	105.70
1	2A	300	C	N3-C2-O2	-5.15	118.29	121.90
13	1R	113	LEU	CA-CB-CG	5.14	127.13	115.30
1	2A	1604	A	P-O3'-C3'	5.14	125.87	119.70
54	1x	14	A	C8-N9-C1'	-5.13	118.46	127.70
7	1H	33	LEU	CA-CB-CG	5.12	127.09	115.30
54	2x	14	A	C4-C5-N7	-5.12	108.14	110.70
1	1A	792	A	O4'-C1'-N9	5.12	112.30	108.20
1	1A	1176	G	N1-C2-N2	-5.11	111.60	116.20
1	2A	300	C	C6-N1-C1'	-5.11	114.67	120.80
1	2A	1806	G	N3-C4-N9	5.10	129.06	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2298	A	N3-C4-C5	5.10	130.37	126.80
54	1x	14	A	C4-C5-N7	-5.10	108.15	110.70
33	2b	187	LEU	CA-CB-CG	5.10	127.03	115.30
1	1A	830	A	OP1-P-O3'	5.08	116.38	105.20
32	2a	516	A	P-O3'-C3'	5.07	125.78	119.70
54	1x	22	G	C5-C6-N1	5.07	114.03	111.50
32	2a	211	U	C2-N1-C1'	5.06	123.77	117.70
1	1A	1358	U	C2-N1-C1'	5.05	123.76	117.70
1	1A	2726	G	O5'-P-OP2	-5.04	101.16	105.70
32	1a	671	A	P-O3'-C3'	5.04	125.75	119.70
1	2A	1359	C	C6-N1-C2	-5.04	118.28	120.30
1	2A	2905	U	N3-C2-O2	-5.04	118.67	122.20
1	2A	1659	A	O5'-P-OP1	-5.04	101.17	105.70
1	2A	1994	G	N1-C6-O6	-5.04	116.88	119.90
1	2A	2604	U	N3-C4-O4	-5.04	115.88	119.40
1	2A	2700	U	P-O3'-C3'	5.04	125.74	119.70
16	2U	74	LEU	CA-CB-CG	5.03	126.88	115.30
32	2a	109	G	P-O3'-C3'	5.03	125.73	119.70
54	1x	14	A	C4-N9-C1'	5.02	135.34	126.30
10	2O	8	LEU	CA-CB-CG	5.02	126.85	115.30
32	2a	982	G	C8-N9-C4	-5.02	104.39	106.40
1	2A	1302	C	C6-N1-C2	-5.02	118.29	120.30
1	1A	2514	A	N1-C2-N3	-5.00	126.80	129.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2F	20	LEU	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	29827	618	0
1	2A	60091	0	30298	807	0
2	1B	2572	0	1306	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2B	2573	0	1306	57	0
3	1D	2136	0	2218	53	0
3	2D	2142	0	2229	48	0
4	1E	1559	0	1618	29	0
4	2E	1559	0	1618	39	0
5	1F	1584	0	1625	30	0
5	2F	1580	0	1619	48	0
6	1G	1425	0	1443	37	0
6	2G	1424	0	1434	58	0
7	1H	1330	0	1407	31	0
7	2H	1330	0	1407	40	0
8	1I	1085	0	1114	26	0
8	2I	1061	0	1080	26	0
9	1N	1117	0	1184	15	0
9	2N	1117	0	1184	18	0
10	1O	933	0	996	13	0
10	2O	933	0	996	19	0
11	1P	1139	0	1223	36	0
11	2P	1135	0	1212	47	0
12	1Q	1122	0	1178	29	0
12	2Q	1122	0	1179	26	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	18	0
14	1S	877	0	938	32	0
14	2S	870	0	923	32	0
15	1T	1091	0	1151	19	0
15	2T	1083	0	1136	23	0
16	1U	959	0	1019	16	0
16	2U	959	0	1018	22	0
17	1V	771	0	830	10	0
17	2V	771	0	830	16	0
18	1W	886	0	940	14	0
18	2W	886	0	940	16	0
19	1X	750	0	814	21	0
19	2X	750	0	814	19	0
20	1Y	806	0	881	28	0
20	2Y	806	0	881	23	0
21	1Z	1470	0	1478	23	0
21	2Z	1454	0	1452	47	0
22	10	598	0	614	7	0
22	20	598	0	614	13	0
23	11	755	0	826	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	21	755	0	826	12	0
24	12	588	0	643	12	0
24	22	588	0	643	16	0
25	13	469	0	518	9	0
25	23	464	0	514	11	0
26	14	558	0	544	24	0
26	24	532	0	503	21	0
27	15	455	0	464	11	0
27	25	455	0	465	9	0
28	16	453	0	473	11	0
28	26	449	0	469	2	0
29	17	418	0	467	16	0
29	27	418	0	467	8	0
30	18	517	0	582	21	0
30	28	517	0	582	24	0
31	19	307	0	335	7	0
31	29	307	0	335	7	0
32	1a	31750	0	16027	0	0
32	2a	31877	0	16088	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	108	0	116	0	0
55	2z	101	0	109	0	0
56	10	6	0	0	0	0
56	11	4	0	0	0	0
56	13	2	0	0	0	0
56	15	3	0	0	0	0
56	16	3	0	0	0	0
56	17	6	0	0	0	0
56	18	4	0	0	0	0
56	19	3	0	0	0	0
56	1A	1096	0	0	0	0
56	1B	27	0	0	0	0
56	1D	13	0	0	0	0
56	1E	8	0	0	0	0
56	1F	7	0	0	0	0
56	1G	3	0	0	0	0
56	1H	3	0	0	0	0
56	1N	8	0	0	0	0
56	1O	3	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1R	6	0	0	0	0
56	1T	6	0	0	0	0
56	1U	6	0	0	0	0
56	1V	1	0	0	0	0
56	1W	5	0	0	0	0
56	1X	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	2	0	0	0	0
56	1a	307	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	3	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	1m	2	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	1u	1	0	0	0	0
56	1x	10	0	0	0	0
56	20	1	0	0	0	0
56	25	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	559	0	0	0	0
56	2B	10	0	0	0	0
56	2D	6	0	0	0	0
56	2E	4	0	0	0	0
56	2F	3	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	2	0	0	0	0
56	2Q	5	0	0	0	0
56	2U	2	0	0	0	0
56	2W	1	0	0	0	0
56	2Y	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	217	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2d	1	0	0	0	0
56	2e	3	0	0	0	0
56	2f	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	4	0	0	0	0
56	2n	1	0	0	0	0
56	2p	1	0	0	0	0
56	2q	2	0	0	0	0
56	2t	1	0	0	0	0
56	2x	5	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	7	0	0	0	0
59	11	9	0	0	0	0
59	12	1	0	0	0	0
59	13	5	0	0	0	0
59	14	1	0	0	0	0
59	15	9	0	0	1	0
59	16	6	0	0	0	0
59	17	3	0	0	0	0
59	18	15	0	0	0	0
59	19	4	0	0	1	0
59	1A	2345	0	0	120	0
59	1B	45	0	0	1	0
59	1D	20	0	0	2	0
59	1E	29	0	0	3	0
59	1F	18	0	0	2	0
59	1G	4	0	0	0	0
59	1H	4	0	0	0	0
59	1I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1N	12	0	0	1	0
59	1O	6	0	0	0	0
59	1P	16	0	0	1	0
59	1Q	12	0	0	0	0
59	1R	10	0	0	1	0
59	1S	1	0	0	0	0
59	1T	14	0	0	3	0
59	1U	11	0	0	0	0
59	1V	5	0	0	1	0
59	1W	9	0	0	0	0
59	1X	6	0	0	0	0
59	1Y	1	0	0	0	0
59	1Z	6	0	0	0	0
59	1a	395	0	0	0	0
59	1b	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	4	0	0	0	0
59	1i	1	0	0	0	0
59	1j	2	0	0	0	0
59	1k	2	0	0	0	0
59	1l	3	0	0	0	0
59	1o	3	0	0	0	0
59	1s	1	0	0	0	0
59	1v	2	0	0	0	0
59	1x	11	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
59	23	2	0	0	0	0
59	28	4	0	0	0	0
59	2A	810	0	0	85	0
59	2B	10	0	0	1	0
59	2D	15	0	0	0	0
59	2E	9	0	0	2	0
59	2F	4	0	0	0	0
59	2O	2	0	0	0	0
59	2P	6	0	0	0	0
59	2Q	2	0	0	0	0
59	2R	2	0	0	0	0
59	2T	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2U	4	0	0	0	0
59	2V	1	0	0	1	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	1	0
59	2a	235	0	0	0	0
59	2d	2	0	0	0	0
59	2e	3	0	0	0	0
59	2i	1	0	0	0	0
59	2m	1	0	0	0	0
59	2n	1	0	0	0	0
59	2p	1	0	0	0	0
59	2t	4	0	0	0	0
59	2x	5	0	0	0	0
59	2z	1	0	0	0	0
All	All	288674	0	189963	2449	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 (2449) 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)
22:10:11:ARG:O	22:10:14:ARG:NH2	2.02	0.93
1:1A:353:A:H2	1:1A:1254:A:HO2'	0.99	0.91
15:2T:55:ASN:H	15:2T:59:THR:HG22	1.35	0.90
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.38	0.89
1:2A:1248:A:H2	1:2A:1286:A:H62	1.20	0.89
1:1A:893:U:O4	1:1A:977:A:N6	2.06	0.88
1:2A:786:U:OP2	59:2A:3601:HOH:O	1.92	0.86
1:1A:2330:G:N7	59:1A:4119:HOH:O	2.08	0.86
20:1Y:54:LYS:HA	20:1Y:56:PRO:HD3	1.59	0.83
1:1A:869:G:OP1	59:1A:4101:HOH:O	1.97	0.83
29:17:24:THR:HG22	29:17:27:GLY:H	1.44	0.83
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.61	0.82
6:2G:33:ARG:HH11	6:2G:33:ARG:HB2	1.44	0.82
1:1A:1735:A:H62	1:1A:1744:A:H2	1.26	0.81
1:2A:655:A:OP1	11:2P:65:ARG:NH1	2.13	0.81
1:2A:1039:C:OP1	16:2U:53:ARG:NH2	2.14	0.81
15:2T:65:LYS:HE2	15:2T:67:SER:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:25:SER:O	59:1P:301:HOH:O	1.99	0.81
1:1A:2466:G:OP2	59:1A:4102:HOH:O	1.98	0.80
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.63	0.80
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.64	0.80
1:1A:1845:A:OP2	3:1D:54:ARG:NH2	2.15	0.79
1:2A:673:G:H4'	30:28:46:ARG:HH22	1.47	0.79
1:2A:1735:A:H62	1:2A:1744:A:H2	1.30	0.79
1:1A:786:U:OP2	59:1A:4103:HOH:O	2.00	0.79
2:2B:4:C:H42	2:2B:117:G:H1	1.30	0.79
1:1A:1316:G:OP2	59:1A:4104:HOH:O	2.00	0.79
1:1A:1694:C:OP1	59:1A:4105:HOH:O	2.01	0.79
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.47	0.78
1:1A:2100:U:OP1	23:11:21:ARG:NH2	2.15	0.78
1:2A:1828:U:OP2	3:2D:274:ARG:NH2	2.16	0.78
1:2A:1310:A:OP2	59:2A:3602:HOH:O	2.01	0.78
1:2A:1083:C:H42	1:2A:1162:G:H1	1.31	0.78
21:2Z:90:VAL:O	59:2Z:3101:HOH:O	2.01	0.78
1:2A:873:U:OP1	59:2A:3603:HOH:O	2.02	0.78
26:14:53:GLU:HB3	26:14:54:GLY:HA2	1.66	0.78
1:2A:554:G:N1	59:2A:3623:HOH:O	2.15	0.78
1:1A:838:G:O6	59:1A:4106:HOH:O	2.02	0.77
1:2A:1188:A:OP1	9:2N:25:ARG:NH2	2.18	0.77
1:2A:821:G:N3	59:2A:3648:HOH:O	2.18	0.77
1:1A:81:G:OP1	59:1A:4107:HOH:O	2.02	0.77
1:2A:2722:A:OP1	59:2A:3604:HOH:O	2.02	0.77
1:2A:1377:G:OP1	59:2A:3605:HOH:O	2.03	0.76
1:1A:1715:A:OP2	59:1A:4108:HOH:O	2.03	0.76
22:20:11:ARG:O	22:20:14:ARG:NH2	2.19	0.76
1:2A:2079:A:N7	59:2A:3650:HOH:O	2.18	0.76
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.66	0.76
1:1A:2510:C:OP2	59:1A:4113:HOH:O	2.05	0.75
1:1A:2561:G:OP1	59:1A:4108:HOH:O	2.05	0.75
1:1A:1354:G:H4'	29:17:7:PRO:HB2	1.68	0.75
1:1A:2768:U:O4	1:1A:2770:A:N6	2.20	0.75
1:2A:186:C:OP2	59:2A:3606:HOH:O	2.04	0.75
1:1A:433:G:OP2	59:1A:4114:HOH:O	2.05	0.75
1:1A:1377:G:OP1	59:1A:4110:HOH:O	2.04	0.75
1:2A:2606:G:N7	59:2A:3656:HOH:O	2.20	0.75
1:2A:2405:C:OP2	30:28:30:ARG:NH1	2.20	0.74
1:1A:238:G:OP2	30:18:13:ARG:NH2	2.19	0.74
1:1A:2698:U:O4	59:1A:4111:HOH:O	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2W:14:PRO:HG2	18:2W:78:GLU:HG2	1.68	0.74
1:1A:2364:G:N7	59:1A:4180:HOH:O	2.20	0.74
22:20:27:GLU:HG3	22:20:68:GLU:HA	1.69	0.74
20:2Y:94:LYS:NZ	59:2Y:301:HOH:O	2.20	0.74
27:15:17:ASP:OD2	59:15:201:HOH:O	2.05	0.74
1:1A:892:C:OP2	59:1A:4115:HOH:O	2.06	0.74
14:2S:84:GLN:HA	14:2S:111:GLU:HB2	1.68	0.74
1:1A:894:G:OP1	59:1A:4112:HOH:O	2.05	0.74
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.70	0.74
2:2B:22:U:H3	2:2B:61:G:H1	1.34	0.74
1:2A:2694:C:OP1	15:2T:53:ARG:NH2	2.21	0.74
1:2A:1638:G:H2'	1:2A:1639:G:C8	2.23	0.73
1:2A:900:G:H2'	1:2A:901:G:H8	1.53	0.73
1:1A:1461:G:N2	1:1A:1628:C:O2	2.19	0.73
1:2A:550:A:OP1	59:2A:3607:HOH:O	2.05	0.73
1:2A:2517:U:OP1	4:2E:144:ARG:NH2	2.22	0.73
3:1D:8:PRO:HB3	3:1D:14:ARG:HB2	1.68	0.73
59:1A:4170:HOH:O	13:1R:3:HIS:NE2	2.21	0.73
1:1A:2298:A:H62	1:1A:2355:U:H3	1.33	0.73
1:1A:2699:U:O4	59:1A:4109:HOH:O	2.04	0.73
1:1A:2718:G:N7	59:1A:4189:HOH:O	2.21	0.73
1:2A:807:A:N7	59:2A:3657:HOH:O	2.20	0.73
1:2A:2456:G:OP1	5:2F:74:ARG:NH2	2.21	0.73
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.22	0.73
19:2X:60:ARG:HH22	29:27:47:ARG:HH22	1.34	0.73
1:2A:206:A:OP2	59:2A:3609:HOH:O	2.07	0.73
1:1A:655:A:OP1	11:1P:65:ARG:NH1	2.21	0.73
1:1A:1841:G:N7	59:1A:4201:HOH:O	2.22	0.72
6:2G:144:ILE:HG23	6:2G:148:MET:HE1	1.69	0.72
20:2Y:44:ILE:HD13	20:2Y:44:ILE:H	1.52	0.72
12:1Q:32:TYR:OH	12:1Q:111:GLU:OE1	2.08	0.72
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.71	0.72
16:2U:49:HIS:HA	16:2U:52:ARG:HG2	1.69	0.72
5:1F:18:ARG:NH2	5:1F:127:GLU:OE2	2.23	0.72
12:1Q:64:ILE:HD12	21:1Z:178:GLU:HG3	1.71	0.72
1:2A:2310:G:H2'	1:2A:2311:G:H8	1.54	0.72
16:2U:76:TYR:OH	16:2U:92:ARG:NH1	2.23	0.72
2:2B:16:G:H1	2:2B:68:C:H42	1.34	0.72
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.71	0.72
1:2A:957:C:OP1	12:2Q:8:LYS:NZ	2.22	0.72
1:2A:1421:C:OP2	59:2A:3610:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1813:A:OP1	59:1A:4103:HOH:O	2.08	0.71
18:1W:14:PRO:HG2	18:1W:78:GLU:HG2	1.71	0.71
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.72	0.71
4:2E:132:HIS:NE2	59:2E:401:HOH:O	2.18	0.71
1:1A:785:G:OP1	59:1A:4120:HOH:O	2.08	0.71
1:2A:2600:A:OP1	59:2A:3608:HOH:O	2.06	0.71
1:2A:2691:C:OP2	4:2E:111:ARG:NH2	2.23	0.71
1:2A:1092:G:H1'	1:2A:1155:G:H22	1.54	0.71
1:1A:474:A:N7	59:1A:4198:HOH:O	2.22	0.71
1:2A:2603:G:OP1	59:2A:3612:HOH:O	2.08	0.71
1:1A:1000:G:OP2	12:1Q:14:ARG:NH2	2.23	0.71
1:1A:1784:C:OP1	15:1T:96:ARG:NH1	2.22	0.71
1:1A:2730:G:OP1	59:1A:4116:HOH:O	2.07	0.71
1:2A:2067:G:H5'	27:25:19:ARG:HA	1.71	0.71
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.64	0.71
1:1A:1068:U:OP2	59:1A:4118:HOH:O	2.07	0.71
5:2F:29:ASN:H	5:2F:112:MET:HE1	1.56	0.71
25:13:3:ARG:NH1	25:13:60:GLU:OE1	2.23	0.70
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.55	0.70
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.72	0.70
1:2A:2696:G:O6	59:2A:3611:HOH:O	2.07	0.70
1:2A:1739:U:O2'	3:2D:14:ARG:NH2	2.24	0.70
1:1A:1809:U:OP2	59:1A:4117:HOH:O	2.07	0.70
1:1A:1342:C:OP1	59:1A:4124:HOH:O	2.09	0.70
1:1A:1378:C:OP1	59:1A:4128:HOH:O	2.10	0.70
1:1A:629:U:OP1	5:1F:102:PRO:HA	1.90	0.70
1:2A:661:A:H5''	11:2P:117:GLU:HG2	1.73	0.70
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.73	0.70
1:2A:2226:G:H3'	1:2A:2227:G:C8	2.27	0.70
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.25	0.70
1:1A:2385:C:OP1	59:1A:4122:HOH:O	2.09	0.70
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.74	0.70
1:2A:2078:A:OP2	59:2A:3614:HOH:O	2.09	0.70
1:2A:1361:U:H2'	1:2A:1362:A:H8	1.55	0.69
1:1A:636:U:O4	1:1A:736:G:O2'	77.62	0.69
1:2A:2488:C:O2	31:29:4:ARG:NH2	2.25	0.69
1:1A:1853:G:OP1	3:1D:54:ARG:NH1	2.26	0.69
1:2A:1064:U:H3	1:2A:1187:A:H62	1.40	0.69
1:2A:1470:G:N2	1:2A:1619:G:N7	2.40	0.69
1:2A:183:A:N7	59:2A:3606:HOH:O	2.24	0.69
1:1A:1229:C:OP2	59:1A:4127:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2510:C:OP2	59:2A:3615:HOH:O	2.10	0.69
1:2A:8:U:H3	1:2A:2640:A:H2	1.39	0.69
4:2E:77:ILE:HD13	4:2E:195:LEU:HD22	1.75	0.69
1:1A:1332:A:OP1	59:1A:4130:HOH:O	2.11	0.69
1:2A:98:G:O2'	24:22:7:ARG:NH2	2.25	0.69
1:2A:836:C:OP2	59:2A:3620:HOH:O	2.11	0.69
1:1A:2230:G:N7	59:1A:4239:HOH:O	2.26	0.69
1:1A:553:A:N1	59:1A:4233:HOH:O	2.25	0.69
1:2A:2848:G:H5'	13:2R:46:GLY:HA2	1.73	0.69
1:1A:1648:A:OP1	59:1A:4123:HOH:O	2.09	0.69
1:2A:1233:A:OP2	59:2A:3616:HOH:O	2.11	0.69
21:2Z:2:GLU:HG2	21:2Z:56:VAL:HB	1.75	0.69
1:1A:1000:G:O6	59:1A:4121:HOH:O	2.08	0.68
1:1A:1360:C:OP2	59:1A:4110:HOH:O	2.11	0.68
1:2A:1185:U:OP2	9:2N:63:THR:OG1	2.10	0.68
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.29	0.68
1:1A:1086:C:H42	1:1A:1159:G:H1	1.38	0.68
1:1A:2670:G:O2'	7:1H:175:LYS:NZ	2.27	0.68
19:1X:60:ARG:HH22	29:17:47:ARG:HH22	1.42	0.68
1:1A:1808:U:OP1	59:1A:4125:HOH:O	2.10	0.68
1:1A:2502:U:OP2	59:1A:4129:HOH:O	2.10	0.68
1:2A:816:G:OP2	59:2A:3621:HOH:O	2.12	0.68
1:1A:1064:U:HO2'	1:1A:1066:A:H2	1.42	0.68
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.12	0.68
1:2A:1512:G:HO2'	1:2A:1592:C:HO2'	1.31	0.68
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.76	0.68
11:2P:95:VAL:HA	11:2P:99:LEU:HD21	1.76	0.68
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.75	0.67
21:1Z:70:LEU:HG	21:1Z:91:LEU:HD21	1.74	0.67
1:2A:2360:G:OP1	59:2A:3619:HOH:O	2.11	0.67
7:2H:46:GLU:HB2	7:2H:49:VAL:HG12	1.76	0.67
1:1A:1312:U:OP1	59:1A:4135:HOH:O	2.13	0.67
1:1A:2586:C:OP2	59:1A:4126:HOH:O	2.10	0.67
1:2A:777:C:OP2	59:2A:3617:HOH:O	2.11	0.67
1:2A:929:G:N2	1:2A:948:C:O2	27.44	0.67
1:2A:2800:C:OP1	4:2E:61:ARG:NH2	2.27	0.67
1:1A:932:C:H2'	1:1A:933:A:H5''	1.76	0.67
1:1A:2327:C:O2'	6:1G:128:ARG:NH1	2.27	0.67
1:2A:1858:G:OP1	59:2A:3622:HOH:O	2.12	0.67
1:2A:2226:G:H5''	1:2A:2227:G:N7	2.09	0.67
7:2H:27:LYS:HA	7:2H:32:GLU:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1100:G:N2	1:1A:1149:C:O2	2.28	0.67
6:2G:135:LEU:HB2	6:2G:155:MET:HG2	1.75	0.67
12:2Q:109:VAL:HG13	12:2Q:113:GLN:HB3	1.75	0.67
1:1A:1317:A:OP1	59:1A:4104:HOH:O	2.13	0.67
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.76	0.67
1:2A:1026:A:OP1	59:2A:3618:HOH:O	2.11	0.67
1:2A:1154:C:H3'	1:2A:1155:G:C8	2.30	0.67
1:2A:1991:A:OP1	59:2A:3625:HOH:O	2.13	0.67
1:2A:610:U:OP2	59:2A:3624:HOH:O	2.13	0.67
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.22	0.67
1:2A:1035:A:OP2	59:2A:3627:HOH:O	2.13	0.67
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.60	0.67
1:2A:396:G:OP2	59:2A:3626:HOH:O	2.13	0.67
1:2A:2375:C:OP1	22:20:55:ARG:NH1	2.28	0.67
1:2A:423:G:N7	59:2A:3696:HOH:O	2.28	0.67
1:2A:1068:U:OP2	59:2A:3630:HOH:O	2.13	0.67
1:2A:1109:C:H42	1:2A:1119:G:H1	1.40	0.67
1:2A:2509:C:OP2	59:2A:3615:HOH:O	2.13	0.67
1:1A:2816:G:N1	1:1A:2901:G:O6	2.20	0.66
21:2Z:134:PRO:O	21:2Z:136:PHE:N	2.28	0.66
1:1A:205:G:OP2	59:1A:4134:HOH:O	2.13	0.66
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.59	0.66
17:1V:98:GLU:OE2	17:1V:100:ARG:NH1	2.29	0.66
1:2A:2043:U:OP1	59:2A:3623:HOH:O	2.12	0.66
1:2A:622:G:N2	1:2A:627:C:O3'	2.28	0.66
10:2O:80:ASP:OD1	15:2T:64:ARG:NH2	2.29	0.66
1:1A:1677:A:OP1	59:1A:4132:HOH:O	2.12	0.66
1:1A:1019:C:OP1	59:1A:4136:HOH:O	2.13	0.66
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.76	0.66
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.76	0.66
1:2A:1910:A:H2'	1:2A:1911:A:C8	2.30	0.66
1:1A:2100:U:O3'	23:11:35:THR:OG1	2.14	0.66
1:1A:2510:C:OP1	59:1A:4133:HOH:O	2.12	0.66
1:1A:817:G:OP1	29:17:10:ARG:NH1	2.28	0.66
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.28	0.66
1:2A:181:U:OP2	59:2A:3629:HOH:O	2.13	0.66
6:2G:13:GLU:O	6:2G:15:VAL:N	2.28	0.66
17:2V:1:MET:HA	17:2V:42:GLY:HA3	1.77	0.66
1:2A:757:G:O3'	3:2D:202:LYS:NZ	43.92	0.66
1:1A:1381:A:OP2	19:1X:64:LYS:NZ	2.29	0.66
7:2H:124:GLU:HB2	7:2H:132:ARG:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1314:A:N7	59:1A:4276:HOH:O	2.29	0.65
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.44	0.65
1:1A:2356:G:OP2	28:16:38:LYS:NZ	2.29	0.65
1:2A:2300:G:OP1	59:2A:3628:HOH:O	2.13	0.65
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.76	0.65
1:1A:481:C:H4'	59:1A:5612:HOH:O	1.97	0.65
1:1A:1479:A:H61	1:1A:1604:A:H62	1.42	0.65
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.29	0.65
1:2A:1430:G:O2'	1:2A:1441:U:O2	2.13	0.65
1:1A:651:A:OP2	59:1A:4137:HOH:O	2.13	0.65
1:2A:2053:G:N7	59:2A:3701:HOH:O	2.30	0.65
1:1A:550:A:OP1	59:1A:4140:HOH:O	2.14	0.65
3:1D:237:GLU:OE2	59:1D:401:HOH:O	2.14	0.65
1:2A:2284:A:H2'	1:2A:2285:A:C8	2.32	0.65
1:2A:829:A:OP2	59:2A:3608:HOH:O	2.13	0.65
3:2D:184:LYS:HE3	3:2D:271:ILE:HD11	1.77	0.65
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.30	0.65
1:1A:2090:G:OP2	59:1A:4141:HOH:O	2.14	0.65
10:1O:35:VAL:HG21	10:1O:69:ILE:HD12	1.79	0.65
1:2A:1360:C:OP2	59:2A:3605:HOH:O	2.14	0.65
12:2Q:29:PHE:O	21:2Z:122:ARG:NH2	2.29	0.65
6:2G:80:PHE:O	6:2G:82:LEU:N	2.23	0.65
2:2B:43:C:O2	6:2G:95:ARG:NH1	2.30	0.65
1:2A:2844:A:N3	59:2A:3699:HOH:O	2.29	0.64
1:1A:2493:G:OP1	59:1A:4144:HOH:O	2.15	0.64
4:1E:127:ASP:OD2	59:1E:401:HOH:O	2.14	0.64
10:1O:35:VAL:HG21	10:1O:105:GLU:HG3	1.79	0.64
1:2A:2043:U:OP1	59:2A:3633:HOH:O	2.14	0.64
1:2A:2100:U:O3'	23:21:35:THR:OG1	2.16	0.64
1:1A:1991:A:OP1	59:1A:4143:HOH:O	2.15	0.64
1:1A:352:G:O6	20:1Y:19:LYS:N	2.30	0.64
1:2A:1184:C:O3'	9:2N:25:ARG:NH1	2.30	0.64
1:2A:1358:U:OP1	59:2A:3635:HOH:O	2.15	0.64
1:1A:2063:A:OP1	59:1A:4146:HOH:O	2.15	0.64
1:1A:2458:G:OP2	59:1A:4139:HOH:O	2.14	0.64
1:2A:585:G:OP2	59:2A:3634:HOH:O	2.15	0.64
1:1A:2338:A:H2'	1:1A:2339:A:C8	2.33	0.64
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.33	0.64
1:2A:1230:G:OP2	59:2A:3627:HOH:O	2.15	0.64
1:2A:524:G:N1	1:2A:527:A:OP2	2.30	0.64
2:2B:44:G:OP1	6:2G:98:ARG:NH2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1359:C:OP1	59:1A:4110:HOH:O	2.15	0.64
1:1A:921:G:H1	1:1A:947:C:H42	1.46	0.64
4:1E:111:ARG:HG3	4:1E:160:TYR:CD2	2.33	0.64
7:2H:3:ARG:HH12	7:2H:6:ARG:H	1.46	0.64
1:1A:2482:C:OP2	59:1A:4145:HOH:O	2.15	0.64
1:1A:2044:G:H5'	1:1A:2628:C:H4'	1.79	0.63
1:2A:2563:U:OP2	59:2A:3636:HOH:O	2.15	0.63
7:2H:42:ARG:NH1	7:2H:53:GLU:OE2	2.29	0.63
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.32	0.63
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.81	0.63
1:1A:258:A:H2'	1:1A:259:A:C8	3.08	0.63
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.63	0.63
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.33	0.63
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	1.80	0.63
21:2Z:92:SER:O	21:2Z:94:GLU:N	2.32	0.63
1:1A:138:A:H8	1:1A:1453:C:HO2'	1.47	0.63
1:2A:900:G:H2'	1:2A:901:G:C8	2.34	0.63
12:1Q:110:THR:HG23	12:1Q:113:GLN:HB2	1.80	0.63
1:1A:1158:U:H2'	1:1A:1159:G:C8	2.34	0.63
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.31	0.63
6:1G:16:ARG:HG2	6:1G:16:ARG:HH11	1.63	0.63
6:2G:33:ARG:NH1	6:2G:33:ARG:HB2	2.13	0.63
1:1A:184:A:H62	11:1P:38:GLN:HE22	1.47	0.63
1:1A:1012:G:O6	59:1A:4131:HOH:O	2.12	0.63
1:1A:555:C:OP2	59:1A:4148:HOH:O	2.16	0.63
1:2A:2731:G:O6	59:2A:3632:HOH:O	2.14	0.63
6:2G:12:TYR:HA	6:2G:16:ARG:HG3	1.79	0.63
1:2A:141:G:H4'	19:2X:35:THR:HG21	1.81	0.63
1:1A:1081:G:OP2	7:1H:59:ARG:NH1	2.31	0.62
1:1A:296:C:H2'	1:1A:297:G:H8	1.64	0.62
1:2A:935:C:O2'	1:2A:936:A:O5'	2.16	0.62
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.81	0.62
1:1A:541:C:OP1	27:15:16:ARG:NH2	2.32	0.62
1:2A:2733:A:OP1	59:2A:3637:HOH:O	2.16	0.62
28:16:13:CYS:SG	28:16:47:THR:HG21	2.39	0.62
1:1A:2323:U:H5'	6:1G:88:ILE:HD11	1.80	0.62
1:1A:536:G:N7	59:1A:4165:HOH:O	2.31	0.62
8:1I:77:LEU:HB3	8:1I:142:VAL:HG13	1.79	0.62
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.81	0.62
28:26:13:CYS:SG	28:26:47:THR:HG21	2.39	0.62
1:2A:609:C:OP2	11:2P:21:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1115:A:N7	1:2A:1141:A:O2'	2.27	0.62
1:2A:2226:G:H8	1:2A:2227:G:N7	1.98	0.62
1:2A:2646:C:O2'	4:2E:48:GLN:NE2	2.31	0.62
23:21:77:ALA:HA	23:21:80:LEU:HD13	1.82	0.62
3:2D:242:ARG:N	3:2D:242:ARG:HD3	2.13	0.62
14:2S:35:ILE:HD13	14:2S:97:ARG:HH21	1.64	0.62
2:2B:75:G:H22	21:2Z:73:GLN:NE2	1.97	0.62
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.33	0.62
1:2A:1576:C:H42	1:2A:1585:G:H1	1.47	0.62
1:1A:2844:A:N3	59:1A:4286:HOH:O	2.31	0.62
6:1G:77:ILE:HD12	6:1G:82:LEU:HD12	1.81	0.62
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.81	0.62
1:2A:2726:G:OP2	59:2A:3638:HOH:O	2.16	0.62
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.32	0.62
1:2A:596:C:OP1	59:2A:3639:HOH:O	2.16	0.62
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.65	0.61
2:2B:40:U:H2'	26:24:2:LYS:HE3	1.82	0.61
6:1G:109:VAL:HG13	26:14:33:VAL:HG11	1.82	0.61
1:2A:929:G:N3	1:2A:948:C:O2'	31.35	0.61
26:24:24:THR:OG1	26:24:25:TYR:N	2.32	0.61
16:2U:92:ARG:HA	16:2U:95:LEU:HB2	1.81	0.61
18:2W:4:LYS:HB2	18:2W:106:ILE:HG12	1.82	0.61
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.33	0.61
1:2A:2302:U:H2'	1:2A:2303:C:C6	2.35	0.61
1:2A:1830:C:OP2	3:2D:183:ARG:NH2	2.33	0.61
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.83	0.61
1:2A:1256:G:N2	1:2A:1257:A:N7	5.54	0.61
1:2A:1685:U:H2'	1:2A:1686:C:H5''	1.82	0.61
1:2A:2278:A:H5''	1:2A:2279:A:H5'	1.81	0.61
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.65	0.61
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.19	0.61
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.01	0.61
1:1A:2858:U:H4'	1:1A:2877:A:C2	2.36	0.61
8:1I:72:LEU:O	8:1I:74:ASN:N	2.33	0.61
1:2A:1042:G:OP1	16:2U:92:ARG:HG2	2.01	0.61
1:2A:1400:G:OP1	3:2D:38:LYS:NZ	2.34	0.61
1:1A:1232:U:H4'	17:1V:79:VAL:HG22	1.81	0.61
1:1A:1939:A:O2'	1:1A:1941:C:N4	2.34	0.61
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.83	0.61
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.82	0.61
1:2A:2805:G:H22	1:2A:2814:C:H1'	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:330:G:H21	1:2A:353:A:H62	1.49	0.61
2:2B:50:G:OP1	14:2S:63:THR:N	2.33	0.61
1:2A:1116:G:H1	1:2A:1124:C:H42	14.96	0.60
1:2A:1311:G:O5'	18:2W:15:ARG:NH2	2.34	0.60
1:1A:137:G:H2'	1:1A:138:A:H8	9.96	0.60
1:1A:2657:C:OP2	1:1A:2744:G:O2'	2.19	0.60
4:1E:54:GLN:HA	4:1E:54:GLN:HE21	1.64	0.60
1:2A:1638:G:H2'	1:2A:1639:G:H8	1.66	0.60
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.83	0.60
11:2P:94:GLU:HG3	11:2P:124:LYS:HD3	1.83	0.60
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.83	0.60
1:2A:2088:G:O2'	1:2A:2090:G:H5''	2.02	0.60
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.82	0.60
1:1A:1500:U:O2'	1:1A:1501:G:N7	2.31	0.60
1:2A:2441:A:OP2	59:2A:3603:HOH:O	2.17	0.60
1:2A:533:C:OP1	59:2A:3641:HOH:O	2.16	0.60
15:2T:64:ARG:HB2	15:2T:73:GLU:HG2	1.82	0.60
1:1A:1846:G:OP2	59:1A:4153:HOH:O	2.17	0.60
21:1Z:92:SER:O	21:1Z:94:GLU:N	2.35	0.60
1:2A:1684:C:H5''	1:2A:2721:C:O2'	2.01	0.60
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.83	0.60
1:1A:1789:A:N3	59:1A:4298:HOH:O	2.32	0.60
1:1A:1039:C:OP1	16:1U:53:ARG:NH2	2.34	0.60
1:2A:624:G:O2'	1:2A:701:A:N6	2.35	0.60
1:2A:82:A:H5''	20:2Y:8:LYS:HE3	1.84	0.60
1:2A:1129:A:N3	1:2A:1150:U:O2'	2.32	0.60
1:2A:775:G:C6	3:2D:208:LYS:HB2	2.36	0.60
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.35	0.60
23:11:77:ALA:HA	23:11:80:LEU:HD13	1.83	0.60
26:14:44:THR:O	26:14:46:GLN:N	2.35	0.60
1:1A:1323:A:OP1	13:1R:36:THR:HG23	2.02	0.60
1:1A:1760:G:N2	1:1A:1774:C:O2	2.33	0.60
1:1A:710:C:O2'	59:1A:4152:HOH:O	2.17	0.60
8:1I:48:GLU:HG2	8:1I:52:ARG:HH22	1.67	0.60
1:2A:1154:C:H3'	1:2A:1155:G:H8	1.66	0.60
1:1A:2622:U:C4	27:15:3:LYS:HG2	2.36	0.59
1:1A:593:A:O2'	17:1V:78:LYS:NZ	2.35	0.59
11:1P:95:VAL:HG22	11:1P:125:VAL:HB	1.84	0.59
13:1R:33:ARG:NH1	13:1R:115:GLU:OE2	2.34	0.59
15:1T:16:ARG:NH2	15:1T:83:ILE:O	2.35	0.59
1:2A:1354:G:H4'	29:27:7:PRO:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1812:C:OP1	59:2A:3642:HOH:O	2.16	0.59
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.35	0.59
1:1A:1038:G:OP1	16:1U:50:ARG:NH2	2.31	0.59
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.84	0.59
1:2A:361:G:OP2	59:2A:3640:HOH:O	2.16	0.59
12:2Q:52:VAL:HG22	21:2Z:183:LEU:HD11	1.83	0.59
1:1A:2694:C:O2	10:1O:70:LYS:NZ	2.26	0.59
1:2A:555:C:OP1	1:2A:583:G:N1	2.34	0.59
2:2B:64:C:H2'	2:2B:65:C:C6	2.37	0.59
2:2B:114:C:H4'	14:2S:46:VAL:HG22	1.85	0.59
1:1A:598:U:H2'	1:1A:599:G:C8	2.36	0.59
11:1P:88:LEU:HD11	11:1P:114:ILE:HD12	1.83	0.59
24:12:32:LEU:HD22	24:12:36:ARG:HH11	1.67	0.59
1:1A:1303:C:OP2	59:1A:4151:HOH:O	2.16	0.59
1:1A:2650:A:OP2	59:1A:4157:HOH:O	2.17	0.59
1:1A:404:C:O2'	59:1A:4155:HOH:O	2.17	0.59
1:1A:929:G:N2	1:1A:948:C:O2	27.38	0.59
1:2A:1002:U:OP2	12:2Q:14:ARG:NH1	2.35	0.59
1:2A:1231:G:H5'	17:2V:81:TYR:CE1	2.38	0.59
21:2Z:157:LEU:HD21	21:2Z:163:LEU:HD13	1.85	0.59
1:1A:183:A:OP1	11:1P:46:LYS:NZ	2.29	0.59
1:2A:69:A:H5''	1:2A:71:A:C8	2.37	0.59
2:2B:62:C:H2'	2:2B:63:G:C8	2.38	0.59
1:1A:1355:G:OP2	29:17:9:ARG:NH1	2.36	0.59
1:1A:663:U:H2'	1:1A:664:C:C6	2.37	0.59
1:2A:1992:A:OP2	3:2D:242:ARG:NH2	2.36	0.59
14:2S:99:LYS:NZ	14:2S:103:GLU:OE2	2.21	0.59
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.83	0.59
12:1Q:32:TYR:CE1	12:1Q:133:ARG:HG3	2.36	0.59
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.84	0.59
1:2A:1717:U:HO2'	1:2A:1719:U:H5	1.51	0.59
1:1A:1514:C:OP1	59:1A:4149:HOH:O	2.16	0.59
1:1A:69:A:N7	19:1X:31:HIS:HE1	2.00	0.59
1:2A:154:C:H42	1:2A:159:G:H1	1.51	0.59
1:2A:2297:A:H4'	1:2A:2298:A:O4'	2.02	0.59
2:2B:66:A:H61	2:2B:109:C:H5''	1.67	0.59
21:2Z:10:ARG:NH1	21:2Z:26:GLY:O	2.36	0.59
26:14:63:TYR:N	26:14:64:GLY:HA2	2.18	0.58
1:1A:1295:G:OP2	11:1P:21:ARG:NH1	2.35	0.58
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	1.85	0.58
12:1Q:52:VAL:O	12:1Q:56:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:130:PRO:HB2	21:2Z:131:ARG:CZ	2.33	0.58
1:1A:1184:C:O3'	9:1N:25:ARG:NH1	2.36	0.58
1:1A:2243:U:O2'	59:1A:4155:HOH:O	2.17	0.58
1:1A:2383:G:N3	59:1A:4303:HOH:O	2.32	0.58
1:2A:1174:A:N6	1:2A:2502:U:OP1	2.36	0.58
23:21:3:LYS:HB2	23:21:61:ARG:HH11	1.68	0.58
2:2B:15:A:OP2	2:2B:69:G:N2	2.34	0.58
8:2I:9:LEU:HD11	8:2I:35:LEU:HD13	1.85	0.58
27:15:16:ARG:HH11	27:15:16:ARG:HG2	1.67	0.58
1:1A:610:U:H2'	1:1A:611:C:C6	2.38	0.58
1:2A:1067:G:N2	1:2A:1068:U:O4	2.36	0.58
1:2A:1416:G:HO2'	1:2A:1417:U:H5	1.51	0.58
1:2A:2601:A:O3'	3:2D:239:ARG:NH2	2.36	0.58
4:1E:1:MET:HE3	4:1E:199:ARG:HB3	1.85	0.58
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.85	0.58
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.84	0.58
1:1A:1868:C:O3'	59:1A:4158:HOH:O	2.17	0.58
14:1S:15:ARG:O	14:1S:19:LYS:HG2	2.04	0.58
1:2A:2327:C:H2'	1:2A:2328:C:H6	1.68	0.58
9:1N:67:LEU:HD13	9:1N:87:LEU:HD13	1.86	0.58
1:2A:641:G:H5'	5:2F:205:ARG:HD2	1.84	0.58
1:2A:885:U:H2'	1:2A:886:C:C6	2.39	0.58
1:1A:2206:C:H2'	1:1A:2207:G:H8	1.69	0.58
1:1A:267:G:OP2	59:1A:4154:HOH:O	2.17	0.58
10:1O:24:VAL:HA	10:1O:39:ILE:HG22	1.84	0.58
1:1A:2330:G:H22	14:1S:3:ARG:HG2	1.68	0.58
16:1U:76:TYR:OH	16:1U:92:ARG:NH1	2.35	0.58
1:2A:1292:A:OP1	5:2F:95:ARG:NH2	2.36	0.58
1:1A:1007:U:OP2	59:1A:4160:HOH:O	2.17	0.58
1:1A:2206:C:H2'	1:1A:2207:G:C8	2.39	0.58
1:2A:1682:C:OP2	59:2A:3647:HOH:O	2.17	0.58
10:2O:7:TYR:HE1	10:2O:20:MET:HE3	1.67	0.58
1:2A:1066:A:H61	1:2A:1187:A:H61	1.50	0.58
1:2A:1854:G:N3	3:2D:254:THR:OG1	2.37	0.58
15:2T:56:GLY:O	15:2T:59:THR:HG23	2.04	0.58
1:1A:830:A:H5'	1:1A:831:G:OP1	2.03	0.57
1:2A:1070:G:C4	1:2A:1179:C:H1'	2.39	0.57
1:2A:1702:C:H2'	1:2A:1703:C:H6	1.69	0.57
19:2X:35:THR:HG22	19:2X:37:THR:H	1.67	0.57
1:1A:2859:A:OP2	1:1A:2875:U:H5	1.88	0.57
1:1A:326:U:O4	59:1A:4156:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2797:C:OP1	4:1E:41:LYS:NZ	2.37	0.57
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.85	0.57
26:24:46:GLN:O	26:24:48:ARG:N	2.36	0.57
11:2P:95:VAL:HG12	11:2P:123:LEU:HD22	1.86	0.57
1:1A:1066:A:H62	1:1A:1185:U:H3	1.50	0.57
1:1A:2803:C:H2'	1:1A:2804:G:H8	1.68	0.57
1:1A:670:A:H2'	1:1A:671:G:O4'	2.04	0.57
1:2A:1823:C:OP1	59:2A:3645:HOH:O	2.17	0.57
11:2P:39:LYS:HA	11:2P:45:LEU:HG	1.86	0.57
1:1A:1713:G:O2'	1:1A:2012:U:O4	2.17	0.57
1:1A:2017:C:H4'	1:1A:2018:G:OP1	2.04	0.57
1:1A:2429:A:H2'	1:1A:2430:U:C6	2.38	0.57
1:1A:2033:G:OP1	18:1W:11:ARG:NH2	2.33	0.57
1:1A:439:C:O2	1:1A:475:G:N2	74.36	0.57
4:1E:54:GLN:HB2	4:1E:76:ARG:HG3	1.85	0.57
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.31	0.57
1:1A:1603:C:OP2	1:1A:1604:A:O2'	2.18	0.57
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.37	0.57
1:2A:704:C:H2'	1:2A:705:C:C6	2.40	0.57
15:2T:55:ASN:N	15:2T:59:THR:HG22	2.14	0.57
1:1A:2626:U:H2'	1:1A:2627:C:H6	1.70	0.57
15:1T:56:GLY:O	15:1T:59:THR:HG23	2.04	0.57
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.23	0.57
3:2D:26:LYS:NZ	3:2D:30:GLU:OE1	2.31	0.57
1:1A:1430:G:O2'	1:1A:1441:U:O2	2.21	0.57
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	1.87	0.57
12:1Q:55:VAL:HG12	12:1Q:64:ILE:HD13	1.86	0.57
1:2A:948:C:H2'	1:2A:949:C:H6	1.70	0.57
1:2A:1052:C:H5''	9:2N:35:ARG:HH11	1.69	0.57
1:2A:2347:A:H61	22:20:43:THR:CG2	2.18	0.57
1:1A:2563:U:OP1	59:1A:4162:HOH:O	2.18	0.57
1:2A:30:C:OP1	59:2A:3646:HOH:O	2.17	0.57
1:2A:172:C:H2'	1:2A:173:U:C6	2.40	0.56
2:2B:90:A:C5	2:2B:91:C:H1'	2.40	0.56
4:1E:29:GLY:HA3	59:1E:404:HOH:O	2.04	0.56
1:2A:1276:G:H2'	1:2A:1277:G:H8	1.70	0.56
1:2A:493:G:N7	29:27:39:ARG:NH2	2.50	0.56
1:1A:1687:A:H2'	1:1A:1688:G:O4'	2.05	0.56
1:1A:2018:G:N7	59:1A:4297:HOH:O	2.32	0.56
1:2A:2238:A:OP2	59:2A:3643:HOH:O	2.16	0.56
1:1A:1697:G:OP1	13:1R:40:LYS:NZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1066:A:H62	1:2A:1185:U:H3	1.53	0.56
1:2A:137:G:H1'	1:2A:138:A:H2	1.68	0.56
1:2A:2375:C:H2'	1:2A:2376:G:O4'	2.06	0.56
12:2Q:12:GLN:HG2	12:2Q:73:PRO:HD2	1.86	0.56
1:1A:1387:A:OP2	59:1A:4142:HOH:O	2.18	0.56
1:1A:1826:U:H2'	1:1A:1827:C:C6	2.40	0.56
15:1T:35:LYS:HD3	15:1T:37:GLY:H	1.70	0.56
16:1U:85:LYS:HD3	16:1U:117:GLN:HA	1.86	0.56
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.23	0.56
2:2B:31:C:H4'	6:2G:29:TRP:HH2	1.69	0.56
1:1A:638:G:OP1	59:1A:4159:HOH:O	2.17	0.56
6:1G:49:ASP:O	6:1G:51:ARG:N	2.29	0.56
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.21	0.56
1:2A:1276:G:H2'	1:2A:1277:G:C8	2.40	0.56
5:2F:53:THR:HG22	5:2F:56:GLU:HG3	1.86	0.56
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.79	0.56
1:1A:1076:G:H21	31:19:36:GLN:HE22	1.53	0.56
1:1A:208:G:O2'	1:1A:221:A:N3	2.34	0.56
3:1D:142:VAL:HG23	3:1D:193:VAL:HA	1.88	0.56
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.88	0.56
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.39	0.56
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	1.87	0.56
28:26:14:THR:OG1	28:26:48:VAL:O	2.22	0.56
1:2A:2122:G:O6	1:2A:2209:C:N4	2.38	0.56
1:1A:1091:A:H3'	1:1A:1092:G:H5'	1.86	0.56
1:1A:2517:U:OP1	4:1E:144:ARG:NH2	2.37	0.56
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.70	0.56
23:21:65:SER:OG	23:21:66:HIS:ND1	2.35	0.56
1:2A:2040:A:OP2	27:25:9:LYS:NZ	2.31	0.56
1:2A:807:A:OP2	59:2A:3644:HOH:O	2.17	0.56
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.87	0.56
1:1A:1409:G:P	23:11:3:LYS:HG3	2.46	0.56
1:1A:301:A:O2'	1:1A:302:C:OP1	2.20	0.56
5:1F:84:VAL:O	59:1F:401:HOH:O	2.18	0.56
1:2A:324:G:OP2	20:2Y:84:ARG:NH2	2.38	0.56
1:1A:1536:G:O2'	3:1D:101:GLU:HB2	2.06	0.56
1:2A:346:G:HO2'	1:2A:1249:U:H3	1.47	0.56
1:2A:2298:A:H62	1:2A:2355:U:H3	1.53	0.56
1:2A:590:U:H5'	1:2A:989:A:N1	2.20	0.56
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.87	0.56
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:16:CYS:SG	26:14:17:GLY:N	2.79	0.55
1:1A:271:U:H4'	8:1I:50:ARG:HH12	1.71	0.55
31:19:2:LYS:NZ	31:19:31:LYS:O	2.34	0.55
1:1A:1090:A:H4'	1:1A:1091:A:H5''	1.87	0.55
1:1A:1257:A:N3	1:1A:1283:G:O2'	2.37	0.55
1:2A:2573:U:H1'	10:2O:23:ARG:HH11	1.71	0.55
1:1A:440:C:H2'	1:1A:441:A:C8	2.41	0.55
1:1A:614:G:H2'	1:1A:615:G:C8	3.78	0.55
6:1G:50:ALA:O	6:1G:52:ILE:N	2.39	0.55
7:1H:3:ARG:HG2	7:1H:6:ARG:HG2	1.88	0.55
20:1Y:68:HIS:ND1	20:1Y:70:SER:HB3	2.21	0.55
1:2A:1154:C:H2'	1:2A:1155:G:C8	3.43	0.55
1:2A:2813:C:H2'	1:2A:2814:C:H6	1.71	0.55
3:2D:75:ILE:HG21	3:2D:99:ASP:HB2	1.88	0.55
11:2P:84:ASN:OD1	11:2P:117:GLU:HB2	2.06	0.55
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.40	0.55
1:1A:1220:G:H21	1:1A:1221:A:H4'	1.71	0.55
1:2A:80:G:N1	1:2A:100:A:OP2	2.36	0.55
1:2A:2785:C:OP1	4:2E:166:THR:OG1	2.24	0.55
5:2F:130:ALA:HB2	5:2F:142:TRP:HD1	1.71	0.55
1:2A:2305:C:H5'	14:2S:10:ARG:HD2	1.89	0.55
1:1A:1450:U:H2'	1:1A:1451:U:C6	2.42	0.55
1:1A:1612:A:OP1	3:1D:211:ARG:NH1	2.39	0.55
1:1A:2117:U:H3	1:1A:2214:G:H1	1.53	0.55
1:1A:2339:A:H2'	1:1A:2340:G:C8	2.42	0.55
12:1Q:21:THR:HG21	12:1Q:101:ARG:HB2	1.88	0.55
1:2A:1070:G:O2'	59:2A:3630:HOH:O	2.18	0.55
1:2A:2012:U:H2'	1:2A:2013:G:H5''	1.89	0.55
1:2A:900:G:N3	1:2A:1381:A:H2	127.15	0.55
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.53	0.55
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.89	0.55
1:1A:1792:A:H2'	59:1A:5846:HOH:O	2.06	0.55
21:1Z:24:LEU:HB2	21:1Z:41:LEU:HD23	1.88	0.55
1:2A:239:A:C5	1:2A:240:G:H1'	2.42	0.55
1:2A:241:C:O2'	59:2A:3652:HOH:O	2.18	0.55
1:2A:839:A:O2'	59:2A:3613:HOH:O	2.09	0.55
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.89	0.55
1:1A:425:G:OP2	59:1A:4163:HOH:O	2.18	0.55
1:2A:1092:G:H1'	1:2A:1155:G:N2	2.21	0.55
1:2A:754:C:H42	1:2A:769:G:H1	1.53	0.55
1:1A:552:A:C2	1:1A:2064:C:H4'	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:239:A:C5	1:1A:240:G:H1'	2.42	0.55
8:1I:72:LEU:C	8:1I:74:ASN:H	2.11	0.55
1:2A:1033:A:N7	59:2A:3715:HOH:O	2.34	0.55
1:2A:656:A:H2'	1:2A:657:A:C8	2.41	0.55
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.07	0.55
11:2P:88:LEU:HD11	11:2P:114:ILE:HD12	1.88	0.55
13:2R:104:ARG:HG3	13:2R:111:LEU:HD21	1.88	0.55
25:13:8:LEU:HD13	25:13:31:LEU:HD23	1.87	0.55
1:2A:1073:A:H2'	1:2A:1074:A:C8	2.41	0.55
1:2A:504:A:N3	1:2A:506:G:H5''	2.22	0.55
2:2B:98:G:H2'	2:2B:99:G:O4'	2.07	0.55
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	1.89	0.55
1:1A:2441:A:H2'	1:1A:2441:A:N3	2.22	0.54
1:2A:1061:G:H2'	1:2A:1062:G:O4'	2.06	0.54
1:2A:2619:G:N7	59:2A:3716:HOH:O	2.34	0.54
1:2A:2641:G:H2'	1:2A:2642:G:C8	2.42	0.54
1:2A:26:G:O2'	1:2A:27:A:OP2	2.24	0.54
24:12:22:GLU:HG2	24:12:64:LEU:HD11	1.89	0.54
26:14:46:GLN:O	26:14:48:ARG:N	2.40	0.54
1:1A:846:A:OP1	1:1A:846:A:H8	1.90	0.54
15:1T:55:ASN:N	15:1T:59:THR:HG22	2.16	0.54
1:2A:2022:A:H2'	1:2A:2023:G:C8	2.42	0.54
1:2A:33:C:H2'	1:2A:34:G:H5'	1.88	0.54
2:2B:49:C:H2'	2:2B:50:G:C8	2.42	0.54
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.89	0.54
1:2A:1110:U:O2	1:2A:1119:G:N2	2.41	0.54
1:2A:1295:G:OP2	11:2P:21:ARG:NH1	2.40	0.54
29:17:24:THR:O	29:17:28:ARG:HG3	2.08	0.54
1:1A:1210:U:H2'	1:1A:1211:C:C6	2.42	0.54
1:1A:741:G:OP1	1:1A:1425:G:O2'	2.25	0.54
1:1A:928:G:H1	1:1A:939:C:H42	1.56	0.54
1:2A:839:A:OP1	59:2A:3649:HOH:O	2.18	0.54
7:2H:118:PRO:HG2	7:2H:121:ILE:HG13	1.90	0.54
1:1A:534:C:OP1	59:1A:4165:HOH:O	2.18	0.54
1:1A:1847:G:OP1	3:1D:88:ARG:NH2	2.40	0.54
1:2A:671:G:O5'	1:2A:671:G:H8	1.90	0.54
1:1A:2316:A:H5''	6:1G:134:GLY:HA3	1.90	0.54
3:1D:108:PRO:HD2	3:1D:111:LEU:HG	1.90	0.54
1:2A:1015:C:OP2	59:2A:3651:HOH:O	2.18	0.54
1:2A:2821:G:H1	1:2A:2897:C:H42	1.54	0.54
1:1A:235:G:H4'	1:1A:412:G:C5	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:358:C:H4'	20:1Y:73:ARG:HD3	1.89	0.54
