



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2017 – 05:18 AM EDT

PDB ID : 5HAU
Title : Crystal structure of antimicrobial peptide Bac7(1-19) bound to the *Thermus thermophilus* 70S ribosome
Authors : Gagnon, M.G.; Roy, R.N.; Lomakin, I.B.; Florin, T.; Mankin, A.S.; Steitz, T.A.
Deposited on : unknown
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

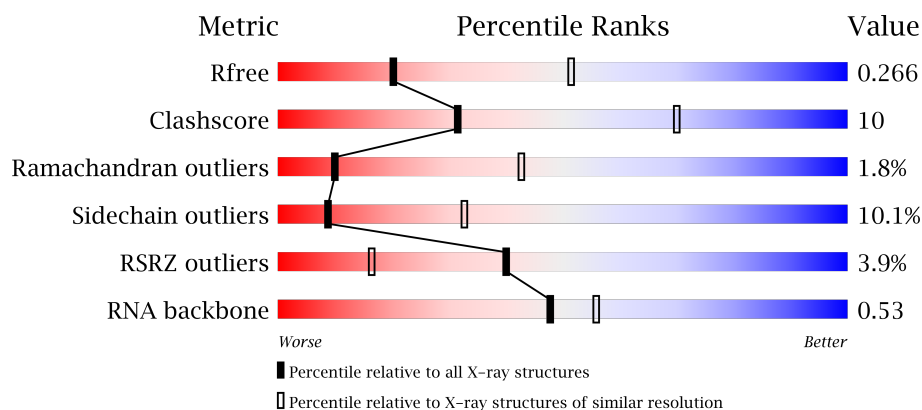
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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













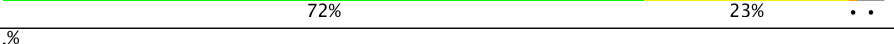
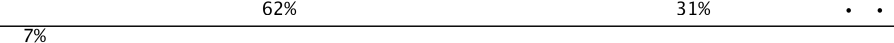
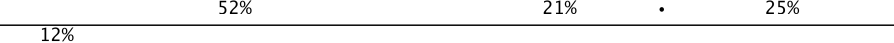

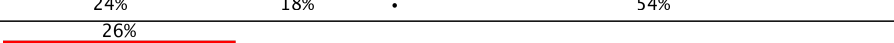
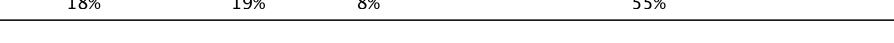
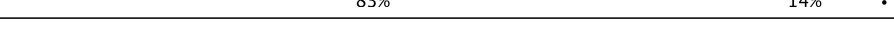

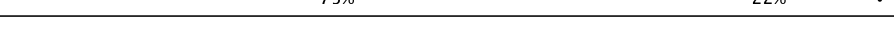






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)
RNA backbone	2435	1007 (3.34-2.66)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>31%</div> <div>7%</div> <div>..</div> </div> </div>
1	2A	2915	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>37%</div> <div>8%</div> <div>..</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>68%</div> <div>31%</div> <div>..</div> </div> </div>
2	2B	121	<div> <div></div> <div> <div></div> <div>59%</div> <div>36%</div> <div>..</div> </div> </div>












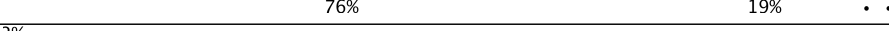







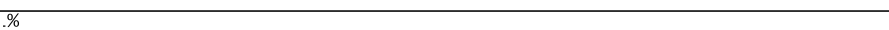

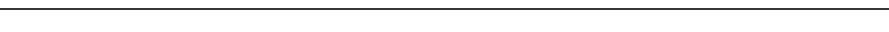
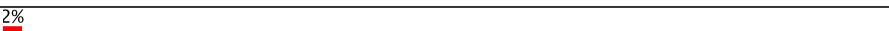


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Mol	Chain	Length	Quality of chain
3	1C	229	
3	2C	229	
4	1D	276	
4	2D	276	
5	1E	206	
5	2E	206	
6	1F	210	
6	2F	210	
7	1G	182	
7	2G	182	
8	1H	180	
8	2H	180	
9	1J	173	
9	2J	173	
10	1K	147	
10	2K	147	
11	1L	140	
11	2L	140	
12	1M	122	
12	2M	122	
13	1N	150	
13	2N	150	
14	1O	141	
14	2O	141	
15	1P	118	

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Mol	Chain	Length	Quality of chain
15	2P	118	
16	1Q	112	
16	2Q	112	
17	1R	146	
17	2R	146	
18	1S	118	
18	2S	118	
19	1T	101	
19	2T	101	
20	1U	113	
20	2U	113	
21	1V	96	
21	2V	96	
22	1W	110	
22	2W	110	
23	1X	206	
23	2X	206	
24	1Y	85	
24	2Y	85	
25	1Z	98	
25	2Z	98	
26	10	72	
26	20	72	
27	11	60	
27	21	60	

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Mol	Chain	Length	Quality of chain
28	12	71	
28	22	71	
29	13	60	
29	23	60	
30	14	54	
30	24	54	
31	15	49	
31	25	49	
32	16	65	
32	26	65	
33	17	37	
33	27	37	
34	1a	1521	
34	2a	1521	
35	1b	256	
35	2b	256	
36	1c	239	
36	2c	239	
37	1d	209	
37	2d	209	
38	1e	162	
38	2e	162	
39	1f	101	
39	2f	101	
40	1g	156	












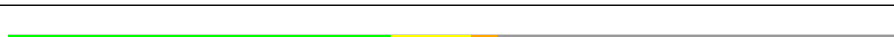
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Mol	Chain	Length	Quality of chain
40	2g	156	
41	1h	138	
41	2h	138	
42	1i	128	
42	2i	128	
43	1j	105	
43	2j	105	
44	1k	129	
44	2k	129	
45	1l	132	
45	2l	132	
46	1m	126	
46	2m	126	
47	1n	61	
47	2n	61	
48	1o	89	
48	2o	89	
49	1p	88	
49	2p	88	
50	1q	105	
50	2q	105	
51	1r	88	
51	2r	88	
52	1s	93	
52	2s	93	

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Mol	Chain	Length	Quality of chain
53	1t	106	
53	2t	106	
54	1u	27	
54	2u	27	
55	1z	758	
55	2z	758	
56	1y	24	
56	2y	24	
57	1w	77	
57	2w	77	
58	1x	35	
58	2x	35	

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
59	MG	11	8001	-	-	-	X
59	MG	13	104	-	-	-	X
59	MG	15	101	-	-	-	X
59	MG	16	102	-	-	-	X
59	MG	1A	3012	-	-	-	X
59	MG	1A	3018	-	-	-	X
59	MG	1A	3019	-	-	-	X
59	MG	1A	3020	-	-	-	X
59	MG	1A	3023	-	-	-	X
59	MG	1A	3028	-	-	-	X
59	MG	1A	3029	-	-	-	X
59	MG	1A	3030	-	-	-	X
59	MG	1A	3032	-	-	-	X
59	MG	1A	3033	-	-	-	X
59	MG	1A	3037	-	-	-	X
59	MG	1A	3040	-	-	-	X
59	MG	1A	3043	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	1A	3048	-	-	-	X
59	MG	1A	3066	-	-	-	X
59	MG	1A	3071	-	-	-	X
59	MG	1A	3078	-	-	-	X
59	MG	1A	3085	-	-	-	X
59	MG	1A	3088	-	-	-	X
59	MG	1A	3090	-	-	-	X
59	MG	1A	3093	-	-	-	X
59	MG	1A	3098	-	-	-	X
59	MG	1A	3105	-	-	-	X
59	MG	1A	3115	-	-	-	X
59	MG	1A	3119	-	-	-	X
59	MG	1A	3125	-	-	-	X
59	MG	1A	3126	-	-	-	X
59	MG	1A	3127	-	-	-	X
59	MG	1A	3130	-	-	-	X
59	MG	1A	3139	-	-	-	X
59	MG	1A	3144	-	-	-	X
59	MG	1A	3148	-	-	-	X
59	MG	1A	3150	-	-	-	X
59	MG	1A	3159	-	-	-	X
59	MG	1A	3175	-	-	-	X
59	MG	1A	3178	-	-	-	X
59	MG	1A	3181	-	-	-	X
59	MG	1A	3190	-	-	-	X
59	MG	1A	3195	-	-	-	X
59	MG	1A	3197	-	-	-	X
59	MG	1A	3202	-	-	-	X
59	MG	1A	3204	-	-	-	X
59	MG	1A	3208	-	-	-	X
59	MG	1A	3210	-	-	-	X
59	MG	1A	3212	-	-	-	X
59	MG	1A	3215	-	-	-	X
59	MG	1A	3217	-	-	-	X
59	MG	1A	3226	-	-	-	X
59	MG	1A	3227	-	-	-	X
59	MG	1A	3236	-	-	-	X
59	MG	1A	3260	-	-	-	X
59	MG	1A	3271	-	-	-	X
59	MG	1A	3273	-	-	-	X
59	MG	1A	3276	-	-	-	X
59	MG	1A	3291	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	1A	3337	-	-	-	X
59	MG	1A	3348	-	-	-	X
59	MG	1A	3349	-	-	-	X
59	MG	1A	3350	-	-	-	X
59	MG	1A	3355	-	-	-	X
59	MG	1A	3382	-	-	-	X
59	MG	1A	3387	-	-	-	X
59	MG	1A	3389	-	-	-	X
59	MG	1A	3411	-	-	-	X
59	MG	1A	3433	-	-	-	X
59	MG	1A	3434	-	-	-	X
59	MG	1A	3435	-	-	-	X
59	MG	1A	3440	-	-	-	X
59	MG	1A	3451	-	-	-	X
59	MG	1A	3452	-	-	-	X
59	MG	1A	3456	-	-	-	X
59	MG	1A	3462	-	-	-	X
59	MG	1A	3468	-	-	-	X
59	MG	1A	3478	-	-	-	X
59	MG	1A	3492	-	-	-	X
59	MG	1A	3499	-	-	-	X
59	MG	1A	3503	-	-	-	X
59	MG	1A	3517	-	-	-	X
59	MG	1A	3525	-	-	-	X
59	MG	1A	3537	-	-	-	X
59	MG	1A	3552	-	-	-	X
59	MG	1A	3576	-	-	-	X
59	MG	1A	3580	-	-	-	X
59	MG	1A	3658	-	-	-	X
59	MG	1A	3669	-	-	-	X
59	MG	1A	3699	-	-	-	X
59	MG	1A	3705	-	-	-	X
59	MG	1A	3713	-	-	-	X
59	MG	1A	3716	-	-	-	X
59	MG	1A	3729	-	-	-	X
59	MG	1A	3730	-	-	-	X
59	MG	1A	3731	-	-	-	X
59	MG	1A	3739	-	-	-	X
59	MG	1A	3742	-	-	-	X
59	MG	1A	3759	-	-	-	X
59	MG	1A	3760	-	-	-	X
59	MG	1A	3761	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	1A	3764	-	-	-	X
59	MG	1A	3774	-	-	-	X
59	MG	1A	3778	-	-	-	X
59	MG	1A	3779	-	-	-	X
59	MG	1A	3780	-	-	-	X
59	MG	1D	301	-	-	-	X
59	MG	1D	302	-	-	-	X
59	MG	1D	304	-	-	-	X
59	MG	1F	301	-	-	-	X
59	MG	1F	302	-	-	-	X
59	MG	1N	202	-	-	-	X
59	MG	1O	3001	-	-	-	X
59	MG	1S	3001	-	-	-	X
59	MG	1S	3002	-	-	-	X
59	MG	1S	3003	-	-	-	X
59	MG	1S	3004	-	-	-	X
59	MG	1U	203	-	-	-	X
59	MG	1Y	103	-	-	-	X
59	MG	1a	1616	-	-	-	X
59	MG	1a	1627	-	-	-	X
59	MG	1a	1630	-	-	-	X
59	MG	1a	1638	-	-	-	X
59	MG	1a	1657	-	-	-	X
59	MG	1a	1672	-	-	-	X
59	MG	1a	1679	-	-	-	X
59	MG	1a	1689	-	-	-	X
59	MG	1a	1691	-	-	-	X
59	MG	1a	1695	-	-	-	X
59	MG	1a	1704	-	-	-	X
59	MG	1a	1720	-	-	-	X
59	MG	1a	1739	-	-	-	X
59	MG	1a	1740	-	-	-	X
59	MG	1a	1741	-	-	-	X
59	MG	1a	1748	-	-	-	X
59	MG	1a	1760	-	-	-	X
59	MG	1a	1767	-	-	-	X
59	MG	1a	1779	-	-	-	X
59	MG	1a	1784	-	-	-	X
59	MG	1a	1793	-	-	-	X
59	MG	1a	1798	-	-	-	X
59	MG	1a	1803	-	-	-	X
59	MG	1t	3001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	2A	3001	-	-	-	X
59	MG	2A	3008	-	-	-	X
59	MG	2A	3013	-	-	-	X
59	MG	2A	3015	-	-	-	X
59	MG	2A	3020	-	-	-	X
59	MG	2A	3024	-	-	-	X
59	MG	2A	3026	-	-	-	X
59	MG	2A	3029	-	-	-	X
59	MG	2A	3031	-	-	-	X
59	MG	2A	3064	-	-	-	X
59	MG	2A	3065	-	-	-	X
59	MG	2A	3073	-	-	-	X
59	MG	2A	3076	-	-	-	X
59	MG	2A	3077	-	-	-	X
59	MG	2A	3080	-	-	-	X
59	MG	2A	3086	-	-	-	X
59	MG	2A	3092	-	-	-	X
59	MG	2A	3093	-	-	-	X
59	MG	2A	3096	-	-	-	X
59	MG	2A	3103	-	-	-	X
59	MG	2A	3110	-	-	-	X
59	MG	2A	3117	-	-	-	X
59	MG	2A	3118	-	-	-	X
59	MG	2A	3128	-	-	-	X
59	MG	2A	3129	-	-	-	X
59	MG	2A	3130	-	-	-	X
59	MG	2A	3143	-	-	-	X
59	MG	2A	3157	-	-	-	X
59	MG	2A	3159	-	-	-	X
59	MG	2A	3161	-	-	-	X
59	MG	2A	3162	-	-	-	X
59	MG	2A	3177	-	-	-	X
59	MG	2A	3185	-	-	-	X
59	MG	2A	3186	-	-	-	X
59	MG	2A	3187	-	-	-	X
59	MG	2A	3188	-	-	-	X
59	MG	2A	3192	-	-	-	X
59	MG	2A	3198	-	-	-	X
59	MG	2A	3199	-	-	-	X
59	MG	2A	3201	-	-	-	X
59	MG	2A	3202	-	-	-	X
59	MG	2A	3207	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	2A	3211	-	-	-	X
59	MG	2A	3214	-	-	-	X
59	MG	2A	3216	-	-	-	X
59	MG	2A	3223	-	-	-	X
59	MG	2A	3236	-	-	-	X
59	MG	2A	3239	-	-	-	X
59	MG	2A	3246	-	-	-	X
59	MG	2A	3251	-	-	-	X
59	MG	2A	3252	-	-	-	X
59	MG	2A	3258	-	-	-	X
59	MG	2A	3267	-	-	-	X
59	MG	2A	3269	-	-	-	X
59	MG	2A	3290	-	-	-	X
59	MG	2A	3300	-	-	-	X
59	MG	2A	3304	-	-	-	X
59	MG	2A	3315	-	-	-	X
59	MG	2A	3322	-	-	-	X
59	MG	2A	3326	-	-	-	X
59	MG	2A	3327	-	-	-	X
59	MG	2A	3330	-	-	-	X
59	MG	2A	3331	-	-	-	X
59	MG	2A	3333	-	-	-	X
59	MG	2A	3335	-	-	-	X
59	MG	2A	3337	-	-	-	X
59	MG	2A	3341	-	-	-	X
59	MG	2A	3354	-	-	-	X
59	MG	2A	3366	-	-	-	X
59	MG	2A	3369	-	-	-	X
59	MG	2A	3390	-	-	-	X
59	MG	2A	3393	-	-	-	X
59	MG	2A	3394	-	-	-	X
59	MG	2A	3396	-	-	-	X
59	MG	2A	3403	-	-	-	X
59	MG	2A	3411	-	-	-	X
59	MG	2A	3419	-	-	-	X
59	MG	2A	3420	-	-	-	X
59	MG	2A	3423	-	-	-	X
59	MG	2A	3455	-	-	-	X
59	MG	2A	3465	-	-	-	X
59	MG	2A	3507	-	-	-	X
59	MG	2A	3518	-	-	-	X
59	MG	2A	3524	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	2A	3526	-	-	-	X
59	MG	2A	3528	-	-	-	X
59	MG	2A	3539	-	-	-	X
59	MG	2A	3542	-	-	-	X
59	MG	2A	3548	-	-	-	X
59	MG	2A	3549	-	-	-	X
59	MG	2A	3558	-	-	-	X
59	MG	2A	3559	-	-	-	X
59	MG	2A	3592	-	-	-	X
59	MG	2A	3594	-	-	-	X
59	MG	2A	3608	-	-	-	X
59	MG	2A	3616	-	-	-	X
59	MG	2A	3619	-	-	-	X
59	MG	2B	207	-	-	-	X
59	MG	2B	208	-	-	-	X
59	MG	2D	303	-	-	-	X
59	MG	2E	303	-	-	-	X
59	MG	2S	201	-	-	-	X
59	MG	2Y	8001	-	-	-	X
59	MG	2a	1628	-	-	-	X
59	MG	2a	1635	-	-	-	X
59	MG	2a	1649	-	-	-	X
59	MG	2a	1653	-	-	-	X
59	MG	2a	1655	-	-	-	X
59	MG	2a	1664	-	-	-	X
59	MG	2a	1669	-	-	-	X
59	MG	2a	1684	-	-	-	X
59	MG	2a	1690	-	-	-	X
59	MG	2a	1693	-	-	-	X
59	MG	2a	1711	-	-	-	X
59	MG	2a	1729	-	-	-	X
59	MG	2a	1738	-	-	-	X
59	MG	2a	1742	-	-	-	X
59	MG	2a	1744	-	-	-	X
59	MG	2n	502	-	-	-	X
59	MG	2t	3001	-	-	-	X
59	MG	2w	3004	-	-	-	X
60	ZN	13	103	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 306384 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	2872	Total	C	N	O	P	0	0	0
			61861	27532	11574	19884	2871			
1	2A	2868	Total	C	N	O	P	0	0	0
			61771	27492	11554	19858	2867			

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

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

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1C	135	Total	C	N	O	S	3	0	0
			1020	641	190	188	1			
3	2C	135	Total	C	N	O	S	3	0	0
			1020	641	190	188	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
4	2D	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
5	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
6	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1G	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
7	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
8	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1J	130	Total	C	N	O		0	0	0
			641	381	130	130				
9	2J	130	Total	C	N	O		0	0	0
			641	381	130	130				

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1K	67	Total	C	N	O	S	0	0	1
			499	310	94	92	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2K	66	Total	C	N	O	S	0	0	0
			498	310	93	92	3			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1L	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
11	2L	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1M	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
12	2M	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1N	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
13	2N	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1O	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
14	2O	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1P	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	2P	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	1Q	110	Total	C	N	O	0	0	0
			877	553	175	149			
16	2Q	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1R	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
17	2R	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1S	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
18	2S	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1T	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
19	2T	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1U	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
20	2U	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1V	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	2V	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1W	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
22	2W	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1X	186	Total	C	N	O	S	0	0	0
			1460	932	259	267	2			
23	2X	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1Y	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
24	2Y	76	Total	C	N	O	S	0	0	0
			602	372	128	101	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1Z	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
25	2Z	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	10	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	20	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	11	59	Total	C	N	O		0	0	0
			469	298	90	81				
27	21	59	Total	C	N	O		0	0	0
			464	296	90	78				

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	12	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
28	22	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	13	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
29	23	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	14	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	24	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	15	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	25	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	16	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	26	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	17	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	27	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1a	1495	Total	C	N	O	P	0	0	0
			32141	14304	5958	10384	1495			
34	2a	1501	Total	C	N	O	P	0	0	0
			32268	14361	5980	10426	1501			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
35	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1c	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
36	2c	206	Total	C	N	O	S	0	0	0
			1544	970	300	273	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1d	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
37	2d	208	Total	C	N	O	S	0	0	0
			1678	1052	333	286	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
38	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1f	100	Total	C	N	O	S	0	0	0
			812	514	146	149	3			
39	2f	100	Total	C	N	O	S	0	0	0
			820	518	147	152	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
40	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
41	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1i	127	Total	C	N	O		0	0	0
			986	626	193	167				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
43	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			
44	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1l	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			
45	2l	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1m	123	Total	C	N	O	S	0	0	0
			966	598	200	166	2			
46	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
47	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
48	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
49	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
50	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
51	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	1s	84	Total	C	N	O	S	0	0	0
			661	423	122	114	2			
52	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
53	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1u	23	Total	C	N	O		0	0	0
			199	122	48	29				
54	2u	23	Total	C	N	O		0	0	0
			199	122	48	29				

- Molecule 55 is a protein called Chimera protein of 50S ribosomal protein L9 and Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1z	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			
55	2z	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1y	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			
56	2y	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 57 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	1w	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
57	2w	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 58 is a protein called Cathelicidin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	1x	19	Total	C	N	O		0	0	0
			168	106	43	19				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	2x	19	Total	C	N	O	0	0	0
			168	106	43	19			

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2E	4	Total	Mg	0	0
			4	4		
59	17	2	Total	Mg	0	0
			2	2		
59	1z	1	Total	Mg	0	0
			1	1		
59	2d	1	Total	Mg	0	0
			1	1		
59	1T	1	Total	Mg	0	0
			1	1		
59	1N	2	Total	Mg	0	0
			2	2		
59	2W	1	Total	Mg	0	0
			1	1		
59	1Y	5	Total	Mg	0	0
			5	5		
59	13	3	Total	Mg	0	0
			3	3		
59	1f	1	Total	Mg	0	0
			1	1		
59	1P	2	Total	Mg	0	0
			2	2		
59	2B	13	Total	Mg	0	0
			13	13		
59	2a	173	Total	Mg	0	0
			173	173		
59	1E	6	Total	Mg	0	0
			6	6		
59	2M	2	Total	Mg	0	0
			2	2		
59	2z	4	Total	Mg	0	0
			4	4		
59	1b	1	Total	Mg	0	0
			1	1		
59	2l	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2F	3	Total 3	Mg 3	0	0
59	16	2	Total 2	Mg 2	0	0
59	1W	1	Total 1	Mg 1	0	0
59	1A	780	Total 780	Mg 780	0	0
59	1t	1	Total 1	Mg 1	0	0
59	2P	1	Total 1	Mg 1	0	0
59	1X	2	Total 2	Mg 2	0	0
59	2w	4	Total 4	Mg 4	0	0
59	1S	4	Total 4	Mg 4	0	0
59	1M	1	Total 1	Mg 1	0	0
59	1D	4	Total 4	Mg 4	0	0
59	2N	1	Total 1	Mg 1	0	0
59	2G	1	Total 1	Mg 1	0	0
59	2f	2	Total 2	Mg 2	0	0
59	1w	6	Total 6	Mg 6	0	0
59	1a	204	Total 204	Mg 204	0	0
59	15	2	Total 2	Mg 2	0	0
59	2j	1	Total 1	Mg 1	0	0
59	1L	2	Total 2	Mg 2	0	0
59	26	2	Total 2	Mg 2	0	0
59	1G	2	Total 2	Mg 2	0	0

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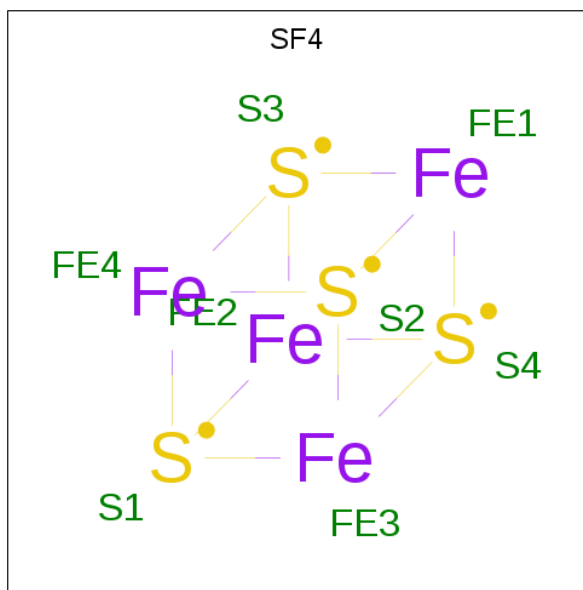
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2O	2	Total 2	Mg 2	0	0
59	11	1	Total 1	Mg 1	0	0
59	1d	2	Total 2	Mg 2	0	0
59	2n	1	Total 1	Mg 1	0	0
59	1H	1	Total 1	Mg 1	0	0
59	2q	1	Total 1	Mg 1	0	0
59	2Y	1	Total 1	Mg 1	0	0
59	23	1	Total 1	Mg 1	0	0
59	2R	1	Total 1	Mg 1	0	0
59	2D	4	Total 4	Mg 4	0	0
59	14	1	Total 1	Mg 1	0	0
59	1U	3	Total 3	Mg 3	0	0
59	1O	2	Total 2	Mg 2	0	0
59	1l	3	Total 3	Mg 3	0	0
59	1F	7	Total 7	Mg 7	0	0
59	10	2	Total 2	Mg 2	0	0
59	2t	1	Total 1	Mg 1	0	0
59	2A	620	Total 620	Mg 620	0	0
59	1B	24	Total 24	Mg 24	0	0
59	2S	2	Total 2	Mg 2	0	0

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

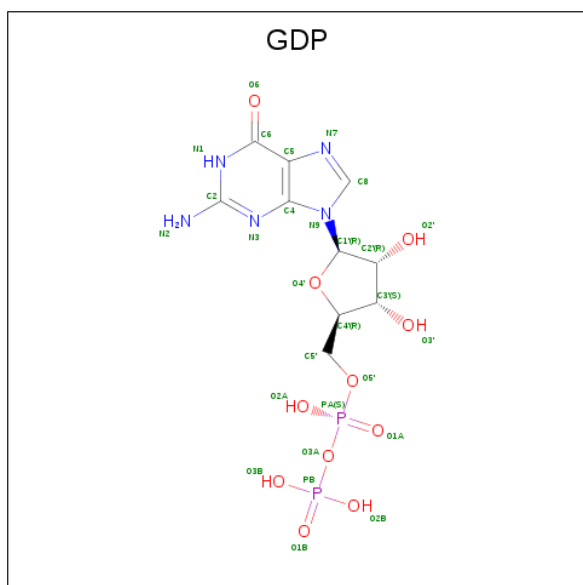
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1W	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	17	1	Total Zn 1 1	0	0
60	12	1	Total Zn 1 1	0	0
60	13	1	Total Zn 1 1	0	0
60	22	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0
60	27	1	Total Zn 1 1	0	0
60	2W	1	Total Zn 1 1	0	0
60	23	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	1z	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
62	2z	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1A	1299	Total	O	0	0
			1299	1299		
63	1B	39	Total	O	0	0
			39	39		
63	1D	15	Total	O	0	0
			15	15		
63	1E	19	Total	O	0	0
			19	19		
63	1F	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1G	3	Total 3	O 3	0	0
63	1H	1	Total 1	O 1	0	0
63	1M	2	Total 2	O 2	0	0
63	1N	12	Total 12	O 12	0	0
63	1O	2	Total 2	O 2	0	0
63	1P	4	Total 4	O 4	0	0
63	1Q	1	Total 1	O 1	0	0
63	1R	2	Total 2	O 2	0	0
63	1S	4	Total 4	O 4	0	0
63	1T	1	Total 1	O 1	0	0
63	1U	2	Total 2	O 2	0	0
63	1V	3	Total 3	O 3	0	0
63	1X	2	Total 2	O 2	0	0
63	1Y	4	Total 4	O 4	0	0
63	1Z	1	Total 1	O 1	0	0
63	11	2	Total 2	O 2	0	0
63	15	2	Total 2	O 2	0	0
63	16	10	Total 10	O 10	0	0
63	17	1	Total 1	O 1	0	0
63	1a	155	Total 155	O 155	0	0
63	1d	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1j	1	Total 1	O 1	0	0
63	1l	2	Total 2	O 2	0	0
63	1o	1	Total 1	O 1	0	0
63	1p	2	Total 2	O 2	0	0
63	1z	5	Total 5	O 5	0	0
63	1w	4	Total 4	O 4	0	0
63	1x	1	Total 1	O 1	0	0
63	2A	650	Total 650	O 650	0	0
63	2B	11	Total 11	O 11	0	0
63	2D	8	Total 8	O 8	0	0
63	2E	7	Total 7	O 7	0	0
63	2F	5	Total 5	O 5	0	0
63	2L	1	Total 1	O 1	0	0
63	2M	2	Total 2	O 2	0	0
63	2N	6	Total 6	O 6	0	0
63	2O	3	Total 3	O 3	0	0
63	2P	1	Total 1	O 1	0	0
63	2R	2	Total 2	O 2	0	0
63	2S	2	Total 2	O 2	0	0
63	2U	1	Total 1	O 1	0	0
63	2V	2	Total 2	O 2	0	0

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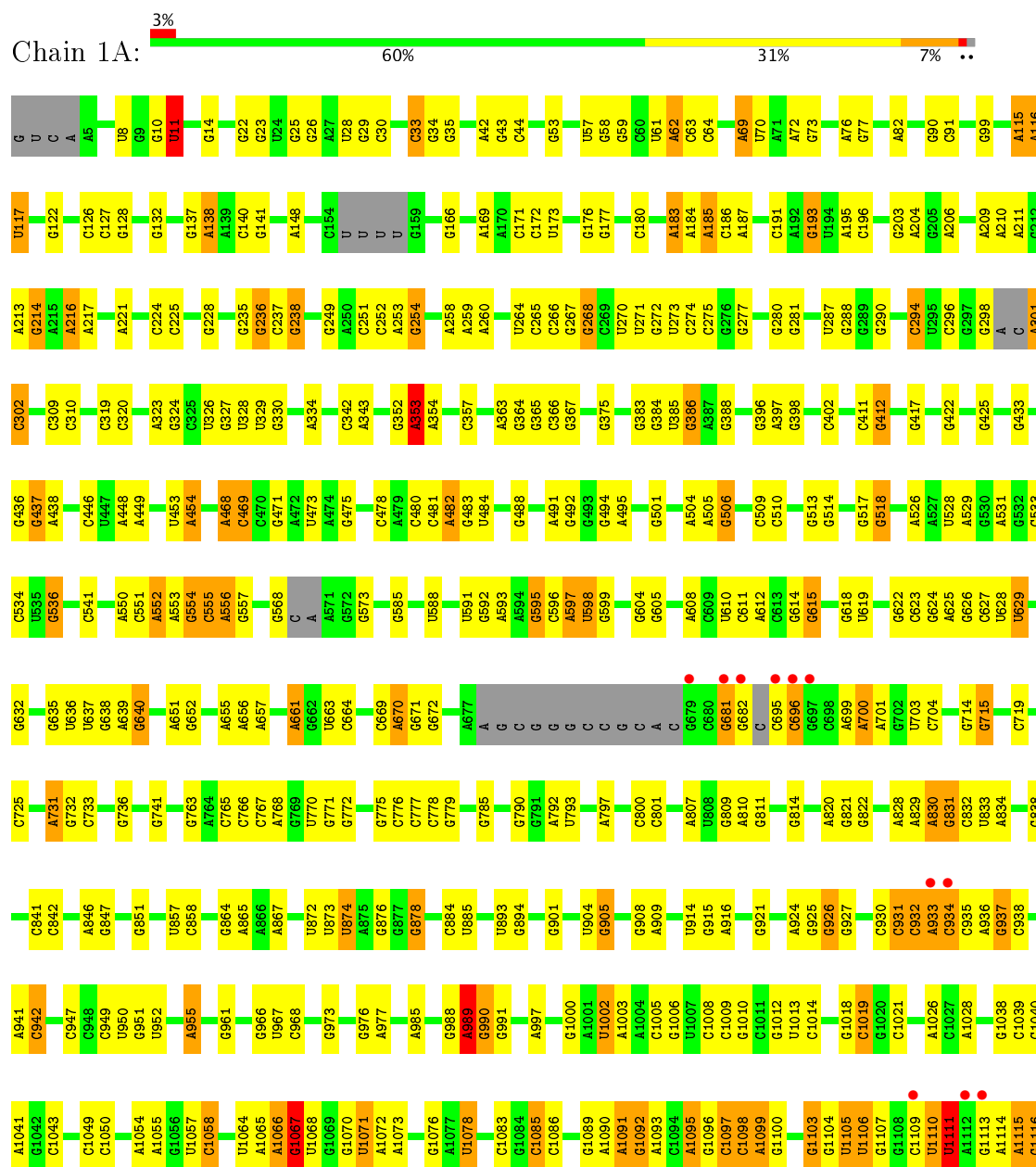
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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63	2Y	5	Total 5	O 5	0	0
63	2Z	2	Total 2	O 2	0	0
63	2I	2	Total 2	O 2	0	0
63	24	1	Total 1	O 1	0	0
63	26	3	Total 3	O 3	0	0
63	2a	122	Total 122	O 122	0	0
63	2f	1	Total 1	O 1	0	0
63	2h	1	Total 1	O 1	0	0
63	2j	1	Total 1	O 1	0	0
63	2n	1	Total 1	O 1	0	0
63	2t	1	Total 1	O 1	0	0
63	2z	1	Total 1	O 1	0	0
63	2y	1	Total 1	O 1	0	0
63	2w	2	Total 2	O 2	0	0

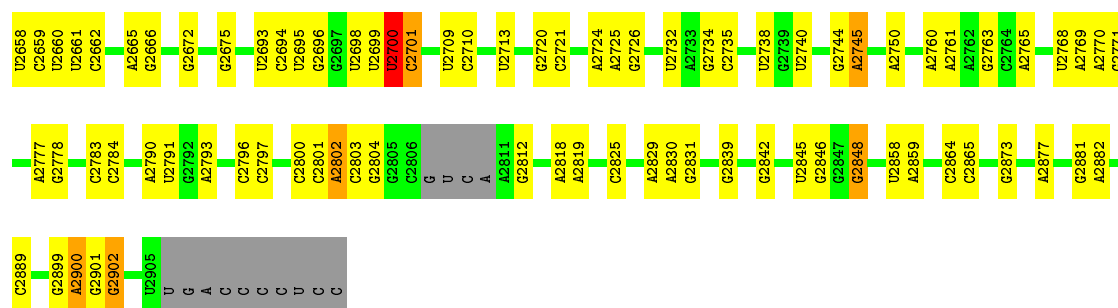
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