1:1A:703:U:H2'	1:1A:704:C:C6	2.43	0.54
1:1A:924:A:H2'	1:1A:925:G:H5'	1.88	0.54
1:1A:708:G:H5''	11:1P:16:ARG:HG3	1.89	0.54
1:2A:2017:C:H4'	1:2A:2018:G:OP1	2.07	0.54
1:2A:560:A:H2'	1:2A:561:C:C6	2.43	0.54
1:2A:1923:C:H5'	3:2D:246:PRO:HD3	1.89	0.54
1:1A:1565:U:H2'	1:1A:1566:G:O4'	2.08	0.54
1:1A:274:C:H2'	1:1A:275:C:C6	2.43	0.54
1:1A:509:C:H2'	1:1A:510:C:C6	2.43	0.54
26:24:59:PHE:HA	26:24:61:ARG:N	2.23	0.54
1:2A:1443:C:H2'	1:2A:1444:C:O4'	2.77	0.54
1:2A:6:G:H2'	1:2A:7:A:O4'	2.07	0.54
1:2A:629:U:OP1	5:2F:102:PRO:HA	2.07	0.54
6:2G:63:ILE:HA	6:2G:143:GLU:HG3	1.88	0.54
19:2X:31:HIS:HD2	19:2X:33:LYS:H	1.55	0.54
1:1A:1026:A:OP1	59:1A:4164:HOH:O	2.18	0.54
1:2A:1465:U:O2'	1:2A:1466:G:OP1	2.24	0.54
1:2A:2858:U:OP2	15:2T:95:ARG:NH1	2.38	0.54
1:2A:323:A:P	20:2Y:86:ARG:HH21	2.31	0.54
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.90	0.54
19:2X:32:PRO:HA	19:2X:77:LYS:HB2	1.89	0.54
1:2A:1381:A:OP2	19:2X:64:LYS:HE3	2.08	0.54
1:1A:1056:G:OP1	16:1U:77:SER:OG	2.25	0.54
1:1A:1066:A:H3'	1:1A:1066:A:C8	2.43	0.54
1:1A:1218:A:H4'	1:1A:1219:U:OP1	2.07	0.54
1:1A:1920:G:N3	1:1A:1920:G:H2'	2.23	0.54
1:2A:2799:C:H1'	4:2E:62:PRO:HG3	1.89	0.54
1:2A:2830:A:H2'	1:2A:2831:G:C8	2.43	0.54
1:2A:323:A:OP1	20:2Y:86:ARG:NH2	2.40	0.54
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.08	0.54
20:2Y:37:VAL:HG21	20:2Y:72:VAL:HG21	1.90	0.54
1:1A:1070:G:C4	1:1A:1179:C:H1'	2.43	0.53
1:1A:2095:U:H2'	1:1A:2096:U:C6	2.42	0.53
1:1A:1176:G:H21	9:1N:73:THR:HG21	1.74	0.53
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.23	0.53
1:2A:1625:A:H2'	1:2A:1626:A:C8	2.43	0.53
1:2A:330:G:N1	1:2A:333:A:OP2	2.38	0.53
2:2B:25:A:H2'	2:2B:26:A:C8	2.44	0.53
1:1A:1017:A:H5'	1:1A:1232:U:H1'	1.90	0.53
1:1A:1510:C:H2'	1:1A:1511:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:550:A:O2'	1:1A:2064:C:O2	2.25	0.53
1:1A:641:G:N2	1:1A:733:C:O2	75.09	0.53
1:1A:922:C:H2'	1:1A:923:U:O4'	2.08	0.53
1:2A:904:U:O2	1:2A:2279:A:H2'	2.09	0.53
1:2A:2072:A:H5'	1:2A:2589:G:O4'	2.07	0.53
1:2A:948:C:H2'	1:2A:949:C:C6	2.43	0.53
16:2U:104:GLN:OE1	16:2U:105:VAL:N	2.28	0.53
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.90	0.53
1:1A:214:G:H21	1:1A:216:A:H62	1.55	0.53
1:2A:2327:C:H2'	1:2A:2328:C:C6	2.43	0.53
5:2F:29:ASN:H	5:2F:112:MET:CE	2.20	0.53
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.89	0.53
31:19:19:ARG:NH2	59:19:601:HOH:O	2.10	0.53
1:1A:1214:G:OP1	59:1A:4166:HOH:O	2.18	0.53
1:1A:2012:U:H2'	1:1A:2013:G:H5''	1.91	0.53
1:1A:296:C:H2'	1:1A:297:G:C8	2.44	0.53
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.07	0.53
1:2A:2568:G:H2'	1:2A:2569:C:H6	1.74	0.53
1:2A:2858:U:H4'	1:2A:2877:A:C2	2.43	0.53
1:2A:33:C:H41	1:2A:472:A:H61	1.57	0.53
1:2A:2735:C:OP2	4:2E:109:LYS:NZ	2.40	0.53
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.89	0.53
5:1F:14:PRO:HD2	5:1F:127:GLU:OE1	2.09	0.53
1:2A:2670:G:O2'	7:2H:175:LYS:NZ	2.34	0.53
1:2A:50:A:OP2	1:2A:114:G:N1	2.27	0.53
1:2A:661:A:H2'	11:2P:117:GLU:OE2	2.09	0.53
1:1A:172:C:H2'	1:1A:173:U:C6	2.44	0.53
1:1A:2284:A:H2'	1:1A:2285:A:C8	2.43	0.53
1:2A:1406:G:H2'	1:2A:1407:C:C6	2.90	0.53
1:2A:2314:G:O2'	6:2G:132:ASN:HB2	2.08	0.53
1:2A:907:A:H2'	1:2A:908:G:O4'	2.09	0.53
5:2F:140:LEU:HD21	5:2F:170:LEU:HD11	1.90	0.53
8:2I:126:TYR:HB2	8:2I:142:VAL:HG23	1.90	0.53
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	1.91	0.53
26:14:14:ILE:HD13	26:14:31:ILE:HB	1.90	0.53
1:1A:1091:A:H5'	1:1A:1092:G:C8	2.44	0.53
6:1G:115:ARG:HG3	6:1G:136:ARG:HH22	1.74	0.53
30:28:63:PRO:HG2	30:28:64:TYR:CD2	2.44	0.53
1:2A:480:C:N3	1:2A:497:A:H2'	2.24	0.53
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.08	0.53
1:1A:2315:G:H22	1:1A:2323:U:H3	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2347:A:H61	22:10:43:THR:CG2	2.22	0.53
1:1A:1924:G:OP1	3:1D:241:PRO:HB2	2.09	0.53
12:1Q:60:ARG:H	12:1Q:60:ARG:NH1	2.07	0.53
1:2A:842:C:H2'	1:2A:843:C:C6	2.44	0.53
5:2F:183:VAL:O	5:2F:187:VAL:HG23	2.09	0.53
19:1X:60:ARG:NH2	29:17:47:ARG:HH22	2.07	0.53
1:1A:1846:G:O6	3:1D:35:LYS:NZ	2.27	0.53
1:1A:302:C:H42	1:1A:384:G:H1	1.57	0.53
1:1A:84:C:H4'	1:1A:101:U:H1'	1.90	0.53
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.91	0.53
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.91	0.53
1:1A:1337:U:H2'	1:1A:1338:C:C6	2.44	0.53
1:1A:233:G:O6	30:18:8:LYS:NZ	2.30	0.53
1:1A:551:C:C5	1:1A:2791:U:H2'	2.44	0.53
1:2A:1513:C:C5	1:2A:1592:C:H2'	2.44	0.53
1:2A:2568:G:H2'	1:2A:2569:C:C6	2.44	0.53
1:2A:1873:C:H5'	3:2D:253:GLN:NE2	2.23	0.53
5:2F:197:ASP:O	5:2F:200:GLU:HB2	2.09	0.53
11:2P:125:VAL:HG13	11:2P:138:LEU:HD21	1.91	0.53
11:2P:114:ILE:HG13	11:2P:125:VAL:HG21	1.91	0.53
1:1A:514:G:N7	18:1W:49:LYS:NZ	2.58	0.52
1:2A:866:A:N3	1:2A:987:U:H4'	2.24	0.52
21:2Z:70:LEU:HG	21:2Z:91:LEU:HD21	1.91	0.52
26:14:26:SER:OG	26:14:27:THR:N	2.43	0.52
1:1A:957:C:OP1	12:1Q:8:LYS:NZ	2.40	0.52
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.90	0.52
1:2A:1685:U:C2'	1:2A:1686:C:H5''	2.38	0.52
1:2A:867:A:H2'	1:2A:990:G:H5''	1.90	0.52
5:2F:36:VAL:HG11	5:2F:183:VAL:HG11	1.92	0.52
26:24:41:PRO:HG3	26:24:49:PHE:CE2	2.45	0.52
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.38	0.52
1:2A:1073:A:N6	1:2A:1170:G:H2'	2.24	0.52
1:2A:135:G:H2'	1:2A:137:G:N7	2.24	0.52
1:2A:309:C:H2'	1:2A:310:C:C6	2.44	0.52
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.91	0.52
1:1A:2330:G:N2	14:1S:3:ARG:HG2	2.24	0.52
1:2A:2704:A:H2'	1:2A:2705:G:H8	1.74	0.52
1:2A:885:U:H2'	1:2A:886:C:H6	1.74	0.52
1:1A:2382:G:O6	59:1A:4150:HOH:O	2.16	0.52
1:1A:955:A:H2'	1:1A:956:A:H5''	4.81	0.52
14:1S:15:ARG:NE	14:1S:88:ASP:OD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:27:24:THR:O	29:27:28:ARG:HG3	2.09	0.52
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.91	0.52
1:2A:2484:U:O2	1:2A:2484:U:H2'	2.08	0.52
1:2A:601:G:H2'	1:2A:602:C:C6	2.45	0.52
1:2A:703:U:H2'	1:2A:704:C:C6	2.44	0.52
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.91	0.52
5:2F:161:GLU:O	5:2F:165:ARG:HB2	2.09	0.52
8:2I:14:ASP:N	8:2I:17:GLN:OE1	2.37	0.52
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.08	0.52
28:16:6:ARG:NE	28:16:24:GLU:OE1	2.35	0.52
1:1A:2429:A:H2'	1:1A:2430:U:H6	1.75	0.52
1:1A:2052:A:C6	1:1A:2509:C:H1'	2.44	0.52
12:1Q:109:VAL:HG13	12:1Q:113:GLN:HB3	1.92	0.52
1:1A:2719:G:H1'	13:1R:71:GLN:HE22	1.72	0.52
10:1O:80:ASP:OD1	15:1T:64:ARG:NH2	2.43	0.52
1:2A:44:C:OP2	1:2A:203:G:H5'	2.10	0.52
8:2I:48:GLU:HG2	8:2I:52:ARG:HH12	1.74	0.52
1:2A:2719:G:H1'	13:2R:71:GLN:HE22	1.75	0.52
1:1A:1054:A:OP2	9:1N:37:LYS:NZ	2.30	0.52
1:1A:964:G:N2	1:1A:2280:A:OP2	2.43	0.52
3:1D:167:GLY:H	3:1D:168:ARG:CZ	7.31	0.52
4:1E:14:ILE:HD11	4:1E:173:VAL:HG11	1.91	0.52
1:1A:1288:G:O2'	11:1P:7:ARG:NH2	2.42	0.52
1:2A:2095:U:H2'	1:2A:2096:U:C6	2.44	0.52
1:2A:2657:C:H2'	1:2A:2658:U:O4'	2.09	0.52
1:2A:780:A:O2'	1:2A:1681:G:H5'	2.10	0.52
8:2I:114:LEU:HD11	8:2I:128:LEU:HD13	1.92	0.52
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.91	0.52
1:1A:1425:G:O2'	1:1A:1426:G:OP1	5.00	0.52
1:1A:1649:C:OP2	59:1A:4123:HOH:O	2.19	0.52
1:1A:173:U:H4'	1:1A:206:A:H4'	1.91	0.52
1:1A:2107:U:H2'	1:1A:2108:G:C8	2.45	0.52
1:1A:1828:U:H5'	3:1D:259:THR:HG23	1.91	0.52
1:1A:2583:A:N7	4:1E:144:ARG:HD2	2.25	0.52
5:1F:140:LEU:HD21	5:1F:170:LEU:HD11	1.92	0.52
7:1H:154:PRO:HB3	7:1H:163:TYR:CE2	2.45	0.52
1:2A:928:G:H1	1:2A:939:C:H42	1.56	0.52
2:2B:95:C:H2'	2:2B:96:U:C6	2.44	0.52
4:2E:134:ILE:HA	4:2E:137:HIS:CD2	2.45	0.52
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.49	0.52
1:1A:1093:A:OP2	1:1A:1154:C:N4	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2297:A:H4'	1:1A:2298:A:O4'	2.10	0.52
1:2A:1232:U:H4'	17:2V:79:VAL:HG22	1.91	0.52
1:2A:160:C:H2'	1:2A:161:G:H8	2.62	0.52
1:2A:1783:G:N1	1:2A:1786:G:OP2	2.42	0.52
1:2A:2282:G:H2'	1:2A:2283:U:H6	1.75	0.52
1:1A:2121:G:H1	1:1A:2210:U:H3	1.58	0.52
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.92	0.52
19:1X:35:THR:HG23	19:1X:37:THR:H	1.75	0.52
2:2B:5:C:H42	2:2B:116:G:H1	1.58	0.52
1:1A:468:A:H1'	1:1A:1245:C:O4'	2.10	0.51
3:1D:68:LYS:HD2	3:1D:70:TRP:CZ2	2.45	0.51
15:1T:16:ARG:NH1	15:1T:18:ASP:OD1	2.43	0.51
25:23:30:ARG:H	25:23:33:GLN:NE2	2.08	0.51
1:2A:1309:G:H2'	1:2A:2035:A:N6	2.25	0.51
1:2A:898:G:H2'	1:2A:899:G:C8	2.44	0.51
5:2F:155:LEU:HD11	5:2F:176:LEU:HD12	1.91	0.51
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.10	0.51
1:1A:552:A:N1	1:1A:2063:A:H2'	2.25	0.51
1:2A:1291:A:OP1	5:2F:38:ARG:NH1	2.42	0.51
1:2A:237:C:O2	30:28:12:LYS:NZ	2.38	0.51
1:2A:647:G:H2'	1:2A:648:C:C6	2.45	0.51
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.44	0.51
7:2H:69:ARG:HG3	7:2H:70:THR:N	2.25	0.51
10:2O:64:ARG:NH1	10:2O:81:ASP:OD1	2.42	0.51
14:2S:10:ARG:HG2	14:2S:13:ARG:NH2	2.26	0.51
27:15:16:ARG:HD2	27:15:20:ARG:NH1	2.26	0.51
1:1A:1064:U:O2'	1:1A:1066:A:H2	1.93	0.51
1:1A:775:G:C6	3:1D:208:LYS:HB2	2.46	0.51
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.93	0.51
7:1H:144:VAL:O	7:1H:148:ILE:HG12	2.10	0.51
1:2A:75:C:H42	1:2A:106:G:H1	1.57	0.51
1:2A:1911:A:OP2	59:2A:3653:HOH:O	2.19	0.51
1:2A:552:A:C2	1:2A:2064:C:H4'	2.46	0.51
1:2A:732:G:N2	1:2A:834:A:H61	2.09	0.51
16:2U:78:THR:O	16:2U:117:GLN:NE2	2.44	0.51
18:2W:18:ARG:HG3	18:2W:76:VAL:HB	1.91	0.51
1:1A:1540:A:H2'	1:1A:1541:A:C8	2.45	0.51
1:1A:1616:A:H2'	1:1A:1617:A:C8	2.45	0.51
22:20:18:ALA:HB3	22:20:20:ARG:HH21	1.75	0.51
23:21:3:LYS:HB2	23:21:61:ARG:NH1	2.25	0.51
1:2A:1084:G:H1	1:2A:1161:C:H42	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1240:C:H2'	1:2A:1241:G:H8	1.74	0.51
1:2A:1894:U:OP1	1:2A:2421:G:O2'	2.28	0.51
5:2F:117:ARG:HH12	11:2P:1:MET:N	2.09	0.51
1:1A:2059:G:O6	59:1A:4167:HOH:O	2.18	0.51
1:1A:286:G:N7	1:1A:447:U:H2'	2.26	0.51
3:1D:9:TYR:CZ	3:1D:13:ARG:HG2	2.46	0.51
21:1Z:110:GLY:HA3	21:1Z:174:VAL:HG11	1.90	0.51
1:2A:1214:G:H1	1:2A:1224:C:H42	1.58	0.51
1:2A:1331:A:N6	1:2A:1356:G:N3	33.77	0.51
1:2A:153:G:H1	1:2A:160:C:H42	1.58	0.51
1:2A:1835:U:O2	3:2D:50:THR:HB	2.10	0.51
1:2A:320:C:OP2	59:2A:3655:HOH:O	2.19	0.51
1:1A:26:G:N2	1:1A:536:G:H1'	2.26	0.51
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.10	0.51
1:2A:2310:G:H2'	1:2A:2311:G:C8	2.41	0.51
1:2A:2554:G:H21	1:2A:2657:C:H5''	1.74	0.51
3:2D:68:LYS:HD2	3:2D:70:TRP:CZ2	2.46	0.51
5:2F:20:LEU:HD13	5:2F:21:ALA:H	1.74	0.51
1:1A:1406:G:OP1	10:1O:49:ARG:NH2	111.55	0.51
1:2A:1361:U:H2'	1:2A:1362:A:C8	2.40	0.51
1:2A:1445:G:H2'	1:2A:1446:G:C8	2.46	0.51
1:2A:1906:A:H2'	1:2A:1907:C:O4'	2.09	0.51
1:2A:786:U:H2'	1:2A:787:G:C8	2.45	0.51
1:1A:1075:G:OP2	12:1Q:128:LYS:NZ	2.40	0.51
1:1A:1520:C:H2'	1:1A:1521:G:C8	2.45	0.51
2:1B:58:A:OP2	59:1B:301:HOH:O	2.20	0.51
1:1A:1828:U:H5'	3:1D:259:THR:CG2	2.41	0.51
14:1S:6:ALA:O	14:1S:10:ARG:HG3	2.09	0.51
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG11	1.93	0.51
1:2A:2658:U:H2'	1:2A:2659:C:C6	2.46	0.51
21:2Z:10:ARG:HB3	21:2Z:36:LYS:HB3	1.93	0.51
1:1A:1691:G:H5''	1:1A:1692:C:H5'	1.92	0.51
1:2A:1735:A:OP2	1:2A:1744:A:N6	2.43	0.51
1:2A:2765:A:N3	31:29:15:LYS:NZ	2.52	0.51
1:2A:309:C:H2'	1:2A:310:C:H6	1.74	0.51
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.76	0.51
1:1A:2783:C:H2'	1:1A:2784:C:C6	2.46	0.51
1:1A:877:G:O2'	11:1P:38:GLN:NE2	2.44	0.51
1:1A:893:U:OP2	59:1A:4168:HOH:O	2.18	0.51
1:2A:2058:G:H2'	1:2A:2059:G:C8	2.46	0.51
1:2A:408:G:OP2	59:2A:3654:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:52:A:N3	2:2B:53:A:N6	2.58	0.51
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.93	0.51
1:1A:1354:G:O6	59:1A:4169:HOH:O	2.19	0.50
1:1A:1873:C:H5'	3:1D:253:GLN:NE2	2.26	0.50
1:1A:286:G:O2'	1:1A:447:U:OP2	2.19	0.50
1:1A:593:A:OP2	59:1A:4171:HOH:O	2.20	0.50
7:1H:124:GLU:HB2	7:1H:132:ARG:HB3	1.92	0.50
1:2A:1403:G:O2'	1:2A:1404:A:H5'	2.11	0.50
1:2A:2278:A:H5''	1:2A:2279:A:C5'	2.41	0.50
6:2G:96:ARG:O	6:2G:99:MET:HB3	2.11	0.50
11:2P:121:LYS:O	11:2P:123:LEU:N	2.45	0.50
16:2U:66:ASN:O	16:2U:70:ARG:HG3	2.11	0.50
1:2A:2376:G:OP1	22:20:55:ARG:HG2	2.11	0.50
1:2A:483:G:C8	29:27:37:LYS:HG2	2.46	0.50
1:2A:2430:U:H5''	30:28:33:ASN:HB2	1.93	0.50
1:2A:1675:G:H2'	1:2A:1676:C:C6	2.45	0.50
1:2A:2272:C:O2'	1:2A:2273:U:H5'	2.12	0.50
1:2A:2611:A:H2'	1:2A:2612:C:C6	2.46	0.50
1:2A:516:A:H2'	1:2A:517:G:O4'	2.11	0.50
7:2H:8:PRO:O	7:2H:69:ARG:NH1	2.44	0.50
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.46	0.50
18:2W:79:GLY:HA3	18:2W:100:THR:HG22	1.93	0.50
1:1A:1559:U:H2'	1:1A:1560:C:C6	2.46	0.50
1:1A:216:A:H3'	1:1A:217:A:C5'	2.41	0.50
1:1A:2831:G:OP2	59:1A:4170:HOH:O	2.19	0.50
1:1A:57:U:H2'	1:1A:58:G:C8	5.64	0.50
1:2A:1856:G:H4'	3:2D:242:ARG:CZ	2.42	0.50
1:2A:898:G:H2'	1:2A:899:G:H8	1.75	0.50
4:2E:52:LEU:O	4:2E:76:ARG:N	2.37	0.50
6:2G:33:ARG:NH1	6:2G:162:THR:OG1	2.45	0.50
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.46	0.50
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.93	0.50
20:2Y:44:ILE:CD1	20:2Y:44:ILE:H	2.21	0.50
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.32	0.50
1:1A:2824:C:H5'	27:15:29:THR:HG21	1.94	0.50
3:1D:126:GLN:NE2	3:1D:127:VAL:H	2.09	0.50
6:1G:16:ARG:HG2	6:1G:16:ARG:NH1	2.22	0.50
1:2A:1210:U:H2'	1:2A:1211:C:C6	2.46	0.50
1:2A:15:G:H2'	1:2A:16:G:H8	1.76	0.50
2:2B:75:G:N1	59:2B:3101:HOH:O	2.25	0.50
5:2F:129:PHE:O	5:2F:132:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:110:THR:HG23	12:2Q:113:GLN:OE1	2.12	0.50
12:2Q:32:TYR:CE1	12:2Q:133:ARG:HG3	2.47	0.50
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.10	0.50
1:1A:2657:C:H2'	1:1A:2658:U:O4'	2.11	0.50
14:1S:3:ARG:C	14:1S:3:ARG:HD3	2.31	0.50
1:2A:2660:U:H2'	1:2A:2661:U:C6	2.47	0.50
1:2A:922:C:H2'	1:2A:923:U:O4'	2.12	0.50
6:2G:43:LEU:HD12	6:2G:45:GLU:HG3	1.93	0.50
31:19:12:ASP:N	31:19:12:ASP:OD2	2.44	0.50
31:19:27:CYS:SG	31:19:28:GLU:N	2.84	0.50
1:1A:1765:G:N7	59:1A:4333:HOH:O	2.34	0.50
1:2A:2698:U:H2'	1:2A:2699:U:O4'	2.12	0.50
1:2A:1302:C:H4'	5:2F:83:PHE:CD1	2.47	0.50
6:2G:35:GLU:HG2	6:2G:36:LYS:NZ	2.27	0.50
26:14:57:GLU:HB3	26:14:58:ARG:HG2	1.94	0.50
1:1A:793:U:O2	1:1A:2035:A:H1'	2.11	0.50
1:1A:2107:U:H2'	1:1A:2108:G:H8	1.76	0.50
1:1A:2254:U:H2'	1:1A:2255:U:C6	2.47	0.50
11:1P:121:LYS:O	11:1P:123:LEU:N	2.44	0.50
18:1W:18:ARG:HG3	18:1W:76:VAL:HB	1.93	0.50
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.46	0.50
1:2A:1278:C:H2'	1:2A:1279:U:H6	1.77	0.50
1:2A:1475:C:H2'	1:2A:1476:U:C6	2.47	0.50
1:2A:1826:U:H2'	1:2A:1827:C:C6	2.47	0.50
1:2A:921:G:O2'	21:2Z:151:HIS:HE1	1.95	0.50
12:2Q:26:TYR:O	12:2Q:67:ARG:NH1	2.43	0.50
27:15:16:ARG:HG2	27:15:16:ARG:NH1	2.26	0.50
1:1A:1066:A:H8	1:1A:1066:A:H3'	1.77	0.50
1:1A:1734:U:O2	1:1A:1746:A:H5'	2.11	0.50
1:1A:222:C:H2'	1:1A:223:U:H6	1.76	0.50
1:1A:2800:C:OP1	4:1E:61:ARG:NH2	2.45	0.50
1:2A:183:A:H5''	1:2A:184:A:O5'	2.11	0.50
1:2A:2315:G:N2	1:2A:2324:C:H5	2.10	0.50
12:1Q:59:ARG:HA	12:1Q:60:ARG:NH2	2.26	0.50
2:1B:7:G:H5'	14:1S:29:PHE:CE2	2.46	0.50
1:2A:2218:U:H1'	1:2A:2219:A:C8	2.47	0.50
1:2A:323:A:H1'	1:2A:342:C:H1'	1.92	0.50
7:2H:44:VAL:HB	7:2H:51:ARG:H	1.77	0.50
23:11:4:VAL:HG22	23:11:11:ARG:HB3	1.93	0.49
1:1A:1098:C:H42	1:1A:1151:G:H1	1.59	0.49
1:2A:1015:C:H2'	1:2A:1016:G:O4'	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1090:A:H5''	1:2A:1092:G:O4'	2.12	0.49
13:2R:55:ALA:HB2	13:2R:79:LEU:HD13	1.93	0.49
1:1A:324:G:OP2	20:1Y:84:ARG:NH2	2.45	0.49
1:2A:2805:G:N2	1:2A:2814:C:H1'	2.28	0.49
1:2A:454:A:H3'	1:2A:455:A:H8	1.78	0.49
7:2H:154:PRO:HB3	7:2H:163:TYR:CE2	2.47	0.49
8:2I:65:ALA:HB1	8:2I:136:VAL:HG11	1.94	0.49
1:1A:206:A:C2	1:1A:223:U:H4'	2.47	0.49
1:1A:935:C:O2'	1:1A:936:A:O4'	2.30	0.49
13:1R:36:THR:HG22	13:1R:37:THR:H	1.76	0.49
18:1W:86:LEU:HD22	18:1W:96:ILE:HD11	1.94	0.49
20:1Y:11:ASP:OD2	20:1Y:97:ARG:NH2	2.44	0.49
1:2A:644:G:N3	1:2A:644:G:H5'	2.27	0.49
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.93	0.49
3:1D:72:LYS:HE3	3:1D:75:ILE:HD12	1.93	0.49
14:1S:61:ASN:O	14:1S:65:VAL:HG23	2.13	0.49
1:2A:2480:A:H2'	1:2A:2481:G:O4'	2.12	0.49
1:2A:2622:U:C4	27:25:3:LYS:HG2	2.47	0.49
6:2G:16:ARG:NH2	6:2G:31:VAL:HG13	2.28	0.49
1:2A:1426:G:O2'	15:2T:122:ASP:OD2	93.34	0.49
1:1A:1067:G:N2	1:1A:1068:U:O4	2.42	0.49
1:1A:1700:A:OP1	59:1A:4172:HOH:O	2.20	0.49
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.44	0.49
2:1B:57:A:H1'	6:1G:29:TRP:HB2	1.93	0.49
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.94	0.49
13:1R:55:ALA:HB2	13:1R:79:LEU:HD13	1.94	0.49
13:1R:51:LEU:HD22	13:1R:66:VAL:HG22	1.94	0.49
1:2A:853:U:OP2	11:2P:41:ARG:NH2	2.45	0.49
1:2A:895:A:H2	25:23:24:LYS:HB3	1.77	0.49
16:2U:97:ASP:OD1	16:2U:101:ARG:HD2	2.13	0.49
1:1A:2205:G:H5'	1:1A:2206:C:OP2	2.12	0.49
1:1A:2880:C:OP1	59:1A:4174:HOH:O	2.20	0.49
1:1A:8:U:H3	1:1A:2640:A:H2	1.61	0.49
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.93	0.49
16:1U:66:ASN:O	16:1U:70:ARG:HG3	2.12	0.49
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.13	0.49
1:2A:1409:G:P	23:21:3:LYS:HG3	2.52	0.49
1:2A:810:A:H5'	3:2D:210:GLY:CA	2.42	0.49
3:2D:227:ASN:O	3:2D:230:ASP:N	2.45	0.49
1:1A:2004:C:H4'	1:1A:2617:C:H4'	1.94	0.49
24:22:32:LEU:HD22	24:22:36:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1240:C:H2'	1:2A:1241:G:C8	2.48	0.49
1:2A:1765:G:H2'	1:2A:1768:G:O6	2.12	0.49
1:2A:2565:U:H2'	1:2A:2566:U:C6	2.46	0.49
1:2A:745:A:H2'	1:2A:746:G:O4'	2.12	0.49
7:2H:54:ARG:HB3	7:2H:65:HIS:CG	2.47	0.49
21:2Z:150:LEU:HD11	21:2Z:172:ALA:HB3	1.94	0.49
1:1A:2481:G:O6	1:1A:2487:A:O2'	2.19	0.49
1:1A:301:A:H2'	1:1A:302:C:C6	2.48	0.49
1:1A:330:G:H21	1:1A:353:A:H62	1.59	0.49
2:1B:50:G:H5''	14:1S:61:ASN:HD22	1.77	0.49
1:2A:118:G:H4'	1:2A:148:A:H5'	1.93	0.49
1:2A:964:G:N2	1:2A:2280:A:OP2	2.46	0.49
1:2A:2554:G:H2'	1:2A:2555:G:C8	2.47	0.49
1:2A:792:A:H2'	1:2A:2623:C:H5''	1.94	0.49
1:2A:861:C:H2'	1:2A:862:C:H6	1.78	0.49
2:2B:32:C:H42	2:2B:50:G:H1	1.60	0.49
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.95	0.49
17:2V:31:ALA:O	17:2V:61:VAL:HG12	2.13	0.49
26:14:63:TYR:CD1	26:14:63:TYR:N	2.81	0.49
1:1A:1231:G:H5''	17:1V:81:TYR:CE1	2.48	0.49
5:1F:129:PHE:CD1	5:1F:163:VAL:HG21	2.47	0.49
14:1S:10:ARG:HH21	14:1S:91:PRO:HB2	1.78	0.49
1:2A:1333:U:O4	13:2R:106:GLY:HA3	2.13	0.49
1:2A:1406:G:OP1	10:2O:49:ARG:NH1	111.47	0.49
1:2A:2389:A:H4'	14:2S:23:ARG:HH11	1.78	0.49
1:2A:2830:A:C2	1:2A:2831:G:C4	3.00	0.49
1:2A:345:A:OP2	5:2F:169:ASN:HB2	2.13	0.49
1:2A:610:U:H2'	1:2A:611:C:C6	2.47	0.49
1:2A:863:C:O2'	1:2A:885:U:H5''	2.13	0.49
26:14:33:VAL:HG12	26:14:34:GLU:H	1.78	0.49
1:1A:1222:C:H2'	1:1A:1223:C:C6	2.47	0.49
1:1A:2535:G:N7	59:1A:4346:HOH:O	2.35	0.49
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.78	0.49
19:1X:11:PRO:HB3	19:1X:92:LEU:HD11	1.95	0.49
1:2A:2309:A:H2'	1:2A:2310:G:O4'	2.13	0.49
1:2A:2333:A:H2'	1:2A:2334:G:O4'	2.12	0.49
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.95	0.49
1:2A:2735:C:H5''	13:2R:1:MET:HE3	1.95	0.49
1:1A:2480:A:O3'	59:1A:4173:HOH:O	2.20	0.48
1:2A:2328:C:H2'	1:2A:2329:G:H8	1.77	0.48
1:2A:2387:A:H8	1:2A:2387:A:OP1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:77:ALA:HA	3:2D:97:TYR:HA	1.95	0.48
10:2O:17:ARG:HG2	10:2O:47:ILE:HG23	1.95	0.48
1:1A:645:A:OP2	11:1P:108:LYS:NZ	2.45	0.48
3:1D:71:ASP:CB	3:1D:103:ARG:HH22	2.26	0.48
1:1A:810:A:H2	3:1D:219:PRO:HG3	1.78	0.48
5:1F:62:ARG:HD3	59:1F:412:HOH:O	2.13	0.48
7:1H:159:GLU:HG3	7:1H:169:VAL:HG11	1.95	0.48
15:1T:65:LYS:HE2	15:1T:67:SER:HB2	1.95	0.48
1:2A:1937:A:H2'	1:2A:1938:U:O4'	2.13	0.48
1:2A:555:C:H4'	1:2A:556:A:H5''	1.94	0.48
1:2A:57:U:H2'	1:2A:58:G:C8	5.46	0.48
1:2A:94:G:H4'	24:22:48:HIS:CD2	2.47	0.48
2:2B:3:C:H2'	2:2B:4:C:C6	2.48	0.48
2:2B:55:U:H1'	6:2G:29:TRP:HE1	1.77	0.48
6:2G:50:ALA:O	6:2G:52:ILE:N	2.46	0.48
1:2A:2760:A:H5'	7:2H:4:ILE:HD12	1.94	0.48
1:1A:1735:A:N6	1:1A:1744:A:H2	2.04	0.48
1:1A:1185:U:OP1	9:1N:25:ARG:NH1	2.46	0.48
1:2A:1000:G:H2'	1:2A:1001:A:H2'	1.94	0.48
1:2A:1536:G:H2'	1:2A:1537:G:H8	1.79	0.48
1:2A:1873:C:H2'	1:2A:1874:C:C6	2.48	0.48
1:2A:2282:G:H2'	1:2A:2283:U:C6	2.48	0.48
1:2A:54:A:H2'	1:2A:55:C:O4'	2.13	0.48
1:2A:919:G:N2	1:2A:950:U:O2	2.46	0.48
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.45	0.48
1:2A:1322:G:O2'	13:2R:24:GLN:HG2	2.13	0.48
14:2S:61:ASN:O	14:2S:65:VAL:HG23	2.13	0.48
16:1U:8:VAL:O	16:1U:12:ARG:HG3	2.13	0.48
1:2A:2588:A:H5'	27:25:3:LYS:HD2	1.95	0.48
1:2A:1759:U:H2'	1:2A:1760:G:H8	1.77	0.48
1:2A:1960:U:OP1	1:2A:2615:U:O2'	2.31	0.48
1:2A:26:G:N2	1:2A:536:G:H1'	2.29	0.48
1:2A:766:C:H2'	1:2A:767:C:C6	2.48	0.48
1:2A:955:A:N3	1:2A:2275:C:O2'	2.39	0.48
1:2A:993:C:H2'	1:2A:994:G:C8	2.49	0.48
3:2D:228:PRO:HD3	3:2D:235:GLY:N	2.29	0.48
6:2G:41:GLN:NE2	6:2G:154:GLY:O	2.45	0.48
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.14	0.48
6:2G:64:THR:HB	6:2G:94:LEU:HD11	1.95	0.48
7:2H:3:ARG:NH1	7:2H:6:ARG:H	2.10	0.48
7:2H:30:LYS:NZ	7:2H:81:GLU:O	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2415:C:O3'	11:2P:77:ARG:NH2	2.47	0.48
1:1A:1643:C:H2'	1:1A:1644:C:H6	1.79	0.48
1:1A:2708:G:OP1	59:1A:4176:HOH:O	2.20	0.48
1:1A:924:A:H2'	1:1A:925:G:C8	5.03	0.48
8:1I:106:GLY:HA2	8:1I:107:VAL:O	2.13	0.48
25:23:12:PRO:HB2	25:23:20:LYS:HG2	1.95	0.48
1:2A:1330:G:N2	1:2A:1373:G:H5''	2.29	0.48
1:2A:1887:G:O2'	1:2A:1906:A:N6	2.42	0.48
4:2E:135:HIS:NE2	59:2E:402:HOH:O	2.35	0.48
1:1A:1093:A:O5'	1:1A:1093:A:H8	2.34	0.48
1:1A:714:G:H5'	1:1A:715:G:OP2	2.13	0.48
1:1A:740:U:OP1	3:1D:59:LYS:NZ	2.46	0.48
1:1A:942:C:H2'	1:1A:943:C:C6	2.49	0.48
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.14	0.48
1:2A:2205:G:H2'	1:2A:2206:C:C6	2.48	0.48
1:2A:2465:G:H1'	59:2A:3701:HOH:O	2.14	0.48
2:2B:72:G:O2'	2:2B:105:A:N6	2.47	0.48
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	1.95	0.48
1:2A:661:A:H8	11:2P:117:GLU:HG3	1.78	0.48
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.13	0.48
24:12:29:LYS:HG2	24:12:57:ILE:HD13	1.95	0.48
1:1A:2405:C:OP2	30:18:30:ARG:NH1	2.46	0.48
1:1A:1833:A:O2'	3:1D:259:THR:HG21	2.14	0.48
1:1A:271:U:H4'	8:1I:50:ARG:NH1	2.28	0.48
1:1A:312:A:N6	1:1A:374:G:O2'	2.43	0.48
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.14	0.48
1:1A:720:G:O2'	5:1F:74:ARG:HD3	2.13	0.48
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.95	0.48
21:1Z:180:VAL:O	21:1Z:183:LEU:HB2	2.14	0.48
1:2A:1673:G:H2'	1:2A:1674:U:C6	2.48	0.48
1:2A:1756:C:H2'	1:2A:1757:C:C6	2.48	0.48
1:2A:2854:G:H2'	1:2A:2855:G:C8	2.49	0.48
1:2A:875:A:N7	1:2A:2259:C:H5'	2.28	0.48
1:2A:2384:G:H2'	1:2A:2385:C:C6	2.49	0.48
1:2A:232:A:C2	1:2A:243:A:C4	3.02	0.48
2:2B:13:A:N1	2:2B:69:G:O2'	2.38	0.48
1:2A:2590:C:H4'	4:2E:134:ILE:HG12	1.95	0.48
11:2P:38:GLN:HG2	11:2P:45:LEU:N	2.29	0.48
12:2Q:58:PHE:CZ	12:2Q:109:VAL:HG21	2.49	0.48
21:2Z:100:VAL:HG21	21:2Z:134:PRO:HG2	1.96	0.48
1:1A:2759:G:O6	1:1A:2767:C:H5''	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:73:GLU:HG3	4:1E:73:GLU:H	1.44	0.48
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.95	0.48
1:2A:1083:C:N4	1:2A:1162:G:H1	2.05	0.48
1:2A:1887:G:C6	1:2A:1888:G:C6	3.02	0.48
10:2O:77:ILE:HB	15:2T:74:ARG:HD3	1.96	0.48
14:2S:67:ARG:O	14:2S:71:ARG:HG3	2.14	0.48
30:28:60:LEU:HA	30:28:60:LEU:HD23	1.74	0.48
1:2A:1423:A:O2'	1:2A:1424:A:H5''	2.14	0.48
1:2A:1643:C:H2'	1:2A:1644:C:H6	1.79	0.48
1:2A:2080:A:O2'	5:2F:69:HIS:HD2	1.95	0.48
1:2A:2715:C:H2'	1:2A:2716:A:O4'	2.14	0.48
1:2A:2845:U:H2'	1:2A:2846:G:C8	2.48	0.48
1:2A:845:G:OP2	1:2A:845:G:H8	3.59	0.48
11:2P:38:GLN:HG2	11:2P:45:LEU:H	1.79	0.48
1:1A:1223:C:H2'	1:1A:1224:C:H6	1.79	0.47
1:1A:1822:G:H5'	3:1D:205:VAL:HG13	1.96	0.47
1:1A:2575:A:C2	1:1A:2658:U:H4'	2.48	0.47
1:1A:2881:G:O2'	1:1A:2882:A:H5'	2.13	0.47
1:1A:26:G:H22	1:1A:536:G:H1'	1.79	0.47
1:1A:661:A:H8	11:1P:117:GLU:HG3	1.79	0.47
11:1P:89:ALA:O	11:1P:121:LYS:NZ	2.39	0.47
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.49	0.47
1:2A:1450:U:H2'	1:2A:1451:U:C6	2.48	0.47
1:2A:1890:G:OP2	1:2A:1890:G:H8	1.97	0.47
1:2A:363:A:H2'	1:2A:364:G:O4'	2.13	0.47
1:2A:56:G:O2'	1:2A:71:A:N1	2.40	0.47
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.49	0.47
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.51	0.47
11:2P:44:GLY:CA	11:2P:45:LEU:HB2	2.44	0.47
14:2S:34:HIS:ND1	14:2S:53:SER:OG	2.45	0.47
15:2T:23:ARG:HG3	15:2T:120:ARG:NH1	2.29	0.47
15:2T:27:THR:HB	15:2T:89:VAL:HG22	1.96	0.47
17:2V:80:GLN:NE2	59:2V:201:HOH:O	2.47	0.47
26:14:40:HIS:O	26:14:43:TYR:N	2.46	0.47
1:1A:2319:G:O2'	1:1A:2321:A:N7	2.46	0.47
1:1A:552:A:C2	1:1A:2063:A:H2'	2.48	0.47
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.95	0.47
1:2A:2077:G:OP2	59:2A:3614:HOH:O	2.20	0.47
1:2A:2347:A:H61	22:20:43:THR:HG22	1.79	0.47
1:2A:2386:G:O2'	1:2A:2388:A:N7	2.35	0.47
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:508:A:O2'	20:2Y:49:VAL:O	2.25	0.47
21:2Z:54:HIS:ND1	21:2Z:101:PRO:HG3	2.29	0.47
1:1A:2358:C:O2'	28:16:21:TYR:OH	2.30	0.47
1:1A:2700:U:H4'	1:1A:2701:C:H5'	1.96	0.47
2:1B:90:A:N7	2:1B:91:C:H1'	2.29	0.47
6:1G:106:LEU:HD12	6:1G:110:ALA:HB3	1.95	0.47
8:1I:79:ILE:HB	8:1I:144:VAL:HG12	1.97	0.47
1:2A:2832:A:OP1	4:2E:113:PHE:HB2	2.14	0.47
1:2A:341:C:OP2	15:2T:39:ARG:NH2	165.85	0.47
2:2B:2:C:H2'	2:2B:3:C:H6	1.80	0.47
14:1S:64:GLU:HB3	26:14:59:PHE:CD1	86.12	0.47
1:1A:1153:U:O2'	1:1A:1154:C:H6	1.97	0.47
1:1A:2330:G:N2	14:1S:3:ARG:HA	2.29	0.47
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.47	0.47
8:1I:40:THR:OG1	8:1I:43:ASN:ND2	2.48	0.47
23:21:82:LEU:HA	23:21:85:LEU:HD12	1.97	0.47
1:2A:346:G:O2'	1:2A:1249:U:N3	2.44	0.47
1:2A:1553:A:H4'	1:2A:1555:A:C5	2.49	0.47
1:2A:2064:C:OP1	1:2A:2789:G:O2'	2.30	0.47
4:2E:1:MET:HE3	4:2E:199:ARG:HD2	1.96	0.47
1:2A:2573:U:H1'	10:2O:23:ARG:HD3	1.97	0.47
1:1A:1409:G:OP2	23:11:3:LYS:HG3	2.14	0.47
1:1A:10:G:H2'	1:1A:11:U:H5''	1.96	0.47
4:1E:143:ASN:HD22	4:1E:147:PRO:CD	2.26	0.47
5:1F:13:SER:HA	5:1F:127:GLU:HG3	1.96	0.47
1:1A:2456:G:OP1	5:1F:74:ARG:NH2	2.47	0.47
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.59	0.47
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.49	0.47
8:1I:6:LEU:HG	8:1I:36:ALA:HA	1.96	0.47
10:1O:103:ALA:HB1	10:1O:105:GLU:HG2	1.96	0.47
20:1Y:28:LYS:HD2	20:1Y:40:GLU:HG3	1.96	0.47
25:23:8:LEU:HD13	25:23:31:LEU:HD23	1.95	0.47
1:2A:1863:U:O2'	1:2A:1990:A:N1	2.40	0.47
1:2A:2813:C:H2'	1:2A:2814:C:C6	2.48	0.47
17:2V:4:ILE:HD12	17:2V:39:LEU:HB3	1.97	0.47
1:1A:1953:A:H2'	1:1A:1954:G:O4'	2.14	0.47
5:1F:102:PRO:HB2	5:1F:105:VAL:HG23	1.95	0.47
12:1Q:60:ARG:CZ	12:1Q:60:ARG:N	2.78	0.47
19:1X:1:MET:HE1	24:12:22:GLU:HA	1.97	0.47
1:2A:1104:G:H3'	1:2A:1105:U:C6	2.50	0.47
1:2A:2331:A:H2'	1:2A:2331:A:N3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:61:LEU:HA	3:2D:61:LEU:HD12	1.80	0.47
1:1A:2478:C:OP2	59:1A:4182:HOH:O	2.20	0.47
4:1E:144:ARG:HB3	4:1E:145:LYS:H	1.41	0.47
7:1H:5:GLY:HA2	7:1H:69:ARG:HB3	1.96	0.47
22:20:19:LYS:HD2	22:20:19:LYS:N	2.29	0.47
1:2A:1475:C:H2'	1:2A:1476:U:H6	1.78	0.47
1:2A:1549:C:H2'	1:2A:1550:C:H6	1.80	0.47
1:2A:514:G:N7	18:2W:49:LYS:NZ	2.60	0.47
8:2I:77:LEU:HD11	8:2I:101:LEU:HB2	1.95	0.47
1:1A:1490:A:H5''	1:1A:1491:C:H5	1.80	0.47
1:1A:1528:G:O6	1:1A:1552:A:N6	2.47	0.47
1:1A:485:A:H2'	1:1A:486:C:O4'	2.15	0.47
3:1D:10:THR:OG1	3:1D:13:ARG:HB2	2.14	0.47
6:1G:3:LEU:HD13	26:14:25:TYR:CZ	2.49	0.47
15:1T:115:ARG:NH2	59:1T:3105:HOH:O	2.47	0.47
16:1U:108:GLU:O	16:1U:112:ARG:HG2	2.15	0.47
1:2A:1136:G:N2	1:2A:1146:U:H1'	2.30	0.47
1:2A:1156:A:N3	1:2A:1157:G:H1'	2.30	0.47
1:2A:2548:U:H2'	1:2A:2549:C:C6	2.49	0.47
1:2A:53:G:H2'	1:2A:54:A:H8	1.79	0.47
1:2A:610:U:H1'	5:2F:90:PHE:CG	2.49	0.47
14:2S:26:LEU:HD22	14:2S:87:PHE:CE1	2.49	0.47
14:2S:10:ARG:NH2	14:2S:91:PRO:O	2.46	0.47
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.15	0.47
1:1A:209:A:N1	1:1A:253:A:O2'	2.43	0.47
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.39	0.47
21:1Z:7:ALA:O	21:1Z:62:PRO:HD3	2.14	0.47
1:1A:1755:U:H2'	1:1A:1756:C:C6	2.50	0.47
1:1A:2257:G:H2'	1:1A:2258:A:C8	2.50	0.47
1:1A:1992:A:C4	3:1D:241:PRO:HD3	2.50	0.47
7:1H:167:GLU:HA	7:1H:168:PRO:HD3	1.77	0.47
14:1S:39:ILE:HB	14:1S:49:VAL:HG13	1.96	0.47
17:1V:69:LYS:NZ	59:1V:301:HOH:O	2.46	0.47
2:2B:24:G:N2	2:2B:27:C:N3	2.56	0.47
3:2D:108:PRO:HB2	3:2D:111:LEU:HB2	1.95	0.47
4:2E:24:THR:HG22	4:2E:186:GLY:O	2.15	0.47
1:1A:1451:U:H2'	1:1A:1452:C:C6	2.50	0.47
1:1A:26:G:C2	1:1A:536:G:N3	2.83	0.47
1:1A:2404:A:H5''	11:1P:63:PRO:HB3	1.96	0.47
1:2A:1820:C:H5''	1:2A:1821:A:OP1	2.15	0.47
1:2A:2421:G:C2	1:2A:2422:A:H1'	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:552:A:O2'	1:2A:553:A:H5'	2.15	0.47
1:2A:55:C:H2'	1:2A:56:G:O4'	2.14	0.47
9:2N:94:HIS:HB3	9:2N:97:ARG:HD3	1.97	0.47
17:2V:43:GLU:N	17:2V:43:GLU:OE2	2.48	0.47
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	1.97	0.47
1:1A:1159:G:H2'	1:1A:1160:G:H8	1.80	0.46
1:1A:2208:G:H4'	1:1A:2209:C:OP1	2.14	0.46
1:1A:558:U:H2'	1:1A:559:C:C6	2.50	0.46
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.27	0.46
6:1G:118:ARG:O	6:1G:181:ARG:HB3	2.16	0.46
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.43	0.46
26:24:58:ARG:HB3	26:24:59:PHE:CD1	2.51	0.46
1:2A:1104:G:H3'	1:2A:1105:U:H6	1.80	0.46
1:2A:1198:C:OP1	16:2U:92:ARG:NH1	2.48	0.46
1:2A:1676:C:H2'	59:2A:3662:HOH:O	2.14	0.46
1:2A:1756:C:H2'	1:2A:1757:C:H6	1.81	0.46
1:2A:241:C:OP2	30:28:5:LYS:NZ	2.28	0.46
1:2A:2690:A:H4'	4:2E:165:VAL:HG11	1.97	0.46
1:2A:468:A:H5''	1:2A:469:C:OP1	2.15	0.46
1:2A:947:C:H2'	1:2A:948:C:C6	2.49	0.46
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.96	0.46
1:1A:1989:G:OP1	59:1A:4177:HOH:O	2.20	0.46
1:1A:777:C:OP2	59:1A:4184:HOH:O	2.21	0.46
59:1A:4279:HOH:O	12:1Q:75:THR:HG23	2.15	0.46
13:1R:13:HIS:CE1	13:1R:16:HIS:HB2	2.50	0.46
59:1A:4116:HOH:O	15:1T:100:TYR:HB2	2.14	0.46
1:2A:2027:C:O5'	1:2A:2027:C:H6	1.99	0.46
1:2A:29:G:C5	1:2A:30:C:C4	3.02	0.46
1:2A:385:U:O2'	1:2A:386:G:H5'	2.15	0.46
1:2A:810:A:N1	1:2A:1819:A:O2'	2.39	0.46
6:2G:48:GLU:O	6:2G:51:ARG:HG3	2.16	0.46
10:2O:23:ARG:HG3	10:2O:24:VAL:N	2.30	0.46
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.96	0.46
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CE1	2.50	0.46
26:14:58:ARG:O	26:14:61:ARG:N	2.47	0.46
1:1A:2588:A:OP2	27:15:3:LYS:NZ	2.41	0.46
4:1E:9:VAL:HG13	4:1E:25:VAL:O	2.15	0.46
1:2A:1314:A:OP1	59:2A:3658:HOH:O	2.20	0.46
1:2A:1698:A:OP1	13:2R:8:ARG:NH1	2.47	0.46
1:2A:200:G:H2'	1:2A:201:A:O4'	2.16	0.46
1:2A:2037:U:H2'	1:2A:2038:U:C6	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2670:G:P	7:2H:158:HIS:HE2	2.38	0.46
1:2A:608:A:N1	1:2A:855:G:O2'	2.38	0.46
1:2A:670:A:H2'	1:2A:671:G:O4'	2.14	0.46
3:2D:159:ALA:HB1	3:2D:198:ASN:HB3	1.97	0.46
8:2I:69:LYS:HG3	8:2I:138:ILE:HG12	1.98	0.46
26:14:9:LEU:HA	26:14:9:LEU:HD23	1.78	0.46
28:16:11:LEU:HB3	28:16:49:HIS:HB3	1.98	0.46
1:1A:1221:A:O2'	1:1A:1222:C:O4'	2.24	0.46
1:1A:1279:U:H2'	1:1A:1280:G:O4'	2.15	0.46
1:1A:864:G:H5'	1:1A:885:U:OP1	2.16	0.46
1:2A:1346:A:H2	1:2A:1671:G:N3	2.14	0.46
1:2A:251:C:H2'	1:2A:252:C:O4'	2.15	0.46
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.97	0.46
1:1A:1821:A:H5'	3:1D:206:LEU:HD12	1.97	0.46
1:1A:266:C:H3'	59:1A:4154:HOH:O	2.14	0.46
1:1A:713:U:O2	30:18:2:PRO:HD2	2.16	0.46
12:1Q:32:TYR:CZ	12:1Q:133:ARG:HG3	2.50	0.46
1:1A:351:U:H4'	20:1Y:68:HIS:CD2	2.51	0.46
21:1Z:40:ASP:HB3	21:1Z:43:GLU:HB2	1.96	0.46
31:29:17:ILE:HG12	31:29:26:ILE:HD11	1.97	0.46
1:2A:263:G:H2'	1:2A:264:U:C6	2.50	0.46
2:2B:19:G:H2'	2:2B:20:C:O4'	2.15	0.46
6:2G:173:LEU:HB3	6:2G:178:PHE:CG	2.49	0.46
8:2I:102:SER:O	8:2I:106:GLY:N	2.42	0.46
1:1A:1248:A:H2	1:1A:1286:A:H62	1.62	0.46
1:1A:1821:A:H3'	1:1A:1822:G:H8	1.81	0.46
1:1A:2811:A:H5''	1:1A:2812:G:C8	2.50	0.46
1:1A:517:G:H2'	1:1A:518:G:O4'	2.16	0.46
2:1B:48:A:H2'	2:1B:49:C:C6	2.51	0.46
12:1Q:60:ARG:CZ	12:1Q:60:ARG:H	2.28	0.46
14:1S:15:ARG:HE	14:1S:88:ASP:CG	2.19	0.46
26:24:57:GLU:HA	26:24:58:ARG:HA	1.58	0.46
1:2A:105:U:H2'	1:2A:106:G:C8	2.51	0.46
1:2A:1072:A:C6	1:2A:1171:A:C4	3.04	0.46
1:2A:754:C:N4	1:2A:769:G:H1	2.13	0.46
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.34	0.46
23:11:86:SER:N	23:11:89:GLU:OE2	2.34	0.46
3:1D:26:LYS:HD3	3:1D:83:GLU:OE2	2.15	0.46
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.97	0.46
6:1G:137:GLU:HB3	6:1G:139:LEU:HD12	1.96	0.46
24:22:64:LEU:O	24:22:68:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:98:ARG:NH2	26:24:1:MET:SD	2.89	0.46
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.98	0.46
1:2A:1116:G:H1	1:2A:1124:C:N4	15.01	0.46
1:2A:1439:U:H2'	1:2A:1440:A:O4'	2.16	0.46
1:2A:1845:A:OP1	1:2A:1845:A:H8	1.98	0.46
1:2A:209:A:O4'	1:2A:221:A:H1'	2.16	0.46
1:2A:228:G:H1'	1:2A:258:A:N1	40.08	0.46
10:2O:120:GLU:HB2	15:2T:68:TYR:HE2	1.79	0.46
11:2P:136:GLU:HG2	11:2P:137:LYS:N	2.31	0.46
1:2A:319:C:O3'	20:2Y:95:LYS:NZ	2.48	0.46
21:2Z:10:ARG:NH1	21:2Z:26:GLY:H	2.13	0.46
30:18:30:ARG:HA	30:18:30:ARG:HD3	1.45	0.46
1:1A:830:A:N6	3:1D:229:VAL:HG11	2.31	0.46
3:1D:27:THR:O	3:1D:27:THR:OG1	2.32	0.46
23:21:56:GLN:HA	23:21:56:GLN:HE21	1.81	0.46
26:24:62:ARG:O	26:24:64:GLY:N	2.44	0.46
1:2A:1108:G:OP2	1:2A:1108:G:H8	1.99	0.46
1:2A:1113:G:O2'	1:2A:1141:A:O2'	2.34	0.46
1:2A:22:G:H2'	1:2A:23:G:C8	3.26	0.46
1:2A:2760:A:H3'	1:2A:2761:A:H8	1.81	0.46
1:2A:592:G:H2'	1:2A:2051:A:C5	2.51	0.46
6:2G:107:LEU:HA	6:2G:111:LEU:HD22	1.98	0.46
6:2G:115:ARG:H	6:2G:136:ARG:HH21	1.64	0.46
6:2G:179:PRO:HG3	26:24:43:TYR:CZ	2.51	0.46
1:1A:1158:U:H2'	1:1A:1159:G:H8	1.80	0.46
1:1A:1520:C:H2'	1:1A:1521:G:H8	1.80	0.46
1:1A:1820:C:H2'	1:1A:1821:A:C5	2.50	0.46
1:1A:214:G:N2	1:1A:216:A:H62	2.14	0.46
1:1A:2210:U:H2'	1:1A:2211:G:H8	1.81	0.46
1:1A:2226:G:H5'	1:1A:2227:G:N7	2.31	0.46
1:1A:1096:G:H4'	1:1A:2764:C:H4'	1.97	0.46
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.16	0.46
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.51	0.46
21:1Z:101:PRO:O	21:1Z:102:LEU:HD12	2.16	0.46
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.72	0.46
1:2A:137:G:H2'	1:2A:138:A:H8	10.00	0.46
1:2A:1474:G:H2'	1:2A:1475:C:C6	2.51	0.46
1:2A:2706:C:H2'	1:2A:2707:U:C6	2.51	0.46
1:2A:2878:G:H2'	1:2A:2879:C:O4'	2.16	0.46
1:2A:857:U:H2'	11:2P:21:ARG:HA	1.97	0.46
2:2B:16:G:H1	2:2B:68:C:N4	2.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:54:G:H21	6:2G:29:TRP:HZ2	1.62	0.46
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.51	0.46
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.19	0.46
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.81	0.46
1:2A:1013:U:H4'	25:23:14:GLY:O	2.16	0.46
1:2A:2325:C:H2'	1:2A:2326:G:H8	1.81	0.46
1:2A:235:G:H4'	1:2A:412:G:C5	2.51	0.46
1:1A:1343:C:N4	1:1A:1344:G:C6	2.84	0.45
1:1A:1757:C:OP2	59:1A:4179:HOH:O	2.20	0.45
1:1A:2523:C:H2'	1:1A:2524:G:O4'	2.16	0.45
1:1A:2568:G:H2'	1:1A:2569:C:C6	2.52	0.45
1:1A:2043:U:O2'	1:1A:2628:C:H5'	2.16	0.45
1:1A:57:U:H2'	1:1A:58:G:H8	5.62	0.45
1:1A:671:G:H2'	1:1A:672:G:O4'	2.16	0.45
9:1N:114:ARG:HD2	59:1N:302:HOH:O	2.16	0.45
19:1X:57:LEU:CD1	19:1X:78:LYS:HB2	2.46	0.45
20:1Y:8:LYS:HD3	20:1Y:97:ARG:NH1	2.31	0.45
1:2A:2115:G:N2	1:2A:2217:C:H1'	2.31	0.45
1:2A:885:U:H1'	1:2A:1235:G:H1'	1.97	0.45
4:2E:144:ARG:HB3	4:2E:145:LYS:H	1.49	0.45
6:2G:44:GLY:N	6:2G:88:ILE:O	2.50	0.45
1:2A:594:A:OP2	17:2V:78:LYS:HE2	2.16	0.45
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.54	0.45
21:2Z:134:PRO:C	21:2Z:136:PHE:H	2.20	0.45
1:1A:1349:C:H2'	1:1A:1350:C:H6	2.57	0.45
1:1A:800:C:H2'	1:1A:801:C:H6	1.80	0.45
1:1A:62:A:O3'	19:1X:71:GLY:HA3	2.16	0.45
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.97	0.45
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG13	1.98	0.45
26:24:16:CYS:SG	26:24:17:GLY:N	2.89	0.45
1:2A:242:G:N7	30:28:5:LYS:HE2	2.31	0.45
1:2A:1459:G:N2	1:2A:1633:C:O2	2.46	0.45
1:2A:2049:U:H2'	1:2A:2050:G:O4'	2.16	0.45
1:2A:5:A:H2	1:2A:6:G:N7	2.14	0.45
1:2A:810:A:H5'	3:2D:210:GLY:HA3	1.98	0.45
6:2G:136:ARG:C	6:2G:136:ARG:HD2	2.36	0.45
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.97	0.45
1:1A:138:A:H8	1:1A:1453:C:O2'	1.96	0.45
1:1A:1633:C:H2'	1:1A:1634:C:H6	1.81	0.45
1:1A:2249:G:H2'	1:1A:2249:G:N3	2.31	0.45
1:1A:2803:C:H2'	1:1A:2804:G:C8	2.50	0.45