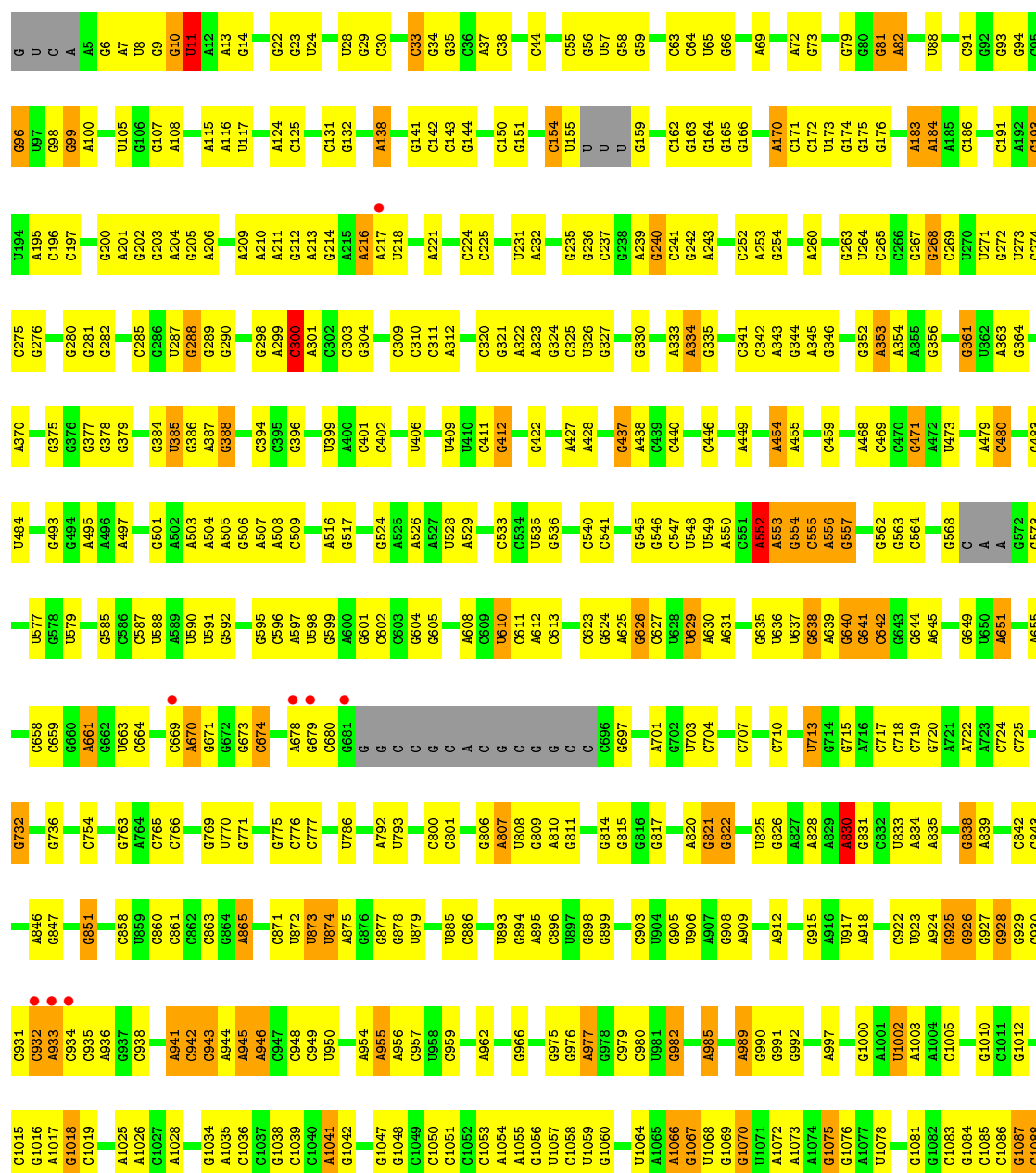
• Molecule 1: 23S Ribosomal RNA



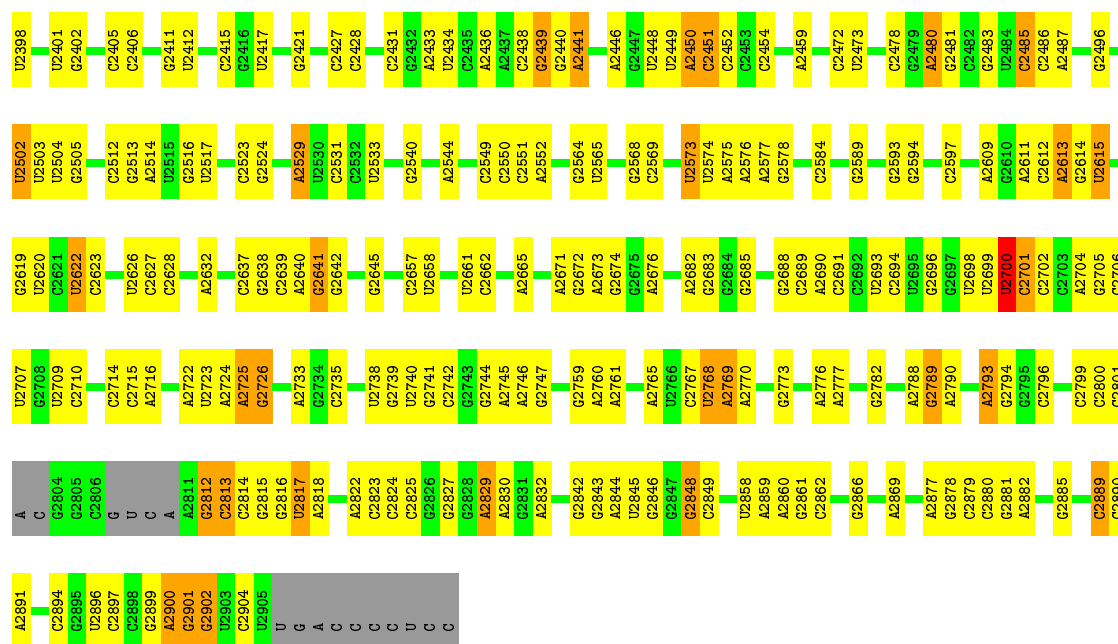




• Molecule 1: 23S Ribosomal RNA

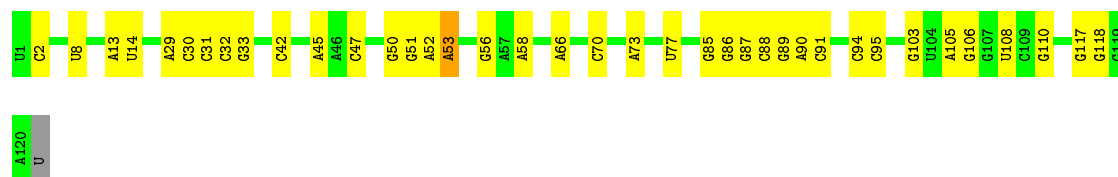


G2319	U2224	A2155	C2065	A1833	G1749	G1671	G1579	G1491	A1314	A1226	A1155	G1089
A2320	C2225	A2156	C2065	C1834	G1753	G1672	U	C1492	C1915	G1227	A1156	A1090
U2323	G2227	C2157	C2071	U1835	U1754	U1673	A	G1493	G1316	G1230	U1158	G1092
C2324	G2227	C2158	A2072	G1840	U1755	G1675	C1582	A1406	A1317	U1231	U1159	A1093
C2325	U2229	C2159	G2076	A1841	U1756	G1676	G1585	A1407	U1318	U1232	G1160	
C2326	G2230	C2160	U1965	G1844	C1757	A1677	U1586	G1408	A1319	A1233	C1161	C1098
C2327	G2231	C2161	U1965	A1845		G1678	U1587	G1409	G1322	G1234	C1162	A1099
C2328		G2162	A1973	G1846	G1761	G1679	A1588	A1410	A1323	G1235	C1163	G1100
G2329	A2237	C2163	U1976	G1847	G1762		A1591	G1413	G1325	A1238	C1164	A1102
G2330	A2238	C2164	U1976	G1848	G1763	C1682	C1592	G1414	G1328	C1244	G1167	G1103
A2331	A2239	C2165	U1976	G1849	U1764	A1683	C1593	G1415	A1329	C1245	U1105	G1104
A2332	G2239	C2166	U1976	G1850	A1765		C1594	G1416	G1330	C1246	U1106	G1105
A2333	U2244	C2167	G1955	G1851	A1766	C1686	C1597	U1417		C1247	A1171	G1107
C2334	G2245	C2168	A1986	C1857	G1767	G1688	C1598	A1418	G1336	A1248	A1172	G1108
C2335	G2246	C2169	A1987	G1858	G1768	G1689	G1598	A1425	U1337	U1249	A1173	G1109
C2336	G2247	C2170	C1988	G1859	A1769	G1690		A1426	C1338	G1250	A1174	U1110
C2337	G2248	C2171	G1989	G1860		C1691	C1603	G1429		C1251	U1175	G1111
A2338	G2249	C2172	A1991	C1861	G1776	G1692	A1604	G1430	U1345	G1252	C1179	G1112
A2339	G2250	C2173	A1992	C1862	G1777	C1693	G1606	C1431	A1346	U1253	U1185	G1113
G2340	U2254	C2174	A1993	G1863		G1694	G1614	G1439	A1347	U1254	G1182	A1114
G2341	U2255	C2175	C1985	G1864	G1784	G1695	G1615	U1443	G1348	G1255	G1183	A1115
G2342	U2256	C2176	C1986	G1865	A1785	G1696	A1616	U1444	U1349	G1256	G1184	G1116
C2343	G2257	C2177	G1987	G1866	G1786	G1697	A1617	U1445	C1350	C1266	U1186	G1117
C2344	A2258	C2178	C1988	G1867	U1787	G1698	A1700	U1446	G1354	A1270	A1187	G1120
C2345	G2259	C2179	U2012	G1868	G1788	C1702	A1701	G1447	G1355	A1271	U1188	G1121
A2346		C2180	G2013	G1869	G1789	G1703	G1619	U1448	G1356	G1276	G1189	G1122
A2347	G2262	C2181	U2014	G1870	G1790	C1704	G1624	U1449	U1357	C1280	A1129	G1123
C2354	U2273	C2182	G2015	G1871	A1792	G1705	U1625	U1450	G1360	G1281	A1130	G1124
U2355	C2274	C2183	C2020	G1872	G1793	C1706	A1626	U1451	G1364	U1285	C1195	G1132
C2356	G2275	C2184	G2021	G1873	G1794	C1707	A1627	U1452	C1366	G1288	C1196	G1133
C2357	C2276	C2185	G2022	G1874	G1795	C1708	U1628	U1453	G1367	G1289	G1197	G1134
C2358	U2278	C2186	G2023	G1875	G1796	C1709	A1629	U1454	U1368	G1293	G1198	G1135
U2359	A2279	C2187	G2024	G1876	U1797	A1710	C1630	U1455	G1369	U1294	G1207	G1136
C2360	G2280	C2188	C2025	G1877	C1797	A1711	C1631	U1456	G1370	G1295	U1210	G1137
C2361	A2281	C2189	G2026	G1878	A1803		A1631	U1457	G1371	G1298	U1211	U1142
C2362	U2282	C2190	C2027	G1879	U1808	A1714	A1632	U1458	C1365	A1299	A1143	A1144
A2363	A2283	C2191	G2028	G1880	U1809	A1715	C1633	G1459	C1366	U1300	G1216	U1145
C2364	C2284	C2192	A2034	G1881	A1810	C1716	C1634	U1460	A1367	G1301	G	U1146
C2365	G2285	C2193	A2035	G1882	C1811	G1720	G1638	U1461	U1368	G1302	A	C1147
C2366	U2286	C2194	G2036	G1883	A1812	G1721	G1639	U1462	G1369	G1303	U	A1148
C2367	G2287	C2195	G2037	G1884	A1813	C1722	A1552	U1463	G1370	G1304	G	C1149
C2368	A2288	C2196	A2041	G1885	A1814	G1723	A1553	U1464	G1371	G1305	A	U1150
C2369	G2289	C2197	C2042	G1886	A1815	C1724	A1554	U1465	G1372		G1222	G1151
C2370	U2290	C2198	U2043	G1887	A1816	C1725	A1555	U1466	G1373	G1312	C1223	U1152
A2371	G2291	C2199	G2044	G1888	G1817	C1726	C1643	U1467	U1374	G1313	C1224	C1154
A2372	C2292	C2200	C2045	G1889	A1818	C1727	C1644	G1470	G1375		G1216	
C2373	G2293	G2201	C2046	G1890	C1820	C1728	C1645	U1471	G1376	U1299	G	U1146
C2374	A2294	G2202	G2047	G1891	A1821	C1729	A1653	U1472	A1381	G1301	A	C1147
C2375	C2295	G2203	A2052	G1892	U1824	C1730	A1654	C1473	G1382	G1302	U	A1148
C2376	G2296	G2204	A2053	G1893	C1825	C1731	A1655	C1474	G1383	G1303	G	C1149
A2387	A2297	C2205	U1936	G1894	U1826	C1732	A1656	C1475	G1384	G1304	A	U1150
	G2298	C2206	U1937	G1895	C1827	C1733	A1657	U1479	U1385	G1305	C1222	G1151
	C2299	G2207	G1938	G1896	U1828	C1734	A1658	G1480	U1386		C1223	U1152
C2390	G2300	C2208	U1939	G1897	C1829	C1735	A1659	G1481			C1224	C1154
C2391	C2301	G2209	A1948	G1898	C1830		A1660	U1570				
C2392	U2307	C2210	A1949	G1899	G1831		A1661	G1571				
C2393	G2307	G2211	C2058	G1900	A1745		A1662					
C2394	G2314	U2218	G2059	G1901	G1746		A1663					
C2395	A2315	A2219	U2062	U1952	A1747							
C2396	G2316		A2063	G1953	G1748							
C2397			C2064	G1954								



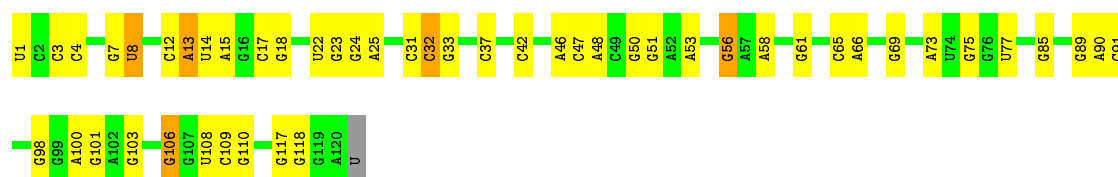
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 68% 31% ..



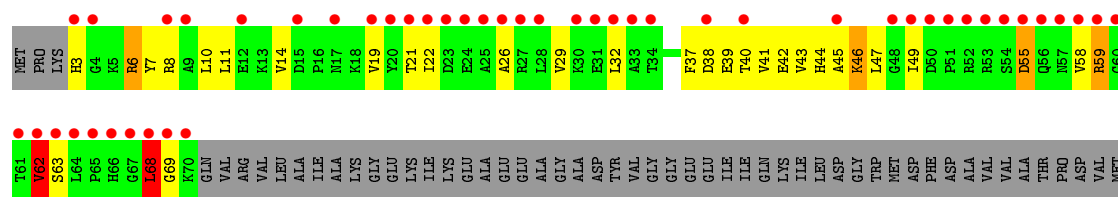
• Molecule 2: 5S Ribosomal RNA

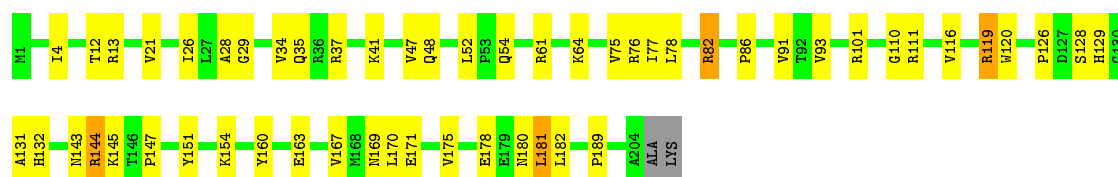
Chain 2B: 59% 36% ..



• Molecule 3: 50S ribosomal protein L1

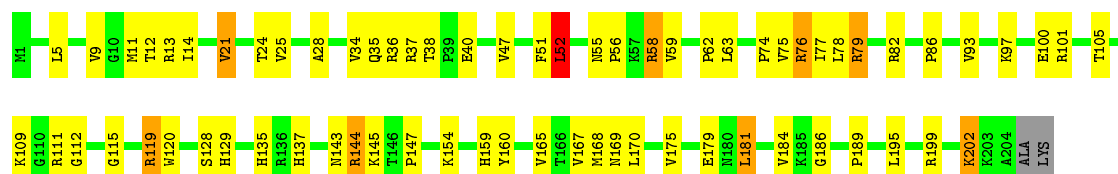
Chain 1C: 45% 29% 24% 5% 41%





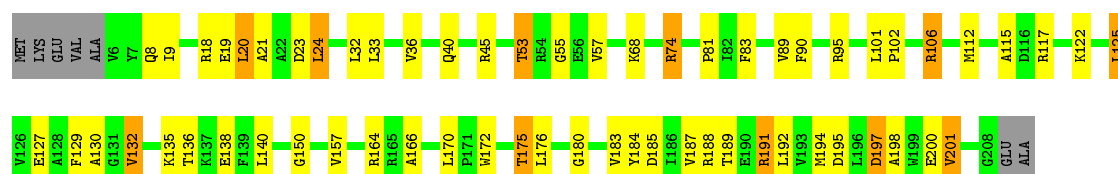
- Molecule 5: 50S ribosomal protein L3

Chain 2E: 66% 29% . .



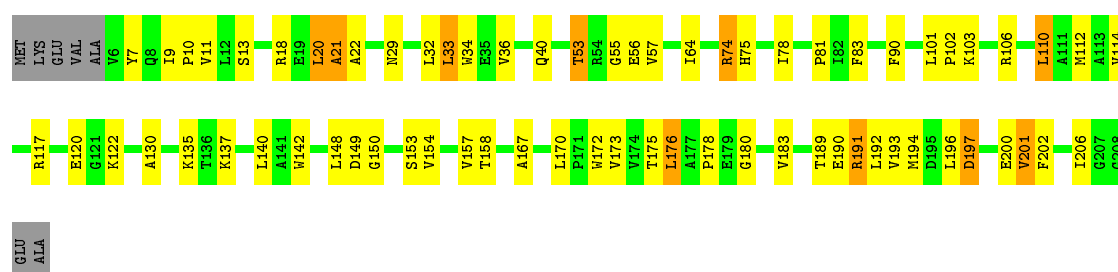
- Molecule 6: 50S ribosomal protein L4

Chain 1F: 67% 24% 5% .



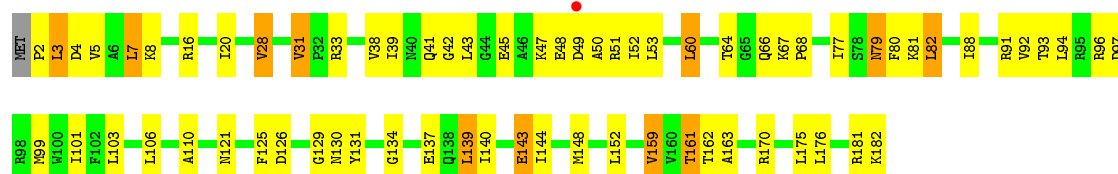
- Molecule 6: 50S ribosomal protein L4

Chain 2F: 64% 28% 5% .

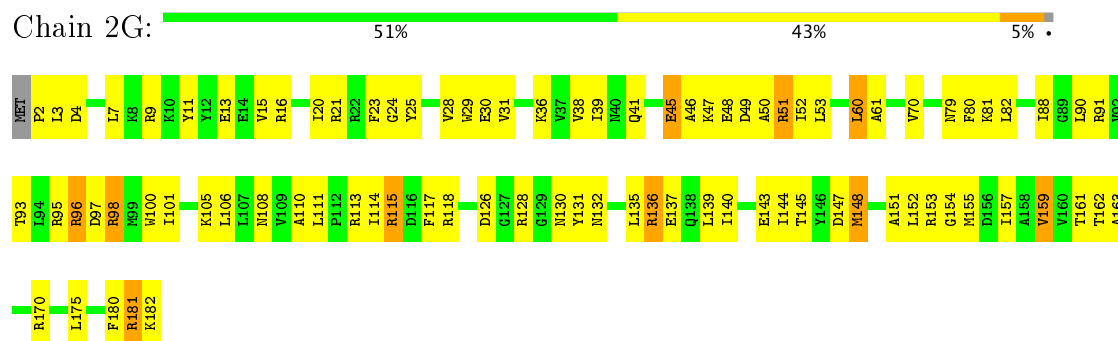


- Molecule 7: 50S ribosomal protein L5

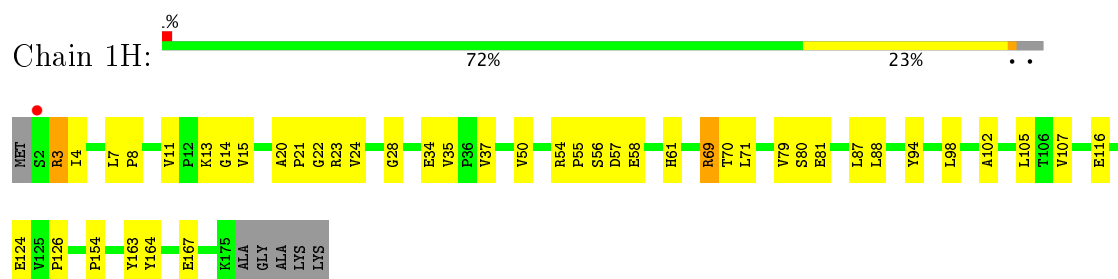
Chain 1G: 62% 32% 6% .



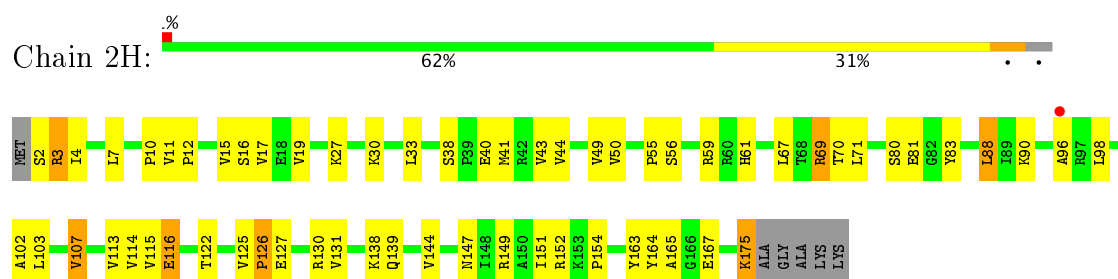
- Molecule 7: 50S ribosomal protein L5



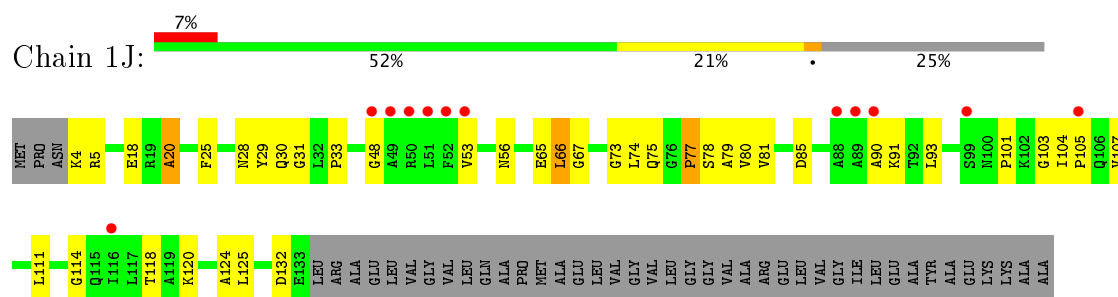
- Molecule 8: 50S ribosomal protein L6



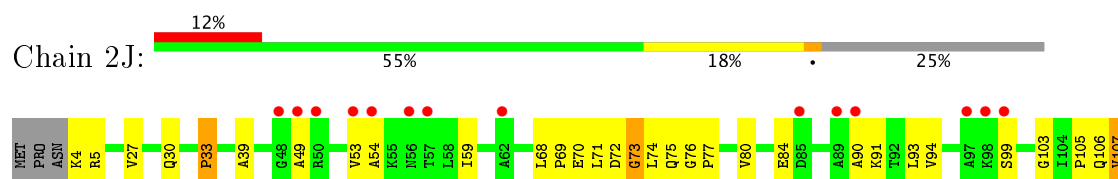
- Molecule 8: 50S ribosomal protein L6

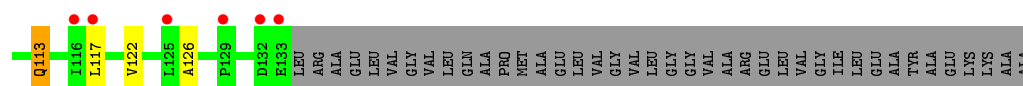


- Molecule 9: 50S ribosomal protein L10

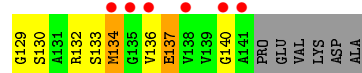
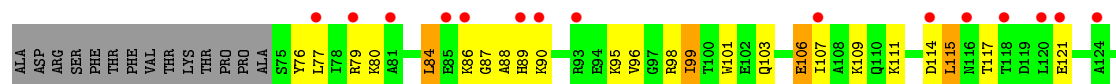


- Molecule 9: 50S ribosomal protein L10

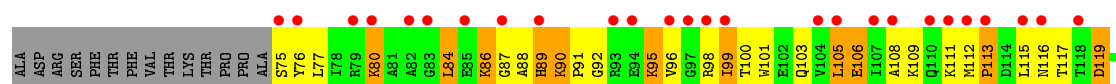
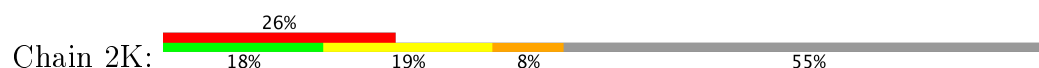




- Molecule 10: 50S ribosomal protein L11



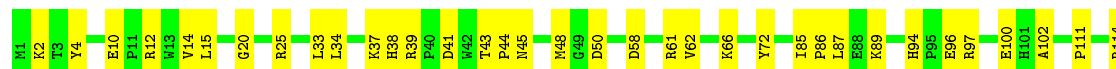
- Molecule 10: 50S ribosomal protein L11



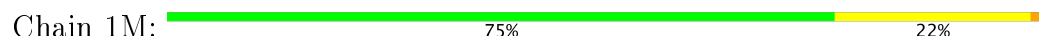
- Molecule 11: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L13

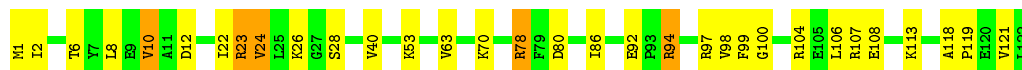
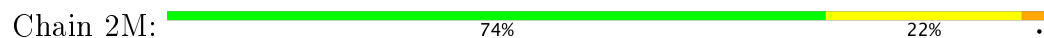


- Molecule 12: 50S ribosomal protein L14

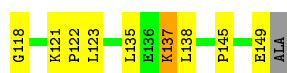
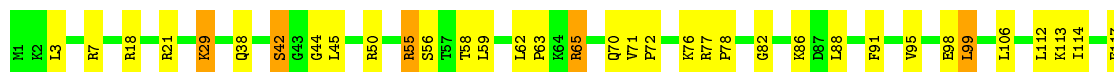




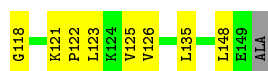
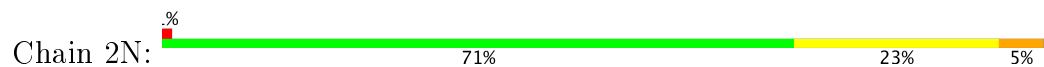
- Molecule 12: 50S ribosomal protein L14



- Molecule 13: 50S ribosomal protein L15



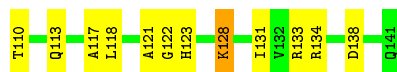
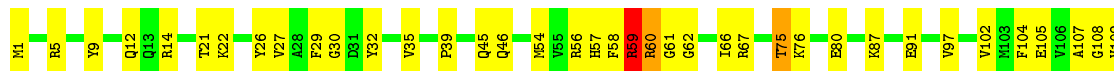
- Molecule 13: 50S ribosomal protein L15



- Molecule 14: 50S ribosomal protein L16

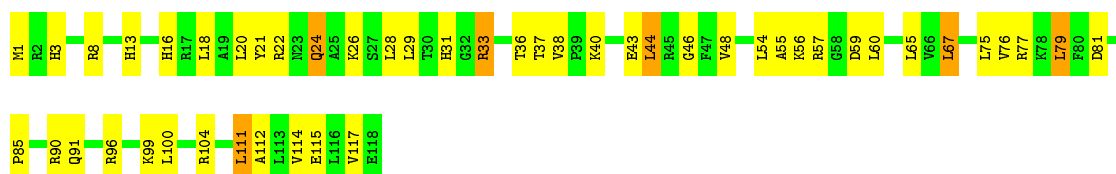


- Molecule 14: 50S ribosomal protein L16



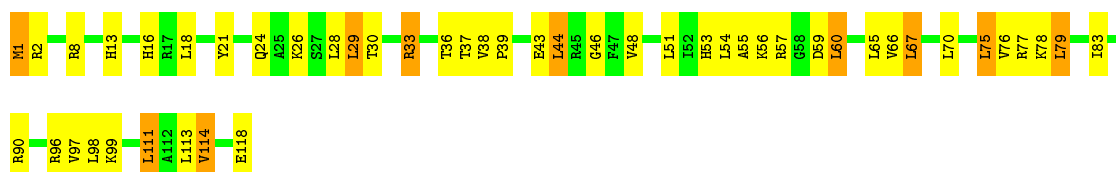
- Molecule 15: 50S ribosomal protein L17





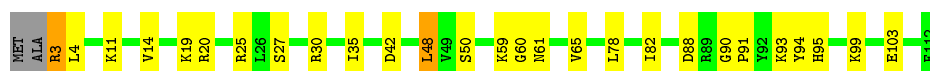
- Molecule 15: 50S ribosomal protein L17

Chain 2P: 59% 32% 8%



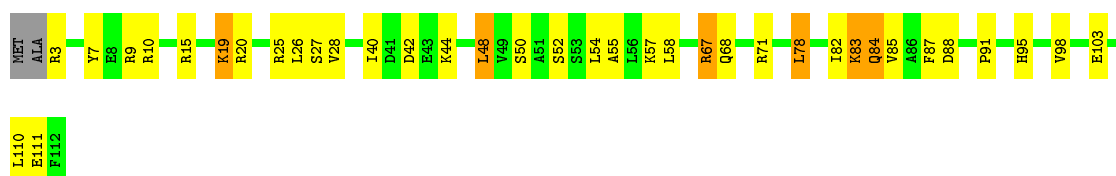
- Molecule 16: 50S ribosomal protein L18

Chain 1Q: 74% 22% ..



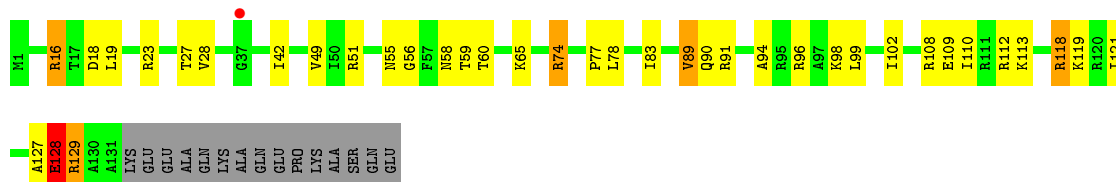
- Molecule 16: 50S ribosomal protein L18

Chain 2Q: 65% 28% 5% ..



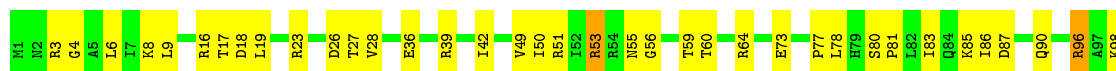
- Molecule 17: 50S ribosomal protein L19

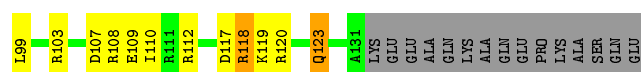
Chain 1R: 64% 22% .. 10%



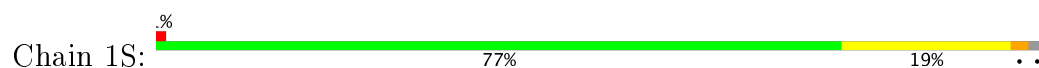
- Molecule 17: 50S ribosomal protein L19

Chain 2R: 56% 31% .. 10%

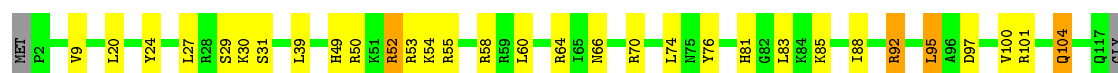




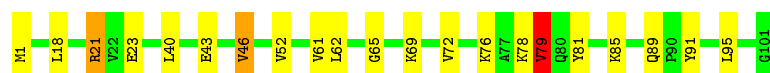
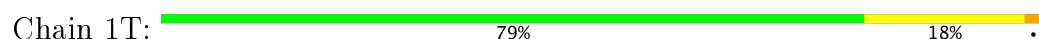
- Molecule 18: 50S ribosomal protein L20



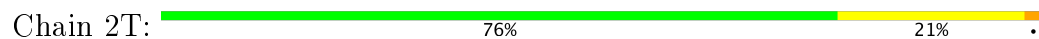
- Molecule 18: 50S ribosomal protein L20



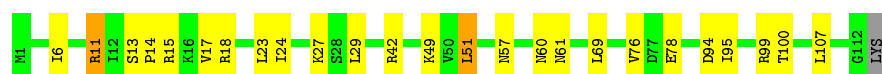
- Molecule 19: 50S ribosomal protein L21



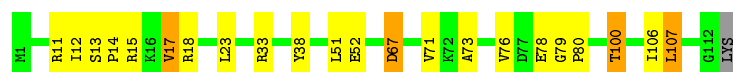
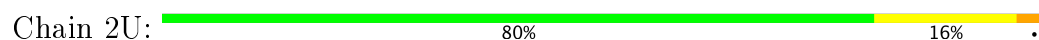
- Molecule 19: 50S ribosomal protein L21



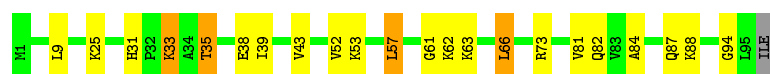
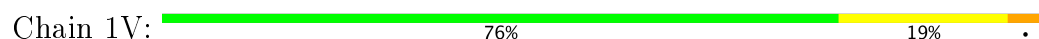
- Molecule 20: 50S ribosomal protein L22



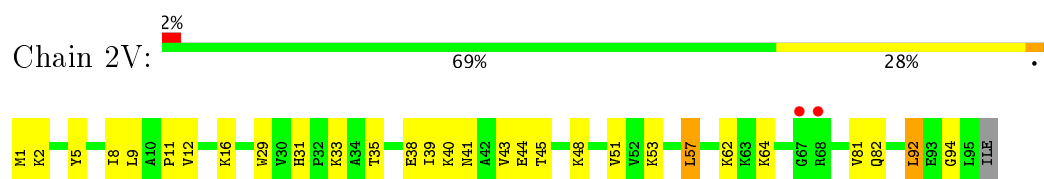
- Molecule 20: 50S ribosomal protein L22



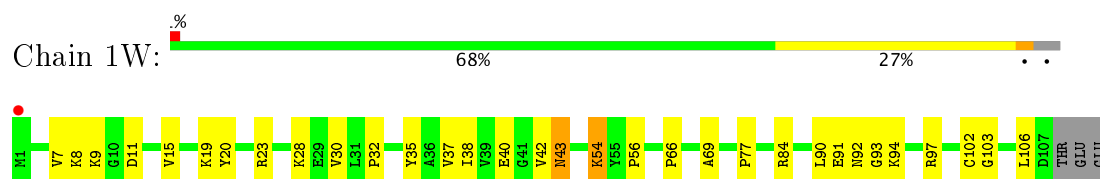
- Molecule 21: 50S ribosomal protein L23



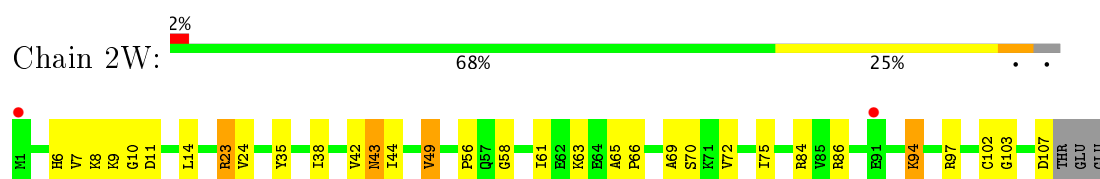
- Molecule 21: 50S ribosomal protein L23



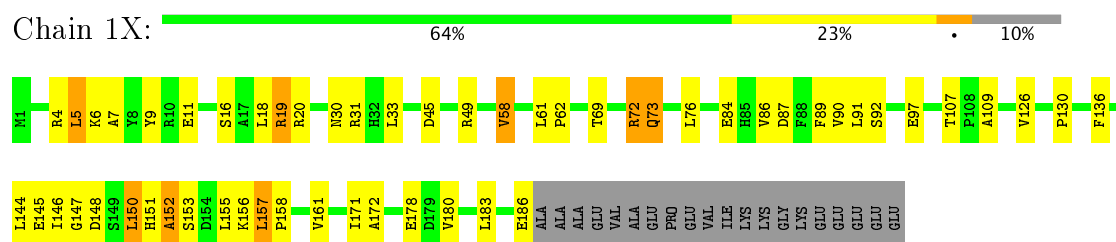
- Molecule 22: 50S ribosomal protein L24



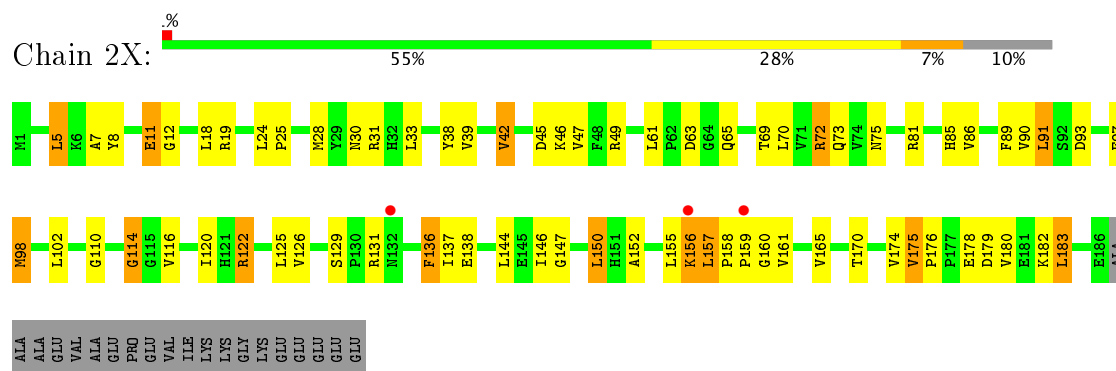
- Molecule 22: 50S ribosomal protein L24



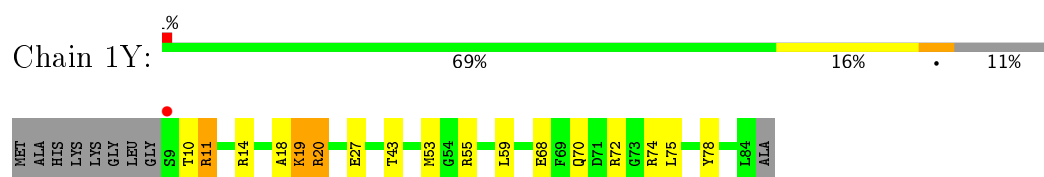
- Molecule 23: 50S ribosomal protein L25



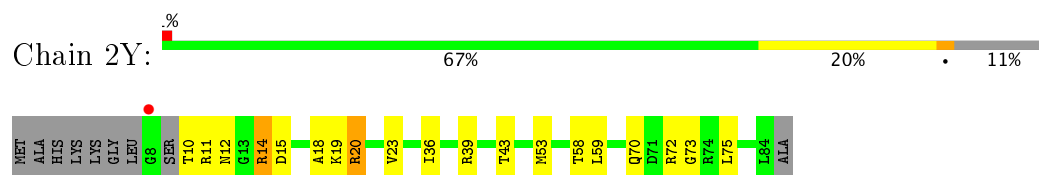
- Molecule 23: 50S ribosomal protein L25



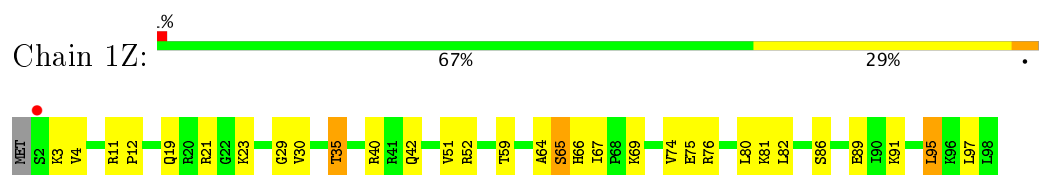
- Molecule 24: 50S ribosomal protein L27



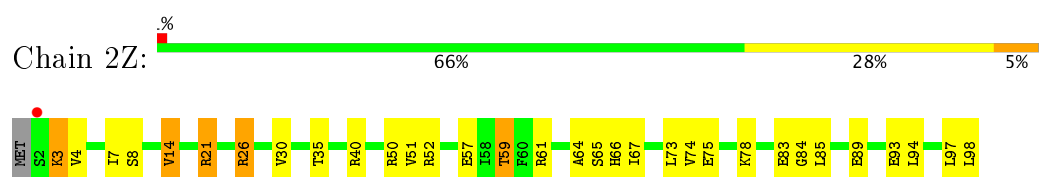
- Molecule 24: 50S ribosomal protein L27



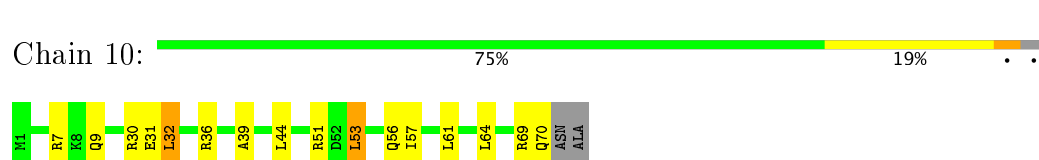
- Molecule 25: 50S ribosomal protein L28



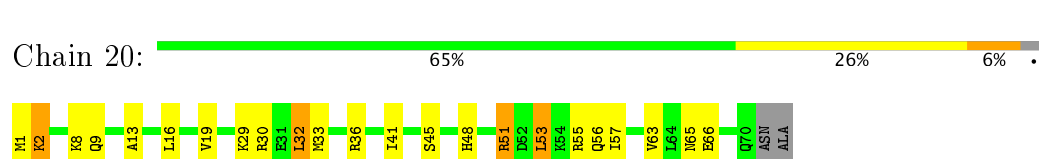
- Molecule 25: 50S ribosomal protein L28



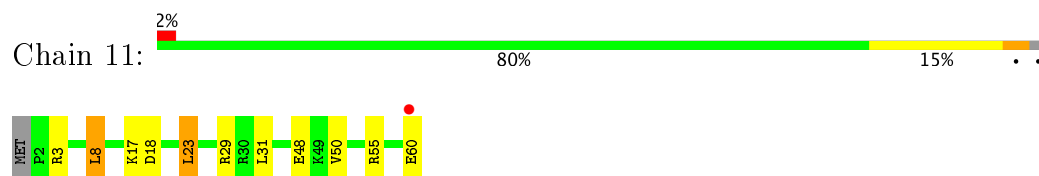
- Molecule 26: 50S ribosomal protein L29



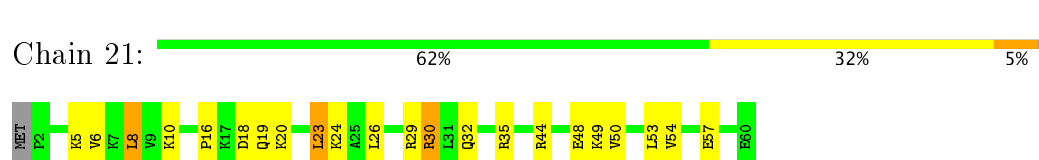
- Molecule 26: 50S ribosomal protein L29



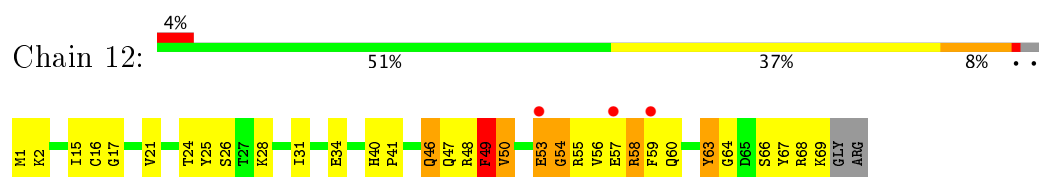
- Molecule 27: 50S ribosomal protein L30



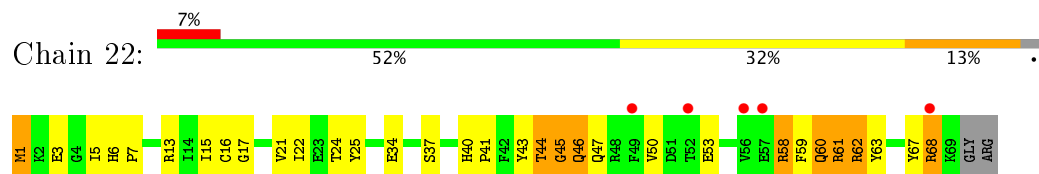
- Molecule 27: 50S ribosomal protein L30



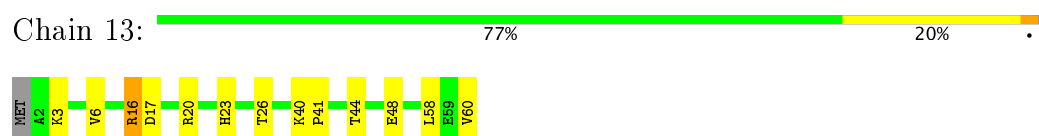
- Molecule 28: 50S ribosomal protein L31



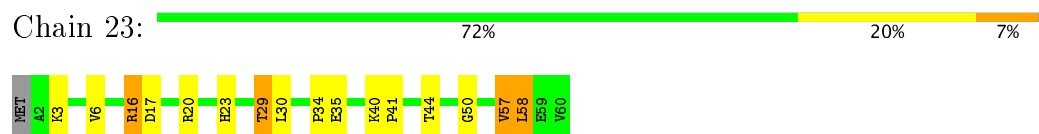
- Molecule 28: 50S ribosomal protein L31



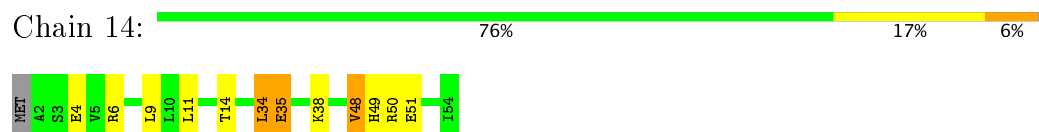
- Molecule 29: 50S ribosomal protein L32



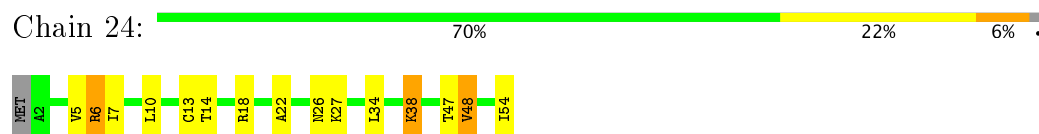
- Molecule 29: 50S ribosomal protein L32



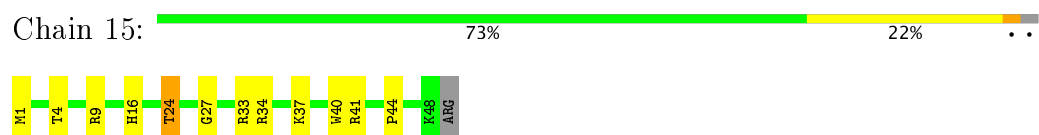
- Molecule 30: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34



- Molecule 31: 50S ribosomal protein L34





- Molecule 32: 50S ribosomal protein L35

Chain 16: 66% 29%



- Molecule 32: 50S ribosomal protein L35

Chain 26: 62% 35%



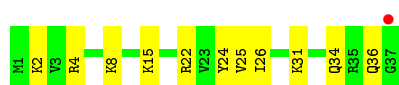
- Molecule 33: 50S ribosomal protein L36

Chain 17: 81% 19%



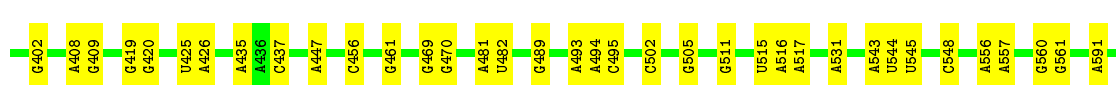
- Molecule 33: 50S ribosomal protein L36

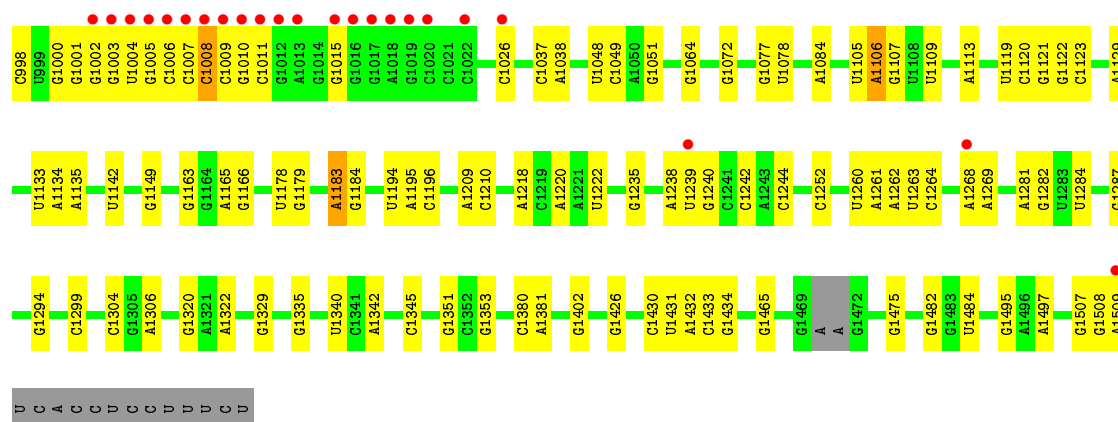
Chain 27: 3% 70% 30%



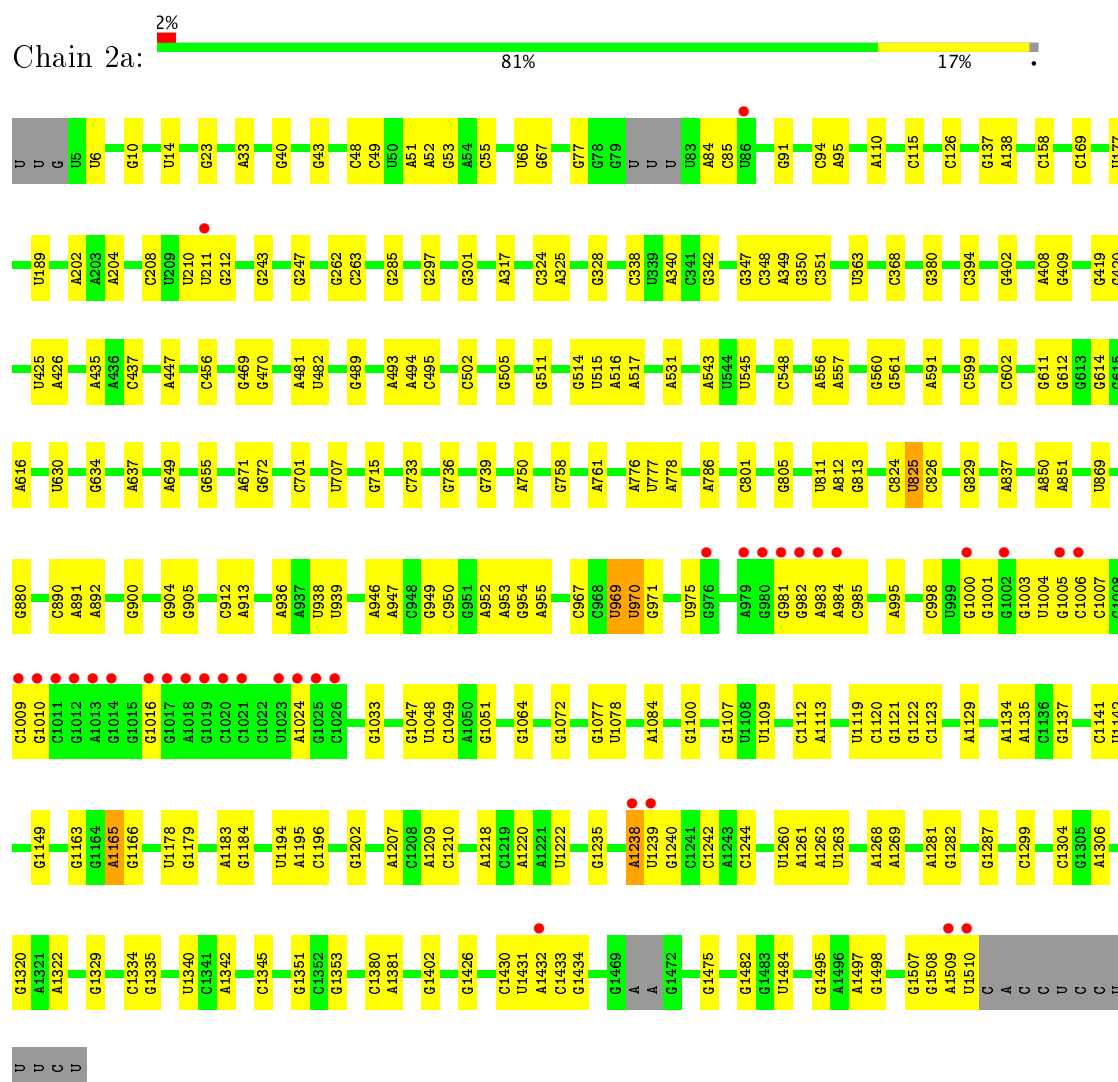
- Molecule 34: 16S Ribosomal RNA

Chain 1a: 2% 80% 18%

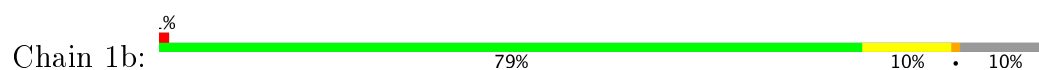


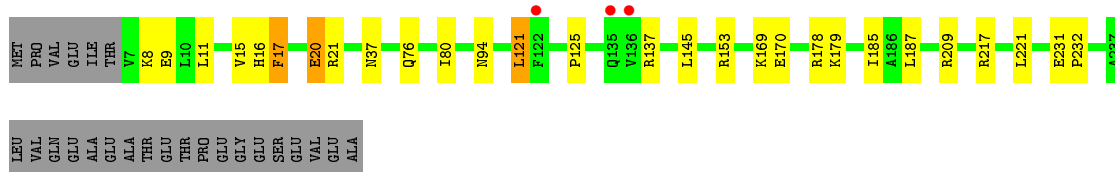


• Molecule 34: 16S Ribosomal RNA

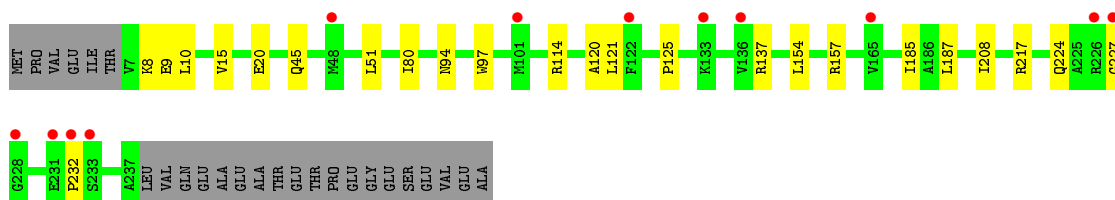
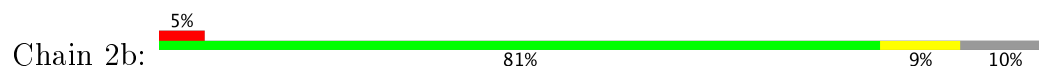


• Molecule 35: 30S ribosomal protein S2

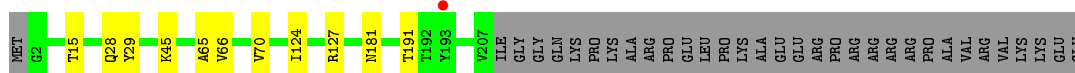
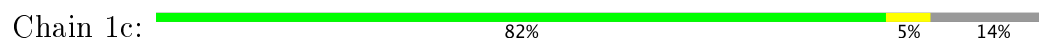




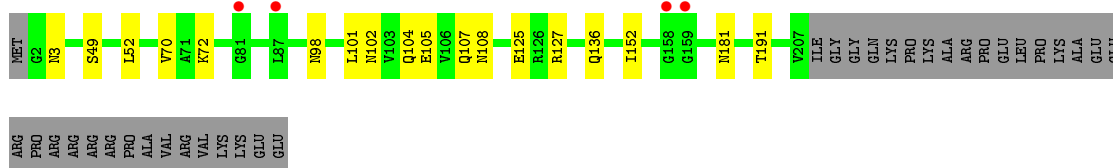
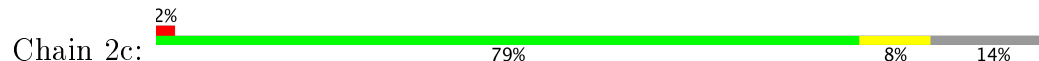
- Molecule 35: 30S ribosomal protein S2



- Molecule 36: 30S ribosomal protein S3



- Molecule 36: 30S ribosomal protein S3



- Molecule 37: 30S ribosomal protein S4



- Molecule 37: 30S ribosomal protein S4



- Molecule 38: 30S ribosomal protein S5





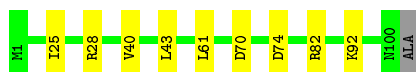
- Molecule 38: 30S ribosomal protein S5

Chain 2e: 86% 6% 9%



- Molecule 39: 30S ribosomal protein S6

Chain 1f: 90% 9% .



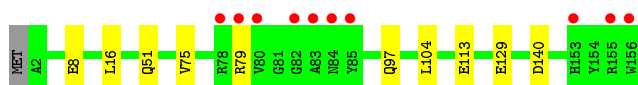
- Molecule 39: 30S ribosomal protein S6

Chain 2f: 92% 7% .



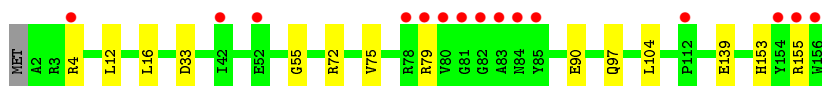
- Molecule 40: 30S ribosomal protein S7

Chain 1g: 6% 93% 6% .



- Molecule 40: 30S ribosomal protein S7

Chain 2g: 10% 90% 9% .



- Molecule 41: 30S ribosomal protein S8

Chain 1h: 88% 11% .



- Molecule 41: 30S ribosomal protein S8

Chain 2h: 86% 13% ..



- Molecule 42: 30S ribosomal protein S9

Chain 1i: 90% 9% ..



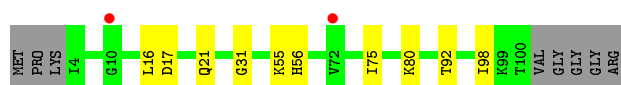
- Molecule 42: 30S ribosomal protein S9

Chain 2i: 5% 87% 13% .



- Molecule 43: 30S ribosomal protein S10

Chain 1j: 2% 83% 10% 8%



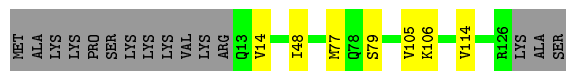
- Molecule 43: 30S ribosomal protein S10

Chain 2j: 10% 87% 5% 9%



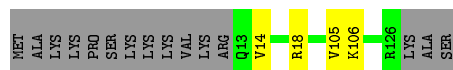
- Molecule 44: 30S ribosomal protein S11

Chain 1k: 83% 5% 12%



- Molecule 44: 30S ribosomal protein S11

Chain 2k: 85% . 12%



- Molecule 45: 30S ribosomal protein S12

Chain 1l: 87% 5% 8%



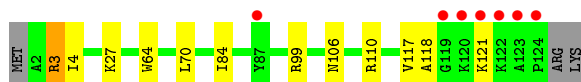
- Molecule 45: 30S ribosomal protein S12

Chain 2l: 86% 7% 8%



- Molecule 46: 30S ribosomal protein S13

Chain 1m: 6% 88% 9% ..



- Molecule 46: 30S ribosomal protein S13

Chain 2m: 7% 88% 9% .



- Molecule 47: 30S ribosomal protein S14 type Z

Chain 1n: 2% 87% 11% .



- Molecule 47: 30S ribosomal protein S14 type Z

Chain 2n: 3% 87% 11% .



- Molecule 48: 30S ribosomal protein S15

Chain 1o: 91% 8% .

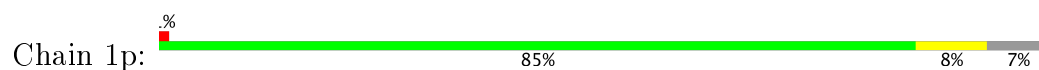


- Molecule 48: 30S ribosomal protein S15

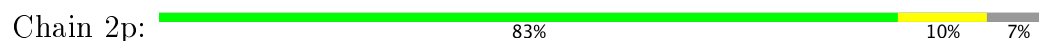
Chain 2o: 88% 11% .



- Molecule 49: 30S ribosomal protein S16



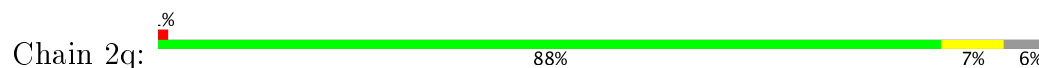
- Molecule 49: 30S ribosomal protein S16



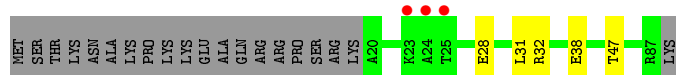
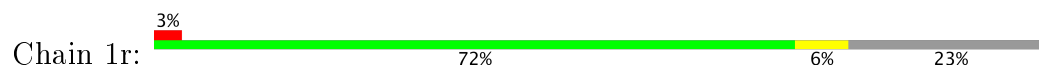
- Molecule 50: 30S ribosomal protein S17



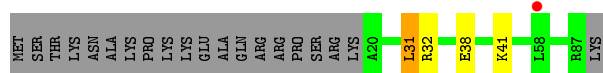
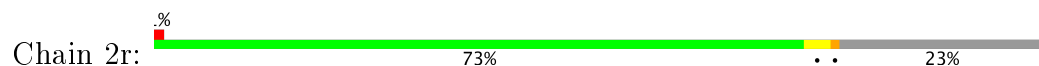
- Molecule 50: 30S ribosomal protein S17



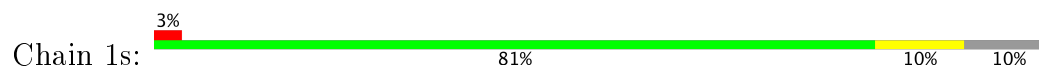
- Molecule 51: 30S ribosomal protein S18

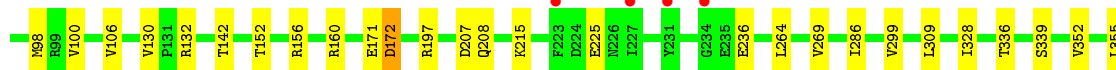


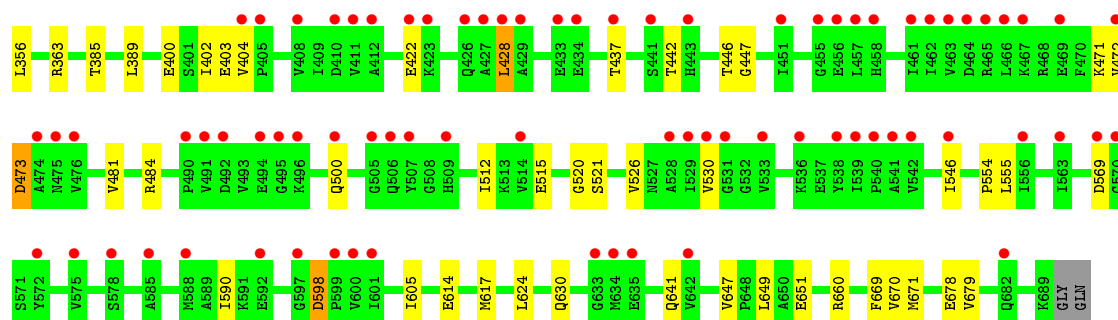
- Molecule 51: 30S ribosomal protein S18



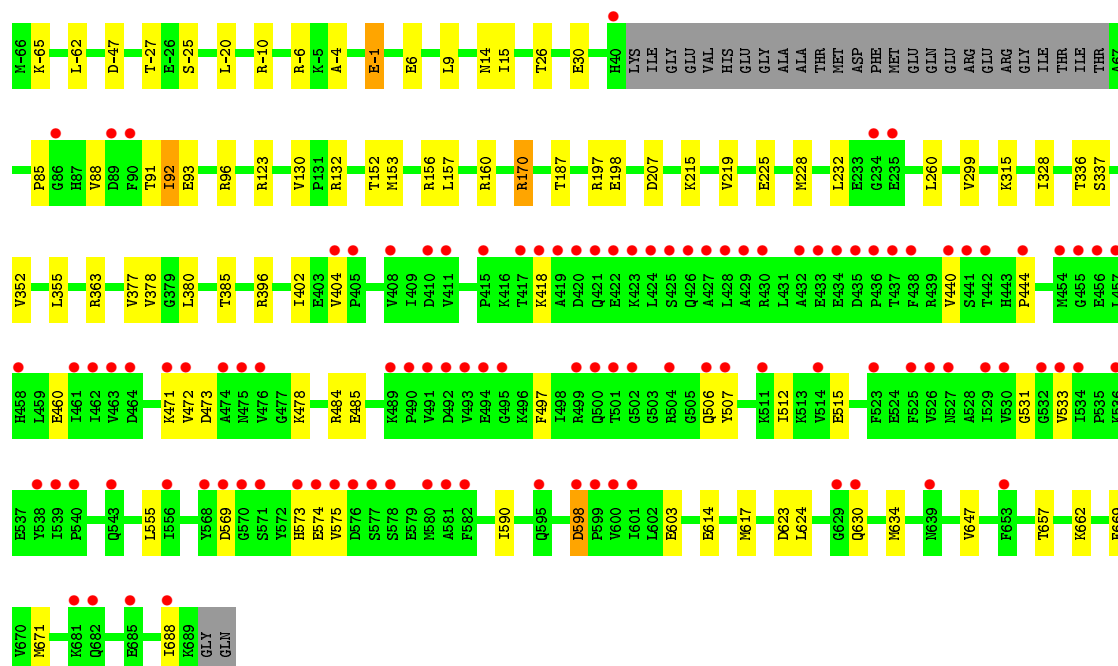
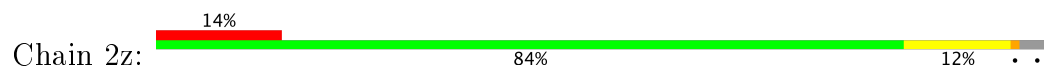
- Molecule 52: 30S ribosomal protein S19







- Molecule 55: Chimera protein of 50S ribosomal protein L9 and Elongation factor G



- Molecule 56: mRNA



- Molecule 56: mRNA

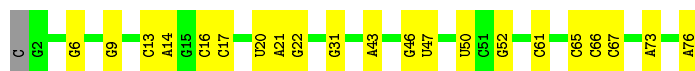


- Molecule 57: P-site tRNA

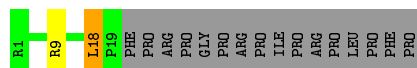




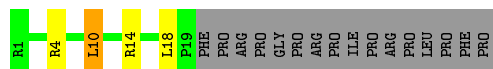
- Molecule 57: P-site tRNA



- Molecule 58: Cathelicidin-3



- Molecule 58: Cathelicidin-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.78Å 449.03Å 619.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 3.00 49.48 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.48-3.00) 99.1 (49.48-3.00)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.265 0.212 , 0.266	Depositor DCC
R_{free} test set	57160 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	306384	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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	4/69281 (0.0%)	0.95	75/108144 (0.1%)
1	2A	0.45	2/69179 (0.0%)	0.92	59/107984 (0.1%)
2	1B	0.47	0/2878	0.93	0/4490
2	2B	0.43	0/2878	0.92	1/4490 (0.0%)
3	1C	0.48	0/1038	0.70	2/1403 (0.1%)
3	2C	0.45	0/1038	0.68	1/1403 (0.1%)
4	1D	0.42	0/2186	0.57	0/2944
4	2D	0.36	0/2192	0.57	0/2951
5	1E	0.42	0/1592	0.56	0/2149
5	2E	0.35	0/1592	0.55	0/2149
6	1F	0.38	0/1619	0.54	0/2193
6	2F	0.34	0/1615	0.55	0/2188
7	1G	0.31	0/1450	0.53	0/1959
7	2G	0.32	0/1449	0.56	0/1958
8	1H	0.34	0/1356	0.53	0/1834
8	2H	0.33	0/1356	0.56	0/1834
9	1J	0.28	0/640	0.59	0/889
9	2J	0.29	0/640	0.55	1/889 (0.1%)
10	1K	0.35	0/504	0.58	0/675
10	2K	0.46	0/503	0.66	0/673
11	1L	0.38	0/1144	0.53	0/1543
11	2L	0.31	0/1144	0.53	0/1543
12	1M	0.40	0/943	0.57	0/1269
12	2M	0.37	0/943	0.54	0/1269
13	1N	0.37	0/1156	0.57	0/1537
13	2N	0.34	0/1152	0.57	0/1533
14	1O	0.41	0/1143	0.52	0/1527
14	2O	0.35	0/1143	0.54	0/1527
15	1P	0.38	0/982	0.59	0/1312
15	2P	0.33	0/982	0.55	0/1312
16	1Q	0.35	0/887	0.57	0/1180
16	2Q	0.33	0/880	0.58	1/1172 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	1R	0.37	0/1105	0.53	0/1477
17	2R	0.33	0/1097	0.54	0/1468
18	1S	0.42	0/977	0.55	0/1301
18	2S	0.32	0/977	0.48	0/1301
19	1T	0.38	0/782	0.54	0/1049
19	2T	0.32	0/782	0.53	0/1049
20	1U	0.39	0/897	0.53	0/1205
20	2U	0.35	0/897	0.52	0/1205
21	1V	0.38	0/764	0.58	1/1025 (0.1%)
21	2V	0.33	0/764	0.55	1/1025 (0.1%)
22	1W	0.39	0/819	0.58	0/1095
22	2W	0.34	0/819	0.56	0/1095
23	1X	0.34	0/1492	0.55	0/2029
23	2X	0.34	0/1486	0.57	0/2022
24	1Y	0.38	0/612	0.57	0/816
24	2Y	0.33	0/609	0.51	0/810
25	1Z	0.37	0/762	0.51	0/1014
25	2Z	0.33	0/762	0.53	0/1014
26	10	0.33	0/590	0.54	0/781
26	20	0.33	0/590	0.51	0/781
27	11	0.41	0/474	0.54	0/635
27	21	0.33	0/469	0.56	0/630
28	12	0.34	0/571	0.64	0/768
28	22	0.37	0/545	0.58	0/737
29	13	0.42	0/469	0.58	0/635
29	23	0.36	0/469	0.53	0/635
30	14	0.46	0/460	0.52	0/613
30	24	0.41	0/456	0.52	0/608
31	15	0.38	0/426	0.54	0/561
31	25	0.34	0/426	0.58	0/561
32	16	0.40	0/525	0.58	0/691
32	26	0.33	0/525	0.52	0/691
33	17	0.43	0/310	0.54	0/407
33	27	0.33	0/310	0.48	0/407
34	1a	0.40	0/35976	0.89	14/56145 (0.0%)
34	2a	0.39	0/36119	0.89	18/56370 (0.0%)
35	1b	0.33	0/1881	0.59	0/2542
35	2b	0.34	0/1860	0.56	0/2518
36	1c	0.29	0/1576	0.50	0/2130
36	2c	0.33	0/1568	0.53	0/2122
37	1d	0.31	0/1689	0.52	0/2267
37	2d	0.30	0/1708	0.54	1/2289 (0.0%)
38	1e	0.32	0/1145	0.52	0/1543

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	2e	0.31	0/1149	0.56	0/1548
39	1f	0.32	0/825	0.53	0/1118
39	2f	0.32	0/833	0.49	0/1128
40	1g	0.29	0/1250	0.48	0/1679
40	2g	0.31	0/1254	0.52	0/1683
41	1h	0.30	0/1108	0.52	0/1494
41	2h	0.29	0/1108	0.55	1/1494 (0.1%)
42	1i	0.30	0/1005	0.51	0/1350
42	2i	0.33	0/997	0.55	0/1343
43	1j	0.29	0/722	0.59	0/982
43	2j	0.33	0/727	0.52	0/988
44	1k	0.33	0/848	0.52	0/1149
44	2k	0.29	0/848	0.52	0/1149
45	1l	0.32	0/946	0.50	0/1274
45	2l	0.33	0/946	0.58	0/1274
46	1m	0.30	0/977	0.55	0/1310
46	2m	0.30	0/961	0.54	0/1291
47	1n	0.31	0/501	0.56	0/664
47	2n	0.31	0/501	0.55	0/664
48	1o	0.32	0/739	0.53	0/985
48	2o	0.31	0/739	0.52	0/985
49	1p	0.30	0/697	0.51	0/939
49	2p	0.30	0/693	0.50	0/935
50	1q	0.33	0/836	0.50	0/1117
50	2q	0.31	0/836	0.50	0/1117
51	1r	0.29	0/560	0.55	1/746 (0.1%)
51	2r	0.31	0/560	0.55	1/746 (0.1%)
52	1s	0.29	0/676	0.53	0/911
52	2s	0.32	0/661	0.60	0/893
53	1t	0.31	0/730	0.54	0/965
53	2t	0.28	0/733	0.49	0/969
54	1u	0.29	0/203	0.54	0/266
54	2u	0.30	0/203	0.48	0/266
55	1z	0.35	0/5792	0.59	1/7844 (0.0%)
55	2z	0.36	0/5792	0.58	0/7844
56	1y	0.47	0/144	0.96	0/222
56	2y	0.59	0/122	1.17	0/188
57	1w	0.57	2/1725 (0.1%)	1.15	22/2689 (0.8%)
57	2w	0.53	0/1725	1.17	20/2689 (0.7%)
58	1x	0.40	0/175	0.68	0/238
58	2x	0.38	0/175	0.98	1/238 (0.4%)
All	All	0.44	8/327047 (0.0%)	0.83	222/487364 (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
28	12	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1187	A	N9-C4	-10.39	1.31	1.37
1	1A	1066	A	N9-C4	-6.00	1.34	1.37
57	1w	22	G	N7-C5	5.90	1.42	1.39
1	1A	353	A	N9-C4	-5.88	1.34	1.37
57	1w	46	G	C6-N1	5.85	1.43	1.39
1	2A	552	A	N9-C4	-5.83	1.34	1.37
1	1A	552	A	N9-C4	-5.61	1.34	1.37
1	2A	1187	A	N9-C4	-5.33	1.34	1.37