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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	0.45
3:1D:67:PHE:HB3	3:1D:153:ALA:H	1.81	0.45
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.97	0.45
30:28:54:GLU:O	30:28:58:ILE:HG13	2.16	0.45
1:2A:1399:A:H2'	1:2A:1400:G:O4'	2.15	0.45
1:2A:2338:A:H2'	1:2A:2339:A:C8	2.51	0.45
1:2A:2358:C:H2'	1:2A:2359:U:C6	2.52	0.45
1:2A:2563:U:H2'	1:2A:2565:U:H5''	1.99	0.45
4:2E:119:ARG:HD2	4:2E:120:TRP:CE2	2.52	0.45
1:2A:1200:A:H5''	16:2U:55:ARG:HD3	1.97	0.45
19:2X:21:PHE:HZ	19:2X:92:LEU:HD12	1.80	0.45
1:1A:1475:C:H2'	1:1A:1476:U:C6	2.51	0.45
1:1A:1735:A:OP2	59:1A:4185:HOH:O	2.21	0.45
1:1A:2375:C:H2'	1:1A:2376:G:O4'	2.16	0.45
1:1A:346:G:C8	5:1F:171:PRO:HG3	2.51	0.45
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.98	0.45
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.98	0.45
1:1A:1200:A:OP1	16:1U:55:ARG:HD3	2.16	0.45
1:2A:1309:G:H8	1:2A:1309:G:O5'	2.00	0.45
1:2A:1649:C:OP2	59:2A:3659:HOH:O	2.21	0.45
1:2A:212:G:H2'	1:2A:213:A:O4'	2.16	0.45
1:2A:243:A:C6	1:2A:244:A:C5	3.04	0.45
1:2A:2483:G:H2'	1:2A:2486:C:H42	1.82	0.45
1:2A:651:A:C6	1:2A:661:A:C8	3.05	0.45
1:2A:984:G:N3	1:2A:1235:G:H4'	2.32	0.45
2:2B:31:C:H42	2:2B:51:G:H1	1.64	0.45
8:2I:14:ASP:O	8:2I:17:GLN:HB3	2.15	0.45
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.17	0.45
14:2S:65:VAL:O	14:2S:68:GLN:HB2	2.16	0.45
1:1A:1369:G:C4	1:1A:1373:G:O6	2.69	0.45
1:1A:1386:U:OP1	1:1A:1442:U:N3	2.44	0.45
1:1A:1652:C:H4'	1:1A:1653:A:O5'	2.16	0.45
1:1A:2588:A:H5''	1:1A:2589:G:H5'	1.97	0.45
1:1A:909:A:H2'	1:1A:910:G:C8	2.51	0.45
6:1G:128:ARG:HB2	6:1G:128:ARG:HE	1.65	0.45
20:1Y:20:TYR:CE1	20:1Y:43:ASN:HA	2.52	0.45
11:2P:65:ARG:HG3	30:28:25:MET:HG3	1.98	0.45
1:2A:1449:C:O2'	1:2A:1450:U:H5'	2.16	0.45
1:2A:2339:A:H2'	1:2A:2340:G:C8	2.52	0.45
1:2A:820:A:H2'	1:2A:820:A:N3	2.30	0.45
3:2D:275:LYS:HA	3:2D:275:LYS:HD2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:98:ARG:H	6:2G:98:ARG:HG2	1.40	0.45
7:2H:71:LEU:HD22	7:2H:71:LEU:HA	1.84	0.45
13:2R:21:TYR:OH	13:2R:43:GLU:HG2	2.16	0.45
24:12:1:MET:N	24:12:52:ASP:OD2	2.46	0.45
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.71	0.45
24:12:32:LEU:HD12	24:12:57:ILE:HD12	1.98	0.45
1:1A:2626:U:H2'	1:1A:2627:C:C6	2.51	0.45
30:28:14:VAL:HG23	30:28:24:ALA:HB2	1.98	0.45
1:2A:1051:C:C2	1:2A:1182:G:N2	2.84	0.45
1:2A:2685:G:H2'	1:2A:2686:A:C8	2.52	0.45
6:2G:56:ALA:N	6:2G:153:ARG:HH21	2.13	0.45
8:2I:45:LYS:O	8:2I:49:ALA:N	2.38	0.45
1:1A:1275:C:H2'	1:1A:1276:G:C8	2.52	0.45
1:1A:266:C:OP2	59:1A:4181:HOH:O	2.20	0.45
1:1A:604:G:H2'	1:1A:605:G:C8	2.52	0.45
1:1A:909:A:H2'	1:1A:910:G:H8	1.81	0.45
1:1A:956:A:H2'	12:1Q:9:TYR:OH	2.17	0.45
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	1.98	0.45
1:2A:1095:A:H2'	1:2A:1096:G:H8	1.82	0.45
1:2A:1873:C:H2'	1:2A:1874:C:H6	1.82	0.45
1:2A:1897:A:H2'	1:2A:1898:A:C8	2.50	0.45
1:2A:2224:U:H2'	1:2A:2225:C:C6	2.51	0.45
1:2A:2489:A:OP2	31:29:2:LYS:NZ	2.44	0.45
1:2A:2704:A:H2'	1:2A:2705:G:C8	2.52	0.45
1:2A:275:C:H2'	1:2A:276:G:O4'	2.17	0.45
1:2A:910:G:C6	1:2A:911:C:N4	2.85	0.45
1:1A:2473:U:H1'	1:1A:2502:U:O4	2.17	0.45
1:1A:334:A:C6	1:1A:351:U:C4	3.04	0.45
1:1A:503:A:C6	1:1A:505:A:C6	3.04	0.45
1:1A:755:U:H2'	1:1A:756:G:C8	2.51	0.45
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.31	0.45
1:1A:1001:A:H5'	12:1Q:76:LYS:HG3	1.98	0.45
1:1A:2829:A:OP2	13:1R:2:ARG:NH2	2.50	0.45
20:1Y:12:THR:HG1	20:1Y:26:LYS:HZ3	1.58	0.45
1:2A:73:G:H4'	24:22:55:ARG:CZ	2.47	0.45
1:2A:1166:C:H2'	1:2A:1167:G:O4'	2.17	0.45
1:2A:1245:C:H2'	1:2A:1246:C:C6	2.82	0.45
1:2A:1333:U:C2	1:2A:1372:C:O2	2.70	0.45
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.52	0.45
1:2A:769:G:H2'	1:2A:770:U:O4'	2.17	0.45
1:2A:903:C:OP2	22:20:77:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:910:G:N2	1:2A:958:U:C2	2.84	0.45
3:2D:134:ARG:HD2	3:2D:135:PHE:CE1	2.52	0.45
11:2P:8:PRO:HB2	11:2P:12:ALA:HB3	1.99	0.45
21:2Z:108:PRO:HG3	21:2Z:141:VAL:HB	1.98	0.45
26:14:68:ARG:HD2	26:14:68:ARG:HA	1.73	0.45
30:18:62:LEU:HB3	30:18:65:GLU:CG	2.46	0.45
1:1A:2578:G:H2'	1:1A:2579:C:C6	2.52	0.45
1:1A:800:C:H2'	1:1A:801:C:C6	2.51	0.45
1:1A:1067:G:N7	9:1N:66:LYS:HE2	2.32	0.45
1:1A:1176:G:H21	9:1N:73:THR:CG2	2.29	0.45
24:22:9:GLN:OE1	24:22:56:GLN:HG2	2.15	0.45
1:2A:1039:C:OP2	16:2U:54:LYS:NZ	2.37	0.45
1:2A:1604:A:H8	59:2A:4206:HOH:O	2.00	0.45
1:2A:1176:G:O6	1:2A:2061:C:H1'	2.16	0.45
1:2A:2854:G:H2'	1:2A:2855:G:H8	1.82	0.45
1:2A:353:A:HO2'	1:2A:354:A:H8	1.65	0.45
1:2A:972:G:H2'	1:2A:973:G:O4'	2.15	0.45
3:2D:13:ARG:HA	3:2D:13:ARG:HD2	1.71	0.45
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.17	0.45
1:2A:623:C:O2'	5:2F:104:LYS:NZ	2.50	0.45
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.99	0.45
1:2A:2428:C:OP1	11:2P:65:ARG:NH2	2.50	0.45
14:2S:87:PHE:CZ	14:2S:102:ALA:HB2	2.52	0.45
1:2A:508:A:O4'	20:2Y:48:ALA:HB1	2.17	0.45
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.32	0.45
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.32	0.45
1:1A:258:A:C6	1:1A:259:A:C6	3.92	0.45
1:1A:2802:A:H5''	1:1A:2803:C:H5'	1.99	0.45
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.82	0.45
4:1E:145:LYS:NZ	59:1E:402:HOH:O	2.28	0.45
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.99	0.45
14:1S:18:ILE:HD13	14:1S:88:ASP:HA	1.99	0.45
1:2A:2397:C:H2'	1:2A:2398:U:C6	2.52	0.45
1:2A:2637:C:H2'	1:2A:2638:G:O4'	2.17	0.45
1:2A:338:G:H2'	1:2A:339:C:C6	2.52	0.45
1:2A:440:C:O2'	1:2A:441:A:H5'	2.17	0.45
1:2A:503:A:C6	1:2A:505:A:C6	3.05	0.45
1:2A:509:C:H2'	1:2A:510:C:C6	2.52	0.45
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.98	0.45
11:2P:21:ARG:HA	11:2P:21:ARG:HD3	1.72	0.45
1:1A:1066:A:H8	1:1A:1067:G:H5''	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1531:A:H2'	1:1A:1532:G:C8	2.52	0.44
1:1A:1633:C:H2'	1:1A:1634:C:C6	2.52	0.44
1:1A:2678:C:N3	7:1H:110:SER:OG	2.42	0.44
2:1B:33:G:C2	2:1B:50:G:C2	3.04	0.44
3:1D:89:SER:HB2	3:1D:201:HIS:CD2	2.52	0.44
6:1G:43:LEU:HD12	6:1G:43:LEU:HA	1.87	0.44
30:28:34:TRP:CE2	30:28:35:GLN:HB2	2.52	0.44
1:2A:1317:A:OP1	59:2A:3660:HOH:O	2.21	0.44
1:2A:170:A:N3	1:2A:459:C:O2'	2.46	0.44
1:2A:1828:U:H5'	3:2D:259:THR:CG2	2.46	0.44
1:2A:2421:G:N2	1:2A:2422:A:H1'	2.32	0.44
1:2A:29:G:H2'	1:2A:30:C:C6	2.51	0.44
3:2D:71:ASP:HB3	3:2D:103:ARG:NH2	2.32	0.44
12:2Q:59:ARG:HD3	12:2Q:60:ARG:HG2	1.99	0.44
14:2S:71:ARG:NE	14:2S:107:GLU:OE1	2.48	0.44
21:2Z:127:LYS:O	21:2Z:128:VAL:HG12	2.17	0.44
1:1A:1262:C:H6	1:1A:1262:C:H5''	1.82	0.44
1:1A:1319:A:N3	1:1A:1342:C:H1'	2.32	0.44
1:1A:2206:C:O2'	1:1A:2207:G:H5'	2.17	0.44
1:1A:2800:C:O2'	1:1A:2818:A:N3	2.44	0.44
1:1A:2881:G:OP2	59:1A:4188:HOH:O	2.21	0.44
4:1E:116:VAL:HG11	4:1E:138:PRO:HB3	1.99	0.44
4:1E:54:GLN:CA	4:1E:54:GLN:HE21	2.30	0.44
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.98	0.44
14:1S:63:THR:OG1	14:1S:64:GLU:N	4.46	0.44
16:1U:46:ALA:O	16:1U:50:ARG:HB2	2.17	0.44
21:1Z:102:LEU:HD13	21:1Z:123:ASP:HA	1.99	0.44
26:24:61:ARG:HD2	26:24:61:ARG:HA	1.70	0.44
1:2A:324:G:N2	1:2A:339:C:O2	2.42	0.44
7:2H:126:PRO:HD2	7:2H:130:ARG:O	2.17	0.44
11:2P:101:VAL:HG12	11:2P:102:ARG:HD3	1.98	0.44
14:2S:11:LYS:O	14:2S:15:ARG:HG3	2.17	0.44
21:2Z:125:LEU:HB3	21:2Z:165:VAL:HG13	1.99	0.44
21:2Z:7:ALA:HB3	21:2Z:61:LEU:HD12	1.99	0.44
25:13:3:ARG:HB2	25:13:60:GLU:HG2	1.99	0.44
1:1A:35:G:N3	1:1A:475:G:O2'	2.49	0.44
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.35	0.44
14:1S:46:VAL:HG12	14:1S:48:LEU:HD12	1.99	0.44
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.98	0.44
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.53	0.44
21:1Z:152:ALA:O	21:1Z:155:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:105:U:H2'	1:2A:106:G:H8	1.81	0.44
1:2A:1076:G:H21	31:29:36:GLN:HE22	1.65	0.44
1:2A:1869:G:C8	1:2A:1948:A:H1'	2.52	0.44
1:2A:2752:A:C6	1:2A:2776:A:C8	3.05	0.44
1:2A:27:A:O2'	1:2A:605:G:H5'	2.18	0.44
6:2G:43:LEU:HB3	6:2G:44:GLY:H	1.56	0.44
14:2S:67:ARG:HG2	14:2S:71:ARG:NH2	2.33	0.44
16:2U:81:HIS:O	16:2U:84:LYS:HB3	2.17	0.44
1:1A:2395:G:OP2	22:10:55:ARG:NH1	2.51	0.44
1:1A:852:C:O2	1:1A:2455:G:O2'	2.33	0.44
2:1B:89:G:H2'	2:1B:90:A:C8	2.53	0.44
12:1Q:84:GLY:O	12:1Q:85:LYS:HB2	2.18	0.44
1:2A:80:G:N2	1:2A:100:A:OP2	2.45	0.44
1:2A:1052:C:H5''	9:2N:35:ARG:NH1	2.33	0.44
1:2A:1056:G:OP2	16:2U:66:ASN:ND2	2.51	0.44
1:2A:1198:C:H2'	1:2A:1199:G:O4'	2.18	0.44
1:2A:1308:U:C4	1:2A:1309:G:C6	3.04	0.44
1:2A:2313:G:N1	1:2A:2326:G:C6	2.86	0.44
1:2A:238:G:C6	1:2A:239:A:C6	3.06	0.44
1:2A:894:G:H2'	1:2A:895:A:C8	2.52	0.44
2:2B:80:U:H2'	2:2B:81:G:C8	2.52	0.44
4:2E:181:LEU:HA	4:2E:181:LEU:HD12	1.80	0.44
4:2E:2:LYS:HA	4:2E:84:PHE:CD1	2.52	0.44
5:2F:192:LEU:HD22	5:2F:194:MET:HG3	1.99	0.44
9:2N:104:LYS:HA	9:2N:107:LEU:HD12	1.98	0.44
12:2Q:27:VAL:HG12	12:2Q:29:PHE:H	1.82	0.44
14:2S:23:ARG:NH2	14:2S:84:GLN:HB3	2.33	0.44
16:2U:86:ALA:O	17:2V:49:THR:HG23	2.17	0.44
21:2Z:110:GLY:HA3	21:2Z:174:VAL:HG11	1.98	0.44
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.86	0.44
22:10:27:GLU:HG3	22:10:68:GLU:HA	2.00	0.44
1:1A:2022:A:H2'	1:1A:2023:G:C8	2.52	0.44
1:1A:1844:G:H4'	3:1D:51:VAL:HG21	2.00	0.44
11:1P:46:LYS:HB3	11:1P:46:LYS:HE3	1.68	0.44
1:2A:1920:G:N3	1:2A:1920:G:H2'	2.33	0.44
1:2A:2381:G:C6	1:2A:2382:G:C6	3.05	0.44
1:2A:250:A:H2'	1:2A:251:C:O4'	2.17	0.44
1:2A:870:A:H2'	1:2A:871:C:C6	2.95	0.44
6:2G:109:VAL:HG21	26:24:14:ILE:HD13	2.00	0.44
12:2Q:30:GLY:O	12:2Q:134:ARG:HD3	2.18	0.44
1:1A:1404:A:N3	1:1A:1404:A:H5'	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2085:C:H2'	1:1A:2086:C:C6	2.53	0.44
1:1A:222:C:H2'	1:1A:223:U:C6	2.52	0.44
1:1A:241:C:OP2	30:18:5:LYS:NZ	2.42	0.44
1:1A:820:A:H2'	1:1A:820:A:N3	2.33	0.44
1:1A:874:U:H4'	1:1A:877:G:N1	2.32	0.44
9:1N:67:LEU:HB3	9:1N:88:GLU:HG3	1.98	0.44
12:1Q:51:ARG:O	12:1Q:55:VAL:HG13	2.18	0.44
1:2A:91:C:H2'	1:2A:92:G:O4'	2.17	0.44
2:2B:40:U:C2	2:2B:43:C:OP2	2.70	0.44
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.98	0.44
14:2S:15:ARG:HB3	14:2S:19:LYS:NZ	2.33	0.44
1:2A:62:A:O3'	19:2X:71:GLY:HA3	2.17	0.44
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.82	0.44
26:14:68:ARG:HH21	26:14:68:ARG:HA	1.83	0.44
1:1A:491:A:P	29:17:34:ARG:HH21	2.41	0.44
1:1A:1674:U:H2'	1:1A:1675:G:C8	2.53	0.44
1:1A:1783:G:N7	59:1A:4359:HOH:O	2.36	0.44
1:1A:1820:C:H5''	1:1A:1821:A:OP1	2.18	0.44
1:1A:228:G:H1'	1:1A:258:A:N1	39.91	0.44
1:1A:2720:G:OP2	59:1A:4192:HOH:O	2.21	0.44
1:1A:2811:A:N3	1:1A:2903:U:H1'	2.33	0.44
1:1A:733:C:H5''	29:17:2:LYS:HE2	1.99	0.44
1:1A:842:C:H2'	1:1A:843:C:C6	2.53	0.44
20:1Y:12:THR:OG1	20:1Y:26:LYS:NZ	2.30	0.44
1:2A:2419:U:H2'	1:2A:2420:G:H8	1.83	0.44
11:2P:95:VAL:HG13	11:2P:125:VAL:HB	2.00	0.44
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.99	0.44
10:2O:104:ARG:HH12	15:2T:43:GLN:HE22	1.66	0.44
21:2Z:26:GLY:HA3	21:2Z:86:VAL:HG23	2.00	0.44
1:1A:2302:U:H2'	1:1A:2303:C:C6	2.53	0.44
1:1A:2855:G:H2'	1:1A:2856:U:O4'	2.18	0.44
6:1G:138:GLN:HE21	6:1G:153:ARG:HH21	1.65	0.44
7:1H:56:SER:OG	7:1H:58:GLU:HG2	2.18	0.44
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.99	0.44
18:1W:79:GLY:HA3	18:1W:100:THR:HG22	1.98	0.44
1:2A:154:C:N4	1:2A:159:G:H1	2.16	0.44
1:2A:2303:C:O2'	1:2A:2304:C:H5'	2.17	0.44
1:2A:2044:G:H5'	1:2A:2628:C:H4'	1.98	0.44
1:2A:2638:G:N2	1:2A:2789:G:OP2	2.51	0.44
1:2A:2848:G:H5'	13:2R:46:GLY:CA	2.43	0.44
6:2G:36:LYS:HE2	6:2G:95:ARG:HH21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:88:LEU:HD23	7:2H:165:ALA:HA	2.00	0.44
15:2T:116:ALA:HB1	15:2T:121:ILE:HD11	1.99	0.44
1:1A:238:G:P	30:18:13:ARG:HH22	2.39	0.44
1:1A:1992:A:OP2	3:1D:242:ARG:NH2	2.51	0.44
1:1A:2331:A:N3	1:1A:2331:A:H2'	2.33	0.44
1:1A:732:G:H4'	1:1A:732:G:OP2	2.18	0.44
1:1A:894:G:H2'	1:1A:895:A:C8	2.53	0.44
8:1I:44:LEU:HD12	8:1I:44:LEU:HA	1.88	0.44
20:1Y:68:HIS:CE1	20:1Y:70:SER:HB3	2.52	0.44
21:1Z:14:LYS:HA	21:1Z:15:PRO:HD3	1.85	0.44
24:22:31:GLU:O	24:22:35:LEU:HD23	2.18	0.44
1:2A:1406:G:H2'	1:2A:1407:C:H6	2.20	0.44
1:2A:1967:U:H2'	1:2A:1968:C:C6	2.52	0.44
1:2A:2494:C:H2'	1:2A:2495:G:O4'	2.18	0.44
1:2A:2641:G:H2'	1:2A:2642:G:H8	1.83	0.44
1:2A:635:G:H2'	1:2A:636:U:O2	2.18	0.44
7:2H:11:VAL:HG13	7:2H:15:VAL:HG22	1.99	0.44
11:2P:46:LYS:HE2	11:2P:46:LYS:HB3	1.87	0.44
1:1A:28:U:H2'	1:1A:29:G:C8	2.53	0.43
1:1A:864:G:H4'	1:1A:884:C:O3'	2.18	0.43
1:1A:867:A:H2'	1:1A:990:G:H5''	2.00	0.43
2:1B:24:G:N7	2:1B:56:G:H2'	2.33	0.43
8:1I:46:ALA:O	8:1I:50:ARG:HG2	2.17	0.43
17:1V:1:MET:HB2	17:1V:43:GLU:OE2	2.18	0.43
18:1W:18:ARG:NH1	18:1W:76:VAL:O	2.51	0.43
1:2A:1098:C:H2'	1:2A:1099:A:H5'	2.00	0.43
1:2A:1272:G:H2'	1:2A:1273:G:H5'	2.59	0.43
1:2A:2325:C:H2'	1:2A:2326:G:C8	2.53	0.43
1:2A:2362:G:HO2'	1:2A:2363:A:H8	1.66	0.43
1:2A:2763:G:C6	7:2H:2:SER:HB2	2.53	0.43
1:2A:457:U:H6	1:2A:457:U:O5'	2.01	0.43
1:2A:82:A:N1	1:2A:96:G:O2'	2.45	0.43
1:2A:861:C:H2'	1:2A:862:C:C6	2.53	0.43
1:2A:955:A:O2'	1:2A:957:C:OP2	9.31	0.43
5:2F:53:THR:CG2	5:2F:55:GLY:H	2.28	0.43
9:2N:43:THR:HA	9:2N:44:PRO:HD3	1.86	0.43
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.18	0.43
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.17	0.43
1:1A:1153:U:O2'	1:1A:1154:C:O5'	2.27	0.43
1:1A:1220:G:H1'	1:1A:1221:A:C5'	2.48	0.43
1:1A:2604:U:H2'	1:1A:2605:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1685:U:H4'	1:1A:2710:C:H4'	2.00	0.43
1:1A:2898:C:OP2	59:1A:4183:HOH:O	2.20	0.43
1:1A:353:A:HO2'	1:1A:354:A:H8	1.62	0.43
1:1A:363:A:H2'	1:1A:364:G:O4'	2.18	0.43
1:1A:77:G:H1'	1:1A:78:G:H8	4.44	0.43
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.17	0.43
14:1S:59:LYS:HD2	14:1S:60:GLY:N	2.32	0.43
15:1T:54:ARG:HA	15:1T:59:THR:HG22	1.99	0.43
1:2A:1114:A:H4'	1:2A:1115:A:O5'	2.18	0.43
1:2A:1488:G:H1	1:2A:1594:C:H42	1.65	0.43
1:2A:1673:G:H2'	1:2A:1674:U:H6	1.82	0.43
1:2A:1958:A:C8	1:2A:1960:U:H2'	2.53	0.43
1:2A:209:A:H5'	1:2A:221:A:O2'	2.19	0.43
1:2A:955:A:N1	1:2A:2288:G:H1'	2.33	0.43
1:2A:2537:G:H2'	1:2A:2538:C:C6	2.53	0.43
1:2A:598:U:H2'	1:2A:599:G:C8	2.53	0.43
1:2A:1833:A:O2'	3:2D:259:THR:HG21	2.18	0.43
11:2P:45:LEU:HD22	11:2P:45:LEU:HA	1.86	0.43
12:2Q:64:ILE:HG12	12:2Q:64:ILE:O	2.17	0.43
19:2X:31:HIS:CD2	19:2X:33:LYS:HB2	2.53	0.43
1:1A:1474:G:H2'	1:1A:1475:C:C6	2.53	0.43
1:1A:914:U:C4	1:1A:915:G:N7	2.86	0.43
1:2A:1565:U:H2'	1:2A:1566:G:O4'	2.18	0.43
1:2A:1792:A:H2'	59:2A:4372:HOH:O	2.18	0.43
1:2A:2386:G:N2	1:2A:2389:A:OP2	2.41	0.43
1:2A:2419:U:H2'	1:2A:2420:G:C8	2.53	0.43
1:2A:2509:C:H3'	59:2A:3615:HOH:O	2.18	0.43
1:2A:2043:U:O2'	1:2A:2628:C:H5'	2.18	0.43
1:2A:1508:C:H4'	1:2A:2714:C:H5'	2.01	0.43
1:2A:320:C:H2'	1:2A:321:G:O4'	2.19	0.43
1:2A:517:G:H2'	1:2A:518:G:O4'	2.19	0.43
1:2A:874:U:H4'	1:2A:877:G:N1	2.33	0.43
5:2F:149:ASP:OD1	5:2F:149:ASP:N	2.46	0.43
6:2G:138:GLN:HG2	6:2G:144:ILE:HG21	1.98	0.43
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	2.00	0.43
6:2G:43:LEU:HA	6:2G:43:LEU:HD12	1.79	0.43
8:2I:44:LEU:HD12	8:2I:44:LEU:HA	1.72	0.43
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.99	0.43
21:2Z:134:PRO:HG3	21:2Z:161:VAL:HG11	2.01	0.43
1:1A:603:C:H2'	1:1A:604:G:C8	2.53	0.43
12:1Q:34:LEU:HD11	12:1Q:129:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:21:82:LEU:O	23:21:85:LEU:HD12	2.19	0.43
1:2A:73:G:H4'	24:22:55:ARG:NH1	2.33	0.43
30:28:30:ARG:HA	30:28:30:ARG:HD3	1.51	0.43
1:2A:1349:C:H2'	1:2A:1350:C:C6	3.14	0.43
1:2A:1361:U:C2	1:2A:1362:A:C8	3.06	0.43
1:2A:1808:U:H2'	1:2A:1814:A:N6	2.34	0.43
1:2A:66:G:H2'	1:2A:67:C:O4'	2.19	0.43
1:2A:491:A:N3	1:2A:729:C:H1'	2.33	0.43
1:2A:1741:G:N7	3:2D:14:ARG:NH2	2.66	0.43
9:2N:120:LEU:HD22	9:2N:122:VAL:HG23	2.01	0.43
14:2S:48:LEU:HD23	14:2S:82:ILE:HD11	2.01	0.43
25:13:23:LEU:HD13	25:13:50:VAL:HG11	2.00	0.43
1:1A:224:C:H2'	1:1A:225:C:C6	2.53	0.43
1:1A:661:A:OP1	11:1P:133:SER:OG	2.31	0.43
2:1B:90:A:C5	2:1B:91:C:H1'	2.54	0.43
11:1P:121:LYS:HG2	11:1P:122:PRO:HD2	1.99	0.43
11:1P:3:LEU:HD12	11:1P:3:LEU:HA	1.78	0.43
15:1T:122:ASP:O	15:1T:126:ALA:N	2.52	0.43
20:1Y:65:ALA:HA	20:1Y:66:PRO:HD3	1.88	0.43
1:2A:142:C:H2'	1:2A:143:C:H6	1.83	0.43
1:2A:1663:A:H5'	59:2A:3707:HOH:O	2.18	0.43
1:2A:665:C:O2'	1:2A:2361:C:OP1	2.20	0.43
1:2A:2547:G:H2'	1:2A:2548:U:O4'	2.18	0.43
1:2A:2549:C:H2'	1:2A:2550:C:H6	1.84	0.43
1:2A:1685:U:O2'	1:2A:2710:C:H4'	2.19	0.43
1:2A:2785:C:H2'	1:2A:2786:C:H6	1.83	0.43
1:2A:2898:C:H2'	1:2A:2899:G:O4'	2.19	0.43
1:2A:310:C:H2'	1:2A:311:C:H6	1.84	0.43
1:2A:822:G:H4'	1:2A:823:A:O5'	2.19	0.43
7:2H:27:LYS:NZ	7:2H:32:GLU:HG3	2.33	0.43
11:2P:101:VAL:HA	11:2P:106:LEU:O	2.19	0.43
11:2P:83:VAL:HG23	11:2P:87:ASP:HB2	2.00	0.43
16:2U:52:ARG:HA	16:2U:55:ARG:HG3	2.00	0.43
21:1Z:5:LEU:O	21:1Z:59:LEU:HA	2.19	0.43
25:23:11:SER:HA	25:23:31:LEU:HD21	1.99	0.43
25:23:52:HIS:CD2	25:23:53:LEU:HG	2.53	0.43
1:2A:1095:A:H2'	1:2A:1096:G:C8	2.54	0.43
1:2A:2578:G:H2'	1:2A:2579:C:C6	2.53	0.43
1:2A:2582:C:H5''	1:2A:2583:A:H5''	2.01	0.43
1:2A:25:G:C6	1:2A:26:G:N1	2.86	0.43
1:2A:509:C:H2'	1:2A:510:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:777:C:OP1	59:2A:3663:HOH:O	2.22	0.43
1:2A:806:G:H2'	1:2A:807:A:O4'	2.18	0.43
1:2A:856:U:OP1	59:2A:3661:HOH:O	2.21	0.43
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.45	0.43
18:2W:6:ILE:HA	18:2W:103:ILE:O	2.19	0.43
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.48	0.43
31:19:14:CYS:HA	31:19:27:CYS:HB2	1.99	0.43
1:1A:1223:C:H2'	1:1A:1224:C:C6	2.54	0.43
1:1A:1526:G:C6	1:1A:1527:U:N3	2.86	0.43
1:1A:1845:A:H8	1:1A:1845:A:OP1	2.01	0.43
1:1A:195:A:H2'	1:1A:196:C:O4'	2.17	0.43
1:1A:2296:C:OP2	28:16:6:ARG:NH1	2.51	0.43
1:1A:2323:U:O2'	6:1G:40:ASN:ND2	2.52	0.43
1:1A:2753:A:OP1	31:19:22:ARG:NH2	2.32	0.43
1:1A:2778:G:N3	1:1A:2778:G:H2'	2.33	0.43
1:1A:482:A:H5''	59:1A:5612:HOH:O	2.17	0.43
1:1A:509:C:H2'	1:1A:510:C:H6	1.83	0.43
1:1A:717:C:H2'	1:1A:718:C:C6	2.53	0.43
1:1A:935:C:O2'	1:1A:936:A:O5'	2.37	0.43
14:1S:39:ILE:HD11	14:1S:110:LEU:HD21	2.01	0.43
14:1S:11:LYS:O	14:1S:15:ARG:HG3	2.17	0.43
14:1S:33:LYS:HB3	14:1S:34:HIS:CD2	2.54	0.43
14:1S:48:LEU:HD23	14:1S:82:ILE:HD11	2.00	0.43
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.66	0.43
30:28:32:LEU:O	30:28:36:LYS:HE3	2.19	0.43
1:2A:1224:C:H2'	1:2A:1225:C:H6	1.82	0.43
1:2A:1252:C:H2'	1:2A:1253:G:H8	2.77	0.43
1:2A:1402:U:H2'	1:2A:1403:G:O4'	2.18	0.43
1:2A:398:G:O2'	1:2A:399:U:OP2	2.36	0.43
1:2A:531:A:H4'	1:2A:532:G:O5'	3.96	0.43
3:2D:108:PRO:HD2	3:2D:111:LEU:HG	1.99	0.43
4:2E:128:SER:OG	4:2E:129:HIS:N	2.48	0.43
6:2G:19:LEU:HG	6:2G:175:LEU:HD22	2.00	0.43
1:1A:1220:G:H1'	1:1A:1221:A:H5'	2.00	0.43
1:1A:1714:A:H4'	1:1A:1715:A:O5'	2.18	0.43
1:1A:2473:U:H2'	1:1A:2474:C:C6	2.53	0.43
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	2.00	0.43
7:1H:60:ARG:HE	7:1H:60:ARG:HB3	1.47	0.43
8:1I:110:ASP:HA	8:1I:111:PRO:HD2	1.76	0.43
13:1R:111:LEU:N	59:1R:302:HOH:O	2.38	0.43
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1020:G:C2	1:2A:1035:A:C8	3.07	0.43
1:2A:2239:G:C5	1:2A:2240:C:C4	3.06	0.43
1:2A:2370:C:H2'	1:2A:2371:A:O4'	2.18	0.43
1:2A:724:C:H2'	1:2A:725:C:C6	2.54	0.43
1:2A:991:G:H2'	1:2A:992:G:H8	1.84	0.43
2:2B:61:G:C6	2:2B:62:C:C4	3.07	0.43
6:2G:3:LEU:H	6:2G:3:LEU:HD23	1.84	0.43
1:2A:2756:G:N2	7:2H:143:GLN:OE1	2.51	0.43
10:2O:24:VAL:HA	10:2O:39:ILE:HG22	2.00	0.43
22:10:10:THR:HB	22:10:11:ARG:H	1.34	0.43
23:11:18:ILE:HG12	23:11:37:ILE:HG23	2.01	0.43
23:11:23:LYS:HB3	23:11:29:GLY:HA3	2.01	0.43
24:12:2:LYS:HG2	24:12:2:LYS:H	1.62	0.43
30:18:61:LEU:O	30:18:63:PRO:HD3	2.18	0.43
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.42	0.43
20:1Y:19:LYS:HE2	20:1Y:20:TYR:CE1	2.54	0.43
20:1Y:81:LYS:HE2	20:1Y:81:LYS:HB3	1.71	0.43
22:20:82:ARG:HA	22:20:83:PRO:HD3	1.70	0.43
1:2A:2077:G:N2	27:25:5:PRO:HA	2.34	0.43
1:2A:1627:G:H2'	1:2A:1628:C:O4'	2.19	0.43
1:2A:1877:A:H4'	1:2A:1878:A:OP2	2.19	0.43
1:2A:2590:C:C4'	4:2E:134:ILE:HG12	2.49	0.43
1:2A:2700:U:P	1:2A:2731:G:H22	2.42	0.43
1:2A:335:G:H4'	1:2A:354:A:C2	2.54	0.43
1:2A:587:C:OP1	17:2V:82:ARG:NH2	2.43	0.43
1:2A:846:A:OP1	1:2A:846:A:H8	2.02	0.43
1:2A:955:A:C6	1:2A:956:A:C6	3.06	0.43
25:13:7:LYS:HA	25:13:33:GLN:O	2.19	0.43
1:1A:1099:A:H62	1:1A:1150:U:H3	1.67	0.43
1:1A:1313:A:C2	1:1A:2034:A:C4	3.07	0.43
1:1A:1383:G:O2'	1:1A:1438:A:N1	2.40	0.43
1:1A:1789:A:H1'	1:1A:2722:A:C2	2.54	0.43
1:1A:309:C:H2'	1:1A:310:C:C6	2.54	0.43
1:1A:44:C:OP2	1:1A:203:G:H2'	2.19	0.43
2:1B:66:A:H61	2:1B:108:U:H2'	1.84	0.43
5:1F:116:ASP:O	5:1F:120:GLU:HG2	2.19	0.43
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.53	0.43
7:1H:7:LEU:HA	7:1H:8:PRO:HD3	1.91	0.43
11:1P:76:LYS:HE2	11:1P:76:LYS:HB3	1.52	0.43
30:28:8:LYS:HB3	30:28:12:LYS:HE3	2.01	0.43
1:2A:1004:A:H5'	1:2A:2468:U:H4'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2226:G:H3'	1:2A:2227:G:H8	1.77	0.43
2:2B:45:A:O2'	2:2B:46:A:OP1	2.36	0.43
5:2F:9:ILE:HA	5:2F:10:PRO:HD3	1.90	0.43
16:2U:19:LYS:HA	16:2U:22:LYS:HZ3	1.84	0.43
19:2X:31:HIS:HA	19:2X:32:PRO:HD3	1.91	0.43
21:2Z:91:LEU:HD13	21:2Z:91:LEU:HA	1.82	0.43
1:1A:1092:G:H1'	1:1A:1155:G:N2	2.34	0.42
1:1A:172:C:H2'	1:1A:173:U:H6	1.83	0.42
1:1A:2376:G:N7	30:18:39:LYS:NZ	2.50	0.42
1:1A:315:C:C2	1:1A:372:G:C2	3.07	0.42
1:1A:663:U:H2'	1:1A:664:C:H6	1.83	0.42
1:1A:77:G:H1'	1:1A:78:G:C8	4.94	0.42
1:1A:943:C:H2'	1:1A:944:A:O4'	2.19	0.42
1:1A:359:C:O2'	20:1Y:35:TYR:OH	2.31	0.42
12:1Q:61:GLY:HA2	21:1Z:177:PRO:HB3	2.01	0.42
1:2A:1682:C:H2'	1:2A:1683:A:C8	2.54	0.42
1:2A:40:C:H2'	1:2A:41:G:H8	1.83	0.42
1:2A:920:G:H2'	1:2A:921:G:O4'	2.19	0.42
2:2B:2:C:H2'	2:2B:3:C:C6	2.53	0.42
1:2A:830:A:O4'	3:2D:227:ASN:ND2	2.52	0.42
1:2A:345:A:H3'	5:2F:169:ASN:HD21	1.84	0.42
7:2H:3:ARG:HB3	7:2H:3:ARG:HH11	1.84	0.42
7:2H:3:ARG:HH12	7:2H:6:ARG:N	2.14	0.42
15:2T:50:ILE:HA	15:2T:99:LEU:HD12	2.01	0.42
21:2Z:102:LEU:HD11	21:2Z:124:ILE:HB	2.00	0.42
21:2Z:70:LEU:HA	21:2Z:70:LEU:HD23	1.80	0.42
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.49	0.42
1:1A:2482:C:H2'	1:1A:2483:G:O4'	2.19	0.42
2:1B:28:C:H2'	2:1B:29:A:O4'	2.19	0.42
1:1A:469:C:H4'	5:1F:49:ALA:HB2	2.01	0.42
19:1X:57:LEU:HD12	19:1X:78:LYS:HB2	2.00	0.42
23:21:73:LEU:HA	23:21:73:LEU:HD23	1.85	0.42
1:2A:2567:C:H2'	1:2A:2568:G:O4'	2.18	0.42
1:2A:1789:A:H4'	1:2A:2727:C:O4'	2.19	0.42
1:2A:2815:G:C6	1:2A:2816:G:C6	3.07	0.42
1:2A:2896:U:H2'	1:2A:2897:C:C6	2.54	0.42
1:2A:786:U:H2'	1:2A:787:G:H8	1.83	0.42
4:2E:175:VAL:O	4:2E:177:PRO:HD3	2.19	0.42
1:2A:2323:U:O2'	6:2G:40:ASN:ND2	2.53	0.42
9:2N:34:LEU:HD12	9:2N:34:LEU:HA	1.87	0.42
1:2A:1973:A:N3	10:2O:22:ILE:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:44:PHE:O	21:2Z:48:PHE:N	2.40	0.42
6:1G:66:GLN:HG3	26:14:1:MET:HE2	2.00	0.42
1:1A:2093:G:N2	59:1A:4572:HOH:O	2.52	0.42
7:1H:44:VAL:HG12	7:1H:46:GLU:HG3	2.01	0.42
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	2.01	0.42
11:1P:100:LEU:HA	11:1P:100:LEU:HD23	1.80	0.42
13:1R:26:LYS:HE2	13:1R:70:LEU:O	2.18	0.42
1:2A:323:A:H1'	1:2A:342:C:C1'	2.50	0.42
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	2.00	0.42
4:2E:78:LEU:O	4:2E:79:ARG:HG2	2.18	0.42
5:2F:152:GLU:HA	5:2F:190:GLU:OE2	2.20	0.42
6:2G:106:LEU:O	6:2G:111:LEU:HD22	2.19	0.42
7:2H:27:LYS:HZ1	7:2H:32:GLU:HG3	1.84	0.42
11:2P:62:LEU:O	30:28:13:ARG:NH1	2.52	0.42
2:2B:75:G:O3'	21:2Z:10:ARG:NH2	2.52	0.42
28:16:40:CYS:HA	28:16:41:PRO:HD3	1.79	0.42
1:1A:1220:G:H1'	1:1A:1221:A:O5'	2.19	0.42
1:1A:230:G:C8	30:18:5:LYS:HG2	2.55	0.42
1:1A:2723:U:OP1	1:1A:2726:G:H4'	2.19	0.42
3:1D:38:LYS:HA	3:1D:38:LYS:HD2	1.81	0.42
13:1R:72:ASP:OD2	13:1R:75:LEU:HB2	2.19	0.42
20:1Y:52:SER:O	20:1Y:54:LYS:N	2.53	0.42
1:2A:104:C:H2'	1:2A:105:U:C6	2.54	0.42
1:2A:1189:G:H2'	1:2A:1190:C:H6	3.26	0.42
1:2A:1776:G:H2'	1:2A:1777:G:H8	1.84	0.42
1:2A:1857:C:OP2	3:2D:222:ARG:NH1	2.52	0.42
1:2A:1910:A:C6	1:2A:1911:A:C6	3.07	0.42
1:2A:2313:G:C2	1:2A:2314:G:C8	3.07	0.42
1:2A:2516:G:H2'	1:2A:2587:G:O6	2.19	0.42
3:2D:146:GLU:HB2	3:2D:189:CYS:HB3	2.01	0.42
6:2G:97:ASP:O	6:2G:101:ILE:HG13	2.19	0.42
7:2H:90:LYS:NZ	7:2H:159:GLU:OE2	2.45	0.42
1:2A:437:G:C5	11:2P:72:PRO:HB3	2.54	0.42
14:2S:84:GLN:CA	14:2S:111:GLU:HB2	2.43	0.42
14:2S:23:ARG:HB3	14:2S:23:ARG:HE	1.60	0.42
1:1A:1065:A:N1	1:1A:1185:U:O2'	2.46	0.42
1:1A:1399:A:H2'	1:1A:1400:G:O4'	2.19	0.42
1:1A:815:G:H5'	1:1A:1424:A:N6	2.35	0.42
1:1A:1902:C:H2'	1:1A:1903:C:H6	1.83	0.42
1:1A:2217:C:OP2	59:1A:4193:HOH:O	2.22	0.42
1:1A:2347:A:H61	22:10:43:THR:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:230:G:O2'	1:1A:242:G:O6	2.29	0.42
1:1A:52:G:O2'	29:17:35:ARG:HD3	2.18	0.42
4:1E:28:ALA:HB3	4:1E:93:VAL:CG1	2.50	0.42
5:1F:129:PHE:O	5:1F:132:VAL:HG13	2.20	0.42
8:1I:127:VAL:HA	8:1I:140:LEU:O	2.19	0.42
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.89	0.42
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.68	0.42
1:2A:1023:G:H2'	1:2A:1024:G:O4'	2.20	0.42
1:2A:1060:G:O2'	1:2A:1061:G:H5'	2.20	0.42
1:2A:1077:A:H2	1:2A:1167:G:H22	1.65	0.42
1:2A:10:G:H2'	1:2A:11:U:H5''	1.99	0.42
2:2B:95:C:H2'	2:2B:96:U:H6	1.83	0.42
5:2F:47:GLY:HA3	5:2F:95:ARG:O	2.20	0.42
6:2G:137:GLU:HG2	6:2G:152:LEU:HD23	2.01	0.42
9:2N:39:ARG:HA	9:2N:40:PRO:HD3	1.92	0.42
9:2N:69:GLN:O	9:2N:71:ILE:HG12	2.20	0.42
11:2P:121:LYS:HE2	11:2P:123:LEU:HD12	2.00	0.42
26:14:48:ARG:O	26:14:50:VAL:N	2.53	0.42
27:15:55:ARG:HH12	27:15:57:VAL:HG13	1.84	0.42
1:1A:1463:G:H1'	1:1A:1627:G:N2	2.35	0.42
1:1A:2283:U:H5''	1:1A:2284:A:OP1	2.20	0.42
1:1A:671:G:H8	1:1A:671:G:O5'	2.02	0.42
1:1A:830:A:C8	1:1A:838:G:C5	3.08	0.42
3:1D:264:LYS:HA	3:1D:265:PRO:HD3	1.93	0.42
3:1D:71:ASP:HB3	3:1D:103:ARG:HH22	1.84	0.42
5:1F:7:TYR:CD1	5:1F:24:LEU:HB2	2.54	0.42
24:22:4:SER:HA	24:22:7:ARG:NH1	2.35	0.42
1:2A:1094:C:H1'	1:2A:1158:U:O2'	2.20	0.42
1:2A:1354:G:HO2'	1:2A:1656:C:HO2'	1.61	0.42
1:2A:227:U:H2'	1:2A:228:G:O4'	2.20	0.42
1:2A:2551:C:H2'	1:2A:2552:A:O4'	2.20	0.42
19:2X:50:LYS:O	19:2X:84:ALA:N	2.53	0.42
20:2Y:43:ASN:ND2	20:2Y:65:ALA:HB3	2.34	0.42
28:16:21:TYR:CE2	28:16:38:LYS:HG2	2.54	0.42
30:18:39:LYS:HA	30:18:42:ARG:NH1	2.35	0.42
1:1A:2086:C:H2'	1:1A:2087:C:C6	2.55	0.42
1:1A:2862:C:H2'	1:1A:2863:G:C8	2.54	0.42
6:1G:103:LEU:HA	6:1G:103:LEU:HD23	1.75	0.42
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.20	0.42
9:1N:131:GLN:O	9:1N:134:ARG:HG2	2.20	0.42
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:85:LEU:HG	11:1P:115:LEU:O	2.20	0.42
20:1Y:38:ILE:HD13	20:1Y:66:PRO:HA	2.00	0.42
25:23:7:LYS:HB2	25:23:34:GLU:HG2	2.02	0.42
1:2A:1056:G:C6	1:2A:1058:C:C4	3.08	0.42
1:2A:1089:G:H21	1:2A:1156:A:H2	1.68	0.42
1:2A:2273:U:H4'	1:2A:2339:A:C2	2.55	0.42
1:2A:644:G:H8	1:2A:646:G:O6	2.02	0.42
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.20	0.42
19:2X:36:LYS:HA	19:2X:39:ILE:HD12	2.00	0.42
24:12:70:GLN:C	24:12:70:GLN:HE21	2.23	0.42
1:1A:1275:C:H2'	1:1A:1276:G:H8	1.83	0.42
1:1A:1639:G:H2'	1:1A:1640:G:O4'	2.20	0.42
1:1A:1869:G:C8	1:1A:1948:A:H1'	2.54	0.42
1:1A:2304:C:H2'	1:1A:2305:C:C6	2.55	0.42
1:1A:2388:A:H2'	1:1A:2389:A:C8	2.55	0.42
1:1A:2641:G:H2'	1:1A:2642:G:C8	2.54	0.42
1:1A:2888:C:OP2	59:1A:4190:HOH:O	2.21	0.42
1:1A:330:G:N2	1:1A:332:G:H3'	2.34	0.42
1:1A:341:C:H2'	1:1A:341:C:O2	2.85	0.42
1:1A:552:A:O2'	1:1A:553:A:H5'	2.20	0.42
1:1A:601:G:H2'	1:1A:602:C:C6	2.55	0.42
2:1B:50:G:H5''	14:1S:61:ASN:ND2	2.34	0.42
2:1B:95:C:H2'	2:1B:96:U:C6	2.54	0.42
3:1D:213:ARG:HA	3:1D:213:ARG:HD2	1.74	0.42
5:1F:110:LEU:HD23	5:1F:110:LEU:HA	1.86	0.42
5:1F:18:ARG:HG2	5:1F:19:GLU:H	1.85	0.42
7:1H:130:ARG:HH12	7:1H:132:ARG:NH2	2.17	0.42
16:1U:17:ILE:HG23	16:1U:39:LEU:HD12	2.02	0.42
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	2.01	0.42
1:2A:2759:G:O6	1:2A:2767:C:H5''	2.20	0.42
1:2A:303:C:H2'	1:2A:304:G:O4'	2.19	0.42
1:2A:713:U:O2	30:28:2:PRO:HD2	2.20	0.42
1:2A:909:A:H2'	1:2A:910:G:C8	2.54	0.42
9:2N:138:LEU:HB3	9:2N:140:VAL:HG13	2.02	0.42
1:2A:2505:G:O2'	12:2Q:80:GLU:HA	2.20	0.42
20:2Y:54:LYS:O	20:2Y:56:PRO:HD3	2.20	0.42
1:1A:1032:G:O2'	1:1A:1045:A:N3	2.48	0.42
1:1A:6:G:H2'	1:1A:7:A:O4'	2.19	0.42
7:1H:83:TYR:CZ	7:1H:138:LYS:HD2	2.54	0.42
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	2.02	0.42
16:1U:52:ARG:HH11	16:1U:52:ARG:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1W:78:GLU:OE1	18:1W:99:ARG:NH1	2.52	0.42
1:2A:108:A:H4'	24:22:69:ARG:NH1	2.34	0.42
1:2A:1101:G:H4'	1:2A:1131:A:H8	1.84	0.42
1:2A:865:A:C4	1:2A:1233:A:C2	3.08	0.42
1:2A:1280:G:C6	1:2A:1281:G:N1	2.87	0.42
1:2A:1494:G:H1'	1:2A:1573:A:N1	2.34	0.42
1:2A:1652:C:H4'	1:2A:1653:A:O5'	2.19	0.42
1:2A:530:G:O3'	1:2A:531:A:H8	2.02	0.42
1:2A:839:A:OP2	1:2A:2092:A:O2'	2.37	0.42
1:2A:981:U:H2'	1:2A:982:G:O4'	2.19	0.42
2:2B:6:C:H42	2:2B:115:G:H1	1.67	0.42
2:2B:78:A:H2'	2:2B:79:C:O4'	2.20	0.42
8:2I:26:ALA:HA	8:2I:30:LEU:HB2	2.00	0.42
8:2I:57:ARG:O	8:2I:61:ARG:HG2	2.20	0.42
14:2S:63:THR:OG1	14:2S:64:GLU:N	3.33	0.42
21:2Z:75:ASN:HB2	21:2Z:85:HIS:HB3	2.01	0.42
29:17:5:TRP:NE1	29:17:7:PRO:HG3	2.35	0.42
1:1A:2842:G:H4'	1:1A:2843:G:OP2	2.19	0.42
1:1A:770:U:H2'	1:1A:771:G:O4'	2.20	0.42
3:1D:221:VAL:HG22	3:1D:226:MET:CE	2.50	0.42
3:1D:69:ARG:C	3:1D:71:ASP:H	2.23	0.42
7:1H:126:PRO:HB2	7:1H:127:GLU:H	1.63	0.42
24:22:1:MET:SD	24:22:56:GLN:NE2	2.93	0.42
1:2A:195:A:H2'	1:2A:196:C:O4'	2.20	0.42
1:2A:196:C:H2'	1:2A:197:C:C6	2.55	0.42
1:2A:2503:U:H2'	1:2A:2504:U:H6	1.84	0.42
1:2A:264:U:H2'	1:2A:265:C:C6	2.55	0.42
1:2A:1781:C:HO2'	1:2A:2870:G:HO2'	1.62	0.42
2:2B:54:G:N2	2:2B:55:U:O2	2.53	0.42
6:2G:125:PHE:O	6:2G:127:GLY:N	2.53	0.42
7:2H:11:VAL:HA	7:2H:12:PRO:HD2	1.85	0.42
9:2N:94:HIS:O	9:2N:97:ARG:HB2	2.20	0.42
16:2U:69:CYS:HB3	16:2U:74:LEU:O	2.20	0.42
17:2V:24:LYS:HA	17:2V:92:THR:OG1	2.20	0.42
21:2Z:8:TYR:HD1	21:2Z:62:PRO:HG3	1.84	0.42
1:1A:1187:A:C4	1:1A:1189:G:C8	3.08	0.41
1:1A:152:C:OP2	23:11:92:LYS:NZ	2.53	0.41
1:1A:2590:C:H2'	1:1A:2591:U:O4'	2.19	0.41
1:1A:2712:C:H2'	1:1A:2713:U:H2'	2.02	0.41
1:1A:921:G:H2'	1:1A:922:C:O4'	2.20	0.41
5:1F:24:LEU:HB3	5:1F:115:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:83:VAL:HG23	11:1P:87:ASP:HB2	2.02	0.41
18:1W:9:TYR:HA	18:1W:100:THR:HG23	2.02	0.41
19:1X:60:ARG:HH22	29:17:47:ARG:NH2	2.14	0.41
26:24:33:VAL:HG12	26:24:34:GLU:H	1.85	0.41
29:27:13:ALA:HB2	29:27:48:LYS:HE2	2.01	0.41
1:2A:113:C:H2'	1:2A:114:G:O4'	2.20	0.41
1:2A:1316:G:OP2	59:2A:3660:HOH:O	2.22	0.41
1:2A:1494:G:O2'	1:2A:1574:A:N1	2.38	0.41
1:2A:1726:U:N3	1:2A:1794:G:OP2	2.48	0.41
1:2A:548:U:H2'	1:2A:549:U:C6	2.55	0.41
1:2A:539:A:H1'	1:2A:603:C:H1'	2.01	0.41
1:2A:894:G:N3	1:2A:977:A:H1'	2.35	0.41
21:2Z:23:LYS:NZ	21:2Z:40:ASP:OD2	2.47	0.41
1:1A:1215:G:C2	1:1A:1224:C:C2	3.08	0.41
1:1A:1470:G:H2'	1:1A:1471:G:O4'	2.20	0.41
1:1A:1524:G:O2'	1:1A:1604:A:N1	2.50	0.41
1:1A:2324:C:H2'	1:1A:2325:C:H6	1.85	0.41
1:1A:873:U:OP1	59:1A:4186:HOH:O	2.21	0.41
3:1D:4:LYS:HB3	3:1D:18:VAL:HG23	2.02	0.41
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	2.01	0.41
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	2.02	0.41
9:1N:85:ILE:HA	9:1N:86:PRO:HD3	1.87	0.41
12:1Q:58:PHE:O	12:1Q:60:ARG:N	2.50	0.41
14:1S:43:GLU:OE1	14:1S:43:GLU:N	6.04	0.41
18:1W:14:PRO:HG2	18:1W:78:GLU:CG	2.45	0.41
21:1Z:44:PHE:CZ	21:1Z:86:VAL:HG11	2.55	0.41
27:25:16:ARG:HG3	27:25:17:ASP:N	2.35	0.41
1:2A:1116:G:H1'	1:2A:1134:G:C8	2.55	0.41
1:2A:138:A:C8	1:2A:1453:C:O2'	2.70	0.41
1:2A:1699:G:C6	13:2R:9:LYS:HB2	2.55	0.41
1:2A:1910:A:N1	1:2A:2245:G:H1'	2.35	0.41
1:2A:2124:C:O2	1:2A:2207:G:N1	2.50	0.41
1:2A:2851:G:H2'	1:2A:2852:G:O4'	2.19	0.41
1:2A:433:G:H2'	1:2A:434:G:C8	2.55	0.41
1:2A:552:A:C2	1:2A:2064:C:H5'	2.54	0.41
1:2A:5:A:C2	1:2A:6:G:C8	3.08	0.41
1:2A:775:G:H2'	1:2A:1805:U:H1'	2.01	0.41
6:2G:16:ARG:NH2	6:2G:33:ARG:HD2	2.35	0.41
12:2Q:29:PHE:HB2	12:2Q:105:GLU:OE2	2.19	0.41
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HB	2.01	0.41
24:12:64:LEU:HD21	24:12:68:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1356:G:O2'	29:17:47:ARG:NH2	2.53	0.41
30:18:28:GLY:O	30:18:36:LYS:NZ	2.43	0.41
1:1A:2359:U:O4	1:1A:2393:G:N1	2.54	0.41
1:1A:2269:C:O2'	1:1A:2438:C:OP2	2.35	0.41
1:1A:2898:C:H2'	1:1A:2899:G:O4'	2.20	0.41
1:1A:301:A:HO2'	1:1A:302:C:P	2.43	0.41
1:1A:825:U:P	1:1A:825:U:H6	3.40	0.41
7:1H:69:ARG:HG3	7:1H:70:THR:N	2.34	0.41
1:1A:857:U:O2'	11:1P:21:ARG:HD3	2.20	0.41
16:1U:104:GLN:H	16:1U:104:GLN:HG3	1.60	0.41
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.54	0.41
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.64	0.41
26:24:15:ILE:HB	26:24:32:TYR:CD1	2.55	0.41
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.21	0.41
1:2A:138:A:H8	1:2A:1453:C:HO2'	1.61	0.41
1:2A:160:C:H2'	1:2A:161:G:C8	3.42	0.41
1:2A:440:C:H2'	1:2A:441:A:C8	2.55	0.41
1:2A:5:A:H2	1:2A:6:G:C8	2.39	0.41
1:2A:766:C:H2'	1:2A:767:C:H6	1.85	0.41
1:2A:966:G:C6	1:2A:967:U:C4	3.09	0.41
4:2E:40:GLU:H	4:2E:40:GLU:HG2	1.56	0.41
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	2.02	0.41
20:2Y:52:SER:HB2	20:2Y:53:PRO:HD2	2.02	0.41
23:11:82:LEU:HA	23:11:85:LEU:HD12	2.02	0.41
1:1A:75:C:OP1	24:12:59:ARG:HD3	2.21	0.41
25:13:18:ASP:OD1	25:13:18:ASP:N	2.53	0.41
1:1A:1845:A:N1	59:1A:4356:HOH:O	2.36	0.41
1:1A:1937:A:H2'	1:1A:1938:U:O4'	2.20	0.41
1:1A:2325:C:H2'	1:1A:2326:G:H8	1.85	0.41
1:1A:241:C:O2'	59:1A:4196:HOH:O	2.22	0.41
1:1A:2505:G:O2'	12:1Q:80:GLU:HA	2.21	0.41
1:1A:904:U:O2	1:1A:2279:A:H2'	2.21	0.41
1:1A:921:G:H1	1:1A:947:C:N4	2.14	0.41
4:1E:5:LEU:HD21	4:1E:79:ARG:HB3	2.03	0.41
7:1H:3:ARG:CG	7:1H:6:ARG:HG2	2.50	0.41
7:1H:8:PRO:O	7:1H:69:ARG:NH1	2.53	0.41
12:1Q:21:THR:HG21	12:1Q:101:ARG:N	2.34	0.41
15:1T:101:PHE:N	59:1T:3102:HOH:O	2.35	0.41
15:1T:51:ARG:NH1	59:1T:3101:HOH:O	2.18	0.41
1:2A:2367:C:O3'	22:20:20:ARG:HD2	2.21	0.41
1:2A:1194:G:H2'	1:2A:1195:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1643:C:H2'	1:2A:1644:C:C6	2.55	0.41
1:2A:1821:A:C8	1:2A:1822:G:C8	3.09	0.41
1:2A:2072:A:OP2	1:2A:2072:A:H8	2.03	0.41
1:2A:2272:C:H1'	1:2A:2399:A:N3	2.36	0.41
1:2A:2416:G:C5'	11:2P:75:ILE:HD13	2.51	0.41
1:2A:2689:C:H2'	1:2A:2690:A:O4'	2.20	0.41
1:2A:2693:U:O2'	15:2T:58:ASN:ND2	2.53	0.41
1:2A:310:C:H2'	1:2A:311:C:C6	2.55	0.41
1:2A:409:U:H2'	1:2A:411:C:H5	1.85	0.41
14:2S:5:THR:O	14:2S:8:GLU:N	2.54	0.41
1:2A:1041:A:H4'	16:2U:91:ASP:OD2	2.20	0.41
1:1A:2210:U:H2'	1:1A:2211:G:C8	2.55	0.41
1:1A:2704:A:H2'	1:1A:2705:G:H8	1.86	0.41
6:1G:39:ILE:HD11	6:1G:102:PHE:CZ	2.56	0.41
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.84	0.41
1:1A:661:A:H5''	11:1P:117:GLU:HG2	2.03	0.41
26:24:14:ILE:CG2	26:24:22:ILE:HB	2.50	0.41
1:2A:75:C:N4	1:2A:106:G:H1	2.19	0.41
1:2A:1313:A:H2'	1:2A:1314:A:O4'	2.20	0.41
1:2A:1677:A:OP1	59:2A:3662:HOH:O	2.21	0.41
1:2A:2107:U:H2'	1:2A:2108:G:C8	2.55	0.41
1:2A:2343:U:O2'	1:2A:2346:A:N3	2.41	0.41
1:2A:2485:C:H5''	1:2A:2486:C:OP2	2.20	0.41
1:2A:285:C:H1'	1:2A:289:G:H1'	2.01	0.41
1:2A:791:G:H2'	1:2A:792:A:H5'	2.03	0.41
1:2A:934:C:H2'	1:2A:935:C:C6	2.56	0.41
2:2B:40:U:N3	2:2B:43:C:OP2	2.53	0.41
4:2E:111:ARG:HA	13:2R:1:MET:SD	2.61	0.41
6:2G:35:GLU:HG2	6:2G:36:LYS:HZ2	1.86	0.41
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	2.02	0.41
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	2.03	0.41
4:2E:9:VAL:HB	15:2T:3:ARG:HG2	2.02	0.41
17:2V:89:GLN:HA	17:2V:90:PRO:HD3	1.90	0.41
20:2Y:20:TYR:CE1	20:2Y:43:ASN:HA	2.56	0.41
25:13:26:LEU:O	25:13:35:ARG:NE	2.54	0.41
18:1W:19:LEU:HB3	27:15:25:LEU:HD11	2.01	0.41
1:1A:1222:C:H2'	1:1A:1223:C:H6	1.86	0.41
1:1A:1224:C:H2'	1:1A:1225:C:C6	2.55	0.41
1:1A:1626:A:OP2	1:1A:1626:A:H8	2.04	0.41
1:1A:873:U:O2	1:1A:2257:G:H4'	2.21	0.41
1:1A:291:G:C6	1:1A:292:C:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:344:G:C4	1:1A:345:A:C8	8.09	0.41
1:1A:68:G:H5''	1:1A:109:U:O2	2.21	0.41
1:1A:765:C:O5'	1:1A:765:C:H6	2.03	0.41
17:1V:49:THR:HG22	17:1V:49:THR:O	2.21	0.41
19:1X:35:THR:O	19:1X:38:GLU:HG2	2.21	0.41
1:2A:1683:A:H4'	1:2A:2722:A:O2'	2.21	0.41
1:2A:2251:C:H2'	1:2A:2252:A:H8	1.86	0.41
1:2A:2503:U:H2'	1:2A:2504:U:C6	2.56	0.41
1:2A:364:G:H2'	1:2A:365:G:O4'	2.20	0.41
1:2A:66:G:N2	1:2A:72:A:O5'	2.53	0.41
1:2A:184:A:C4	1:2A:851:G:C6	3.09	0.41
3:2D:142:VAL:HG23	3:2D:193:VAL:HA	2.02	0.41
1:2A:2798:U:O2'	4:2E:65:GLY:HA3	2.21	0.41
1:2A:706:G:H5'	5:2F:99:TYR:CE2	2.55	0.41
7:2H:118:PRO:O	7:2H:121:ILE:HB	2.20	0.41
7:2H:7:LEU:O	7:2H:69:ARG:HD3	2.20	0.41
16:2U:110:VAL:O	16:2U:113:ALA:HB3	2.21	0.41
18:2W:82:LEU:HB3	18:2W:84:ARG:NH1	2.36	0.41
20:2Y:23:ARG:HG2	20:2Y:42:VAL:HG22	2.03	0.41
59:1A:4570:HOH:O	28:16:2:ALA:N	2.54	0.41
29:17:31:LEU:HD22	29:17:42:LEU:HB3	2.02	0.41
1:1A:6:G:H2'	1:1A:7:A:C8	2.56	0.41
4:1E:21:VAL:HA	4:1E:22:PRO:HD3	1.90	0.41
5:1F:93:LYS:HD3	5:1F:93:LYS:HA	1.96	0.41
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	2.03	0.41
7:1H:67:LEU:HG	7:1H:71:LEU:HD22	2.03	0.41
1:2A:98:G:HO2'	24:22:7:ARG:HH22	1.64	0.41
1:2A:1816:A:C4	1:2A:1959:A:C6	3.09	0.41
1:2A:2860:A:H2'	1:2A:2861:G:O4'	2.21	0.41
1:2A:346:G:H1'	1:2A:1249:U:O2	2.20	0.41
1:2A:653:G:H1'	1:2A:663:U:O2'	2.20	0.41
3:2D:10:THR:OG1	3:2D:13:ARG:HG2	2.21	0.41
7:2H:24:VAL:HG11	7:2H:43:VAL:HG11	2.03	0.41
20:2Y:19:LYS:HE2	20:2Y:20:TYR:CE1	2.55	0.41
26:14:46:GLN:HB2	26:14:48:ARG:CZ	2.51	0.41
1:1A:1956:G:H1'	1:1A:1985:G:N2	2.36	0.41
1:1A:2282:G:OP1	22:10:18:ALA:HB1	2.21	0.41
1:1A:554:G:N3	1:1A:554:G:O4'	2.52	0.41
1:1A:623:C:OP1	5:1F:108:LYS:HE3	2.21	0.41
1:1A:271:U:H4'	8:1I:50:ARG:HH22	1.86	0.41
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:69:PHE:HA	12:1Q:70:PRO:HD3	1.98	0.41
21:1Z:155:LEU:HD12	21:1Z:155:LEU:HA	1.85	0.41
21:1Z:67:LEU:HA	21:1Z:68:PRO:HD3	1.92	0.41
24:22:9:GLN:HE22	24:22:56:GLN:HB3	1.86	0.41
18:2W:34:ASN:ND2	27:25:39:MET:HG3	2.36	0.41
1:2A:917:U:H5''	1:2A:918:A:OP1	2.20	0.41
2:2B:32:C:N4	2:2B:50:G:H1	2.19	0.41
8:2I:61:ARG:HD3	8:2I:61:ARG:HA	1.89	0.41
12:2Q:73:PRO:HA	12:2Q:93:TYR:CD1	2.56	0.41
1:2A:1041:A:H5'	16:2U:93:LYS:HD3	2.02	0.41
19:2X:21:PHE:CZ	19:2X:92:LEU:HD12	2.56	0.41
1:1A:1047:G:H2'	1:1A:1048:G:O4'	2.21	0.41
1:1A:1726:U:H2'	1:1A:1727:G:O4'	2.21	0.41
1:1A:2723:U:O2'	1:1A:2725:A:H5'	2.21	0.41
1:1A:210:A:H5''	1:1A:447:U:OP1	2.21	0.41
1:1A:492:G:OP1	29:17:33:ARG:HD2	2.21	0.41
1:1A:885:U:H2'	1:1A:886:C:C6	2.55	0.41
1:1A:982:G:OP1	30:18:52:LYS:HD2	2.21	0.41
3:1D:33:LEU:HA	3:1D:33:LEU:HD23	1.95	0.41
6:1G:125:PHE:O	6:1G:127:GLY:N	2.54	0.41
7:1H:4:ILE:O	7:1H:69:ARG:HG2	2.21	0.41
11:1P:70:GLN:HE21	11:1P:70:GLN:HB3	1.68	0.41
15:1T:45:PHE:CE1	15:1T:65:LYS:HD3	2.55	0.41
30:28:34:TRP:CG	30:28:35:GLN:N	2.89	0.41
1:2A:1777:G:H2'	1:2A:1778:G:H8	1.86	0.41
1:2A:2326:G:H2'	1:2A:2327:C:C6	2.56	0.41
1:2A:298:G:N3	1:2A:540:C:H4'	110.28	0.41
1:2A:33:C:H2'	1:2A:34:G:C5'	2.51	0.41
1:2A:668:A:C2	1:2A:2380:A:H1'	2.55	0.41
1:2A:821:G:C4	1:2A:840:G:C8	3.08	0.41
2:2B:84:C:H2'	2:2B:85:G:O4'	2.21	0.41
1:2A:720:G:O2'	5:2F:74:ARG:HD3	2.21	0.41
7:2H:127:GLU:C	7:2H:129:THR:H	2.23	0.41
14:2S:110:LEU:HA	14:2S:110:LEU:HD12	1.94	0.41
25:13:39:ASP:OD2	25:13:44:ARG:NH2	2.53	0.41
26:14:14:ILE:HB	26:14:22:ILE:HB	2.02	0.41
1:1A:1947:U:O2'	1:1A:1949:A:N7	2.45	0.41
1:1A:2103:A:H2'	1:1A:2104:G:O4'	2.20	0.41
1:1A:2356:G:H4'	1:1A:2357:A:H5''	2.02	0.41
1:1A:2503:U:H2'	1:1A:2504:U:C6	2.56	0.41
1:1A:2768:U:H1'	1:1A:2769:A:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:237:GLU:OE2	59:1D:402:HOH:O	2.22	0.41
5:1F:176:LEU:HD23	5:1F:176:LEU:HA	1.89	0.41
6:1G:142:PRO:HG2	6:1G:143:GLU:OE1	2.21	0.41
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.60	0.41
14:1S:34:HIS:ND1	14:1S:53:SER:OG	2.42	0.41
20:1Y:56:PRO:C	20:1Y:58:GLY:H	2.24	0.41
1:2A:1713:G:O2'	1:2A:2012:U:O4	2.33	0.41
1:2A:2767:C:HO2'	1:2A:2768:U:H6	1.68	0.41
1:2A:2879:C:H2'	1:2A:2880:C:O4'	2.21	0.41
1:2A:628:U:H4'	1:2A:704:C:H4'	2.02	0.41
1:2A:638:G:H5''	1:2A:639:A:OP1	2.20	0.41
1:2A:69:A:N7	19:2X:31:HIS:HE1	2.19	0.41
1:2A:979:C:O2'	1:2A:980:C:H5'	2.20	0.41
1:2A:982:G:N3	1:2A:982:G:H3'	4.29	0.41
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	2.02	0.41
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	2.02	0.41
2:2B:55:U:C1'	6:2G:29:TRP:HE1	2.33	0.41
11:2P:48:PRO:O	30:28:57:ARG:NH2	2.50	0.41
1:2A:998:G:H5''	12:2Q:13:GLN:HB3	2.03	0.41
13:2R:28:LEU:HD23	13:2R:28:LEU:HA	1.92	0.41
14:2S:33:LYS:HB3	14:2S:34:HIS:CD2	2.56	0.41
18:2W:92:ARG:HD2	18:2W:93:ALA:N	2.36	0.41
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	2.02	0.41
12:2Q:141:GLN:NE2	21:2Z:74:VAL:O	2.51	0.41
11:1P:63:PRO:O	30:18:13:ARG:HG2	2.20	0.41
1:1A:1067:G:C5	1:1A:1184:C:C4	3.09	0.41
1:1A:1731:C:H2'	1:1A:1732:C:H6	1.85	0.41
1:1A:2744:G:H3'	1:1A:2745:A:O4'	2.21	0.41
1:1A:2896:U:H2'	1:1A:2897:C:C6	2.55	0.41
1:1A:710:C:H2'	1:1A:711:C:H6	1.86	0.41
1:1A:931:C:H3'	1:1A:932:C:H5''	2.02	0.41
3:1D:175:LEU:HD12	3:1D:185:VAL:HG21	2.03	0.41
4:1E:2:LYS:HA	4:1E:84:PHE:CG	2.57	0.41
14:1S:59:LYS:H	14:1S:59:LYS:HE3	1.85	0.41
24:22:1:MET:HE3	24:22:5:GLU:HB3	2.03	0.41
1:2A:1732:C:H2'	1:2A:1733:G:O4'	2.21	0.41
1:2A:870:A:H1'	1:2A:2369:G:N7	2.35	0.41
1:2A:38:C:H2'	1:2A:39:C:C6	2.56	0.41
1:2A:732:G:H21	1:2A:834:A:H61	1.68	0.41
3:2D:137:PRO:O	3:2D:140:THR:HG23	2.21	0.41
8:2I:140:LEU:HA	8:2I:140:LEU:HD23	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2N:99:LEU:HA	9:2N:99:LEU:HD22	1.92	0.41
10:2O:122:LEU:HD13	15:2T:72:VAL:HG11	2.02	0.41
1:2A:794:G:O6	18:2W:90:ARG:NH1	2.54	0.41
21:2Z:128:VAL:HB	21:2Z:161:VAL:HA	2.02	0.41
28:16:34:LEU:HB2	28:16:51:GLU:HB2	2.03	0.40
1:1A:1461:G:O2'	1:1A:1462:C:OP2	2.33	0.40
1:1A:2124:C:O2	1:1A:2208:G:N2	2.55	0.40
1:1A:2734:G:H2'	1:1A:2735:C:C6	2.56	0.40
1:1A:204:A:C4	1:1A:458:A:C2	3.09	0.40
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	2.03	0.40
19:1X:31:HIS:HA	19:1X:32:PRO:HD3	1.92	0.40
1:2A:2367:C:H5'	22:20:24:LYS:HZ1	1.85	0.40
25:23:18:ASP:OD1	25:23:18:ASP:N	2.54	0.40
1:2A:1056:G:C5	1:2A:1058:C:C4	3.09	0.40
1:2A:1072:A:C2	1:2A:2499:A:H5'	2.56	0.40
1:2A:1411:A:H2'	1:2A:1412:A:O4'	2.22	0.40
1:2A:1534:U:HO2'	1:2A:1535:A:H8	1.68	0.40
1:2A:211:A:N1	1:2A:433:G:O2'	2.45	0.40
1:2A:2347:A:H61	22:20:43:THR:HG21	1.85	0.40
1:2A:2353:C:O2'	1:2A:2385:C:OP1	2.24	0.40
1:2A:2668:A:O3'	7:2H:160:LYS:NZ	2.53	0.40
1:2A:563:G:H2'	1:2A:564:C:C6	2.56	0.40
1:2A:861:C:C2	1:2A:1237:G:C2	3.09	0.40
1:2A:905:G:N2	1:2A:962:A:OP2	2.41	0.40
5:2F:164:ARG:O	5:2F:168:ARG:HG3	2.20	0.40
8:2I:43:ASN:HD22	8:2I:43:ASN:C	2.23	0.40
5:2F:188:ARG:HA	11:2P:3:LEU:HD23	2.01	0.40
1:2A:2857:G:C8	15:2T:97:ALA:HB2	2.56	0.40
1:1A:115:A:C8	1:1A:116:A:C8	3.09	0.40
1:1A:1732:C:H2'	1:1A:1733:G:O4'	2.21	0.40
1:1A:2514:A:H4'	1:1A:2515:U:OP1	2.22	0.40
1:1A:25:G:C6	1:1A:26:G:C6	3.08	0.40
1:1A:603:C:H2'	1:1A:604:G:H8	1.87	0.40
1:1A:751:A:H2'	1:1A:752:A:O4'	2.29	0.40
1:1A:839:A:OP2	1:1A:2092:A:O2'	2.36	0.40
1:1A:908:G:H2'	1:1A:909:A:O4'	2.22	0.40
2:1B:42:C:OP1	6:1G:67:LYS:NZ	2.48	0.40
2:1B:4:C:H2'	2:1B:5:C:O4'	2.21	0.40
6:1G:64:THR:HB	6:1G:94:LEU:HD11	2.03	0.40
7:1H:71:LEU:HD12	7:1H:71:LEU:HA	1.87	0.40
10:1O:7:TYR:CE1	10:1O:20:MET:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2574:U:H4'	10:1O:28:SER:HA	2.03	0.40
11:1P:130:PHE:HB2	11:1P:135:LEU:HG	2.04	0.40
1:2A:1244:C:H5'	59:2A:3667:HOH:O	2.21	0.40
1:2A:1332:A:C5	1:2A:1333:U:C4	3.09	0.40
1:2A:1807:U:O2'	1:2A:1808:U:H5'	2.21	0.40
1:2A:223:U:H2'	1:2A:224:C:C6	2.57	0.40
1:2A:243:A:N6	1:2A:244:A:C6	2.89	0.40
1:2A:755:U:H2'	1:2A:756:G:C8	2.56	0.40
2:2B:20:C:N4	2:2B:21:G:C6	2.89	0.40
7:2H:89:ILE:O	7:2H:129:THR:HG22	2.21	0.40
8:2I:118:LYS:HA	8:2I:119:PRO:HD3	1.91	0.40
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.54	0.40
25:13:15:TYR:CE2	25:13:53:LEU:HD21	2.56	0.40
1:1A:1067:G:C5	1:1A:1068:U:C4	6.59	0.40
1:1A:1086:C:N4	1:1A:1159:G:H1	2.13	0.40
1:1A:141:G:H1'	19:1X:37:THR:HG21	2.03	0.40
1:1A:210:A:OP2	59:1A:4194:HOH:O	2.22	0.40
1:1A:2227:G:O2'	1:1A:2228:A:OP1	2.35	0.40
1:1A:2244:U:H2'	1:1A:2245:G:C8	2.57	0.40
1:1A:229:A:H5''	59:1A:5710:HOH:O	2.21	0.40
1:1A:2710:C:H2'	1:1A:2711:C:O4'	2.22	0.40
1:1A:2771:G:OP2	59:1A:4187:HOH:O	2.21	0.40
1:1A:818:C:H2'	1:1A:819:U:C6	2.56	0.40
1:1A:825:U:H6	1:1A:825:U:OP2	3.59	0.40
6:1G:181:ARG:HG3	6:1G:182:LYS:H	1.86	0.40
9:1N:99:LEU:HD23	9:1N:99:LEU:HA	1.93	0.40
25:23:6:VAL:HG23	25:23:35:ARG:O	2.21	0.40
1:2A:1003:A:N6	1:2A:1004:A:N1	2.70	0.40
1:2A:1101:G:H4'	1:2A:1131:A:C8	2.56	0.40
1:2A:1272:G:C5	1:2A:1273:G:C8	3.51	0.40
1:2A:142:C:H2'	1:2A:143:C:C6	2.57	0.40
1:2A:1634:C:H2'	1:2A:1635:U:C6	2.56	0.40
1:2A:2037:U:H2'	1:2A:2038:U:H6	1.86	0.40
1:2A:2752:A:C6	1:2A:2753:A:C6	3.10	0.40
1:2A:602:C:H2'	1:2A:603:C:C6	2.57	0.40
1:2A:901:G:H2'	1:2A:902:C:C6	2.56	0.40
1:2A:991:G:H2'	1:2A:992:G:C8	2.56	0.40
2:2B:73:A:C4	2:2B:105:A:C2	3.09	0.40
2:2B:28:C:H2'	2:2B:29:A:O4'	2.21	0.40
4:2E:32:PRO:HD2	4:2E:50:GLY:O	2.20	0.40
6:2G:109:VAL:O	6:2G:113:ARG:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:100:GLY:O	10:2O:119:PRO:HD2	2.21	0.40
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.21	0.40
11:2P:144:GLU:HA	11:2P:145:PRO:HD3	1.87	0.40
1:2A:1232:U:C4'	17:2V:79:VAL:HG22	2.51	0.40
26:14:8:LYS:HE2	26:14:8:LYS:HB3	1.91	0.40
1:1A:141:G:N2	1:1A:172:C:C4	54.83	0.40
1:1A:2059:G:H2'	1:1A:2060:C:O4'	2.22	0.40
1:1A:235:G:H4'	1:1A:412:G:C6	2.56	0.40
1:1A:2536:G:C2	1:1A:2550:C:C2	3.09	0.40
1:1A:830:A:C6	3:1D:229:VAL:HG11	2.56	0.40
8:1I:75:LEU:HD22	8:1I:105:HIS:ND1	2.37	0.40
10:1O:105:GLU:HG2	10:1O:105:GLU:H	1.53	0.40
16:1U:112:ARG:HG2	16:1U:112:ARG:H	1.74	0.40
1:2A:1409:G:OP2	23:21:3:LYS:HG3	2.21	0.40
1:2A:1415:C:N4	1:2A:1416:G:C6	2.89	0.40
1:2A:1480:G:H2'	1:2A:1481:G:O4'	2.22	0.40
1:2A:179:A:N1	59:2A:3736:HOH:O	2.37	0.40
1:2A:1921:A:O2'	1:2A:1922:A:OP1	2.30	0.40
1:2A:2411:G:N2	1:2A:2428:C:C2	2.89	0.40
1:2A:330:G:H21	1:2A:353:A:N6	2.15	0.40
1:2A:483:G:O2'	29:27:39:ARG:HD3	2.22	0.40
1:2A:639:A:C4	5:2F:180:GLY:HA3	2.57	0.40
1:2A:83:G:C5	1:2A:96:G:C2	3.10	0.40
2:2B:78:A:C2	2:2B:100:A:C4	3.09	0.40
3:2D:72:LYS:CG	3:2D:103:ARG:HH21	2.35	0.40
3:2D:145:VAL:HG12	3:2D:146:GLU:O	2.21	0.40
6:2G:108:ASN:HD22	26:24:37:SER:HB2	1.86	0.40
6:2G:23:PHE:HB2	6:2G:25:TYR:CZ	2.55	0.40
11:2P:98:GLU:O	11:2P:101:VAL:HG12	2.20	0.40
13:2R:70:LEU:HA	13:2R:70:LEU:HD23	1.80	0.40
26:14:24:THR:OG1	26:14:25:TYR:N	2.52	0.40
30:18:23:VAL:CG2	30:18:47:LYS:HB3	2.52	0.40
1:1A:1159:G:H2'	1:1A:1160:G:C8	2.57	0.40
1:1A:1827:C:H4'	3:1D:257:LEU:O	2.21	0.40
1:1A:2114:G:C6	1:1A:2236:A:C8	3.10	0.40
1:1A:2330:G:H22	14:1S:3:ARG:CG	2.32	0.40
3:1D:68:LYS:O	3:1D:69:ARG:HB2	2.21	0.40
13:1R:70:LEU:O	13:1R:72:ASP:N	2.53	0.40
18:1W:88:ARG:HG3	18:1W:92:ARG:HH21	1.85	0.40
27:25:20:ARG:HG2	27:25:23:HIS:CE1	2.57	0.40
1:2A:1135:U:H2'	1:2A:1136:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1098:C:H42	1:2A:1151:G:H1	1.70	0.40
1:2A:1556:A:H2'	1:2A:1557:G:C8	2.57	0.40
1:2A:2080:A:O2'	5:2F:69:HIS:CD2	2.74	0.40
1:2A:2602:C:H2'	1:2A:2603:G:C8	2.56	0.40
1:2A:263:G:C2	1:2A:264:U:C2	3.10	0.40
1:2A:2700:U:H4'	1:2A:2701:C:H5'	2.04	0.40
1:2A:718:C:H2'	1:2A:719:C:C6	2.56	0.40
1:2A:830:A:C8	1:2A:838:G:C5	3.10	0.40
3:2D:132:PRO:HG3	3:2D:190:TYR:CE1	2.56	0.40
1:2A:1924:G:OP1	3:2D:241:PRO:HB2	2.21	0.40
3:2D:264:LYS:HA	3:2D:265:PRO:HD3	1.92	0.40
1:2A:2669:C:H5''	7:2H:158:HIS:CD2	2.56	0.40
21:2Z:35:ARG:HA	21:2Z:35:ARG:HD2	1.78	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	254 (93%)	17 (6%)	2 (1%)	26	62
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	34	69
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	34	69
5	1F	201/210 (96%)	189 (94%)	11 (6%)	1 (0%)	34	69
5	2F	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	19	52
6	1G	179/182 (98%)	158 (88%)	17 (10%)	4 (2%)	8	28
6	2G	179/182 (98%)	154 (86%)	20 (11%)	5 (3%)	6	21
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	30	65
7	2H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	16	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	1I	144/148 (97%)	121 (84%)	19 (13%)	4 (3%)	6	21
8	2I	144/148 (97%)	122 (85%)	20 (14%)	2 (1%)	14	42
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	26	62
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	26	62
11	2P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
12	1Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	26	62
12	2Q	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
13	1R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	21	55
14	2S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	21	55
15	1T	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	24	58
15	2T	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	19	52
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	19	52
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	17	50
19	2X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	17	50
20	1Y	105/110 (96%)	94 (90%)	9 (9%)	2 (2%)	10	32
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	19	52
21	1Z	184/206 (89%)	167 (91%)	15 (8%)	2 (1%)	17	50
21	2Z	184/206 (89%)	163 (89%)	16 (9%)	5 (3%)	6	21
22	10	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
22	20	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	17	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	50
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	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%)	10 (15%)	8 (12%)	0	1
26	24	67/71 (94%)	50 (75%)	10 (15%)	7 (10%)	1	1
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%)	1 (2%)	0	100	100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	182 (80%)	36 (16%)	11 (5%)	3	9
33	2b	229/256 (90%)	187 (82%)	33 (14%)	9 (4%)	4	12
34	1c	204/239 (85%)	173 (85%)	28 (14%)	3 (2%)	13	40
34	2c	204/239 (85%)	166 (81%)	36 (18%)	2 (1%)	19	52
35	1d	206/209 (99%)	185 (90%)	20 (10%)	1 (0%)	34	69
35	2d	206/209 (99%)	188 (91%)	16 (8%)	2 (1%)	19	52
36	1e	146/162 (90%)	128 (88%)	15 (10%)	3 (2%)	9	29
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	14	42
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	130 (85%)	23 (15%)	0	100	100
38	2g	153/156 (98%)	130 (85%)	23 (15%)	0	100	100
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	26	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	1i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	24	58
40	2i	125/128 (98%)	104 (83%)	19 (15%)	2 (2%)	12	38
41	1j	95/105 (90%)	82 (86%)	6 (6%)	7 (7%)	1	3
41	2j	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	5	17
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	11	34
42	2k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	11	34
43	1l	120/132 (91%)	115 (96%)	4 (3%)	1 (1%)	24	58
43	2l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
44	1m	116/126 (92%)	105 (90%)	8 (7%)	3 (3%)	7	22
44	2m	114/126 (90%)	100 (88%)	10 (9%)	4 (4%)	4	15
45	1n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	11	36
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	16	47
46	2o	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	8	26
47	1p	80/88 (91%)	65 (81%)	15 (19%)	0	100	100
47	2p	80/88 (91%)	65 (81%)	15 (19%)	0	100	100
48	1q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	19	52
48	2q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
49	1r	66/88 (75%)	59 (89%)	6 (9%)	1 (2%)	13	40
49	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	13	40
50	1s	82/93 (88%)	68 (83%)	14 (17%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	16	47
51	1t	94/106 (89%)	80 (85%)	12 (13%)	2 (2%)	9	29
51	2t	94/106 (89%)	79 (84%)	13 (14%)	2 (2%)	9	29
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
55	1z	11/19 (58%)	10 (91%)	0	1 (9%)	1	2
55	2z	10/19 (53%)	10 (100%)	0	0	100	100
All	All	11431/12166 (94%)	10441 (91%)	856 (8%)	134 (1%)	16	47