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1w	46	G	C6-N1-C2	-11.71	118.07	125.10
57	2w	46	G	C6-N1-C2	-10.97	118.52	125.10
1	1A	1149	C	OP1-P-O3'	-10.93	81.15	105.20
57	1w	22	G	C5-N7-C8	-10.78	98.91	104.30
57	2w	22	G	C5-N7-C8	-10.15	99.22	104.30
1	1A	1066	A	C2-N3-C4	-9.37	105.92	110.60
1	1A	1187	A	C2-N3-C4	-9.16	106.02	110.60
1	1A	1149	C	OP2-P-O3'	-9.00	85.40	105.20
1	1A	2161	C	N1-C2-O2	8.95	124.27	118.90
1	1A	353	A	C2-N3-C4	-8.94	106.13	110.60
1	1A	552	A	C2-N3-C4	-8.91	106.14	110.60
1	2A	552	A	C2-N3-C4	-8.88	106.16	110.60
1	1A	2161	C	N3-C2-O2	-8.67	115.83	121.90
57	2w	14	A	C5-N7-C8	8.64	108.22	103.90
1	1A	1187	A	N3-C4-C5	8.49	132.74	126.80
57	2w	46	G	N3-C2-N2	-8.34	114.06	119.90
1	2A	2164	C	C2-N3-C4	8.33	124.07	119.90
1	1A	2161	C	C2-N1-C1'	8.27	127.90	118.80
1	1A	847	G	O5'-P-OP2	-8.17	98.34	105.70
57	1w	22	G	N7-C8-N9	8.07	117.14	113.10
1	1A	1066	A	N1-C2-N3	8.05	133.32	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	989	A	N1-C6-N6	8.00	123.40	118.60
34	2a	825	U	C5-C6-N1	7.96	126.68	122.70
34	2a	1238	A	N1-C6-N6	7.92	123.35	118.60
57	2w	14	A	C4-C5-C6	7.90	120.95	117.00
1	1A	989	A	N1-C6-N6	7.89	123.34	118.60
57	2w	46	G	N9-C4-C5	7.86	108.55	105.40
1	1A	1153	U	C5-C6-N1	7.80	126.60	122.70
1	1A	138	A	N7-C8-N9	7.79	117.69	113.80
57	1w	46	G	C5-C6-N1	7.76	115.38	111.50
57	2w	22	G	N7-C8-N9	7.75	116.97	113.10
1	2A	11	U	C2-N1-C1'	7.62	126.85	117.70
57	1w	22	G	C4-C5-C6	-7.59	114.25	118.80
1	2A	2124	C	C2-N3-C4	7.58	123.69	119.90
1	2A	11	U	N1-C2-O2	7.52	128.07	122.80
1	1A	1310	A	O5'-P-OP2	-7.51	98.94	105.70
1	1A	2161	C	C6-N1-C2	-7.50	117.30	120.30
1	2A	2188	U	N3-C2-O2	-7.46	116.98	122.20
1	1A	1694	C	O5'-P-OP1	-7.33	99.10	105.70
57	1w	46	G	C5-C6-O6	-7.30	124.22	128.60
1	1A	1187	A	N3-C4-N9	-7.29	121.56	127.40
1	1A	2609	A	O5'-P-OP1	-7.25	99.17	105.70
3	2C	209	LEU	CA-CB-CG	7.19	131.84	115.30
1	2A	2188	U	N1-C2-O2	7.15	127.81	122.80
34	2a	1137	G	C5-C6-O6	7.13	132.88	128.60
1	2A	11	U	N3-C2-O2	-7.11	117.22	122.20
55	1z	428	LEU	CA-CB-CG	6.97	131.33	115.30
57	1w	22	G	N1-C6-O6	-6.93	115.74	119.90
1	2A	2157	C	N1-C2-O2	6.89	123.03	118.90
34	2a	1238	A	N9-C4-C5	-6.88	103.05	105.80
1	1A	1358	U	C2-N1-C1'	6.87	125.95	117.70
57	1w	14	A	C4-C5-C6	6.87	120.44	117.00
1	1A	536	G	O4'-C1'-N9	6.86	113.69	108.20
34	1a	1011	C	C2-N1-C1'	6.82	126.31	118.80
1	1A	138	A	C8-N9-C4	-6.81	103.08	105.80
1	2A	989	A	C4-C5-N7	6.80	114.10	110.70
57	1w	14	A	C5-N7-C8	6.79	107.29	103.90
1	1A	1538	C	N1-C2-O2	6.78	122.97	118.90
34	1a	975	U	C5-C4-O4	6.78	129.97	125.90
1	2A	138	A	C8-N9-C4	-6.77	103.09	105.80
1	1A	989	A	C6-C5-N7	-6.72	127.60	132.30
57	2w	46	G	C4-C5-N7	-6.70	108.12	110.80
1	1A	1111	U	N3-C2-O2	-6.69	117.52	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1359	C	C2-N1-C1'	6.69	126.16	118.80
1	2A	989	A	O4'-C1'-N9	6.65	113.52	108.20
1	2A	2197	A	N1-C6-N6	-6.65	114.61	118.60
1	1A	1150	U	OP1-P-OP2	6.61	129.51	119.60
1	2A	1187	A	C2-N3-C4	-6.57	107.31	110.60
1	1A	1111	U	N1-C2-O2	6.54	127.38	122.80
57	2w	22	G	C4-C5-C6	-6.51	114.89	118.80
1	1A	1067	G	N3-C4-N9	-6.51	122.09	126.00
1	2A	2188	U	C2-N1-C1'	6.50	125.50	117.70
34	1a	1133	U	C2-N3-C4	6.48	130.89	127.00
34	2a	1238	A	C5-C6-N6	-6.47	118.53	123.70
1	2A	2197	A	C5-C6-N6	6.43	128.85	123.70
1	2A	138	A	N7-C8-N9	6.40	117.00	113.80
1	2A	989	A	C5-N7-C8	-6.33	100.73	103.90
34	2a	1141	C	C2-N1-C1'	6.32	125.75	118.80
34	1a	1106	A	C6-N1-C2	6.24	122.35	118.60
1	2A	989	A	C6-C5-N7	-6.24	127.93	132.30
57	2w	22	G	C4-C5-N7	6.24	113.30	110.80
57	2w	22	G	C5-C6-N1	6.23	114.62	111.50
1	1A	138	A	C5-N7-C8	-6.18	100.81	103.90
34	1a	1011	C	C6-N1-C2	-6.12	117.85	120.30
34	2a	983	A	O4'-C1'-N9	6.11	113.09	108.20
16	2Q	78	LEU	CA-CB-CG	6.10	129.34	115.30
1	2A	2512	C	C2-N1-C1'	-6.09	112.10	118.80
1	1A	2013	G	P-O3'-C3'	6.09	127.01	119.70
1	2A	138	A	O4'-C1'-N9	6.08	113.07	108.20
57	2w	46	G	C5-C6-N1	6.08	114.54	111.50
1	1A	1066	A	C5-N7-C8	-6.07	100.86	103.90
1	2A	2164	C	C5-C6-N1	6.05	124.03	121.00
1	1A	2700	U	N3-C2-O2	-6.03	117.98	122.20
57	2w	46	G	N1-C2-N3	6.02	127.51	123.90
1	2A	2485	C	C2-N1-C1'	6.02	125.42	118.80
1	1A	1066	A	N7-C8-N9	5.99	116.80	113.80
3	1C	62	VAL	CB-CA-C	5.97	122.75	111.40
1	1A	1538	C	N3-C2-O2	-5.97	117.72	121.90
1	1A	11	U	C2-N1-C1'	5.95	124.84	117.70
57	1w	22	G	N3-C4-N9	-5.93	122.44	126.00
1	1A	1153	U	C2-N1-C1'	5.91	124.80	117.70
1	1A	989	A	N9-C4-C5	-5.90	103.44	105.80
1	1A	2696	G	N1-C6-O6	-5.90	116.36	119.90
34	2a	66	U	P-O3'-C3'	5.90	126.78	119.70
34	2a	1238	A	O4'-C1'-N9	-5.90	103.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1248	A	O4'-C1'-N9	5.89	112.92	108.20
57	1w	22	G	C5-C6-N1	5.87	114.44	111.50
1	1A	977	A	C5-N7-C8	-5.86	100.97	103.90
1	2A	2169	G	C6-N1-C2	5.83	128.59	125.10
34	1a	1015	G	C5-C6-O6	5.82	132.09	128.60
1	1A	214	G	O4'-C1'-N9	5.81	112.85	108.20
34	1a	1026	C	C2-N1-C1'	5.78	125.16	118.80
1	2A	552	A	N1-C2-N3	5.78	132.19	129.30
34	1a	981	G	N3-C4-N9	5.76	129.46	126.00
57	2w	14	A	C5-C6-N1	-5.76	114.82	117.70
1	1A	2297	A	N7-C8-N9	5.73	116.66	113.80
34	2a	1141	C	N1-C2-O2	5.72	122.33	118.90
57	1w	22	G	C4-C5-N7	5.71	113.08	110.80
2	2B	1	U	C2-N1-C1'	5.71	124.55	117.70
34	2a	891	A	P-O3'-C3'	5.69	126.53	119.70
21	1V	57	LEU	CA-CB-CG	5.67	128.33	115.30
1	1A	2057	C	O5'-P-OP1	-5.64	100.62	105.70
1	1A	552	A	N3-C4-N9	-5.64	122.89	127.40
1	1A	1439	U	O5'-P-OP1	-5.62	100.64	105.70
57	2w	22	G	C8-N9-C1'	5.61	134.30	127.00
1	2A	300	C	C2-N1-C1'	5.61	124.97	118.80
1	2A	989	A	N9-C4-C5	-5.60	103.56	105.80
1	1A	598	U	O5'-P-OP1	-5.59	100.67	105.70
1	1A	989	A	C2-N3-C4	-5.59	107.80	110.60
1	1A	1404	A	N1-C2-N3	-5.59	126.50	129.30
58	2x	10	LEU	CA-CB-CG	5.59	128.15	115.30
1	1A	989	A	C4-C5-N7	5.57	113.48	110.70
1	1A	1066	A	C8-N9-C4	-5.57	103.57	105.80
9	2J	76	GLY	C-N-CA	5.57	145.37	122.00
1	2A	2485	C	N1-C2-O2	5.55	122.23	118.90
1	1A	2402	G	O4'-C1'-N9	5.54	112.64	108.20
34	2a	1047	G	P-O3'-C3'	5.54	126.35	119.70
1	2A	1358	U	C2-N1-C1'	5.54	124.35	117.70
1	1A	2512	C	C2-N1-C1'	-5.53	112.72	118.80
34	2a	514	G	C4-N9-C1'	5.52	133.67	126.50
1	1A	1219	U	P-O3'-C3'	5.49	126.29	119.70
1	1A	2263	G	N3-C4-N9	-5.49	122.70	126.00
1	2A	2450	A	O4'-C1'-N9	-5.48	103.82	108.20
1	1A	1067	G	N9-C4-C5	5.46	107.58	105.40
57	1w	46	G	N1-C2-N3	5.46	127.17	123.90
1	2A	552	A	N3-C4-C5	5.46	130.62	126.80
1	2A	1604	A	P-O3'-C3'	5.46	126.25	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1w	46	G	N3-C2-N2	-5.45	116.08	119.90
1	1A	2203	G	C5-C6-O6	5.44	131.87	128.60
1	1A	1417	U	C5-C4-O4	-5.44	122.64	125.90
1	1A	353	A	N1-C2-N3	5.43	132.02	129.30
1	1A	1440	A	O4'-C1'-N9	5.43	112.55	108.20
57	1w	14	A	C5-C6-N1	-5.43	114.99	117.70
1	2A	2204	C	C2-N3-C4	5.42	122.61	119.90
37	2d	194	LEU	CA-CB-CG	5.41	127.74	115.30
1	2A	2485	C	C6-N1-C1'	-5.40	114.32	120.80
34	2a	970	U	P-O3'-C3'	5.40	126.18	119.70
21	2V	57	LEU	CA-CB-CG	5.40	127.71	115.30
1	2A	942	C	N1-C2-O2	5.39	122.13	118.90
34	1a	732	C	P-O3'-C3'	5.38	126.16	119.70
34	1a	1008	C	C5-C4-N4	5.37	123.96	120.20
57	1w	14	A	C4-C5-N7	-5.36	108.02	110.70
57	1w	46	G	N9-C4-C5	5.36	107.55	105.40
1	1A	1067	G	N3-C2-N2	-5.36	116.15	119.90
57	2w	22	G	C8-N9-C4	-5.36	104.26	106.40
1	2A	2700	U	P-O3'-C3'	5.35	126.12	119.70
34	2a	969	U	P-O3'-C3'	5.35	126.12	119.70
41	2h	107	LEU	CA-CB-CG	5.35	127.61	115.30
1	2A	1066	A	C2-N3-C4	-5.34	107.93	110.60
1	2A	1659	A	O5'-P-OP1	-5.32	100.91	105.70
1	1A	2297	A	C5-N7-C8	-5.32	101.24	103.90
57	2w	14	A	C4-C5-N7	-5.32	108.04	110.70
1	1A	1461	G	O4'-C1'-N9	5.30	112.44	108.20
1	2A	2082	G	O5'-P-OP2	-5.29	100.94	105.70
57	2w	14	A	C4-N9-C1'	5.29	135.81	126.30
1	2A	11	U	C6-N1-C1'	-5.28	113.81	121.20
1	1A	989	A	C5-C6-N6	-5.27	119.49	123.70
34	1a	262	G	P-O3'-C3'	5.26	126.01	119.70
34	2a	1334	C	N1-C2-O2	-5.26	115.75	118.90
1	2A	1958	A	O4'-C1'-N9	5.25	112.40	108.20
1	2A	977	A	C5-N7-C8	-5.25	101.28	103.90
34	1a	1183	A	P-O3'-C3'	5.25	126.00	119.70
57	2w	14	A	C8-N9-C1'	-5.25	118.25	127.70
1	2A	2149	C	N1-C2-O2	5.24	122.05	118.90
57	1w	14	A	C4-N9-C1'	5.24	135.73	126.30
57	1w	22	G	C8-N9-C1'	5.24	133.81	127.00
1	2A	2080	A	O4'-C1'-N9	5.24	112.39	108.20
1	1A	2208	G	C5-C6-O6	5.23	131.74	128.60
1	2A	1145	C	C2-N1-C1'	5.23	124.55	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	11	U	O4'-C1'-N1	-5.22	104.03	108.20
1	1A	1744	A	O4'-C1'-N9	5.21	112.37	108.20
1	1A	1122	A	O4'-C1'-N9	5.21	112.37	108.20
1	2A	191	C	N1-C2-O2	-5.21	115.77	118.90
34	1a	899	U	C2-N3-C4	5.21	130.12	127.00
1	1A	253	A	O4'-C1'-N9	5.20	112.36	108.20
1	2A	989	A	C5-C6-N6	-5.20	119.54	123.70
1	2A	193	G	C8-N9-C4	5.20	108.48	106.40
1	2A	977	A	N7-C8-N9	5.19	116.40	113.80
34	1a	825	U	C5-C6-N1	5.19	125.29	122.70
57	1w	52	G	N3-C4-C5	-5.18	126.01	128.60
1	2A	2198	C	C6-N1-C2	-5.15	118.24	120.30
3	1C	62	VAL	CA-C-N	5.15	128.53	117.20
57	1w	14	A	C8-N9-C1'	-5.13	118.47	127.70
1	1A	2197	A	N1-C6-N6	-5.12	115.53	118.60
1	2A	138	A	C5-N7-C8	-5.12	101.34	103.90
51	2r	31	LEU	CA-CB-CG	5.12	127.08	115.30
1	1A	552	A	N1-C2-N3	5.12	131.86	129.30
51	1r	31	LEU	CA-CB-CG	5.11	127.06	115.30
1	2A	1699	G	P-O3'-C3'	5.10	125.81	119.70
34	2a	1165	A	P-O3'-C3'	5.09	125.81	119.70
1	2A	830	A	O4'-C1'-N9	5.09	112.27	108.20
1	1A	2161	C	C6-N1-C1'	-5.08	114.71	120.80
34	2a	975	U	C5-C4-O4	5.06	128.94	125.90
1	2A	2169	G	C5-C6-O6	5.06	131.64	128.60
57	1w	22	G	C8-N9-C4	-5.06	104.38	106.40
1	2A	1404	A	N1-C2-N3	-5.06	126.77	129.30
57	2w	46	G	C8-N9-C4	-5.05	104.38	106.40
1	1A	1220	G	P-O3'-C3'	5.04	125.75	119.70
1	2A	2122	G	N3-C4-C5	-5.03	126.08	128.60
1	2A	2904	C	N1-C2-O2	5.03	121.92	118.90
1	1A	353	A	N3-C4-C5	5.02	130.31	126.80
1	2A	2207	G	C6-N1-C2	5.01	128.11	125.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	12	59	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61861	0	31188	760	0
1	2A	61771	0	31145	923	0
2	1B	2573	0	1306	23	0
2	2B	2573	0	1306	25	0
3	1C	1020	0	1013	58	0
3	2C	1020	0	1013	69	0
4	1D	2136	0	2218	48	0
4	2D	2142	0	2229	55	0
5	1E	1559	0	1618	37	0
5	2E	1559	0	1618	45	0
6	1F	1584	0	1625	45	0
6	2F	1580	0	1619	52	0
7	1G	1425	0	1443	42	0
7	2G	1424	0	1434	50	0
8	1H	1330	0	1407	23	0
8	2H	1330	0	1407	34	0
9	1J	641	0	309	13	0
9	2J	641	0	309	10	0
10	1K	499	0	521	20	0
10	2K	498	0	521	40	0
11	1L	1117	0	1184	16	0
11	2L	1117	0	1184	27	0
12	1M	933	0	996	21	0
12	2M	933	0	996	20	0
13	1N	1139	0	1223	32	0
13	2N	1135	0	1212	40	0
14	1O	1122	0	1179	21	0
14	2O	1122	0	1179	38	0
15	1P	968	0	1033	24	0
15	2P	968	0	1033	36	0
16	1Q	877	0	938	12	0
16	2Q	870	0	923	25	0
17	1R	1091	0	1151	23	0
17	2R	1083	0	1136	34	0
18	1S	959	0	1019	12	0
18	2S	959	0	1019	25	0
19	1T	771	0	830	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2T	771	0	830	11	0
20	1U	886	0	940	15	0
20	2U	886	0	940	15	0
21	1V	750	0	814	13	0
21	2V	750	0	814	18	0
22	1W	806	0	881	18	0
22	2W	806	0	881	19	0
23	1X	1460	0	1463	33	0
23	2X	1454	0	1452	53	0
24	1Y	604	0	619	13	0
24	2Y	602	0	616	16	0
25	1Z	755	0	826	20	0
25	2Z	755	0	826	19	0
26	10	588	0	643	10	0
26	20	588	0	643	16	0
27	11	469	0	518	7	0
27	21	464	0	514	14	0
28	12	558	0	544	17	0
28	22	532	0	503	19	0
29	13	455	0	465	7	0
29	23	455	0	465	13	0
30	14	453	0	473	6	0
30	24	449	0	469	10	0
31	15	418	0	467	11	0
31	25	418	0	467	9	0
32	16	517	0	582	15	0
32	26	517	0	582	22	0
33	17	307	0	335	5	0
33	27	307	0	335	7	0
34	1a	32141	0	16223	0	0
34	2a	32268	0	16287	0	0
35	1b	1846	0	1867	0	0
35	2b	1825	0	1828	0	0
36	1c	1552	0	1546	0	0
36	2c	1544	0	1524	0	0
37	1d	1659	0	1676	0	0
37	2d	1678	0	1718	0	0
38	1e	1129	0	1185	0	0
38	2e	1133	0	1191	0	0
39	1f	812	0	804	0	0
39	2f	820	0	814	0	0
40	1g	1231	0	1238	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2g	1235	0	1249	0	0
41	1h	1088	0	1126	0	0
41	2h	1088	0	1126	0	0
42	1i	986	0	995	0	0
42	2i	978	0	966	0	0
43	1j	709	0	650	0	0
43	2j	714	0	672	0	0
44	1k	833	0	836	0	0
44	2k	833	0	836	0	0
45	1l	930	0	980	0	0
45	2l	930	0	980	0	0
46	1m	966	0	1024	0	0
46	2m	950	0	988	0	0
47	1n	492	0	529	0	0
47	2n	492	0	529	0	0
48	1o	728	0	760	0	0
48	2o	728	0	760	0	0
49	1p	681	0	697	0	0
49	2p	677	0	686	0	0
50	1q	823	0	891	0	0
50	2q	823	0	891	0	0
51	1r	555	0	618	0	0
51	2r	555	0	618	0	0
52	1s	661	0	675	0	0
52	2s	646	0	644	0	0
53	1t	728	0	798	0	0
53	2t	731	0	807	0	0
54	1u	199	0	208	0	0
54	2u	199	0	208	0	0
55	1z	5690	0	5783	0	0
55	2z	5690	0	5783	0	0
56	1y	129	0	65	0	0
56	2y	109	0	55	0	0
57	1w	1625	0	829	0	0
57	2w	1625	0	829	0	0
58	1x	168	0	195	0	0
58	2x	168	0	195	0	0
59	10	2	0	0	0	0
59	11	1	0	0	0	0
59	13	3	0	0	0	0
59	14	1	0	0	0	0
59	15	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	16	2	0	0	0	0
59	17	2	0	0	0	0
59	1A	780	0	0	0	0
59	1B	24	0	0	0	0
59	1D	4	0	0	0	0
59	1E	6	0	0	0	0
59	1F	7	0	0	0	0
59	1G	2	0	0	0	0
59	1H	1	0	0	0	0
59	1L	2	0	0	0	0
59	1M	1	0	0	0	0
59	1N	2	0	0	0	0
59	1O	2	0	0	0	0
59	1P	2	0	0	0	0
59	1S	4	0	0	0	0
59	1T	1	0	0	0	0
59	1U	3	0	0	0	0
59	1W	1	0	0	0	0
59	1X	2	0	0	0	0
59	1Y	5	0	0	0	0
59	1a	204	0	0	0	0
59	1b	1	0	0	0	0
59	1d	2	0	0	0	0
59	1f	1	0	0	0	0
59	1l	3	0	0	0	0
59	1t	1	0	0	0	0
59	1w	6	0	0	0	0
59	1z	1	0	0	0	0
59	23	1	0	0	0	0
59	26	2	0	0	0	0
59	2A	620	0	0	0	0
59	2B	13	0	0	0	0
59	2D	4	0	0	0	0
59	2E	4	0	0	0	0
59	2F	3	0	0	0	0
59	2G	1	0	0	0	0
59	2M	2	0	0	0	0
59	2N	1	0	0	0	0
59	2O	2	0	0	0	0
59	2P	1	0	0	0	0
59	2R	1	0	0	0	0
59	2S	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2W	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2a	173	0	0	0	0
59	2d	1	0	0	0	0
59	2f	2	0	0	0	0
59	2j	1	0	0	0	0
59	2l	1	0	0	0	0
59	2n	1	0	0	0	0
59	2q	1	0	0	0	0
59	2t	1	0	0	0	0
59	2w	4	0	0	0	0
59	2z	4	0	0	0	0
60	12	1	0	0	0	0
60	13	1	0	0	0	0
60	14	1	0	0	0	0
60	17	1	0	0	0	0
60	1W	1	0	0	0	0
60	1n	1	0	0	0	0
60	22	1	0	0	0	0
60	23	1	0	0	0	0
60	24	1	0	0	0	0
60	27	1	0	0	0	0
60	2W	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	1z	28	0	12	0	0
62	2z	28	0	12	0	0
63	11	2	0	0	0	0
63	15	2	0	0	1	0
63	16	10	0	0	0	0
63	17	1	0	0	0	0
63	1A	1299	0	0	118	0
63	1B	39	0	0	1	0
63	1D	15	0	0	1	0
63	1E	19	0	0	4	0
63	1F	12	0	0	2	0
63	1G	3	0	0	1	0
63	1H	1	0	0	0	0
63	1M	2	0	0	0	0
63	1N	12	0	0	1	0
63	1O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	1P	4	0	0	0	0
63	1Q	1	0	0	0	0
63	1R	2	0	0	0	0
63	1S	4	0	0	0	0
63	1T	1	0	0	0	0
63	1U	2	0	0	0	0
63	1V	3	0	0	0	0
63	1X	2	0	0	0	0
63	1Y	4	0	0	0	0
63	1Z	1	0	0	0	0
63	1a	155	0	0	0	0
63	1d	1	0	0	0	0
63	1j	1	0	0	0	0
63	1l	2	0	0	0	0
63	1o	1	0	0	0	0
63	1p	2	0	0	0	0
63	1w	4	0	0	0	0
63	1x	1	0	0	0	0
63	1z	5	0	0	0	0
63	21	2	0	0	0	0
63	24	1	0	0	1	0
63	26	3	0	0	0	0
63	2A	650	0	0	63	0
63	2B	11	0	0	0	0
63	2D	8	0	0	2	0
63	2E	7	0	0	1	0
63	2F	5	0	0	0	0
63	2L	1	0	0	0	0
63	2M	2	0	0	0	0
63	2N	6	0	0	2	0
63	2O	3	0	0	1	0
63	2P	1	0	0	0	0
63	2R	2	0	0	0	0
63	2S	2	0	0	0	0
63	2U	1	0	0	0	0
63	2V	2	0	0	0	0
63	2W	1	0	0	0	0
63	2Y	5	0	0	0	0
63	2Z	2	0	0	0	0
63	2a	122	0	0	0	0
63	2f	1	0	0	0	0
63	2h	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	2j	1	0	0	0	0
63	2n	1	0	0	0	0
63	2t	1	0	0	0	0
63	2w	2	0	0	0	0
63	2y	1	0	0	0	0
63	2z	1	0	0	0	0
All	All	306384	0	207797	2823	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 (2823) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1828:U:H5'	4:1D:259:THR:HG22	1.48	0.95
1:2A:2158:C:H42	1:2A:2175:G:H1	0.98	0.94
1:1A:478:C:OP1	63:1A:3801:HOH:O	1.86	0.94
14:2O:62:GLY:HA2	23:2X:116:VAL:HG21	1.49	0.94
1:1A:1006:G:OP1	63:1A:3802:HOH:O	1.86	0.93
1:1A:1355:G:OP2	31:15:9:ARG:NH1	2.04	0.91
1:1A:2154:G:N3	1:1A:2179:A:N6	2.20	0.90
1:1A:1064:U:HO2'	1:1A:1066:A:H2	1.05	0.90
1:2A:2158:C:N4	1:2A:2175:G:H1	1.68	0.89
1:1A:1058:C:OP2	63:1A:3803:HOH:O	1.91	0.88
1:1A:1735:A:H62	1:1A:1744:A:H2	1.22	0.88
1:2A:183:A:N7	63:2A:4903:HOH:O	2.07	0.87
1:2A:2155:A:H62	1:2A:2178:G:H4'	1.41	0.86
1:2A:1735:A:H62	1:2A:1744:A:H2	1.23	0.86
1:1A:1054:A:OP2	11:1L:37:LYS:NZ	2.08	0.86
17:1R:55:ASN:H	17:1R:59:THR:HG22	1.40	0.86
1:1A:655:A:OP1	13:1N:65:ARG:NH1	2.09	0.85
1:2A:1649:C:OP2	63:2A:4901:HOH:O	1.94	0.85
1:1A:2144:G:H1	1:1A:2196:C:H42	1.23	0.85
1:1A:681:G:H1	1:1A:696:C:H42	1.24	0.85
1:1A:2456:G:OP1	6:1F:74:ARG:NH2	2.09	0.85
7:2G:80:PHE:O	7:2G:82:LEU:N	2.10	0.85
1:1A:1038:G:OP1	18:1S:50:ARG:NH2	2.09	0.84
13:2N:36:LYS:O	63:2N:301:HOH:O	1.94	0.84
31:15:24:THR:HG22	31:15:27:GLY:H	1.43	0.84
7:2G:180:PHE:O	7:2G:182:LYS:N	2.13	0.82
1:2A:1991:A:OP1	63:2A:4902:HOH:O	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1316:G:OP2	63:1A:3805:HOH:O	1.98	0.81
1:1A:2585:G:OP1	63:1A:3806:HOH:O	1.98	0.81
1:1A:2510:C:OP1	63:1A:3804:HOH:O	1.97	0.81
3:1C:41:VAL:HA	3:1C:216:THR:HA	1.63	0.80
1:1A:1002:U:OP2	14:1O:14:ARG:NH1	2.14	0.80
19:2T:98:GLU:OE1	19:2T:100:ARG:NH1	2.13	0.80
1:1A:2771:G:OP2	63:1A:3807:HOH:O	1.99	0.80
1:2A:2152:G:H4'	1:2A:2153:U:H3'	1.63	0.80
10:1K:134:MET:HG3	10:1K:136:VAL:HG12	1.63	0.80
1:1A:682:G:N2	1:1A:695:C:O2	2.15	0.80
63:1E:401:HOH:O	15:1P:3:HIS:NE2	2.14	0.80
1:2A:1125:C:N4	1:2A:1133:A:OP2	2.15	0.80
1:2A:2144:G:O2'	3:2C:172:HIS:O	2.00	0.79
1:2A:2296:C:OP2	30:24:6:ARG:NH1	2.15	0.79
5:2E:11:MET:HG2	5:2E:24:THR:HG22	1.63	0.79
3:2C:26:ALA:HB1	3:2C:185:LEU:HB3	1.65	0.79
1:2A:2127:G:O6	1:2A:2204:C:N3	2.15	0.79
30:24:6:ARG:NH2	63:24:5001:HOH:O	2.11	0.79
1:1A:1698:A:OP1	15:1P:8:ARG:NH1	2.15	0.79
28:22:44:THR:O	28:22:46:GLN:N	2.16	0.79
1:1A:1715:A:OP2	63:1A:3808:HOH:O	1.99	0.78
2:2B:22:U:H3	2:2B:61:G:H1	1.30	0.78
2:1B:31:C:O2	2:1B:53:A:N6	2.16	0.78
1:1A:1150:U:H2'	1:1A:1151:G:H8	1.48	0.78
16:1Q:27:SER:HA	16:1Q:88:ASP:HB3	1.65	0.78
1:2A:2694:C:OP1	17:2R:53:ARG:NH2	2.17	0.78
1:2A:2817:U:O2	1:2A:2900:A:N6	2.15	0.78
1:1A:2694:C:O2	12:1M:70:LYS:NZ	2.15	0.78
1:2A:1765:G:H8	1:2A:1769:A:H62	1.30	0.78
1:2A:2135:A:N6	1:2A:2140:A:N7	2.31	0.78
5:2E:28:ALA:HB3	5:2E:93:VAL:HG12	1.65	0.78
22:1W:54:LYS:HA	22:1W:56:PRO:HD3	1.66	0.77
1:2A:1064:U:H3	1:2A:1187:A:H62	1.31	0.77
1:2A:186:C:OP2	63:2A:4903:HOH:O	2.00	0.77
1:1A:2529:A:OP2	63:1A:3810:HOH:O	2.02	0.77
7:1G:161:THR:HG23	7:1G:163:ALA:H	1.49	0.77
1:1A:991:G:OP2	63:1A:3811:HOH:O	2.03	0.77
22:1W:92:ASN:HB2	22:1W:94:LYS:H	1.49	0.77
1:2A:893:U:O4	1:2A:977:A:N6	2.18	0.77
16:2Q:27:SER:HA	16:2Q:88:ASP:HB3	1.64	0.77
13:2N:59:LEU:HD11	32:26:10:ALA:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2P:33:ARG:NH2	29:23:57:VAL:O	2.18	0.76
1:1A:1043:C:OP1	63:1A:3812:HOH:O	2.03	0.76
6:1F:185:ASP:HA	6:1F:188:ARG:HD3	1.67	0.76
1:1A:1229:C:OP2	63:1A:3809:HOH:O	2.01	0.76
1:1A:238:G:OP2	32:16:13:ARG:NH2	2.17	0.76
1:1A:1404:A:H61	1:1A:1417:U:H3	1.34	0.76
1:2A:346:G:HO2'	1:2A:1249:U:H3	1.32	0.76
1:2A:2197:A:H5'	3:2C:215:THR:HG21	1.67	0.76
1:2A:2298:A:H62	1:2A:2355:U:H3	1.34	0.76
1:1A:324:G:OP2	22:1W:84:ARG:NH2	2.19	0.76
1:2A:1107:G:O2'	10:2K:133:SER:O	2.04	0.76
17:2R:55:ASN:H	17:2R:59:THR:HG22	1.50	0.75
3:2C:32:LEU:HD22	3:2C:220:PRO:HD2	1.67	0.75
1:1A:1516:G:N7	63:1A:3872:HOH:O	2.18	0.75
1:2A:1035:A:OP2	63:2A:4904:HOH:O	2.04	0.75
22:2W:23:ARG:HG2	22:2W:42:VAL:HG22	1.67	0.75
1:1A:1150:U:H2'	1:1A:1151:G:C8	2.21	0.75
3:2C:40:THR:HA	3:2C:177:LYS:HA	1.68	0.75
1:1A:10:G:H2'	1:1A:11:U:H5''	1.69	0.75
28:22:16:CYS:SG	28:22:17:GLY:N	2.59	0.75
11:2L:123:TYR:HH	11:2L:130:HIS:HE2	1.26	0.75
15:1P:55:ALA:HB2	15:1P:79:LEU:HD13	1.68	0.75
1:2A:550:A:OP1	63:2A:4905:HOH:O	2.04	0.74
10:1K:106:GLU:HA	10:1K:109:LYS:HD3	1.68	0.74
1:1A:1019:C:OP1	63:1A:3815:HOH:O	2.05	0.74
1:2A:941:A:H5''	23:2X:147:GLY:HA3	1.69	0.74
28:12:15:ILE:HG23	28:12:21:VAL:HG22	1.69	0.74
1:2A:1127:U:H1'	10:2K:116:ASN:HB3	1.69	0.74
1:1A:2100:U:OP1	25:1Z:21:ARG:NH2	2.19	0.74
1:2A:1108:G:H4'	10:2K:87:GLY:HA3	1.68	0.74
1:2A:2162:G:O6	1:2A:2171:U:O2	2.06	0.74
3:2C:163:PHE:HB2	3:2C:171:ILE:HD11	1.70	0.74
1:1A:2298:A:H62	1:1A:2355:U:H3	1.33	0.74
1:1A:2552:A:N7	63:1A:3878:HOH:O	2.19	0.74
1:2A:1036:C:OP2	63:2A:4904:HOH:O	2.05	0.74
1:2A:1404:A:H61	1:2A:1417:U:H3	1.36	0.74
1:1A:1113:G:O6	1:1A:1114:A:N6	2.20	0.74
1:2A:2815:G:H2'	1:2A:2816:G:C8	2.23	0.74
16:2Q:48:LEU:HD23	16:2Q:82:ILE:HD11	1.68	0.74
1:2A:2671:A:N7	8:2H:175:LYS:NZ	2.36	0.73
23:2X:5:LEU:HG	23:2X:47:VAL:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:154:C:H42	1:2A:159:G:H1	1.36	0.73
1:2A:2760:A:H5'	8:2H:4:ILE:HD12	1.70	0.73