All (134) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
6	1G	126	ASP
8	1I	106	GLY
21	1Z	93	ASP
23	11	3	LYS
26	14	45	GLY
26	14	48	ARG
26	14	50	VAL
26	14	53	GLU
33	1b	16	HIS
33	1b	121	LEU
33	1b	125	PRO
34	1c	107	GLN
40	1i	54	ASP
41	1j	55	LYS
41	1j	56	HIS
42	1k	49	GLY
44	1m	4	ILE
45	1n	3	ARG
48	1q	68	ARG
6	2G	14	GLU
6	2G	47	LYS
6	2G	51	ARG
6	2G	126	ASP
7	2H	55	PRO
7	2H	126	PRO
8	2I	10	GLU
17	2V	79	VAL
21	2Z	93	ASP
21	2Z	128	VAL
21	2Z	135	GLU
26	24	45	GLY
26	24	62	ARG
26	24	68	ARG
33	2b	17	PHE
33	2b	93	VAL
33	2b	124	SER
40	2i	54	ASP
42	2k	49	GLY
44	2m	106	ASN
51	2t	99	LEU
5	1F	130	ALA
7	1H	126	PRO
12	1Q	58	PHE

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Mol	Chain	Res	Type
14	1S	60	GLY
17	1V	79	VAL
19	1X	94	GLY
33	1b	17	PHE
33	1b	95	GLN
33	1b	128	GLU
41	1j	31	GLY
43	1l	29	GLY
5	2F	130	ALA
6	2G	81	LYS
19	2X	94	GLY
20	2Y	54	LYS
26	24	54	GLY
33	2b	121	LEU
33	2b	125	PRO
36	2e	37	ARG
44	2m	4	ILE
44	2m	21	TYR
44	2m	107	ALA
6	1G	47	LYS
6	1G	51	ARG
8	1I	42	SER
8	1I	73	GLU
26	14	62	ARG
33	1b	22	LYS
33	1b	23	ARG
33	1b	231	GLU
41	1j	77	PRO
44	1m	106	ASN
51	1t	47	GLY
9	2N	2	LYS
23	21	3	LYS
26	24	47	GLN
40	2i	39	GLY
41	2j	77	PRO
41	2j	78	ASN
49	2r	25	THR
4	1E	52	LEU
20	1Y	53	PRO
20	1Y	54	LYS
26	14	49	PHE
33	1b	20	GLU

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Mol	Chain	Res	Type
44	1m	21	TYR
49	1r	25	THR
55	1z	9	ARG
4	2E	52	LEU
5	2F	18	ARG
8	2I	42	SER
26	24	63	TYR
34	2c	61	ALA
34	2c	187	ALA
35	2d	47	ARG
50	2s	30	LEU
51	2t	47	GLY
8	1I	107	VAL
21	1Z	101	PRO
26	14	46	GLN
26	14	47	GLN
33	1b	202	PRO
34	1c	3	ASN
41	1j	78	ASN
41	1j	82	ILE
3	2D	3	VAL
14	2S	84	GLN
21	2Z	101	PRO
21	2Z	127	LYS
33	2b	20	GLU
33	2b	202	PRO
33	2b	230	VAL
35	2d	45	GLN
46	2o	88	ARG
6	1G	50	ALA
34	1c	61	ALA
36	1e	69	VAL
41	1j	32	ALA
36	2e	69	VAL
46	2o	19	PRO
35	1d	8	VAL
3	2D	125	ILE
26	24	50	VAL
36	1e	85	GLY
42	1k	105	VAL
42	2k	105	VAL
46	1o	19	PRO

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Mol	Chain	Res	Type
33	2b	151	GLY
41	2j	82	ILE
11	1P	122	PRO
15	1T	37	GLY
36	1e	96	PRO
51	1t	102	GLY
39	2h	73	ASP

### 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%)	189 (88%)	26 (12%)	6	18
3	2D	216/218 (99%)	194 (90%)	22 (10%)	9	26
4	1E	164/166 (99%)	144 (88%)	20 (12%)	6	18
4	2E	164/166 (99%)	149 (91%)	15 (9%)	12	33
5	1F	160/166 (96%)	146 (91%)	14 (9%)	12	35
5	2F	159/166 (96%)	146 (92%)	13 (8%)	14	38
6	1G	143/156 (92%)	130 (91%)	13 (9%)	12	33
6	2G	142/156 (91%)	122 (86%)	20 (14%)	4	12
7	1H	144/148 (97%)	134 (93%)	10 (7%)	19	48
7	2H	144/148 (97%)	127 (88%)	17 (12%)	6	19
8	1I	110/124 (89%)	90 (82%)	20 (18%)	2	6
8	2I	104/124 (84%)	90 (86%)	14 (14%)	5	14
9	1N	118/119 (99%)	104 (88%)	14 (12%)	6	19
9	2N	118/119 (99%)	103 (87%)	15 (13%)	5	16
10	1O	100/100 (100%)	93 (93%)	7 (7%)	19	47
10	2O	100/100 (100%)	95 (95%)	5 (5%)	30	64
11	1P	116/116 (100%)	101 (87%)	15 (13%)	5	16
11	2P	115/116 (99%)	98 (85%)	17 (15%)	4	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	22	53
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	22	53
13	1R	101/101 (100%)	87 (86%)	14 (14%)	4	13
13	2R	101/101 (100%)	90 (89%)	11 (11%)	8	23
14	1S	87/88 (99%)	80 (92%)	7 (8%)	15	40
14	2S	85/88 (97%)	74 (87%)	11 (13%)	5	16
15	1T	115/127 (91%)	105 (91%)	10 (9%)	13	35
15	2T	113/127 (89%)	105 (93%)	8 (7%)	18	46
16	1U	93/94 (99%)	84 (90%)	9 (10%)	10	29
16	2U	93/94 (99%)	87 (94%)	6 (6%)	21	52
17	1V	80/82 (98%)	68 (85%)	12 (15%)	3	11
17	2V	80/82 (98%)	71 (89%)	9 (11%)	7	22
18	1W	90/92 (98%)	84 (93%)	6 (7%)	20	50
18	2W	90/92 (98%)	84 (93%)	6 (7%)	20	50
19	1X	77/78 (99%)	75 (97%)	2 (3%)	54	86
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%)	150 (94%)	9 (6%)	25	58
21	2Z	156/179 (87%)	144 (92%)	12 (8%)	16	41
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%)	74 (92%)	6 (8%)	17	43
24	12	65/67 (97%)	62 (95%)	3 (5%)	33	67
24	22	65/67 (97%)	61 (94%)	4 (6%)	23	54
25	13	51/52 (98%)	47 (92%)	4 (8%)	16	41
25	23	50/52 (96%)	45 (90%)	5 (10%)	9	27
26	14	60/63 (95%)	53 (88%)	7 (12%)	7	20
26	24	53/63 (84%)	47 (89%)	6 (11%)	7	22
27	15	50/52 (96%)	46 (92%)	4 (8%)	15	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	25	50/52 (96%)	46 (92%)	4 (8%)	15	40
28	16	51/52 (98%)	46 (90%)	5 (10%)	10	28
28	26	50/52 (96%)	45 (90%)	5 (10%)	9	27
29	17	41/42 (98%)	37 (90%)	4 (10%)	10	28
29	27	41/42 (98%)	40 (98%)	1 (2%)	57	87
30	18	54/55 (98%)	49 (91%)	5 (9%)	11	32
30	28	54/55 (98%)	51 (94%)	3 (6%)	26	59
31	19	34/34 (100%)	33 (97%)	1 (3%)	50	83
31	29	34/34 (100%)	33 (97%)	1 (3%)	50	83
33	1b	177/220 (80%)	149 (84%)	28 (16%)	3	9
33	2b	158/220 (72%)	132 (84%)	26 (16%)	3	8
34	1c	127/188 (68%)	115 (91%)	12 (9%)	11	31
34	2c	108/188 (57%)	96 (89%)	12 (11%)	8	23
35	1d	161/181 (89%)	142 (88%)	19 (12%)	6	19
35	2d	164/181 (91%)	149 (91%)	15 (9%)	12	33
36	1e	113/123 (92%)	104 (92%)	9 (8%)	15	40
36	2e	106/123 (86%)	94 (89%)	12 (11%)	7	22
37	1f	83/90 (92%)	78 (94%)	5 (6%)	24	56
37	2f	86/90 (96%)	83 (96%)	3 (4%)	43	77
38	1g	111/127 (87%)	98 (88%)	13 (12%)	7	20
38	2g	107/127 (84%)	92 (86%)	15 (14%)	4	13
39	1h	114/119 (96%)	104 (91%)	10 (9%)	12	35
39	2h	111/119 (93%)	99 (89%)	12 (11%)	8	23
40	1i	89/99 (90%)	79 (89%)	10 (11%)	7	22
40	2i	80/99 (81%)	71 (89%)	9 (11%)	7	22
41	1j	60/92 (65%)	51 (85%)	9 (15%)	3	11
41	2j	62/92 (67%)	52 (84%)	10 (16%)	3	9
42	1k	82/99 (83%)	72 (88%)	10 (12%)	6	18
42	2k	82/99 (83%)	75 (92%)	7 (8%)	13	36
43	1l	95/109 (87%)	91 (96%)	4 (4%)	36	71
43	2l	94/109 (86%)	91 (97%)	3 (3%)	46	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	1m	90/101 (89%)	80 (89%)	10 (11%)	8	23
44	2m	87/101 (86%)	74 (85%)	13 (15%)	4	11
45	1n	47/50 (94%)	43 (92%)	4 (8%)	13	36
45	2n	43/50 (86%)	36 (84%)	7 (16%)	3	8
46	1o	75/80 (94%)	69 (92%)	6 (8%)	15	40
46	2o	78/80 (98%)	74 (95%)	4 (5%)	29	63
47	1p	67/74 (90%)	57 (85%)	10 (15%)	4	11
47	2p	68/74 (92%)	60 (88%)	8 (12%)	6	19
48	1q	91/97 (94%)	85 (93%)	6 (7%)	21	51
48	2q	94/97 (97%)	89 (95%)	5 (5%)	28	61
49	1r	59/77 (77%)	55 (93%)	4 (7%)	20	49
49	2r	59/77 (77%)	53 (90%)	6 (10%)	9	26
50	1s	65/80 (81%)	56 (86%)	9 (14%)	4	13
50	2s	67/80 (84%)	59 (88%)	8 (12%)	6	19
51	1t	66/82 (80%)	61 (92%)	5 (8%)	16	42
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	13/19 (68%)	13 (100%)	0	100	100
55	2z	12/19 (63%)	11 (92%)	1 (8%)	14	38
All	All	9160/10104 (91%)	8276 (90%)	884 (10%)	10	29

All (884) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	13	ARG
3	1D	14	ARG
3	1D	27	THR
3	1D	54	ARG
3	1D	61	LEU
3	1D	71	ASP
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG

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Mol	Chain	Res	Type
3	1D	111	LEU
3	1D	113	VAL
3	1D	115	GLN
3	1D	116	GLN
3	1D	138	VAL
3	1D	142	VAL
3	1D	171	ASP
3	1D	193	VAL
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
3	1D	260	ARG
3	1D	275	LYS
4	1E	7	VAL
4	1E	12	THR
4	1E	14	ILE
4	1E	21	VAL
4	1E	40	GLU
4	1E	49	LEU
4	1E	54	GLN
4	1E	73	GLU
4	1E	75	VAL
4	1E	82	ARG
4	1E	111	ARG
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	154	LYS
4	1E	163	GLU
4	1E	167	VAL
4	1E	175	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	20	LEU
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG

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Mol	Chain	Res	Type
5	1F	106	ARG
5	1F	110	LEU
5	1F	112	MET
5	1F	125	LEU
5	1F	170	LEU
5	1F	191	ARG
5	1F	192	LEU
5	1F	195	ASP
6	1G	4	ASP
6	1G	7	LEU
6	1G	16	ARG
6	1G	43	LEU
6	1G	45	GLU
6	1G	91	ARG
6	1G	139	LEU
6	1G	143	GLU
6	1G	148	MET
6	1G	159	VAL
6	1G	162	THR
6	1G	170	ARG
6	1G	181	ARG
7	1H	3	ARG
7	1H	45	VAL
7	1H	49	VAL
7	1H	59	ARG
7	1H	60	ARG
7	1H	69	ARG
7	1H	71	LEU
7	1H	127	GLU
7	1H	129	THR
7	1H	175	LYS
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU
8	1I	43	ASN
8	1I	50	ARG
8	1I	57	ARG
8	1I	61	ARG
8	1I	66	GLU
8	1I	68	LEU

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Mol	Chain	Res	Type
8	1I	75	LEU
8	1I	77	LEU
8	1I	92	VAL
8	1I	101	LEU
8	1I	103	ARG
8	1I	109	ILE
8	1I	116	LEU
8	1I	140	LEU
8	1I	142	VAL
9	1N	8	GLN
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET
9	1N	61	ARG
9	1N	73	THR
9	1N	87	LEU
9	1N	97	ARG
9	1N	99	LEU
9	1N	120	LEU
9	1N	131	GLN
9	1N	133	GLN
9	1N	138	LEU
10	1O	10	VAL
10	1O	23	ARG
10	1O	24	VAL
10	1O	69	ILE
10	1O	94	ARG
10	1O	105	GLU
10	1O	113	LYS
11	1P	3	LEU
11	1P	21	ARG
11	1P	55	ARG
11	1P	59	LEU
11	1P	70	GLN
11	1P	76	LYS
11	1P	83	VAL
11	1P	95	VAL
11	1P	98	GLU
11	1P	99	LEU
11	1P	106	LEU
11	1P	112	LEU

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Mol	Chain	Res	Type
11	1P	125	VAL
11	1P	148	LEU
11	1P	149	GLU
12	1Q	1	MET
12	1Q	45	GLN
12	1Q	55	VAL
12	1Q	60	ARG
12	1Q	64	ILE
12	1Q	109	VAL
12	1Q	110	THR
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	60	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	75	LEU
13	1R	79	LEU
13	1R	91	GLN
13	1R	111	LEU
14	1S	3	ARG
14	1S	14	VAL
14	1S	20	ARG
14	1S	59	LYS
14	1S	61	ASN
14	1S	69	VAL
14	1S	85	VAL
15	1T	6	LEU
15	1T	13	ARG
15	1T	35	LYS
15	1T	49	VAL
15	1T	78	LEU
15	1T	89	VAL
15	1T	96	ARG
15	1T	107	ASP
15	1T	108	ARG
15	1T	118	ARG
16	1U	8	VAL

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Mol	Chain	Res	Type
16	1U	36	ARG
16	1U	52	ARG
16	1U	60	LEU
16	1U	74	LEU
16	1U	77	SER
16	1U	92	ARG
16	1U	95	LEU
16	1U	104	GLN
17	1V	18	LEU
17	1V	21	ARG
17	1V	28	GLU
17	1V	35	LEU
17	1V	38	LEU
17	1V	43	GLU
17	1V	46	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	95	LEU
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	51	LEU
18	1W	107	LEU
19	1X	35	THR
19	1X	88	LYS
20	1Y	9	LYS
20	1Y	23	ARG
20	1Y	43	ASN
20	1Y	70	SER
20	1Y	90	LEU
21	1Z	11	GLU
21	1Z	31	ARG
21	1Z	86	VAL
21	1Z	107	THR
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	162	GLU
21	1Z	170	THR
21	1Z	182	LYS

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Mol	Chain	Res	Type
22	10	10	THR
22	10	11	ARG
22	10	20	ARG
22	10	49	LYS
22	10	55	ARG
23	11	21	ARG
23	11	35	THR
23	11	40	ARG
23	11	59	THR
23	11	78	LYS
23	11	89	GLU
23	11	95	LEU
24	12	19	VAL
24	12	53	LEU
24	12	70	GLN
25	13	6	VAL
25	13	8	LEU
25	13	23	LEU
25	13	54	VAL
26	14	47	GLN
26	14	49	PHE
26	14	58	ARG
26	14	60	GLN
26	14	61	ARG
26	14	63	TYR
26	14	68	ARG
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	40	LYS
28	16	4	GLU
28	16	6	ARG
28	16	14	THR
28	16	38	LYS
28	16	48	VAL
29	17	1	MET
29	17	23	ARG
29	17	24	THR
29	17	43	THR
30	18	14	VAL
30	18	31	HIS
30	18	32	LEU

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Mol	Chain	Res	Type
30	18	34	TRP
30	18	46	ARG
31	19	26	ILE
33	1b	7	VAL
33	1b	8	LYS
33	1b	10	LEU
33	1b	16	HIS
33	1b	17	PHE
33	1b	21	ARG
33	1b	24	TRP
33	1b	60	ASP
33	1b	67	THR
33	1b	76	GLN
33	1b	80	ILE
33	1b	93	VAL
33	1b	96	ARG
33	1b	112	VAL
33	1b	124	SER
33	1b	127	ILE
33	1b	128	GLU
33	1b	156	LYS
33	1b	169	LYS
33	1b	185	ILE
33	1b	187	LEU
33	1b	189	ASP
33	1b	190	THR
33	1b	208	ILE
33	1b	215	LEU
33	1b	217	ARG
33	1b	221	LEU
33	1b	226	ARG
34	1c	15	THR
34	1c	29	TYR
34	1c	47	LEU
34	1c	52	LEU
34	1c	54	ARG
34	1c	59	ARG
34	1c	70	VAL
34	1c	82	GLU
34	1c	115	LEU
34	1c	131	ARG
34	1c	150	LYS

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Mol	Chain	Res	Type
34	1c	204	LEU
35	1d	5	ILE
35	1d	15	GLU
35	1d	28	SER
35	1d	31	CYS
35	1d	45	GLN
35	1d	49	ARG
35	1d	58	LEU
35	1d	66	ARG
35	1d	73	ARG
35	1d	101	LEU
35	1d	107	ARG
35	1d	122	ARG
35	1d	141	ARG
35	1d	160	GLN
35	1d	162	LEU
35	1d	168	ARG
35	1d	181	MET
35	1d	188	LEU
35	1d	194	LEU
36	1e	18	ARG
36	1e	24	ARG
36	1e	31	LEU
36	1e	41	VAL
36	1e	47	LYS
36	1e	51	VAL
36	1e	73	ASN
36	1e	75	THR
36	1e	79	GLU
37	1f	69	GLU
37	1f	72	VAL
37	1f	74	ASP
37	1f	75	LEU
37	1f	89	MET
38	1g	6	ARG
38	1g	8	GLU
38	1g	13	GLN
38	1g	15	ASP
38	1g	21	VAL
38	1g	45	ASP
38	1g	50	ILE
38	1g	52	GLU

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Mol	Chain	Res	Type
38	1g	56	GLN
38	1g	57	GLU
38	1g	75	VAL
38	1g	104	LEU
38	1g	131	LYS
39	1h	21	LYS
39	1h	26	VAL
39	1h	50	ARG
39	1h	51	VAL
39	1h	63	LEU
39	1h	64	LYS
39	1h	75	ARG
39	1h	78	GLN
39	1h	91	ARG
39	1h	137	VAL
40	1i	23	ASN
40	1i	27	THR
40	1i	42	ARG
40	1i	81	ILE
40	1i	86	VAL
40	1i	102	LEU
40	1i	104	ARG
40	1i	108	VAL
40	1i	113	LYS
40	1i	127	LYS
41	1j	17	ASP
41	1j	30	SER
41	1j	43	ARG
41	1j	49	VAL
41	1j	84	GLN
41	1j	85	LEU
41	1j	94	VAL
41	1j	95	GLU
41	1j	98	ILE
42	1k	14	VAL
42	1k	18	ARG
42	1k	31	THR
42	1k	48	ILE
42	1k	78	GLN
42	1k	84	VAL
42	1k	87	THR
42	1k	106	LYS

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Mol	Chain	Res	Type
42	1k	109	VAL
42	1k	114	VAL
43	1l	27	LEU
43	1l	33	ARG
43	1l	60	LEU
43	1l	67	THR
44	1m	4	ILE
44	1m	11	ARG
44	1m	19	LEU
44	1m	56	LEU
44	1m	69	GLU
44	1m	70	LEU
44	1m	102	ARG
44	1m	109	THR
44	1m	110	ARG
44	1m	117	VAL
45	1n	11	LYS
45	1n	18	VAL
45	1n	33	VAL
45	1n	46	GLU
46	1o	3	ILE
46	1o	5	LYS
46	1o	22	THR
46	1o	39	LEU
46	1o	71	GLN
46	1o	83	GLU
47	1p	1	MET
47	1p	2	VAL
47	1p	5	ARG
47	1p	19	ILE
47	1p	20	VAL
47	1p	45	THR
47	1p	47	ASP
47	1p	54	GLU
47	1p	67	THR
47	1p	72	ARG
48	1q	49	GLU
48	1q	68	ARG
48	1q	74	LEU
48	1q	79	SER
48	1q	89	LEU
48	1q	98	LEU

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Mol	Chain	Res	Type
49	1r	26	LEU
49	1r	38	GLU
49	1r	68	LYS
49	1r	76	LEU
50	1s	3	ARG
50	1s	22	LEU
50	1s	28	LYS
50	1s	37	ARG
50	1s	63	THR
50	1s	65	ASN
50	1s	77	THR
50	1s	81	ARG
50	1s	83	HIS
51	1t	9	ASN
51	1t	24	LEU
51	1t	60	GLU
51	1t	62	LEU
51	1t	84	LEU
3	2D	13	ARG
3	2D	54	ARG
3	2D	61	LEU
3	2D	94	LEU
3	2D	103	ARG
3	2D	106	ILE
3	2D	113	VAL
3	2D	134	ARG
3	2D	141	VAL
3	2D	142	VAL
3	2D	154	LYS
3	2D	164	GLN
3	2D	183	ARG
3	2D	193	VAL
3	2D	217	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	257	LEU
3	2D	260	ARG
3	2D	262	ARG
3	2D	276	LYS
4	2E	12	THR
4	2E	21	VAL

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Mol	Chain	Res	Type
4	2E	40	GLU
4	2E	49	LEU
4	2E	52	LEU
4	2E	75	VAL
4	2E	82	ARG
4	2E	111	ARG
4	2E	116	VAL
4	2E	119	ARG
4	2E	144	ARG
4	2E	154	LYS
4	2E	163	GLU
4	2E	175	VAL
4	2E	202	LYS
5	2F	15	SER
5	2F	20	LEU
5	2F	24	LEU
5	2F	53	THR
5	2F	57	VAL
5	2F	74	ARG
5	2F	106	ARG
5	2F	135	LYS
5	2F	191	ARG
5	2F	192	LEU
5	2F	196	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	9	ARG
6	2G	13	GLU
6	2G	28	VAL
6	2G	31	VAL
6	2G	33	ARG
6	2G	60	LEU
6	2G	91	ARG
6	2G	98	ARG
6	2G	111	LEU
6	2G	113	ARG
6	2G	136	ARG
6	2G	139	LEU
6	2G	140	ILE
6	2G	143	GLU
6	2G	148	MET
6	2G	153	ARG

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Mol	Chain	Res	Type
6	2G	159	VAL
6	2G	162	THR
6	2G	165	THR
6	2G	170	ARG
7	2H	3	ARG
7	2H	27	LYS
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	69	ARG
7	2H	71	LEU
7	2H	98	LEU
7	2H	129	THR
7	2H	134	SER
7	2H	136	ILE
7	2H	139	GLN
7	2H	171	LEU
8	2I	15	VAL
8	2I	38	LEU
8	2I	43	ASN
8	2I	57	ARG
8	2I	61	ARG
8	2I	68	LEU
8	2I	75	LEU
8	2I	76	THR
8	2I	77	LEU
8	2I	102	SER
8	2I	116	LEU
8	2I	117	GLU
8	2I	140	LEU
8	2I	142	VAL
9	2N	33	LEU
9	2N	34	LEU
9	2N	43	THR
9	2N	48	MET
9	2N	59	LYS
9	2N	61	ARG
9	2N	62	VAL

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Mol	Chain	Res	Type
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	133	GLN
9	2N	137	LYS
10	2O	10	VAL
10	2O	23	ARG
10	2O	24	VAL
10	2O	69	ILE
10	2O	94	ARG
11	2P	3	LEU
11	2P	15	ARG
11	2P	21	ARG
11	2P	45	LEU
11	2P	55	ARG
11	2P	59	LEU
11	2P	65	ARG
11	2P	83	VAL
11	2P	96	THR
11	2P	101	VAL
11	2P	102	ARG
11	2P	112	LEU
11	2P	121	LYS
11	2P	123	LEU
11	2P	133	SER
11	2P	136	GLU
11	2P	148	LEU
12	2Q	5	ARG
12	2Q	21	THR
12	2Q	22	LYS
12	2Q	38	GLU
12	2Q	45	GLN
12	2Q	64	ILE
12	2Q	110	THR
13	2R	1	MET
13	2R	6	SER
13	2R	18	LEU
13	2R	28	LEU
13	2R	29	LEU

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Mol	Chain	Res	Type
13	2R	44	LEU
13	2R	60	LEU
13	2R	65	LEU
13	2R	79	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	4	LEU
14	2S	14	VAL
14	2S	20	ARG
14	2S	23	ARG
14	2S	35	ILE
14	2S	44	LYS
14	2S	67	ARG
14	2S	69	VAL
14	2S	75	GLU
14	2S	83	LYS
14	2S	85	VAL
15	2T	6	LEU
15	2T	8	LYS
15	2T	34	VAL
15	2T	49	VAL
15	2T	89	VAL
15	2T	96	ARG
15	2T	98	LYS
15	2T	118	ARG
16	2U	36	ARG
16	2U	60	LEU
16	2U	74	LEU
16	2U	92	ARG
16	2U	104	GLN
16	2U	108	GLU
17	2V	18	LEU
17	2V	21	ARG
17	2V	35	LEU
17	2V	43	GLU
17	2V	46	VAL
17	2V	52	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
18	2W	1	MET
18	2W	11	ARG

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Mol	Chain	Res	Type
18	2W	15	ARG
18	2W	17	VAL
18	2W	51	LEU
18	2W	107	LEU
19	2X	57	LEU
19	2X	92	LEU
20	2Y	9	LYS
20	2Y	43	ASN
20	2Y	44	ILE
20	2Y	70	SER
20	2Y	92	ASN
20	2Y	99	CYS
20	2Y	101	LYS
21	2Z	73	GLN
21	2Z	86	VAL
21	2Z	87	ASP
21	2Z	107	THR
21	2Z	126	VAL
21	2Z	131	ARG
21	2Z	132	ASN
21	2Z	135	GLU
21	2Z	136	PHE
21	2Z	150	LEU
21	2Z	175	VAL
21	2Z	185	GLU
22	20	10	THR
22	20	19	LYS
22	20	55	ARG
22	20	82	ARG
23	21	21	ARG
23	21	35	THR
23	21	40	ARG
23	21	56	GLN
23	21	59	THR
23	21	95	LEU
24	22	34	GLU
24	22	35	LEU
24	22	53	LEU
24	22	70	GLN
25	23	6	VAL
25	23	8	LEU
25	23	31	LEU

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Mol	Chain	Res	Type
25	23	54	VAL
25	23	56	VAL
26	24	1	MET
26	24	58	ARG
26	24	61	ARG
26	24	63	TYR
26	24	68	ARG
26	24	69	LYS
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
27	25	40	LYS
28	26	6	ARG
28	26	14	THR
28	26	28	ARG
28	26	38	LYS
28	26	48	VAL
29	27	46	VAL
30	28	14	VAL
30	28	31	HIS
30	28	34	TRP
31	29	17	ILE
33	2b	7	VAL
33	2b	8	LYS
33	2b	17	PHE
33	2b	19	HIS
33	2b	24	TRP
33	2b	35	GLU
33	2b	44	LEU
33	2b	48	MET
33	2b	51	LEU
33	2b	56	ARG
33	2b	60	ASP
33	2b	63	MET
33	2b	67	THR
33	2b	71	VAL
33	2b	90	MET
33	2b	93	VAL
33	2b	117	GLU
33	2b	126	GLU
33	2b	128	GLU
33	2b	179	LYS

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Mol	Chain	Res	Type
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP
33	2b	191	ASP
33	2b	222	ILE
33	2b	224	GLN
34	2c	3	ASN
34	2c	5	ILE
34	2c	14	ILE
34	2c	16	ARG
34	2c	29	TYR
34	2c	47	LEU
34	2c	52	LEU
34	2c	59	ARG
34	2c	70	VAL
34	2c	125	GLU
34	2c	178	LEU
34	2c	182	ILE
35	2d	3	ARG
35	2d	8	VAL
35	2d	26	CYS
35	2d	34	GLU
35	2d	38	TYR
35	2d	47	ARG
35	2d	58	LEU
35	2d	61	LYS
35	2d	73	ARG
35	2d	96	LEU
35	2d	135	LEU
35	2d	157	LEU
35	2d	170	VAL
35	2d	187	ARG
35	2d	194	LEU
36	2e	24	ARG
36	2e	27	ARG
36	2e	31	LEU
36	2e	40	ARG
36	2e	41	VAL
36	2e	47	LYS
36	2e	50	GLU
36	2e	51	VAL
36	2e	68	GLU

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Mol	Chain	Res	Type
36	2e	78	HIS
36	2e	115	VAL
36	2e	121	LYS
37	2f	28	ARG
37	2f	46	ARG
37	2f	69	GLU
38	2g	8	GLU
38	2g	11	GLN
38	2g	15	ASP
38	2g	16	LEU
38	2g	21	VAL
38	2g	42	ILE
38	2g	52	GLU
38	2g	57	GLU
38	2g	72	ARG
38	2g	75	VAL
38	2g	104	LEU
38	2g	110	GLN
38	2g	114	ARG
38	2g	120	ILE
38	2g	129	GLU
39	2h	10	LEU
39	2h	21	LYS
39	2h	26	VAL
39	2h	51	VAL
39	2h	63	LEU
39	2h	78	GLN
39	2h	84	ARG
39	2h	91	ARG
39	2h	111	ILE
39	2h	120	THR
39	2h	125	ARG
39	2h	137	VAL
40	2i	3	GLN
40	2i	12	GLU
40	2i	38	GLN
40	2i	50	LEU
40	2i	81	ILE
40	2i	89	ASN
40	2i	102	LEU
40	2i	104	ARG
40	2i	124	GLN

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Mol	Chain	Res	Type
41	2j	8	LEU
41	2j	16	LEU
41	2j	21	GLN
41	2j	46	ARG
41	2j	48	THR
41	2j	57	LYS
41	2j	68	HIS
41	2j	84	GLN
41	2j	94	VAL
41	2j	95	GLU
42	2k	18	ARG
42	2k	48	ILE
42	2k	75	TYR
42	2k	78	GLN
42	2k	103	LEU
42	2k	109	VAL
42	2k	114	VAL
43	2l	33	ARG
43	2l	115	LYS
43	2l	123	LYS
44	2m	47	ASP
44	2m	49	THR
44	2m	52	GLU
44	2m	55	ARG
44	2m	65	LYS
44	2m	80	ARG
44	2m	81	LEU
44	2m	82	MET
44	2m	90	LEU
44	2m	102	ARG
44	2m	106	ASN
44	2m	109	THR
44	2m	110	ARG
45	2n	11	LYS
45	2n	17	LYS
45	2n	18	VAL
45	2n	27	CYS
45	2n	32	SER
45	2n	33	VAL
45	2n	46	GLU
46	2o	3	ILE
46	2o	5	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
46	2o	24	SER
46	2o	39	LEU
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG
47	2p	11	SER
47	2p	54	GLU
47	2p	67	THR
47	2p	72	ARG
47	2p	74	LEU
48	2q	6	LEU
48	2q	49	GLU
48	2q	63	ARG
48	2q	74	LEU
48	2q	79	SER
49	2r	25	THR
49	2r	26	LEU
49	2r	29	PHE
49	2r	35	ARG
49	2r	38	GLU
49	2r	76	LEU
50	2s	3	ARG
50	2s	27	GLU
50	2s	28	LYS
50	2s	30	LEU
50	2s	41	VAL
50	2s	63	THR
50	2s	65	ASN
50	2s	77	THR
51	2t	10	LEU
51	2t	24	LEU
51	2t	71	THR
52	2u	10	ARG
55	2z	7	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	1D	126	GLN
3	1D	253	GLN
4	1E	54	GLN
5	1F	69	HIS

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Mol	Chain	Res	Type
5	1F	203	GLN
6	1G	40	ASN
6	1G	79	ASN
8	1I	43	ASN
9	1N	8	GLN
9	1N	133	GLN
11	1P	38	GLN
11	1P	70	GLN
12	1Q	45	GLN
13	1R	71	GLN
14	1S	95	HIS
15	1T	43	GLN
15	1T	123	GLN
16	1U	104	GLN
16	1U	117	GLN
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
26	14	47	GLN
30	18	35	GLN
31	19	36	GLN
33	1b	16	HIS
33	1b	94	ASN
34	1c	6	HIS
34	1c	37	GLN
34	1c	176	HIS
35	1d	43	HIS
35	1d	45	GLN
35	1d	77	ASN
35	1d	123	HIS
35	1d	160	GLN
36	1e	38	GLN
36	1e	141	GLN
37	1f	100	ASN
38	1g	86	GLN
38	1g	97	GLN
38	1g	110	GLN
39	1h	82	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	1i	31	GLN
40	1i	38	GLN
40	1i	58	HIS
40	1i	73	GLN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
41	1j	84	GLN
42	1k	93	GLN
43	1l	78	GLN
43	1l	99	HIS
48	1q	16	GLN
48	1q	26	GLN
50	1s	14	HIS
50	1s	47	HIS
50	1s	56	GLN
50	1s	65	ASN
50	1s	69	HIS
51	1t	9	ASN
51	1t	16	HIS
51	1t	26	ASN
51	1t	45	GLN
3	2D	87	ASN
3	2D	253	GLN
5	2F	69	HIS
5	2F	169	ASN
5	2F	203	GLN
6	2G	108	ASN
6	2G	132	ASN
8	2I	43	ASN
8	2I	54	GLN
9	2N	8	GLN
10	2O	5	GLN
11	2P	38	GLN
12	2Q	45	GLN
13	2R	71	GLN
14	2S	68	GLN
14	2S	95	HIS
15	2T	43	GLN
15	2T	58	ASN
15	2T	123	GLN
17	2V	64	HIS

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Mol	Chain	Res	Type
19	2X	31	HIS
20	2Y	43	ASN
20	2Y	92	ASN
21	2Z	73	GLN
21	2Z	151	HIS
23	21	56	GLN
24	22	38	GLN
25	23	33	GLN
28	26	32	ASN
30	28	35	GLN
31	29	36	GLN
33	2b	19	HIS
33	2b	45	GLN
33	2b	146	GLN
34	2c	3	ASN
34	2c	6	HIS
34	2c	123	GLN
34	2c	136	GLN
35	2d	74	GLN
35	2d	77	ASN
35	2d	123	HIS
35	2d	125	HIS
35	2d	201	GLN
38	2g	28	ASN
38	2g	86	GLN
38	2g	97	GLN
38	2g	110	GLN
38	2g	122	HIS
38	2g	148	ASN
39	2h	15	ASN
40	2i	38	GLN
40	2i	73	GLN
41	2j	21	GLN
41	2j	56	HIS
41	2j	84	GLN
42	2k	22	HIS
42	2k	78	GLN
42	2k	93	GLN
42	2k	104	GLN
43	2l	75	HIS
43	2l	78	GLN
44	2m	40	ASN

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Mol	Chain	Res	Type
44	2m	77	ASN
44	2m	106	ASN
46	2o	28	GLN
46	2o	62	GLN
50	2s	56	GLN
50	2s	69	HIS
51	2t	18	GLN
51	2t	42	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	383 (13%)	21 (0%)
1	2A	2781/2915 (95%)	467 (16%)	21 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	24 (20%)	2 (1%)
32	1a	1472/1521 (96%)	263 (17%)	0
32	2a	1479/1521 (97%)	283 (19%)	0
53	1v	4/24 (16%)	1 (25%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	17 (22%)	0
54	2x	75/77 (97%)	15 (20%)	0
All	All	8865/9316 (95%)	1464 (16%)	44 (0%)

All (1464) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	33	C
1	1A	44	C
1	1A	53	G
1	1A	62	A
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	122	G

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Mol	Chain	Res	Type
1	1A	135	G
1	1A	137	G
1	1A	148	A
1	1A	160	C
1	1A	169	A
1	1A	170	A
1	1A	184	A
1	1A	187	A
1	1A	193	G
1	1A	203	G
1	1A	204	A
1	1A	210	A
1	1A	214	G
1	1A	216	A
1	1A	217	A
1	1A	221	A
1	1A	236	G
1	1A	268	G
1	1A	271	U
1	1A	272	G
1	1A	273	U
1	1A	274	C
1	1A	287	U
1	1A	288	G
1	1A	294	C
1	1A	295	U
1	1A	302	C
1	1A	334	A
1	1A	347	A
1	1A	352	G
1	1A	353	A
1	1A	375	G
1	1A	386	G
1	1A	388	G
1	1A	398	G
1	1A	406	U
1	1A	412	G
1	1A	422	G
1	1A	431	U
1	1A	433	G
1	1A	437	G
1	1A	438	A

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Mol	Chain	Res	Type
1	1A	447	U
1	1A	454	A
1	1A	467	G
1	1A	468	A
1	1A	469	C
1	1A	473	U
1	1A	476	C
1	1A	482	A
1	1A	495	A
1	1A	500	U
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
1	1A	597	A
1	1A	624	G
1	1A	625	A
1	1A	626	G
1	1A	629	U
1	1A	638	G
1	1A	640	G
1	1A	658	C
1	1A	661	A
1	1A	669	C
1	1A	670	A
1	1A	681	G
1	1A	682	G
1	1A	696	C
1	1A	700	A
1	1A	714	G
1	1A	715	G
1	1A	732	G
1	1A	763	G
1	1A	765	C
1	1A	776	C

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Mol	Chain	Res	Type
1	1A	785	G
1	1A	797	A
1	1A	803	U
1	1A	810	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	851	G
1	1A	857	U
1	1A	858	C
1	1A	873	U
1	1A	874	U
1	1A	876	G
1	1A	901	G
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
1	1A	934	C
1	1A	935	C
1	1A	936	A
1	1A	937	G
1	1A	938	C
1	1A	939	C
1	1A	941	A
1	1A	942	C
1	1A	952	U
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

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Mol	Chain	Res	Type
1	1A	1018	G
1	1A	1019	C
1	1A	1028	A
1	1A	1041	A
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	1090	A
1	1A	1091	A
1	1A	1092	G
1	1A	1150	U
1	1A	1154	C
1	1A	1156	A
1	1A	1159	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	1194	G
1	1A	1200	A
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	1264	A
1	1A	1265	C
1	1A	1285	U
1	1A	1286	A
1	1A	1293	G
1	1A	1298	A
1	1A	1301	G
1	1A	1316	G
1	1A	1317	A
1	1A	1318	U

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Mol	Chain	Res	Type
1	1A	1345	U
1	1A	1346	A
1	1A	1348	G
1	1A	1397	U
1	1A	1404	A
1	1A	1405	A
1	1A	1410	A
1	1A	1418	A
1	1A	1429	A
1	1A	1430	G
1	1A	1461	G
1	1A	1462	C
1	1A	1465	U
1	1A	1466	G
1	1A	1473	C
1	1A	1482	C
1	1A	1490	A
1	1A	1496	G
1	1A	1501	G
1	1A	1505	G
1	1A	1511	G
1	1A	1513	C
1	1A	1524	G
1	1A	1528	G
1	1A	1535	A
1	1A	1538	C
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	1605	G
1	1A	1612	A
1	1A	1615	A
1	1A	1624	U
1	1A	1627	G
1	1A	1630	C
1	1A	1631	A

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Mol	Chain	Res	Type
1	1A	1632	A
1	1A	1653	A
1	1A	1654	A
1	1A	1655	A
1	1A	1694	C
1	1A	1700	A
1	1A	1704	C
1	1A	1720	G
1	1A	1746	A
1	1A	1747	A
1	1A	1766	A
1	1A	1767	U
1	1A	1776	G
1	1A	1793	G
1	1A	1794	G
1	1A	1799	G
1	1A	1803	A
1	1A	1810	A
1	1A	1821	A
1	1A	1830	C
1	1A	1831	G
1	1A	1846	G
1	1A	1859	A
1	1A	1869	G
1	1A	1877	A
1	1A	1899	G
1	1A	1910	A
1	1A	1917	G
1	1A	1921	A
1	1A	1927	G
1	1A	1934	A
1	1A	1940	A
1	1A	1948	A
1	1A	1950	G
1	1A	1951	G
1	1A	1958	A
1	1A	1959	A
1	1A	1976	U
1	1A	1984	U
1	1A	1988	C
1	1A	1991	A
1	1A	1992	A

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Mol	Chain	Res	Type
1	1A	1993	A
1	1A	2013	G
1	1A	2014	U
1	1A	2018	G
1	1A	2041	A
1	1A	2044	G
1	1A	2052	A
1	1A	2053	G
1	1A	2054	A
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	2101	G
1	1A	2114	G
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	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	2336	G

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Mol	Chain	Res	Type
1	1A	2338	A
1	1A	2345	G
1	1A	2347	A
1	1A	2354	C
1	1A	2358	C
1	1A	2361	C
1	1A	2365	G
1	1A	2394	G
1	1A	2396	C
1	1A	2416	G
1	1A	2417	U
1	1A	2433	A
1	1A	2434	U
1	1A	2436	A
1	1A	2440	G
1	1A	2441	A
1	1A	2442	U
1	1A	2446	A
1	1A	2450	A
1	1A	2452	C
1	1A	2459	A
1	1A	2487	A
1	1A	2489	A
1	1A	2501	G
1	1A	2513	G
1	1A	2516	G
1	1A	2517	U
1	1A	2529	A
1	1A	2540	G
1	1A	2565	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	2634	G
1	1A	2639	C
1	1A	2640	A

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Mol	Chain	Res	Type
1	1A	2641	G
1	1A	2665	A
1	1A	2690	A
1	1A	2700	U
1	1A	2701	C
1	1A	2702	C
1	1A	2713	U
1	1A	2718	G
1	1A	2724	A
1	1A	2725	A
1	1A	2726	G
1	1A	2738	U
1	1A	2745	A
1	1A	2769	A
1	1A	2770	A
1	1A	2776	A
1	1A	2777	A
1	1A	2778	G
1	1A	2790	A
1	1A	2802	A
1	1A	2806	C
1	1A	2812	G
1	1A	2829	A
1	1A	2830	A
1	1A	2844	A
1	1A	2867	C
1	1A	2881	G
1	1A	2882	A
1	1A	2889	C
1	1A	2900	A
1	1A	2902	G
1	1A	2903	U
1	1A	2905	U
2	1B	2	C
2	1B	13	A
2	1B	25	A
2	1B	56	G
2	1B	65	C
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	106	G

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Mol	Chain	Res	Type
2	1B	110	G
32	1a	6	U
32	1a	10	G
32	1a	33	A
32	1a	40	G
32	1a	44	C
32	1a	45	G
32	1a	48	C
32	1a	49	C
32	1a	51	A
32	1a	52	A
32	1a	62	G
32	1a	65	G
32	1a	66	U
32	1a	74	G
32	1a	76	G
32	1a	77	G
32	1a	78	G
32	1a	89	G
32	1a	91	G
32	1a	92	G
32	1a	95	A
32	1a	110	A
32	1a	115	C
32	1a	126	C
32	1a	132	C
32	1a	133	G
32	1a	139	G
32	1a	146	A
32	1a	149	C
32	1a	150	C
32	1a	156	A
32	1a	161	G
32	1a	162	G
32	1a	168	U
32	1a	169	C
32	1a	177	U
32	1a	189	U
32	1a	202	A
32	1a	204	A
32	1a	206	G
32	1a	208	C

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Mol	Chain	Res	Type
32	1a	210	U
32	1a	211	U
32	1a	212	G
32	1a	219	U
32	1a	243	G
32	1a	246	A
32	1a	247	G
32	1a	254	G
32	1a	258	A
32	1a	262	G
32	1a	263	C
32	1a	264	C
32	1a	277	G
32	1a	285	G
32	1a	297	G
32	1a	313	G
32	1a	317	A
32	1a	324	C
32	1a	325	A
32	1a	326	C
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	351	C
32	1a	363	U
32	1a	368	C
32	1a	369	A
32	1a	380	G
32	1a	386	C
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	431	C

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Mol	Chain	Res	Type
32	1a	435	A
32	1a	437	C
32	1a	447	A
32	1a	449	C
32	1a	455	A
32	1a	456	C
32	1a	457	G
32	1a	470	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	502	C
32	1a	511	G
32	1a	516	A
32	1a	517	A
32	1a	531	A
32	1a	543	A
32	1a	545	U
32	1a	556	A
32	1a	557	A
32	1a	560	G
32	1a	561	G
32	1a	574	C
32	1a	576	G
32	1a	602	C
32	1a	614	G
32	1a	625	U
32	1a	637	A
32	1a	649	A
32	1a	671	A
32	1a	672	G
32	1a	677	G
32	1a	701	C
32	1a	707	U
32	1a	731	C
32	1a	733	C
32	1a	739	G
32	1a	743	A
32	1a	757	G

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Mol	Chain	Res	Type
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	812	A
32	1a	813	G
32	1a	820	G
32	1a	824	C
32	1a	825	U
32	1a	826	C
32	1a	829	G
32	1a	837	A
32	1a	838	A
32	1a	848	U
32	1a	850	A
32	1a	851	A
32	1a	880	G
32	1a	892	A
32	1a	904	G
32	1a	905	G
32	1a	909	C
32	1a	912	C
32	1a	913	A
32	1a	914	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	970	U
32	1a	971	G
32	1a	972	A
32	1a	977	C
32	1a	980	G

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Mol	Chain	Res	Type
32	1a	982	G
32	1a	983	A
32	1a	984	A
32	1a	987	C
32	1a	988	G
32	1a	989	G
32	1a	990	G
32	1a	995	A
32	1a	999	U
32	1a	1025	G
32	1a	1026	C
32	1a	1027	A
32	1a	1034	C
32	1a	1036	G
32	1a	1037	C
32	1a	1047	G
32	1a	1048	U
32	1a	1049	C
32	1a	1064	G
32	1a	1069	U
32	1a	1077	G
32	1a	1078	U
32	1a	1084	A
32	1a	1091	G
32	1a	1094	A
32	1a	1106	A
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	1122	G
32	1a	1135	A
32	1a	1142	U
32	1a	1143	G
32	1a	1149	G
32	1a	1164	G
32	1a	1165	A
32	1a	1166	G
32	1a	1175	G
32	1a	1178	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1179	G
32	1a	1184	G
32	1a	1194	U
32	1a	1195	A
32	1a	1196	C
32	1a	1209	A
32	1a	1220	A
32	1a	1222	U
32	1a	1238	A
32	1a	1239	U
32	1a	1240	G
32	1a	1252	C
32	1a	1255	G
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	1287	G
32	1a	1294	G
32	1a	1301	A
32	1a	1304	C
32	1a	1320	G
32	1a	1322	A
32	1a	1329	G
32	1a	1335	G
32	1a	1342	A
32	1a	1345	C
32	1a	1353	G
32	1a	1360	A
32	1a	1361	C
32	1a	1362	G
32	1a	1364	U
32	1a	1379	A
32	1a	1380	C
32	1a	1392	C
32	1a	1402	G
32	1a	1424	G
32	1a	1425	G

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Mol	Chain	Res	Type
32	1a	1426	G
32	1a	1432	A
32	1a	1433	C
32	1a	1465	G
32	1a	1475	G
32	1a	1480	A
32	1a	1481	A
32	1a	1482	G
32	1a	1484	U
32	1a	1495	G
32	1a	1507	G
32	1a	1508	G
53	1v	15	A
54	1x	6	G
54	1x	9	G
54	1x	13	C
54	1x	16	C
54	1x	17	C
54	1x	17(A)	U
54	1x	20	U
54	1x	21	A
54	1x	31	G
54	1x	42	G
54	1x	47	U
54	1x	54	5MU
54	1x	55	PSU
54	1x	56	C
54	1x	65	C
54	1x	70	G
54	1x	76	A
1	2A	7	A
1	2A	11	U
1	2A	12	A
1	2A	13	A
1	2A	14	G
1	2A	34	G
1	2A	44	C
1	2A	53	G
1	2A	59	G
1	2A	69	A
1	2A	72	A
1	2A	73	G

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Mol	Chain	Res	Type
1	2A	81	G
1	2A	82	A
1	2A	88	U
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	128	G
1	2A	137	G
1	2A	138	A
1	2A	154	C
1	2A	155	U
1	2A	160	C
1	2A	169	A
1	2A	170	A
1	2A	184	A
1	2A	187	A
1	2A	193	G
1	2A	201	A
1	2A	203	G
1	2A	204	A
1	2A	209	A
1	2A	210	A
1	2A	212	G
1	2A	217	A
1	2A	223	U
1	2A	224	C
1	2A	225	C
1	2A	236	G
1	2A	238	G
1	2A	252	C
1	2A	253	A
1	2A	268	G
1	2A	270	U
1	2A	271	U
1	2A	272	G
1	2A	274	C
1	2A	287	U
1	2A	288	G
1	2A	301	A