1:1A:830:A:OP2	63:1A:3817:HOH:O	2.06	0.73
1:2A:2155:A:O2'	1:2A:2180:G:N3	2.21	0.73
1:2A:1136:G:O6	1:2A:1145:C:N4	2.21	0.73
5:2E:77:ILE:HD11	5:2E:79:ARG:HH11	1.54	0.73
3:2C:209:LEU:HB2	3:2C:226:PRO:HG2	1.71	0.73
1:1A:1283:G:OP2	63:1A:3819:HOH:O	2.07	0.73
23:1X:151:HIS:O	23:1X:153:SER:N	2.19	0.73
25:1Z:51:VAL:HG11	25:1Z:74:VAL:HG21	1.71	0.73
4:1D:69:ARG:NH2	4:1D:128:GLY:O	2.22	0.72
1:1A:1540:A:OP2	63:1A:3816:HOH:O	2.06	0.72
1:2A:2226:G:H3'	1:2A:2227:G:H8	1.54	0.72
1:1A:2050:G:OP2	63:1A:3814:HOH:O	2.05	0.72
6:1F:90:PHE:N	63:1F:5001:HOH:O	2.19	0.72
13:2N:63:PRO:HD3	32:26:27:THR:HG22	1.69	0.72
1:1A:2417:U:OP1	63:1A:3818:HOH:O	2.06	0.72
1:1A:588:U:H5''	13:1N:29:LYS:HE3	1.72	0.72
4:2D:24:ILE:HG23	4:2D:83:GLU:HA	1.71	0.71
1:1A:1070:G:O2'	63:1A:3813:HOH:O	2.03	0.71
4:2D:238:GLY:O	63:2D:401:HOH:O	2.08	0.71
6:2F:53:THR:HG23	6:2F:55:GLY:H	1.55	0.71
1:1A:1717:U:OP2	63:1A:3820:HOH:O	2.08	0.71
1:2A:894:G:H2'	1:2A:895:A:C8	2.25	0.71
6:2F:154:VAL:HG12	6:2F:191:ARG:HB2	1.72	0.71
1:2A:1295:G:N7	13:2N:18:ARG:NH2	2.38	0.71
13:2N:42:SER:O	63:2N:302:HOH:O	2.07	0.71
12:2M:86:ILE:HG22	12:2M:94:ARG:HG3	1.71	0.71
1:1A:2378:G:N7	63:1A:3895:HOH:O	2.23	0.71
29:23:40:LYS:NZ	29:23:44:THR:O	2.23	0.71
1:1A:1111:U:N3	1:1A:1113:G:OP2	2.23	0.71
1:2A:1116:G:H1'	1:2A:1134:G:H2'	1.71	0.71
1:2A:878:G:OP1	63:2A:4907:HOH:O	2.08	0.71
9:2J:49:ALA:H	9:2J:90:ALA:HB1	1.54	0.71
1:1A:534:C:OP1	63:1A:3822:HOH:O	2.08	0.71
1:1A:807:A:N7	63:1A:3900:HOH:O	2.23	0.71
1:2A:1378:C:HO2'	1:2A:1384:G:HO2'	24.70	0.71
1:2A:807:A:N7	63:2A:4954:HOH:O	2.23	0.71
1:2A:1679:G:OP2	63:2A:4906:HOH:O	2.07	0.71
1:1A:330:G:H21	1:1A:353:A:H62	1.36	0.70
1:2A:1099:A:H61	1:2A:1150:U:H3	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:163:PHE:HB2	3:1C:171:ILE:HD11	1.72	0.70
1:1A:878:G:H5'	13:1N:45:LEU:HD21	1.73	0.70
1:2A:1858:G:OP1	63:2A:4911:HOH:O	2.09	0.70
1:2A:1075:G:OP2	14:2O:128:LYS:NZ	2.25	0.70
1:2A:2704:A:H2'	1:2A:2705:G:H8	1.56	0.70
1:2A:2733:A:OP1	63:2A:4908:HOH:O	2.08	0.70
1:1A:2132:C:OP2	1:1A:2166:C:N4	2.24	0.70
1:2A:1847:G:OP1	4:2D:88:ARG:NH2	2.24	0.70
1:2A:1127:U:O2'	10:2K:116:ASN:O	2.08	0.70
1:1A:186:C:OP2	63:1A:3823:HOH:O	2.08	0.70
1:2A:1360:C:OP2	63:2A:4909:HOH:O	2.10	0.70
25:2Z:50:ARG:HG2	25:2Z:59:THR:HB	1.73	0.70
1:1A:536:G:N7	63:1A:3822:HOH:O	2.24	0.70
1:2A:2441:A:OP2	63:2A:4910:HOH:O	2.08	0.70
1:2A:786:U:OP2	63:2A:4912:HOH:O	2.10	0.70
14:2O:60:ARG:HH12	14:2O:113:GLN:HE22	1.39	0.70
1:2A:1698:A:OP1	15:2P:8:ARG:NH1	2.25	0.69
1:2A:2161:C:N3	1:2A:2172:G:O6	2.25	0.69
1:2A:2693:U:OP2	63:2A:4908:HOH:O	2.09	0.69
1:1A:1377:G:OP1	63:1A:3824:HOH:O	2.09	0.69
1:1A:893:U:OP2	63:1A:3825:HOH:O	2.09	0.69
1:2A:1109:C:H5'	10:2K:89:HIS:HD2	1.57	0.69
13:1N:63:PRO:HD3	32:16:27:THR:HG22	1.74	0.69
1:1A:1099:A:H62	1:1A:1150:U:H3	1.39	0.69
9:2J:27:VAL:HA	9:2J:113:GLN:HA	1.75	0.69
10:2K:119:ASP:N	10:2K:119:ASP:OD2	2.24	0.69
1:1A:2458:G:OP2	63:1A:3827:HOH:O	2.10	0.69
18:1S:76:TYR:OH	18:1S:92:ARG:NH1	2.24	0.69
1:2A:1614:G:N7	63:2A:4960:HOH:O	2.24	0.69
1:1A:1369:G:O6	63:1A:3829:HOH:O	2.10	0.69
1:2A:655:A:OP1	13:2N:65:ARG:NH1	2.25	0.69
1:2A:1377:G:OP1	63:2A:4909:HOH:O	2.08	0.69
1:1A:2494:C:N3	14:1O:124:LYS:NZ	2.37	0.69
11:2L:15:LEU:HD12	11:2L:137:LYS:HG2	1.73	0.69
1:1A:1680:A:OP2	63:1A:3826:HOH:O	2.09	0.69
23:1X:19:ARG:NH1	23:1X:84:GLU:O	2.25	0.69
1:2A:541:C:OP1	29:23:16:ARG:NH2	2.25	0.69
1:1A:180:C:OP1	63:1A:3832:HOH:O	2.11	0.69
1:1A:2161:C:O2'	1:1A:2173:G:N2	2.25	0.69
9:2J:73:GLY:O	9:2J:75:GLN:N	2.26	0.69
26:20:1:MET:SD	26:20:56:GLN:NE2	2.66	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1516:G:N2	1:1A:1567:G:OP2	2.24	0.68
1:1A:831:G:OP2	63:1A:3828:HOH:O	2.10	0.68
1:2A:1870:G:OP2	63:2A:4913:HOH:O	2.10	0.68
1:2A:2657:C:OP2	1:2A:2744:G:O2'	2.11	0.68
1:2A:2739:G:O2'	12:2M:70:LYS:NZ	2.26	0.68
3:2C:20:TYR:HB2	3:2C:224:ILE:HG22	1.75	0.68
1:1A:1220:G:N2	1:1A:1222:C:OP2	2.25	0.68
5:1E:76:ARG:HB2	5:1E:77:ILE:HD12	1.75	0.68
9:1J:48:GLY:HA2	9:1J:90:ALA:HB1	1.74	0.68
1:2A:1068:U:OP2	63:2A:4914:HOH:O	2.11	0.68
18:2S:76:TYR:OH	18:2S:92:ARG:NH1	2.26	0.68
21:2V:2:LYS:NZ	21:2V:38:GLU:OE2	2.25	0.68
1:1A:1086:C:H42	1:1A:1159:G:H1	1.39	0.68
1:1A:1911:A:OP2	63:1A:3831:HOH:O	2.11	0.68
1:2A:2848:G:H5'	15:2P:46:GLY:HA2	1.75	0.68
1:1A:1026:A:OP1	63:1A:3834:HOH:O	2.12	0.68
1:2A:2126:C:H42	1:2A:2204:C:H42	1.41	0.68
1:2A:2858:U:O4	17:2R:23:ARG:NH2	2.27	0.68
6:1F:18:ARG:NH2	6:1F:127:GLU:OE1	2.26	0.68
17:1R:51:ARG:HG3	17:1R:98:LYS:HD2	1.76	0.68
1:2A:1026:A:OP1	63:2A:4917:HOH:O	2.12	0.68
1:2A:1067:G:H22	1:2A:1187:A:H2	1.39	0.68
25:2Z:51:VAL:HG21	25:2Z:74:VAL:HG21	1.75	0.68
1:1A:1684:C:OP2	63:1A:3835:HOH:O	2.12	0.68
1:1A:1739:U:O2'	4:1D:14:ARG:NH2	2.27	0.68
1:1A:448:A:OP2	63:1A:3837:HOH:O	2.12	0.68
1:1A:991:G:OP1	63:1A:3830:HOH:O	2.11	0.68
1:2A:2622:U:C4	29:23:3:LYS:HG2	2.28	0.68
1:2A:2327:C:O2'	7:2G:128:ARG:NH2	2.27	0.68
7:1G:125:PHE:O	63:1G:3101:HOH:O	2.11	0.68
1:2A:2825:C:O3'	15:2P:99:LYS:NZ	2.27	0.68
2:1B:58:A:OP2	63:1B:301:HOH:O	2.11	0.67
2:1B:105:A:OP1	23:1X:72:ARG:NH1	2.27	0.67
1:2A:1311:G:O2'	1:2A:2033:G:O6	2.06	0.67
1:1A:1109:C:N4	1:1A:1115:A:OP1	2.26	0.67
1:1A:777:C:OP2	63:1A:3836:HOH:O	2.12	0.67
1:2A:1081:G:H1	1:2A:1164:C:H42	1.41	0.67
1:2A:2144:G:H1'	3:2C:172:HIS:HB2	1.75	0.67
3:1C:55:ASP:N	3:1C:55:ASP:OD1	2.27	0.67
1:2A:2184:C:H3'	1:2A:2185:C:H4'	1.77	0.67
1:2A:2275:C:N4	24:2Y:15:ASP:OD2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1104:G:O2'	10:2K:126:MET:O	2.10	0.67
14:2O:60:ARG:H	14:2O:60:ARG:HD3	1.58	0.67
27:11:8:LEU:HD13	27:11:31:LEU:HD23	1.75	0.67
1:1A:1402:U:OP2	63:1A:3838:HOH:O	2.13	0.67
5:1E:110:GLY:O	63:1E:401:HOH:O	2.11	0.67
1:2A:1443:C:OP2	17:2R:108:ARG:NH2	84.43	0.67
1:1A:99:G:OP1	26:10:7:ARG:NH2	2.27	0.67
1:2A:2594:G:OP2	63:2A:4916:HOH:O	2.12	0.67
3:2C:41:VAL:HG22	3:2C:216:THR:HG22	1.76	0.67
25:1Z:3:LYS:HG2	25:1Z:4:VAL:HG23	1.76	0.67
28:22:59:PHE:HA	28:22:61:ARG:N	2.09	0.67
1:1A:2382:G:O6	63:1A:3821:HOH:O	2.08	0.67
6:1F:157:VAL:HB	6:1F:194:MET:HG2	1.76	0.67
1:2A:1108:G:H1	1:2A:1120:C:H42	1.42	0.67
1:2A:1814:A:OP2	63:2A:4912:HOH:O	2.12	0.67
1:1A:1716:C:OP1	63:1A:3833:HOH:O	2.12	0.67
1:1A:1071:U:OP1	63:1A:3813:HOH:O	2.12	0.67
16:1Q:11:LYS:HG3	16:1Q:91:PRO:HD3	1.77	0.66
1:2A:777:C:OP2	63:2A:4918:HOH:O	2.12	0.66
1:1A:2144:G:H1	1:1A:2196:C:N4	1.92	0.66
1:1A:2157:C:N4	1:1A:2176:G:H1	1.92	0.66
1:1A:454:A:OP1	63:1A:3839:HOH:O	2.13	0.66
1:2A:2134:U:H2'	1:2A:2135:A:H8	1.56	0.66
1:2A:833:U:OP1	63:2A:4919:HOH:O	2.13	0.66
1:1A:2148:G:H21	1:1A:2194:A:H1'	1.59	0.66
1:2A:826:G:OP1	4:2D:218:ARG:NH2	2.29	0.66
21:1V:9:LEU:HA	26:10:36:ARG:HH21	1.60	0.66
1:2A:1198:C:OP1	18:2S:92:ARG:NH1	2.28	0.66
1:2A:1512:G:HO2'	1:2A:1592:C:HO2'	1.40	0.66
1:1A:777:C:OP1	63:1A:3841:HOH:O	2.13	0.66
6:1F:32:LEU:HB3	6:1F:112:MET:HE1	1.77	0.66
1:1A:2377:A:OP1	63:1A:3845:HOH:O	2.14	0.66
1:2A:1105:U:H5''	10:2K:75:SER:N	2.10	0.66
1:2A:394:C:OP2	63:2A:4921:HOH:O	2.14	0.66
2:2B:77:U:OP1	23:2X:19:ARG:NH2	2.29	0.66
1:1A:8:U:H3	1:1A:2640:A:H2	1.43	0.66
7:2G:41:GLN:HG3	7:2G:60:LEU:HD21	1.78	0.66
15:1P:33:ARG:NH1	15:1P:115:GLU:OE2	2.23	0.66
1:2A:1109:C:N4	1:2A:1115:A:OP2	2.28	0.66
1:2A:2262:G:OP1	63:2A:4920:HOH:O	2.14	0.66
1:2A:79:G:N7	63:2A:4971:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2606:G:N7	63:1A:3925:HOH:O	2.28	0.65
1:2A:873:U:OP1	63:2A:4910:HOH:O	2.13	0.65
7:2G:39:ILE:HG13	7:2G:157:ILE:HG12	1.78	0.65
1:1A:1390:C:OP2	63:1A:3840:HOH:O	2.13	0.65
5:1E:143:ASN:HD22	5:1E:147:PRO:HD3	1.61	0.65
17:1R:56:GLY:O	17:1R:59:THR:HG23	1.96	0.65
17:1R:60:THR:HG22	17:1R:77:PRO:HA	1.78	0.65
1:2A:241:C:O2'	63:2A:4923:HOH:O	2.14	0.65
6:2F:157:VAL:HB	6:2F:194:MET:HG2	1.77	0.65
1:1A:1294:U:OP1	63:1A:3846:HOH:O	2.14	0.65
3:1C:19:VAL:HG22	3:1C:223:ARG:HD2	1.77	0.65
23:2X:72:ARG:HG2	23:2X:89:PHE:HB2	1.77	0.65
1:1A:2594:G:OP1	63:1A:3848:HOH:O	2.15	0.65
1:2A:154:C:N4	1:2A:159:G:H1	1.94	0.65
1:2A:1638:G:H2'	1:2A:1639:G:C8	2.30	0.65
1:2A:2197:A:H4'	3:2C:44:HIS:CD2	2.32	0.65
20:2U:18:ARG:HG3	20:2U:76:VAL:HB	1.77	0.65
11:2L:128:HIS:O	11:2L:131:GLN:NE2	2.29	0.65
18:2S:9:VAL:HG21	28:22:61:ARG:HH22	162.74	0.65
1:1A:1105:U:H4'	1:1A:1106:U:H5'	1.79	0.65
1:1A:475:G:OP2	63:1A:3847:HOH:O	2.14	0.65
5:2E:179:GLU:HB3	5:2E:181:LEU:HD22	1.79	0.65
1:1A:2595:U:O4	63:1A:3842:HOH:O	2.13	0.65
1:1A:640:G:OP1	6:1F:40:GLN:NE2	2.27	0.65
1:1A:236:G:OP1	63:1A:3851:HOH:O	2.15	0.65
1:1A:725:C:OP1	63:1A:3844:HOH:O	2.14	0.65
27:21:5:LYS:HB3	27:21:57:GLU:HG3	1.79	0.65
1:2A:2696:G:O6	63:2A:4915:HOH:O	2.11	0.65
1:1A:132:G:N7	63:1A:3939:HOH:O	2.30	0.65
3:2C:47:LEU:HB2	3:2C:49:ILE:HD12	1.80	0.65
22:2W:49:VAL:HG21	22:2W:61:ILE:HG23	1.79	0.65
1:1A:2831:G:OP2	63:1E:401:HOH:O	2.15	0.64
1:2A:2158:C:N3	1:2A:2175:G:N2	2.41	0.64
22:2W:11:ASP:OD2	22:2W:97:ARG:NH2	2.30	0.64
1:1A:550:A:OP1	63:1A:3843:HOH:O	2.14	0.64
1:1A:2043:U:O2'	1:1A:2628:C:H5'	1.97	0.64
1:2A:324:G:OP2	22:2W:84:ARG:NH2	2.29	0.64
1:2A:1520:C:H2'	1:2A:1521:G:C8	2.33	0.64
1:2A:1288:G:O2'	13:2N:7:ARG:NH2	2.30	0.64
1:1A:191:C:OP2	63:1A:3849:HOH:O	2.15	0.64
10:1K:77:LEU:HB2	10:1K:107:ILE:HG23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:640:G:OP1	6:2F:40:GLN:NE2	2.26	0.64
3:1C:180:PHE:HB3	3:1C:185:LEU:HD23	1.79	0.64
1:2A:2057:C:OP1	63:2A:4926:HOH:O	2.15	0.64
1:2A:588:U:H5'	13:2N:29:LYS:HE3	1.80	0.64
6:2F:20:LEU:HD13	6:2F:21:ALA:H	1.62	0.64
1:1A:1103:G:H22	1:1A:1126:U:H1'	1.62	0.64
1:1A:1360:C:OP2	63:1A:3824:HOH:O	2.14	0.64
10:1K:115:LEU:HD13	10:1K:117:THR:HG22	1.80	0.64
17:2R:56:GLY:O	17:2R:59:THR:HG23	1.97	0.64
20:2U:18:ARG:NH1	20:2U:76:VAL:O	2.30	0.64
14:2O:134:ARG:HD2	23:2X:122:ARG:HH21	1.63	0.64
3:1C:58:VAL:HG11	3:1C:196:LEU:HD12	1.78	0.64
4:1D:17:THR:O	4:1D:211:ARG:NH2	2.31	0.64
23:1X:183:LEU:HA	23:1X:186:GLU:HB2	1.80	0.64
10:2K:84:LEU:HD23	10:2K:96:VAL:HB	1.78	0.64
1:2A:1761:G:H2'	1:2A:1762:G:H8	1.62	0.64
1:2A:2891:A:OP1	15:2P:96:ARG:NE	2.21	0.64
1:1A:2226:G:H3'	1:1A:2227:G:H8	1.62	0.64
1:1A:481:C:H4'	63:1A:4651:HOH:O	1.97	0.64
19:1T:76:LYS:HB2	19:1T:81:TYR:HB3	1.80	0.64
1:2A:2134:U:H2'	1:2A:2135:A:C8	2.33	0.64
1:1A:614:G:H2'	1:1A:615:G:H8	3.00	0.63
1:2A:2704:A:H2'	1:2A:2705:G:C8	2.33	0.63
1:1A:2123:U:H2'	1:1A:2124:C:H6	1.63	0.63
1:2A:2131:G:O2'	1:2A:2141:G:OP2	2.15	0.63
7:2G:161:THR:HG22	7:2G:163:ALA:H	1.63	0.63
1:1A:294:C:H42	1:1A:388:G:H1	1.47	0.63
1:2A:1830:C:OP2	4:2D:183:ARG:NH2	2.31	0.63
17:1R:16:ARG:NH2	17:1R:83:ILE:O	2.31	0.63
1:1A:138:A:H8	1:1A:1453:C:HO2'	1.44	0.63
1:1A:2204:C:H2'	1:1A:2205:G:H8	1.64	0.63
1:1A:829:A:OP2	63:1A:3850:HOH:O	2.15	0.63
17:2R:51:ARG:HG3	17:2R:98:LYS:HE3	1.81	0.63
14:2O:61:GLY:HA3	23:2X:178:GLU:HB2	1.81	0.63
1:1A:2131:G:OP1	1:1A:2139:U:N3	2.30	0.63
2:1B:14:U:OP2	2:1B:70:C:O2'	2.15	0.63
5:1E:47:VAL:HG11	5:1E:86:PRO:HD2	1.80	0.63
2:1B:8:U:O3'	16:1Q:25:ARG:NH2	2.30	0.63
17:1R:55:ASN:N	17:1R:59:THR:HG22	2.13	0.63
1:2A:663:U:H2'	1:2A:664:C:C6	2.34	0.63
1:1A:2043:U:OP1	63:1A:3852:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2831:G:N7	63:1A:3942:HOH:O	2.30	0.63
1:2A:2799:C:H1'	5:2E:62:PRO:HG3	1.81	0.63
1:1A:70:U:OP1	63:1A:3854:HOH:O	2.15	0.63
1:2A:879:U:O2	13:2N:55:ARG:NH2	2.32	0.62
1:1A:785:G:OP1	63:1A:3853:HOH:O	2.15	0.62
1:2A:2238:A:OP2	63:2A:4925:HOH:O	2.15	0.62
1:2A:2198:C:H1'	3:2C:170:ALA:HB2	1.81	0.62
3:2C:6:ARG:NH1	3:2C:218:MET:HB2	2.14	0.62
1:2A:1739:U:O2'	4:2D:14:ARG:NH2	2.31	0.62
23:1X:69:THR:HG22	23:1X:90:VAL:HA	1.79	0.62
1:2A:10:G:H2'	1:2A:11:U:H5''	1.80	0.62
3:2C:43:VAL:HG11	3:2C:193:ILE:HD11	1.80	0.62
1:1A:2648:U:H5''	5:1E:82:ARG:HH21	1.65	0.62
1:1A:1009:C:N3	1:1A:1010:G:O2'	7.93	0.62
1:1A:1098:C:H2'	1:1A:1099:A:H5''	1.82	0.62
1:1A:1067:G:OP2	11:1L:65:LYS:NZ	2.33	0.62
1:2A:1144:G:H2'	1:2A:1145:C:O4'	1.99	0.62
6:2F:117:ARG:NH2	6:2F:189:THR:O	2.32	0.62
8:2H:88:LEU:HD22	8:2H:165:ALA:HA	1.82	0.62
1:1A:2229:U:O4'	25:1Z:52:ARG:NH2	2.32	0.62
1:2A:1835:U:O2	4:2D:50:THR:HB	2.00	0.62
1:2A:2127:G:N1	1:2A:2204:C:O2	2.25	0.62
1:1A:1724:G:N7	63:1A:3944:HOH:O	2.30	0.62
1:1A:2157:C:H42	1:1A:2176:G:H1	1.46	0.62
1:1A:552:A:C2	1:1A:2063:A:H2'	2.34	0.62
3:1C:14:VAL:HG21	3:1C:220:PRO:HB2	1.82	0.62
1:2A:493:G:N7	31:25:39:ARG:NH2	2.47	0.62
1:2A:1092:G:O2'	1:2A:1154:C:N4	2.33	0.62
1:2A:2363:A:N6	1:2A:2376:G:O2'	2.33	0.62
1:2A:636:U:O4	1:2A:736:G:O2'	77.54	0.62
7:2G:114:ILE:HG23	7:2G:136:ARG:HH22	1.64	0.62
10:2K:95:LYS:NZ	10:2K:137:GLU:OE1	2.30	0.62
14:2O:57:HIS:HD2	14:2O:117:ALA:HB2	1.64	0.62
1:1A:211:A:O2'	1:1A:446:C:O2	2.15	0.61
28:22:61:ARG:O	28:22:63:TYR:N	2.30	0.61
3:1C:212:VAL:HG21	3:1C:226:PRO:HB3	1.82	0.61
19:1T:72:VAL:HG13	19:1T:85:LYS:HB3	1.81	0.61
1:2A:2338:A:H2'	1:2A:2339:A:C8	2.35	0.61
1:2A:2685:G:H5''	12:2M:26:LYS:HE3	1.82	0.61
13:2N:38:GLN:HG2	13:2N:45:LEU:H	1.65	0.61
23:2X:69:THR:HG22	23:2X:90:VAL:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:40:THR:HG23	3:1C:175:VAL:HG23	1.82	0.61
3:1C:42:GLU:N	3:1C:215:THR:O	2.33	0.61
13:1N:118:GLY:O	13:1N:137:LYS:NZ	2.33	0.61
20:1U:18:ARG:HG3	20:1U:76:VAL:HB	1.83	0.61
1:2A:1042:G:OP1	18:2S:92:ARG:HG2	2.00	0.61
1:2A:2254:U:H2'	1:2A:2255:U:C6	2.35	0.61
10:2K:99:ILE:O	10:2K:139:VAL:N	2.25	0.61
19:2T:40:LEU:HB2	19:2T:46:VAL:HG13	1.83	0.61
1:1A:2144:G:H2'	1:1A:2145:G:C8	2.36	0.61
3:1C:175:VAL:HG13	3:1C:176:GLY:H	1.65	0.61
23:2X:137:ILE:HD13	23:2X:157:LEU:HD22	1.82	0.61
1:1A:1217:G:O2'	1:1A:1218:A:O4'	2.19	0.61
1:2A:1867:C:O2'	1:2A:1948:A:N3	2.32	0.61
1:2A:30:C:OP1	63:2A:4928:HOH:O	2.16	0.61
13:1N:65:ARG:HG3	32:16:25:MET:HG3	1.82	0.61
4:1D:37:LEU:HD13	4:1D:62:TYR:HB2	1.83	0.61
28:22:24:THR:OG1	28:22:25:TYR:N	2.34	0.61
1:2A:1768:G:H2'	1:2A:1769:A:H8	1.65	0.61
1:2A:454:A:H3'	1:2A:455:A:H8	1.65	0.61
1:2A:235:G:H4'	1:2A:412:G:C5	2.35	0.61
1:2A:846:A:OP1	1:2A:846:A:H8	1.83	0.61
1:1A:1039:C:OP2	18:1S:54:LYS:NZ	2.34	0.60
1:1A:1694:C:OP1	63:1A:3805:HOH:O	2.16	0.60
1:1A:2162:G:N7	1:1A:2172:G:N2	2.49	0.60
1:2A:2360:G:OP1	63:2A:4929:HOH:O	2.16	0.60
1:2A:2700:U:H4'	1:2A:2701:C:H5'	1.83	0.60
23:2X:158:PRO:O	23:2X:161:VAL:HG12	2.01	0.60
1:1A:1198:C:OP1	18:1S:92:ARG:NH1	2.31	0.60
1:1A:1524:G:H2'	1:1A:1525:G:H8	1.66	0.60
1:2A:1130:A:O2'	1:2A:1149:C:O2	2.19	0.60
1:2A:2740:U:H5'	12:2M:70:LYS:HZ3	1.66	0.60
28:12:54:GLY:H	28:12:56:VAL:HG22	1.66	0.60
1:1A:1089:G:O2'	1:1A:1156:A:N6	2.34	0.60
1:2A:1135:U:H2'	1:2A:1136:G:C8	2.36	0.60
1:2A:1319:A:N1	1:2A:1690:C:O2'	2.34	0.60
1:2A:264:U:H2'	1:2A:265:C:C6	2.37	0.60
1:2A:354:A:OP1	1:2A:1253:G:N2	2.26	0.60
23:2X:45:ASP:OD2	23:2X:49:ARG:NH1	2.35	0.60
1:1A:2261:G:OP1	14:1O:85:LYS:NZ	2.30	0.60
1:1A:2335:C:H5''	1:1A:2336:G:H5'	1.82	0.60
1:2A:2815:G:H2'	1:2A:2816:G:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:172:C:H2'	1:1A:173:U:C6	2.36	0.60
1:2A:1104:G:H1	1:2A:1124:C:H42	1.50	0.60
1:1A:1424:A:H4'	1:1A:1425:G:OP2	2.02	0.60
6:2F:11:VAL:HB	6:2F:18:ARG:HB2	1.82	0.60
1:2A:1295:G:OP2	13:2N:21:ARG:NH1	2.35	0.60
1:1A:2354:C:OP1	63:1A:3856:HOH:O	2.16	0.60
1:1A:2800:C:OP1	5:1E:61:ARG:NH2	2.33	0.60
1:2A:1479:A:H61	1:2A:1604:A:N6	1.99	0.60
1:1A:1093:A:OP2	1:1A:1154:C:N4	2.35	0.60
1:1A:1404:A:N6	1:1A:1417:U:H3	1.99	0.60
1:1A:793:U:O2	1:1A:2035:A:H1'	2.01	0.60
1:1A:425:G:OP2	63:1A:3858:HOH:O	2.17	0.60
7:1G:28:VAL:O	7:1G:31:VAL:HG13	2.01	0.60
23:1X:156:LYS:HG3	23:1X:157:LEU:H	1.65	0.60
26:20:51:ARG:HH21	26:20:55:ARG:HH11	1.49	0.60
1:2A:1064:U:HO2'	1:2A:1066:A:H2	1.49	0.60
1:2A:1710:A:OP2	63:2A:4927:HOH:O	2.16	0.60
1:2A:2626:U:H2'	1:2A:2627:C:H6	1.65	0.60
1:2A:1232:U:H4'	19:2T:79:VAL:HG22	1.84	0.60
1:1A:1502:G:OP2	63:1A:3857:HOH:O	2.16	0.60
1:1A:2796:C:H1'	5:1E:37:ARG:HH12	1.67	0.60
15:1P:20:LEU:HD21	15:1P:40:LYS:HD3	1.82	0.60
1:2A:1126:U:N3	1:2A:1127:U:O4	2.34	0.60
1:2A:2022:A:H2'	1:2A:2023:G:C8	2.37	0.60
1:2A:955:A:H62	14:2O:12:GLN:HA	1.66	0.60
18:2S:29:SER:OG	18:2S:30:LYS:NZ	2.35	0.60
1:1A:1013:U:OP1	27:11:17:LYS:HG3	2.02	0.60
1:1A:2825:C:O3'	15:1P:99:LYS:NZ	2.35	0.60
5:1E:35:GLN:HB3	5:1E:48:GLN:HB3	1.84	0.60
1:1A:629:U:OP1	6:1F:102:PRO:HA	2.01	0.60
28:22:45:GLY:O	28:22:47:GLN:N	2.35	0.60
1:2A:231:U:OP1	32:26:6:THR:OG1	2.14	0.60
1:2A:2298:A:N6	1:2A:2355:U:H3	2.00	0.60
1:2A:2845:U:H2'	1:2A:2846:G:C8	2.37	0.60
1:2A:341:C:OP2	17:2R:39:ARG:NH2	166.36	0.59
9:2J:99:SER:O	9:2J:103:GLY:N	2.32	0.59
1:1A:830:A:H5'	1:1A:831:G:OP1	2.02	0.59
4:1D:242:ARG:O	63:1D:401:HOH:O	2.17	0.59
1:2A:1090:A:O4'	1:2A:1092:G:H8	1.85	0.59
4:1D:61:LEU:O	4:1D:63:ARG:NH1	2.35	0.59
1:2A:1386:U:OP1	1:2A:1442:U:N3	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2E:119:ARG:HB3	5:2E:120:TRP:CD1	2.37	0.59
1:1A:2763:G:H4'	8:1H:4:ILE:HD11	1.85	0.59
7:1G:5:VAL:HG13	7:1G:8:LYS:HE2	1.84	0.59
11:2L:15:LEU:HB2	11:2L:135:PRO:HB2	1.84	0.59
11:1L:130:HIS:HB3	11:1L:133:GLN:HE21	1.67	0.59
1:1A:2298:A:N6	1:1A:2355:U:H3	2.00	0.59
1:1A:2415:C:O3'	13:1N:77:ARG:NH2	2.35	0.59
1:2A:401:C:H2'	1:2A:402:C:C6	2.38	0.59
17:2R:55:ASN:N	17:2R:59:THR:HG22	2.17	0.59
21:2V:43:VAL:HG21	21:2V:81:VAL:HG11	1.84	0.59
13:1N:50:ARG:HD3	32:16:7:HIS:CD2	2.37	0.59
1:1A:1430:G:O2'	1:1A:1441:U:O2	2.18	0.59
1:2A:1233:A:OP2	63:2A:4930:HOH:O	2.17	0.59
1:2A:2230:G:H2'	1:2A:2231:G:H8	1.67	0.59
31:15:33:ARG:NH2	63:15:5001:HOH:O	2.21	0.59
1:1A:2338:A:H2'	1:1A:2339:A:C8	2.37	0.59
26:20:13:ALA:HA	26:20:16:LEU:HD12	1.83	0.59
4:2D:10:THR:OG1	4:2D:13:ARG:HG2	2.03	0.59
6:2F:34:TRP:CE2	13:2N:8:PRO:HG3	2.38	0.59
14:2O:57:HIS:O	14:2O:59:ARG:NH1	2.35	0.59
1:2A:2694:C:O2	12:2M:70:LYS:NZ	2.34	0.59
1:2A:1093:A:N1	1:2A:1157:G:O2'	2.32	0.59
3:2C:212:VAL:HG21	3:2C:226:PRO:HG3	1.85	0.59
1:1A:1009:C:H2'	1:1A:1010:G:H4'	4.29	0.58
1:1A:703:U:H2'	1:1A:704:C:C6	2.38	0.58
11:1L:73:THR:HG23	11:1L:82:LEU:HD11	1.85	0.58
1:2A:1649:C:OP1	63:2A:4931:HOH:O	2.17	0.58
1:2A:1597:C:H2'	1:2A:1598:G:O4'	2.03	0.58
1:2A:1816:A:H1'	1:2A:1959:A:N6	2.18	0.58
4:2D:148:GLU:HB2	4:2D:151:LYS:HD2	1.85	0.58
15:2P:97:VAL:HG22	15:2P:114:VAL:HG13	1.85	0.58
1:1A:2012:U:H2'	1:1A:2013:G:H5''	1.85	0.58
1:1A:636:U:O4	1:1A:736:G:O2'	77.70	0.58
3:1C:179:SER:HA	3:1C:180:PHE:C	2.23	0.58
6:1F:184:TYR:CE2	6:1F:188:ARG:HD2	2.37	0.58
13:1N:42:SER:O	63:1N:301:HOH:O	2.17	0.58
1:2A:1102:A:C6	1:2A:1131:A:H2'	2.39	0.58
1:2A:1450:U:H2'	1:2A:1451:U:C6	2.38	0.58
1:2A:2611:A:H2'	1:2A:2612:C:C6	2.38	0.58
9:2J:70:GLU:O	9:2J:72:ASP:N	2.32	0.58
28:12:56:VAL:O	28:12:60:GLN:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1107:G:OP1	1:1A:1115:A:H4'	2.02	0.58
22:1W:35:TYR:CE2	22:1W:69:ALA:HB3	2.39	0.58
3:2C:14:VAL:HG21	3:2C:32:LEU:HD21	1.85	0.58
1:1A:1078:U:OP1	33:17:9:ARG:NH2	2.37	0.58
1:1A:2459:A:OP1	63:1A:3860:HOH:O	2.17	0.58
1:2A:1000:G:OP2	14:2O:14:ARG:NH2	2.35	0.58
1:2A:1265:C:H2'	1:2A:1266:C:H6	1.68	0.58
1:2A:991:G:H2'	1:2A:992:G:H8	1.69	0.58
15:2P:57:ARG:HB3	15:2P:59:ASP:OD1	2.04	0.58
1:2A:2168:G:C2	1:2A:2169:G:H1'	2.38	0.58
1:2A:237:C:O2	32:26:12:LYS:NZ	2.28	0.58
1:1A:2148:G:N2	1:1A:2194:A:H1'	2.19	0.58
1:2A:1426:G:C8	17:2R:118:ARG:HG2	88.26	0.58
7:2G:25:TYR:HD2	7:2G:30:GLU:HB3	1.69	0.58
1:1A:1808:U:OP1	63:1A:3862:HOH:O	2.17	0.58
1:1A:930:C:H42	1:1A:937:G:H1	1.51	0.58
7:1G:47:LYS:HG3	7:1G:48:GLU:H	1.68	0.58
17:1R:127:ALA:O	17:1R:129:ARG:N	2.35	0.58
1:2A:645:A:OP2	13:2N:108:LYS:NZ	2.37	0.58
1:1A:1614:G:P	4:1D:63:ARG:HH22	2.27	0.58
1:1A:471:G:OP2	63:1A:3863:HOH:O	2.17	0.58
1:2A:1104:G:H1	1:2A:1124:C:N4	2.01	0.58
1:1A:1331:A:N6	1:1A:1356:G:N3	33.80	0.57
1:1A:402:C:OP1	63:1A:3864:HOH:O	2.17	0.57
1:2A:670:A:H2'	1:2A:671:G:O4'	2.03	0.57
1:2A:777:C:OP1	63:2A:4932:HOH:O	2.17	0.57
4:2D:275:LYS:HA	4:2D:276:LYS:C	2.23	0.57
5:2E:101:ARG:NH1	5:2E:169:ASN:O	2.37	0.57
1:1A:141:G:H1	1:1A:171:C:H42	51.24	0.57
1:1A:635:G:N2	1:1A:639:A:O2'	2.37	0.57
1:2A:2709:U:H2'	1:2A:2710:C:C6	2.39	0.57
1:2A:327:G:O6	63:2A:4922:HOH:O	2.14	0.57
10:2K:92:GLY:HA2	10:2K:132:ARG:HG2	1.85	0.57
3:1C:6:ARG:CZ	3:1C:218:MET:HB3	2.33	0.57
18:1S:78:THR:HG23	18:1S:117:GLN:HE22	1.69	0.57
1:2A:2023:G:N7	63:2A:4989:HOH:O	2.33	0.57
1:2A:2593:G:OP2	63:2A:4934:HOH:O	2.17	0.57
4:2D:24:ILE:HD13	4:2D:84:TYR:HB2	1.85	0.57