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Mol	Chain	Res	Type
1	2A	334	A
1	2A	347	A
1	2A	350	G
1	2A	352	G
1	2A	353	A
1	2A	355	A
1	2A	357	C
1	2A	358	C
1	2A	361	G
1	2A	365	G
1	2A	375	G
1	2A	385	U
1	2A	386	G
1	2A	389	G
1	2A	412	G
1	2A	422	G
1	2A	431	U
1	2A	433	G
1	2A	437	G
1	2A	438	A
1	2A	441	A
1	2A	453	U
1	2A	454	A
1	2A	460	U
1	2A	468	A
1	2A	469	C
1	2A	471	G
1	2A	479	A
1	2A	480	C
1	2A	481	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	573	G

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Mol	Chain	Res	Type
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	615	G
1	2A	625	A
1	2A	626	G
1	2A	629	U
1	2A	637	U
1	2A	638	G
1	2A	639	A
1	2A	640	G
1	2A	651	A
1	2A	658	C
1	2A	661	A
1	2A	669	C
1	2A	670	A
1	2A	673	G
1	2A	678	A
1	2A	679	G
1	2A	697	G
1	2A	732	G
1	2A	763	G
1	2A	772	G
1	2A	776	C
1	2A	811	G
1	2A	817	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	838	G
1	2A	848	A
1	2A	851	G
1	2A	858	C
1	2A	865	A
1	2A	873	U
1	2A	874	U

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Mol	Chain	Res	Type
1	2A	903	C
1	2A	905	G
1	2A	906	U
1	2A	912	A
1	2A	915	G
1	2A	918	A
1	2A	924	A
1	2A	925	G
1	2A	926	G
1	2A	928	G
1	2A	930	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	945	A
1	2A	946	A
1	2A	955	A
1	2A	956	A
1	2A	960	C
1	2A	962	A
1	2A	975	G
1	2A	976	G
1	2A	980	C
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	1025	A
1	2A	1028	A
1	2A	1041	A
1	2A	1050	C
1	2A	1057	U

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Mol	Chain	Res	Type
1	2A	1058	C
1	2A	1066	A
1	2A	1067	G
1	2A	1070	G
1	2A	1078	U
1	2A	1088	C
1	2A	1090	A
1	2A	1091	A
1	2A	1092	G
1	2A	1093	A
1	2A	1103	G
1	2A	1104	G
1	2A	1105	U
1	2A	1106	U
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	1126	U
1	2A	1128	U
1	2A	1132	G
1	2A	1133	A
1	2A	1136	G
1	2A	1142	U
1	2A	1152	G
1	2A	1156	A
1	2A	1157	G
1	2A	1158	U
1	2A	1159	G
1	2A	1167	G
1	2A	1175	U
1	2A	1179	C
1	2A	1180	G
1	2A	1183	G
1	2A	1187	A
1	2A	1216	G
1	2A	1249	U
1	2A	1264	A

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Mol	Chain	Res	Type
1	2A	1265	C
1	2A	1266	C
1	2A	1276	G
1	2A	1281	G
1	2A	1284	G
1	2A	1295	G
1	2A	1297	G
1	2A	1298	A
1	2A	1301	G
1	2A	1316	G
1	2A	1317	A
1	2A	1318	U
1	2A	1345	U
1	2A	1346	A
1	2A	1348	G
1	2A	1350	C
1	2A	1359	C
1	2A	1374	U
1	2A	1387	A
1	2A	1399	A
1	2A	1400	G
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	1448	C
1	2A	1461	G
1	2A	1462	C
1	2A	1465	U
1	2A	1466	G
1	2A	1472	A
1	2A	1473	C
1	2A	1486	G
1	2A	1490	A
1	2A	1495	A
1	2A	1496	G
1	2A	1501	G
1	2A	1502	G

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Mol	Chain	Res	Type
1	2A	1507	G
1	2A	1513	C
1	2A	1517	A
1	2A	1524	G
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	1589	C
1	2A	1604	A
1	2A	1605	G
1	2A	1612	A
1	2A	1615	A
1	2A	1624	U
1	2A	1626	A
1	2A	1630	C
1	2A	1631	A
1	2A	1653	A
1	2A	1654	A
1	2A	1655	A
1	2A	1663	A
1	2A	1667	G
1	2A	1686	C
1	2A	1687	A
1	2A	1694	C
1	2A	1715	A
1	2A	1720	G
1	2A	1746	A
1	2A	1765	G
1	2A	1766	A
1	2A	1786	G
1	2A	1792	A
1	2A	1793	G
1	2A	1794	G
1	2A	1803	A
1	2A	1810	A
1	2A	1812	C
1	2A	1821	A

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Mol	Chain	Res	Type
1	2A	1830	C
1	2A	1831	G
1	2A	1846	G
1	2A	1859	A
1	2A	1869	G
1	2A	1877	A
1	2A	1889	A
1	2A	1898	A
1	2A	1899	G
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	1958	A
1	2A	1962	C
1	2A	1976	U
1	2A	1984	U
1	2A	1985	G
1	2A	1988	C
1	2A	1991	A
1	2A	1992	A
1	2A	1993	A
1	2A	2014	U
1	2A	2018	G
1	2A	2041	A
1	2A	2044	G
1	2A	2052	A
1	2A	2054	A
1	2A	2057	C
1	2A	2064	C
1	2A	2067	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	2120	U

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Mol	Chain	Res	Type
1	2A	2206	C
1	2A	2209	C
1	2A	2210	U
1	2A	2213	G
1	2A	2219	A
1	2A	2226	G
1	2A	2227	G
1	2A	2228	A
1	2A	2236	A
1	2A	2246	G
1	2A	2250	G
1	2A	2278	A
1	2A	2279	A
1	2A	2280	A
1	2A	2286	C
1	2A	2289	A
1	2A	2290	G
1	2A	2294	C
1	2A	2298	A
1	2A	2299	A
1	2A	2300	G
1	2A	2304	C
1	2A	2308	C
1	2A	2316	A
1	2A	2318	G
1	2A	2319	G
1	2A	2322	A
1	2A	2323	U
1	2A	2329	G
1	2A	2330	G
1	2A	2331	A
1	2A	2336	G
1	2A	2345	G
1	2A	2347	A
1	2A	2354	C
1	2A	2358	C
1	2A	2361	C
1	2A	2377	A
1	2A	2390	G
1	2A	2394	G
1	2A	2396	C
1	2A	2398	U

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Mol	Chain	Res	Type
1	2A	2413	C
1	2A	2417	U
1	2A	2421	G
1	2A	2430	U
1	2A	2433	A
1	2A	2436	A
1	2A	2439	G
1	2A	2440	G
1	2A	2441	A
1	2A	2446	A
1	2A	2450	A
1	2A	2452	C
1	2A	2456	G
1	2A	2459	A
1	2A	2476	C
1	2A	2480	A
1	2A	2485	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	2554	G
1	2A	2565	U
1	2A	2566	U
1	2A	2577	A
1	2A	2578	G
1	2A	2585	G
1	2A	2590	C
1	2A	2613	A
1	2A	2620	U
1	2A	2622	U
1	2A	2623	C
1	2A	2640	A
1	2A	2641	G
1	2A	2657	C
1	2A	2665	A

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Mol	Chain	Res	Type
1	2A	2700	U
1	2A	2701	C
1	2A	2714	C
1	2A	2724	A
1	2A	2725	A
1	2A	2726	G
1	2A	2738	U
1	2A	2745	A
1	2A	2756	G
1	2A	2763	G
1	2A	2769	A
1	2A	2776	A
1	2A	2777	A
1	2A	2778	G
1	2A	2790	A
1	2A	2795	G
1	2A	2801	C
1	2A	2805	G
1	2A	2812	G
1	2A	2817	U
1	2A	2827	G
1	2A	2829	A
1	2A	2830	A
1	2A	2842	G
1	2A	2843	G
1	2A	2845	U
1	2A	2869	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	2905	U
2	2B	2	C
2	2B	7	G
2	2B	9	G
2	2B	13	A
2	2B	16	G
2	2B	28	C
2	2B	34	U

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Mol	Chain	Res	Type
2	2B	43	C
2	2B	45	A
2	2B	46	A
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	59	A
2	2B	63	G
2	2B	67	G
2	2B	73	A
2	2B	85	G
2	2B	90	A
2	2B	110	G
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	6	U
32	2a	10	G
32	2a	15	U
32	2a	16	G
32	2a	23	G
32	2a	33	A
32	2a	39	G
32	2a	40	G
32	2a	48	C
32	2a	49	C
32	2a	51	A
32	2a	52	A
32	2a	66	U
32	2a	67	G
32	2a	74	G
32	2a	79	G
32	2a	84	A
32	2a	85	C
32	2a	91	G
32	2a	95	A
32	2a	110	A
32	2a	115	C
32	2a	123	U
32	2a	124	G
32	2a	126	C

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Mol	Chain	Res	Type
32	2a	138	A
32	2a	141	G
32	2a	151	G
32	2a	158	C
32	2a	169	C
32	2a	177	U
32	2a	202	A
32	2a	204	A
32	2a	211	U
32	2a	212	G
32	2a	213	C
32	2a	243	G
32	2a	247	G
32	2a	262	G
32	2a	263	C
32	2a	277	G
32	2a	285	G
32	2a	297	G
32	2a	317	A
32	2a	324	C
32	2a	326	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	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
32	2a	408	A
32	2a	418	C
32	2a	425	U
32	2a	426	A
32	2a	435	A
32	2a	437	C
32	2a	447	A

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Mol	Chain	Res	Type
32	2a	455	A
32	2a	456	C
32	2a	457	G
32	2a	463	A
32	2a	466	G
32	2a	470	G
32	2a	481	A
32	2a	482	U
32	2a	489	G
32	2a	495	C
32	2a	496	U
32	2a	497	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	529	C
32	2a	531	A
32	2a	543	A
32	2a	545	U
32	2a	546	C
32	2a	552	G
32	2a	556	A
32	2a	557	A
32	2a	560	G
32	2a	561	G
32	2a	575	U
32	2a	576	G
32	2a	580	C
32	2a	581	G
32	2a	591	A
32	2a	610	U
32	2a	614	G
32	2a	636	U
32	2a	637	A
32	2a	641	G
32	2a	649	A
32	2a	658	G
32	2a	671	A
32	2a	672	G

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Mol	Chain	Res	Type
32	2a	677	G
32	2a	679	A
32	2a	686	A
32	2a	696	A
32	2a	705	G
32	2a	707	U
32	2a	708	G
32	2a	715	G
32	2a	733	C
32	2a	737	A
32	2a	738	C
32	2a	739	G
32	2a	744	G
32	2a	754	C
32	2a	758	G
32	2a	761	A
32	2a	777	U
32	2a	778	A
32	2a	783	G
32	2a	800	A
32	2a	801	C
32	2a	805	G
32	2a	811	U
32	2a	812	A
32	2a	813	G
32	2a	824	C
32	2a	825	U
32	2a	826	C
32	2a	827	C
32	2a	831	G
32	2a	836	G
32	2a	837	A
32	2a	852	G
32	2a	880	G
32	2a	892	A
32	2a	904	G
32	2a	905	G
32	2a	909	C
32	2a	912	C
32	2a	913	A
32	2a	916	A
32	2a	920	G

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Mol	Chain	Res	Type
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	963	C
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	983	A
32	2a	984	A
32	2a	986	C
32	2a	988	G
32	2a	1000	G
32	2a	1001	G
32	2a	1002	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	1093	A
32	2a	1096	C
32	2a	1099	C
32	2a	1101	C
32	2a	1104	U
32	2a	1105	U

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Mol	Chain	Res	Type
32	2a	1107	G
32	2a	1110	G
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	1123	C
32	2a	1129	A
32	2a	1140	A
32	2a	1141	C
32	2a	1142	U
32	2a	1146	C
32	2a	1149	G
32	2a	1158	A
32	2a	1165	A
32	2a	1168	G
32	2a	1172	G
32	2a	1173	A
32	2a	1178	U
32	2a	1184	G
32	2a	1191	C
32	2a	1193	U
32	2a	1194	U
32	2a	1196	C
32	2a	1210	C
32	2a	1218	A
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	1243	A
32	2a	1244	C
32	2a	1255	G
32	2a	1260	U

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Mol	Chain	Res	Type
32	2a	1262	A
32	2a	1263	U
32	2a	1264	C
32	2a	1268	A
32	2a	1269	A
32	2a	1281	A
32	2a	1285	C
32	2a	1287	G
32	2a	1293	G
32	2a	1301	A
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	1335	G
32	2a	1341	C
32	2a	1342	A
32	2a	1345	C
32	2a	1347	U
32	2a	1353	G
32	2a	1359	U
32	2a	1380	C
32	2a	1381	A
32	2a	1402	G
32	2a	1425	G
32	2a	1426	G
32	2a	1427	A
32	2a	1430	C
32	2a	1431	U
32	2a	1432	A
32	2a	1433	C
32	2a	1434	G
32	2a	1469	G
32	2a	1480	A
32	2a	1481	A
32	2a	1482	G
32	2a	1483	G
32	2a	1484	U

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Mol	Chain	Res	Type
32	2a	1495	G
32	2a	1498	G
32	2a	1507	G
32	2a	1508	G
32	2a	1509	A
32	2a	1510	U
53	2v	15	A
54	2x	6	G
54	2x	9	G
54	2x	13	C
54	2x	16	C
54	2x	17	C
54	2x	17(A)	U
54	2x	21	A
54	2x	31	G
54	2x	42	G
54	2x	47	U
54	2x	55	PSU
54	2x	56	C
54	2x	65	C
54	2x	70	G
54	2x	76	A

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	183	A
1	1A	184	A
1	1A	270	U
1	1A	301	A
1	1A	516	A
1	1A	792	A
1	1A	873	U
1	1A	1018	G
1	1A	1047	G
1	1A	1153	U
1	1A	1218	A
1	1A	1220	G
1	1A	1285	U
1	1A	1425	G
1	1A	1653	A
1	1A	2013	G

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Mol	Chain	Res	Type
1	1A	2208	G
1	1A	2417	U
1	1A	2441	A
1	1A	2700	U
1	1A	2768	U
1	2A	183	A
1	2A	184	A
1	2A	203	G
1	2A	357	C
1	2A	516	A
1	2A	810	A
1	2A	902	C
1	2A	945	A
1	2A	1114	A
1	2A	1238	A
1	2A	1425	G
1	2A	1465	U
1	2A	1604	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
1	2A	2762	A
1	2A	2768	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	1.28	1 (7%)	17,32,35	1.04	1 (5%)
54	5MU	1x	54	54	13,22,23	0.63	1 (7%)	16,32,35	2.87	2 (12%)
54	PSU	1x	55	54	15,21,22	1.39	1 (6%)	16,30,33	2.40	4 (25%)
54	4SU	1x	8	54	12,21,22	0.89	1 (8%)	15,30,33	1.45	1 (6%)
54	5MC	2x	32	54	14,22,23	1.27	1 (7%)	17,32,35	0.96	1 (5%)
54	5MU	2x	54	54	13,22,23	0.55	0	16,32,35	2.87	2 (12%)
54	PSU	2x	55	54	15,21,22	1.16	1 (6%)	16,30,33	2.22	4 (25%)
54	4SU	2x	8	54	12,21,22	0.90	1 (8%)	15,30,33	1.66	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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	55	PSU	C5-C1'	-4.19	1.48	1.52
54	2x	55	PSU	C5-C1'	-3.29	1.49	1.52
54	1x	8	4SU	C2-N3	-2.78	1.32	1.38
54	2x	8	4SU	C2-N3	-2.75	1.32	1.38
54	1x	54	5MU	C2-N3	-2.03	1.34	1.38
54	2x	32	5MC	C5-C4	4.46	1.48	1.41
54	1x	32	5MC	C5-C4	4.51	1.48	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	54	5MU	C5-C4-N3	-8.19	118.47	125.35
54	1x	54	5MU	C5-C4-N3	-7.84	118.77	125.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	8	4SU	C5-C4-N3	-5.89	117.32	123.56
54	1x	8	4SU	C5-C4-N3	-5.16	118.09	123.56
54	2x	55	PSU	C5-C6-N1	-3.40	119.64	124.38
54	1x	55	PSU	C5-C6-N1	-2.63	120.71	124.38
54	2x	55	PSU	C5-C1'-C2'	-2.40	111.36	115.44
54	1x	55	PSU	C5-C1'-C2'	-2.26	111.60	115.44
54	2x	32	5MC	N4-C4-N3	2.40	120.44	116.92
54	2x	55	PSU	O4'-C1'-C2'	2.52	107.41	104.69
54	1x	55	PSU	O4'-C1'-C2'	2.54	107.44	104.69
54	1x	32	5MC	N4-C4-N3	2.75	120.94	116.92
54	2x	55	PSU	C4-N3-C2	6.94	120.95	115.16
54	2x	54	5MU	C4-N3-C2	7.75	121.62	115.16
54	1x	55	PSU	C4-N3-C2	8.09	121.91	115.16
54	1x	54	5MU	C4-N3-C2	8.11	121.93	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2436 ligands modelled in this entry, 2434 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	501	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	501	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2746/2915 (94%)	-0.07	16 (0%) 90 86	20, 42, 84, 108	0
1	2A	2790/2915 (95%)	-0.34	41 (1%) 76 68	24, 46, 91, 108	0
2	1B	120/121 (99%)	-0.22	0 100 100	35, 63, 80, 89	0
2	2B	120/121 (99%)	-0.06	1 (0%) 87 81	41, 68, 82, 91	0
3	1D	275/276 (99%)	-0.35	0 100 100	21, 40, 56, 78	0
3	2D	275/276 (99%)	-0.45	1 (0%) 93 90	22, 42, 59, 78	0
4	1E	204/206 (99%)	-0.21	0 100 100	21, 44, 65, 84	0
4	2E	204/206 (99%)	-0.25	0 100 100	23, 47, 67, 85	0
5	1F	203/210 (96%)	-0.24	0 100 100	22, 50, 74, 88	0
5	2F	203/210 (96%)	-0.31	1 (0%) 91 88	23, 54, 77, 90	0
6	1G	181/182 (99%)	-0.20	3 (1%) 73 63	50, 67, 79, 91	0
6	2G	181/182 (99%)	0.42	18 (9%) 9 4	54, 71, 81, 92	0
7	1H	174/180 (96%)	-0.13	1 (0%) 90 86	48, 63, 75, 85	0
7	2H	174/180 (96%)	0.74	22 (12%) 5 2	52, 68, 79, 86	0
8	1I	146/148 (98%)	0.06	1 (0%) 89 84	46, 74, 84, 90	0
8	2I	146/148 (98%)	0.47	6 (4%) 41 29	48, 74, 84, 90	0
9	1N	140/140 (100%)	-0.24	0 100 100	29, 47, 65, 76	0
9	2N	140/140 (100%)	-0.05	0 100 100	33, 50, 68, 78	0
10	1O	122/122 (100%)	-0.32	0 100 100	32, 44, 61, 74	0
10	2O	122/122 (100%)	-0.40	0 100 100	34, 47, 62, 74	0
11	1P	149/150 (99%)	-0.20	0 100 100	22, 53, 74, 81	0
11	2P	149/150 (99%)	0.23	6 (4%) 42 30	24, 56, 76, 83	0
12	1Q	141/141 (100%)	-0.09	1 (0%) 89 84	32, 48, 61, 79	0
12	2Q	141/141 (100%)	-0.37	1 (0%) 89 84	35, 51, 64, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.21	0 100 100	27, 39, 50, 64	0
13	2R	118/118 (100%)	-0.36	0 100 100	30, 42, 54, 66	0
14	1S	110/112 (98%)	-0.09	0 100 100	43, 61, 71, 77	0
14	2S	110/112 (98%)	0.59	9 (8%) 14 7	48, 63, 76, 79	0
15	1T	131/146 (89%)	-0.27	0 100 100	37, 49, 72, 84	0
15	2T	131/146 (89%)	-0.39	0 100 100	40, 50, 73, 83	0
16	1U	116/118 (98%)	-0.19	0 100 100	27, 39, 56, 74	0
16	2U	116/118 (98%)	-0.34	1 (0%) 85 79	29, 43, 61, 74	0
17	1V	101/101 (100%)	-0.24	0 100 100	28, 47, 65, 75	0
17	2V	101/101 (100%)	-0.05	0 100 100	32, 53, 69, 76	0
18	1W	112/113 (99%)	-0.35	1 (0%) 85 79	27, 36, 55, 89	0
18	2W	112/113 (99%)	-0.26	0 100 100	28, 39, 57, 90	0
19	1X	95/96 (98%)	-0.19	0 100 100	26, 46, 66, 81	0
19	2X	95/96 (98%)	-0.09	3 (3%) 51 39	29, 49, 68, 81	0
20	1Y	107/110 (97%)	-0.03	1 (0%) 85 79	42, 59, 76, 86	0
20	2Y	107/110 (97%)	0.61	6 (5%) 28 18	47, 62, 79, 88	0
21	1Z	186/206 (90%)	-0.38	0 100 100	48, 66, 79, 89	0
21	2Z	186/206 (90%)	0.43	11 (5%) 26 16	53, 69, 81, 91	0
22	10	75/85 (88%)	-0.49	0 100 100	18, 36, 48, 61	0
22	20	75/85 (88%)	0.27	4 (5%) 30 20	46, 62, 73, 80	0
23	11	97/98 (98%)	-0.19	1 (1%) 84 77	28, 48, 72, 77	0
23	21	97/98 (98%)	-0.16	1 (1%) 84 77	31, 51, 72, 75	0
24	12	70/72 (97%)	-0.16	0 100 100	43, 56, 70, 74	0
24	22	70/72 (97%)	0.05	1 (1%) 78 69	46, 60, 73, 74	0
25	13	59/60 (98%)	-0.13	0 100 100	32, 44, 64, 77	0
25	23	59/60 (98%)	0.54	1 (1%) 73 63	35, 48, 66, 77	0
26	14	69/71 (97%)	0.05	6 (8%) 13 6	47, 71, 93, 97	0
26	24	69/71 (97%)	0.71	11 (15%) 3 1	56, 89, 96, 98	0
27	15	59/60 (98%)	-0.60	0 100 100	16, 28, 46, 72	0
27	25	59/60 (98%)	-0.35	0 100 100	29, 49, 66, 75	0
28	16	53/54 (98%)	-0.46	0 100 100	24, 38, 54, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	-0.29	0 100 100	41, 58, 74, 79	0
29	17	48/49 (97%)	-0.18	1 (2%) 67 56	24, 32, 64, 78	0
29	27	48/49 (97%)	-0.13	3 (6%) 23 14	27, 34, 66, 77	0
30	18	64/65 (98%)	-0.14	0 100 100	32, 39, 49, 60	0
30	28	64/65 (98%)	-0.07	1 (1%) 74 66	35, 43, 54, 62	0
31	19	37/37 (100%)	0.07	0 100 100	38, 49, 66, 70	0
31	29	37/37 (100%)	0.39	3 (8%) 15 7	44, 52, 67, 72	0
32	1a	1477/1521 (97%)	-0.11	32 (2%) 65 54	32, 70, 96, 113	0
32	2a	1483/1521 (97%)	-0.04	28 (1%) 70 59	44, 77, 98, 111	0
33	1b	231/256 (90%)	0.35	18 (7%) 16 8	66, 81, 93, 101	0
33	2b	231/256 (90%)	0.54	22 (9%) 10 5	68, 86, 96, 102	0
34	1c	206/239 (86%)	0.23	14 (6%) 20 12	65, 81, 88, 95	0
34	2c	206/239 (86%)	0.47	16 (7%) 16 8	69, 82, 89, 93	0
35	1d	208/209 (99%)	0.18	10 (4%) 34 23	51, 75, 88, 96	0
35	2d	208/209 (99%)	-0.02	1 (0%) 91 88	58, 73, 85, 90	0
36	1e	148/162 (91%)	-0.21	0 100 100	45, 67, 77, 84	0
36	2e	148/162 (91%)	-0.19	0 100 100	56, 74, 83, 89	0
37	1f	100/101 (99%)	-0.23	0 100 100	57, 72, 80, 88	0
37	2f	100/101 (99%)	-0.24	2 (2%) 68 58	58, 73, 83, 87	0
38	1g	155/156 (99%)	0.34	12 (7%) 16 8	67, 77, 91, 95	0
38	2g	155/156 (99%)	0.68	13 (8%) 14 6	67, 78, 90, 93	0
39	1h	137/138 (99%)	-0.06	0 100 100	53, 69, 77, 85	0
39	2h	137/138 (99%)	0.11	2 (1%) 76 68	65, 76, 83, 89	0
40	1i	127/128 (99%)	0.51	10 (7%) 15 8	64, 83, 91, 95	0
40	2i	127/128 (99%)	1.21	25 (19%) 1 1	65, 84, 92, 98	0
41	1j	97/105 (92%)	0.90	13 (13%) 4 2	67, 85, 93, 97	0
41	2j	96/105 (91%)	1.07	14 (14%) 3 2	69, 86, 94, 97	0
42	1k	114/129 (88%)	-0.07	2 (1%) 71 61	43, 67, 80, 88	0
42	2k	114/129 (88%)	0.25	3 (2%) 59 47	56, 76, 86, 91	0
43	1l	122/132 (92%)	-0.17	1 (0%) 87 81	43, 61, 72, 79	0
43	2l	122/132 (92%)	-0.05	3 (2%) 61 48	52, 67, 75, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	118/126 (93%)	0.11	0 100 100	59, 77, 85, 94	0
44	2m	116/126 (92%)	0.34	12 (10%) 9 4	66, 80, 86, 93	0
45	1n	60/61 (98%)	0.30	3 (5%) 32 21	62, 73, 83, 84	0
45	2n	60/61 (98%)	1.29	14 (23%) 1 1	76, 84, 90, 92	0
46	1o	88/89 (98%)	0.03	1 (1%) 82 74	47, 64, 80, 90	0
46	2o	88/89 (98%)	0.11	1 (1%) 82 74	58, 72, 83, 86	0
47	1p	82/88 (93%)	0.57	5 (6%) 25 15	61, 76, 87, 94	0
47	2p	82/88 (93%)	0.28	2 (2%) 62 50	57, 70, 82, 90	0
48	1q	99/105 (94%)	-0.02	0 100 100	47, 67, 78, 82	0
48	2q	99/105 (94%)	0.16	3 (3%) 54 41	56, 72, 80, 87	0
49	1r	68/88 (77%)	0.40	3 (4%) 38 26	54, 68, 81, 87	0
49	2r	68/88 (77%)	0.60	7 (10%) 9 4	61, 72, 82, 92	0
50	1s	84/93 (90%)	0.58	3 (3%) 46 34	66, 78, 86, 97	0
50	2s	83/93 (89%)	1.48	23 (27%) 1 0	73, 89, 96, 103	0
51	1t	96/106 (90%)	0.25	1 (1%) 84 77	58, 73, 81, 88	0
51	2t	96/106 (90%)	0.20	0 100 100	57, 71, 81, 86	0
52	1u	23/27 (85%)	0.71	1 (4%) 39 27	68, 75, 80, 84	0
52	2u	23/27 (85%)	1.40	6 (26%) 1 0	69, 76, 83, 85	0
53	1v	5/24 (20%)	0.22	0 100 100	63, 66, 85, 92	0
53	2v	5/24 (20%)	0.95	1 (20%) 1 1	66, 69, 85, 93	0
54	1x	72/77 (93%)	-0.15	0 100 100	32, 66, 81, 96	0
54	2x	72/77 (93%)	0.03	1 (1%) 78 69	34, 69, 83, 97	0
55	1z	13/19 (68%)	0.14	0 100 100	26, 36, 52, 56	0
55	2z	12/19 (63%)	-0.05	0 100 100	28, 39, 53, 55	0
All	All	20521/21482 (95%)	-0.03	512 (2%) 61 48	16, 61, 89, 113	0

All (512) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	1a	980	G	8.6
32	1a	981	G	7.6
1	2A	2812	G	6.4
38	1g	81	GLY	6.3
32	1a	979	A	6.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	2Y	1	MET	5.8
32	2a	981	G	5.7
41	1j	10	GLY	5.6
38	1g	79	ARG	5.6
40	2i	21	PRO	5.6
20	1Y	1	MET	5.5
32	2a	980	G	5.4
38	2g	82	GLY	5.4
32	2a	979	A	5.4
40	2i	7	THR	5.3
38	2g	83	ALA	5.3
52	2u	14	TRP	5.2
32	1a	982	G	5.1
38	2g	156	TRP	5.0
31	29	37	GLY	4.7
1	2A	2811	A	4.7
41	1j	98	ILE	4.7
45	2n	25	VAL	4.7
38	1g	80	VAL	4.6
1	1A	2815	G	4.5
1	1A	1554	C	4.5
7	2H	112	PRO	4.4
32	1a	209	U	4.4
34	2c	189	ALA	4.4
38	2g	78	ARG	4.4
38	1g	156	TRP	4.4
41	2j	75	ILE	4.3
29	17	48	LYS	4.3
26	24	49	PHE	4.3
38	1g	82	GLY	4.3
32	1a	211	U	4.3
41	2j	6	ILE	4.3
50	2s	12	ASP	4.3
1	2A	2815	G	4.3
33	2b	152	PHE	4.3
33	1b	214	ILE	4.2
33	2b	132	LYS	4.2
50	2s	31	ILE	4.2
7	2H	115	VAL	4.2
45	2n	49	HIS	4.2
1	2A	1091	A	4.2
26	24	68	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
52	2u	6	ARG	4.1
7	2H	111	HIS	4.0
40	2i	8	GLY	4.0
40	1i	15	ALA	4.0
40	2i	15	ALA	4.0
33	2b	133	LYS	3.9
40	2i	61	ALA	3.9
49	1r	25	THR	3.9
6	2G	28	VAL	3.9
26	24	45	GLY	3.9
41	2j	63	PHE	3.9
32	1a	978	U	3.8
1	2A	2904	C	3.8
14	2S	58	LEU	3.8
38	2g	154	TYR	3.7
34	1c	81	GLY	3.7
7	2H	113	VAL	3.7
50	2s	16	LEU	3.7
1	2A	2813	C	3.7
32	2a	1509	A	3.7
49	2r	66	LEU	3.7
1	2A	1554	C	3.7
1	2A	2805	G	3.7
32	2a	1510	U	3.7
32	2a	978	U	3.6
41	2j	20	ALA	3.6
33	2b	187	LEU	3.6
32	2a	982	G	3.6
34	2c	159	GLY	3.6
40	2i	66	ARG	3.6
33	2b	131	PRO	3.6
45	2n	36	PHE	3.5
49	2r	46	GLU	3.5
33	1b	227	GLY	3.5
35	1d	23	GLY	3.5
41	1j	85	LEU	3.5
1	2A	678	A	3.5
26	14	55	ARG	3.5
38	2g	80	VAL	3.4
34	1c	87	LEU	3.4
45	2n	39	LEU	3.4
21	2Z	5	LEU	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	1i	19	LEU	3.4
40	2i	36	TYR	3.4
19	2X	92	LEU	3.3
50	2s	8	GLY	3.3
38	2g	84	ASN	3.3
41	1j	90	LEU	3.3
33	1b	28	PHE	3.3
34	2c	180	ALA	3.3
41	1j	72	VAL	3.3
50	2s	38	SER	3.3
35	2d	130	GLY	3.3
48	2q	8	GLY	3.3
40	2i	41	VAL	3.3
26	24	67	TYR	3.3
41	1j	96	ILE	3.3
32	1a	1025	G	3.3
33	2b	97	TRP	3.3
20	2Y	5	MET	3.2
19	2X	69	TYR	3.2
32	2a	1239	U	3.2
41	2j	72	VAL	3.2
34	2c	57	ILE	3.2
32	2a	1000	G	3.2
32	1a	1023	U	3.2
1	2A	2902	G	3.2
40	2i	62	TYR	3.2
1	2A	2806	C	3.2
7	2H	103	LEU	3.2
41	2j	85	LEU	3.2
1	2A	1106	U	3.2
6	2G	137	GLU	3.2
1	1A	2206	C	3.2
1	1A	2806	C	3.2
1	2A	217	A	3.2
31	29	5	ALA	3.2
8	2I	11	ASN	3.2
25	23	26	LEU	3.2
40	2i	9	ARG	3.1
32	1a	1024	A	3.1
40	1i	98	PRO	3.1
21	2Z	160	GLY	3.1
39	2h	122	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	1A	2205	G	3.1
32	2a	1025	G	3.1
33	1b	135	GLN	3.1
40	1i	33	PHE	3.1
40	2i	37	PHE	3.1
34	2c	179	ARG	3.1
50	1s	56	GLN	3.1
32	2a	1265	G	3.1
50	2s	80	TYR	3.1
50	2s	20	LEU	3.1
50	2s	43	GLU	3.1
1	1A	2814	C	3.1
6	2G	25	TYR	3.1
38	1g	78	ARG	3.1
34	2c	154	SER	3.0
50	2s	40	ILE	3.0
50	2s	52	TYR	3.0
7	2H	114	VAL	3.0
1	1A	2813	C	3.0
32	2a	1021	C	3.0
32	2a	1022	C	3.0
1	1A	2805	G	3.0
33	2b	232	PRO	3.0
41	2j	98	ILE	3.0
42	1k	13	GLN	3.0
44	2m	82	MET	3.0
6	2G	2	PRO	3.0
45	2n	35	ARG	3.0
46	2o	87	ILE	3.0
32	1a	88	C	3.0
41	1j	71	LEU	3.0
42	2k	31	THR	3.0
42	2k	13	GLN	3.0
7	2H	107	VAL	3.0
6	1G	51	ARG	3.0
38	2g	16	LEU	3.0
49	2r	85	LEU	3.0
1	2A	2816	G	3.0
32	1a	208	C	3.0
45	2n	37	PHE	2.9
1	2A	2121	G	2.9
1	2A	1130	A	2.9

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Mol	Chain	Res	Type	RSRZ
32	1a	984	A	2.9
49	2r	43	PHE	2.9
38	2g	86	GLN	2.9
47	1p	51	VAL	2.9
53	2v	14	A	2.9
38	1g	153	HIS	2.9
7	2H	6	ARG	2.9
44	2m	102	ARG	2.9
34	2c	155	GLY	2.9
44	2m	95	GLY	2.9
41	1j	66	ARG	2.9
32	2a	211	U	2.9
49	2r	23	LYS	2.9
8	2I	14	ASP	2.9
7	2H	102	ALA	2.9
33	1b	232	PRO	2.9
50	2s	76	PRO	2.9
50	2s	13	ASP	2.9
50	2s	53	ASN	2.9
1	2A	1149	C	2.9
50	2s	34	TRP	2.9
32	2a	1268	A	2.9
34	2c	39	ILE	2.9
41	2j	8	LEU	2.9
41	2j	81	THR	2.9
32	1a	1239	U	2.9
33	2b	227	GLY	2.9
34	1c	206	GLU	2.8
32	1a	1002	G	2.8
49	2r	58	LEU	2.8
24	22	1	MET	2.8
41	1j	4	ILE	2.8
35	1d	152	SER	2.8
1	2A	1104	G	2.8
6	2G	48	GLU	2.8
19	2X	68	ARG	2.8
1	1A	2905	U	2.8
50	2s	49	ILE	2.8
32	1a	977	C	2.8
1	2A	697	G	2.8
7	2H	110	SER	2.8
50	2s	41	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
11	2P	91	PHE	2.7
34	2c	77	ILE	2.7
7	2H	105	LEU	2.7
33	2b	197	VAL	2.7
34	1c	78	GLY	2.7
7	1H	2	SER	2.7
38	2g	79	ARG	2.7
49	1r	31	LEU	2.7
50	2s	71	LEU	2.7
38	2g	105	VAL	2.7
40	2i	20	ARG	2.7
52	2u	9	ARG	2.7
20	2Y	45	VAL	2.7
47	2p	59	TRP	2.7
40	1i	36	TYR	2.7
21	2Z	143	GLY	2.7
26	24	59	PHE	2.6
1	2A	1129	A	2.6
1	2A	2814	C	2.6
32	1a	72	C	2.6
1	2A	1089	G	2.6
32	1a	999	U	2.6
47	1p	19	ILE	2.6
50	2s	24	ALA	2.6
33	1b	16	HIS	2.6
50	2s	35	SER	2.6
32	2a	983	A	2.6
32	2a	1024	A	2.6
44	2m	75	ALA	2.6
6	2G	27	ASN	2.6
26	14	53	GLU	2.6
8	2I	77	LEU	2.6
40	2i	5	TYR	2.6
20	2Y	2	ARG	2.6
22	20	72	ARG	2.6
14	2S	54	LEU	2.6
35	1d	167	GLY	2.6
21	2Z	96	VAL	2.6
34	2c	66	VAL	2.6
1	2A	2905	U	2.6
32	1a	985	C	2.6
33	2b	101	MET	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	2I	19	VAL	2.6
34	1c	100	ALA	2.6
52	1u	18	TYR	2.6
14	2S	29	PHE	2.6
45	2n	42	ILE	2.5
41	1j	97	GLU	2.5
50	1s	16	LEU	2.5
6	1G	49	ASP	2.5
32	1a	87	C	2.5
43	2l	64	TYR	2.5
41	2j	27	ALA	2.5
41	1j	78	ASN	2.5
32	2a	1023	U	2.5
34	2c	6	HIS	2.5
43	2l	62	SER	2.5
1	1A	1220	G	2.5
33	2b	118	LEU	2.5
35	1d	176	LEU	2.5
52	2u	22	ARG	2.5
6	2G	86	MET	2.5
54	2x	47	U	2.5
32	1a	1026	C	2.5
34	1c	65	ALA	2.5
38	1g	83	ALA	2.5
12	2Q	59	ARG	2.5
45	2n	38	GLY	2.5
1	2A	1128	U	2.5
7	2H	106	THR	2.5
44	2m	7	VAL	2.5
34	2c	186	PHE	2.5
37	2f	97	PHE	2.5
1	1A	1149	C	2.5
7	2H	128	PRO	2.5
1	2A	2804	G	2.5
52	2u	17	THR	2.5
22	20	69	PHE	2.5
33	2b	31	TYR	2.5
6	2G	142	PRO	2.5
14	2S	84	GLN	2.5
32	2a	1002	G	2.5
34	2c	87	LEU	2.5
22	20	45	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
44	2m	94	ARG	2.4
7	2H	44	VAL	2.4
33	1b	122	PHE	2.4
11	2P	116	GLY	2.4
20	2Y	58	GLY	2.4
26	24	46	GLN	2.4
6	2G	29	TRP	2.4
21	2Z	161	VAL	2.4
33	1b	233	SER	2.4
1	2A	1132	G	2.4
14	2S	34	HIS	2.4
33	1b	222	ILE	2.4
3	2D	273	ARG	2.4
11	2P	90	ARG	2.4
21	2Z	164	ALA	2.4
21	2Z	171	ILE	2.4
33	1b	201	ILE	2.4
11	2P	122	PRO	2.4
32	2a	209	U	2.4
32	2a	999	U	2.4
32	2a	977	C	2.4
32	2a	986	C	2.4
45	2n	2	ALA	2.4
1	2A	2125	G	2.4
49	2r	56	THR	2.4
33	1b	225	ALA	2.4
32	1a	1022	C	2.4
40	2i	63	ILE	2.4
20	2Y	51	VAL	2.4
26	14	59	PHE	2.4
31	29	13	LYS	2.4
45	2n	8	GLU	2.4
47	1p	39	TYR	2.4
7	2H	95	ARG	2.4
12	1Q	59	ARG	2.4
44	2m	92	HIS	2.4
38	2g	130	GLY	2.4
26	24	52	THR	2.4
1	2A	1102	A	2.4
23	11	2	SER	2.4
45	1n	2	ALA	2.4
16	2U	88	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
21	2Z	133	ILE	2.4
33	1b	130	ARG	2.4
50	1s	40	ILE	2.4
1	1A	2904	C	2.4
33	2b	122	PHE	2.3
32	1a	86	U	2.3
1	2A	1101	G	2.3
43	2l	28	LYS	2.3
33	2b	162	ILE	2.3
40	2i	79	LEU	2.3
51	1t	55	ILE	2.3
1	2A	300	C	2.3
32	1a	1268	A	2.3
1	1A	2209	C	2.3
34	1c	64	VAL	2.3
40	2i	88	TYR	2.3
34	2c	160	ALA	2.3
6	2G	19	LEU	2.3
38	1g	84	ASN	2.3
6	2G	42	GLY	2.3
33	2b	228	GLY	2.3
1	1A	2804	G	2.3
6	2G	26	GLN	2.3
40	2i	28	VAL	2.3
32	1a	707	U	2.3
26	14	57	GLU	2.3
14	2S	35	ILE	2.3
44	2m	103	THR	2.3
1	2A	1553	A	2.3
32	2a	1026	C	2.3
45	2n	48	ALA	2.3
34	1c	39	ILE	2.3
41	1j	6	ILE	2.3
33	2b	48	MET	2.3
40	2i	92	TYR	2.3
38	1g	3	ARG	2.3
40	2i	6	GLY	2.3
40	2i	10	ARG	2.3
45	1n	7	ILE	2.3
33	2b	37	ASN	2.3
35	1d	175	SER	2.3
40	2i	26	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
5	2F	14	PRO	2.3
7	2H	96	ALA	2.3
22	20	75	LEU	2.3
18	1W	111	HIS	2.3
32	2a	998	C	2.3
34	2c	124	ILE	2.3
39	2h	131	GLY	2.3
40	2i	72	GLY	2.3
41	2j	74	ILE	2.3
43	1l	64	TYR	2.3
32	2a	976	G	2.3
1	2A	2817	U	2.2
6	2G	17	PRO	2.2
14	2S	26	LEU	2.2
33	2b	10	LEU	2.2
6	2G	160	VAL	2.2
2	2B	118	G	2.2
32	1a	1121	G	2.2
1	2A	1071	U	2.2
33	2b	62	ALA	2.2
40	1i	63	ILE	2.2
47	2p	19	ILE	2.2
37	2f	6	VAL	2.2
30	28	21	LYS	2.2
41	1j	69	ASN	2.2
32	1a	825	U	2.2
44	2m	78	ILE	2.2
1	1A	1098	C	2.2
48	2q	100	LYS	2.2
41	2j	78	ASN	2.2
50	2s	42	PRO	2.2
42	1k	25	TYR	2.2
32	1a	1120	C	2.2
26	14	49	PHE	2.2
32	1a	983	A	2.2
40	1i	37	PHE	2.2
26	24	8	LYS	2.2
34	1c	193	TYR	2.2
7	2H	52	VAL	2.2
35	1d	104	VAL	2.2
7	2H	101	ARG	2.2
21	2Z	125	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
21	2Z	163	LEU	2.2
34	1c	160	ALA	2.2
34	1c	2	GLY	2.2
11	2P	85	LEU	2.2
50	2s	23	ASN	2.2
1	2A	1120	C	2.2
6	2G	139	LEU	2.2
33	2b	70	PHE	2.2
6	2G	39	ILE	2.2
35	1d	158	ILE	2.2
38	1g	77	SER	2.2
29	27	47	ARG	2.2
45	2n	18	VAL	2.2
34	1c	80	GLY	2.1
1	2A	2903	U	2.1
32	2a	707	U	2.1
47	1p	59	TRP	2.1
32	2a	1148	C	2.1
46	1o	89	GLY	2.1
1	2A	1087	G	2.1
26	24	66	SER	2.1
32	1a	1000	G	2.1
40	1i	28	VAL	2.1
40	2i	27	THR	2.1
7	2H	164	TYR	2.1
7	2H	97	ARG	2.1
44	2m	110	ARG	2.1
45	2n	7	ILE	2.1
6	1G	2	PRO	2.1
35	1d	169	LYS	2.1
40	2i	99	LEU	2.1
44	2m	80	ARG	2.1
44	2m	104	ARG	2.1
7	2H	92	ILE	2.1
1	2A	2206	C	2.1
8	2I	13	GLY	2.1
26	14	50	VAL	2.1
40	2i	30	GLY	2.1
33	1b	33	TYR	2.1
33	1b	70	PHE	2.1
33	2b	134	GLU	2.1
48	2q	22	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
50	2s	64	GLU	2.1
1	2A	1090	A	2.1
29	27	48	LYS	2.1
26	24	54	GLY	2.1
8	2I	81	VAL	2.1
29	27	46	VAL	2.1
40	1i	41	VAL	2.1
41	2j	34	VAL	2.1
50	2s	45	VAL	2.1
33	1b	221	LEU	2.1
49	1r	29	PHE	2.1
7	2H	45	VAL	2.1
1	1A	695	C	2.1
38	2g	77	SER	2.1
6	2G	161	THR	2.1
45	2n	34	TYR	2.1
35	1d	180	GLY	2.1
40	1i	8	GLY	2.1
14	2S	31	SER	2.1
33	2b	233	SER	2.1
21	2Z	146	ILE	2.1
26	24	44	THR	2.1
34	1c	179	ARG	2.1
33	1b	229	VAL	2.1
35	1d	165	MET	2.1
32	1a	986	C	2.0
47	1p	38	TYR	2.0
52	2u	13	ILE	2.0
1	2A	1088	C	2.0
11	2P	2	LYS	2.0
33	1b	129	GLU	2.0
34	1c	201	TYR	2.0
38	1g	130	GLY	2.0
45	1n	8	GLU	2.0
6	2G	15	VAL	2.0
8	1I	35	LEU	2.0
42	2k	125	PHE	2.0
1	2A	934	C	2.0
33	1b	187	LEU	2.0
41	2j	38	ILE	2.0
23	21	2	SER	2.0
1	2A	1103	G	2.0