6:1F:9:ILE:HG21	6:1F:125:LEU:HD22	1.86	0.57
25:1Z:23:LYS:HB3	25:1Z:29:GLY:HA3	1.87	0.57
28:22:40:HIS:O	28:22:44:THR:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1697:G:H5'	15:2P:39:PRO:HG2	1.85	0.57
1:2A:943:C:H2'	1:2A:944:A:O4'	2.04	0.57
1:2A:81:G:O2'	1:2A:99:G:N2	2.37	0.57
1:2A:661:A:H8	13:2N:117:GLU:HG3	1.69	0.57
1:1A:2750:A:OP2	63:1A:3859:HOH:O	2.17	0.57
1:2A:200:G:H2'	1:2A:201:A:O4'	2.05	0.57
3:2C:41:VAL:HA	3:2C:216:THR:HA	1.85	0.57
6:2F:34:TRP:CZ2	13:2N:8:PRO:HG3	2.39	0.57
19:2T:4:ILE:HG22	19:2T:38:LEU:HD23	1.85	0.57
1:1A:1231:G:H5''	19:1T:81:TYR:CE1	2.40	0.57
1:1A:1500:U:OP1	15:1P:77:ARG:NH1	2.31	0.57
11:1L:62:VAL:HG13	11:1L:66:LYS:HD2	1.84	0.57
1:2A:1002:U:H5''	14:2O:14:ARG:HD3	1.87	0.57
1:2A:1087:G:O2'	1:2A:1088:C:OP1	2.20	0.57
1:2A:2137:G:H22	1:2A:2182:C:H5'	1.68	0.57
1:1A:772:G:N7	63:1A:3959:HOH:O	2.32	0.57
1:1A:82:A:H3'	22:1W:8:LYS:HG3	1.87	0.57
1:2A:1088:C:O2'	1:2A:1093:A:O2'	2.21	0.57
1:2A:2150:C:OP2	3:2C:6:ARG:NH1	2.37	0.57
1:2A:1039:C:OP1	18:2S:53:ARG:NH2	2.38	0.57
1:1A:2151:U:H4'	1:1A:2154:G:H5''	1.87	0.57
3:1C:186:ALA:HA	3:1C:189:ILE:HG22	1.87	0.57
1:2A:1345:U:H4'	1:2A:1346:A:H5''	1.87	0.57
1:2A:9:G:H2'	1:2A:10:G:C8	2.40	0.57
1:1A:2803:C:H2'	1:1A:2804:G:H8	1.69	0.57
15:1P:36:THR:HG22	15:1P:37:THR:H	1.70	0.57
21:2V:8:ILE:O	26:20:36:ARG:NH2	2.37	0.57
1:2A:1828:U:H5'	4:2D:259:THR:HG22	1.85	0.57
19:2T:76:LYS:HB2	19:2T:81:TYR:HB3	1.87	0.57
1:1A:1107:G:N2	1:1A:1121:C:H42	2.03	0.57
1:1A:2143:U:O2'	3:1C:166:ASP:OD2	2.21	0.57
10:1K:99:ILE:HG12	10:1K:103:GLN:NE2	2.20	0.57
1:2A:172:C:H2'	1:2A:173:U:C6	2.40	0.57
1:2A:629:U:OP1	6:2F:102:PRO:HA	2.05	0.57
1:1A:1404:A:N1	1:1A:1417:U:O4	2.38	0.56
3:2C:188:ASN:O	3:2C:188:ASN:ND2	2.38	0.56
1:2A:484:U:OP2	31:25:39:ARG:NH1	2.37	0.56
1:2A:2012:U:H2'	1:2A:2013:G:H5''	1.87	0.56
16:2Q:52:SER:HB2	16:2Q:55:ALA:H	1.69	0.56
1:1A:2848:G:H5'	15:1P:46:GLY:HA2	1.86	0.56
20:2U:38:TYR:HE2	29:23:40:LYS:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1227:G:O3'	27:21:29:ARG:NH1	2.38	0.56
1:2A:516:A:H2'	1:2A:517:G:O4'	2.06	0.56
1:2A:851:G:OP1	63:2A:4933:HOH:O	2.17	0.56
5:2E:55:ASN:HB3	5:2E:58:ARG:HG2	1.86	0.56
6:2F:7:TYR:O	6:2F:22:ALA:N	2.37	0.56
11:2L:96:GLU:HB2	11:2L:122:VAL:HG12	1.86	0.56
1:1A:2339:A:H2'	1:1A:2340:G:C8	2.41	0.56
1:1A:2698:U:H2'	1:1A:2699:U:O4'	2.05	0.56
7:1G:50:ALA:O	7:1G:52:ILE:N	2.39	0.56
26:20:9:GLN:HE22	26:20:56:GLN:HB3	1.70	0.56
1:1A:2803:C:H2'	1:1A:2804:G:C8	2.40	0.56
23:1X:144:LEU:HD21	23:1X:150:LEU:HD13	1.87	0.56
1:2A:2143:U:O4	1:2A:2197:A:N1	2.39	0.56
5:2E:24:THR:HG23	5:2E:186:GLY:O	2.05	0.56
1:1A:932:C:OP1	1:1A:932:C:H4'	2.06	0.56
21:1V:31:HIS:CD2	21:1V:33:LYS:H	2.23	0.56
1:2A:1123:U:H4'	1:2A:1133:A:H2	1.71	0.56
1:2A:1381:A:OP2	21:2V:64:LYS:HE3	2.05	0.56
1:2A:1439:U:O2	21:2V:16:LYS:NZ	2.35	0.56
1:2A:211:A:O2'	1:2A:446:C:O2	2.23	0.56
5:2E:128:SER:OG	5:2E:129:HIS:N	2.34	0.56
23:2X:63:ASP:OD2	23:2X:65:GLN:NE2	2.32	0.56
7:1G:129:GLY:O	7:1G:161:THR:HG22	2.05	0.56
25:1Z:64:ALA:HA	25:1Z:67:ILE:HG13	1.87	0.56
1:1A:2588:A:H5'	29:13:3:LYS:HD2	1.88	0.56
1:1A:330:G:H21	1:1A:353:A:N6	2.03	0.56
1:1A:931:C:H3'	1:1A:932:C:H5''	1.88	0.56
1:1A:2197:A:H5''	3:1C:215:THR:HG21	1.87	0.56
1:2A:2187:G:N7	1:2A:2189:G:N2	2.54	0.56
14:2O:118:LEU:HD12	14:2O:131:ILE:HG23	1.88	0.56
1:1A:1480:G:H21	1:1A:1524:G:H5'	1.70	0.56
7:1G:39:ILE:HG21	7:1G:60:LEU:HD11	1.87	0.56
22:1W:15:VAL:HG21	22:1W:42:VAL:HG11	1.86	0.56
33:27:15:LYS:HD3	33:27:26:ILE:HD11	1.87	0.56
6:2F:101:LEU:O	6:2F:106:ARG:NH1	2.39	0.56
17:2R:27:THR:HB	17:2R:90:GLN:HB3	1.87	0.56
22:1W:28:LYS:HD2	22:1W:40:GLU:HG3	1.87	0.56
1:2A:929:G:N2	1:2A:948:C:O2	26.74	0.56
1:1A:2041:A:O2'	1:1A:2042:C:H5'	2.06	0.55
1:1A:1479:A:H61	1:1A:1604:A:H62	1.52	0.55
1:1A:1953:A:H2'	1:1A:1954:G:O4'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:741:G:OP1	1:1A:1425:G:O2'	2.18	0.55
3:2C:179:SER:HA	3:2C:180:PHE:O	2.06	0.55
1:2A:2239:G:OP1	4:2D:261:LYS:NZ	2.38	0.55
1:1A:2587:G:OP1	63:1A:3861:HOH:O	2.17	0.55
1:2A:1833:A:O2'	4:2D:259:THR:HG21	2.06	0.55
4:2D:71:ASP:OD2	4:2D:103:ARG:NH2	2.39	0.55
6:2F:21:ALA:HB3	6:2F:22:ALA:HA	1.89	0.55
23:2X:146:ILE:H	23:2X:146:ILE:HD12	1.72	0.55
5:1E:12:THR:HG22	5:1E:13:ARG:H	1.72	0.55
1:2A:1042:G:OP2	18:2S:58:ARG:NH1	2.36	0.55
1:2A:1154:C:H2'	1:2A:1155:G:H8	3.41	0.55
1:2A:2226:G:H3'	1:2A:2227:G:C8	2.38	0.55
10:2K:88:ALA:O	10:2K:90:LYS:N	2.39	0.55
1:1A:258:A:H2'	1:1A:259:A:C8	3.03	0.55
1:1A:2765:A:N3	33:17:15:LYS:NZ	2.50	0.55
14:1O:16:ARG:HE	14:1O:18:LYS:HE3	1.71	0.55
22:1W:19:LYS:HE3	22:1W:20:TYR:CE1	2.41	0.55
25:1Z:65:SER:OG	25:1Z:66:HIS:ND1	2.38	0.55
1:2A:1081:G:H1	1:2A:1164:C:N4	2.04	0.55
1:2A:2187:G:H3'	1:2A:2188:U:H5''	1.89	0.55
1:2A:2043:U:O2'	1:2A:2628:C:H5'	2.07	0.55
1:2A:454:A:H3'	1:2A:455:A:C8	2.41	0.55
1:2A:596:C:N3	5:2E:145:LYS:NZ	2.43	0.55
1:1A:1313:A:H2'	1:1A:1314:A:O4'	2.07	0.55
1:1A:33:C:H5''	1:1A:34:G:OP2	2.06	0.55
7:1G:131:TYR:HB3	7:1G:159:VAL:HG13	1.88	0.55
22:1W:92:ASN:N	22:1W:93:GLY:HA2	2.20	0.55
1:2A:2401:U:P	32:26:35:GLN:HE22	2.30	0.55
1:2A:2155:A:N6	1:2A:2178:G:H4'	2.17	0.55
1:1A:117:U:OP2	63:1A:3865:HOH:O	2.18	0.55
4:1D:147:LEU:HD13	4:1D:155:LEU:HD11	1.88	0.55
1:1A:610:U:H1'	6:1F:90:PHE:HB3	1.89	0.55
13:1N:121:LYS:O	13:1N:123:LEU:N	2.40	0.55
29:23:41:PRO:HG2	29:23:44:THR:HG21	1.88	0.55
1:2A:2859:A:N7	1:2A:2877:A:O2'	2.34	0.55
6:2F:130:ALA:HB3	6:2F:142:TRP:HD1	1.72	0.55
1:1A:541:C:OP1	29:13:16:ARG:NH2	2.39	0.55
1:1A:1420:C:N4	63:1A:4002:HOH:O	2.39	0.55
1:1A:1716:C:OP1	63:1A:3820:HOH:O	2.18	0.55
1:1A:2131:G:C2	1:1A:2141:G:H1'	2.42	0.55
1:1A:925:G:H2'	1:1A:926:G:O4'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:3:LEU:O	7:1G:8:LYS:NZ	2.31	0.55
1:1A:2032:U:OP1	20:1U:42:ARG:NH1	2.39	0.55
1:2A:1159:G:H2'	1:2A:1160:G:H8	1.70	0.55
15:2P:67:LEU:HG	15:2P:76:VAL:HG21	1.88	0.55
1:1A:1633:C:H2'	1:1A:1634:C:C6	2.42	0.55
14:1O:59:ARG:HA	23:1X:180:VAL:HG23	1.89	0.55
1:2A:1188:A:OP1	11:2L:25:ARG:NH2	2.40	0.55
1:1A:2128:C:H42	1:1A:2203:G:H1	1.54	0.55
1:1A:2415:C:OP2	63:1A:3873:HOH:O	2.18	0.55
1:2A:1463:G:N7	63:2A:4990:HOH:O	2.33	0.55
1:2A:1699:G:H3'	15:2P:2:ARG:HD3	1.89	0.55
1:2A:800:C:H2'	1:2A:801:C:C6	2.41	0.55
23:2X:28:MET:HE1	23:2X:61:LEU:HD21	1.89	0.55
1:1A:1765:G:H5'	1:1A:1766:A:OP2	2.07	0.54
1:1A:596:C:N3	5:1E:145:LYS:NZ	2.52	0.54
3:1C:39:GLU:HG2	3:1C:217:THR:HB	1.87	0.54
5:1E:178:GLU:OE2	5:1E:178:GLU:N	2.37	0.54
9:1J:28:ASN:O	9:1J:30:GLN:N	2.40	0.54
14:1O:104:PHE:HE2	14:1O:125:LEU:HD11	1.72	0.54
25:1Z:80:LEU:HB3	25:1Z:82:LEU:HG	1.89	0.54
1:2A:894:G:C4	1:2A:977:A:H8	2.25	0.54
28:12:48:ARG:O	28:12:50:VAL:N	2.40	0.54
1:1A:238:G:P	32:16:13:ARG:HH22	2.30	0.54
1:1A:1994:G:OP1	63:1A:3870:HOH:O	2.18	0.54
3:1C:14:VAL:HG23	3:1C:32:LEU:HD21	1.88	0.54
3:1C:45:ALA:HA	3:1C:211:SER:O	2.07	0.54
1:1A:2583:A:N7	5:1E:144:ARG:HD2	2.22	0.54
13:2N:65:ARG:HG3	32:26:25:MET:HG3	1.88	0.54
6:2F:122:LYS:HE3	6:2F:191:ARG:HG2	1.88	0.54
31:15:34:ARG:NH1	31:15:41:ARG:O	2.40	0.54
1:1A:1341:G:OP1	1:1A:2720:G:O2'	2.16	0.54
1:1A:1451:U:H2'	1:1A:1452:C:C6	2.43	0.54
1:1A:1826:U:H2'	1:1A:1827:C:C6	2.42	0.54
1:1A:2463:C:OP1	23:1X:4:ARG:NH2	85.44	0.54
12:1M:36:GLY:HA3	12:1M:109:LYS:HD2	1.90	0.54
1:2A:1457:A:H2'	1:2A:1458:G:C8	2.42	0.54
1:2A:2473:U:H1'	1:2A:2502:U:O4	2.07	0.54
1:2A:309:C:H2'	1:2A:310:C:C6	2.42	0.54
1:2A:552:A:C2	1:2A:2063:A:H2'	2.42	0.54
1:2A:2735:C:OP2	5:2E:109:LYS:NZ	2.39	0.54
7:2G:28:VAL:O	7:2G:31:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1295:G:OP2	13:1N:21:ARG:NH1	2.41	0.54
1:1A:138:A:C8	1:1A:1453:C:O2'	2.60	0.54
1:1A:2456:G:N7	63:1A:3969:HOH:O	2.34	0.54
4:1D:168:ARG:H	4:1D:168:ARG:NH1	6.07	0.54
26:20:51:ARG:HH21	26:20:55:ARG:NH1	2.04	0.54
30:24:6:ARG:NH1	30:24:26:ASN:HB2	2.21	0.54
1:2A:1106:U:H4'	1:2A:1115:A:H1'	1.89	0.54
1:2A:894:G:N3	1:2A:977:A:H1'	2.22	0.54
2:2B:15:A:OP2	2:2B:69:G:N2	2.38	0.54
8:2H:69:ARG:HG3	8:2H:70:THR:N	2.22	0.54
11:2L:39:ARG:NH2	11:2L:41:ASP:OD2	2.40	0.54
1:1A:2709:U:H2'	1:1A:2710:C:C6	2.43	0.54
1:2A:599:G:O2'	1:2A:1299:A:OP1	2.24	0.54
1:2A:1386:U:OP2	1:2A:1439:U:O2'	2.17	0.54
1:2A:1632:A:H2'	1:2A:1633:C:C6	2.43	0.54
1:2A:1856:G:H4'	4:2D:242:ARG:CZ	2.37	0.54
1:2A:2339:A:H2'	1:2A:2340:G:C8	2.42	0.54
11:2L:4:TYR:CD2	18:2S:100:VAL:HG11	2.43	0.54
19:2T:6:LYS:HB2	19:2T:38:LEU:HD21	1.90	0.54
1:1A:1072:A:C2	1:1A:2499:A:H5'	2.42	0.54
1:1A:1219:U:O3'	1:1A:1220:G:H4'	2.07	0.54
22:1W:11:ASP:OD2	22:1W:97:ARG:NH2	2.40	0.54
1:2A:1404:A:N1	1:2A:1417:U:O4	2.40	0.54
12:2M:107:ARG:NE	17:2R:36:GLU:HG2	2.23	0.54
1:2A:82:A:H5''	22:2W:8:LYS:HG2	1.88	0.54
1:1A:1218:A:H1'	1:1A:1219:U:H5''	1.90	0.54
1:1A:551:C:C5	1:1A:2791:U:H2'	2.42	0.54
32:26:9:GLY:O	32:26:13:ARG:HG2	2.07	0.54
1:2A:1355:G:OP2	31:25:9:ARG:NH1	2.35	0.54
1:2A:860:C:H2'	1:2A:861:C:H6	1.73	0.54
3:2C:212:VAL:O	3:2C:224:ILE:HG12	2.08	0.54
3:2C:51:PRO:O	3:2C:53:ARG:N	2.37	0.54
23:2X:144:LEU:HD21	23:2X:150:LEU:HD13	1.90	0.54
1:1A:1512:G:H2'	1:1A:1593:C:H41	1.73	0.54
25:1Z:91:LYS:HG2	25:1Z:95:LEU:HD22	1.90	0.54
14:2O:35:VAL:HG12	14:2O:102:VAL:HG22	1.89	0.54
20:2U:79:GLY:HA3	20:2U:100:THR:HG22	1.89	0.54
1:1A:128:G:OP2	63:1A:3875:HOH:O	2.19	0.54
1:2A:1542:U:H5''	1:2A:1543:C:H5	1.73	0.54
1:1A:1107:G:H1	1:1A:1120:C:N4	2.06	0.54
1:1A:2254:U:H2'	1:1A:2255:U:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2323:U:H5'	7:1G:88:ILE:HD11	1.90	0.54
1:1A:2362:G:O6	32:16:39:LYS:HG3	2.08	0.54
1:1A:614:G:H2'	1:1A:615:G:C8	3.64	0.54
2:2B:33:G:H5'	7:2G:2:PRO:HD3	1.90	0.54
1:1A:1103:G:N2	1:1A:1126:U:H1'	2.23	0.53
1:1A:1198:C:H2'	1:1A:1199:G:O4'	2.08	0.53
1:1A:1903:C:H2'	1:1A:1904:G:O4'	2.08	0.53
12:1M:2:ILE:HD12	12:1M:6:THR:HG21	1.89	0.53
1:2A:713:U:O2	32:26:2:PRO:HD2	2.07	0.53
1:2A:1336:C:H2'	1:2A:1337:U:C6	2.44	0.53
1:2A:1417:U:H2'	1:2A:1418:A:H5'	1.89	0.53
1:2A:2127:G:H3'	1:2A:2128:C:C6	2.43	0.53
1:2A:1155:G:N3	1:2A:1155:G:H2'	2.23	0.53
1:2A:1457:A:H2'	1:2A:1458:G:H8	1.73	0.53
10:2K:77:LEU:HD12	10:2K:111:LYS:HE2	1.90	0.53
1:2A:1109:C:H4'	10:2K:89:HIS:HA	1.90	0.53
1:1A:1614:G:OP2	4:1D:63:ARG:NH2	2.41	0.53
1:1A:2563:U:OP2	63:1A:3871:HOH:O	2.18	0.53
1:1A:2578:G:H2'	1:1A:2579:C:C6	2.43	0.53
1:2A:1337:U:H2'	1:2A:1338:C:C6	2.43	0.53
1:2A:2127:G:C6	1:2A:2204:C:N3	2.77	0.53
3:2C:49:ILE:HB	3:2C:56:GLN:HB3	1.91	0.53
17:2R:18:ASP:OD1	17:2R:18:ASP:N	2.34	0.53
1:1A:1097:C:H2'	1:1A:1098:C:H6	1.72	0.53
1:1A:1113:G:N2	1:1A:1140:A:O2'	2.39	0.53
1:1A:2459:A:N6	63:1A:4023:HOH:O	2.42	0.53
1:2A:1159:G:H2'	1:2A:1160:G:C8	2.43	0.53
23:2X:45:ASP:O	23:2X:49:ARG:HG3	2.08	0.53
1:1A:2666:G:O2'	1:1A:2675:G:O6	2.22	0.53
12:1M:10:VAL:HG21	12:1M:16:ALA:HB3	1.91	0.53
1:2A:171:C:H2'	1:2A:172:C:H6	2.71	0.53
29:13:41:PRO:O	29:13:44:THR:OG1	2.21	0.53
1:1A:2858:U:O4	17:1R:23:ARG:NH2	2.42	0.53
1:1A:309:C:H2'	1:1A:310:C:C6	2.44	0.53
26:20:32:LEU:HD13	26:20:36:ARG:HH11	1.73	0.53
1:2A:1085:C:H2'	1:2A:1086:C:O4'	2.09	0.53
1:2A:1126:U:H5'	10:2K:125:ARG:HD3	1.91	0.53
1:2A:1512:G:N2	1:2A:1593:C:N3	2.56	0.53
1:2A:170:A:N3	1:2A:459:C:O2'	2.37	0.53
29:13:48:GLU:O	29:13:60:VAL:HG11	2.08	0.53
1:1A:236:G:H5'	1:1A:238:G:N7	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:651:A:H4'	1:1A:652:G:H5'	1.89	0.53
1:2A:1223:C:H2'	1:2A:1224:C:H6	1.73	0.53
1:2A:2020:C:H5''	1:2A:2735:C:O2'	2.09	0.53
1:2A:885:U:H1'	1:2A:1235:G:H1'	1.91	0.53
7:2G:50:ALA:O	7:2G:52:ILE:N	2.41	0.53
15:2P:36:THR:HG22	15:2P:37:THR:H	1.73	0.53
4:1D:85:ASP:OD2	4:1D:88:ARG:NH1	2.41	0.53
7:1G:106:LEU:HD12	7:1G:110:ALA:HB3	1.90	0.53
1:2A:2256:U:H5''	1:2A:2257:G:H5'	1.90	0.53
13:2N:95:VAL:HG23	13:2N:99:LEU:HD11	1.90	0.53
1:1A:1000:G:O6	63:1A:3855:HOH:O	2.16	0.53
12:1M:35:VAL:HG21	12:1M:105:GLU:HG3	1.91	0.53
21:1V:43:VAL:HG21	21:1V:81:VAL:HG11	1.91	0.53
23:1X:152:ALA:H	23:1X:171:ILE:HG12	1.73	0.53
1:2A:1424:A:H4'	1:2A:1425:G:OP2	2.08	0.53
1:2A:2483:G:H2'	1:2A:2486:C:H42	1.74	0.53
3:1C:68:LEU:HD13	3:1C:175:VAL:HG11	1.90	0.53
1:2A:1265:C:H2'	1:2A:1266:C:C6	2.43	0.53
1:2A:1323:A:OP1	15:2P:36:THR:HG23	2.09	0.53
1:2A:1358:U:OP1	63:2A:4938:HOH:O	2.19	0.53
1:2A:2323:U:H5'	7:2G:88:ILE:HD11	1.90	0.53
1:2A:991:G:H2'	1:2A:992:G:C8	2.44	0.53
3:2C:39:GLU:O	3:2C:178:ALA:N	2.42	0.53
1:1A:492:G:OP1	31:15:33:ARG:NH1	2.40	0.52
1:1A:931:C:H3'	1:1A:932:C:C5'	2.38	0.52
16:1Q:93:LYS:HE2	16:1Q:95:HIS:HB2	1.91	0.52
1:2A:1070:G:C4	1:2A:1179:C:H1'	2.44	0.52
1:2A:309:C:H2'	1:2A:310:C:H6	1.74	0.52
1:2A:948:C:H2'	1:2A:949:C:H6	1.74	0.52
1:1A:2146:G:O2'	1:1A:2194:A:N6	2.42	0.52
1:1A:1122:A:O2'	10:1K:132:ARG:O	2.20	0.52
1:2A:1138:G:C2'	1:2A:1143:A:H61	2.22	0.52
11:2L:14:VAL:HG13	11:2L:138:LEU:HB2	1.90	0.52
1:2A:1067:G:N7	11:2L:66:LYS:HE2	2.24	0.52
15:2P:33:ARG:HE	15:2P:113:LEU:HD22	1.73	0.52
26:10:31:GLU:HB2	26:10:53:LEU:HD11	1.91	0.52
1:1A:1188:A:OP1	11:1L:25:ARG:NH2	2.43	0.52
1:1A:1691:G:H5''	1:1A:1692:C:H5'	1.91	0.52
1:2A:1155:G:HO2'	1:2A:1156:A:H8	1.56	0.52
1:2A:1443:C:H2'	1:2A:1444:C:O4'	2.78	0.52
1:2A:1480:G:H2'	1:2A:1481:G:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2H:154:PRO:HB3	8:2H:163:TYR:CZ	2.45	0.52
1:1A:138:A:H8	1:1A:1453:C:O2'	1.93	0.52
1:1A:2016:U:OP1	63:1A:3868:HOH:O	2.18	0.52
1:1A:1715:A:H5''	1:1A:2561:G:OP1	2.09	0.52
1:1A:598:U:H2'	1:1A:599:G:C8	2.45	0.52
12:1M:115:VAL:HG13	12:1M:121:VAL:HG21	1.91	0.52
23:1X:152:ALA:O	23:1X:155:LEU:HB2	2.08	0.52
1:2A:1184:C:O3'	11:2L:25:ARG:NH1	2.43	0.52
1:2A:2118:C:H2'	1:2A:2119:U:O4'	2.09	0.52
5:2E:11:MET:CG	5:2E:24:THR:HG22	2.37	0.52
13:2N:101:VAL:HA	13:2N:106:LEU:O	2.09	0.52
14:2O:66:ILE:HG12	14:2O:104:PHE:CD1	2.44	0.52
29:13:20:ARG:HG2	29:13:23:HIS:CE1	2.45	0.52
1:1A:2204:C:H2'	1:1A:2205:G:C8	2.45	0.52
1:1A:921:G:H1	1:1A:947:C:H42	1.56	0.52
1:1A:437:G:C5	13:1N:72:PRO:HB3	2.45	0.52
1:2A:1092:G:O2'	1:2A:1155:G:O6	2.21	0.52
1:2A:955:A:N1	1:2A:2288:G:H1'	2.24	0.52
3:2C:211:SER:HB3	3:2C:213:TYR:HE2	1.73	0.52
1:2A:2478:C:H4'	14:2O:123:HIS:CD2	2.45	0.52
18:2S:27:LEU:HB3	18:2S:31:SER:HB3	1.91	0.52
18:2S:83:LEU:HG	18:2S:88:ILE:HB	1.92	0.52
1:1A:2622:U:C4	29:13:3:LYS:HG2	2.45	0.52
1:1A:932:C:H2'	1:1A:933:A:H5''	1.92	0.52
3:1C:59:ARG:HE	3:1C:164:ARG:HH22	1.57	0.52
2:2B:8:U:O2'	16:2Q:40:ILE:HD13	2.10	0.52
1:1A:814:G:O2'	1:1A:1424:A:N1	2.40	0.52
1:1A:1715:A:OP1	63:1A:3867:HOH:O	2.18	0.52
1:1A:1960:U:OP1	1:1A:2615:U:O2'	2.21	0.52
1:1A:2226:G:H3'	1:1A:2227:G:C8	2.44	0.52
9:1J:118:THR:O	9:1J:120:LYS:N	2.42	0.52
13:1N:82:GLY:HA2	13:1N:113:LYS:O	2.10	0.52
7:2G:108:ASN:HA	28:22:37:SER:HB2	1.90	0.52
1:2A:239:A:C5	1:2A:240:G:H1'	2.45	0.52
7:2G:115:ARG:HB3	7:2G:115:ARG:NH1	2.24	0.52
8:2H:56:SER:HB3	8:2H:61:HIS:ND1	2.25	0.52
26:10:32:LEU:HD13	26:10:36:ARG:HH11	1.75	0.52
32:16:28:GLY:O	32:16:36:LYS:NZ	2.36	0.52
1:1A:1153:U:O2'	1:1A:1154:C:H5''	2.10	0.52
1:1A:1855:A:OP1	4:1D:249:PRO:HD3	2.10	0.52
1:2A:590:U:O4	63:2A:4936:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2F:36:VAL:HG11	6:2F:183:VAL:HG11	1.92	0.52
17:2R:50:ILE:HA	17:2R:99:LEU:HD12	1.90	0.52
28:12:53:GLU:HB3	28:12:54:GLY:HA2	1.91	0.52
1:1A:2574:U:H4'	12:1M:28:SER:HA	1.92	0.52
23:1X:7:ALA:O	23:1X:62:PRO:HD3	2.09	0.52
1:2A:1136:G:H2'	1:2A:1137:C:O4'	2.10	0.52
1:2A:1520:C:H2'	1:2A:1521:G:H8	1.73	0.52
1:2A:639:A:C4	6:2F:180:GLY:HA3	2.45	0.52
1:2A:806:G:OP1	63:2A:4937:HOH:O	2.19	0.52
7:2G:145:THR:HG22	7:2G:148:MET:SD	2.50	0.52
1:1A:1833:A:O2'	4:1D:259:THR:HG21	2.09	0.52
1:1A:2139:U:OP1	1:1A:2169:G:H4'	2.09	0.52
20:2U:38:TYR:CE2	29:23:41:PRO:HD3	2.45	0.52
1:2A:1561:U:H2'	1:2A:1562:G:H8	1.75	0.52
1:2A:1648:A:OP1	63:2A:4940:HOH:O	2.19	0.52
1:2A:554:G:C5	1:2A:2043:U:H5''	2.44	0.52
7:2G:70:VAL:HA	7:2G:90:LEU:HD23	1.92	0.52
17:2R:117:ASP:OD2	17:2R:120:ARG:NE	2.42	0.52
1:1A:1085:C:H2'	1:1A:1086:C:O4'	2.11	0.51
1:1A:1116:G:O2'	1:1A:1134:G:H2'	2.10	0.51
1:1A:1345:U:H4'	1:1A:1346:A:H5''	1.92	0.51
1:1A:904:U:O2	1:1A:2279:A:H2'	2.10	0.51
3:1C:10:LEU:HD22	3:1C:32:LEU:HA	1.91	0.51
6:1F:150:GLY:HA2	6:1F:172:TRP:CE3	2.45	0.51
9:1J:65:GLU:O	9:1J:67:GLY:N	2.43	0.51
1:2A:1349:C:H2'	1:2A:1350:C:C6	3.21	0.51
3:2C:33:ALA:HB2	3:2C:216:THR:HG21	1.92	0.51
4:2D:8:PRO:HB3	4:2D:14:ARG:HB2	1.92	0.51
5:2E:9:VAL:HG13	5:2E:25:VAL:O	2.10	0.51
10:2K:99:ILE:HG22	10:2K:103:GLN:HB2	1.92	0.51
1:1A:604:G:H2'	1:1A:605:G:C8	2.45	0.51
7:1G:41:GLN:HB3	7:1G:43:LEU:HD13	1.92	0.51
11:1L:48:MET:HE2	11:1L:48:MET:H	1.75	0.51
15:1P:38:VAL:HG22	15:1P:112:ALA:HB2	1.90	0.51
1:2A:1072:A:C6	1:2A:1171:A:C4	2.99	0.51
1:2A:141:G:H2'	1:2A:142:C:C6	2.46	0.51
1:2A:212:G:H2'	1:2A:213:A:O4'	2.10	0.51
1:2A:2129:C:H2'	1:2A:2130:U:C6	2.46	0.51
1:2A:2307:U:OP2	16:2Q:9:ARG:NH2	2.34	0.51
1:2A:344:G:OP2	6:2F:135:LYS:HE2	2.09	0.51
26:10:9:GLN:HE22	26:10:56:GLN:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1129:A:N3	1:1A:1150:U:O2'	2.41	0.51
1:1A:1402:U:H2'	1:1A:1403:G:O4'	2.10	0.51
11:1L:128:HIS:O	11:1L:131:GLN:NE2	2.44	0.51
1:2A:1199:G:O5'	1:2A:1199:G:H8	1.93	0.51
13:2N:52:GLU:HG2	32:26:57:ARG:HH22	1.75	0.51
23:2X:180:VAL:HA	23:2X:183:LEU:HD22	1.91	0.51
1:1A:1153:U:H6	1:1A:1154:C:C6	2.28	0.51
1:1A:775:G:C8	4:1D:208:LYS:HD2	2.45	0.51
5:1E:128:SER:OG	5:1E:129:HIS:N	2.42	0.51
6:1F:150:GLY:HA2	6:1F:172:TRP:CD2	2.46	0.51
28:22:59:PHE:N	28:22:60:GLN:HB2	2.26	0.51
1:2A:1765:G:H8	1:2A:1769:A:N6	2.04	0.51
1:2A:322:A:N1	1:2A:345:A:O2'	2.34	0.51
3:2C:42:GLU:HB2	3:2C:44:HIS:NE2	2.26	0.51
5:2E:47:VAL:HG11	5:2E:86:PRO:HD2	1.92	0.51
10:2K:76:TYR:O	10:2K:80:LYS:NZ	2.28	0.51
1:1A:1311:G:O5'	20:1U:15:ARG:NH2	2.44	0.51
1:1A:183:A:C8	1:1A:185:A:OP1	2.63	0.51
1:1A:2583:A:C8	5:1E:144:ARG:HD2	2.46	0.51
1:1A:1109:C:H4'	10:1K:86:LYS:HE3	1.91	0.51
15:1P:96:ARG:NH1	15:1P:115:GLU:OE1	2.42	0.51
1:1A:398:G:OP2	25:1Z:69:LYS:HE2	2.11	0.51
28:22:40:HIS:HB3	28:22:43:TYR:HB2	1.92	0.51
33:27:2:LYS:HE2	33:27:31:LYS:O	2.11	0.51
5:2E:111:ARG:HG3	5:2E:160:TYR:CD2	2.46	0.51
15:1P:67:LEU:HD13	15:1P:76:VAL:HG21	1.91	0.51
1:2A:1101:G:H5''	1:2A:1102:A:H5'	1.93	0.51
1:2A:1154:C:H2'	1:2A:1155:G:C8	3.05	0.51
1:2A:1920:G:N3	1:2A:1920:G:H2'	2.26	0.51
1:2A:471:G:OP2	1:2A:471:G:H8	1.94	0.51
1:1A:2172:G:H2'	1:1A:2173:G:C8	2.45	0.51
27:21:26:LEU:O	27:21:35:ARG:NE	2.44	0.51
1:2A:1828:U:OP2	4:2D:274:ARG:NH2	2.44	0.51
1:2A:1853:G:OP1	4:2D:54:ARG:NH1	2.44	0.51
1:2A:353:A:H2	1:2A:1254:A:HO2'	1.57	0.51
18:2S:49:HIS:O	18:2S:53:ARG:N	2.44	0.51
1:1A:2187:G:N7	1:1A:2189:G:N2	2.59	0.51
1:1A:277:G:OP1	25:1Z:76:ARG:NE	2.36	0.51
1:1A:924:A:H2'	1:1A:925:G:C8	4.44	0.51
6:1F:164:ARG:HD2	6:1F:175:THR:HG23	1.93	0.51
7:1G:33:ARG:O	7:1G:161:THR:OG1	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1T:40:LEU:HB2	19:1T:46:VAL:HG13	1.92	0.51
1:2A:2226:G:H5''	1:2A:2227:G:N7	2.26	0.51
1:2A:2688:G:H2'	1:2A:2689:C:C6	2.44	0.51
1:2A:267:G:HO2'	1:2A:268:G:H8	1.59	0.51
1:2A:719:C:H5''	6:2F:81:PRO:HD2	1.93	0.51
18:2S:52:ARG:HA	18:2S:55:ARG:HG3	1.92	0.51
1:1A:1076:G:H21	33:17:36:GLN:HE22	1.58	0.51
1:1A:2174:G:H2'	1:1A:2175:G:H8	1.76	0.51
4:1D:27:THR:O	4:1D:27:THR:OG1	2.28	0.51
8:1H:28:GLY:HA3	8:1H:79:VAL:HB	1.93	0.51
16:1Q:30:ARG:HG3	16:1Q:35:ILE:HD12	1.93	0.51
20:1U:29:LEU:HD22	20:1U:69:LEU:HD12	1.93	0.51
23:1X:92:SER:O	23:1X:130:PRO:HG2	2.11	0.51
1:2A:1565:U:H2'	1:2A:1566:G:O4'	2.10	0.51
1:2A:195:A:H2'	1:2A:196:C:O4'	2.10	0.51
1:2A:2198:C:H2'	1:2A:2199:C:O4'	2.11	0.51
1:2A:553:A:H62	1:2A:2062:U:H3	1.59	0.51
1:2A:847:G:O6	6:2F:53:THR:OG1	2.29	0.51
1:2A:894:G:N9	1:2A:977:A:H8	2.09	0.51
3:2C:3:HIS:HA	3:2C:7:TYR:HB3	1.93	0.51
3:1C:43:VAL:HG22	3:1C:214:VAL:HG22	1.92	0.51
10:1K:88:ALA:O	10:1K:90:LYS:N	2.44	0.51
1:2A:94:G:H4'	26:20:48:HIS:CD2	2.46	0.51
1:2A:1194:G:H2'	1:2A:1195:C:C6	2.46	0.51
1:2A:82:A:N1	1:2A:96:G:O2'	2.32	0.51
7:2G:145:THR:HG23	7:2G:147:ASP:H	1.75	0.51
25:2Z:89:GLU:O	25:2Z:93:GLU:HG2	2.11	0.51
1:1A:885:U:H1'	1:1A:1235:G:H1'	1.93	0.50
1:1A:1951:G:O2'	1:1A:1989:G:O6	2.20	0.50
1:1A:2063:A:OP1	63:1A:3877:HOH:O	2.19	0.50
1:1A:2123:U:H2'	1:1A:2124:C:C6	2.44	0.50
1:1A:552:A:O2'	1:1A:553:A:H5'	2.11	0.50
3:1C:47:LEU:O	3:1C:210:ARG:HD3	2.10	0.50
1:2A:1826:U:H2'	1:2A:1827:C:C6	2.46	0.50
1:2A:1994:G:H2'	1:2A:1995:C:C6	2.46	0.50
1:2A:524:G:N2	1:2A:526:A:H3'	2.26	0.50
1:2A:908:G:H2'	1:2A:909:A:O4'	2.12	0.50
28:12:63:TYR:N	28:12:64:GLY:HA2	2.24	0.50
1:1A:1295:G:N7	13:1N:18:ARG:NH2	2.59	0.50
1:1A:1729:C:H2'	1:1A:1730:C:C6	2.46	0.50
1:1A:1986:C:H3'	1:1A:1987:A:H2'	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2095:U:OP1	63:1A:3874:HOH:O	2.18	0.50
1:2A:1207:G:H2'	1:2A:1208:G:H8	1.77	0.50
1:2A:1354:G:P	31:25:9:ARG:HD3	2.51	0.50
1:2A:1525:G:O2'	1:2A:1604:A:H5'	2.10	0.50
1:2A:2155:A:H3'	1:2A:2156:A:H8	1.76	0.50
1:2A:2176:G:C5	1:2A:2177:G:H1'	2.46	0.50
1:2A:2176:G:H2'	1:2A:2177:G:O4'	2.10	0.50
1:2A:2331:A:H2'	1:2A:2331:A:N3	2.27	0.50
2:2B:90:A:N7	2:2B:91:C:H1'	2.26	0.50
6:2F:153:SER:N	6:2F:190:GLU:OE2	2.33	0.50
6:2F:53:THR:HG22	6:2F:56:GLU:HG3	1.93	0.50
12:2M:2:ILE:HD12	12:2M:6:THR:HG21	1.92	0.50
19:2T:62:LEU:HD11	19:2T:95:LEU:HD12	1.91	0.50
1:1A:1218:A:H4'	1:1A:1219:U:OP1	2.10	0.50
1:1A:1357:U:H4'	1:1A:1358:U:O5'	2.11	0.50
1:1A:2018:G:N7	63:1A:3976:HOH:O	2.35	0.50
1:1A:2348:G:OP1	63:1A:3879:HOH:O	2.20	0.50
3:1C:171:ILE:HG23	3:1C:172:HIS:H	1.76	0.50
4:1D:68:LYS:O	4:1D:70:TRP:N	2.39	0.50
8:1H:69:ARG:HG3	8:1H:70:THR:N	2.26	0.50
12:1M:87:ILE:HD12	12:1M:91:LEU:HA	1.93	0.50
13:2N:63:PRO:HG2	32:26:25:MET:HB2	1.93	0.50
1:2A:1828:U:OP2	4:2D:273:ARG:NH2	2.44	0.50
1:2A:2186:G:H1	1:2A:2193:U:H5	1.58	0.50
1:2A:361:G:O6	63:2A:4935:HOH:O	2.18	0.50
5:2E:135:HIS:NE2	63:2E:401:HOH:O	2.34	0.50
6:2F:150:GLY:HA2	6:2F:172:TRP:CE3	2.46	0.50
1:1A:1845:A:H8	1:1A:1845:A:OP1	1.95	0.50
1:1A:2235:G:H4'	1:1A:2237:C:C2	2.47	0.50
1:1A:468:A:H5''	1:1A:469:C:OP1	2.12	0.50
4:1D:12:SER:HB3	4:1D:208:LYS:HB3	1.92	0.50
19:1T:23:GLU:OE1	19:1T:89:GLN:NE2	2.45	0.50
1:1A:2100:U:O3'	25:1Z:35:THR:OG1	2.28	0.50
1:2A:724:C:H2'	1:2A:725:C:C6	2.47	0.50
6:2F:167:ALA:HB1	6:2F:173:VAL:HG11	1.93	0.50
10:2K:80:LYS:H	10:2K:80:LYS:HE2	1.76	0.50
1:1A:35:G:N3	1:1A:475:G:O2'	2.41	0.50
1:1A:719:C:H5''	6:1F:81:PRO:HD2	1.94	0.50
23:1X:158:PRO:O	23:1X:161:VAL:HG12	2.12	0.50
1:2A:1224:C:H2'	1:2A:1225:C:C6	2.47	0.50
1:2A:1687:A:H2'	1:2A:1688:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1953:A:H2'	1:2A:1954:G:O4'	2.12	0.50
5:2E:143:ASN:HD22	5:2E:147:PRO:HD3	1.75	0.50
1:2A:2505:G:H4'	14:2O:80:GLU:HG2	1.93	0.50
26:10:53:LEU:O	26:10:57:ILE:HG13	2.11	0.50
1:1A:1066:A:H2'	1:1A:1068:U:H5'	1.92	0.50
1:1A:1066:A:H62	1:1A:1185:U:H3	1.60	0.50
1:1A:1261:C:OP1	18:1S:15:LYS:NZ	2.37	0.50
1:1A:1816:A:H1'	1:1A:1959:A:N6	2.26	0.50
1:1A:2144:G:OP1	3:1C:164:ARG:HD3	2.12	0.50
1:1A:2244:U:H2'	1:1A:2245:G:C8	2.47	0.50
1:1A:235:G:H4'	1:1A:412:G:C5	2.46	0.50
1:1A:2548:U:H2'	1:1A:2549:C:C6	2.46	0.50
2:1B:45:A:OP2	7:1G:96:ARG:NH2	2.43	0.50
7:1G:137:GLU:HG2	7:1G:152:LEU:HD13	1.93	0.50
15:1P:57:ARG:HB3	15:1P:59:ASP:OD1	2.11	0.50
20:1U:18:ARG:NH1	20:1U:76:VAL:O	2.45	0.50
1:2A:1824:U:H2'	1:2A:1825:C:C6	2.47	0.50
1:2A:2156:A:C6	1:2A:2157:C:N4	2.80	0.50
1:2A:2427:C:H2'	1:2A:2428:C:H6	1.77	0.50
1:2A:2142:G:N2	3:2C:168:THR:OG1	2.45	0.50
23:2X:93:ASP:HA	23:2X:131:ARG:NH2	2.26	0.50
1:1A:554:G:C5	1:1A:2043:U:H5''	2.47	0.50
1:1A:302:C:H42	1:1A:384:G:H1	1.59	0.50
1:1A:2740:U:H5'	12:1M:70:LYS:HZ1	1.77	0.50
24:1Y:53:MET:HG3	24:1Y:59:LEU:HD23	1.94	0.50
1:2A:1603:C:OP2	1:2A:1604:A:O2'	2.24	0.50
3:2C:22:ILE:HG21	3:2C:190:ARG:HG3	1.92	0.50
18:2S:97:ASP:OD1	18:2S:101:ARG:HD2	2.12	0.50
1:1A:1664:G:N7	63:1A:3974:HOH:O	2.34	0.50
1:1A:2406:C:O2'	25:1Z:30:VAL:HG13	2.12	0.50
1:2A:174:G:H2'	1:2A:175:G:H8	1.75	0.50
1:2A:2173:G:H2'	1:2A:2174:G:O4'	2.12	0.50
1:2A:2356:G:N3	1:2A:2392:C:H2'	2.27	0.50
1:2A:2698:U:H2'	1:2A:2699:U:O4'	2.12	0.50
2:2B:46:A:H2'	2:2B:47:C:C6	2.47	0.50
5:2E:170:LEU:HB3	5:2E:184:VAL:HG22	1.93	0.50
6:2F:101:LEU:HD12	6:2F:102:PRO:HD2	1.93	0.50
21:2V:12:VAL:HG22	21:2V:29:TRP:CE2	2.46	0.50
24:2Y:11:ARG:O	24:2Y:14:ARG:NH2	2.44	0.50
1:1A:1065:A:N1	1:1A:1185:U:O2'	2.34	0.50
1:1A:2167:C:O2	1:1A:2168:G:N1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2227:G:O2'	1:1A:2228:A:OP1	2.30	0.50
1:1A:833:U:H5''	1:1A:834:A:H5'	1.94	0.50
1:2A:2371:A:H2'	1:2A:2372:A:O4'	2.11	0.50
1:2A:37:A:H2'	1:2A:38:C:C6	2.47	0.50
4:2D:208:LYS:HG3	4:2D:211:ARG:H	1.76	0.50
17:2R:16:ARG:HD2	17:2R:19:LEU:HG	1.94	0.50
1:1A:1153:U:O2'	1:1A:1154:C:H6	1.94	0.49
1:1A:1514:C:OP1	63:1A:3881:HOH:O	2.20	0.49
1:1A:1792:A:H2'	63:1A:4565:HOH:O	2.12	0.49
1:1A:2659:C:H2'	1:1A:2660:U:H6	1.76	0.49
1:2A:1223:C:H2'	1:2A:1224:C:C6	2.47	0.49
1:2A:1586:U:H2'	1:2A:1587:G:O4'	2.12	0.49
1:2A:1735:A:N6	1:2A:1744:A:H2	2.02	0.49
6:2F:120:GLU:HB2	6:2F:122:LYS:HG2	1.93	0.49
1:2A:2573:U:H1'	12:2M:23:ARG:HH11	1.76	0.49
23:2X:24:LEU:HD12	23:2X:25:PRO:HD2	1.93	0.49
27:11:18:ASP:N	27:11:18:ASP:OD1	2.44	0.49
1:1A:1066:A:H3'	1:1A:1066:A:C8	2.47	0.49
1:1A:1140:A:H2'	1:1A:1141:A:C8	2.47	0.49
10:1K:98:ARG:HB3	10:1K:137:GLU:HG3	1.94	0.49
12:1M:23:ARG:HG3	12:1M:24:VAL:N	2.27	0.49
15:1P:104:ARG:HG3	15:1P:111:LEU:HD21	1.94	0.49
18:1S:58:ARG:HA	18:1S:61:TRP:CE3	2.48	0.49
1:2A:1103:G:N2	1:2A:1126:U:O2'	2.45	0.49
1:2A:1210:U:H2'	1:2A:1211:C:C6	2.47	0.49
1:2A:1280:G:OP1	63:2A:4941:HOH:O	2.20	0.49
1:2A:2472:C:H2'	1:2A:2473:U:C6	2.47	0.49
1:2A:2503:U:H2'	1:2A:2504:U:C6	2.48	0.49
8:2H:96:ALA:HB1	8:2H:103:LEU:HD11	1.94	0.49
1:1A:518:G:H4'	20:1U:6:ILE:HB	1.95	0.49
1:2A:1250:G:H2'	1:2A:1251:C:C6	2.46	0.49
1:2A:1473:C:N4	1:2A:1616:A:OP2	2.44	0.49
1:2A:1753:G:H1	1:2A:1781:C:H42	1.60	0.49
1:2A:2356:G:OP2	30:24:38:LYS:HG3	2.12	0.49
1:2A:2544:A:OP1	1:2A:2676:A:O2'	2.25	0.49
1:2A:2735:C:H5''	15:2P:1:MET:HE2	1.95	0.49
1:1A:224:C:H2'	1:1A:225:C:C6	2.47	0.49
1:1A:2657:C:OP2	1:1A:2744:G:O2'	2.24	0.49
4:1D:71:ASP:OD2	4:1D:103:ARG:NH2	2.45	0.49
9:1J:73:GLY:O	9:1J:75:GLN:N	2.45	0.49
14:2O:29:PHE:HB2	14:2O:105:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2174:G:H2'	1:1A:2175:G:C8	2.48	0.49
1:2A:1356:G:H5''	7:2G:36:LYS:HB2	145.47	0.49
1:2A:1404:A:H5'	1:2A:1404:A:N3	2.27	0.49
1:2A:1500:U:OP1	15:2P:77:ARG:NH1	2.43	0.49
1:2A:1561:U:H2'	1:2A:1562:G:C8	2.48	0.49
11:2L:111:PRO:HA	11:2L:114:ARG:NH1	2.27	0.49
24:2Y:36:ILE:HD12	24:2Y:58:THR:HG21	1.95	0.49
25:2Z:21:ARG:HD3	25:2Z:35:THR:HG21	1.95	0.49
1:1A:1633:C:H2'	1:1A:1634:C:H6	1.76	0.49
1:1A:624:G:O2'	1:1A:701:A:N6	2.45	0.49
3:1C:6:ARG:NE	3:1C:218:MET:O	2.45	0.49
14:1O:64:ILE:HG13	23:1X:178:GLU:HG3	1.93	0.49
23:1X:4:ARG:HG2	23:1X:58:VAL:HG13	1.95	0.49
29:23:29:THR:O	29:23:30:LEU:HD23	2.13	0.49
1:2A:945:A:O2'	1:2A:946:A:OP1	2.26	0.49
4:2D:153:ALA:O	4:2D:157:ARG:NH1	2.45	0.49
7:2G:101:ILE:HG22	7:2G:105:LYS:HE2	1.93	0.49
7:2G:7:LEU:HD23	7:2G:100:TRP:HE3	1.78	0.49
9:2J:49:ALA:N	9:2J:90:ALA:HB1	2.27	0.49
1:1A:846:A:OP1	1:1A:846:A:H8	1.95	0.49
3:1C:26:ALA:HA	3:1C:29:VAL:HG22	1.93	0.49
1:2A:2503:U:H2'	1:2A:2504:U:H6	1.77	0.49
7:2G:38:VAL:HG22	7:2G:93:THR:HG23	1.94	0.49
8:2H:7:LEU:HD23	8:2H:69:ARG:CZ	2.43	0.49
15:2P:55:ALA:HB2	15:2P:79:LEU:HD13	1.94	0.49
17:2R:107:ASP:HA	17:2R:110:ILE:HD12	1.94	0.49
32:16:23:VAL:HG11	32:16:47:LYS:HD3	1.94	0.49
1:1A:1222:C:H2'	1:1A:1223:C:C6	2.48	0.49
1:1A:1404:A:N3	1:1A:1404:A:H5'	2.28	0.49
1:1A:1848:U:H2'	4:1D:157:ARG:HG3	1.94	0.49
1:1A:955:A:N1	1:1A:2288:G:H1'	2.28	0.49
8:1H:20:ALA:HB1	8:1H:21:PRO:HD2	1.94	0.49
1:1A:1357:U:OP2	21:1V:63:LYS:HD2	2.13	0.49
25:1Z:19:GLN:HB3	25:1Z:35:THR:HG23	1.95	0.49
1:2A:2813:C:H2'	1:2A:2814:C:H6	1.76	0.49
1:2A:346:G:O2'	1:2A:1249:U:N3	2.26	0.49
5:2E:34:VAL:HG21	5:2E:78:LEU:HD11	1.95	0.49
1:2A:2330:G:N2	16:2Q:3:ARG:HA	2.27	0.49
2:2B:37:C:O2	16:2Q:95:HIS:NE2	2.46	0.49
21:2V:40:LYS:HG3	21:2V:51:VAL:HB	1.95	0.49
28:12:24:THR:OG1	28:12:25:TYR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1450:U:H2'	1:1A:1451:U:C6	2.48	0.49
1:1A:670:A:H2'	1:1A:671:G:O4'	2.12	0.49
1:1A:908:G:H2'	1:1A:909:A:O4'	2.13	0.49
22:1W:77:PRO:HD3	22:1W:106:LEU:HD23	1.94	0.49
28:22:59:PHE:HA	28:22:61:ARG:H	1.75	0.49
1:2A:1150:U:H2'	1:2A:1151:G:C8	2.47	0.49
1:2A:2284:A:O2'	1:2A:2285:A:H5'	2.13	0.49
1:2A:2286:C:H6	1:2A:2286:C:H5'	1.78	0.49
1:2A:33:C:H5''	1:2A:34:G:OP2	2.13	0.49
20:2U:12:ILE:HD13	20:2U:17:VAL:HG13	1.95	0.49
23:2X:110:GLY:HA3	23:2X:174:VAL:HG11	1.94	0.49
1:1A:1337:U:H2'	1:1A:1338:C:C6	2.47	0.49
1:1A:1809:U:H2'	63:1A:4171:HOH:O	2.12	0.49
1:2A:2661:U:H2'	1:2A:2662:C:C6	2.48	0.49
4:2D:106:ILE:O	4:2D:108:PRO:HD3	2.13	0.49
4:2D:108:PRO:HD2	4:2D:111:LEU:HG	1.95	0.49
1:1A:1383:G:N7	21:1V:62:LYS:NZ	2.44	0.48
1:1A:1559:U:H2'	1:1A:1560:C:C6	2.47	0.48
1:1A:699:A:H2'	1:1A:700:A:C8	3.36	0.48
4:1D:72:LYS:HD3	4:1D:97:TYR:CE2	2.48	0.48
6:1F:135:LYS:HB2	6:1F:138:GLU:CD	2.34	0.48
6:1F:185:ASP:OD1	6:1F:188:ARG:NH1	2.39	0.48
14:1O:57:HIS:HD2	14:1O:117:ALA:HB2	1.77	0.48
13:2N:62:LEU:HD11	32:26:50:LEU:HD11	1.95	0.48
1:2A:552:A:OP2	11:2L:114:ARG:NH1	2.46	0.48
1:2A:906:U:C2	1:2A:2279:A:C8	3.01	0.48
3:2C:211:SER:HB3	3:2C:213:TYR:CE2	2.48	0.48
13:2N:50:ARG:HD3	32:26:7:HIS:CD2	2.48	0.48
17:2R:77:PRO:HB2	17:2R:80:SER:HB2	1.94	0.48
18:2S:92:ARG:HA	18:2S:95:LEU:HB2	1.95	0.48
1:1A:1000:G:OP2	14:1O:14:ARG:NH2	2.46	0.48
1:1A:1070:G:C4	1:1A:1179:C:H1'	2.49	0.48
1:1A:2122:G:H2'	1:1A:2123:U:O4'	2.13	0.48
1:1A:2443:A:OP2	63:1A:3883:HOH:O	2.20	0.48
22:1W:102:CYS:SG	22:1W:103:GLY:N	2.86	0.48
29:23:20:ARG:HA	29:23:23:HIS:CD2	2.48	0.48
1:2A:172:C:H2'	1:2A:173:U:H6	1.78	0.48
1:2A:1808:U:H2'	1:2A:1814:A:N6	2.27	0.48
1:2A:224:C:H2'	1:2A:225:C:H6	1.78	0.48
1:2A:775:G:C8	4:2D:208:LYS:HD3	2.48	0.48
17:2R:19:LEU:HD13	17:2R:86:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:16:31:HIS:ND1	32:16:32:LEU:HD13	2.28	0.48
1:1A:267:G:HO2'	1:1A:268:G:H8	1.60	0.48
1:1A:2700:U:H4'	1:1A:2701:C:H5'	1.93	0.48
3:1C:166:ASP:OD1	3:1C:170:ALA:HB3	2.13	0.48
7:1G:3:LEU:HD13	7:1G:5:VAL:HG12	1.95	0.48
1:2A:1018:G:C6	1:2A:1230:G:C6	3.01	0.48
1:2A:263:G:C6	1:2A:264:U:C4	3.01	0.48
1:2A:800:C:H2'	1:2A:801:C:H6	1.77	0.48
1:2A:927:G:H2'	1:2A:928:G:O4'	2.14	0.48
8:2H:90:LYS:HD2	8:2H:163:TYR:CD1	2.49	0.48
16:2Q:15:ARG:HB3	16:2Q:19:LYS:NZ	2.27	0.48
1:1A:1113:G:O2'	1:1A:1141:A:O2'	2.12	0.48
1:1A:22:G:H2'	1:1A:23:G:C8	2.95	0.48
1:1A:790:G:OP1	5:1E:132:HIS:ND1	2.47	0.48
21:1V:35:THR:HG23	21:1V:38:GLU:HB2	1.95	0.48
24:1Y:18:ALA:HB3	24:1Y:20:ARG:HH21	1.78	0.48
1:2A:2529:A:OP2	63:2A:4942:HOH:O	2.20	0.48
4:2D:96:HIS:CD2	4:2D:102:LYS:HG2	2.47	0.48
6:2F:21:ALA:CB	6:2F:22:ALA:HA	2.44	0.48
1:2A:1107:G:H4'	10:2K:133:SER:HB3	1.94	0.48
15:2P:56:LYS:NZ	15:2P:90:ARG:O	2.47	0.48
23:2X:152:ALA:O	23:2X:155:LEU:HB2	2.13	0.48
1:2A:1048:G:O2'	1:2A:1055:A:N1	2.33	0.48
1:2A:1336:C:H2'	1:2A:1337:U:H6	1.77	0.48
1:2A:587:C:H2'	1:2A:588:U:O4'	2.13	0.48
3:2C:68:LEU:HA	3:2C:175:VAL:HG11	1.94	0.48
17:2R:109:GLU:HG2	17:2R:112:ARG:HH22	1.77	0.48
17:2R:83:ILE:HD13	17:2R:86:ILE:HD11	1.95	0.48
1:2A:1038:G:OP1	18:2S:50:ARG:NH2	2.46	0.48
21:2V:53:LYS:HB3	21:2V:82:GLN:HB3	1.96	0.48
32:16:23:VAL:CG1	32:16:47:LYS:HD3	2.43	0.48
1:1A:1638:G:H2'	1:1A:1639:G:C8	2.47	0.48
1:1A:2189:G:O6	1:1A:2192:A:H2'	2.14	0.48
2:1B:77:U:OP1	23:1X:19:ARG:NH2	2.45	0.48
4:1D:175:LEU:HD12	4:1D:185:VAL:HG21	1.96	0.48
14:1O:30:GLY:HA2	14:1O:107:ALA:HB2	1.95	0.48
27:21:23:LEU:HD13	27:21:50:VAL:HG11	1.96	0.48
1:2A:1128:U:O2'	1:2A:1130:A:N7	2.42	0.48
1:2A:1494:G:H4'	1:2A:1588:A:OP1	2.14	0.48
1:2A:2151:U:H1'	1:2A:2179:A:N1	2.29	0.48
1:2A:2427:C:H2'	1:2A:2428:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2F:148:LEU:HD11	6:2F:193:VAL:HG21	1.95	0.48
1:1A:663:U:H2'	1:1A:664:C:C6	2.49	0.48
1:1A:2224:U:O4'	4:1D:151:LYS:HE2	2.14	0.48
6:1F:183:VAL:O	6:1F:187:VAL:HG23	2.12	0.48
7:1G:97:ASP:O	7:1G:101:ILE:HG13	2.14	0.48
7:1G:126:ASP:HB2	7:1G:130:ASN:HB2	1.95	0.48
30:24:14:THR:OG1	30:24:48:VAL:HG13	2.14	0.48
1:2A:1494:G:H2'	1:2A:1495:A:C8	2.49	0.48
1:2A:171:C:H2'	1:2A:172:C:C6	3.50	0.48
1:2A:1768:G:H2'	1:2A:1769:A:C8	2.46	0.48
1:2A:2141:G:O6	1:2A:2199:C:N3	2.47	0.48
1:2A:637:U:H4'	1:2A:638:G:H5''	1.96	0.48
8:2H:102:ALA:HB2	8:2H:116:GLU:HG3	1.95	0.48
1:1A:1010:G:H2'	1:1A:1012:G:OP2	6.42	0.48
1:1A:2139:U:H5	1:1A:2169:G:N3	2.11	0.48
1:1A:2554:G:H2'	1:1A:2555:G:C8	2.48	0.48
3:1C:62:VAL:HG11	3:1C:192:PHE:HD1	1.79	0.48
7:1G:77:ILE:HG22	7:1G:80:PHE:H	1.77	0.48
23:1X:9:TYR:OH	23:1X:61:LEU:HD23	2.14	0.48
1:2A:1073:A:N6	1:2A:1170:G:H2'	2.28	0.48
1:2A:1104:G:H3'	1:2A:1105:U:H2'	1.95	0.48
1:2A:1106:U:C5	10:2K:75:SER:HB2	2.48	0.48
1:2A:2159:C:H42	1:2A:2174:G:H1	1.62	0.48
3:2C:213:TYR:HA	3:2C:222:VAL:O	2.13	0.48
14:2O:122:GLY:O	63:2O:3101:HOH:O	2.20	0.48
25:2Z:83:GLU:OE1	25:2Z:83:GLU:N	2.42	0.48
1:1A:1248:A:H2	1:1A:1286:A:H62	1.60	0.48
1:1A:2298:A:C4	1:1A:2300:G:C8	3.02	0.48
6:1F:125:LEU:HD12	6:1F:194:MET:HB2	1.96	0.48
1:2A:1653:A:H1'	1:2A:1655:A:OP2	2.14	0.48
1:2A:206:A:OP2	63:2A:4939:HOH:O	2.19	0.48
1:2A:2480:A:H2'	1:2A:2481:G:O4'	2.14	0.48
1:2A:658:C:H2'	1:2A:659:C:C6	2.48	0.48
1:2A:863:C:O2'	1:2A:885:U:H5''	2.14	0.48
17:2R:4:GLY:O	17:2R:8:LYS:HG3	2.14	0.48
24:2Y:70:GLN:HG2	24:2Y:72:ARG:HG3	1.96	0.48
1:1A:1107:G:H22	1:1A:1121:C:H42	1.62	0.48
1:1A:115:A:N3	1:1A:166:G:H1'	2.28	0.48
1:1A:2119:U:H3	1:1A:2212:G:H1	1.62	0.48
1:1A:2473:U:H1'	1:1A:2502:U:O4	2.14	0.48
1:1A:2859:A:N7	1:1A:2877:A:O2'	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2858:U:H4'	1:1A:2877:A:C2	2.48	0.48
1:2A:1054:A:OP2	11:2L:37:LYS:NZ	2.42	0.48
1:2A:1948:A:H2'	1:2A:1949:A:C8	2.48	0.48
1:2A:793:U:O2	1:2A:2035:A:H1'	2.14	0.48
1:2A:2742:C:H4'	5:2E:168:MET:O	2.14	0.48
1:2A:922:C:H2'	1:2A:923:U:O4'	2.14	0.48
1:2A:956:A:H2'	14:2O:9:TYR:OH	2.13	0.48
2:2B:24:G:N7	2:2B:56:G:H2'	2.29	0.48
3:2C:22:ILE:HG21	3:2C:190:ARG:HB2	1.95	0.48
7:2G:47:LYS:HE2	7:2G:47:LYS:HB3	1.59	0.48
8:2H:38:SER:HB3	8:2H:41:MET:HG2	1.96	0.48
10:2K:106:GLU:HA	10:2K:109:LYS:HD3	1.96	0.48
1:2A:1103:G:H21	10:2K:126:MET:HG2	1.79	0.48
1:2A:1109:C:OP1	10:2K:86:LYS:HE3	2.13	0.48
33:17:2:LYS:HE2	33:17:31:LYS:O	2.14	0.47
1:1A:1820:C:H5''	1:1A:1821:A:OP1	2.13	0.47
6:1F:53:THR:HG23	6:1F:55:GLY:H	1.78	0.47
14:1O:118:LEU:HD12	14:1O:131:ILE:HG23	1.96	0.47
15:1P:13:HIS:CE1	15:1P:16:HIS:HB2	2.49	0.47
1:2A:2375:C:H2'	1:2A:2376:G:O4'	2.14	0.47
4:2D:76:PRO:HB2	4:2D:116:GLN:HE21	1.77	0.47
7:2G:136:ARG:HD2	7:2G:137:GLU:N	2.29	0.47
15:2P:26:LYS:HE2	15:2P:70:LEU:O	2.13	0.47
23:2X:93:ASP:HA	23:2X:131:ARG:HH22	1.77	0.47
23:2X:8:TYR:HB2	23:2X:38:TYR:CE2	2.49	0.47
1:1A:573:G:O2'	1:1A:1264:A:N3	2.39	0.47
1:1A:1799:G:O2'	1:1A:1979:C:OP1	2.21	0.47
1:1A:2197:A:H2'	1:1A:2198:C:C6	2.49	0.47
1:1A:2278:A:H5''	1:1A:2279:A:H5'	1.96	0.47
1:1A:2330:G:H22	16:1Q:3:ARG:CZ	2.27	0.47
1:1A:2801:C:O2'	1:1A:2802:A:H4'	2.14	0.47
1:1A:57:U:H2'	1:1A:58:G:C8	5.62	0.47
5:1E:29:GLY:HA3	63:1E:408:HOH:O	2.14	0.47
1:1A:1444:C:OP1	21:1V:25:LYS:NZ	2.44	0.47
1:2A:176:G:H5'	25:2Z:14:VAL:HG21	1.96	0.47
1:2A:2741:G:N3	63:2A:4997:HOH:O	2.35	0.47
1:2A:945:A:HO2'	1:2A:946:A:P	2.36	0.47
23:2X:138:GLU:H	23:2X:156:LYS:NZ	2.13	0.47
1:1A:237:C:O2	32:16:12:LYS:NZ	2.39	0.47
1:1A:504:A:N3	1:1A:506:G:H5''	2.29	0.47
1:1A:618:G:H2'	1:1A:619:U:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:45:ASP:O	23:1X:49:ARG:HG3	2.13	0.47
1:2A:1470:G:H2'	1:2A:1471:G:C8	2.49	0.47
1:2A:1682:C:H2'	1:2A:1683:A:C8	2.50	0.47
1:2A:1755:U:H2'	1:2A:1756:C:C6	2.50	0.47
1:2A:2593:G:C2	1:2A:2594:G:C8	3.02	0.47
1:2A:2575:A:C2	1:2A:2658:U:H4'	2.50	0.47
1:2A:2723:U:OP1	1:2A:2726:G:H4'	2.14	0.47
1:2A:285:C:O2	1:2A:288:G:N2	2.44	0.47
1:2A:2733:A:H1'	1:2A:2882:A:O2'	2.15	0.47
1:2A:311:C:H2'	1:2A:312:A:H8	1.80	0.47
1:2A:323:A:HO2'	1:2A:341:C:HO2'	1.62	0.47
1:2A:535:U:O4	1:2A:536:G:N1	2.47	0.47
3:2C:10:LEU:O	3:2C:220:PRO:HG2	2.15	0.47
3:2C:179:SER:HA	3:2C:180:PHE:C	2.35	0.47
1:2A:1182:G:O2'	11:2L:102:ALA:O	2.32	0.47
12:2M:63:VAL:HG12	12:2M:106:LEU:HD11	1.96	0.47
23:2X:157:LEU:HB3	23:2X:161:VAL:HG13	1.96	0.47
1:1A:1091:A:H3'	1:1A:1092:G:H5'	1.96	0.47
1:1A:1313:A:OP1	63:1A:3884:HOH:O	2.20	0.47
1:1A:2796:C:H1'	5:1E:37:ARG:NH1	2.28	0.47
1:1A:90:G:H2'	1:1A:91:C:H6	1.79	0.47
1:1A:2761:A:P	8:1H:3:ARG:HH21	2.37	0.47
9:1J:25:PHE:O	9:1J:85:ASP:N	2.46	0.47
1:1A:661:A:H8	13:1N:117:GLU:HG3	1.80	0.47
1:2A:1076:G:H21	33:27:36:GLN:HE22	1.61	0.47
1:2A:2339:A:H2'	1:2A:2340:G:H8	1.79	0.47
1:2A:2449:U:O2'	1:2A:2451:C:OP1	2.22	0.47
1:2A:330:G:N7	63:2A:5000:HOH:O	2.36	0.47
1:2A:933:A:OP1	1:2A:934:C:N4	2.41	0.47
3:2C:217:THR:HG22	3:2C:218:MET:HE2	1.96	0.47
13:2N:126:VAL:HG12	13:2N:148:LEU:HD22	1.96	0.47
1:1A:1090:A:C8	1:1A:1092:G:C2	3.02	0.47
1:1A:1244:C:H2'	1:1A:1245:C:C6	2.97	0.47
1:1A:2223:C:H2'	1:1A:2224:U:O4'	2.14	0.47
1:1A:26:G:N2	1:1A:536:G:H1'	2.30	0.47
1:1A:595:G:O2'	1:1A:596:C:H3'	2.14	0.47
3:1C:10:LEU:HB3	3:1C:32:LEU:HD22	1.95	0.47
3:1C:3:HIS:HA	3:1C:7:TYR:CD2	2.50	0.47
5:1E:101:ARG:CZ	5:1E:171:GLU:HB2	2.44	0.47
10:1K:76:TYR:HD2	10:1K:77:LEU:HD23	1.80	0.47
17:1R:91:ARG:HB2	17:1R:121:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:21:16:PRO:HB2	27:21:18:ASP:OD1	2.14	0.47
1:2A:1252:C:H2'	1:2A:1253:G:H8	2.74	0.47
1:2A:1734:U:O2	1:2A:1746:A:H5'	2.14	0.47
1:2A:1820:C:H5''	1:2A:1821:A:OP1	2.14	0.47
1:2A:1824:U:H2'	1:2A:1825:C:H6	1.79	0.47
1:2A:2072:A:OP1	5:2E:137:HIS:ND1	2.39	0.47
1:2A:2154:G:O2'	1:2A:2178:G:N2	2.48	0.47
1:2A:2866:G:N2	1:2A:2869:A:OP2	2.34	0.47
2:2B:100:A:H3'	2:2B:101:G:H8	1.79	0.47
7:2G:23:PHE:HB2	7:2G:25:TYR:CE1	2.49	0.47
7:2G:61:ALA:O	28:22:7:PRO:HG2	2.14	0.47
30:14:35:GLU:OE1	30:14:50:ARG:NH2	2.48	0.47
1:1A:1219:U:OP1	1:1A:1221:A:N6	2.47	0.47
1:1A:2283:U:H5''	1:1A:2284:A:OP1	2.15	0.47
2:1B:42:C:OP2	28:12:2:LYS:NZ	2.35	0.47
5:1E:28:ALA:HB3	5:1E:93:VAL:HG22	1.96	0.47
2:1B:33:G:H5'	7:1G:2:PRO:HD3	1.97	0.47
1:2A:1161:C:H2'	1:2A:1162:G:H8	1.80	0.47
1:2A:1915:C:H2'	1:2A:1916:C:H6	1.79	0.47
1:2A:196:C:H2'	1:2A:197:C:C6	2.49	0.47
1:2A:2347:A:H61	24:2Y:43:THR:CG2	2.27	0.47
1:2A:2842:G:H4'	1:2A:2843:G:OP2	2.14	0.47
1:2A:924:A:H2'	1:2A:925:G:C8	5.32	0.47
3:2C:37:PHE:HD1	3:2C:37:PHE:H	1.63	0.47
7:2G:115:ARG:HB3	7:2G:115:ARG:HH11	1.80	0.47
8:2H:164:TYR:HB2	8:2H:167:GLU:HB2	1.95	0.47
23:2X:97:GLU:HA	23:2X:126:VAL:O	2.13	0.47
1:2A:1409:G:P	25:2Z:3:LYS:HG3	2.55	0.47
1:1A:1499:A:OP2	63:1A:3880:HOH:O	2.20	0.47
1:1A:1925:G:H2'	1:1A:1926:C:O4'	2.15	0.47
1:1A:770:U:H2'	1:1A:771:G:O4'	2.15	0.47
7:1G:121:ASN:ND2	7:1G:181:ARG:HH12	2.13	0.47
1:2A:1764:U:H2'	1:2A:1765:G:O4'	2.14	0.47
1:2A:2124:C:N3	1:2A:2207:G:O6	2.48	0.47
1:2A:2788:A:H4'	1:2A:2789:G:H5''	1.97	0.47
1:1A:1013:U:H2'	1:1A:1014:C:C6	2.49	0.47
1:1A:140:C:H2'	1:1A:141:G:O4'	2.14	0.47
1:1A:2161:C:H2'	1:1A:2161:C:O2	2.13	0.47
1:1A:2052:A:C6	1:1A:2509:C:H1'	2.49	0.47
1:1A:258:A:C6	1:1A:259:A:C6	4.08	0.47
1:1A:264:U:H2'	1:1A:265:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:301:A:H4'	1:1A:302:C:OP1	2.15	0.47
1:1A:949:C:H2'	1:1A:950:U:C6	2.50	0.47
24:1Y:18:ALA:HB3	24:1Y:20:ARG:NH2	2.30	0.47
33:27:22:ARG:HB2	33:27:24:TYR:CE1	2.49	0.47
1:2A:1127:U:H5'	10:2K:122:ALA:HB1	1.96	0.47
1:2A:1525:G:C6	1:2A:1526:G:C5	3.02	0.47
1:2A:1659:A:H8	1:2A:1659:A:P	2.38	0.47
1:2A:1856:G:H4'	4:2D:242:ARG:NH1	2.29	0.47
1:2A:224:C:H2'	1:2A:225:C:C6	2.50	0.47
1:2A:547:C:H4'	1:2A:564:C:O2	2.14	0.47
5:2E:105:THR:OG1	5:2E:199:ARG:NH2	2.45	0.47
6:2F:150:GLY:HA2	6:2F:172:TRP:CD2	2.50	0.47
16:2Q:67:ARG:O	16:2Q:71:ARG:HG2	2.15	0.47
20:2U:80:PRO:O	20:2U:100:THR:HB	2.15	0.47
22:2W:43:ASN:CG	22:2W:65:ALA:HB3	2.35	0.47
1:1A:1247:G:OP2	1:1A:1248:A:O2'	2.25	0.47
1:1A:2121:G:H1'	1:1A:2211:G:N2	2.30	0.47
1:1A:513:G:O2'	20:1U:49:LYS:NZ	2.31	0.47
2:1B:87:G:N2	2:1B:90:A:OP2	2.34	0.47
10:1K:101:TRP:CE2	10:1K:140:GLY:HA3	2.50	0.47
1:2A:1183:G:O2'	1:2A:1188:A:N1	2.38	0.47
1:2A:1311:G:O5'	20:2U:15:ARG:NH2	2.48	0.47
1:2A:2163:C:H2'	1:2A:2164:C:C6	2.50	0.47
1:2A:562:G:H2'	1:2A:563:G:H8	1.79	0.47
1:2A:825:U:OP2	1:2A:825:U:H6	3.90	0.47
5:2E:77:ILE:HD11	5:2E:79:ARG:NH1	2.23	0.47
8:2H:80:SER:OG	8:2H:81:GLU:N	2.48	0.47
1:2A:1109:C:P	10:2K:86:LYS:HE3	2.55	0.47
1:1A:1972:U:O4	63:1A:3885:HOH:O	2.21	0.47
1:1A:2354:C:HO2'	1:1A:2384:G:HO2'	1.61	0.47
3:1C:171:ILE:HG23	3:1C:172:HIS:N	2.30	0.47
3:1C:212:VAL:O	3:1C:224:ILE:HG12	2.15	0.47
10:1K:111:LYS:HG2	10:1K:114:ASP:OD2	2.14	0.47