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Mol	Chain	Res	Type	RSRZ
32	1a	212	G	2.0
34	2c	167	TRP	2.0
14	2S	110	LEU	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	4SU	1x	8	20/21	0.95	0.13	-	58,63,74,74	0
54	5MU	1x	54	21/22	0.95	0.14	-	55,62,73,81	0
54	PSU	1x	55	20/21	0.93	0.15	-	51,64,77,80	0
54	PSU	2x	55	20/21	0.87	0.14	-	54,68,77,91	0
54	5MU	2x	54	21/22	0.92	0.17	-	68,73,80,91	0
54	4SU	2x	8	20/21	0.94	0.12	-	73,78,85,87	0
54	5MC	2x	32	21/22	0.94	0.21	-	61,75,84,88	0
54	5MC	1x	32	21/22	0.97	0.17	-	40,61,68,75	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(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3918	1/1	0.73	0.82	105.36	47,47,47,47	0
56	MG	1A	3510	1/1	0.80	0.69	50.41	62,62,62,62	0
56	MG	1A	3079	1/1	0.93	0.53	44.39	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	3432	1/1	0.95	0.42	42.86	52,52,52,52	0
56	MG	1A	3305	1/1	0.90	0.41	40.44	52,52,52,52	0
56	MG	1A	3485	1/1	0.80	0.74	39.05	58,58,58,58	0
56	MG	1A	3375	1/1	0.89	0.47	37.53	62,62,62,62	0
56	MG	1A	4093	1/1	0.88	0.69	33.16	39,39,39,39	0
56	MG	2A	3100	1/1	0.94	0.39	32.64	38,38,38,38	0
56	MG	1A	4055	1/1	0.90	0.74	30.75	53,53,53,53	0
56	MG	2A	3140	1/1	0.99	0.38	30.68	35,35,35,35	0
56	MG	1A	3186	1/1	0.92	0.47	29.92	36,36,36,36	0
56	MG	1A	3730	1/1	0.93	0.42	27.78	59,59,59,59	0
56	MG	1A	3140	1/1	0.96	0.58	25.11	38,38,38,38	0
56	MG	1A	3509	1/1	0.94	0.41	24.24	43,43,43,43	0
56	MG	2A	3186	1/1	0.89	0.28	23.64	35,35,35,35	0
56	MG	1A	3360	1/1	0.94	0.41	21.88	48,48,48,48	0
56	MG	2A	3493	1/1	0.92	0.29	21.86	57,57,57,57	0
56	MG	2a	1799	1/1	0.93	0.48	21.58	56,56,56,56	0
56	MG	1N	202	1/1	0.93	0.46	21.54	49,49,49,49	0
56	MG	1A	3498	1/1	0.89	0.39	21.53	44,44,44,44	0
56	MG	1A	3847	1/1	0.90	0.59	20.50	40,40,40,40	0
56	MG	2A	3196	1/1	0.97	0.38	20.49	51,51,51,51	0
56	MG	1U	204	1/1	0.90	0.49	20.28	33,33,33,33	0
56	MG	2A	3105	1/1	0.97	0.35	20.27	29,29,29,29	0
56	MG	1A	3007	1/1	0.94	0.44	20.23	43,43,43,43	0
56	MG	1A	3148	1/1	0.80	0.41	20.21	43,43,43,43	0
56	MG	1A	4045	1/1	0.94	0.40	19.88	34,34,34,34	0
56	MG	2A	3555	1/1	0.81	0.37	19.83	50,50,50,50	0
56	MG	1A	3035	1/1	0.93	0.44	19.36	59,59,59,59	0
56	MG	1A	3262	1/1	0.96	0.69	19.25	43,43,43,43	0
56	MG	1A	4073	1/1	0.90	0.44	18.83	47,47,47,47	0
56	MG	2A	3145	1/1	0.95	0.32	18.71	33,33,33,33	0
56	MG	1a	1723	1/1	0.97	0.32	18.51	48,48,48,48	0
56	MG	2A	3356	1/1	0.74	0.27	18.24	41,41,41,41	0
56	MG	1A	3512	1/1	0.96	0.34	18.20	34,34,34,34	0
56	MG	2a	1701	1/1	0.94	0.33	17.68	46,46,46,46	0
56	MG	1a	1732	1/1	0.95	0.44	17.54	42,42,42,42	0
56	MG	1A	3839	1/1	0.94	0.31	17.33	28,28,28,28	0
56	MG	1A	3241	1/1	0.96	0.32	17.23	30,30,30,30	0
56	MG	2A	3315	1/1	0.97	0.25	17.12	50,50,50,50	0
56	MG	2a	1817	1/1	0.86	0.78	16.59	84,84,84,84	0
56	MG	1A	3610	1/1	0.94	0.26	16.44	27,27,27,27	0
56	MG	1A	4074	1/1	0.94	0.47	16.41	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4088	1/1	0.94	0.47	16.28	35,35,35,35	0
56	MG	2A	3277	1/1	0.93	0.31	16.08	42,42,42,42	0
56	MG	2A	3532	1/1	0.93	0.39	15.98	43,43,43,43	0
56	MG	1A	3473	1/1	0.92	0.52	15.96	47,47,47,47	0
56	MG	2A	3419	1/1	0.94	0.21	15.96	45,45,45,45	0
56	MG	1A	4092	1/1	0.97	0.48	15.92	33,33,33,33	0
56	MG	2a	1704	1/1	0.80	0.39	15.72	57,57,57,57	0
56	MG	2A	3322	1/1	0.97	0.30	15.48	41,41,41,41	0
56	MG	2A	3176	1/1	0.93	0.30	15.29	37,37,37,37	0
56	MG	1a	1753	1/1	0.95	0.55	15.20	53,53,53,53	0
56	MG	2a	1806	1/1	0.90	0.33	15.16	57,57,57,57	0
56	MG	1A	3948	1/1	0.95	0.35	15.14	56,56,56,56	0
56	MG	1A	3996	1/1	0.97	0.47	14.96	32,32,32,32	0
56	MG	1A	3136	1/1	0.86	0.45	14.56	39,39,39,39	0
56	MG	1Q	3004	1/1	0.85	0.65	14.54	51,51,51,51	0
56	MG	2A	3064	1/1	0.94	0.24	14.52	33,33,33,33	0
56	MG	1A	3218	1/1	0.98	0.42	14.51	28,28,28,28	0
56	MG	2A	3221	1/1	0.93	0.29	14.47	30,30,30,30	0
56	MG	1A	3001	1/1	0.98	0.27	14.34	30,30,30,30	0
56	MG	1q	3301	1/1	0.92	0.29	13.88	49,49,49,49	0
56	MG	2A	3229	1/1	0.97	0.32	13.81	64,64,64,64	0
56	MG	2A	3533	1/1	0.93	0.35	13.74	28,28,28,28	0
56	MG	2A	3388	1/1	0.82	0.36	13.48	57,57,57,57	0
56	MG	2A	3421	1/1	0.81	0.27	13.44	61,61,61,61	0
56	MG	1A	3185	1/1	0.95	0.41	13.37	29,29,29,29	0
56	MG	2A	3173	1/1	0.94	0.37	13.28	54,54,54,54	0
56	MG	1A	3611	1/1	0.87	0.28	12.53	31,31,31,31	0
56	MG	1A	3731	1/1	0.95	0.26	12.40	58,58,58,58	0
56	MG	2A	3378	1/1	0.94	0.23	12.37	34,34,34,34	0
56	MG	1A	3578	1/1	0.92	0.36	12.35	47,47,47,47	0
56	MG	1A	4057	1/1	0.97	0.32	12.25	40,40,40,40	0
56	MG	2A	3156	1/1	0.97	0.25	12.14	28,28,28,28	0
56	MG	2a	1812	1/1	0.94	0.27	12.07	42,42,42,42	0
56	MG	2A	3422	1/1	0.94	0.35	12.03	53,53,53,53	0
56	MG	1A	3151	1/1	0.96	0.28	12.00	26,26,26,26	0
56	MG	1A	3128	1/1	0.97	0.26	11.94	27,27,27,27	0
56	MG	2a	1786	1/1	0.88	0.39	11.85	71,71,71,71	0
56	MG	1A	4090	1/1	0.95	0.41	11.78	38,38,38,38	0
56	MG	2A	3190	1/1	0.96	0.28	11.72	44,44,44,44	0
56	MG	1A	3200	1/1	0.96	0.24	11.38	28,28,28,28	0
56	MG	1H	203	1/1	0.52	0.68	11.28	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3311	1/1	0.93	0.25	11.25	32,32,32,32	0
56	MG	2A	3138	1/1	0.93	0.22	11.17	36,36,36,36	0
56	MG	2A	3491	1/1	0.91	0.29	11.17	53,53,53,53	0
56	MG	2A	3187	1/1	0.97	0.21	11.13	40,40,40,40	0
56	MG	2A	3090	1/1	0.97	0.28	11.13	33,33,33,33	0
56	MG	2A	3189	1/1	0.92	0.25	10.73	45,45,45,45	0
56	MG	1A	3078	1/1	0.91	0.31	10.72	56,56,56,56	0
56	MG	1X	3001	1/1	0.92	0.27	10.72	43,43,43,43	0
56	MG	1A	3597	1/1	0.96	0.23	10.72	36,36,36,36	0
56	MG	1A	3582	1/1	0.94	0.28	10.64	45,45,45,45	0
56	MG	1D	311	1/1	0.75	0.45	10.64	58,58,58,58	0
56	MG	1A	3155	1/1	0.96	0.28	10.56	27,27,27,27	0
56	MG	17	101	1/1	0.94	0.45	10.35	35,35,35,35	0
56	MG	10	101	1/1	0.81	0.31	10.24	64,64,64,64	0
56	MG	2A	3290	1/1	0.97	0.21	10.23	40,40,40,40	0
56	MG	1A	3282	1/1	0.91	0.26	10.21	36,36,36,36	0
56	MG	1U	206	1/1	0.88	0.46	10.12	46,46,46,46	0
56	MG	2A	3286	1/1	0.91	0.23	10.08	32,32,32,32	0
56	MG	1A	3253	1/1	0.90	0.28	10.06	54,54,54,54	0
56	MG	1A	3222	1/1	0.96	0.20	9.84	21,21,21,21	0
56	MG	2A	3391	1/1	0.94	0.27	9.81	47,47,47,47	0
56	MG	1A	3059	1/1	0.97	0.24	9.77	43,43,43,43	0
56	MG	1P	206	1/1	0.95	0.34	9.55	44,44,44,44	0
56	MG	2A	3260	1/1	0.94	0.23	9.49	63,63,63,63	0
56	MG	1a	1671	1/1	0.95	0.24	9.41	54,54,54,54	0
56	MG	2a	1631	1/1	0.96	0.51	9.37	51,51,51,51	0
56	MG	1A	3202	1/1	0.99	0.33	9.37	33,33,33,33	0
56	MG	2A	3249	1/1	0.93	0.23	9.27	53,53,53,53	0
56	MG	1U	205	1/1	0.91	0.39	9.25	30,30,30,30	0
56	MG	2A	3553	1/1	0.97	0.41	9.22	42,42,42,42	0
56	MG	2A	3257	1/1	0.92	0.21	9.19	35,35,35,35	0
56	MG	1F	304	1/1	0.96	0.35	9.17	19,19,19,19	0
56	MG	1A	3443	1/1	0.96	0.27	9.17	50,50,50,50	0
56	MG	2A	3395	1/1	0.97	0.23	9.15	51,51,51,51	0
56	MG	1A	3205	1/1	0.97	0.21	9.07	40,40,40,40	0
56	MG	1A	4048	1/1	0.94	0.29	9.07	41,41,41,41	0
56	MG	2A	3320	1/1	0.98	0.29	9.03	46,46,46,46	0
56	MG	2e	202	1/1	0.78	0.50	8.99	74,74,74,74	0
56	MG	2A	3179	1/1	0.92	0.20	8.96	47,47,47,47	0
56	MG	1A	3054	1/1	0.98	0.31	8.84	50,50,50,50	0
56	MG	11	101	1/1	0.94	0.41	8.72	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	1R	205	1/1	0.79	0.53	8.71	55,55,55,55	0
56	MG	2A	3146	1/1	0.96	0.21	8.71	32,32,32,32	0
56	MG	1A	3511	1/1	0.96	0.25	8.62	47,47,47,47	0
56	MG	1A	3303	1/1	0.85	0.27	8.58	43,43,43,43	0
56	MG	1A	3199	1/1	0.95	0.25	8.51	36,36,36,36	0
56	MG	1V	201	1/1	0.96	0.32	8.45	39,39,39,39	0
56	MG	2A	3281	1/1	0.84	0.22	8.43	41,41,41,41	0
56	MG	1A	3945	1/1	0.97	0.27	8.40	36,36,36,36	0
56	MG	2A	3289	1/1	0.98	0.23	8.34	49,49,49,49	0
56	MG	2a	1682	1/1	0.91	0.29	8.31	48,48,48,48	0
56	MG	2A	3020	1/1	0.98	0.37	8.24	44,44,44,44	0
56	MG	2A	3408	1/1	0.95	0.23	8.21	46,46,46,46	0
56	MG	1a	1770	1/1	0.94	0.21	8.15	60,60,60,60	0
56	MG	1A	4080	1/1	0.97	0.34	8.12	45,45,45,45	0
56	MG	1A	3475	1/1	0.85	0.34	7.98	50,50,50,50	0
56	MG	2A	3486	1/1	0.93	0.21	7.96	70,70,70,70	0
56	MG	2a	1788	1/1	0.95	0.29	7.88	68,68,68,68	0
56	MG	1A	3219	1/1	0.85	0.34	7.87	62,62,62,62	0
56	MG	1A	3442	1/1	0.93	0.51	7.86	64,64,64,64	0
56	MG	1a	1829	1/1	0.96	0.28	7.73	37,37,37,37	0
56	MG	1a	1729	1/1	0.95	0.22	7.47	38,38,38,38	0
56	MG	1A	3590	1/1	0.97	0.21	7.43	40,40,40,40	0
56	MG	1A	3667	1/1	0.96	0.21	7.37	19,19,19,19	0
56	MG	2A	3217	1/1	0.80	0.31	7.24	46,46,46,46	0
56	MG	1a	1663	1/1	0.94	0.24	7.24	64,64,64,64	0
56	MG	1a	1827	1/1	0.96	0.24	7.18	55,55,55,55	0
56	MG	2a	1604	1/1	0.97	0.40	7.18	47,47,47,47	0
56	MG	1A	4041	1/1	0.99	0.22	7.15	12,12,12,12	0
56	MG	1A	3138	1/1	0.96	0.24	7.13	32,32,32,32	0
56	MG	1A	4046	1/1	0.90	0.40	7.05	50,50,50,50	0
56	MG	1A	3941	1/1	0.90	0.24	6.82	50,50,50,50	0
56	MG	1A	3299	1/1	0.98	0.28	6.76	16,16,16,16	0
56	MG	2A	3347	1/1	0.97	0.25	6.75	60,60,60,60	0
56	MG	2U	202	1/1	0.98	0.41	6.63	48,48,48,48	0
56	MG	2D	303	1/1	0.87	0.25	6.58	46,46,46,46	0
56	MG	1D	308	1/1	0.89	0.31	6.45	16,16,16,16	0
56	MG	1A	3949	1/1	0.90	0.34	6.36	37,37,37,37	0
56	MG	1A	3789	1/1	0.95	0.22	6.33	21,21,21,21	0
56	MG	2A	3556	1/1	0.96	0.39	6.30	40,40,40,40	0
56	MG	1A	3139	1/1	0.97	0.23	6.23	21,21,21,21	0
56	MG	2a	1816	1/1	0.82	0.27	6.17	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	3302	1/1	0.96	0.28	6.16	28,28,28,28	0
56	MG	2A	3052	1/1	0.96	0.22	6.15	37,37,37,37	0
56	MG	2A	3180	1/1	0.99	0.31	6.13	34,34,34,34	0
56	MG	1U	202	1/1	0.92	0.40	6.13	56,56,56,56	0
56	MG	1A	3003	1/1	0.84	0.23	6.12	41,41,41,41	0
56	MG	2E	302	1/1	0.93	0.28	6.12	45,45,45,45	0
56	MG	1q	3302	1/1	0.95	0.26	6.10	53,53,53,53	0
56	MG	2A	3292	1/1	0.99	0.21	6.05	43,43,43,43	0
56	MG	2A	3270	1/1	0.97	0.25	5.99	27,27,27,27	0
56	MG	1A	4089	1/1	0.97	0.22	5.90	34,34,34,34	0
56	MG	1A	4042	1/1	0.97	0.31	5.89	32,32,32,32	0
56	MG	2A	3379	1/1	0.94	0.22	5.88	64,64,64,64	0
56	MG	2A	3387	1/1	0.89	0.22	5.85	37,37,37,37	0
56	MG	1P	204	1/1	0.98	0.31	5.84	34,34,34,34	0
56	MG	2D	305	1/1	0.98	0.33	5.72	27,27,27,27	0
56	MG	1D	310	1/1	0.98	0.33	5.65	31,31,31,31	0
56	MG	2a	1620	1/1	0.89	0.23	5.65	66,66,66,66	0
56	MG	2A	3324	1/1	0.98	0.20	5.64	24,24,24,24	0
56	MG	2A	3314	1/1	0.90	0.18	5.64	49,49,49,49	0
56	MG	1B	212	1/1	0.91	0.30	5.63	50,50,50,50	0
56	MG	2A	3365	1/1	0.78	0.17	5.61	49,49,49,49	0
56	MG	2A	3299	1/1	0.89	0.28	5.56	65,65,65,65	0
56	MG	2a	1684	1/1	0.87	0.41	5.53	60,60,60,60	0
56	MG	2A	3248	1/1	0.98	0.25	5.50	45,45,45,45	0
56	MG	1a	1702	1/1	0.91	0.20	5.48	43,43,43,43	0
56	MG	2a	1760	1/1	0.91	0.26	5.47	59,59,59,59	0
56	MG	2a	1712	1/1	0.90	0.22	5.33	67,67,67,67	0
56	MG	2A	3470	1/1	0.97	0.20	5.30	67,67,67,67	0
56	MG	1A	3405	1/1	0.90	0.27	5.29	36,36,36,36	0
56	MG	1A	3790	1/1	0.89	0.23	5.21	38,38,38,38	0
56	MG	1A	3655	1/1	0.93	0.27	5.20	36,36,36,36	0
56	MG	1A	4067	1/1	0.94	0.29	5.17	37,37,37,37	0
56	MG	2A	3222	1/1	0.97	0.17	5.14	34,34,34,34	0
56	MG	1A	3863	1/1	0.98	0.24	5.11	45,45,45,45	0
56	MG	1A	3910	1/1	0.86	0.21	5.11	37,37,37,37	0
56	MG	2A	3362	1/1	0.94	0.22	5.08	62,62,62,62	0
56	MG	1A	3245	1/1	0.97	0.23	5.02	25,25,25,25	0
56	MG	2A	3353	1/1	0.94	0.17	4.90	59,59,59,59	0
56	MG	1E	308	1/1	0.93	0.29	4.85	28,28,28,28	0
56	MG	2A	3043	1/1	0.97	0.19	4.80	46,46,46,46	0
56	MG	2A	3021	1/1	0.97	0.29	4.79	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	2A	3025	1/1	0.92	0.20	4.78	45,45,45,45	0
56	MG	1A	4028	1/1	0.92	0.20	4.75	87,87,87,87	0
56	MG	1A	3270	1/1	0.97	0.25	4.74	41,41,41,41	0
56	MG	1A	3993	1/1	0.97	0.21	4.43	30,30,30,30	0
56	MG	1A	3668	1/1	0.97	0.20	4.38	31,31,31,31	0
56	MG	1A	3293	1/1	0.87	0.26	4.29	50,50,50,50	0
56	MG	1A	3660	1/1	0.95	0.20	4.27	30,30,30,30	0
56	MG	1A	3125	1/1	0.91	0.17	4.27	56,56,56,56	0
56	MG	1A	3154	1/1	0.97	0.22	4.16	34,34,34,34	0
56	MG	2A	3551	1/1	0.90	0.20	4.14	32,32,32,32	0
56	MG	2A	3540	1/1	0.95	0.21	4.13	45,45,45,45	0
56	MG	1a	1756	1/1	0.87	0.19	4.08	74,74,74,74	0
56	MG	1A	3646	1/1	0.91	0.20	3.98	49,49,49,49	0
56	MG	2A	3197	1/1	0.94	0.18	3.98	47,47,47,47	0
56	MG	2A	3123	1/1	0.94	0.14	3.97	53,53,53,53	0
56	MG	1A	3460	1/1	0.88	0.21	3.95	61,61,61,61	0
56	MG	2A	3358	1/1	0.97	0.22	3.90	47,47,47,47	0
56	MG	1a	1632	1/1	0.94	0.17	3.90	47,47,47,47	0
56	MG	1A	3770	1/1	0.96	0.24	3.88	26,26,26,26	0
56	MG	1A	3803	1/1	0.95	0.16	3.75	53,53,53,53	0
56	MG	1A	3130	1/1	0.96	0.32	3.74	35,35,35,35	0
56	MG	2A	3296	1/1	0.95	0.19	3.71	40,40,40,40	0
56	MG	1A	4084	1/1	0.93	0.25	3.61	36,36,36,36	0
56	MG	1A	3571	1/1	0.97	0.18	3.61	42,42,42,42	0
56	MG	2A	3046	1/1	0.99	0.17	3.58	38,38,38,38	0
56	MG	2B	3005	1/1	0.96	0.20	3.57	51,51,51,51	0
56	MG	1Q	3002	1/1	0.92	0.22	3.56	36,36,36,36	0
56	MG	1A	3751	1/1	0.85	0.22	3.56	20,20,20,20	0
56	MG	2A	3216	1/1	0.86	0.17	3.51	44,44,44,44	0
56	MG	1A	3820	1/1	0.96	0.20	3.48	45,45,45,45	0
56	MG	1A	3110	1/1	0.82	0.27	3.43	52,52,52,52	0
56	MG	2A	3485	1/1	0.93	0.15	3.38	48,48,48,48	0
56	MG	2A	3285	1/1	0.85	0.17	3.36	48,48,48,48	0
56	MG	2A	3323	1/1	0.96	0.22	3.36	56,56,56,56	0
56	MG	1A	3127	1/1	0.97	0.24	3.35	39,39,39,39	0
56	MG	1a	1662	1/1	0.84	0.20	3.35	61,61,61,61	0
56	MG	2A	3174	1/1	0.93	0.17	3.33	32,32,32,32	0
56	MG	2A	3330	1/1	0.94	0.17	3.30	37,37,37,37	0
56	MG	2A	3459	1/1	0.92	0.21	3.29	46,46,46,46	0
56	MG	1A	3703	1/1	0.85	0.23	3.26	29,29,29,29	0
56	MG	1A	3690	1/1	0.89	0.21	3.19	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1720	1/1	0.90	0.20	3.15	40,40,40,40	0
56	MG	1A	3166	1/1	0.94	0.20	3.10	29,29,29,29	0
56	MG	1a	1711	1/1	0.97	0.20	3.10	60,60,60,60	0
56	MG	2A	3386	1/1	0.95	0.17	3.08	68,68,68,68	0
56	MG	2A	3525	1/1	0.91	0.16	3.06	40,40,40,40	0
56	MG	1a	1793	1/1	0.97	0.18	3.05	29,29,29,29	0
56	MG	2a	1715	1/1	0.71	0.23	3.04	82,82,82,82	0
56	MG	1a	1858	1/1	0.98	0.21	3.01	35,35,35,35	0
56	MG	1Q	3006	1/1	0.98	0.29	2.93	37,37,37,37	0
56	MG	2a	1752	1/1	0.85	0.20	2.91	59,59,59,59	0
56	MG	2A	3062	1/1	0.92	0.16	2.88	43,43,43,43	0
56	MG	2a	1771	1/1	0.96	0.23	2.85	50,50,50,50	0
56	MG	1A	3152	1/1	0.99	0.20	2.84	29,29,29,29	0
56	MG	1R	201	1/1	0.92	0.27	2.83	55,55,55,55	0
56	MG	1a	1844	1/1	0.86	0.18	2.77	53,53,53,53	0
56	MG	1A	3584	1/1	0.96	0.21	2.76	33,33,33,33	0
56	MG	1A	3178	1/1	0.89	0.18	2.72	48,48,48,48	0
56	MG	1a	1708	1/1	0.93	0.20	2.69	40,40,40,40	0
56	MG	1W	3005	1/1	0.93	0.25	2.66	32,32,32,32	0
56	MG	2A	3184	1/1	0.90	0.21	2.65	43,43,43,43	0
56	MG	2a	1618	1/1	0.90	0.27	2.65	74,74,74,74	0
56	MG	2A	3451	1/1	0.95	0.17	2.64	53,53,53,53	0
56	MG	2A	3503	1/1	0.96	0.16	2.60	50,50,50,50	0
56	MG	1h	3003	1/1	0.85	0.27	2.57	70,70,70,70	0
56	MG	1A	3956	1/1	0.85	0.22	2.52	17,17,17,17	0
56	MG	2A	3256	1/1	0.94	0.18	2.51	36,36,36,36	0
56	MG	1a	1604	1/1	0.85	0.17	2.47	63,63,63,63	0
56	MG	1a	1836	1/1	0.90	0.20	2.45	52,52,52,52	0
56	MG	2A	3390	1/1	0.64	0.19	2.45	55,55,55,55	0
56	MG	1A	4094	1/1	0.98	0.23	2.44	27,27,27,27	0
56	MG	2A	3298	1/1	0.95	0.17	2.42	31,31,31,31	0
56	MG	2A	3529	1/1	0.90	0.18	2.38	43,43,43,43	0
56	MG	1A	4061	1/1	0.94	0.21	2.37	48,48,48,48	0
56	MG	2a	1732	1/1	0.95	0.21	2.36	75,75,75,75	0
56	MG	1A	3959	1/1	0.97	0.23	2.35	27,27,27,27	0
56	MG	2A	3199	1/1	0.96	0.19	2.33	42,42,42,42	0
56	MG	1A	3771	1/1	0.95	0.20	2.28	11,11,11,11	0
56	MG	1A	3583	1/1	0.97	0.20	2.24	47,47,47,47	0
56	MG	1t	3001	1/1	0.95	0.37	2.23	53,53,53,53	0
56	MG	1a	1900	1/1	0.95	0.23	2.16	68,68,68,68	0
56	MG	1D	307	1/1	0.83	0.20	2.14	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	2A	3203	1/1	0.87	0.19	2.11	19,19,19,19	0
56	MG	2A	3048	1/1	0.88	0.17	2.08	43,43,43,43	0
56	MG	2A	3120	1/1	0.91	0.18	2.06	33,33,33,33	0
56	MG	2F	303	1/1	0.95	0.23	2.04	50,50,50,50	0
56	MG	1A	4056	1/1	0.97	0.21	2.03	30,30,30,30	0
56	MG	1A	3161	1/1	0.98	0.18	2.03	27,27,27,27	0
56	MG	1A	3144	1/1	0.94	0.22	2.00	34,34,34,34	0
56	MG	2W	201	1/1	0.94	0.27	1.99	42,42,42,42	0
56	MG	1A	3662	1/1	0.90	0.22	1.95	22,22,22,22	0
56	MG	1a	1690	1/1	0.83	0.17	1.94	78,78,78,78	0
56	MG	1A	3446	1/1	0.94	0.18	1.93	43,43,43,43	0
56	MG	1A	3652	1/1	0.88	0.19	1.89	48,48,48,48	0
56	MG	1a	1868	1/1	0.97	0.14	1.87	41,41,41,41	0
56	MG	1A	3685	1/1	0.95	0.19	1.87	31,31,31,31	0
56	MG	1D	304	1/1	0.88	0.23	1.84	44,44,44,44	0
56	MG	1A	3674	1/1	0.90	0.20	1.84	37,37,37,37	0
56	MG	2t	3001	1/1	0.88	0.31	1.83	53,53,53,53	0
56	MG	2A	3405	1/1	0.97	0.16	1.83	53,53,53,53	0
57	ZN	16	102	1/1	0.96	0.18	1.79	57,57,57,57	0
56	MG	1A	3481	1/1	0.85	0.22	1.77	56,56,56,56	0
56	MG	1a	1831	1/1	0.98	0.17	1.76	32,32,32,32	0
56	MG	2A	3119	1/1	0.97	0.15	1.75	25,25,25,25	0
56	MG	2a	1685	1/1	0.97	0.20	1.73	53,53,53,53	0
56	MG	1A	3745	1/1	0.87	0.19	1.71	69,69,69,69	0
56	MG	1A	3868	1/1	0.89	0.16	1.70	65,65,65,65	0
56	MG	15	102	1/1	0.94	0.17	1.63	45,45,45,45	0
56	MG	2A	3355	1/1	0.94	0.18	1.60	22,22,22,22	0
56	MG	2A	3546	1/1	0.86	0.26	1.57	48,48,48,48	0
56	MG	2a	1784	1/1	0.90	0.20	1.55	71,71,71,71	0
56	MG	2A	3231	1/1	0.99	0.15	1.54	42,42,42,42	0
56	MG	1A	3129	1/1	0.87	0.19	1.48	41,41,41,41	0
56	MG	2A	3207	1/1	0.94	0.21	1.47	41,41,41,41	0
56	MG	1D	302	1/1	0.89	0.23	1.47	63,63,63,63	0
56	MG	1A	3954	1/1	0.88	0.18	1.43	42,42,42,42	0
56	MG	2U	201	1/1	0.93	0.17	1.41	30,30,30,30	0
56	MG	1D	313	1/1	0.97	0.18	1.40	39,39,39,39	0
56	MG	1N	203	1/1	0.84	0.24	1.39	47,47,47,47	0
56	MG	1A	3619	1/1	0.94	0.22	1.38	24,24,24,24	0
56	MG	2A	3177	1/1	0.93	0.16	1.37	40,40,40,40	0
56	MG	2a	1754	1/1	0.94	0.17	1.35	44,44,44,44	0
56	MG	1b	3001	1/1	0.96	0.22	1.34	63,63,63,63	0
56	MG	1A	3972	1/1	0.93	0.17	1.34	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3869	1/1	0.85	0.24	1.34	81,81,81,81	0
56	MG	1a	1668	1/1	0.73	0.18	1.33	81,81,81,81	0
56	MG	2A	3557	1/1	0.97	0.18	1.33	52,52,52,52	0
56	MG	2A	3518	1/1	0.97	0.22	1.31	58,58,58,58	0
56	MG	1A	3640	1/1	0.93	0.18	1.31	42,42,42,42	0
56	MG	1A	3824	1/1	0.97	0.21	1.27	19,19,19,19	0
56	MG	1A	3454	1/1	0.93	0.19	1.26	42,42,42,42	0
56	MG	1A	3240	1/1	0.94	0.18	1.25	37,37,37,37	0
56	MG	1A	3759	1/1	0.98	0.18	1.22	41,41,41,41	0
56	MG	2A	3548	1/1	0.91	0.19	1.21	53,53,53,53	0
56	MG	1A	3163	1/1	0.94	0.16	1.20	38,38,38,38	0
56	MG	1P	201	1/1	0.96	0.22	1.16	56,56,56,56	0
56	MG	2A	3247	1/1	0.97	0.16	1.15	47,47,47,47	0
56	MG	2A	3091	1/1	0.93	0.16	1.13	52,52,52,52	0
56	MG	1A	3179	1/1	0.96	0.21	1.11	38,38,38,38	0
56	MG	1A	3656	1/1	0.96	0.21	1.11	46,46,46,46	0
56	MG	1A	3841	1/1	0.98	0.18	1.10	17,17,17,17	0
56	MG	1A	4012	1/1	0.96	0.22	1.07	42,42,42,42	0
56	MG	2a	1758	1/1	0.76	0.18	1.07	59,59,59,59	0
56	MG	2A	3287	1/1	0.86	0.21	1.05	55,55,55,55	0
56	MG	2A	3282	1/1	0.95	0.13	0.99	39,39,39,39	0
56	MG	1A	3801	1/1	0.93	0.19	0.99	15,15,15,15	0
56	MG	1e	202	1/1	0.97	0.25	0.90	81,81,81,81	0
56	MG	1a	1851	1/1	0.97	0.20	0.89	64,64,64,64	0
56	MG	1A	3091	1/1	0.98	0.18	0.80	46,46,46,46	0
56	MG	1a	1740	1/1	0.96	0.27	0.79	46,46,46,46	0
56	MG	2A	3520	1/1	0.95	0.16	0.75	25,25,25,25	0
56	MG	1A	3145	1/1	0.98	0.19	0.72	29,29,29,29	0
56	MG	1A	3289	1/1	0.93	0.18	0.70	32,32,32,32	0
56	MG	15	103	1/1	0.94	0.18	0.70	33,33,33,33	0
56	MG	1R	204	1/1	0.93	0.23	0.69	58,58,58,58	0
56	MG	2A	3158	1/1	0.97	0.17	0.67	39,39,39,39	0
56	MG	1A	3594	1/1	0.96	0.17	0.65	36,36,36,36	0
56	MG	1A	3591	1/1	0.97	0.18	0.61	52,52,52,52	0
56	MG	1A	3137	1/1	0.84	0.15	0.49	58,58,58,58	0
56	MG	2A	3531	1/1	0.93	0.11	0.48	47,47,47,47	0
56	MG	1A	3775	1/1	0.94	0.20	0.47	14,14,14,14	0
56	MG	2A	3041	1/1	0.95	0.17	0.45	28,28,28,28	0
56	MG	1A	3677	1/1	0.92	0.17	0.41	16,16,16,16	0
56	MG	1a	1736	1/1	0.96	0.20	0.37	59,59,59,59	0
56	MG	2A	3112	1/1	0.97	0.12	0.36	40,40,40,40	0
56	MG	2A	3516	1/1	0.94	0.16	0.35	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	2A	3088	1/1	0.86	0.14	0.35	46,46,46,46	0
56	MG	1A	3494	1/1	0.93	0.19	0.34	63,63,63,63	0
56	MG	1A	3369	1/1	0.94	0.16	0.34	38,38,38,38	0
56	MG	1U	203	1/1	0.97	0.20	0.34	42,42,42,42	0
56	MG	2A	3552	1/1	0.97	0.16	0.32	47,47,47,47	0
56	MG	1A	3651	1/1	0.87	0.19	0.30	23,23,23,23	0
56	MG	2A	3474	1/1	0.89	0.14	0.28	63,63,63,63	0
56	MG	2E	301	1/1	0.96	0.16	0.28	30,30,30,30	0
56	MG	1A	3710	1/1	0.88	0.18	0.27	25,25,25,25	0
56	MG	1A	3752	1/1	0.94	0.20	0.27	25,25,25,25	0
56	MG	2a	1669	1/1	0.91	0.14	0.22	43,43,43,43	0
56	MG	2D	301	1/1	0.87	0.13	0.18	50,50,50,50	0
56	MG	1A	3818	1/1	0.98	0.19	0.14	19,19,19,19	0
56	MG	1A	3812	1/1	0.95	0.16	0.07	59,59,59,59	0
57	ZN	15	101	1/1	0.99	0.13	0.06	48,48,48,48	0
56	MG	1A	3233	1/1	0.93	0.14	0.02	42,42,42,42	0
56	MG	1a	1837	1/1	0.96	0.13	0.01	46,46,46,46	0
56	MG	1A	3817	1/1	0.98	0.17	-0.04	49,49,49,49	0
56	MG	1A	4058	1/1	0.95	0.17	-0.06	56,56,56,56	0
56	MG	2A	3309	1/1	0.93	0.14	-0.06	39,39,39,39	0
56	MG	1a	1867	1/1	0.96	0.13	-0.07	56,56,56,56	0
56	MG	1A	4019	1/1	0.89	0.15	-0.07	59,59,59,59	0
56	MG	2q	3002	1/1	0.80	0.23	-0.08	59,59,59,59	0
56	MG	2A	3160	1/1	0.88	0.12	-0.08	52,52,52,52	0
56	MG	1E	301	1/1	0.96	0.16	-0.11	14,14,14,14	0
56	MG	2A	3152	1/1	0.97	0.14	-0.11	30,30,30,30	0
56	MG	2A	3071	1/1	0.93	0.12	-0.14	42,42,42,42	0
56	MG	11	103	1/1	0.92	0.16	-0.16	50,50,50,50	0
56	MG	2A	3130	1/1	0.98	0.12	-0.22	43,43,43,43	0
56	MG	1D	305	1/1	0.96	0.19	-0.25	46,46,46,46	0
56	MG	2O	3001	1/1	0.95	0.14	-0.29	49,49,49,49	0
56	MG	2Q	3003	1/1	0.96	0.12	-0.31	37,37,37,37	0
56	MG	2a	1699	1/1	0.97	0.15	-0.33	71,71,71,71	0
56	MG	1A	3741	1/1	0.98	0.18	-0.38	13,13,13,13	0
56	MG	2a	1674	1/1	0.94	0.14	-0.38	50,50,50,50	0
56	MG	1N	206	1/1	0.90	0.17	-0.40	37,37,37,37	0
56	MG	2A	3538	1/1	0.86	0.14	-0.43	56,56,56,56	0
56	MG	1A	3023	1/1	0.90	0.14	-0.43	47,47,47,47	0
56	MG	1a	1666	1/1	0.88	0.15	-0.43	61,61,61,61	0
56	MG	1A	3390	1/1	0.92	0.14	-0.44	56,56,56,56	0
56	MG	2x	3003	1/1	0.97	0.14	-0.44	48,48,48,48	0
56	MG	1A	3214	1/1	0.95	0.11	-0.45	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3122	1/1	0.92	0.14	-0.46	44,44,44,44	0
56	MG	1A	4047	1/1	0.88	0.18	-0.47	44,44,44,44	0
56	MG	1a	1808	1/1	0.93	0.17	-0.49	57,57,57,57	0
56	MG	1A	3804	1/1	0.95	0.15	-0.49	58,58,58,58	0
56	MG	1a	1709	1/1	0.95	0.14	-0.53	66,66,66,66	0
56	MG	2A	3305	1/1	0.96	0.14	-0.53	41,41,41,41	0
56	MG	1A	3688	1/1	0.95	0.17	-0.56	21,21,21,21	0
56	MG	1A	3877	1/1	0.82	0.13	-0.57	41,41,41,41	0
57	ZN	25	501	1/1	0.99	0.11	-0.58	47,47,47,47	0
56	MG	1A	3592	1/1	0.97	0.12	-0.59	35,35,35,35	0
56	MG	2A	3102	1/1	0.85	0.12	-0.60	53,53,53,53	0
56	MG	2D	302	1/1	0.95	0.11	-0.60	48,48,48,48	0
56	MG	1q	3303	1/1	0.95	0.15	-0.61	60,60,60,60	0
56	MG	1A	4075	1/1	0.92	0.17	-0.63	36,36,36,36	0
56	MG	1a	1640	1/1	0.97	0.17	-0.64	57,57,57,57	0
56	MG	1A	3172	1/1	0.96	0.11	-0.64	56,56,56,56	0
56	MG	2A	3438	1/1	0.76	0.14	-0.65	39,39,39,39	0
56	MG	2A	3336	1/1	0.97	0.14	-0.65	38,38,38,38	0
56	MG	1A	3729	1/1	0.91	0.18	-0.67	43,43,43,43	0
56	MG	1A	3263	1/1	0.95	0.18	-0.68	31,31,31,31	0
56	MG	1A	3769	1/1	0.95	0.15	-0.71	44,44,44,44	0
56	MG	1a	1659	1/1	0.92	0.13	-0.75	68,68,68,68	0
57	ZN	1n	501	1/1	0.97	0.12	-0.76	84,84,84,84	0
56	MG	1A	3482	1/1	0.91	0.17	-0.77	55,55,55,55	0
56	MG	1A	3269	1/1	0.98	0.18	-0.78	17,17,17,17	0
56	MG	2A	3361	1/1	0.90	0.13	-0.80	53,53,53,53	0
56	MG	2a	1773	1/1	0.97	0.14	-0.83	53,53,53,53	0
56	MG	1D	303	1/1	0.94	0.16	-0.85	37,37,37,37	0
56	MG	2a	1661	1/1	0.87	0.16	-0.87	58,58,58,58	0
56	MG	2A	3544	1/1	0.83	0.12	-0.90	48,48,48,48	0
56	MG	2A	3232	1/1	0.94	0.13	-0.92	47,47,47,47	0
56	MG	1d	502	1/1	0.95	0.10	-0.92	60,60,60,60	0
56	MG	1a	1658	1/1	0.62	0.12	-0.92	69,69,69,69	0
56	MG	1A	3120	1/1	0.96	0.16	-0.94	28,28,28,28	0
56	MG	1A	3932	1/1	0.87	0.16	-0.94	58,58,58,58	0
56	MG	1A	3968	1/1	0.98	0.16	-0.95	21,21,21,21	0
56	MG	1a	1694	1/1	0.94	0.12	-0.96	45,45,45,45	0
56	MG	2A	3558	1/1	0.96	0.17	-0.96	40,40,40,40	0
56	MG	1A	3036	1/1	0.97	0.17	-1.00	41,41,41,41	0
57	ZN	26	501	1/1	0.91	0.10	-1.01	62,62,62,62	0
56	MG	2f	3001	1/1	0.89	0.14	-1.03	54,54,54,54	0
56	MG	1A	3633	1/1	0.96	0.15	-1.03	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3030	1/1	0.90	0.12	-1.03	45,45,45,45	0
56	MG	1a	1774	1/1	0.93	0.11	-1.05	75,75,75,75	0
56	MG	2A	3368	1/1	0.89	0.12	-1.07	43,43,43,43	0
57	ZN	29	501	1/1	0.97	0.07	-1.07	58,58,58,58	0
56	MG	1a	1660	1/1	0.95	0.12	-1.07	57,57,57,57	0
56	MG	2A	3271	1/1	0.94	0.12	-1.08	42,42,42,42	0
56	MG	2a	1803	1/1	0.96	0.09	-1.08	60,60,60,60	0
56	MG	2A	3366	1/1	0.90	0.12	-1.11	51,51,51,51	0
56	MG	1Q	3005	1/1	0.98	0.15	-1.11	38,38,38,38	0
56	MG	1a	1704	1/1	0.99	0.14	-1.12	40,40,40,40	0
56	MG	1A	3312	1/1	0.92	0.12	-1.12	59,59,59,59	0
56	MG	1A	3097	1/1	0.95	0.14	-1.12	55,55,55,55	0
58	SF4	1d	501	8/8	0.99	0.13	-1.13	56,73,76,77	0
56	MG	1A	4054	1/1	0.95	0.15	-1.13	40,40,40,40	0
56	MG	1a	1652	1/1	0.95	0.12	-1.16	63,63,63,63	0
58	SF4	2d	501	8/8	0.99	0.12	-1.17	56,71,81,82	0
56	MG	2A	3019	1/1	0.94	0.10	-1.21	45,45,45,45	0
56	MG	1A	3663	1/1	0.93	0.17	-1.22	20,20,20,20	0
57	ZN	14	501	1/1	0.96	0.10	-1.24	75,75,75,75	0
57	ZN	19	102	1/1	0.99	0.13	-1.25	46,46,46,46	0
56	MG	1A	3239	1/1	0.94	0.17	-1.26	25,25,25,25	0
56	MG	1W	3003	1/1	0.96	0.16	-1.29	43,43,43,43	0
56	MG	2a	1678	1/1	0.92	0.09	-1.31	58,58,58,58	0
56	MG	1a	1905	1/1	0.96	0.12	-1.34	52,52,52,52	0
57	ZN	1Y	202	1/1	0.97	0.11	-1.35	65,65,65,65	0
56	MG	1A	3231	1/1	0.97	0.13	-1.35	42,42,42,42	0
56	MG	1A	3283	1/1	0.90	0.15	-1.36	47,47,47,47	0
56	MG	1A	3958	1/1	0.98	0.16	-1.37	18,18,18,18	0
56	MG	1a	1898	1/1	0.96	0.12	-1.39	47,47,47,47	0
56	MG	1N	205	1/1	0.94	0.15	-1.40	42,42,42,42	0
56	MG	2A	3394	1/1	0.85	0.12	-1.40	57,57,57,57	0
56	MG	1A	3220	1/1	0.97	0.14	-1.42	30,30,30,30	0
56	MG	2A	3061	1/1	0.94	0.12	-1.42	44,44,44,44	0
56	MG	2A	3250	1/1	0.94	0.12	-1.46	70,70,70,70	0
56	MG	2A	3303	1/1	0.92	0.10	-1.49	30,30,30,30	0
56	MG	2A	3278	1/1	0.93	0.12	-1.50	52,52,52,52	0
56	MG	1B	219	1/1	0.98	0.12	-1.51	25,25,25,25	0
56	MG	2A	3517	1/1	0.97	0.09	-1.51	36,36,36,36	0
56	MG	1A	3234	1/1	0.90	0.13	-1.52	52,52,52,52	0
57	ZN	2Y	202	1/1	0.92	0.05	-1.54	80,80,80,80	0
56	MG	2A	3306	1/1	0.87	0.13	-1.54	32,32,32,32	0
56	MG	1A	3037	1/1	0.96	0.14	-1.54	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	1748	1/1	0.91	0.14	-1.56	50,50,50,50	0
56	MG	1a	1742	1/1	0.85	0.12	-1.56	69,69,69,69	0
56	MG	1A	3800	1/1	0.97	0.15	-1.58	25,25,25,25	0
56	MG	2A	3412	1/1	0.93	0.10	-1.60	53,53,53,53	0
56	MG	2A	3097	1/1	0.90	0.10	-1.62	51,51,51,51	0
56	MG	1A	3658	1/1	0.98	0.12	-1.62	36,36,36,36	0
56	MG	1A	3997	1/1	0.91	0.14	-1.64	48,48,48,48	0
56	MG	1G	3001	1/1	0.87	0.10	-1.65	45,45,45,45	0
56	MG	1A	3783	1/1	0.95	0.16	-1.68	22,22,22,22	0
56	MG	1a	1879	1/1	0.95	0.14	-1.70	43,43,43,43	0
56	MG	1A	4095	1/1	0.99	0.14	-1.70	32,32,32,32	0
56	MG	1A	3580	1/1	0.97	0.14	-1.73	22,22,22,22	0
56	MG	2A	3153	1/1	0.85	0.13	-1.74	45,45,45,45	0
56	MG	1a	1899	1/1	0.95	0.09	-1.77	43,43,43,43	0
56	MG	1A	3603	1/1	0.99	0.14	-1.81	45,45,45,45	0
56	MG	2A	3205	1/1	0.98	0.13	-1.82	46,46,46,46	0
56	MG	1n	502	1/1	0.95	0.10	-1.83	55,55,55,55	0
56	MG	1A	3840	1/1	0.96	0.16	-1.83	59,59,59,59	0
56	MG	2A	3442	1/1	0.94	0.12	-1.89	60,60,60,60	0
56	MG	1a	1638	1/1	0.93	0.10	-1.90	56,56,56,56	0
56	MG	2A	3053	1/1	0.95	0.10	-1.95	47,47,47,47	0
57	ZN	2n	501	1/1	0.90	0.06	-1.97	93,93,93,93	0
56	MG	1a	1904	1/1	0.94	0.12	-1.98	60,60,60,60	0
56	MG	1A	3696	1/1	0.91	0.13	-2.03	34,34,34,34	0
56	MG	1A	3256	1/1	0.93	0.11	-2.03	37,37,37,37	0
56	MG	1A	3930	1/1	0.94	0.10	-2.04	28,28,28,28	0
56	MG	1A	3085	1/1	0.96	0.14	-2.05	28,28,28,28	0
56	MG	2A	3080	1/1	0.94	0.10	-2.08	41,41,41,41	0
56	MG	1A	3909	1/1	0.93	0.12	-2.09	54,54,54,54	0
56	MG	2G	3001	1/1	0.86	0.17	-2.10	49,49,49,49	0
56	MG	1B	205	1/1	0.94	0.10	-2.19	57,57,57,57	0
57	ZN	24	501	1/1	0.64	0.07	-2.20	114,114,114,114	0
56	MG	2A	3288	1/1	0.94	0.11	-2.21	35,35,35,35	0
56	MG	2B	3003	1/1	0.90	0.12	-2.23	60,60,60,60	0
56	MG	1e	201	1/1	0.96	0.07	-2.24	75,75,75,75	0
56	MG	1A	3716	1/1	0.87	0.09	-2.25	52,52,52,52	0
56	MG	2a	1687	1/1	0.76	0.10	-2.25	62,62,62,62	0
56	MG	1A	3781	1/1	0.95	0.14	-2.25	19,19,19,19	0
56	MG	1A	3666	1/1	0.92	0.10	-2.26	28,28,28,28	0
56	MG	2A	3413	1/1	0.89	0.12	-2.27	63,63,63,63	0
56	MG	1r	102	1/1	0.93	0.12	-2.28	47,47,47,47	0
56	MG	2l	202	1/1	0.86	0.13	-2.29	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	1691	1/1	0.95	0.11	-2.29	59,59,59,59	0
56	MG	1A	3193	1/1	0.92	0.14	-2.30	50,50,50,50	0
56	MG	1A	3671	1/1	0.97	0.14	-2.31	16,16,16,16	0
56	MG	2A	3056	1/1	0.91	0.11	-2.32	37,37,37,37	0
56	MG	1A	4078	1/1	0.97	0.14	-2.33	23,23,23,23	0
56	MG	1A	3831	1/1	0.94	0.14	-2.33	42,42,42,42	0
56	MG	1A	3808	1/1	0.92	0.12	-2.36	31,31,31,31	0
56	MG	2x	3004	1/1	0.95	0.06	-2.37	76,76,76,76	0
56	MG	2A	3045	1/1	0.93	0.09	-2.39	38,38,38,38	0
56	MG	1A	3661	1/1	0.98	0.16	-2.40	16,16,16,16	0
56	MG	1A	3676	1/1	0.91	0.10	-2.41	22,22,22,22	0
56	MG	2A	3304	1/1	0.94	0.08	-2.42	40,40,40,40	0
56	MG	2A	3157	1/1	0.94	0.12	-2.44	40,40,40,40	0
56	MG	1a	1713	1/1	0.94	0.11	-2.46	54,54,54,54	0
56	MG	1a	1678	1/1	0.97	0.11	-2.48	54,54,54,54	0
56	MG	1A	3556	1/1	0.81	0.14	-2.51	67,67,67,67	0
56	MG	2A	3218	1/1	0.95	0.08	-2.53	37,37,37,37	0
56	MG	2a	1790	1/1	0.97	0.06	-2.58	72,72,72,72	0
56	MG	1A	4021	1/1	0.96	0.14	-2.58	18,18,18,18	0
56	MG	1a	1672	1/1	0.94	0.10	-2.59	53,53,53,53	0
56	MG	1a	1777	1/1	0.93	0.11	-2.60	64,64,64,64	0
56	MG	1A	3788	1/1	0.97	0.14	-2.60	27,27,27,27	0
56	MG	1A	3985	1/1	0.96	0.14	-2.66	22,22,22,22	0
56	MG	2a	1725	1/1	0.79	0.10	-2.67	58,58,58,58	0
56	MG	1A	3873	1/1	0.85	0.13	-2.69	48,48,48,48	0
56	MG	1G	3003	1/1	0.97	0.04	-2.72	45,45,45,45	0
56	MG	1a	1703	1/1	0.87	0.09	-2.82	66,66,66,66	0
56	MG	1A	3778	1/1	0.96	0.16	-2.86	30,30,30,30	0
56	MG	1A	4070	1/1	0.94	0.13	-2.90	25,25,25,25	0
56	MG	1D	312	1/1	0.94	0.09	-2.91	44,44,44,44	0
56	MG	1A	3150	1/1	0.96	0.14	-2.92	39,39,39,39	0
56	MG	1A	3116	1/1	0.98	0.12	-2.94	21,21,21,21	0
56	MG	1a	1626	1/1	0.90	0.08	-2.94	62,62,62,62	0
56	MG	2A	3473	1/1	0.85	0.12	-2.95	42,42,42,42	0
56	MG	1A	3118	1/1	0.98	0.07	-2.98	33,33,33,33	0
56	MG	2A	3475	1/1	0.95	0.08	-2.99	53,53,53,53	0
56	MG	1a	1766	1/1	0.90	0.10	-3.01	82,82,82,82	0
56	MG	2a	1658	1/1	0.93	0.13	-3.01	53,53,53,53	0
56	MG	1P	202	1/1	0.97	0.14	-3.02	41,41,41,41	0
56	MG	1A	3999	1/1	0.96	0.13	-3.03	27,27,27,27	0
56	MG	1A	3632	1/1	0.94	0.14	-3.06	27,27,27,27	0
56	MG	1A	3833	1/1	0.93	0.12	-3.07	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	3456	1/1	0.96	0.09	-3.14	31,31,31,31	0
56	MG	1R	202	1/1	0.89	0.13	-3.17	64,64,64,64	0
56	MG	1a	1696	1/1	0.91	0.12	-3.25	59,59,59,59	0
56	MG	2A	3462	1/1	0.88	0.10	-3.25	44,44,44,44	0
56	MG	1A	3620	1/1	0.99	0.14	-3.27	7,7,7,7	0
56	MG	1A	3726	1/1	0.98	0.11	-3.31	23,23,23,23	0
56	MG	1A	3669	1/1	0.98	0.13	-3.31	17,17,17,17	0
56	MG	1A	3142	1/1	0.87	0.08	-3.33	62,62,62,62	0
56	MG	2A	3384	1/1	0.93	0.09	-3.33	33,33,33,33	0
56	MG	1A	3830	1/1	0.87	0.10	-3.36	38,38,38,38	0
56	MG	1A	4091	1/1	0.96	0.07	-3.46	45,45,45,45	0
56	MG	2a	1680	1/1	0.98	0.09	-3.48	49,49,49,49	0
56	MG	1r	101	1/1	0.79	0.14	-3.61	65,65,65,65	0
56	MG	1A	3872	1/1	0.95	0.13	-3.62	28,28,28,28	0
56	MG	1a	1717	1/1	0.94	0.09	-3.65	73,73,73,73	0
56	MG	1a	1628	1/1	0.97	0.11	-3.67	35,35,35,35	0
56	MG	2A	3434	1/1	0.92	0.06	-3.74	49,49,49,49	0
56	MG	1A	3117	1/1	0.96	0.16	-3.76	29,29,29,29	0
56	MG	1A	3215	1/1	0.87	0.10	-3.80	50,50,50,50	0
56	MG	1x	104	1/1	0.96	0.06	-3.82	40,40,40,40	0
56	MG	1A	3876	1/1	0.98	0.09	-3.82	26,26,26,26	0
56	MG	1A	3861	1/1	0.94	0.15	-3.84	34,34,34,34	0
56	MG	2A	3329	1/1	0.94	0.10	-3.86	36,36,36,36	0
56	MG	1A	3595	1/1	0.97	0.12	-3.87	27,27,27,27	0
56	MG	2a	1719	1/1	0.96	0.10	-3.87	63,63,63,63	0
56	MG	1A	3519	1/1	0.83	0.07	-3.91	62,62,62,62	0
56	MG	1A	3782	1/1	0.96	0.11	-3.92	27,27,27,27	0
56	MG	2a	1689	1/1	0.96	0.07	-3.94	43,43,43,43	0
56	MG	2a	1737	1/1	0.92	0.10	-3.95	74,74,74,74	0
56	MG	1A	4044	1/1	0.85	0.11	-3.95	27,27,27,27	0
56	MG	1A	3015	1/1	0.93	0.12	-4.04	52,52,52,52	0
56	MG	1A	3246	1/1	0.95	0.16	-4.04	23,23,23,23	0
56	MG	2A	3539	1/1	0.96	0.09	-4.07	29,29,29,29	0
56	MG	1B	208	1/1	0.95	0.13	-4.07	30,30,30,30	0
56	MG	1A	3843	1/1	0.99	0.10	-4.12	29,29,29,29	0
56	MG	2a	1650	1/1	0.94	0.08	-4.33	70,70,70,70	0
56	MG	1a	1605	1/1	0.77	0.15	-4.37	83,83,83,83	0
56	MG	1A	4036	1/1	0.94	0.09	-4.39	61,61,61,61	0
56	MG	1B	211	1/1	0.90	0.09	-4.41	46,46,46,46	0
56	MG	1A	3838	1/1	0.96	0.10	-4.47	28,28,28,28	0
56	MG	2a	1709	1/1	0.97	0.10	-4.52	64,64,64,64	0
56	MG	17	104	1/1	0.97	0.10	-4.84	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3283	1/1	0.97	0.07	-4.85	57,57,57,57	0
56	MG	1a	1681	1/1	0.96	0.07	-4.88	52,52,52,52	0
56	MG	1A	3625	1/1	0.96	0.09	-4.88	43,43,43,43	0
56	MG	1A	4043	1/1	0.96	0.09	-4.92	24,24,24,24	0
56	MG	1a	1746	1/1	0.98	0.11	-5.05	54,54,54,54	0
56	MG	1A	3408	1/1	0.94	0.04	-5.13	43,43,43,43	0
56	MG	1A	3728	1/1	0.99	0.12	-5.29	17,17,17,17	0
56	MG	2A	3279	1/1	0.92	0.06	-5.35	55,55,55,55	0
56	MG	1B	221	1/1	0.92	0.10	-5.38	57,57,57,57	0
56	MG	1D	301	1/1	0.98	0.12	-5.43	31,31,31,31	0
56	MG	1A	3980	1/1	0.91	0.09	-5.53	33,33,33,33	0
56	MG	1A	3618	1/1	0.96	0.08	-5.55	39,39,39,39	0
56	MG	2a	1663	1/1	0.92	0.07	-5.64	51,51,51,51	0
56	MG	1A	3146	1/1	0.96	0.11	-5.70	39,39,39,39	0
56	MG	1A	3915	1/1	0.98	0.09	-5.79	13,13,13,13	0
56	MG	1A	3613	1/1	0.92	0.10	-5.82	30,30,30,30	0
56	MG	1a	1656	1/1	0.96	0.12	-5.86	56,56,56,56	0
56	MG	1A	3226	1/1	0.84	0.12	-5.95	31,31,31,31	0
56	MG	2a	1801	1/1	0.96	0.06	-6.02	63,63,63,63	0
56	MG	1A	3648	1/1	0.99	0.09	-6.13	24,24,24,24	0
56	MG	2A	3399	1/1	0.91	0.07	-6.21	58,58,58,58	0
56	MG	2A	3537	1/1	0.96	0.07	-6.41	45,45,45,45	0
56	MG	1A	4083	1/1	0.96	0.15	-6.47	34,34,34,34	0
56	MG	1A	4020	1/1	0.99	0.07	-6.70	30,30,30,30	0
56	MG	2A	3264	1/1	0.93	0.11	-7.15	36,36,36,36	0
56	MG	1A	4053	1/1	0.98	0.12	-8.03	29,29,29,29	0
56	MG	1a	1657	1/1	0.92	0.10	-8.14	25,25,25,25	0
56	MG	1A	3718	1/1	0.98	0.10	-8.26	8,8,8,8	0
56	MG	2A	3259	1/1	0.97	0.07	-9.25	36,36,36,36	0
56	MG	1A	3763	1/1	0.95	0.10	-9.44	41,41,41,41	0
56	MG	1A	3705	1/1	0.98	0.08	-9.73	16,16,16,16	0
56	MG	1A	3854	1/1	0.95	0.13	-10.14	35,35,35,35	0
56	MG	2a	1640	1/1	0.96	0.08	-12.25	81,81,81,81	0
56	MG	1a	1803	1/1	0.98	0.05	-12.55	57,57,57,57	0
56	MG	2a	1774	1/1	0.91	0.07	-13.11	69,69,69,69	0
56	MG	1A	4085	1/1	0.95	0.11	-	46,46,46,46	0
56	MG	1A	3520	1/1	0.91	0.07	-	53,53,53,53	0
56	MG	1B	203	1/1	0.90	0.20	-	53,53,53,53	0
56	MG	2a	1626	1/1	0.90	0.17	-	55,55,55,55	0
56	MG	1A	3714	1/1	0.88	0.14	-	54,54,54,54	0
56	MG	1a	1613	1/1	0.84	0.12	-	44,44,44,44	0
56	MG	1A	3294	1/1	0.79	0.20	-	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	2a	1778	1/1	0.94	0.12	-	69,69,69,69	0
56	MG	1A	3225	1/1	0.85	0.12	-	49,49,49,49	0
56	MG	1A	3424	1/1	0.89	0.10	-	45,45,45,45	0
56	MG	1A	3974	1/1	0.93	0.19	-	46,46,46,46	0
56	MG	1a	1758	1/1	0.93	0.12	-	50,50,50,50	0
56	MG	1a	1674	1/1	0.97	0.12	-	46,46,46,46	0
56	MG	2A	3506	1/1	0.93	0.11	-	37,37,37,37	0
56	MG	1A	3373	1/1	0.92	0.14	-	58,58,58,58	0
56	MG	1A	3259	1/1	0.97	0.09	-	52,52,52,52	0
56	MG	1A	3412	1/1	0.97	0.13	-	77,77,77,77	0
56	MG	2a	1734	1/1	0.84	0.10	-	69,69,69,69	0
56	MG	1A	3434	1/1	0.98	0.17	-	47,47,47,47	0
56	MG	1A	3018	1/1	0.86	0.18	-	46,46,46,46	0
56	MG	1A	3636	1/1	0.96	0.15	-	35,35,35,35	0
56	MG	1A	3653	1/1	0.96	0.14	-	25,25,25,25	0
56	MG	1f	3001	1/1	0.95	0.24	-	56,56,56,56	0
56	MG	1A	3682	1/1	0.93	0.15	-	37,37,37,37	0
56	MG	1a	1839	1/1	0.95	0.14	-	70,70,70,70	0
56	MG	2a	1652	1/1	0.95	0.06	-	45,45,45,45	0
56	MG	1A	3344	1/1	0.83	0.31	-	73,73,73,73	0
56	MG	1A	3316	1/1	0.90	0.20	-	48,48,48,48	0
56	MG	1a	1866	1/1	0.96	0.12	-	55,55,55,55	0
56	MG	2A	3076	1/1	0.95	0.07	-	42,42,42,42	0
56	MG	1A	3342	1/1	0.81	0.14	-	49,49,49,49	0
56	MG	2A	3244	1/1	0.97	0.10	-	55,55,55,55	0
56	MG	2a	1722	1/1	0.97	0.23	-	47,47,47,47	0
56	MG	2a	1688	1/1	0.90	0.12	-	49,49,49,49	0
56	MG	1A	3734	1/1	0.98	0.05	-	45,45,45,45	0
56	MG	1O	203	1/1	0.83	0.33	-	60,60,60,60	0
56	MG	1A	3271	1/1	0.91	0.19	-	36,36,36,36	0
56	MG	2A	3334	1/1	0.93	0.16	-	57,57,57,57	0
56	MG	1a	1644	1/1	0.92	0.17	-	60,60,60,60	0
56	MG	1A	4002	1/1	0.91	0.18	-	70,70,70,70	0
56	MG	2a	1700	1/1	0.90	0.15	-	55,55,55,55	0
56	MG	1a	1718	1/1	0.91	0.15	-	67,67,67,67	0
56	MG	1A	3542	1/1	0.85	0.30	-	53,53,53,53	0
56	MG	1A	3709	1/1	0.97	0.13	-	15,15,15,15	0
56	MG	1A	3921	1/1	0.79	0.10	-	52,52,52,52	0
56	MG	1a	1642	1/1	0.95	0.31	-	95,95,95,95	0
56	MG	2A	3210	1/1	0.85	0.33	-	52,52,52,52	0
56	MG	1A	3229	1/1	0.91	0.16	-	57,57,57,57	0
56	MG	1a	1846	1/1	0.97	0.15	-	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	1T	205	1/1	0.85	0.27	-	76,76,76,76	0
56	MG	1A	3798	1/1	0.95	0.15	-	23,23,23,23	0
56	MG	1D	306	1/1	0.88	0.21	-	50,50,50,50	0
56	MG	1A	3132	1/1	0.96	0.15	-	39,39,39,39	0
56	MG	1A	3845	1/1	0.96	0.20	-	53,53,53,53	0
56	MG	1A	3275	1/1	0.88	0.27	-	58,58,58,58	0
56	MG	1A	3141	1/1	0.91	0.29	-	37,37,37,37	0
56	MG	1a	1618	1/1	0.98	0.16	-	58,58,58,58	0
56	MG	1a	1833	1/1	0.96	0.13	-	51,51,51,51	0
56	MG	1A	3836	1/1	0.98	0.40	-	57,57,57,57	0
56	MG	2A	3167	1/1	0.93	0.14	-	40,40,40,40	0
56	MG	1A	3983	1/1	0.94	0.19	-	53,53,53,53	0
56	MG	1A	3288	1/1	0.97	0.07	-	82,82,82,82	0
56	MG	1A	3532	1/1	0.84	0.12	-	54,54,54,54	0
56	MG	1a	1602	1/1	0.91	0.25	-	81,81,81,81	0
56	MG	1a	1813	1/1	0.96	0.10	-	56,56,56,56	0
56	MG	2A	3085	1/1	0.91	0.16	-	31,31,31,31	0
56	MG	1a	1687	1/1	0.95	0.11	-	51,51,51,51	0
56	MG	1A	3187	1/1	0.91	0.15	-	42,42,42,42	0
56	MG	1A	3065	1/1	0.92	0.44	-	53,53,53,53	0
56	MG	1a	1790	1/1	0.92	0.20	-	68,68,68,68	0
56	MG	1a	1636	1/1	0.96	0.12	-	66,66,66,66	0
56	MG	1a	1778	1/1	0.96	0.07	-	70,70,70,70	0
56	MG	1a	1824	1/1	0.97	0.33	-	52,52,52,52	0
56	MG	2B	3006	1/1	0.93	0.18	-	40,40,40,40	0
56	MG	1A	3335	1/1	0.97	0.11	-	46,46,46,46	0
56	MG	1A	3016	1/1	0.95	0.31	-	41,41,41,41	0
56	MG	1A	4001	1/1	0.95	0.09	-	49,49,49,49	0
56	MG	2A	3058	1/1	0.88	0.20	-	46,46,46,46	0
56	MG	10	102	1/1	0.95	0.05	-	51,51,51,51	0
56	MG	1A	3173	1/1	0.98	0.27	-	44,44,44,44	0
56	MG	1a	1785	1/1	0.93	0.16	-	66,66,66,66	0
56	MG	2A	3341	1/1	0.97	0.06	-	54,54,54,54	0
56	MG	1A	3315	1/1	0.89	0.17	-	50,50,50,50	0
56	MG	1A	3842	1/1	0.98	0.09	-	47,47,47,47	0
56	MG	1m	202	1/1	0.79	0.42	-	71,71,71,71	0
56	MG	1A	3565	1/1	0.93	0.18	-	67,67,67,67	0
56	MG	1A	3203	1/1	0.96	0.13	-	19,19,19,19	0
56	MG	1A	3557	1/1	0.96	0.11	-	48,48,48,48	0
56	MG	2A	3513	1/1	0.91	0.19	-	66,66,66,66	0
56	MG	1A	4039	1/1	0.77	0.20	-	81,81,81,81	0
56	MG	1A	3946	1/1	0.95	0.21	-	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	4063	1/1	0.93	0.14	-	38,38,38,38	0
56	MG	2A	3501	1/1	0.94	0.09	-	52,52,52,52	0
56	MG	1A	3697	1/1	0.97	0.10	-	23,23,23,23	0
56	MG	2A	3327	1/1	0.94	0.13	-	56,56,56,56	0
56	MG	1A	3025	1/1	0.92	0.28	-	44,44,44,44	0
56	MG	2A	3349	1/1	0.97	0.04	-	63,63,63,63	0
56	MG	2A	3427	1/1	0.89	0.09	-	43,43,43,43	0
56	MG	1A	3296	1/1	0.98	0.20	-	42,42,42,42	0
56	MG	1A	3255	1/1	0.92	0.08	-	61,61,61,61	0
56	MG	2a	1785	1/1	0.88	0.14	-	68,68,68,68	0
56	MG	1A	3470	1/1	0.88	0.40	-	43,43,43,43	0
56	MG	1A	3740	1/1	0.99	0.20	-	23,23,23,23	0
56	MG	2a	1622	1/1	0.95	0.16	-	53,53,53,53	0
56	MG	1A	3760	1/1	0.94	0.15	-	36,36,36,36	0
56	MG	2A	3522	1/1	0.94	0.16	-	50,50,50,50	0
56	MG	1A	3027	1/1	0.91	0.14	-	42,42,42,42	0
56	MG	2a	1691	1/1	0.95	0.14	-	55,55,55,55	0
56	MG	1A	3704	1/1	0.95	0.13	-	26,26,26,26	0
56	MG	1A	3799	1/1	0.96	0.09	-	39,39,39,39	0
56	MG	1a	1761	1/1	0.91	0.29	-	77,77,77,77	0
56	MG	1A	3896	1/1	0.88	0.12	-	47,47,47,47	0
56	MG	1a	1667	1/1	0.91	0.61	-	51,51,51,51	0
56	MG	2A	3559	1/1	0.93	0.12	-	58,58,58,58	0
56	MG	2A	3206	1/1	0.98	0.35	-	55,55,55,55	0
56	MG	18	101	1/1	0.97	0.15	-	30,30,30,30	0
56	MG	2A	3453	1/1	0.91	0.16	-	67,67,67,67	0
56	MG	1a	1789	1/1	0.88	0.10	-	62,62,62,62	0
56	MG	2a	1633	1/1	0.70	0.12	-	86,86,86,86	0
56	MG	2A	3148	1/1	0.95	0.09	-	54,54,54,54	0
56	MG	1A	3922	1/1	0.90	0.25	-	52,52,52,52	0
56	MG	2A	3510	1/1	0.95	0.19	-	49,49,49,49	0
56	MG	1A	3244	1/1	0.98	0.07	-	14,14,14,14	0
56	MG	1A	3631	1/1	0.95	0.10	-	43,43,43,43	0
56	MG	1A	3744	1/1	0.92	0.16	-	59,59,59,59	0
56	MG	1A	3707	1/1	0.97	0.17	-	50,50,50,50	0
56	MG	2a	1759	1/1	0.94	0.11	-	68,68,68,68	0
56	MG	1a	1801	1/1	0.77	0.16	-	58,58,58,58	0
56	MG	1A	3235	1/1	0.91	0.08	-	36,36,36,36	0
56	MG	2A	3479	1/1	0.82	0.17	-	56,56,56,56	0
56	MG	2A	3360	1/1	0.95	0.32	-	41,41,41,41	0
56	MG	2E	304	1/1	0.95	0.12	-	58,58,58,58	0
56	MG	1D	309	1/1	0.90	0.12	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3432	1/1	0.93	0.24	-	48,48,48,48	0
56	MG	2A	3371	1/1	0.89	0.26	-	61,61,61,61	0
56	MG	2a	1740	1/1	0.88	0.90	-	101,101,101,101	0
56	MG	1A	3067	1/1	0.88	0.19	-	48,48,48,48	0
56	MG	1A	3276	1/1	0.95	0.28	-	37,37,37,37	0
56	MG	1A	3555	1/1	0.96	0.29	-	47,47,47,47	0
56	MG	1A	3588	1/1	0.94	0.21	-	14,14,14,14	0
56	MG	1a	1714	1/1	0.83	0.35	-	56,56,56,56	0
56	MG	1A	3249	1/1	0.94	0.27	-	43,43,43,43	0
56	MG	1A	3735	1/1	0.98	0.13	-	32,32,32,32	0
56	MG	2a	1710	1/1	0.96	0.15	-	71,71,71,71	0
56	MG	2A	3057	1/1	0.92	0.15	-	54,54,54,54	0
56	MG	1A	3787	1/1	0.97	0.18	-	33,33,33,33	0
56	MG	2A	3441	1/1	0.97	0.07	-	43,43,43,43	0
56	MG	1a	1673	1/1	0.97	0.05	-	51,51,51,51	0
56	MG	1A	3742	1/1	0.97	0.30	-	37,37,37,37	0
56	MG	1B	220	1/1	0.90	0.11	-	52,52,52,52	0
56	MG	1a	1621	1/1	0.96	0.11	-	68,68,68,68	0
56	MG	2A	3170	1/1	0.95	0.11	-	40,40,40,40	0
56	MG	1A	3484	1/1	0.96	0.08	-	54,54,54,54	0
56	MG	1A	3074	1/1	0.97	0.25	-	34,34,34,34	0
56	MG	2A	3338	1/1	0.96	0.08	-	53,53,53,53	0
56	MG	1A	3458	1/1	0.75	0.18	-	71,71,71,71	0
56	MG	2A	3554	1/1	0.66	0.24	-	70,70,70,70	0
56	MG	1A	3070	1/1	0.95	0.18	-	52,52,52,52	0
56	MG	1A	3414	1/1	0.92	0.22	-	55,55,55,55	0
56	MG	1A	3113	1/1	0.97	0.13	-	27,27,27,27	0
56	MG	2a	1639	1/1	0.87	0.09	-	80,80,80,80	0
56	MG	1A	3176	1/1	0.95	0.16	-	38,38,38,38	0
56	MG	1A	3026	1/1	0.96	0.21	-	49,49,49,49	0
56	MG	2A	3354	1/1	0.94	0.11	-	49,49,49,49	0
56	MG	2Q	3002	1/1	0.96	0.14	-	44,44,44,44	0
56	MG	2A	3087	1/1	0.88	0.28	-	49,49,49,49	0
56	MG	1A	3092	1/1	0.96	0.27	-	47,47,47,47	0
56	MG	1A	3534	1/1	0.70	0.15	-	64,64,64,64	0
56	MG	2A	3034	1/1	0.96	0.11	-	44,44,44,44	0
56	MG	1A	3047	1/1	0.93	0.16	-	40,40,40,40	0
56	MG	1A	3969	1/1	0.98	0.12	-	40,40,40,40	0
56	MG	1A	4062	1/1	0.90	0.23	-	62,62,62,62	0
56	MG	1a	1838	1/1	1.00	0.09	-	34,34,34,34	0
56	MG	1A	3423	1/1	0.86	0.17	-	59,59,59,59	0
56	MG	2A	3017	1/1	0.89	0.19	-	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	2A	3312	1/1	0.94	0.10	-	27,27,27,27	0
56	MG	1A	3100	1/1	0.99	0.19	-	34,34,34,34	0
56	MG	1A	3853	1/1	0.95	0.12	-	44,44,44,44	0
56	MG	1a	1743	1/1	0.97	0.08	-	73,73,73,73	0
56	MG	1A	3695	1/1	0.97	0.22	-	29,29,29,29	0
56	MG	16	101	1/1	0.97	0.15	-	42,42,42,42	0
56	MG	1B	201	1/1	0.94	0.25	-	72,72,72,72	0
56	MG	2A	3463	1/1	0.87	0.13	-	57,57,57,57	0
56	MG	1A	3701	1/1	0.93	0.07	-	28,28,28,28	0
56	MG	1a	1679	1/1	0.95	0.16	-	54,54,54,54	0
56	MG	2A	3068	1/1	0.91	0.13	-	50,50,50,50	0
56	MG	2A	3414	1/1	0.98	0.31	-	67,67,67,67	0
56	MG	2A	3511	1/1	0.94	0.23	-	45,45,45,45	0
56	MG	2A	3450	1/1	0.92	0.19	-	52,52,52,52	0
56	MG	1A	3784	1/1	0.96	0.13	-	27,27,27,27	0
56	MG	1a	1624	1/1	0.92	0.34	-	64,64,64,64	0
56	MG	1A	3112	1/1	0.94	0.14	-	45,45,45,45	0
56	MG	1A	3051	1/1	0.95	0.31	-	47,47,47,47	0
56	MG	1A	3994	1/1	0.78	0.39	-	33,33,33,33	0
56	MG	1N	201	1/1	0.70	0.46	-	73,73,73,73	0
56	MG	1A	3212	1/1	0.92	0.07	-	50,50,50,50	0
56	MG	1A	3183	1/1	0.98	0.29	-	43,43,43,43	0
56	MG	2a	1804	1/1	0.95	0.28	-	60,60,60,60	0
56	MG	1A	3046	1/1	0.93	0.05	-	51,51,51,51	0
56	MG	1x	103	1/1	0.96	0.14	-	68,68,68,68	0
56	MG	2a	1681	1/1	0.95	0.16	-	53,53,53,53	0
56	MG	2D	306	1/1	0.94	0.14	-	55,55,55,55	0
56	MG	2A	3272	1/1	0.97	0.27	-	44,44,44,44	0
56	MG	1A	3020	1/1	0.97	0.25	-	47,47,47,47	0
56	MG	1a	1782	1/1	0.95	0.20	-	61,61,61,61	0
56	MG	2A	3155	1/1	0.98	0.14	-	33,33,33,33	0
56	MG	1A	3347	1/1	0.78	0.11	-	47,47,47,47	0
56	MG	2a	1614	1/1	0.74	0.42	-	55,55,55,55	0
56	MG	1A	3628	1/1	0.98	0.08	-	26,26,26,26	0
56	MG	1a	1857	1/1	0.95	0.32	-	47,47,47,47	0
56	MG	2A	3049	1/1	0.97	0.14	-	35,35,35,35	0
56	MG	1B	224	1/1	0.87	0.22	-	58,58,58,58	0
56	MG	1A	3599	1/1	0.94	0.12	-	47,47,47,47	0
56	MG	1F	301	1/1	0.97	0.23	-	36,36,36,36	0
56	MG	1A	3850	1/1	0.96	0.20	-	43,43,43,43	0
56	MG	1a	1883	1/1	0.96	0.20	-	47,47,47,47	0
56	MG	1A	3167	1/1	0.94	0.16	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3059	1/1	0.79	0.29	-	64,64,64,64	0
56	MG	2A	3385	1/1	0.96	0.16	-	42,42,42,42	0
56	MG	10	103	1/1	0.88	0.26	-	59,59,59,59	0
56	MG	2a	1765	1/1	0.96	0.25	-	52,52,52,52	0
56	MG	1A	3400	1/1	0.74	0.30	-	69,69,69,69	0
56	MG	2a	1670	1/1	0.96	0.10	-	60,60,60,60	0
56	MG	1A	3075	1/1	0.94	0.59	-	57,57,57,57	0
56	MG	2A	3418	1/1	0.95	0.20	-	56,56,56,56	0
56	MG	2a	1629	1/1	0.91	0.07	-	72,72,72,72	0
56	MG	2A	3507	1/1	0.96	0.29	-	63,63,63,63	0
56	MG	1A	3317	1/1	0.81	0.26	-	56,56,56,56	0
56	MG	2A	3268	1/1	0.87	0.30	-	75,75,75,75	0
56	MG	1A	3174	1/1	0.95	0.12	-	47,47,47,47	0
56	MG	2A	3003	1/1	0.96	0.11	-	44,44,44,44	0
56	MG	1E	304	1/1	0.95	0.14	-	44,44,44,44	0
56	MG	1A	3881	1/1	0.94	0.15	-	43,43,43,43	0
56	MG	1a	1901	1/1	0.73	0.25	-	65,65,65,65	0
56	MG	2a	1606	1/1	0.93	0.09	-	78,78,78,78	0
56	MG	1A	3409	1/1	0.75	0.38	-	51,51,51,51	0
56	MG	2A	3258	1/1	0.87	0.23	-	52,52,52,52	0
56	MG	1A	3421	1/1	0.95	0.11	-	52,52,52,52	0
56	MG	1A	3604	1/1	0.94	0.16	-	30,30,30,30	0
56	MG	1a	1819	1/1	0.69	0.40	-	59,59,59,59	0
56	MG	1A	3837	1/1	0.90	0.09	-	44,44,44,44	0
56	MG	1A	3068	1/1	0.97	0.04	-	53,53,53,53	0
56	MG	1A	3776	1/1	0.97	0.23	-	42,42,42,42	0
56	MG	2A	3465	1/1	0.98	0.34	-	52,52,52,52	0
56	MG	1a	1630	1/1	0.89	0.20	-	59,59,59,59	0
56	MG	2A	3011	1/1	0.97	0.48	-	50,50,50,50	0
56	MG	2A	3067	1/1	0.95	0.36	-	56,56,56,56	0
56	MG	2A	3094	1/1	0.75	0.23	-	45,45,45,45	0
56	MG	1A	3433	1/1	0.90	0.15	-	53,53,53,53	0
56	MG	1e	203	1/1	0.93	0.14	-	61,61,61,61	0
56	MG	1a	1612	1/1	0.83	0.15	-	58,58,58,58	0
56	MG	2A	3392	1/1	0.96	0.15	-	24,24,24,24	0
56	MG	2A	3342	1/1	0.92	0.34	-	56,56,56,56	0
56	MG	1A	3050	1/1	0.97	0.31	-	62,62,62,62	0
56	MG	2A	3114	1/1	0.92	0.29	-	45,45,45,45	0
56	MG	1A	3544	1/1	0.90	0.60	-	67,67,67,67	0
56	MG	2A	3142	1/1	0.90	0.55	-	53,53,53,53	0
56	MG	1A	3536	1/1	0.96	0.12	-	45,45,45,45	0
56	MG	28	8001	1/1	0.85	0.41	-	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	1781	1/1	0.96	0.46	-	68,68,68,68	0
56	MG	1A	3374	1/1	0.94	0.14	-	48,48,48,48	0
56	MG	2A	3077	1/1	0.90	0.26	-	54,54,54,54	0
56	MG	1A	3189	1/1	0.90	0.23	-	37,37,37,37	0
56	MG	1A	3153	1/1	0.98	0.21	-	36,36,36,36	0
56	MG	1A	4016	1/1	0.97	0.17	-	26,26,26,26	0
56	MG	1A	3468	1/1	0.87	0.53	-	64,64,64,64	0
56	MG	1A	3821	1/1	0.92	0.17	-	59,59,59,59	0
56	MG	1U	201	1/1	0.98	0.11	-	33,33,33,33	0
56	MG	1A	3053	1/1	0.93	0.61	-	41,41,41,41	0
56	MG	1B	216	1/1	0.96	0.16	-	33,33,33,33	0
56	MG	2A	3171	1/1	0.97	0.20	-	40,40,40,40	0
56	MG	1A	3989	1/1	0.98	0.14	-	38,38,38,38	0
56	MG	2A	3335	1/1	0.94	0.14	-	38,38,38,38	0
56	MG	1a	1705	1/1	0.97	0.15	-	38,38,38,38	0
56	MG	2a	1777	1/1	0.97	0.09	-	66,66,66,66	0
56	MG	2A	3213	1/1	0.92	0.15	-	53,53,53,53	0
56	MG	1A	3474	1/1	0.91	0.11	-	49,49,49,49	0
56	MG	1A	3691	1/1	0.96	0.11	-	8,8,8,8	0
56	MG	1A	3960	1/1	0.95	0.20	-	47,47,47,47	0
56	MG	1A	3678	1/1	0.96	0.28	-	44,44,44,44	0
56	MG	1A	3334	1/1	0.97	0.30	-	37,37,37,37	0
56	MG	2A	3211	1/1	0.95	0.09	-	58,58,58,58	0
56	MG	2A	3331	1/1	0.90	0.23	-	58,58,58,58	0
56	MG	1a	1752	1/1	0.94	0.53	-	60,60,60,60	0
56	MG	1a	1840	1/1	0.93	0.26	-	57,57,57,57	0
56	MG	2A	3098	1/1	0.87	0.25	-	50,50,50,50	0
56	MG	1A	4086	1/1	0.90	0.12	-	51,51,51,51	0
56	MG	1a	1847	1/1	0.86	0.18	-	45,45,45,45	0
56	MG	1A	3479	1/1	0.78	0.34	-	75,75,75,75	0
56	MG	1A	3413	1/1	0.94	0.27	-	53,53,53,53	0
56	MG	1A	3398	1/1	0.84	0.48	-	58,58,58,58	0
56	MG	1A	3162	1/1	0.97	0.45	-	35,35,35,35	0
56	MG	1A	3095	1/1	0.88	0.13	-	60,60,60,60	0
56	MG	2a	1619	1/1	0.94	0.21	-	53,53,53,53	0
56	MG	1A	3796	1/1	0.88	0.23	-	59,59,59,59	0
56	MG	1A	3605	1/1	0.98	0.09	-	42,42,42,42	0
56	MG	1r	103	1/1	0.90	0.12	-	51,51,51,51	0
56	MG	1A	3338	1/1	0.96	0.17	-	61,61,61,61	0
56	MG	2A	3027	1/1	0.96	0.18	-	53,53,53,53	0
56	MG	1a	1617	1/1	0.86	0.19	-	60,60,60,60	0
56	MG	1A	3758	1/1	0.95	0.12	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3436	1/1	0.99	0.17	-	32,32,32,32	0
56	MG	1A	3206	1/1	0.93	0.17	-	37,37,37,37	0
56	MG	1a	1848	1/1	0.97	0.13	-	45,45,45,45	0
56	MG	1a	1873	1/1	0.97	0.17	-	52,52,52,52	0
56	MG	1A	3339	1/1	0.88	0.19	-	73,73,73,73	0
56	MG	1x	106	1/1	0.92	0.17	-	46,46,46,46	0
56	MG	2a	1714	1/1	0.89	0.18	-	65,65,65,65	0
56	MG	18	102	1/1	0.87	0.39	-	48,48,48,48	0
56	MG	1A	3706	1/1	0.92	0.34	-	68,68,68,68	0
56	MG	1A	3109	1/1	0.87	0.11	-	60,60,60,60	0
56	MG	1A	3923	1/1	0.92	0.17	-	46,46,46,46	0
56	MG	2A	3195	1/1	0.97	0.31	-	38,38,38,38	0
56	MG	2A	3415	1/1	0.98	0.19	-	47,47,47,47	0
56	MG	1A	4010	1/1	0.96	0.16	-	37,37,37,37	0
56	MG	1A	3725	1/1	0.97	0.14	-	56,56,56,56	0
56	MG	1A	3550	1/1	0.75	0.21	-	81,81,81,81	0
56	MG	1a	1907	1/1	0.94	0.23	-	37,37,37,37	0
56	MG	1A	3284	1/1	0.96	0.35	-	41,41,41,41	0
56	MG	2A	3144	1/1	0.96	0.07	-	43,43,43,43	0
56	MG	2a	1750	1/1	0.92	0.38	-	54,54,54,54	0
56	MG	1A	3055	1/1	0.88	0.31	-	41,41,41,41	0
56	MG	1u	8001	1/1	0.92	0.21	-	69,69,69,69	0
56	MG	1a	1845	1/1	0.93	0.07	-	70,70,70,70	0
56	MG	2A	3224	1/1	0.93	0.11	-	37,37,37,37	0
56	MG	1A	3257	1/1	0.93	0.34	-	55,55,55,55	0
56	MG	1a	1637	1/1	0.93	0.14	-	51,51,51,51	0
56	MG	1A	3465	1/1	0.90	0.15	-	49,49,49,49	0
56	MG	1a	1735	1/1	0.96	0.37	-	43,43,43,43	0
56	MG	1W	3002	1/1	0.94	0.24	-	40,40,40,40	0
56	MG	1a	1641	1/1	0.92	0.81	-	64,64,64,64	0
56	MG	1A	3361	1/1	0.96	0.36	-	53,53,53,53	0
56	MG	1A	3629	1/1	0.97	0.17	-	40,40,40,40	0
56	MG	2A	3125	1/1	0.87	0.39	-	55,55,55,55	0
56	MG	1A	3039	1/1	0.90	0.17	-	51,51,51,51	0
56	MG	1a	1906	1/1	0.93	0.07	-	75,75,75,75	0
56	MG	1A	3436	1/1	0.82	0.33	-	66,66,66,66	0
56	MG	1A	3331	1/1	0.96	0.10	-	39,39,39,39	0
56	MG	2A	3410	1/1	0.93	0.12	-	56,56,56,56	0
56	MG	1A	3024	1/1	0.95	0.11	-	48,48,48,48	0
56	MG	1A	3396	1/1	0.96	0.17	-	39,39,39,39	0
56	MG	1A	3430	1/1	0.85	0.26	-	58,58,58,58	0
56	MG	1A	3210	1/1	0.98	0.14	-	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	2A	3166	1/1	0.97	0.14	-	40,40,40,40	0
56	MG	2A	3228	1/1	0.91	0.19	-	52,52,52,52	0
56	MG	1a	1853	1/1	0.98	0.08	-	31,31,31,31	0
56	MG	2a	1638	1/1	0.88	0.21	-	59,59,59,59	0
56	MG	1A	3816	1/1	0.93	0.17	-	56,56,56,56	0
56	MG	1A	3353	1/1	0.76	0.62	-	63,63,63,63	0
56	MG	2a	1603	1/1	0.95	0.29	-	50,50,50,50	0
56	MG	2A	3208	1/1	0.95	0.18	-	43,43,43,43	0
56	MG	1a	1806	1/1	0.88	0.17	-	79,79,79,79	0
56	MG	1o	3001	1/1	0.94	0.08	-	64,64,64,64	0
56	MG	2A	3452	1/1	0.78	0.44	-	69,69,69,69	0
56	MG	1a	1832	1/1	0.95	0.15	-	65,65,65,65	0
56	MG	1A	3908	1/1	0.97	0.16	-	49,49,49,49	0
56	MG	1a	1631	1/1	0.94	0.40	-	45,45,45,45	0
56	MG	2A	3280	1/1	0.93	0.11	-	46,46,46,46	0
56	MG	1A	3243	1/1	0.97	0.25	-	51,51,51,51	0
56	MG	2a	1742	1/1	0.92	0.28	-	71,71,71,71	0
56	MG	1A	3395	1/1	0.90	0.10	-	61,61,61,61	0
56	MG	1A	4008	1/1	0.91	0.23	-	68,68,68,68	0
56	MG	1A	3765	1/1	0.96	0.06	-	36,36,36,36	0
56	MG	1A	3490	1/1	0.85	0.38	-	56,56,56,56	0
56	MG	2A	3416	1/1	0.95	0.09	-	50,50,50,50	0
56	MG	2a	1717	1/1	0.88	0.22	-	57,57,57,57	0
56	MG	2A	3254	1/1	0.95	0.18	-	55,55,55,55	0
56	MG	1A	3693	1/1	0.92	0.12	-	25,25,25,25	0
56	MG	1A	3917	1/1	0.98	0.13	-	58,58,58,58	0
56	MG	2a	1755	1/1	0.89	0.14	-	82,82,82,82	0
56	MG	2A	3494	1/1	0.91	0.24	-	54,54,54,54	0
56	MG	1A	4033	1/1	0.91	0.12	-	71,71,71,71	0
56	MG	1A	3089	1/1	0.91	0.17	-	50,50,50,50	0
56	MG	1A	3169	1/1	0.89	0.33	-	48,48,48,48	0
56	MG	15	104	1/1	0.90	0.26	-	54,54,54,54	0
56	MG	1a	1861	1/1	0.90	0.13	-	48,48,48,48	0
56	MG	1A	3615	1/1	0.98	0.17	-	16,16,16,16	0
56	MG	2A	3122	1/1	0.92	0.08	-	54,54,54,54	0
56	MG	1A	3250	1/1	0.98	0.13	-	52,52,52,52	0
56	MG	1A	3248	1/1	0.89	0.17	-	42,42,42,42	0
56	MG	1A	3875	1/1	0.97	0.13	-	19,19,19,19	0
56	MG	2F	301	1/1	0.96	0.12	-	39,39,39,39	0
56	MG	2A	3209	1/1	0.93	0.21	-	49,49,49,49	0
56	MG	1A	3370	1/1	0.95	0.15	-	43,43,43,43	0
56	MG	2A	3101	1/1	0.98	0.15	-	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	16	103	1/1	0.86	0.13	-	36,36,36,36	0
56	MG	2A	3403	1/1	0.98	0.33	-	53,53,53,53	0
56	MG	1A	3504	1/1	0.96	0.13	-	64,64,64,64	0
56	MG	1A	3621	1/1	0.91	0.13	-	79,79,79,79	0
56	MG	1x	109	1/1	0.99	0.05	-	78,78,78,78	0
56	MG	1A	3285	1/1	0.95	0.14	-	47,47,47,47	0
56	MG	2A	3433	1/1	0.94	0.13	-	56,56,56,56	0
56	MG	1A	3343	1/1	0.81	0.17	-	54,54,54,54	0
56	MG	1A	3105	1/1	0.87	0.13	-	43,43,43,43	0
56	MG	2a	1705	1/1	0.93	0.28	-	68,68,68,68	0
56	MG	1a	1646	1/1	0.80	0.30	-	60,60,60,60	0
56	MG	1A	4015	1/1	0.93	0.10	-	29,29,29,29	0
56	MG	1T	206	1/1	0.94	0.22	-	69,69,69,69	0
56	MG	1A	3383	1/1	0.94	0.20	-	43,43,43,43	0
56	MG	1a	1701	1/1	0.94	0.13	-	60,60,60,60	0
56	MG	2D	304	1/1	0.95	0.18	-	27,27,27,27	0
56	MG	1a	1897	1/1	0.93	0.42	-	53,53,53,53	0
56	MG	1a	1816	1/1	0.95	0.07	-	56,56,56,56	0
56	MG	2A	3397	1/1	0.96	0.26	-	27,27,27,27	0
56	MG	2A	3092	1/1	0.90	0.20	-	52,52,52,52	0
56	MG	2a	1766	1/1	0.82	0.21	-	83,83,83,83	0
56	MG	1A	4082	1/1	0.91	0.16	-	44,44,44,44	0
56	MG	1A	3503	1/1	0.92	0.13	-	56,56,56,56	0
56	MG	2N	8001	1/1	0.93	0.18	-	56,56,56,56	0
56	MG	1A	3546	1/1	0.97	0.18	-	62,62,62,62	0
56	MG	2a	1601	1/1	0.91	0.39	-	54,54,54,54	0
56	MG	1A	3940	1/1	0.92	0.14	-	48,48,48,48	0
56	MG	1A	3858	1/1	0.94	0.23	-	44,44,44,44	0
56	MG	1A	4027	1/1	0.94	0.15	-	50,50,50,50	0
56	MG	2A	3460	1/1	0.97	0.24	-	44,44,44,44	0
56	MG	1A	3455	1/1	0.90	0.11	-	59,59,59,59	0
56	MG	1A	3228	1/1	0.94	0.29	-	33,33,33,33	0
56	MG	1A	3040	1/1	0.96	0.22	-	34,34,34,34	0
56	MG	2A	3302	1/1	0.97	0.19	-	48,48,48,48	0
56	MG	1a	1849	1/1	0.96	0.06	-	59,59,59,59	0
56	MG	1A	3404	1/1	0.98	0.13	-	38,38,38,38	0
56	MG	1A	3019	1/1	0.94	0.28	-	46,46,46,46	0
56	MG	1A	3012	1/1	0.95	0.36	-	46,46,46,46	0
56	MG	2a	1608	1/1	0.93	0.09	-	67,67,67,67	0
56	MG	1A	3819	1/1	0.95	0.14	-	80,80,80,80	0
56	MG	2A	3464	1/1	0.85	0.29	-	59,59,59,59	0
56	MG	2a	1735	1/1	0.93	0.15	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3527	1/1	0.97	0.16	-	37,37,37,37	0
56	MG	1A	3449	1/1	0.95	0.29	-	54,54,54,54	0
56	MG	1A	3700	1/1	0.79	0.13	-	31,31,31,31	0
56	MG	1A	3426	1/1	0.99	0.17	-	56,56,56,56	0
56	MG	1A	3267	1/1	0.96	0.50	-	51,51,51,51	0
56	MG	1A	3851	1/1	0.97	0.28	-	52,52,52,52	0
56	MG	2A	3033	1/1	0.95	0.10	-	57,57,57,57	0
56	MG	1A	3951	1/1	0.92	0.14	-	40,40,40,40	0
56	MG	1A	3093	1/1	0.97	0.31	-	54,54,54,54	0
56	MG	2a	1637	1/1	0.96	0.22	-	71,71,71,71	0
56	MG	2a	1615	1/1	0.99	0.10	-	56,56,56,56	0
56	MG	1a	1616	1/1	0.83	0.24	-	63,63,63,63	0
56	MG	20	8001	1/1	0.75	0.22	-	67,67,67,67	0
56	MG	1A	4009	1/1	0.95	0.19	-	40,40,40,40	0
56	MG	1A	3535	1/1	0.92	0.22	-	57,57,57,57	0
56	MG	2a	1796	1/1	0.87	0.15	-	73,73,73,73	0
56	MG	2A	3373	1/1	0.91	0.13	-	41,41,41,41	0
56	MG	1B	207	1/1	0.97	0.11	-	43,43,43,43	0
56	MG	2A	3235	1/1	0.98	0.37	-	54,54,54,54	0
56	MG	1A	3121	1/1	0.95	0.14	-	30,30,30,30	0
56	MG	1A	3827	1/1	0.93	0.24	-	44,44,44,44	0
56	MG	2A	3198	1/1	0.95	0.16	-	51,51,51,51	0
56	MG	1A	3515	1/1	0.97	0.10	-	57,57,57,57	0
56	MG	1A	3204	1/1	0.99	0.19	-	36,36,36,36	0
56	MG	1A	3415	1/1	0.88	0.33	-	58,58,58,58	0
56	MG	1A	3562	1/1	0.90	0.11	-	63,63,63,63	0
56	MG	1h	3002	1/1	0.97	0.09	-	63,63,63,63	0
56	MG	1A	3497	1/1	0.98	0.14	-	36,36,36,36	0
56	MG	2A	3488	1/1	0.95	0.16	-	57,57,57,57	0
56	MG	2A	3147	1/1	0.90	0.17	-	33,33,33,33	0
56	MG	1A	3522	1/1	0.90	0.10	-	73,73,73,73	0
56	MG	1A	3033	1/1	0.96	0.13	-	39,39,39,39	0
56	MG	1A	3084	1/1	0.93	0.26	-	32,32,32,32	0
56	MG	1A	3221	1/1	0.95	0.12	-	36,36,36,36	0
56	MG	1A	3529	1/1	0.88	0.13	-	46,46,46,46	0
56	MG	2A	3063	1/1	0.95	0.31	-	47,47,47,47	0
56	MG	1A	3359	1/1	0.82	0.31	-	43,43,43,43	0
56	MG	1A	3322	1/1	0.83	0.23	-	55,55,55,55	0
56	MG	2a	1610	1/1	0.91	0.25	-	60,60,60,60	0
56	MG	1a	1619	1/1	0.94	0.15	-	82,82,82,82	0
56	MG	1A	3170	1/1	0.95	0.23	-	23,23,23,23	0
56	MG	1a	1821	1/1	0.96	0.10	-	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	1F	305	1/1	0.94	0.18	-	48,48,48,48	0
56	MG	1A	3066	1/1	0.94	0.09	-	56,56,56,56	0
56	MG	1a	1798	1/1	0.94	0.13	-	52,52,52,52	0
56	MG	1A	3967	1/1	0.82	0.14	-	51,51,51,51	0
56	MG	2a	1767	1/1	0.97	0.06	-	57,57,57,57	0
56	MG	1A	3191	1/1	0.96	0.23	-	37,37,37,37	0
56	MG	1A	3453	1/1	0.95	0.09	-	48,48,48,48	0
56	MG	1A	3724	1/1	0.96	0.08	-	50,50,50,50	0
56	MG	1a	1645	1/1	0.94	0.07	-	59,59,59,59	0
56	MG	1A	3495	1/1	0.83	0.15	-	61,61,61,61	0
56	MG	2a	1761	1/1	0.95	0.04	-	45,45,45,45	0
56	MG	1a	1864	1/1	0.94	0.30	-	61,61,61,61	0
56	MG	1A	3083	1/1	0.90	0.29	-	48,48,48,48	0
56	MG	2A	3263	1/1	0.98	0.29	-	41,41,41,41	0
56	MG	2A	3319	1/1	0.91	0.13	-	55,55,55,55	0
56	MG	1A	3878	1/1	0.98	0.08	-	20,20,20,20	0
56	MG	1B	206	1/1	0.93	0.21	-	38,38,38,38	0
56	MG	1A	3852	1/1	0.96	0.14	-	41,41,41,41	0
56	MG	2Q	3001	1/1	0.93	0.35	-	39,39,39,39	0
56	MG	2A	3200	1/1	0.84	0.21	-	41,41,41,41	0
56	MG	1A	3626	1/1	0.92	0.21	-	27,27,27,27	0
56	MG	1A	3184	1/1	0.97	0.29	-	35,35,35,35	0
56	MG	2A	3054	1/1	0.92	0.15	-	44,44,44,44	0
56	MG	1A	3048	1/1	0.94	0.33	-	43,43,43,43	0
56	MG	1A	3711	1/1	0.96	0.24	-	63,63,63,63	0
56	MG	1B	225	1/1	0.95	0.09	-	51,51,51,51	0
56	MG	1a	1822	1/1	0.85	0.18	-	76,76,76,76	0
56	MG	2a	1707	1/1	0.97	0.10	-	58,58,58,58	0
56	MG	2A	3446	1/1	0.95	0.13	-	52,52,52,52	0
56	MG	2A	3008	1/1	0.96	0.18	-	58,58,58,58	0
56	MG	1A	3182	1/1	0.95	0.18	-	33,33,33,33	0
56	MG	1a	1834	1/1	0.92	0.27	-	48,48,48,48	0
56	MG	1a	1763	1/1	0.85	0.12	-	57,57,57,57	0
56	MG	1A	3355	1/1	0.93	0.11	-	54,54,54,54	0
56	MG	2a	1660	1/1	0.94	0.07	-	62,62,62,62	0
56	MG	1A	3870	1/1	0.97	0.10	-	47,47,47,47	0
56	MG	2a	1776	1/1	0.94	0.18	-	54,54,54,54	0
56	MG	2A	3294	1/1	0.88	0.21	-	41,41,41,41	0
56	MG	1a	1755	1/1	0.79	0.20	-	68,68,68,68	0
56	MG	1A	3017	1/1	0.96	0.54	-	53,53,53,53	0
56	MG	1a	1669	1/1	0.91	0.17	-	45,45,45,45	0
56	MG	1A	3274	1/1	0.80	0.15	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3846	1/1	0.96	0.13	-	21,21,21,21	0
56	MG	1A	3194	1/1	0.88	0.29	-	50,50,50,50	0
56	MG	1A	3371	1/1	0.92	0.26	-	46,46,46,46	0
56	MG	1A	3828	1/1	0.87	0.19	-	22,22,22,22	0
56	MG	1A	3966	1/1	0.98	0.14	-	56,56,56,56	0
56	MG	1A	3638	1/1	0.97	0.16	-	56,56,56,56	0
56	MG	1a	1653	1/1	0.91	0.15	-	54,54,54,54	0
56	MG	1a	1722	1/1	0.95	0.14	-	65,65,65,65	0
56	MG	1B	218	1/1	0.98	0.12	-	43,43,43,43	0
56	MG	1A	3438	1/1	0.92	0.21	-	54,54,54,54	0
56	MG	2a	1718	1/1	0.91	0.40	-	53,53,53,53	0
56	MG	1a	1779	1/1	0.85	0.18	-	47,47,47,47	0
56	MG	2A	3376	1/1	0.99	0.19	-	48,48,48,48	0
56	MG	1Z	301	1/1	0.93	0.16	-	44,44,44,44	0
56	MG	1A	3689	1/1	0.81	0.16	-	34,34,34,34	0
56	MG	1a	1710	1/1	0.80	0.13	-	59,59,59,59	0
56	MG	1A	4096	1/1	0.98	0.29	-	69,69,69,69	0
56	MG	1A	3435	1/1	0.81	0.17	-	71,71,71,71	0
56	MG	1A	3813	1/1	0.95	0.14	-	37,37,37,37	0
56	MG	2A	3103	1/1	0.96	0.24	-	50,50,50,50	0
56	MG	1a	1611	1/1	0.94	0.07	-	76,76,76,76	0
56	MG	1a	1859	1/1	0.86	0.21	-	65,65,65,65	0
56	MG	1A	3736	1/1	0.96	0.17	-	34,34,34,34	0
56	MG	1A	3814	1/1	0.98	0.16	-	35,35,35,35	0
56	MG	1A	3890	1/1	0.90	0.21	-	63,63,63,63	0
56	MG	2A	3357	1/1	0.98	0.10	-	55,55,55,55	0
56	MG	1A	4034	1/1	0.93	0.13	-	50,50,50,50	0
56	MG	1A	3564	1/1	0.75	0.11	-	72,72,72,72	0
56	MG	2A	3431	1/1	0.97	0.05	-	59,59,59,59	0
56	MG	2a	1609	1/1	0.98	0.38	-	60,60,60,60	0
56	MG	1A	3216	1/1	0.88	0.17	-	41,41,41,41	0
56	MG	17	102	1/1	0.89	0.21	-	40,40,40,40	0
56	MG	2A	3348	1/1	0.93	0.14	-	49,49,49,49	0
56	MG	2a	1605	1/1	0.84	0.15	-	66,66,66,66	0
56	MG	1a	1884	1/1	0.97	0.12	-	44,44,44,44	0
56	MG	2A	3078	1/1	0.96	0.19	-	51,51,51,51	0
56	MG	1a	1855	1/1	0.93	0.31	-	58,58,58,58	0
56	MG	1A	3483	1/1	0.87	0.27	-	75,75,75,75	0
56	MG	1A	3011	1/1	0.92	0.20	-	49,49,49,49	0
56	MG	1A	3970	1/1	0.96	0.14	-	28,28,28,28	0
56	MG	11	102	1/1	0.93	0.14	-	58,58,58,58	0
56	MG	1A	3292	1/1	0.78	0.27	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3081	1/1	0.95	0.13	-	57,57,57,57	0
56	MG	1A	3323	1/1	0.96	0.11	-	40,40,40,40	0
56	MG	1A	3514	1/1	0.96	0.36	-	46,46,46,46	0
56	MG	1a	1738	1/1	0.93	0.21	-	53,53,53,53	0
56	MG	1a	1835	1/1	0.98	0.14	-	54,54,54,54	0
56	MG	1A	3780	1/1	0.92	0.21	-	23,23,23,23	0
56	MG	2A	3308	1/1	0.96	0.13	-	44,44,44,44	0
56	MG	1A	3774	1/1	0.94	0.14	-	63,63,63,63	0
56	MG	1A	3090	1/1	0.96	0.08	-	36,36,36,36	0
56	MG	2A	3535	1/1	0.76	0.11	-	51,51,51,51	0
56	MG	2A	3543	1/1	0.97	0.06	-	47,47,47,47	0
56	MG	2a	1811	1/1	0.88	0.16	-	66,66,66,66	0
56	MG	1A	3664	1/1	0.95	0.12	-	37,37,37,37	0
56	MG	1A	3180	1/1	0.86	0.17	-	39,39,39,39	0
56	MG	2A	3239	1/1	0.95	0.12	-	59,59,59,59	0
56	MG	1A	3785	1/1	0.97	0.12	-	21,21,21,21	0
56	MG	1A	3906	1/1	0.95	0.06	-	67,67,67,67	0
56	MG	1B	202	1/1	0.96	0.14	-	56,56,56,56	0
56	MG	1A	3624	1/1	0.84	0.12	-	50,50,50,50	0
56	MG	1A	3577	1/1	0.86	0.18	-	32,32,32,32	0
56	MG	1a	1889	1/1	0.73	0.22	-	68,68,68,68	0
56	MG	2a	1692	1/1	0.97	0.08	-	67,67,67,67	0
56	MG	1A	3397	1/1	0.91	0.15	-	46,46,46,46	0
56	MG	1A	3466	1/1	0.92	0.27	-	57,57,57,57	0
56	MG	2A	3461	1/1	0.96	0.23	-	64,64,64,64	0
56	MG	1A	3261	1/1	0.88	0.17	-	43,43,43,43	0
56	MG	2A	3165	1/1	0.89	0.10	-	35,35,35,35	0
56	MG	1A	3687	1/1	0.87	0.23	-	53,53,53,53	0
56	MG	1A	3230	1/1	0.94	0.18	-	28,28,28,28	0
56	MG	2A	3181	1/1	0.93	0.21	-	38,38,38,38	0
56	MG	2A	3519	1/1	0.93	0.15	-	44,44,44,44	0
56	MG	1a	1650	1/1	0.98	0.14	-	42,42,42,42	0
56	MG	1A	3794	1/1	0.95	0.06	-	57,57,57,57	0
56	MG	1A	3175	1/1	0.96	0.17	-	21,21,21,21	0
56	MG	2a	1762	1/1	0.96	0.08	-	70,70,70,70	0
56	MG	1Y	201	1/1	0.93	0.29	-	39,39,39,39	0
56	MG	1A	3445	1/1	0.98	0.17	-	55,55,55,55	0
56	MG	2a	1744	1/1	0.89	0.30	-	63,63,63,63	0
56	MG	2a	1662	1/1	0.88	0.09	-	83,83,83,83	0
56	MG	2A	3029	1/1	0.81	0.30	-	54,54,54,54	0
56	MG	2A	3291	1/1	0.69	0.13	-	48,48,48,48	0
56	MG	1A	3406	1/1	0.93	0.14	-	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	1q	3304	1/1	0.95	0.15	-	47,47,47,47	0
56	MG	2A	3139	1/1	0.96	0.16	-	40,40,40,40	0
56	MG	2A	3536	1/1	0.94	0.18	-	37,37,37,37	0
56	MG	2a	1664	1/1	0.95	0.37	-	51,51,51,51	0
56	MG	1A	4032	1/1	0.96	0.08	-	35,35,35,35	0
56	MG	1A	3181	1/1	0.97	0.08	-	41,41,41,41	0
56	MG	1A	3805	1/1	0.95	0.18	-	21,21,21,21	0
56	MG	1A	3549	1/1	0.87	0.27	-	64,64,64,64	0
56	MG	1A	3501	1/1	0.82	0.34	-	66,66,66,66	0
56	MG	1A	3290	1/1	0.89	0.14	-	55,55,55,55	0
56	MG	1A	3541	1/1	0.97	0.11	-	44,44,44,44	0
56	MG	2A	3150	1/1	0.97	0.24	-	39,39,39,39	0
56	MG	1A	3844	1/1	0.91	0.14	-	56,56,56,56	0
56	MG	1A	3779	1/1	0.90	0.19	-	36,36,36,36	0
56	MG	1A	3211	1/1	0.94	0.15	-	43,43,43,43	0
56	MG	1a	1688	1/1	0.84	0.13	-	72,72,72,72	0
56	MG	1A	4040	1/1	0.93	0.15	-	51,51,51,51	0
56	MG	1A	3995	1/1	0.94	0.23	-	16,16,16,16	0
56	MG	1A	3964	1/1	0.93	0.18	-	20,20,20,20	0
56	MG	1A	3723	1/1	0.95	0.14	-	51,51,51,51	0
56	MG	1A	3014	1/1	0.93	0.31	-	46,46,46,46	0
56	MG	2A	3084	1/1	0.82	0.24	-	39,39,39,39	0
56	MG	1A	3201	1/1	0.94	0.18	-	49,49,49,49	0
56	MG	1A	3114	1/1	0.95	0.13	-	36,36,36,36	0
56	MG	1A	3616	1/1	0.98	0.17	-	32,32,32,32	0
56	MG	2A	3325	1/1	0.96	0.20	-	70,70,70,70	0
56	MG	2a	1764	1/1	0.90	0.30	-	52,52,52,52	0
56	MG	2A	3428	1/1	0.95	0.32	-	58,58,58,58	0
56	MG	2x	3001	1/1	0.97	0.09	-	57,57,57,57	0
56	MG	2a	1721	1/1	0.86	0.12	-	49,49,49,49	0
56	MG	1A	3171	1/1	0.94	0.09	-	45,45,45,45	0
56	MG	2A	3169	1/1	0.93	0.34	-	54,54,54,54	0
56	MG	1A	3903	1/1	0.93	0.27	-	50,50,50,50	0
56	MG	2a	1791	1/1	0.93	0.36	-	71,71,71,71	0
56	MG	2A	3134	1/1	0.94	0.12	-	40,40,40,40	0
56	MG	2A	3273	1/1	0.93	0.10	-	70,70,70,70	0
56	MG	1A	3004	1/1	0.96	0.10	-	49,49,49,49	0
56	MG	1A	3385	1/1	0.75	0.51	-	56,56,56,56	0
56	MG	1A	3953	1/1	0.94	0.20	-	44,44,44,44	0
56	MG	2A	3420	1/1	0.95	0.10	-	54,54,54,54	0
56	MG	2A	3541	1/1	0.95	0.22	-	31,31,31,31	0
56	MG	1A	3357	1/1	0.97	0.06	-	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	3567	1/1	0.92	0.25	-	47,47,47,47	0
56	MG	1A	3786	1/1	0.99	0.13	-	31,31,31,31	0
56	MG	1A	4049	1/1	0.96	0.36	-	18,18,18,18	0
56	MG	1a	1677	1/1	0.97	0.27	-	45,45,45,45	0
56	MG	1A	3480	1/1	0.94	0.18	-	47,47,47,47	0
56	MG	1A	3428	1/1	0.96	0.11	-	36,36,36,36	0
56	MG	1A	3859	1/1	0.98	0.26	-	41,41,41,41	0
56	MG	1A	3237	1/1	0.94	0.11	-	27,27,27,27	0
56	MG	2a	1679	1/1	0.97	0.23	-	52,52,52,52	0
56	MG	2A	3375	1/1	0.97	0.09	-	57,57,57,57	0
56	MG	1A	3195	1/1	0.97	0.24	-	38,38,38,38	0
56	MG	1a	1802	1/1	0.94	0.14	-	56,56,56,56	0
56	MG	1A	3767	1/1	0.93	0.15	-	71,71,71,71	0
56	MG	2A	3050	1/1	0.89	0.33	-	47,47,47,47	0
56	MG	1A	3238	1/1	0.94	0.09	-	63,63,63,63	0
56	MG	2A	3042	1/1	0.95	0.23	-	50,50,50,50	0
56	MG	1A	3311	1/1	0.91	0.13	-	67,67,67,67	0
56	MG	1A	4007	1/1	0.96	0.13	-	68,68,68,68	0
56	MG	2a	1814	1/1	0.88	0.13	-	79,79,79,79	0
56	MG	2A	3439	1/1	0.85	0.10	-	65,65,65,65	0
56	MG	2A	3172	1/1	0.91	0.45	-	58,58,58,58	0
56	MG	1A	3517	1/1	0.97	0.06	-	55,55,55,55	0
56	MG	1A	3209	1/1	0.97	0.15	-	45,45,45,45	0
56	MG	2a	1613	1/1	0.91	0.49	-	63,63,63,63	0
56	MG	1A	3028	1/1	0.87	0.29	-	52,52,52,52	0
56	MG	19	101	1/1	0.94	0.21	-	55,55,55,55	0
56	MG	2a	1675	1/1	0.98	0.13	-	59,59,59,59	0
56	MG	2a	1731	1/1	0.94	0.12	-	68,68,68,68	0
56	MG	17	106	1/1	0.78	0.16	-	40,40,40,40	0
56	MG	1A	3644	1/1	0.95	0.12	-	60,60,60,60	0
56	MG	1A	3938	1/1	0.92	0.13	-	34,34,34,34	0
56	MG	1A	3056	1/1	0.98	0.29	-	57,57,57,57	0
56	MG	2A	3032	1/1	0.87	0.26	-	59,59,59,59	0
56	MG	2A	3445	1/1	0.90	0.18	-	56,56,56,56	0
56	MG	1a	1825	1/1	0.94	0.16	-	64,64,64,64	0
56	MG	1A	3254	1/1	0.95	0.28	-	29,29,29,29	0
56	MG	1A	3914	1/1	0.90	0.20	-	51,51,51,51	0
56	MG	1A	3777	1/1	0.90	0.15	-	41,41,41,41	0
56	MG	1A	3900	1/1	0.93	0.25	-	49,49,49,49	0
56	MG	2A	3070	1/1	0.94	0.14	-	53,53,53,53	0
56	MG	1E	305	1/1	0.85	0.36	-	45,45,45,45	0
56	MG	2B	3010	1/1	0.98	0.21	-	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	3509	1/1	0.95	0.18	-	44,44,44,44	0
56	MG	1A	4052	1/1	0.95	0.43	-	43,43,43,43	0
56	MG	2A	3487	1/1	0.82	0.10	-	67,67,67,67	0
56	MG	1A	3559	1/1	0.97	0.20	-	47,47,47,47	0
56	MG	1A	3072	1/1	0.90	0.29	-	44,44,44,44	0
56	MG	1A	3984	1/1	0.98	0.14	-	51,51,51,51	0
56	MG	1A	3378	1/1	0.87	0.24	-	36,36,36,36	0
56	MG	1A	3528	1/1	0.95	0.21	-	64,64,64,64	0
56	MG	2A	3253	1/1	0.90	0.27	-	29,29,29,29	0
56	MG	2A	3262	1/1	0.97	0.13	-	35,35,35,35	0
56	MG	1a	1762	1/1	0.96	0.13	-	59,59,59,59	0
56	MG	1A	3627	1/1	0.95	0.15	-	50,50,50,50	0
56	MG	1A	3337	1/1	0.97	0.07	-	39,39,39,39	0
56	MG	1a	1865	1/1	0.94	0.10	-	55,55,55,55	0
56	MG	1A	4030	1/1	0.76	0.31	-	77,77,77,77	0
56	MG	1a	1820	1/1	0.83	0.30	-	50,50,50,50	0
56	MG	1A	3372	1/1	0.93	0.19	-	52,52,52,52	0
56	MG	1A	3431	1/1	0.81	0.19	-	64,64,64,64	0
56	MG	2A	3215	1/1	0.96	0.14	-	43,43,43,43	0
56	MG	1A	3111	1/1	0.96	0.18	-	35,35,35,35	0
56	MG	1A	3924	1/1	0.91	0.21	-	23,23,23,23	0
56	MG	1A	4065	1/1	0.86	0.15	-	42,42,42,42	0
56	MG	2a	1756	1/1	0.99	0.18	-	47,47,47,47	0
56	MG	1a	1633	1/1	0.97	0.26	-	51,51,51,51	0
56	MG	1A	3942	1/1	0.26	0.17	-	53,53,53,53	0
56	MG	2a	1768	1/1	0.91	0.25	-	70,70,70,70	0
56	MG	2A	3115	1/1	0.89	0.25	-	49,49,49,49	0
56	MG	1a	1895	1/1	0.88	0.28	-	47,47,47,47	0
56	MG	1A	3874	1/1	0.94	0.10	-	33,33,33,33	0
56	MG	2A	3113	1/1	0.91	0.27	-	44,44,44,44	0
56	MG	1a	1665	1/1	0.95	0.17	-	54,54,54,54	0
56	MG	1P	205	1/1	0.90	0.47	-	75,75,75,75	0
56	MG	2A	3393	1/1	0.91	0.25	-	44,44,44,44	0
56	MG	2a	1729	1/1	0.82	0.10	-	58,58,58,58	0
56	MG	2A	3363	1/1	0.97	0.28	-	52,52,52,52	0
56	MG	1a	1664	1/1	0.90	0.12	-	50,50,50,50	0
56	MG	1A	3642	1/1	0.94	0.16	-	39,39,39,39	0
56	MG	1A	4013	1/1	0.82	0.38	-	55,55,55,55	0
56	MG	1a	1812	1/1	0.88	0.28	-	66,66,66,66	0
56	MG	1A	3692	1/1	0.96	0.06	-	61,61,61,61	0
56	MG	2a	1672	1/1	0.87	0.38	-	57,57,57,57	0
56	MG	1N	207	1/1	0.98	0.05	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1624	1/1	0.94	0.14	-	62,62,62,62	0
56	MG	1A	3992	1/1	0.91	0.14	-	70,70,70,70	0
56	MG	1A	3976	1/1	0.93	0.18	-	46,46,46,46	0
56	MG	1A	3963	1/1	0.98	0.04	-	33,33,33,33	0
56	MG	2A	3204	1/1	0.87	0.21	-	46,46,46,46	0
56	MG	1A	3071	1/1	0.97	0.10	-	41,41,41,41	0
56	MG	1A	3617	1/1	0.98	0.17	-	38,38,38,38	0
56	MG	1A	3469	1/1	0.97	0.17	-	16,16,16,16	0
56	MG	1a	1697	1/1	0.64	0.19	-	67,67,67,67	0
56	MG	1A	3913	1/1	0.83	0.15	-	73,73,73,73	0
56	MG	2a	1724	1/1	0.93	0.22	-	64,64,64,64	0
56	MG	1A	3061	1/1	0.95	0.15	-	51,51,51,51	0
56	MG	1A	3491	1/1	0.98	0.10	-	45,45,45,45	0
56	MG	2a	1802	1/1	0.90	0.33	-	68,68,68,68	0
56	MG	2a	1720	1/1	0.97	0.28	-	60,60,60,60	0
56	MG	1A	4081	1/1	0.94	0.64	-	27,27,27,27	0
56	MG	2A	3051	1/1	0.87	0.35	-	62,62,62,62	0
56	MG	1A	3540	1/1	0.86	0.20	-	69,69,69,69	0
56	MG	2A	3093	1/1	0.90	0.35	-	52,52,52,52	0
56	MG	2a	1745	1/1	0.90	0.31	-	54,54,54,54	0
56	MG	2A	3457	1/1	0.95	0.06	-	68,68,68,68	0
56	MG	2A	3380	1/1	0.93	0.10	-	37,37,37,37	0
56	MG	1x	101	1/1	0.67	0.67	-	89,89,89,89	0
56	MG	2A	3372	1/1	0.94	0.07	-	58,58,58,58	0
56	MG	2A	3318	1/1	0.88	0.33	-	58,58,58,58	0
56	MG	2a	1655	1/1	0.95	0.10	-	60,60,60,60	0
56	MG	1A	3566	1/1	0.85	0.11	-	64,64,64,64	0
56	MG	1a	1817	1/1	0.84	0.14	-	71,71,71,71	0
56	MG	1a	1881	1/1	0.94	0.21	-	40,40,40,40	0
56	MG	1a	1896	1/1	0.97	0.15	-	72,72,72,72	0
56	MG	1a	1635	1/1	0.78	0.25	-	66,66,66,66	0
56	MG	1A	3099	1/1	0.94	0.26	-	53,53,53,53	0
56	MG	2A	3240	1/1	0.94	0.16	-	46,46,46,46	0
56	MG	2a	1769	1/1	0.92	0.23	-	56,56,56,56	0
56	MG	1A	3602	1/1	0.91	0.16	-	46,46,46,46	0
56	MG	1A	3493	1/1	0.78	0.25	-	54,54,54,54	0
56	MG	1d	503	1/1	0.96	0.12	-	56,56,56,56	0
56	MG	1A	3038	1/1	0.98	0.15	-	51,51,51,51	0
56	MG	1A	3156	1/1	0.91	0.31	-	40,40,40,40	0
56	MG	1A	3579	1/1	0.92	0.07	-	51,51,51,51	0
56	MG	2A	3014	1/1	0.85	0.31	-	59,59,59,59	0
56	MG	1A	3411	1/1	0.92	0.14	-	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	2a	1611	1/1	0.91	0.10	-	68,68,68,68	0
56	MG	1A	3539	1/1	0.89	0.18	-	56,56,56,56	0
56	MG	1A	3324	1/1	0.91	0.07	-	62,62,62,62	0
56	MG	2A	3099	1/1	0.95	0.05	-	57,57,57,57	0
56	MG	1a	1791	1/1	0.87	0.19	-	71,71,71,71	0
56	MG	1A	3883	1/1	0.93	0.16	-	45,45,45,45	0
56	MG	2A	3110	1/1	0.97	0.34	-	44,44,44,44	0
56	MG	1a	1878	1/1	0.95	0.21	-	64,64,64,64	0
56	MG	2A	3476	1/1	0.95	0.12	-	72,72,72,72	0
56	MG	1A	3645	1/1	0.95	0.25	-	44,44,44,44	0
56	MG	2a	1625	1/1	0.94	0.26	-	42,42,42,42	0
56	MG	2A	3497	1/1	0.93	0.22	-	62,62,62,62	0
56	MG	1A	3609	1/1	0.95	0.26	-	26,26,26,26	0
56	MG	1A	3286	1/1	0.88	0.25	-	63,63,63,63	0
56	MG	2a	1634	1/1	0.96	0.13	-	94,94,94,94	0
56	MG	2a	1730	1/1	0.96	0.13	-	66,66,66,66	0
56	MG	17	103	1/1	0.90	0.26	-	49,49,49,49	0
56	MG	1A	3894	1/1	0.94	0.13	-	49,49,49,49	0
56	MG	2A	3016	1/1	0.95	0.11	-	58,58,58,58	0
56	MG	1a	1902	1/1	0.60	0.59	-	92,92,92,92	0
56	MG	2Z	3001	1/1	0.89	0.05	-	73,73,73,73	0
56	MG	1A	3929	1/1	0.94	0.20	-	47,47,47,47	0
56	MG	2A	3400	1/1	0.95	0.22	-	34,34,34,34	0
56	MG	1A	3977	1/1	0.96	0.21	-	54,54,54,54	0
56	MG	1A	3326	1/1	0.91	0.09	-	62,62,62,62	0
56	MG	1a	1781	1/1	0.96	0.18	-	48,48,48,48	0
56	MG	2A	3382	1/1	0.97	0.26	-	47,47,47,47	0
56	MG	1A	3899	1/1	0.49	0.12	-	80,80,80,80	0
56	MG	1A	4006	1/1	0.94	0.23	-	51,51,51,51	0
56	MG	1a	1712	1/1	0.99	0.19	-	53,53,53,53	0
56	MG	1a	1737	1/1	0.91	0.07	-	70,70,70,70	0
56	MG	1a	1854	1/1	0.96	0.10	-	41,41,41,41	0
56	MG	1A	3825	1/1	0.98	0.20	-	13,13,13,13	0
56	MG	1A	4000	1/1	0.92	0.26	-	50,50,50,50	0
56	MG	1a	1614	1/1	0.98	0.06	-	74,74,74,74	0
56	MG	1A	3391	1/1	0.88	0.16	-	44,44,44,44	0
56	MG	2a	1728	1/1	0.97	0.10	-	75,75,75,75	0
56	MG	1A	3654	1/1	0.92	0.15	-	20,20,20,20	0
56	MG	2A	3515	1/1	0.93	0.10	-	53,53,53,53	0
56	MG	1A	3507	1/1	0.86	0.24	-	40,40,40,40	0
56	MG	1a	1863	1/1	0.89	0.14	-	64,64,64,64	0
56	MG	2A	3547	1/1	0.88	0.38	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1733	1/1	0.86	0.12	-	67,67,67,67	0
56	MG	2a	1627	1/1	0.86	0.43	-	68,68,68,68	0
56	MG	1A	3030	1/1	0.98	0.08	-	38,38,38,38	0
56	MG	2A	3126	1/1	0.94	0.17	-	44,44,44,44	0
56	MG	1a	1655	1/1	0.98	0.18	-	50,50,50,50	0
56	MG	1A	3505	1/1	0.66	0.28	-	58,58,58,58	0
56	MG	2A	3233	1/1	0.98	0.16	-	58,58,58,58	0
56	MG	1A	3753	1/1	0.93	0.17	-	21,21,21,21	0
56	MG	1a	1643	1/1	0.82	0.18	-	47,47,47,47	0
56	MG	1a	1741	1/1	0.96	0.37	-	58,58,58,58	0
56	MG	2A	3251	1/1	0.97	0.21	-	40,40,40,40	0
56	MG	2a	1632	1/1	0.81	0.17	-	76,76,76,76	0
56	MG	1A	3768	1/1	0.95	0.16	-	39,39,39,39	0
56	MG	1a	1767	1/1	0.94	0.19	-	63,63,63,63	0
56	MG	1A	4066	1/1	0.74	0.23	-	51,51,51,51	0
56	MG	2A	3458	1/1	0.97	0.08	-	64,64,64,64	0
56	MG	2a	1648	1/1	0.91	0.13	-	68,68,68,68	0
56	MG	1A	3791	1/1	0.97	0.18	-	19,19,19,19	0
56	MG	2a	1647	1/1	0.95	0.12	-	64,64,64,64	0
56	MG	1a	1733	1/1	0.97	0.11	-	41,41,41,41	0
56	MG	1R	206	1/1	0.90	0.19	-	37,37,37,37	0
56	MG	2A	3374	1/1	0.99	0.12	-	41,41,41,41	0
56	MG	2A	3550	1/1	0.91	0.14	-	51,51,51,51	0
56	MG	1A	3488	1/1	0.91	0.16	-	43,43,43,43	0
56	MG	2A	3151	1/1	0.91	0.33	-	40,40,40,40	0
56	MG	1x	108	1/1	0.86	0.09	-	59,59,59,59	0
56	MG	1A	3207	1/1	0.95	0.23	-	47,47,47,47	0
56	MG	1A	3042	1/1	0.93	0.25	-	44,44,44,44	0
56	MG	2A	3350	1/1	0.98	0.09	-	55,55,55,55	0
56	MG	1A	3328	1/1	0.83	0.11	-	78,78,78,78	0
56	MG	1A	3002	1/1	0.93	0.11	-	48,48,48,48	0
56	MG	1b	3002	1/1	0.94	0.38	-	82,82,82,82	0
56	MG	1A	4035	1/1	0.97	0.19	-	57,57,57,57	0
56	MG	1A	4031	1/1	0.92	0.66	-	64,64,64,64	0
56	MG	1A	3006	1/1	0.86	0.32	-	48,48,48,48	0
56	MG	1c	3001	1/1	0.88	0.13	-	64,64,64,64	0
56	MG	2A	3406	1/1	0.94	0.09	-	58,58,58,58	0
56	MG	1x	107	1/1	0.96	0.10	-	50,50,50,50	0
56	MG	1a	1891	1/1	0.88	0.15	-	52,52,52,52	0
56	MG	1A	3407	1/1	0.93	0.17	-	67,67,67,67	0
56	MG	2a	1789	1/1	0.97	0.04	-	88,88,88,88	0
56	MG	1H	201	1/1	0.97	0.30	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3937	1/1	0.90	0.15	-	51,51,51,51	0
56	MG	2A	3265	1/1	0.96	0.09	-	49,49,49,49	0
56	MG	1A	3197	1/1	0.93	0.17	-	44,44,44,44	0
56	MG	1A	3273	1/1	0.97	0.10	-	16,16,16,16	0
56	MG	1A	3399	1/1	0.92	0.13	-	39,39,39,39	0
56	MG	1a	1768	1/1	0.98	0.09	-	56,56,56,56	0
56	MG	2A	3499	1/1	0.97	0.16	-	56,56,56,56	0
56	MG	1a	1754	1/1	0.77	0.28	-	60,60,60,60	0
56	MG	2A	3109	1/1	0.86	0.26	-	57,57,57,57	0
56	MG	1a	1809	1/1	0.95	0.15	-	75,75,75,75	0
56	MG	2A	3002	1/1	0.97	0.16	-	47,47,47,47	0
56	MG	2B	3009	1/1	0.94	0.35	-	58,58,58,58	0
56	MG	2A	3426	1/1	0.95	0.09	-	43,43,43,43	0
56	MG	1A	3321	1/1	0.95	0.18	-	28,28,28,28	0
56	MG	2A	3447	1/1	0.89	0.09	-	57,57,57,57	0
56	MG	1a	1719	1/1	0.87	0.14	-	53,53,53,53	0
56	MG	1A	3855	1/1	0.96	0.10	-	51,51,51,51	0
56	MG	2A	3133	1/1	0.97	0.11	-	33,33,33,33	0
56	MG	18	103	1/1	0.93	0.26	-	59,59,59,59	0
56	MG	1a	1654	1/1	0.94	0.14	-	72,72,72,72	0
56	MG	1A	3895	1/1	0.93	0.20	-	57,57,57,57	0
56	MG	2A	3044	1/1	0.98	0.11	-	32,32,32,32	0
56	MG	1A	3862	1/1	0.97	0.07	-	45,45,45,45	0
56	MG	2A	3036	1/1	0.90	0.25	-	61,61,61,61	0
56	MG	2A	3489	1/1	0.93	0.24	-	60,60,60,60	0
56	MG	1A	4071	1/1	0.95	0.11	-	40,40,40,40	0
56	MG	2a	1743	1/1	0.96	0.23	-	35,35,35,35	0
56	MG	1a	1843	1/1	0.29	0.14	-	69,69,69,69	0
56	MG	1a	1872	1/1	0.90	0.07	-	50,50,50,50	0
56	MG	2A	3295	1/1	0.90	0.20	-	32,32,32,32	0
56	MG	1A	3516	1/1	0.97	0.08	-	54,54,54,54	0
56	MG	2a	1641	1/1	0.96	0.12	-	64,64,64,64	0
56	MG	1W	3001	1/1	0.96	0.20	-	43,43,43,43	0
56	MG	1A	3892	1/1	0.97	0.12	-	44,44,44,44	0
56	MG	2a	1659	1/1	0.93	0.26	-	60,60,60,60	0
56	MG	1A	3429	1/1	0.97	0.12	-	45,45,45,45	0
56	MG	1A	3268	1/1	0.97	0.16	-	51,51,51,51	0
56	MG	2A	3012	1/1	0.85	0.18	-	57,57,57,57	0
56	MG	1a	1780	1/1	0.93	0.27	-	62,62,62,62	0
56	MG	2A	3528	1/1	0.72	0.37	-	60,60,60,60	0
56	MG	2Q	3005	1/1	0.94	0.30	-	46,46,46,46	0
56	MG	1a	1893	1/1	0.97	0.36	-	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	1A	3961	1/1	0.95	0.12	-	54,54,54,54	0
56	MG	2A	3472	1/1	0.82	0.22	-	53,53,53,53	0
56	MG	1a	1639	1/1	0.89	0.15	-	76,76,76,76	0
56	MG	2A	3423	1/1	0.91	0.10	-	65,65,65,65	0
56	MG	2A	3095	1/1	0.88	0.23	-	54,54,54,54	0
56	MG	1A	3757	1/1	0.96	0.27	-	33,33,33,33	0
56	MG	1A	3635	1/1	0.95	0.12	-	83,83,83,83	0
56	MG	1a	1874	1/1	0.98	0.15	-	48,48,48,48	0
56	MG	1a	1680	1/1	0.91	0.24	-	45,45,45,45	0
56	MG	1A	3069	1/1	0.68	0.14	-	58,58,58,58	0
56	MG	1A	3077	1/1	0.92	0.17	-	59,59,59,59	0
56	MG	1A	3665	1/1	0.97	0.10	-	40,40,40,40	0
56	MG	2A	3230	1/1	0.97	0.16	-	45,45,45,45	0
56	MG	2A	3466	1/1	0.92	0.13	-	45,45,45,45	0
56	MG	2A	3381	1/1	0.92	0.10	-	52,52,52,52	0
56	MG	2A	3202	1/1	0.95	0.09	-	47,47,47,47	0
56	MG	2a	1727	1/1	0.96	0.14	-	45,45,45,45	0
56	MG	1A	3888	1/1	0.93	0.12	-	87,87,87,87	0
56	MG	1a	1603	1/1	0.97	0.17	-	56,56,56,56	0
56	MG	2A	3245	1/1	0.87	0.23	-	23,23,23,23	0
56	MG	1A	3387	1/1	0.93	0.27	-	33,33,33,33	0
56	MG	1A	4077	1/1	0.88	0.10	-	62,62,62,62	0
56	MG	2a	1642	1/1	0.90	0.46	-	87,87,87,87	0
56	MG	1A	3063	1/1	0.96	0.12	-	41,41,41,41	0
56	MG	1A	3737	1/1	0.95	0.12	-	60,60,60,60	0
56	MG	2a	1753	1/1	0.82	0.10	-	63,63,63,63	0
56	MG	1a	1725	1/1	0.91	0.21	-	59,59,59,59	0
56	MG	2A	3252	1/1	0.86	0.24	-	58,58,58,58	0
56	MG	2A	3284	1/1	0.83	0.12	-	45,45,45,45	0
56	MG	1A	3076	1/1	0.98	0.18	-	40,40,40,40	0
56	MG	1a	1888	1/1	0.92	0.28	-	46,46,46,46	0
56	MG	1a	1727	1/1	0.95	0.25	-	66,66,66,66	0
56	MG	2A	3409	1/1	0.87	0.12	-	68,68,68,68	0
56	MG	1A	3506	1/1	0.84	0.20	-	57,57,57,57	0
56	MG	1A	3576	1/1	0.83	0.13	-	45,45,45,45	0
56	MG	1A	3887	1/1	0.86	0.10	-	44,44,44,44	0
56	MG	1a	1706	1/1	0.99	0.11	-	53,53,53,53	0
56	MG	13	101	1/1	0.95	0.16	-	46,46,46,46	0
56	MG	1A	3217	1/1	0.93	0.14	-	43,43,43,43	0
56	MG	1A	3530	1/1	0.98	0.07	-	41,41,41,41	0
56	MG	2a	1690	1/1	0.97	0.34	-	55,55,55,55	0
56	MG	1A	3452	1/1	0.86	0.23	-	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	1651	1/1	0.93	0.13	-	52,52,52,52	0
56	MG	1A	3287	1/1	0.69	0.36	-	43,43,43,43	0
56	MG	1A	3224	1/1	0.97	0.11	-	37,37,37,37	0
56	MG	1A	3630	1/1	0.97	0.21	-	47,47,47,47	0
56	MG	1A	3010	1/1	0.96	0.20	-	46,46,46,46	0
56	MG	1A	3981	1/1	0.91	0.34	-	43,43,43,43	0
56	MG	1A	3190	1/1	0.97	0.07	-	55,55,55,55	0
56	MG	1A	3346	1/1	0.43	0.18	-	76,76,76,76	0
56	MG	2A	3161	1/1	0.97	0.18	-	37,37,37,37	0
56	MG	2a	1676	1/1	0.94	0.31	-	60,60,60,60	0
56	MG	1A	3043	1/1	0.97	0.10	-	36,36,36,36	0
56	MG	2A	3261	1/1	0.97	0.28	-	66,66,66,66	0
56	MG	1O	201	1/1	0.83	0.33	-	47,47,47,47	0
56	MG	2A	3297	1/1	0.91	0.33	-	49,49,49,49	0
56	MG	2A	3136	1/1	0.95	0.10	-	44,44,44,44	0
56	MG	1A	3916	1/1	0.96	0.23	-	49,49,49,49	0
56	MG	2A	3526	1/1	0.94	0.31	-	46,46,46,46	0
56	MG	1A	3971	1/1	0.82	0.30	-	82,82,82,82	0
56	MG	2A	3267	1/1	0.97	0.29	-	50,50,50,50	0
56	MG	1a	1805	1/1	0.90	0.28	-	77,77,77,77	0
56	MG	1A	3990	1/1	0.94	0.18	-	47,47,47,47	0
56	MG	2e	203	1/1	0.94	0.19	-	78,78,78,78	0
56	MG	1A	3857	1/1	0.91	0.18	-	51,51,51,51	0
56	MG	2A	3310	1/1	0.96	0.13	-	55,55,55,55	0
56	MG	2A	3477	1/1	0.90	0.09	-	52,52,52,52	0
56	MG	2A	3398	1/1	0.91	0.24	-	45,45,45,45	0
56	MG	1A	3743	1/1	0.97	0.19	-	69,69,69,69	0
56	MG	1A	3147	1/1	0.99	0.13	-	33,33,33,33	0
56	MG	1A	3041	1/1	0.93	0.24	-	50,50,50,50	0
56	MG	1A	3119	1/1	0.98	0.12	-	31,31,31,31	0
56	MG	1A	3978	1/1	0.93	0.12	-	67,67,67,67	0
56	MG	1a	1856	1/1	0.92	0.20	-	68,68,68,68	0
56	MG	1A	3192	1/1	0.96	0.29	-	47,47,47,47	0
56	MG	1a	1695	1/1	0.96	0.10	-	40,40,40,40	0
56	MG	1a	1700	1/1	0.84	0.22	-	62,62,62,62	0
56	MG	1a	1683	1/1	0.95	0.50	-	51,51,51,51	0
56	MG	1a	1869	1/1	0.84	0.19	-	66,66,66,66	0
56	MG	1a	1787	1/1	0.93	0.12	-	61,61,61,61	0
56	MG	1A	3623	1/1	0.86	0.08	-	61,61,61,61	0
56	MG	1A	3569	1/1	0.86	0.21	-	36,36,36,36	0
56	MG	1A	3659	1/1	0.89	0.14	-	25,25,25,25	0
56	MG	1A	3158	1/1	0.92	0.21	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1764	1/1	0.92	0.10	-	85,85,85,85	0
56	MG	1A	3232	1/1	0.97	0.68	-	39,39,39,39	0
56	MG	1A	3080	1/1	0.95	0.23	-	38,38,38,38	0
56	MG	1A	3060	1/1	0.90	0.15	-	46,46,46,46	0
56	MG	2A	3194	1/1	0.82	0.30	-	48,48,48,48	0
56	MG	18	104	1/1	0.93	0.27	-	41,41,41,41	0
56	MG	1A	3401	1/1	0.97	0.12	-	46,46,46,46	0
56	MG	2A	3246	1/1	0.97	0.20	-	56,56,56,56	0
56	MG	1a	1800	1/1	0.96	0.32	-	67,67,67,67	0
56	MG	1A	3587	1/1	0.92	0.10	-	38,38,38,38	0
56	MG	1A	4005	1/1	0.97	0.11	-	65,65,65,65	0
56	MG	1A	3987	1/1	0.92	0.15	-	54,54,54,54	0
56	MG	1A	3650	1/1	0.83	0.18	-	30,30,30,30	0
56	MG	1A	3545	1/1	0.63	0.47	-	61,61,61,61	0
56	MG	2A	3345	1/1	0.97	0.24	-	51,51,51,51	0
56	MG	1A	3538	1/1	0.81	0.10	-	67,67,67,67	0
56	MG	2A	3185	1/1	0.91	0.15	-	46,46,46,46	0
56	MG	1H	202	1/1	0.84	0.18	-	53,53,53,53	0
56	MG	2a	1654	1/1	0.98	0.07	-	49,49,49,49	0
56	MG	2A	3055	1/1	0.86	0.15	-	57,57,57,57	0
56	MG	1a	1880	1/1	0.93	0.12	-	68,68,68,68	0
56	MG	2a	1800	1/1	0.98	0.41	-	73,73,73,73	0
56	MG	1A	3885	1/1	0.98	0.09	-	51,51,51,51	0
56	MG	2A	3411	1/1	0.94	0.20	-	65,65,65,65	0
56	MG	2A	3274	1/1	0.88	0.14	-	46,46,46,46	0
56	MG	1A	3797	1/1	0.97	0.17	-	15,15,15,15	0
56	MG	2A	3549	1/1	0.96	0.23	-	49,49,49,49	0
56	MG	2A	3004	1/1	0.82	0.17	-	55,55,55,55	0
56	MG	1A	3133	1/1	0.98	0.14	-	28,28,28,28	0
56	MG	2a	1794	1/1	0.94	0.12	-	68,68,68,68	0
56	MG	1A	3134	1/1	0.94	0.43	-	35,35,35,35	0
56	MG	1A	3440	1/1	0.93	0.06	-	45,45,45,45	0
56	MG	1a	1728	1/1	0.90	0.26	-	49,49,49,49	0
56	MG	1A	3223	1/1	0.98	0.15	-	24,24,24,24	0
56	MG	1a	1882	1/1	0.95	0.12	-	40,40,40,40	0
56	MG	11	104	1/1	0.95	0.19	-	59,59,59,59	0
56	MG	2A	3108	1/1	0.88	0.25	-	59,59,59,59	0
56	MG	2Y	201	1/1	0.95	0.09	-	58,58,58,58	0
56	MG	2a	1711	1/1	0.93	0.15	-	61,61,61,61	0
56	MG	1a	1887	1/1	0.88	0.16	-	64,64,64,64	0
56	MG	1A	3352	1/1	0.97	0.15	-	37,37,37,37	0
56	MG	2l	204	1/1	0.96	0.18	-	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	3647	1/1	0.86	0.16	-	41,41,41,41	0
56	MG	2A	3013	1/1	0.93	0.12	-	52,52,52,52	0
56	MG	1A	3320	1/1	0.91	0.10	-	52,52,52,52	0
56	MG	1a	1826	1/1	0.97	0.24	-	47,47,47,47	0
56	MG	1A	3551	1/1	0.89	0.16	-	85,85,85,85	0
56	MG	1A	3826	1/1	0.94	0.22	-	42,42,42,42	0
56	MG	1Q	3003	1/1	0.96	0.33	-	59,59,59,59	0
56	MG	1A	3834	1/1	0.96	0.14	-	51,51,51,51	0
56	MG	1A	3021	1/1	0.93	0.19	-	43,43,43,43	0
56	MG	1A	3581	1/1	0.95	0.20	-	51,51,51,51	0
56	MG	1A	3928	1/1	0.94	0.10	-	57,57,57,57	0
56	MG	1A	3291	1/1	0.90	0.22	-	33,33,33,33	0
56	MG	1A	3107	1/1	0.87	0.20	-	53,53,53,53	0
56	MG	1a	1745	1/1	0.92	0.21	-	50,50,50,50	0
56	MG	1A	3543	1/1	0.93	0.10	-	41,41,41,41	0
56	MG	2A	3104	1/1	0.85	0.13	-	52,52,52,52	0
56	MG	2A	3117	1/1	0.93	0.14	-	41,41,41,41	0
56	MG	1A	3738	1/1	0.96	0.13	-	46,46,46,46	0
56	MG	2A	3124	1/1	0.93	0.23	-	48,48,48,48	0
56	MG	2a	1798	1/1	0.96	0.14	-	69,69,69,69	0
56	MG	1A	4051	1/1	0.90	0.13	-	45,45,45,45	0
56	MG	2A	3448	1/1	0.94	0.27	-	53,53,53,53	0
56	MG	1T	204	1/1	0.87	0.20	-	68,68,68,68	0
56	MG	1a	1699	1/1	0.90	0.27	-	68,68,68,68	0
56	MG	1A	3715	1/1	0.89	0.25	-	57,57,57,57	0
56	MG	2A	3367	1/1	0.84	0.24	-	41,41,41,41	0
56	MG	1A	3720	1/1	0.95	0.22	-	67,67,67,67	0
56	MG	1A	3643	1/1	0.91	0.23	-	34,34,34,34	0
56	MG	1A	3962	1/1	0.96	0.09	-	42,42,42,42	0
56	MG	1A	3680	1/1	0.92	0.09	-	45,45,45,45	0
56	MG	2A	3454	1/1	0.96	0.08	-	61,61,61,61	0
56	MG	2A	3234	1/1	0.97	0.27	-	55,55,55,55	0
56	MG	1A	3975	1/1	0.92	0.20	-	50,50,50,50	0
56	MG	10	104	1/1	0.97	0.06	-	46,46,46,46	0
56	MG	2a	1815	1/1	0.92	0.13	-	56,56,56,56	0
56	MG	1A	3679	1/1	0.93	0.15	-	41,41,41,41	0
56	MG	1A	4072	1/1	0.94	0.15	-	70,70,70,70	0
56	MG	2A	3035	1/1	0.95	0.11	-	57,57,57,57	0
56	MG	1A	3699	1/1	0.90	0.18	-	49,49,49,49	0
56	MG	2a	1810	1/1	0.88	0.20	-	84,84,84,84	0
56	MG	1A	3298	1/1	0.94	0.11	-	46,46,46,46	0
56	MG	2A	3023	1/1	0.93	0.18	-	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	1634	1/1	0.85	0.21	-	41,41,41,41	0
56	MG	1A	3049	1/1	0.86	0.14	-	60,60,60,60	0
56	MG	2A	3086	1/1	0.94	0.12	-	36,36,36,36	0
56	MG	1A	3537	1/1	0.96	0.07	-	43,43,43,43	0
56	MG	1A	3673	1/1	0.97	0.26	-	32,32,32,32	0
56	MG	2A	3435	1/1	0.95	0.25	-	59,59,59,59	0
56	MG	1A	3717	1/1	0.96	0.04	-	48,48,48,48	0
56	MG	1A	3264	1/1	0.94	0.12	-	51,51,51,51	0
56	MG	2a	1751	1/1	0.95	0.36	-	55,55,55,55	0
56	MG	2A	3444	1/1	0.91	0.07	-	58,58,58,58	0
56	MG	2a	1666	1/1	0.67	0.21	-	65,65,65,65	0
56	MG	2A	3024	1/1	0.94	0.16	-	46,46,46,46	0
56	MG	2A	3193	1/1	0.90	0.20	-	50,50,50,50	0
56	MG	1A	3164	1/1	0.97	0.40	-	20,20,20,20	0
56	MG	1A	3330	1/1	0.94	0.07	-	56,56,56,56	0
56	MG	1A	3381	1/1	0.89	0.25	-	38,38,38,38	0
56	MG	1A	3366	1/1	0.88	0.12	-	48,48,48,48	0
56	MG	1A	3608	1/1	0.94	0.18	-	32,32,32,32	0
56	MG	2A	3321	1/1	0.93	0.15	-	32,32,32,32	0
56	MG	1A	3907	1/1	0.95	0.23	-	15,15,15,15	0
56	MG	2A	3514	1/1	0.92	0.20	-	53,53,53,53	0
56	MG	1A	3388	1/1	0.96	0.20	-	60,60,60,60	0
56	MG	2A	3534	1/1	0.95	0.31	-	45,45,45,45	0
56	MG	1a	1629	1/1	0.98	0.14	-	33,33,33,33	0
56	MG	1A	3420	1/1	0.86	0.14	-	72,72,72,72	0
56	MG	1A	3463	1/1	0.89	0.22	-	54,54,54,54	0
56	MG	1A	3518	1/1	0.94	0.12	-	57,57,57,57	0
56	MG	1k	201	1/1	0.93	0.11	-	68,68,68,68	0
56	MG	2A	3495	1/1	0.85	0.13	-	44,44,44,44	0
56	MG	2a	1782	1/1	0.99	0.27	-	46,46,46,46	0
56	MG	2x	3002	1/1	0.93	0.06	-	57,57,57,57	0
56	MG	2a	1630	1/1	0.78	0.12	-	60,60,60,60	0
56	MG	1A	3005	1/1	0.93	0.19	-	57,57,57,57	0
56	MG	2A	3191	1/1	0.87	0.30	-	51,51,51,51	0
56	MG	2A	3075	1/1	0.95	0.20	-	26,26,26,26	0
56	MG	1A	4004	1/1	0.94	0.16	-	53,53,53,53	0
56	MG	1a	1776	1/1	0.92	0.08	-	54,54,54,54	0
56	MG	1Q	3001	1/1	0.97	0.25	-	31,31,31,31	0
56	MG	1A	3614	1/1	0.82	0.12	-	58,58,58,58	0
56	MG	1A	3410	1/1	0.95	0.22	-	47,47,47,47	0
56	MG	1B	214	1/1	0.82	0.18	-	69,69,69,69	0
56	MG	2a	1716	1/1	0.92	0.14	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3102	1/1	0.87	0.21	-	51,51,51,51	0
56	MG	2A	3484	1/1	0.93	0.14	-	53,53,53,53	0
56	MG	1A	3523	1/1	0.90	0.54	-	77,77,77,77	0
56	MG	1A	3104	1/1	0.85	0.15	-	52,52,52,52	0
56	MG	1A	3547	1/1	0.91	0.11	-	56,56,56,56	0
56	MG	1a	1698	1/1	0.54	0.30	-	64,64,64,64	0
56	MG	2A	3508	1/1	0.94	0.07	-	45,45,45,45	0
56	MG	1A	3467	1/1	0.98	0.11	-	50,50,50,50	0
56	MG	2A	3482	1/1	0.93	0.37	-	59,59,59,59	0
56	MG	2A	3175	1/1	0.93	0.35	-	30,30,30,30	0
56	MG	1A	3681	1/1	0.89	0.15	-	43,43,43,43	0
56	MG	1A	3247	1/1	0.93	0.17	-	62,62,62,62	0
56	MG	1A	3499	1/1	0.94	0.12	-	42,42,42,42	0
56	MG	1A	3384	1/1	0.88	0.55	-	48,48,48,48	0
56	MG	1a	1892	1/1	0.95	0.16	-	49,49,49,49	0
56	MG	1A	3354	1/1	0.98	0.06	-	56,56,56,56	0
56	MG	2A	3031	1/1	0.93	0.21	-	49,49,49,49	0
56	MG	2A	3128	1/1	0.97	0.12	-	46,46,46,46	0
56	MG	2A	3219	1/1	0.81	0.13	-	61,61,61,61	0
56	MG	2A	3370	1/1	0.88	0.10	-	49,49,49,49	0
56	MG	1A	3552	1/1	0.96	0.13	-	53,53,53,53	0
56	MG	2A	3490	1/1	0.90	0.15	-	48,48,48,48	0
56	MG	2A	3275	1/1	0.95	0.20	-	45,45,45,45	0
56	MG	1A	3889	1/1	0.97	0.14	-	46,46,46,46	0
56	MG	1A	3761	1/1	0.97	0.12	-	47,47,47,47	0
56	MG	1a	1749	1/1	0.81	0.23	-	72,72,72,72	0
56	MG	1A	3441	1/1	0.90	0.24	-	59,59,59,59	0
56	MG	1A	3871	1/1	0.76	0.27	-	45,45,45,45	0
56	MG	2A	3089	1/1	0.87	0.10	-	47,47,47,47	0
56	MG	1a	1724	1/1	0.94	0.09	-	47,47,47,47	0
56	MG	1A	3749	1/1	0.96	0.05	-	48,48,48,48	0
56	MG	2A	3201	1/1	0.94	0.09	-	62,62,62,62	0
56	MG	1a	1707	1/1	0.86	0.15	-	65,65,65,65	0
56	MG	2A	3135	1/1	0.92	0.15	-	46,46,46,46	0
56	MG	2a	1636	1/1	0.96	0.08	-	92,92,92,92	0
56	MG	1A	3348	1/1	0.98	0.21	-	20,20,20,20	0
56	MG	1A	3422	1/1	0.86	0.20	-	63,63,63,63	0
56	MG	1A	3045	1/1	0.98	0.33	-	42,42,42,42	0
56	MG	1A	3394	1/1	0.97	0.06	-	60,60,60,60	0
56	MG	2A	3469	1/1	0.89	0.20	-	60,60,60,60	0
56	MG	1a	1841	1/1	0.96	0.10	-	37,37,37,37	0
56	MG	1A	3865	1/1	0.88	0.24	-	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	1A	4069	1/1	0.97	0.15	-	38,38,38,38	0
56	MG	2A	3339	1/1	0.83	0.09	-	78,78,78,78	0
56	MG	1A	3795	1/1	0.94	0.12	-	37,37,37,37	0
56	MG	2A	3116	1/1	0.94	0.16	-	33,33,33,33	0
56	MG	1a	1750	1/1	0.79	0.34	-	73,73,73,73	0
56	MG	2A	3192	1/1	0.86	0.11	-	49,49,49,49	0
56	MG	2A	3351	1/1	0.96	0.11	-	52,52,52,52	0
56	MG	1A	3062	1/1	0.82	0.25	-	50,50,50,50	0
56	MG	1A	3533	1/1	0.93	0.16	-	57,57,57,57	0
56	MG	1A	3135	1/1	0.96	0.30	-	36,36,36,36	0
56	MG	1A	3936	1/1	0.97	0.10	-	37,37,37,37	0
56	MG	2a	1651	1/1	0.88	0.60	-	56,56,56,56	0
56	MG	1R	203	1/1	0.97	0.19	-	24,24,24,24	0
56	MG	2A	3316	1/1	0.97	0.20	-	33,33,33,33	0
56	MG	1a	1804	1/1	0.92	0.15	-	66,66,66,66	0
56	MG	1A	3332	1/1	0.92	0.12	-	54,54,54,54	0
56	MG	1a	1771	1/1	0.96	0.21	-	52,52,52,52	0
56	MG	13	102	1/1	0.77	0.25	-	72,72,72,72	0
56	MG	2a	1706	1/1	0.96	0.36	-	58,58,58,58	0
56	MG	1A	3457	1/1	0.92	0.16	-	52,52,52,52	0
56	MG	2E	303	1/1	0.94	0.40	-	42,42,42,42	0
56	MG	1A	3471	1/1	0.86	0.28	-	58,58,58,58	0
56	MG	1A	3756	1/1	0.73	0.18	-	43,43,43,43	0
56	MG	2A	3183	1/1	0.92	0.19	-	44,44,44,44	0
56	MG	1E	307	1/1	0.93	0.14	-	64,64,64,64	0
56	MG	1a	1811	1/1	0.88	0.15	-	90,90,90,90	0
56	MG	1A	3492	1/1	0.88	0.23	-	59,59,59,59	0
56	MG	1A	3810	1/1	0.96	0.06	-	43,43,43,43	0
56	MG	2A	3293	1/1	0.99	0.17	-	36,36,36,36	0
56	MG	1A	3500	1/1	0.91	0.23	-	60,60,60,60	0
56	MG	1A	3554	1/1	0.95	0.15	-	61,61,61,61	0
56	MG	1a	1661	1/1	0.91	0.28	-	58,58,58,58	0
56	MG	1A	3754	1/1	0.84	0.08	-	61,61,61,61	0
56	MG	1A	3864	1/1	0.96	0.11	-	53,53,53,53	0
56	MG	1A	3898	1/1	0.95	0.06	-	50,50,50,50	0
56	MG	2A	3223	1/1	0.84	0.11	-	82,82,82,82	0
56	MG	2a	1775	1/1	0.97	0.33	-	42,42,42,42	0
56	MG	1a	1876	1/1	0.91	0.18	-	47,47,47,47	0
56	MG	2A	3081	1/1	0.81	0.31	-	60,60,60,60	0
56	MG	1A	3748	1/1	0.94	0.12	-	64,64,64,64	0
56	MG	2A	3340	1/1	0.89	0.05	-	58,58,58,58	0
56	MG	1A	3417	1/1	0.92	0.30	-	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	1627	1/1	0.97	0.07	-	36,36,36,36	0
56	MG	2A	3018	1/1	0.78	0.15	-	50,50,50,50	0
56	MG	1A	3168	1/1	0.95	0.29	-	38,38,38,38	0
56	MG	1a	1862	1/1	0.95	0.15	-	58,58,58,58	0
56	MG	2A	3480	1/1	0.95	0.13	-	74,74,74,74	0
56	MG	2A	3137	1/1	0.96	0.25	-	63,63,63,63	0
56	MG	1A	3341	1/1	0.90	0.13	-	49,49,49,49	0
56	MG	2n	502	1/1	0.92	0.47	-	56,56,56,56	0
56	MG	2a	1656	1/1	0.92	0.20	-	50,50,50,50	0
56	MG	2A	3401	1/1	0.92	0.25	-	60,60,60,60	0
56	MG	2A	3129	1/1	0.96	0.11	-	43,43,43,43	0
56	MG	1a	1842	1/1	0.97	0.29	-	39,39,39,39	0
56	MG	1A	3277	1/1	0.96	0.11	-	33,33,33,33	0
56	MG	2A	3241	1/1	0.88	0.20	-	35,35,35,35	0
56	MG	2A	3162	1/1	0.94	0.31	-	42,42,42,42	0
56	MG	1A	3157	1/1	0.95	0.13	-	40,40,40,40	0
56	MG	1A	4014	1/1	0.85	0.31	-	47,47,47,47	0
56	MG	1A	3308	1/1	0.95	0.14	-	40,40,40,40	0
56	MG	2a	1677	1/1	0.98	0.09	-	55,55,55,55	0
56	MG	1A	3879	1/1	0.89	0.13	-	48,48,48,48	0
56	MG	2a	1780	1/1	0.86	0.15	-	64,64,64,64	0
56	MG	2Y	203	1/1	0.97	0.10	-	41,41,41,41	0
56	MG	1A	3982	1/1	0.92	0.19	-	40,40,40,40	0
56	MG	1A	3260	1/1	0.96	0.17	-	50,50,50,50	0
56	MG	1A	3086	1/1	0.96	0.23	-	39,39,39,39	0
56	MG	1a	1759	1/1	0.89	0.15	-	58,58,58,58	0
56	MG	2a	1698	1/1	0.94	0.29	-	57,57,57,57	0
56	MG	2a	1617	1/1	0.86	0.17	-	67,67,67,67	0
56	MG	1A	3866	1/1	0.96	0.16	-	53,53,53,53	0
56	MG	1a	1783	1/1	0.58	0.15	-	78,78,78,78	0
56	MG	1A	3601	1/1	0.92	0.14	-	24,24,24,24	0
56	MG	1B	215	1/1	0.97	0.09	-	36,36,36,36	0
56	MG	1A	3477	1/1	0.83	0.12	-	56,56,56,56	0
56	MG	1A	3386	1/1	0.97	0.11	-	34,34,34,34	0
56	MG	1A	3641	1/1	0.97	0.10	-	36,36,36,36	0
56	MG	2A	3106	1/1	0.84	0.14	-	58,58,58,58	0
56	MG	1A	3606	1/1	0.96	0.10	-	58,58,58,58	0
56	MG	1a	1769	1/1	0.95	0.21	-	58,58,58,58	0
56	MG	2a	1657	1/1	0.97	0.17	-	61,61,61,61	0
56	MG	1A	3103	1/1	0.89	0.10	-	53,53,53,53	0
56	MG	2A	3524	1/1	0.94	0.16	-	46,46,46,46	0
56	MG	1A	3860	1/1	0.97	0.15	-	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	3380	1/1	0.85	0.28	-	49,49,49,49	0
56	MG	1A	3188	1/1	0.95	0.21	-	50,50,50,50	0
56	MG	2A	3481	1/1	0.86	0.07	-	83,83,83,83	0
56	MG	2O	3002	1/1	0.96	0.09	-	36,36,36,36	0
56	MG	2A	3227	1/1	0.86	0.17	-	59,59,59,59	0
56	MG	1a	1610	1/1	0.97	0.04	-	48,48,48,48	0
56	MG	1A	3884	1/1	0.91	0.14	-	47,47,47,47	0
56	MG	1A	3739	1/1	0.98	0.16	-	16,16,16,16	0
56	MG	1a	1726	1/1	0.97	0.16	-	53,53,53,53	0
56	MG	1O	202	1/1	0.98	0.10	-	52,52,52,52	0
56	MG	1A	3524	1/1	0.94	0.60	-	63,63,63,63	0
56	MG	1A	3379	1/1	0.95	0.19	-	41,41,41,41	0
56	MG	2A	3443	1/1	0.94	0.09	-	53,53,53,53	0
56	MG	1a	1795	1/1	0.91	0.21	-	56,56,56,56	0
56	MG	19	103	1/1	0.94	0.11	-	40,40,40,40	0
56	MG	1A	3364	1/1	0.96	0.21	-	41,41,41,41	0
56	MG	1A	3886	1/1	0.91	0.27	-	65,65,65,65	0
56	MG	1A	4017	1/1	0.96	0.11	-	42,42,42,42	0
56	MG	1T	201	1/1	0.82	0.23	-	57,57,57,57	0
56	MG	1A	3165	1/1	0.93	0.12	-	35,35,35,35	0
56	MG	1A	3639	1/1	0.95	0.15	-	57,57,57,57	0
56	MG	1A	3957	1/1	0.95	0.13	-	20,20,20,20	0
56	MG	1a	1807	1/1	0.81	0.28	-	74,74,74,74	0
56	MG	2A	3074	1/1	0.90	0.16	-	50,50,50,50	0
56	MG	1A	3427	1/1	0.95	0.12	-	44,44,44,44	0
56	MG	2a	1649	1/1	0.86	0.24	-	51,51,51,51	0
56	MG	2A	3430	1/1	0.95	0.15	-	59,59,59,59	0
56	MG	1A	3527	1/1	0.97	0.18	-	68,68,68,68	0
56	MG	1A	3764	1/1	0.96	0.08	-	41,41,41,41	0
56	MG	1A	3459	1/1	0.92	0.12	-	44,44,44,44	0
56	MG	1A	3773	1/1	0.98	0.06	-	49,49,49,49	0
56	MG	1A	3931	1/1	0.94	0.10	-	42,42,42,42	0
56	MG	1A	4024	1/1	0.96	0.25	-	61,61,61,61	0
56	MG	1a	1730	1/1	0.94	0.18	-	49,49,49,49	0
56	MG	1E	302	1/1	0.98	0.18	-	55,55,55,55	0
56	MG	1A	3988	1/1	0.97	0.39	-	37,37,37,37	0
56	MG	1m	201	1/1	0.93	0.25	-	73,73,73,73	0
56	MG	2a	1612	1/1	0.80	0.20	-	67,67,67,67	0
56	MG	1A	3589	1/1	0.99	0.14	-	31,31,31,31	0
56	MG	1A	3612	1/1	0.99	0.15	-	37,37,37,37	0
56	MG	1a	1716	1/1	0.92	0.16	-	77,77,77,77	0
56	MG	2A	3471	1/1	0.96	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	3083	1/1	0.95	0.12	-	51,51,51,51	0
56	MG	1a	1675	1/1	0.86	0.25	-	59,59,59,59	0
56	MG	1A	3755	1/1	0.95	0.05	-	51,51,51,51	0
56	MG	1A	3502	1/1	0.96	0.34	-	61,61,61,61	0
56	MG	1A	3393	1/1	0.92	0.08	-	54,54,54,54	0
56	MG	2a	1736	1/1	0.95	0.08	-	74,74,74,74	0
56	MG	2A	3504	1/1	0.84	0.15	-	56,56,56,56	0
56	MG	2A	3429	1/1	0.96	0.10	-	58,58,58,58	0
56	MG	2A	3118	1/1	0.94	0.11	-	37,37,37,37	0
56	MG	1a	1796	1/1	0.94	0.14	-	54,54,54,54	0
56	MG	2a	1809	1/1	0.94	0.19	-	64,64,64,64	0
56	MG	1A	3807	1/1	0.99	0.15	-	47,47,47,47	0
56	MG	2A	3159	1/1	0.92	0.23	-	71,71,71,71	0
56	MG	1A	3911	1/1	0.96	0.11	-	46,46,46,46	0
56	MG	2A	3164	1/1	0.97	0.14	-	37,37,37,37	0
56	MG	2A	3301	1/1	0.91	0.12	-	43,43,43,43	0
56	MG	1a	1860	1/1	0.93	0.08	-	49,49,49,49	0
56	MG	2a	1763	1/1	0.85	0.13	-	57,57,57,57	0
56	MG	1Z	302	1/1	0.95	0.11	-	56,56,56,56	0
56	MG	1A	3451	1/1	0.86	0.07	-	52,52,52,52	0
56	MG	1A	3698	1/1	0.91	0.14	-	26,26,26,26	0
56	MG	1A	3266	1/1	0.78	0.19	-	57,57,57,57	0
56	MG	1A	3622	1/1	0.97	0.08	-	61,61,61,61	0
56	MG	1a	1620	1/1	0.96	0.12	-	72,72,72,72	0
56	MG	2A	3149	1/1	0.94	0.14	-	39,39,39,39	0
56	MG	1A	3159	1/1	0.93	0.15	-	69,69,69,69	0
56	MG	2A	3121	1/1	0.91	0.20	-	35,35,35,35	0
56	MG	1a	1792	1/1	0.89	0.27	-	63,63,63,63	0
56	MG	2p	101	1/1	0.96	0.26	-	62,62,62,62	0
56	MG	1a	1852	1/1	0.91	0.12	-	51,51,51,51	0
56	MG	1A	3902	1/1	0.93	0.16	-	70,70,70,70	0
56	MG	2a	1665	1/1	0.97	0.27	-	41,41,41,41	0
56	MG	1A	4023	1/1	0.95	0.14	-	39,39,39,39	0
56	MG	1A	3034	1/1	0.94	0.17	-	57,57,57,57	0
56	MG	1B	226	1/1	0.96	0.12	-	47,47,47,47	0
56	MG	2a	1739	1/1	0.82	0.25	-	73,73,73,73	0
56	MG	2a	1741	1/1	0.50	0.24	-	89,89,89,89	0
56	MG	1A	3521	1/1	0.80	0.31	-	51,51,51,51	0
56	MG	1A	3600	1/1	0.96	0.12	-	50,50,50,50	0
56	MG	1A	3419	1/1	0.94	0.13	-	47,47,47,47	0
56	MG	1A	3531	1/1	0.93	0.06	-	68,68,68,68	0
56	MG	1A	3943	1/1	0.93	0.12	-	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	2a	1747	1/1	0.78	0.14	-	45,45,45,45	0
56	MG	1A	3350	1/1	0.93	0.27	-	67,67,67,67	0
56	MG	2a	1708	1/1	0.94	0.15	-	59,59,59,59	0
56	MG	1A	3496	1/1	0.72	0.15	-	57,57,57,57	0
56	MG	1A	3281	1/1	0.93	0.16	-	53,53,53,53	0
56	MG	1A	3279	1/1	0.92	0.40	-	53,53,53,53	0
56	MG	1A	3101	1/1	0.96	0.19	-	46,46,46,46	0
56	MG	2A	3449	1/1	0.95	0.12	-	52,52,52,52	0
56	MG	2A	3437	1/1	0.77	0.19	-	56,56,56,56	0
56	MG	2A	3455	1/1	0.97	0.09	-	45,45,45,45	0
56	MG	2A	3111	1/1	0.93	0.13	-	36,36,36,36	0
56	MG	1A	3486	1/1	0.81	0.34	-	70,70,70,70	0
56	MG	1A	3856	1/1	0.83	0.12	-	48,48,48,48	0
56	MG	1A	3849	1/1	0.92	0.08	-	55,55,55,55	0
56	MG	2A	3364	1/1	0.92	0.18	-	42,42,42,42	0
56	MG	1A	3306	1/1	0.88	0.19	-	47,47,47,47	0
56	MG	2A	3300	1/1	0.98	0.15	-	50,50,50,50	0
56	MG	2a	1607	1/1	0.88	0.22	-	54,54,54,54	0
56	MG	2l	203	1/1	0.82	0.09	-	55,55,55,55	0
56	MG	2a	1807	1/1	0.96	0.18	-	46,46,46,46	0
56	MG	1A	3450	1/1	0.95	0.16	-	54,54,54,54	0
56	MG	1F	306	1/1	0.91	0.26	-	49,49,49,49	0
56	MG	2A	3276	1/1	0.82	0.09	-	58,58,58,58	0
56	MG	10	105	1/1	0.77	0.15	-	61,61,61,61	0
56	MG	2A	3131	1/1	0.97	0.10	-	46,46,46,46	0
56	MG	2a	1695	1/1	0.80	0.16	-	58,58,58,58	0
56	MG	2A	3236	1/1	0.98	0.14	-	55,55,55,55	0
56	MG	1A	3213	1/1	0.92	0.09	-	63,63,63,63	0
56	MG	1A	3295	1/1	0.97	0.28	-	50,50,50,50	0
56	MG	1a	1684	1/1	0.96	0.08	-	52,52,52,52	0
56	MG	1a	1751	1/1	0.90	0.22	-	60,60,60,60	0
56	MG	1A	3986	1/1	0.90	0.18	-	38,38,38,38	0
56	MG	1A	3258	1/1	0.93	0.22	-	43,43,43,43	0
56	MG	1N	204	1/1	0.97	0.19	-	36,36,36,36	0
56	MG	1a	1885	1/1	0.97	0.21	-	49,49,49,49	0
56	MG	1A	3829	1/1	0.91	0.19	-	49,49,49,49	0
56	MG	1A	3508	1/1	0.90	0.23	-	52,52,52,52	0
56	MG	1A	4011	1/1	0.94	0.12	-	48,48,48,48	0
56	MG	1A	3416	1/1	0.86	0.22	-	56,56,56,56	0
56	MG	1A	3478	1/1	0.95	0.32	-	50,50,50,50	0
56	MG	1A	3087	1/1	0.94	0.29	-	52,52,52,52	0
56	MG	1x	102	1/1	0.98	0.14	-	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	2a	1787	1/1	0.96	0.20	-	67,67,67,67	0
56	MG	2a	1757	1/1	0.94	0.17	-	60,60,60,60	0
56	MG	1A	3573	1/1	0.97	0.11	-	38,38,38,38	0
56	MG	1a	1815	1/1	0.96	0.12	-	72,72,72,72	0
56	MG	1a	1686	1/1	0.91	0.15	-	48,48,48,48	0
56	MG	2A	3467	1/1	0.97	0.18	-	39,39,39,39	0
56	MG	1Q	3007	1/1	0.84	0.22	-	60,60,60,60	0
56	MG	1A	3336	1/1	0.53	0.25	-	62,62,62,62	0
56	MG	2A	3026	1/1	0.94	0.44	-	54,54,54,54	0
56	MG	1W	3004	1/1	0.96	0.23	-	34,34,34,34	0
56	MG	1A	3356	1/1	0.87	0.35	-	56,56,56,56	0
56	MG	1a	1615	1/1	0.91	0.13	-	66,66,66,66	0
56	MG	2A	3022	1/1	0.93	0.12	-	42,42,42,42	0
56	MG	1a	1784	1/1	0.70	0.23	-	95,95,95,95	0
56	MG	1A	3880	1/1	0.95	0.08	-	76,76,76,76	0
56	MG	1a	1623	1/1	0.89	0.29	-	71,71,71,71	0
56	MG	1A	3822	1/1	0.92	0.07	-	48,48,48,48	0
56	MG	1A	3123	1/1	0.88	0.20	-	43,43,43,43	0
56	MG	2A	3238	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	2A	3269	1/1	0.88	0.21	-	52,52,52,52	0
56	MG	1x	105	1/1	0.77	0.15	-	65,65,65,65	0
56	MG	1A	4076	1/1	0.97	0.16	-	36,36,36,36	0
56	MG	1A	3310	1/1	0.96	0.16	-	51,51,51,51	0
56	MG	1A	3683	1/1	0.98	0.21	-	48,48,48,48	0
56	MG	1B	209	1/1	0.89	0.19	-	66,66,66,66	0
56	MG	2A	3040	1/1	0.89	0.18	-	60,60,60,60	0
56	MG	2a	1616	1/1	0.86	0.17	-	61,61,61,61	0
56	MG	1a	1788	1/1	0.97	0.12	-	71,71,71,71	0
56	MG	1A	3727	1/1	0.96	0.20	-	43,43,43,43	0
56	MG	1A	3657	1/1	0.94	0.17	-	48,48,48,48	0
56	MG	1A	3973	1/1	0.94	0.14	-	29,29,29,29	0
56	MG	1E	303	1/1	0.98	0.20	-	14,14,14,14	0
56	MG	2A	3242	1/1	0.91	0.27	-	53,53,53,53	0
56	MG	1A	3345	1/1	0.90	0.13	-	51,51,51,51	0
56	MG	1A	3750	1/1	0.90	0.26	-	41,41,41,41	0
56	MG	17	105	1/1	0.87	0.20	-	44,44,44,44	0
56	MG	1A	3560	1/1	0.96	0.18	-	37,37,37,37	0
56	MG	2a	1703	1/1	0.87	0.17	-	57,57,57,57	0
56	MG	2a	1797	1/1	0.97	0.14	-	57,57,57,57	0
56	MG	1A	3712	1/1	0.95	0.24	-	29,29,29,29	0
56	MG	1A	3596	1/1	0.89	0.18	-	45,45,45,45	0
56	MG	1P	203	1/1	0.96	0.28	-	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	1786	1/1	0.78	0.16	-	71,71,71,71	0
56	MG	1A	3920	1/1	0.93	0.32	-	87,87,87,87	0
56	MG	1A	3772	1/1	0.95	0.24	-	51,51,51,51	0
56	MG	2A	3079	1/1	0.86	0.08	-	45,45,45,45	0
56	MG	2A	3039	1/1	0.93	0.43	-	45,45,45,45	0
56	MG	1A	3402	1/1	0.93	0.20	-	51,51,51,51	0
56	MG	1A	3955	1/1	0.92	0.17	-	46,46,46,46	0
56	MG	2A	3214	1/1	0.94	0.11	-	42,42,42,42	0
56	MG	1A	3057	1/1	0.94	0.20	-	49,49,49,49	0
56	MG	2A	3225	1/1	0.85	0.23	-	50,50,50,50	0
56	MG	1A	4087	1/1	0.96	0.10	-	37,37,37,37	0
56	MG	2k	3001	1/1	0.97	0.07	-	60,60,60,60	0
56	MG	1A	3031	1/1	0.91	0.14	-	60,60,60,60	0
56	MG	1A	3979	1/1	0.98	0.22	-	32,32,32,32	0
56	MG	1A	3965	1/1	0.88	0.14	-	39,39,39,39	0
56	MG	1A	4059	1/1	0.78	0.24	-	52,52,52,52	0
56	MG	1A	3349	1/1	0.86	0.13	-	46,46,46,46	0
56	MG	2A	3492	1/1	0.71	0.18	-	43,43,43,43	0
56	MG	2A	3521	1/1	0.96	0.20	-	38,38,38,38	0
56	MG	1A	3747	1/1	0.95	0.14	-	64,64,64,64	0
56	MG	25	502	1/1	0.96	0.52	-	52,52,52,52	0
56	MG	1A	3912	1/1	0.79	0.17	-	55,55,55,55	0
56	MG	1A	3702	1/1	0.93	0.22	-	48,48,48,48	0
56	MG	1A	3272	1/1	0.94	0.16	-	60,60,60,60	0
56	MG	1A	4064	1/1	0.81	0.21	-	69,69,69,69	0
56	MG	2A	3072	1/1	0.97	0.35	-	40,40,40,40	0
56	MG	1A	3447	1/1	0.90	0.23	-	47,47,47,47	0
56	MG	1A	3809	1/1	0.92	0.12	-	43,43,43,43	0
56	MG	1a	1689	1/1	0.97	0.05	-	61,61,61,61	0
56	MG	1a	1775	1/1	0.98	0.16	-	55,55,55,55	0
56	MG	1A	3301	1/1	0.83	0.17	-	85,85,85,85	0
56	MG	2A	3226	1/1	0.89	0.15	-	72,72,72,72	0
56	MG	1A	3376	1/1	0.67	0.31	-	55,55,55,55	0
56	MG	1A	3733	1/1	0.94	0.14	-	44,44,44,44	0
56	MG	1A	3304	1/1	0.89	0.20	-	72,72,72,72	0
56	MG	1F	307	1/1	0.97	0.18	-	41,41,41,41	0
56	MG	2A	3498	1/1	0.93	0.12	-	63,63,63,63	0
56	MG	1A	3403	1/1	0.96	0.07	-	38,38,38,38	0
56	MG	1A	3368	1/1	0.93	0.12	-	53,53,53,53	0
56	MG	2a	1628	1/1	0.92	0.54	-	66,66,66,66	0
56	MG	2a	1644	1/1	0.93	0.12	-	47,47,47,47	0
56	MG	2B	3002	1/1	0.91	0.09	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3351	1/1	0.93	0.29	-	47,47,47,47	0
56	MG	2A	3007	1/1	0.93	0.26	-	57,57,57,57	0
56	MG	2A	3132	1/1	0.90	0.09	-	52,52,52,52	0
56	MG	2A	3127	1/1	0.96	0.57	-	45,45,45,45	0
56	MG	2A	3530	1/1	0.96	0.14	-	46,46,46,46	0
56	MG	1A	3925	1/1	0.97	0.15	-	50,50,50,50	0
56	MG	1A	3476	1/1	0.88	0.14	-	61,61,61,61	0
56	MG	1a	1810	1/1	0.87	0.11	-	69,69,69,69	0
56	MG	1A	3313	1/1	0.96	0.08	-	50,50,50,50	0
56	MG	2A	3005	1/1	0.92	0.18	-	59,59,59,59	0
56	MG	1a	1894	1/1	0.81	0.39	-	72,72,72,72	0
56	MG	1A	3835	1/1	0.91	0.13	-	57,57,57,57	0
56	MG	1B	213	1/1	0.73	0.10	-	68,68,68,68	0
56	MG	1a	1608	1/1	0.97	0.12	-	73,73,73,73	0
56	MG	1A	3198	1/1	0.98	0.12	-	46,46,46,46	0
56	MG	1T	203	1/1	0.87	0.30	-	50,50,50,50	0
56	MG	16	104	1/1	0.95	0.28	-	43,43,43,43	0
56	MG	2a	1792	1/1	0.91	0.16	-	44,44,44,44	0
56	MG	1A	3389	1/1	0.77	0.34	-	50,50,50,50	0
56	MG	1A	3108	1/1	0.86	0.20	-	51,51,51,51	0
56	MG	1A	3815	1/1	0.92	0.10	-	52,52,52,52	0
56	MG	2A	3096	1/1	0.94	0.14	-	43,43,43,43	0
56	MG	2a	1697	1/1	0.89	0.09	-	60,60,60,60	0
56	MG	1A	3766	1/1	0.94	0.13	-	43,43,43,43	0
56	MG	1A	3462	1/1	0.92	0.15	-	62,62,62,62	0
56	MG	1A	3793	1/1	0.96	0.22	-	50,50,50,50	0
56	MG	2A	3188	1/1	0.89	0.14	-	54,54,54,54	0
56	MG	2A	3010	1/1	0.90	0.12	-	46,46,46,46	0
56	MG	1A	3672	1/1	0.98	0.11	-	17,17,17,17	0
56	MG	1A	3073	1/1	0.89	0.27	-	49,49,49,49	0
56	MG	2I	201	1/1	0.96	0.10	-	66,66,66,66	0
56	MG	1A	3722	1/1	0.84	0.14	-	62,62,62,62	0
56	MG	1A	3236	1/1	0.96	0.06	-	50,50,50,50	0
56	MG	2Q	3004	1/1	0.92	0.22	-	38,38,38,38	0
56	MG	1a	1747	1/1	0.97	0.13	-	43,43,43,43	0
56	MG	1A	3131	1/1	0.98	0.27	-	50,50,50,50	0
56	MG	2A	3502	1/1	0.93	0.09	-	47,47,47,47	0
56	MG	1a	1828	1/1	0.97	0.16	-	45,45,45,45	0
56	MG	1A	3525	1/1	0.95	0.24	-	54,54,54,54	0
56	MG	1A	3919	1/1	0.94	0.18	-	48,48,48,48	0
56	MG	1A	3563	1/1	0.81	0.18	-	62,62,62,62	0
56	MG	2A	3343	1/1	0.92	0.16	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3684	1/1	0.95	0.15	-	21,21,21,21	0
56	MG	1A	3252	1/1	0.95	0.18	-	29,29,29,29	0
56	MG	1A	3897	1/1	0.95	0.16	-	46,46,46,46	0
56	MG	1A	3208	1/1	0.94	0.20	-	51,51,51,51	0
56	MG	2A	3182	1/1	0.95	0.14	-	47,47,47,47	0
56	MG	1A	4060	1/1	0.94	0.18	-	56,56,56,56	0
56	MG	1a	1850	1/1	0.94	0.17	-	47,47,47,47	0
56	MG	1A	3333	1/1	0.94	0.11	-	53,53,53,53	0
56	MG	1A	3607	1/1	0.98	0.09	-	27,27,27,27	0
56	MG	2A	3107	1/1	0.75	0.26	-	54,54,54,54	0
56	MG	2A	3468	1/1	0.87	0.19	-	57,57,57,57	0
56	MG	2a	1667	1/1	0.83	0.36	-	69,69,69,69	0
56	MG	1A	3802	1/1	0.95	0.16	-	36,36,36,36	0
56	MG	1a	1799	1/1	0.96	0.15	-	39,39,39,39	0
56	MG	2A	3168	1/1	0.95	0.12	-	43,43,43,43	0
56	MG	1A	4038	1/1	0.84	0.26	-	63,63,63,63	0
56	MG	2A	3377	1/1	0.96	0.18	-	39,39,39,39	0
56	MG	1A	3160	1/1	0.90	0.22	-	53,53,53,53	0
56	MG	2A	3359	1/1	0.91	0.13	-	49,49,49,49	0
56	MG	1A	3686	1/1	0.94	0.08	-	36,36,36,36	0
56	MG	1A	3585	1/1	0.95	0.14	-	20,20,20,20	0
56	MG	1A	3363	1/1	0.89	0.19	-	65,65,65,65	0
56	MG	2A	3337	1/1	0.94	0.32	-	59,59,59,59	0
56	MG	1A	3598	1/1	0.92	0.16	-	48,48,48,48	0
56	MG	1a	1772	1/1	0.76	0.09	-	83,83,83,83	0
56	MG	1A	3088	1/1	0.94	0.09	-	47,47,47,47	0
56	MG	2A	3483	1/1	0.93	0.09	-	43,43,43,43	0
56	MG	2A	3015	1/1	0.92	0.12	-	57,57,57,57	0
56	MG	1a	1676	1/1	0.96	0.23	-	49,49,49,49	0
56	MG	1A	3489	1/1	0.88	0.12	-	41,41,41,41	0
56	MG	1A	3242	1/1	0.86	0.23	-	30,30,30,30	0
56	MG	1A	3425	1/1	0.97	0.22	-	62,62,62,62	0
56	MG	1A	3448	1/1	0.94	0.10	-	58,58,58,58	0
56	MG	1B	204	1/1	0.82	0.17	-	59,59,59,59	0
56	MG	1A	3904	1/1	0.95	0.08	-	64,64,64,64	0
56	MG	1A	4037	1/1	0.87	0.35	-	54,54,54,54	0
56	MG	1A	3719	1/1	0.97	0.12	-	34,34,34,34	0
56	MG	10	106	1/1	0.93	0.52	-	72,72,72,72	0
56	MG	1A	3553	1/1	0.94	0.21	-	50,50,50,50	0
56	MG	2a	1793	1/1	0.96	0.11	-	58,58,58,58	0
56	MG	1A	3444	1/1	0.96	0.15	-	63,63,63,63	0
56	MG	2A	3542	1/1	0.89	0.09	-	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	3933	1/1	0.96	0.07	-	42,42,42,42	0
56	MG	1A	3265	1/1	0.93	0.19	-	52,52,52,52	0
56	MG	2A	3212	1/1	0.77	0.27	-	64,64,64,64	0
56	MG	2A	3237	1/1	0.90	0.14	-	46,46,46,46	0
56	MG	1a	1886	1/1	0.94	0.13	-	60,60,60,60	0
56	MG	2a	1779	1/1	0.96	0.10	-	39,39,39,39	0
56	MG	1A	3935	1/1	0.83	0.23	-	69,69,69,69	0
56	MG	1F	303	1/1	0.98	0.08	-	35,35,35,35	0
56	MG	2a	1671	1/1	0.93	0.35	-	53,53,53,53	0
56	MG	1a	1794	1/1	0.95	0.12	-	60,60,60,60	0
56	MG	1A	4026	1/1	0.97	0.22	-	45,45,45,45	0
56	MG	2B	3001	1/1	0.93	0.20	-	57,57,57,57	0
56	MG	1A	3926	1/1	0.97	0.06	-	52,52,52,52	0
56	MG	2A	3060	1/1	0.87	0.14	-	50,50,50,50	0
56	MG	1A	3358	1/1	0.94	0.14	-	55,55,55,55	0
56	MG	1A	3096	1/1	0.98	0.07	-	46,46,46,46	0
56	MG	1a	1734	1/1	0.94	0.33	-	54,54,54,54	0
56	MG	1A	3944	1/1	0.94	0.50	-	50,50,50,50	0
56	MG	1a	1830	1/1	0.90	0.14	-	59,59,59,59	0
56	MG	1A	3377	1/1	0.95	0.39	-	43,43,43,43	0
56	MG	1A	3721	1/1	0.96	0.10	-	51,51,51,51	0
56	MG	2B	3007	1/1	0.97	0.14	-	48,48,48,48	0
56	MG	1a	1625	1/1	0.96	0.15	-	51,51,51,51	0
56	MG	2A	3313	1/1	0.90	0.06	-	57,57,57,57	0
56	MG	2B	3004	1/1	0.88	0.23	-	45,45,45,45	0
56	MG	1a	1823	1/1	0.94	0.19	-	54,54,54,54	0
56	MG	1A	3568	1/1	0.94	0.30	-	53,53,53,53	0
56	MG	1A	3472	1/1	0.95	0.09	-	46,46,46,46	0
56	MG	1a	1797	1/1	0.91	0.17	-	54,54,54,54	0
56	MG	2A	3346	1/1	0.93	0.12	-	44,44,44,44	0
56	MG	1A	4079	1/1	0.96	0.41	-	49,49,49,49	0
56	MG	1A	3811	1/1	0.95	0.15	-	34,34,34,34	0
56	MG	1A	3570	1/1	0.71	0.13	-	32,32,32,32	0
56	MG	1A	3013	1/1	0.96	0.06	-	50,50,50,50	0
56	MG	1A	3009	1/1	0.86	0.10	-	47,47,47,47	0
56	MG	1A	3362	1/1	0.95	0.31	-	41,41,41,41	0
56	MG	1A	3732	1/1	0.84	0.12	-	67,67,67,67	0
56	MG	1a	1773	1/1	0.91	0.12	-	65,65,65,65	0
56	MG	1A	3513	1/1	0.92	0.20	-	58,58,58,58	0
56	MG	2a	1621	1/1	0.87	0.30	-	53,53,53,53	0
56	MG	1A	3297	1/1	0.94	0.15	-	41,41,41,41	0
56	MG	2a	1749	1/1	0.73	0.23	-	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	2A	3047	1/1	0.92	0.22	-	48,48,48,48	0
56	MG	2a	1686	1/1	0.94	0.08	-	49,49,49,49	0
56	MG	1A	3893	1/1	0.84	0.17	-	53,53,53,53	0
56	MG	1A	3746	1/1	0.87	0.12	-	38,38,38,38	0
56	MG	2A	3478	1/1	0.89	0.05	-	42,42,42,42	0
56	MG	1A	3939	1/1	0.96	0.35	-	30,30,30,30	0
56	MG	1a	1609	1/1	0.84	0.32	-	56,56,56,56	0
56	MG	1a	1871	1/1	0.94	0.13	-	50,50,50,50	0
56	MG	1a	1875	1/1	0.93	0.19	-	61,61,61,61	0
56	MG	2A	3006	1/1	0.90	0.13	-	54,54,54,54	0
56	MG	1a	1622	1/1	0.94	0.18	-	59,59,59,59	0
56	MG	2A	3326	1/1	0.94	0.28	-	50,50,50,50	0
56	MG	2A	3317	1/1	0.94	0.11	-	37,37,37,37	0
56	MG	1A	3064	1/1	0.96	0.07	-	57,57,57,57	0
56	MG	2a	1653	1/1	0.94	0.08	-	60,60,60,60	0
56	MG	2a	1772	1/1	0.94	0.32	-	63,63,63,63	0
56	MG	2A	3352	1/1	0.76	0.14	-	62,62,62,62	0
56	MG	1F	302	1/1	0.96	0.07	-	42,42,42,42	0
56	MG	1a	1748	1/1	0.88	0.24	-	56,56,56,56	0
56	MG	1A	3558	1/1	0.83	0.25	-	65,65,65,65	0
56	MG	1E	306	1/1	0.96	0.12	-	51,51,51,51	0
56	MG	2A	3001	1/1	0.85	0.20	-	39,39,39,39	0
56	MG	2a	1673	1/1	0.97	0.45	-	52,52,52,52	0
56	MG	1A	3487	1/1	0.97	0.12	-	41,41,41,41	0
56	MG	1A	4029	1/1	0.83	0.20	-	61,61,61,61	0
56	MG	2A	3009	1/1	0.93	0.42	-	45,45,45,45	0
56	MG	2A	3512	1/1	0.94	0.36	-	32,32,32,32	0
56	MG	1A	3044	1/1	0.90	0.54	-	38,38,38,38	0
56	MG	1A	3094	1/1	0.96	0.11	-	42,42,42,42	0
56	MG	2A	3082	1/1	0.91	0.20	-	55,55,55,55	0
56	MG	1a	1744	1/1	0.97	0.09	-	53,53,53,53	0
56	MG	1A	3106	1/1	0.96	0.17	-	57,57,57,57	0
56	MG	2A	3255	1/1	0.95	0.15	-	42,42,42,42	0
56	MG	1a	1877	1/1	0.95	0.05	-	65,65,65,65	0
56	MG	2A	3496	1/1	0.59	0.42	-	66,66,66,66	0
56	MG	2a	1668	1/1	0.91	0.31	-	42,42,42,42	0
56	MG	2A	3307	1/1	0.96	0.07	-	63,63,63,63	0
56	MG	1A	3058	1/1	0.98	0.37	-	63,63,63,63	0
56	MG	1A	3365	1/1	0.95	0.13	-	57,57,57,57	0
56	MG	2a	1623	1/1	0.81	0.50	-	63,63,63,63	0
56	MG	2a	1693	1/1	0.97	0.19	-	67,67,67,67	0
56	MG	1A	3461	1/1	0.80	0.24	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3066	1/1	0.95	0.26	-	59,59,59,59	0
56	MG	1A	3300	1/1	0.83	0.27	-	28,28,28,28	0
56	MG	2q	3001	1/1	0.87	0.23	-	54,54,54,54	0
56	MG	2a	1813	1/1	0.92	0.33	-	72,72,72,72	0
56	MG	1a	1890	1/1	0.94	0.34	-	66,66,66,66	0
56	MG	2a	1694	1/1	0.89	0.07	-	61,61,61,61	0
56	MG	1A	4025	1/1	0.98	0.18	-	30,30,30,30	0
56	MG	1a	1685	1/1	0.88	0.12	-	37,37,37,37	0
56	MG	1a	1903	1/1	0.96	0.16	-	72,72,72,72	0
56	MG	19	104	1/1	0.93	0.13	-	46,46,46,46	0
56	MG	1A	3848	1/1	0.97	0.11	-	69,69,69,69	0
56	MG	1A	3126	1/1	0.92	0.26	-	44,44,44,44	0
56	MG	1A	3675	1/1	0.96	0.20	-	21,21,21,21	0
56	MG	1A	3670	1/1	0.92	0.17	-	19,19,19,19	0
56	MG	2A	3333	1/1	0.97	0.16	-	45,45,45,45	0
56	MG	1a	1739	1/1	0.86	0.13	-	54,54,54,54	0
56	MG	1A	3124	1/1	0.89	0.35	-	49,49,49,49	0
56	MG	1A	3637	1/1	0.99	0.31	-	31,31,31,31	0
56	MG	1a	1607	1/1	0.96	0.20	-	62,62,62,62	0
56	MG	2a	1723	1/1	0.94	0.39	-	67,67,67,67	0
56	MG	1A	3367	1/1	0.96	0.24	-	53,53,53,53	0
56	MG	1A	3832	1/1	0.94	0.12	-	36,36,36,36	0
56	MG	2A	3038	1/1	0.97	0.20	-	46,46,46,46	0
56	MG	1A	3882	1/1	0.93	0.06	-	49,49,49,49	0
56	MG	1A	3561	1/1	0.83	0.29	-	55,55,55,55	0
56	MG	1A	3177	1/1	0.87	0.11	-	52,52,52,52	0
56	MG	2a	1702	1/1	0.96	0.14	-	64,64,64,64	0
56	MG	1B	222	1/1	0.92	0.13	-	62,62,62,62	0
56	MG	2a	1683	1/1	0.99	0.12	-	43,43,43,43	0
56	MG	1A	3227	1/1	0.98	0.14	-	27,27,27,27	0
56	MG	1A	3806	1/1	0.93	0.07	-	65,65,65,65	0
56	MG	2A	3028	1/1	0.93	0.21	-	45,45,45,45	0
56	MG	1B	210	1/1	0.93	0.11	-	50,50,50,50	0
56	MG	1A	3649	1/1	0.96	0.13	-	54,54,54,54	0
56	MG	2A	3154	1/1	0.95	0.31	-	39,39,39,39	0
56	MG	2e	201	1/1	0.84	0.24	-	71,71,71,71	0
56	MG	1a	1670	1/1	0.89	0.38	-	60,60,60,60	0
56	MG	1B	223	1/1	0.98	0.18	-	48,48,48,48	0
56	MG	1A	3713	1/1	0.91	0.17	-	48,48,48,48	0
56	MG	1a	1606	1/1	0.77	0.09	-	62,62,62,62	0
56	MG	1o	3002	1/1	0.93	0.13	-	57,57,57,57	0
56	MG	2a	1808	1/1	0.90	0.08	-	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	3425	1/1	0.95	0.10	-	46,46,46,46	0
56	MG	1G	3002	1/1	0.83	0.12	-	48,48,48,48	0
56	MG	1A	3115	1/1	0.96	0.19	-	48,48,48,48	0
56	MG	2A	3220	1/1	0.92	0.15	-	43,43,43,43	0
56	MG	1h	3001	1/1	0.70	0.12	-	70,70,70,70	0
56	MG	1a	1601	1/1	0.86	0.28	-	62,62,62,62	0
56	MG	1A	3991	1/1	0.87	0.28	-	94,94,94,94	0
56	MG	1l	201	1/1	0.52	0.13	-	74,74,74,74	0
56	MG	2A	3396	1/1	0.90	0.18	-	64,64,64,64	0
56	MG	1B	227	1/1	0.71	0.52	-	70,70,70,70	0
56	MG	1A	3867	1/1	0.97	0.25	-	48,48,48,48	0
56	MG	1A	3032	1/1	0.94	0.21	-	66,66,66,66	0
56	MG	1A	3905	1/1	0.87	0.21	-	43,43,43,43	0
56	MG	2A	3407	1/1	0.94	0.20	-	68,68,68,68	0
56	MG	1A	3586	1/1	0.94	0.18	-	55,55,55,55	0
56	MG	1A	3329	1/1	0.86	0.13	-	52,52,52,52	0
56	MG	1a	1818	1/1	0.90	0.33	-	69,69,69,69	0
56	MG	2A	3178	1/1	0.90	0.06	-	52,52,52,52	0
56	MG	1A	3575	1/1	0.96	0.09	-	62,62,62,62	0
56	MG	1A	3392	1/1	0.88	0.14	-	44,44,44,44	0
56	MG	1x	110	1/1	0.90	0.09	-	53,53,53,53	0
56	MG	1A	3082	1/1	0.97	0.37	-	65,65,65,65	0
56	MG	2A	3065	1/1	0.93	0.22	-	56,56,56,56	0
56	MG	1T	202	1/1	0.95	0.08	-	38,38,38,38	0
56	MG	1a	1692	1/1	0.92	0.05	-	61,61,61,61	0
56	MG	1A	3319	1/1	0.84	0.15	-	50,50,50,50	0
56	MG	1A	3950	1/1	0.93	0.41	-	68,68,68,68	0
56	MG	1A	3318	1/1	0.93	0.23	-	53,53,53,53	0
56	MG	1A	3891	1/1	0.76	0.28	-	65,65,65,65	0
56	MG	2a	1783	1/1	0.95	0.20	-	59,59,59,59	0
56	MG	1A	3251	1/1	0.96	0.15	-	58,58,58,58	0
56	MG	1A	3998	1/1	0.81	0.11	-	47,47,47,47	0
56	MG	2A	3500	1/1	0.97	0.35	-	53,53,53,53	0
56	MG	1a	1721	1/1	0.95	0.34	-	36,36,36,36	0
56	MG	2a	1646	1/1	0.99	0.14	-	70,70,70,70	0
56	MG	1A	3934	1/1	0.98	0.06	-	52,52,52,52	0
56	MG	2a	1738	1/1	0.94	0.10	-	58,58,58,58	0
56	MG	2A	3141	1/1	0.97	0.23	-	37,37,37,37	0
56	MG	2a	1746	1/1	0.96	0.14	-	46,46,46,46	0
56	MG	2A	3073	1/1	0.89	0.40	-	43,43,43,43	0
56	MG	1a	1757	1/1	0.96	0.07	-	50,50,50,50	0
56	MG	1a	1682	1/1	0.95	0.21	-	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	1648	1/1	0.92	0.23	-	60,60,60,60	0
56	MG	1A	3439	1/1	0.96	0.12	-	64,64,64,64	0
56	MG	1A	3901	1/1	0.97	0.07	-	40,40,40,40	0
56	MG	2A	3369	1/1	0.97	0.34	-	45,45,45,45	0
56	MG	1A	3143	1/1	0.95	0.22	-	41,41,41,41	0
56	MG	1A	3437	1/1	0.87	0.15	-	51,51,51,51	0
56	MG	1A	3694	1/1	0.69	0.16	-	76,76,76,76	0
56	MG	1A	3008	1/1	0.93	0.22	-	53,53,53,53	0
56	MG	2A	3417	1/1	0.95	0.09	-	42,42,42,42	0
56	MG	1A	3029	1/1	0.97	0.28	-	40,40,40,40	0
56	MG	1A	4003	1/1	0.83	0.19	-	53,53,53,53	0
56	MG	1a	1814	1/1	0.98	0.11	-	61,61,61,61	0
56	MG	2A	3037	1/1	0.93	0.13	-	44,44,44,44	0
56	MG	2d	502	1/1	0.96	0.30	-	48,48,48,48	0
56	MG	2a	1635	1/1	0.90	0.14	-	88,88,88,88	0
56	MG	1A	3149	1/1	0.97	0.13	-	35,35,35,35	0
56	MG	2A	3069	1/1	0.97	0.36	-	52,52,52,52	0
56	MG	1a	1647	1/1	0.94	0.10	-	45,45,45,45	0
56	MG	1A	3382	1/1	0.95	0.56	-	59,59,59,59	0
56	MG	1A	3823	1/1	0.94	0.13	-	62,62,62,62	0
56	MG	2a	1602	1/1	0.92	0.17	-	41,41,41,41	0
56	MG	2A	3523	1/1	0.95	0.18	-	57,57,57,57	0
56	MG	1A	3327	1/1	0.90	0.07	-	64,64,64,64	0
56	MG	1B	217	1/1	0.99	0.14	-	55,55,55,55	0
56	MG	2A	3266	1/1	0.90	0.19	-	76,76,76,76	0
56	MG	1A	3526	1/1	0.97	0.40	-	41,41,41,41	0
56	MG	1A	3548	1/1	0.97	0.13	-	44,44,44,44	0
56	MG	1A	3022	1/1	0.92	0.15	-	46,46,46,46	0
56	MG	2A	3424	1/1	0.92	0.14	-	44,44,44,44	0
56	MG	1A	3280	1/1	0.74	0.11	-	76,76,76,76	0
56	MG	2A	3389	1/1	0.92	0.11	-	52,52,52,52	0
56	MG	1A	3574	1/1	0.93	0.23	-	29,29,29,29	0
56	MG	1A	3052	1/1	0.93	0.18	-	49,49,49,49	0
56	MG	2B	3008	1/1	0.94	0.20	-	69,69,69,69	0
56	MG	2A	3328	1/1	0.99	0.05	-	47,47,47,47	0
56	MG	2A	3243	1/1	0.92	0.14	-	27,27,27,27	0
56	MG	1A	3418	1/1	0.96	0.10	-	53,53,53,53	0
56	MG	1a	1731	1/1	0.98	0.44	-	42,42,42,42	0
56	MG	1A	3098	1/1	0.94	0.19	-	44,44,44,44	0
56	MG	2a	1795	1/1	0.89	0.15	-	53,53,53,53	0
56	MG	1A	3952	1/1	0.94	0.07	-	66,66,66,66	0
56	MG	1A	4022	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	3792	1/1	0.88	0.20	-	26,26,26,26	0
56	MG	2A	3505	1/1	0.92	0.09	-	42,42,42,42	0
56	MG	2A	3332	1/1	0.93	0.21	-	48,48,48,48	0
56	MG	2a	1726	1/1	0.81	0.39	-	59,59,59,59	0
56	MG	1N	208	1/1	0.98	0.08	-	47,47,47,47	0
56	MG	1A	3708	1/1	0.95	0.14	-	46,46,46,46	0
56	MG	2a	1696	1/1	0.98	0.15	-	43,43,43,43	0
56	MG	2A	3402	1/1	0.95	0.15	-	44,44,44,44	0
56	MG	2x	3005	1/1	0.84	0.08	-	80,80,80,80	0
56	MG	1a	1715	1/1	0.94	0.20	-	47,47,47,47	0
56	MG	1A	4050	1/1	0.80	0.37	-	55,55,55,55	0
56	MG	2A	3143	1/1	0.97	0.32	-	49,49,49,49	0
56	MG	2A	3404	1/1	0.93	0.25	-	55,55,55,55	0
56	MG	1A	4018	1/1	0.93	0.18	-	49,49,49,49	0
56	MG	1A	3456	1/1	0.87	0.15	-	52,52,52,52	0
56	MG	2A	3163	1/1	0.92	0.17	-	52,52,52,52	0
56	MG	1A	3307	1/1	0.62	0.49	-	61,61,61,61	0
56	MG	1A	3309	1/1	0.95	0.10	-	48,48,48,48	0
56	MG	2F	302	1/1	0.90	0.06	-	36,36,36,36	0
56	MG	2A	3545	1/1	0.91	0.14	-	69,69,69,69	0
56	MG	1a	1693	1/1	0.93	0.19	-	55,55,55,55	0
56	MG	1A	3340	1/1	0.97	0.07	-	43,43,43,43	0
56	MG	1A	3762	1/1	0.79	0.08	-	60,60,60,60	0
56	MG	1A	3593	1/1	0.99	0.13	-	38,38,38,38	0
56	MG	2a	1643	1/1	0.93	0.33	-	69,69,69,69	0
56	MG	1A	3927	1/1	0.94	0.16	-	61,61,61,61	0
56	MG	1A	3947	1/1	0.97	0.15	-	32,32,32,32	0
56	MG	1A	3314	1/1	0.95	0.14	-	52,52,52,52	0
56	MG	1a	1649	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	1A	3325	1/1	0.92	0.29	-	59,59,59,59	0
56	MG	1A	3278	1/1	0.97	0.10	-	28,28,28,28	0
56	MG	1A	3196	1/1	0.97	0.10	-	54,54,54,54	0
56	MG	2A	3344	1/1	0.98	0.12	-	43,43,43,43	0
56	MG	1A	4068	1/1	0.96	0.16	-	36,36,36,36	0
56	MG	1A	3572	1/1	0.95	0.14	-	56,56,56,56	0
56	MG	2a	1713	1/1	0.94	0.10	-	60,60,60,60	0
56	MG	2a	1645	1/1	0.86	0.26	-	57,57,57,57	0
56	MG	1a	1765	1/1	0.89	0.29	-	69,69,69,69	0
56	MG	1a	1760	1/1	0.88	0.08	-	48,48,48,48	0
56	MG	1A	3464	1/1	0.93	0.28	-	25,25,25,25	0
56	MG	1a	1870	1/1	0.86	0.24	-	58,58,58,58	0
56	MG	2A	3383	1/1	0.99	0.17	-	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	2A	3440	1/1	0.98	0.33	-	56,56,56,56	0
56	MG	2a	1805	1/1	0.96	0.09	-	52,52,52,52	0
56	MG	2a	1770	1/1	0.78	0.11	-	63,63,63,63	0
56	MG	1A	3634	1/1	0.98	0.05	-	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.