1:1A:216:A:OP1	13:1N:76:LYS:NZ	2.48	0.47
24:1Y:70:GLN:HG2	24:1Y:72:ARG:HG3	1.97	0.47
1:2A:214:G:H21	1:2A:216:A:H62	1.63	0.47
1:2A:2203:G:H2'	1:2A:2204:C:C6	2.49	0.47
1:2A:2278:A:H5''	1:2A:2279:A:H5'	1.97	0.47
1:2A:437:G:C5	13:2N:72:PRO:HB3	2.50	0.47
3:2C:23:ASP:HB2	3:2C:190:ARG:HH22	1.80	0.47
15:2P:60:LEU:HA	15:2P:60:LEU:HD13	3.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2P:78:LYS:HE2	15:2P:83:ILE:HD11	1.96	0.47
1:1A:1066:A:H8	1:1A:1066:A:H3'	1.80	0.47
1:1A:1399:A:H2'	1:1A:1400:G:O4'	2.15	0.47
1:1A:363:A:H2'	1:1A:364:G:O4'	2.15	0.47
1:1A:448:A:H2'	1:1A:449:A:C8	2.49	0.47
1:1A:610:U:H2'	1:1A:611:C:C6	2.50	0.47
8:2H:12:PRO:O	8:2H:15:VAL:HG12	2.15	0.47
15:2P:29:LEU:HB3	15:2P:75:LEU:HD21	1.97	0.47
18:2S:49:HIS:HA	18:2S:52:ARG:HG2	1.97	0.47
1:1A:1159:G:H2'	1:1A:1160:G:C8	2.50	0.46
1:1A:1313:A:C2	1:1A:2034:A:C4	3.03	0.46
1:1A:1685:U:O2'	1:1A:1686:C:H5'	2.15	0.46
1:1A:260:A:N1	1:1A:290:G:O2'	2.35	0.46
7:1G:143:GLU:OE2	28:12:26:SER:OG	2.26	0.46
9:1J:103:GLY:HA2	9:1J:111:LEU:H	1.80	0.46
1:2A:1066:A:H62	1:2A:1185:U:H3	1.61	0.46
1:2A:1404:A:N6	1:2A:1417:U:H3	2.09	0.46
1:2A:2157:C:N4	1:2A:2176:G:H1	2.13	0.46
4:2D:69:ARG:NH2	4:2D:128:GLY:O	2.48	0.46
6:2F:32:LEU:HB3	6:2F:112:MET:HE1	1.97	0.46
7:2G:106:LEU:O	7:2G:110:ALA:HB3	2.16	0.46
7:2G:144:ILE:HG23	7:2G:148:MET:HE1	1.96	0.46
1:1A:2160:C:H2'	1:1A:2161:C:H4'	1.96	0.46
1:1A:214:G:H21	1:1A:216:A:H62	1.63	0.46
1:1A:411:C:O2	13:1N:71:VAL:HG21	2.15	0.46
3:1C:32:LEU:HD22	3:1C:220:PRO:HD2	1.98	0.46
1:2A:1381:A:H2'	1:2A:1382:G:C8	2.50	0.46
1:2A:1992:A:C4	4:2D:241:PRO:HD3	2.50	0.46
1:2A:2324:C:H2'	1:2A:2325:C:H6	1.80	0.46
1:2A:2701:C:N4	1:2A:2725:A:H1'	2.30	0.46
1:2A:401:C:H2'	1:2A:402:C:H6	1.78	0.46
5:2E:5:LEU:HD12	5:2E:51:PHE:HB2	1.97	0.46
11:2L:62:VAL:HG11	11:2L:66:LYS:HB2	1.96	0.46
14:2O:76:LYS:HB3	14:2O:91:GLU:HG3	1.97	0.46
15:2P:21:TYR:OH	15:2P:43:GLU:HG2	2.14	0.46
1:1A:468:A:H1'	1:1A:1245:C:O4'	2.16	0.46
1:1A:2049:U:H2'	1:1A:2050:G:O4'	2.16	0.46
4:1D:106:ILE:O	4:1D:108:PRO:HD3	2.16	0.46
1:1A:1992:A:C4	4:1D:241:PRO:HD3	2.49	0.46
8:1H:54:ARG:NH2	8:1H:57:ASP:OD1	2.34	0.46
17:1R:102:ILE:HB	17:1R:110:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1107:G:H2'	1:2A:1108:G:C8	2.49	0.46
1:2A:1430:G:H4'	1:2A:1431:C:OP1	2.15	0.46
1:2A:1585:G:H2'	1:2A:1586:U:O4'	2.15	0.46
1:2A:2117:U:H2'	1:2A:2118:C:C6	2.50	0.46
1:2A:2370:C:H2'	1:2A:2371:A:O4'	2.14	0.46
1:2A:2746:A:H2'	1:2A:2747:G:O4'	2.15	0.46
1:2A:948:C:H2'	1:2A:949:C:C6	2.49	0.46
1:2A:720:G:O2'	6:2F:74:ARG:HD3	2.16	0.46
12:2M:78:ARG:HG2	17:2R:73:GLU:HB2	1.97	0.46
1:1A:1323:A:OP1	15:1P:36:THR:HG23	2.16	0.46
1:1A:1768:G:H2'	1:1A:1769:A:C8	2.51	0.46
1:1A:1824:U:H2'	1:1A:1825:C:H6	1.80	0.46
1:1A:1844:G:O6	63:1A:3869:HOH:O	2.18	0.46
1:1A:2239:G:OP2	4:1D:263:ARG:NH1	2.40	0.46
2:1B:86:G:H1	2:1B:91:C:H42	1.62	0.46
7:1G:82:LEU:HD21	7:1G:88:ILE:HG21	1.97	0.46
8:1H:13:LYS:HA	8:1H:14:GLY:HA2	1.63	0.46
13:1N:86:LYS:HB3	13:1N:118:GLY:HA3	1.98	0.46
22:1W:92:ASN:HB2	22:1W:94:LYS:N	2.25	0.46
27:21:19:GLN:O	27:21:23:LEU:HD22	2.16	0.46
31:25:12:ARG:NH2	31:25:44:PRO:HB3	2.31	0.46
1:2A:105:U:H4'	1:2A:370:A:H2	1.81	0.46
1:2A:1928:G:H2'	1:2A:1929:C:C6	2.50	0.46
1:2A:2551:C:H2'	1:2A:2552:A:O4'	2.16	0.46
1:2A:2027:C:O2'	1:2A:2832:A:N3	2.48	0.46
1:2A:2879:C:H2'	1:2A:2880:C:O4'	2.16	0.46
1:2A:775:G:O2'	1:2A:809:G:H4'	2.16	0.46
1:2A:894:G:OP1	63:2A:4944:HOH:O	2.21	0.46
8:2H:17:VAL:HG11	8:2H:50:VAL:HG21	1.96	0.46
13:2N:86:LYS:HB3	13:2N:118:GLY:HA3	1.97	0.46
1:1A:1822:G:O2'	1:1A:1860:C:OP1	2.29	0.46
1:1A:2017:C:H4'	1:1A:2018:G:OP1	2.15	0.46
1:1A:2107:U:H2'	1:1A:2108:G:C8	2.51	0.46
1:1A:2622:U:H5'	1:1A:2622:U:H6	1.80	0.46
1:1A:2657:C:H2'	1:1A:2658:U:O4'	2.15	0.46
1:1A:301:A:H2'	1:1A:302:C:C6	2.50	0.46
1:1A:383:G:H2'	1:1A:384:G:O4'	2.16	0.46
1:1A:482:A:H5''	63:1A:4651:HOH:O	2.16	0.46
1:1A:593:A:O2'	19:1T:78:LYS:HE2	2.16	0.46
3:1C:62:VAL:HG11	3:1C:192:PHE:CD1	2.50	0.46
20:1U:57:ASN:O	20:1U:61:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:19:LYS:HA	24:1Y:19:LYS:HD2	1.71	0.46
1:2A:342:C:H2'	1:2A:343:A:O4'	2.15	0.46
1:2A:1833:A:H4'	4:2D:259:THR:HG23	1.98	0.46
12:2M:10:VAL:HG23	12:2M:12:ASP:OD1	2.16	0.46
17:2R:64:ARG:NH1	17:2R:103:ARG:HA	2.31	0.46
22:2W:56:PRO:C	22:2W:58:GLY:H	2.19	0.46
30:14:14:THR:HG21	30:14:48:VAL:HG13	1.98	0.46
1:1A:1152:G:N2	1:1A:1153:U:H3	2.13	0.46
1:1A:1288:G:O2'	13:1N:7:ARG:NH2	2.49	0.46
1:1A:1649:C:H5'	63:1A:4182:HOH:O	2.16	0.46
1:1A:2659:C:H2'	1:1A:2660:U:C6	2.50	0.46
1:1A:555:C:H4'	1:1A:556:A:H5''	1.96	0.46
1:1A:924:A:H2'	1:1A:925:G:H5'	1.97	0.46
3:1C:38:ASP:OD2	3:1C:177:LYS:HD3	2.16	0.46
4:1D:10:THR:OG1	4:1D:13:ARG:HG2	2.15	0.46
6:1F:101:LEU:O	6:1F:106:ARG:HD3	2.16	0.46
1:1A:2454:C:OP1	6:1F:68:LYS:HD3	2.15	0.46
12:1M:53:LYS:HG3	12:1M:56:ASP:OD2	2.16	0.46
1:2A:1115:A:N1	1:2A:1142:U:O2'	2.48	0.46
1:2A:1313:A:H2'	1:2A:1314:A:O4'	2.16	0.46
1:2A:2147:A:N6	1:2A:2184:C:H5'	2.31	0.46
1:2A:1708:C:O2'	1:2A:2698:U:OP1	2.33	0.46
1:2A:2759:G:O6	1:2A:2767:C:H5''	2.15	0.46
1:2A:363:A:H2'	1:2A:364:G:O4'	2.15	0.46
17:2R:60:THR:HG22	17:2R:77:PRO:HA	1.98	0.46
1:1A:484:U:H5''	31:15:40:TRP:CD2	2.50	0.46
1:1A:2086:C:H2'	1:1A:2087:C:C6	2.50	0.46
1:1A:2156:A:N6	1:1A:2177:G:O2'	2.48	0.46
1:1A:2575:A:C2	1:1A:2658:U:H4'	2.50	0.46
1:1A:2693:U:O2'	17:1R:58:ASN:ND2	2.49	0.46
1:1A:695:C:N3	1:1A:696:C:N4	2.64	0.46
22:1W:43:ASN:HD22	22:1W:43:ASN:HA	1.53	0.46
24:1Y:11:ARG:H	24:1Y:11:ARG:HD2	1.81	0.46
1:2A:1101:G:H4'	1:2A:1131:A:N7	2.31	0.46
1:2A:1235:G:H1	1:2A:1266:C:H42	31.89	0.46
1:2A:1643:C:H2'	1:2A:1644:C:H6	1.80	0.46
1:2A:1761:G:H2'	1:2A:1762:G:C8	2.48	0.46
1:2A:2161:C:O2	1:2A:2172:G:N1	2.34	0.46
1:2A:22:G:H2'	1:2A:23:G:C8	3.23	0.46
1:2A:2657:C:H2'	1:2A:2658:U:O4'	2.15	0.46
1:2A:2715:C:H2'	1:2A:2716:A:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:624:G:O2'	1:2A:626:G:O2'	2.26	0.46
2:2B:13:A:N1	2:2B:69:G:O2'	2.31	0.46
11:2L:72:TYR:N	11:2L:85:ILE:O	2.48	0.46
15:2P:13:HIS:CE1	15:2P:16:HIS:HB2	2.50	0.46
33:17:25:VAL:HB	33:17:34:GLN:HB2	1.98	0.46
1:1A:1140:A:N1	1:1A:1160:G:N2	51.32	0.46
1:1A:1524:G:O2'	1:1A:1604:A:H2	1.99	0.46
1:1A:807:A:OP1	63:1A:3836:HOH:O	2.20	0.46
2:1B:117:G:H2'	2:1B:118:G:O4'	2.15	0.46
1:2A:143:C:H2'	1:2A:144:G:H8	1.81	0.46
1:2A:253:A:N6	1:2A:454:A:H1'	2.31	0.46
20:2U:67:ASP:N	20:2U:67:ASP:OD2	2.49	0.46
1:1A:1120:C:H5'	1:1A:1121:C:OP2	2.16	0.46
1:1A:1734:U:O2	1:1A:1746:A:H5'	2.16	0.46
1:1A:417:G:O2'	1:1A:436:G:OP1	2.26	0.46
1:1A:894:G:O6	1:1A:973:G:H2'	2.15	0.46
1:2A:2273:U:H4'	1:2A:2339:A:C2	2.51	0.46
1:2A:2405:C:H1'	63:2A:5138:HOH:O	2.16	0.46
1:2A:2613:A:OP2	1:2A:2614:G:H5''	2.16	0.46
7:2G:15:VAL:HG22	7:2G:175:LEU:HB3	1.98	0.46
8:2H:144:VAL:HA	8:2H:147:ASN:ND2	2.31	0.46
21:2V:44:GLU:O	21:2V:48:LYS:N	2.49	0.46
23:2X:11:GLU:HB3	23:2X:12:GLY:H	1.61	0.46
1:1A:1153:U:HO2'	1:1A:1154:C:H6	1.64	0.46
1:1A:2192:A:H1'	1:1A:2193:U:C6	2.50	0.46
3:1C:40:THR:N	3:1C:217:THR:OG1	2.49	0.46
5:1E:143:ASN:HB2	5:1E:147:PRO:HD2	1.98	0.46
5:1E:144:ARG:HB3	5:1E:145:LYS:H	1.48	0.46
13:1N:58:THR:O	13:1N:62:LEU:HG	2.16	0.46
1:2A:1055:A:H1'	1:2A:1198:C:H1'	1.98	0.46
1:2A:1108:G:H1'	10:2K:91:PRO:CG	2.46	0.46
1:2A:2699:U:O2'	1:2A:2733:A:N6	2.49	0.46
5:2E:35:GLN:HG3	5:2E:36:ARG:N	2.31	0.46
32:16:62:LEU:HB3	32:16:65:GLU:HG2	1.98	0.45
1:1A:1457:A:H2'	1:1A:1458:G:C8	2.51	0.45
1:1A:2187:G:H5'	1:1A:2188:U:OP2	2.17	0.45
1:1A:326:U:H2'	1:1A:327:G:C8	2.50	0.45
1:1A:494:G:O6	31:15:37:LYS:HE2	2.16	0.45
32:26:7:HIS:HB3	32:26:61:LEU:HB3	1.98	0.45
1:2A:1587:G:OP2	1:2A:1588:A:O2'	2.34	0.45
1:2A:1633:C:H2'	1:2A:1634:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2203:G:H2'	1:2A:2204:C:H6	1.81	0.45
1:2A:260:A:N7	1:2A:282:G:N2	2.58	0.45
1:2A:1302:C:H4'	6:2F:83:PHE:CD1	2.51	0.45
1:1A:1147:C:H2'	1:1A:1148:A:C8	2.51	0.45
1:1A:328:U:H2'	1:1A:329:U:C6	2.52	0.45
1:1A:254:G:N2	1:1A:453:U:H1'	2.31	0.45
1:1A:656:A:H2'	1:1A:657:A:C8	2.52	0.45
2:1B:32:C:C2	2:1B:51:G:N2	2.84	0.45
3:1C:179:SER:HA	3:1C:180:PHE:O	2.16	0.45
15:1P:24:GLN:HE21	15:1P:44:LEU:HG	1.81	0.45
1:2A:1138:G:H2'	1:2A:1143:A:H61	1.80	0.45
1:2A:885:U:O2'	1:2A:1235:G:N3	2.42	0.45
1:2A:2082:G:H5''	1:2A:2514:A:C2	2.51	0.45
1:2A:2151:U:OP1	3:2C:5:LYS:N	2.37	0.45
1:2A:2768:U:H4'	1:2A:2769:A:OP1	2.14	0.45
1:2A:2890:C:H2'	1:2A:2891:A:O4'	2.15	0.45
1:2A:610:U:H1'	6:2F:90:PHE:HB3	1.98	0.45
3:2C:200:LYS:HG2	3:2C:203:GLY:N	2.32	0.45
6:2F:33:LEU:HD22	6:2F:112:MET:HE3	1.99	0.45
7:2G:47:LYS:HG2	7:2G:48:GLU:N	2.31	0.45
1:2A:1081:G:OP2	8:2H:59:ARG:NH1	2.49	0.45
1:2A:1107:G:H4'	10:2K:133:SER:CB	2.46	0.45
16:2Q:54:LEU:O	16:2Q:57:LYS:HG3	2.16	0.45
2:2B:48:A:H4'	16:2Q:95:HIS:CD2	2.51	0.45
1:2A:1200:A:OP1	18:2S:55:ARG:HD3	2.16	0.45
1:2A:2342:G:O2'	24:2Y:43:THR:HG22	2.17	0.45
24:2Y:53:MET:HA	24:2Y:58:THR:O	2.16	0.45
31:15:24:THR:HG22	31:15:27:GLY:N	2.22	0.45
1:1A:1109:C:H2'	1:1A:1110:U:O4'	2.17	0.45
1:1A:1571:G:C6	1:1A:1572:G:C2	3.04	0.45
1:1A:552:A:C2	1:1A:2064:C:H4'	2.51	0.45
1:1A:2654:G:O6	63:1A:3876:HOH:O	2.19	0.45
1:1A:2801:C:O2	1:1A:2902:G:N2	2.38	0.45
1:1A:57:U:H2'	1:1A:58:G:H8	5.64	0.45
3:1C:46:LYS:O	3:1C:210:ARG:HB2	2.16	0.45
1:1A:2630:C:H4'	5:1E:151:TYR:O	2.16	0.45
9:1J:66:LEU:O	9:1J:73:GLY:HA2	2.16	0.45
17:1R:118:ARG:HD2	17:1R:118:ARG:HA	1.60	0.45
30:24:10:LEU:HD23	30:24:22:ALA:HB2	1.97	0.45
1:2A:2431:C:P	32:26:33:ASN:H	2.39	0.45
1:2A:1051:C:C2	1:2A:1182:G:N2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1474:G:H2'	1:2A:1475:C:C6	2.50	0.45
1:2A:1568:U:H2'	1:2A:1569:G:H8	1.80	0.45
1:2A:1732:C:H2'	1:2A:1733:G:O4'	2.16	0.45
1:2A:2824:C:H5'	29:23:29:THR:HG21	1.98	0.45
1:1A:1524:G:H2'	1:1A:1525:G:C8	2.47	0.45
1:1A:2139:U:H6	1:1A:2169:G:O2'	2.00	0.45
1:1A:2144:G:H2'	1:1A:2145:G:H8	1.79	0.45
1:1A:622:G:N2	1:1A:627:C:O3'	2.50	0.45
1:1A:468:A:C5	6:1F:45:ARG:HD2	2.52	0.45
13:1N:138:LEU:HD23	13:1N:145:PRO:HG3	1.98	0.45
17:1R:27:THR:O	17:1R:89:VAL:HG22	2.15	0.45
19:1T:65:GLY:HA3	19:1T:91:TYR:CZ	2.52	0.45
27:21:20:LYS:HE3	27:21:20:LYS:HB2	1.81	0.45
1:2A:1137:C:H2'	1:2A:1138:G:O4'	2.16	0.45
1:2A:1099:A:N6	1:2A:1150:U:H3	2.09	0.45
1:2A:2574:U:O2	1:2A:2576:A:H8	1.99	0.45
1:2A:2800:C:O2'	1:2A:2818:A:N3	2.46	0.45
7:2G:98:ARG:H	7:2G:98:ARG:HG2	1.39	0.45
22:2W:44:ILE:HA	22:2W:63:LYS:O	2.15	0.45
1:1A:1187:A:C4	1:1A:1189:G:C8	3.04	0.45
1:1A:2302:U:H2'	1:1A:2303:C:C6	2.52	0.45
1:1A:267:G:O2'	1:1A:268:G:H8	2.00	0.45
1:1A:951:G:OP1	14:1O:26:TYR:OH	2.32	0.45
5:1E:119:ARG:HB3	5:1E:120:TRP:CD1	2.52	0.45
6:1F:132:VAL:HA	6:1F:138:GLU:HB3	1.98	0.45
26:20:53:LEU:O	26:20:57:ILE:HG13	2.15	0.45
1:2A:1317:A:N7	1:2A:1663:A:H1'	2.32	0.45
1:2A:1616:A:H2'	1:2A:1617:A:C8	2.51	0.45
1:2A:2071:C:H2'	1:2A:2072:A:O4'	2.17	0.45
1:2A:2741:G:H2'	1:2A:2742:C:C6	2.51	0.45
1:2A:503:A:N1	1:2A:524:G:H4'	2.32	0.45
1:2A:765:C:H2'	1:2A:766:C:C6	2.52	0.45
2:2B:17:C:H2'	2:2B:18:G:O4'	2.17	0.45
6:2F:20:LEU:HD22	6:2F:20:LEU:HA	1.66	0.45
12:2M:23:ARG:HG3	12:2M:24:VAL:N	2.31	0.45
1:2A:1039:C:H3'	18:2S:54:LYS:HE3	1.98	0.45
1:1A:1100:G:H1	1:1A:1149:C:H42	1.63	0.45
1:1A:2356:G:OP2	30:14:38:LYS:HG3	2.16	0.45
1:1A:1684:C:OP1	1:1A:2721:C:O2'	2.35	0.45
1:1A:509:C:H2'	1:1A:510:C:C6	2.52	0.45
1:1A:501:G:H4'	1:1A:526:A:N1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:26:ALA:HB3	3:1C:186:ALA:HB2	1.99	0.45
5:1E:167:VAL:HG22	5:1E:189:PRO:HD3	1.98	0.45
7:1G:106:LEU:HA	7:1G:110:ALA:HB3	1.98	0.45
18:1S:24:TYR:HB2	18:1S:29:SER:HB3	1.99	0.45
1:1A:23:G:O2'	20:1U:78:GLU:O	2.30	0.45
23:1X:144:LEU:HD11	23:1X:150:LEU:HD22	1.98	0.45
27:21:10:LYS:HB3	27:21:53:LEU:HA	1.99	0.45
1:2A:1284:G:H2'	1:2A:1285:U:O4'	2.16	0.45
1:2A:1356:G:O6	31:25:9:ARG:NH2	2.49	0.45
1:2A:2183:G:O3'	1:2A:2193:U:H2'	2.16	0.45
1:2A:2829:A:OP1	15:2P:2:ARG:NH2	2.48	0.45
1:2A:875:A:N7	1:2A:2259:C:H5'	2.32	0.45
5:2E:52:LEU:O	5:2E:76:ARG:N	2.41	0.45
6:2F:197:ASP:O	6:2F:201:VAL:HG13	2.16	0.45
6:2F:202:PHE:CZ	6:2F:206:ILE:HD13	2.52	0.45
7:2G:135:LEU:HB2	7:2G:155:MET:HG2	1.98	0.45
1:2A:707:C:H4'	13:2N:13:ASN:OD1	2.17	0.45
1:1A:90:G:H2'	1:1A:91:C:C6	2.51	0.45
8:1H:164:TYR:HB2	8:1H:167:GLU:HB2	1.98	0.45
1:2A:2894:C:O2'	29:23:34:PRO:HG3	2.16	0.45
1:2A:1716:C:OP1	63:2A:4943:HOH:O	2.21	0.45
1:2A:2244:U:H2'	1:2A:2245:G:C8	2.52	0.45
1:2A:2273:U:H4'	1:2A:2339:A:H2	1.81	0.45
1:2A:2626:U:H2'	1:2A:2627:C:C6	2.50	0.45
1:2A:323:A:OP1	22:2W:86:ARG:NH2	2.50	0.45
1:2A:504:A:H4'	1:2A:505:A:OP1	2.15	0.45
1:2A:703:U:H2'	1:2A:704:C:C6	2.51	0.45
1:2A:732:G:H21	1:2A:834:A:H61	1.64	0.45
1:2A:896:C:O3'	27:21:49:LYS:HE2	2.16	0.45
2:2B:65:C:N4	2:2B:109:C:C2	2.85	0.45
1:2A:2151:U:P	3:2C:5:LYS:H	2.40	0.45
6:2F:135:LYS:HG2	6:2F:137:LYS:HG2	1.99	0.45
23:2X:110:GLY:O	23:2X:114:GLY:N	2.42	0.45
1:1A:1835:U:O2	4:1D:50:THR:HB	2.16	0.45
1:1A:2197:A:H2'	1:1A:2198:C:C5	2.51	0.45
1:1A:2330:G:O6	16:1Q:4:LEU:HD13	2.17	0.45
7:1G:79:ASN:N	7:1G:79:ASN:OD1	2.49	0.45
25:1Z:76:ARG:HB2	25:1Z:97:LEU:HD13	1.99	0.45
28:22:13:ARG:HA	28:22:22:ILE:O	2.17	0.45
1:2A:1633:C:H2'	1:2A:1634:C:H6	1.82	0.45
1:2A:2126:C:N4	1:2A:2204:C:H42	2.11	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:671:G:O5'	1:2A:671:G:H8	2.00	0.45
7:2G:97:ASP:O	7:2G:101:ILE:HG13	2.16	0.45
1:2A:2314:G:H1'	7:2G:132:ASN:HD22	1.81	0.45
8:2H:98:LEU:HD22	8:2H:125:VAL:HG23	1.99	0.45
9:2J:4:LYS:HA	9:2J:5:ARG:HA	1.70	0.45
10:2K:112:MET:HB2	10:2K:113:PRO:HD3	1.99	0.45
25:2Z:73:LEU:HA	25:2Z:73:LEU:HD23	1.78	0.45
1:1A:2508:A:H5''	63:1A:4191:HOH:O	2.16	0.45
5:1E:78:LEU:HA	5:1E:78:LEU:HD12	1.80	0.45
10:1K:129:GLY:HA2	10:1K:132:ARG:HH22	1.82	0.45
12:1M:64:ARG:HB2	12:1M:83:ALA:HB3	1.99	0.45
1:2A:330:G:H22	1:2A:333:A:H5''	1.81	0.45
1:2A:579:U:O2	11:2L:45:ASN:HB2	2.16	0.45
1:2A:770:U:H2'	1:2A:771:G:O4'	2.17	0.45
3:2C:171:ILE:HG23	3:2C:172:HIS:N	2.32	0.45
6:2F:176:LEU:HD23	6:2F:176:LEU:HA	1.71	0.45
14:2O:138:ASP:OD2	23:2X:81:ARG:NH1	2.50	0.45
1:1A:1210:U:H2'	1:1A:1211:C:C6	2.52	0.45
1:1A:1232:U:H4'	19:1T:79:VAL:HG22	1.99	0.45
1:1A:195:A:H2'	1:1A:196:C:O4'	2.16	0.45
1:1A:552:A:N1	1:1A:2063:A:H2'	2.31	0.45
1:1A:612:A:OP1	6:1F:95:ARG:NH1	2.47	0.45
3:1C:59:ARG:NE	3:1C:164:ARG:HH22	2.15	0.45
5:1E:26:ILE:O	5:1E:182:LEU:N	2.44	0.45
6:1F:136:THR:HA	6:1F:166:ALA:O	2.17	0.45
7:1G:16:ARG:O	7:1G:20:ILE:HG13	2.16	0.45
12:1M:98:VAL:HG22	12:1M:118:ALA:HA	1.99	0.45
18:1S:102:GLU:HB3	18:1S:104:GLN:HE22	1.82	0.45
1:1A:2347:A:H61	24:1Y:43:THR:CG2	2.29	0.45
28:22:15:ILE:HG23	28:22:21:VAL:HG22	1.99	0.45
1:2A:1304:G:H2'	1:2A:1305:G:C8	2.52	0.45
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.82	0.45
1:2A:2072:A:H5'	1:2A:2589:G:O4'	2.17	0.45
1:2A:2672:G:H2'	1:2A:2673:A:O4'	2.16	0.45
1:2A:280:G:H2'	1:2A:281:G:H8	2.16	0.45
1:2A:396:G:N7	63:2A:5003:HOH:O	2.36	0.45
3:2C:44:HIS:O	3:2C:212:VAL:HG13	2.17	0.45
8:2H:30:LYS:NZ	8:2H:81:GLU:O	2.27	0.45
14:2O:75:THR:HG21	14:2O:87:LYS:NZ	2.32	0.45
20:2U:71:VAL:HA	20:2U:107:LEU:HD12	1.99	0.45
22:2W:9:LYS:HA	22:2W:10:GLY:HA2	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:16:50:LEU:HA	32:16:50:LEU:HD23	1.83	0.44
1:1A:1632:A:H2'	1:1A:1633:C:C6	2.52	0.44
1:1A:914:U:C4	1:1A:915:G:N7	2.85	0.44
4:1D:167:GLY:H	4:1D:168:ARG:HH12	8.30	0.44
17:1R:113:LYS:HA	17:1R:113:LYS:HD3	1.76	0.44
1:2A:1529:G:C2	1:2A:1551:C:C2	3.05	0.44
1:2A:1587:G:H3'	1:2A:1588:A:H2'	2.00	0.44
1:2A:1845:A:OP2	4:2D:54:ARG:NH2	2.50	0.44
1:2A:2151:U:H1'	1:2A:2179:A:C2	2.52	0.44
1:2A:2533:U:O2'	1:2A:2658:U:OP1	2.28	0.44
1:2A:2726:G:OP2	63:2A:4946:HOH:O	2.21	0.44
1:2A:598:U:H2'	1:2A:599:G:C8	2.52	0.44
1:2A:63:C:H2'	1:2A:64:C:C6	2.53	0.44
3:2C:171:ILE:HG23	3:2C:172:HIS:H	1.83	0.44
4:2D:264:LYS:HA	4:2D:265:PRO:HD3	1.89	0.44
8:2H:10:PRO:O	8:2H:12:PRO:HD3	2.17	0.44
11:2L:58:ASP:OD1	11:2L:58:ASP:N	2.50	0.44
22:2W:102:CYS:SG	22:2W:103:GLY:N	2.90	0.44
23:2X:136:PHE:HA	23:2X:136:PHE:HD1	1.74	0.44
28:12:16:CYS:SG	28:12:17:GLY:N	2.90	0.44
1:1A:1129:A:N6	1:1A:1130:A:C6	2.85	0.44
1:1A:115:A:C8	1:1A:116:A:C8	3.05	0.44
1:1A:1217:G:O2'	1:1A:1218:A:O5'	2.35	0.44
1:1A:1271:A:OP1	18:1S:16:LYS:NZ	2.51	0.44
1:1A:326:U:H2'	1:1A:327:G:H8	1.83	0.44
1:1A:867:A:O2'	1:1A:990:G:OP2	2.24	0.44
5:1E:12:THR:HG22	5:1E:13:ARG:N	2.32	0.44
8:1H:7:LEU:HA	8:1H:8:PRO:HD3	1.79	0.44
11:1L:62:VAL:CG1	11:1L:66:LYS:HB2	2.46	0.44
12:1M:68:GLU:HB3	12:1M:78:ARG:HB2	1.98	0.44
13:1N:91:PHE:CE1	13:1N:99:LEU:HD12	2.52	0.44
23:1X:5:LEU:HD22	23:1X:6:LYS:N	2.32	0.44
28:22:58:ARG:N	28:22:60:GLN:OE1	2.50	0.44
1:2A:1018:G:C4	1:2A:1034:G:C2	3.05	0.44
1:2A:1108:G:C6	1:2A:1109:C:C2	3.05	0.44
1:2A:131:C:H2'	1:2A:132:G:O4'	2.16	0.44
1:2A:289:G:H2'	1:2A:290:G:O4'	2.17	0.44
2:2B:12:C:H2'	24:2Y:73:GLY:HA3	1.99	0.44
6:2F:178:PRO:HB2	6:2F:201:VAL:HG21	2.00	0.44
14:2O:26:TYR:O	14:2O:67:ARG:NH1	2.43	0.44
19:2T:16:PRO:HD3	19:2T:99:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1055:A:N3	1:1A:1198:C:H1'	2.32	0.44
1:1A:1857:C:O2'	1:1A:1991:A:N3	2.45	0.44
1:1A:1994:G:H2'	1:1A:1995:C:C6	2.52	0.44
1:1A:2578:G:H2'	1:1A:2579:C:H6	1.81	0.44
1:1A:63:C:H2'	1:1A:64:C:H6	1.83	0.44
7:1G:7:LEU:HD13	7:1G:176:LEU:HD22	1.99	0.44
16:1Q:25:ARG:NH1	16:1Q:42:ASP:OD1	2.49	0.44
23:1X:109:ALA:HB3	23:1X:145:GLU:HG3	1.98	0.44
1:2A:1102:A:N6	1:2A:1132:G:OP2	2.33	0.44
1:2A:1244:C:H2'	1:2A:1245:C:C6	2.99	0.44
1:2A:1910:A:N1	1:2A:2245:G:H1'	2.33	0.44
1:2A:1928:G:H2'	1:2A:1929:C:H6	1.83	0.44
1:2A:2438:C:H5''	1:2A:2439:G:OP1	2.17	0.44
1:2A:298:G:O2'	1:2A:540:C:H5''	109.96	0.44
1:2A:55:C:H2'	1:2A:56:G:O4'	2.18	0.44
8:2H:107:VAL:O	8:2H:152:ARG:NH2	2.50	0.44
14:2O:58:PHE:HB3	14:2O:61:GLY:HA2	1.99	0.44
1:2A:1426:G:N2	17:2R:119:LYS:HB2	92.41	0.44
23:2X:175:VAL:HG12	23:2X:176:PRO:O	2.17	0.44
1:2A:2367:C:O3'	24:2Y:20:ARG:HD3	2.17	0.44
30:14:9:LEU:HD13	30:14:51:GLU:HG3	1.99	0.44
1:1A:1378:C:H2'	1:1A:1379:G:H8	1.81	0.44
1:1A:2331:A:N3	1:1A:2331:A:H2'	2.31	0.44
1:1A:909:A:P	14:1O:22:LYS:HG3	2.58	0.44
2:1B:30:C:H2'	2:1B:31:C:H5'	2.00	0.44
1:2A:1100:G:H3'	1:2A:1101:G:C8	2.53	0.44
1:2A:1714:A:H4'	1:2A:1715:A:O5'	2.18	0.44
1:2A:1921:A:OP2	63:2A:4947:HOH:O	2.21	0.44
1:2A:2122:G:C4	1:2A:2123:U:H1'	2.52	0.44
1:2A:2574:U:H4'	12:2M:28:SER:HA	1.99	0.44
1:2A:2044:G:H5'	1:2A:2628:C:H4'	1.98	0.44
1:2A:399:U:H1'	1:2A:449:A:C2	2.53	0.44
1:2A:409:U:H2'	1:2A:411:C:H5	1.83	0.44
1:2A:555:C:H4'	1:2A:556:A:H5''	1.99	0.44
1:2A:649:G:O6	13:2N:107:LYS:NZ	2.50	0.44
1:2A:2197:A:OP1	3:2C:221:SER:HB3	2.17	0.44
4:2D:143:HIS:HD1	4:2D:194:GLY:C	2.21	0.44
12:2M:22:ILE:HD11	12:2M:40:VAL:HG12	1.99	0.44
13:2N:44:GLY:CA	13:2N:45:LEU:HB2	2.48	0.44
1:1A:274:C:H2'	1:1A:275:C:C6	2.53	0.44
1:1A:488:G:N1	1:1A:491:A:OP2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:62:A:C5	21:1V:66:LEU:HD12	2.53	0.44
3:1C:21:THR:HG22	3:1C:22:ILE:H	1.81	0.44
13:1N:77:ARG:HB2	13:1N:78:PRO:HD2	1.98	0.44
22:1W:30:VAL:HG22	22:1W:37:VAL:HG12	2.00	0.44
23:1X:72:ARG:NH2	23:1X:97:GLU:O	2.45	0.44
1:2A:1059:U:H2'	1:2A:1060:G:H8	1.83	0.44
1:2A:1638:G:H2'	1:2A:1639:G:H8	1.81	0.44
1:2A:1861:G:H2'	1:2A:1862:C:C6	2.52	0.44
1:2A:2149:C:H5'	1:2A:2194:A:C2	2.52	0.44
1:2A:2326:G:H2'	1:2A:2327:C:C6	2.53	0.44
1:2A:2361:C:H2'	1:2A:2362:G:O4'	2.18	0.44
1:2A:2682:A:H2'	1:2A:2683:G:O4'	2.18	0.44
1:2A:326:U:H2'	1:2A:327:G:H8	1.83	0.44
1:2A:473:U:O4	1:2A:605:G:H1'	2.17	0.44
8:2H:83:TYR:CE2	8:2H:138:LYS:HB2	2.53	0.44
13:2N:52:GLU:HB3	13:2N:55:ARG:HH11	1.82	0.44
14:2O:128:LYS:HB3	14:2O:128:LYS:NZ	2.32	0.44
14:2O:58:PHE:HB3	14:2O:61:GLY:CA	2.47	0.44
18:2S:66:ASN:O	18:2S:70:ARG:HG3	2.18	0.44
21:2V:31:HIS:CD2	21:2V:33:LYS:H	2.35	0.44
25:2Z:83:GLU:HA	25:2Z:84:GLY:HA2	1.67	0.44
1:1A:1230:G:H2'	1:1A:1231:G:O4'	2.18	0.44
1:1A:206:A:OP2	63:1A:3887:HOH:O	2.21	0.44
1:1A:2131:G:P	1:1A:2139:U:H3	2.37	0.44
1:1A:2044:G:H5'	1:1A:2628:C:H4'	1.98	0.44
15:1P:81:ASP:O	15:1P:85:PRO:HG2	2.17	0.44
1:2A:2411:G:H4'	30:24:18:ARG:HG2	2.00	0.44
33:27:2:LYS:HD3	33:27:4:ARG:NH2	2.33	0.44
1:2A:1105:U:H4'	1:2A:1106:U:H5''	2.00	0.44
1:2A:1377:G:HO2'	1:2A:1654:A:H2	1.64	0.44
1:2A:1451:U:H2'	1:2A:1452:C:C6	2.53	0.44
1:2A:2397:C:H2'	1:2A:2398:U:C6	2.53	0.44
1:2A:440:C:H1'	1:2A:1894:U:H1'	1.99	0.44
1:2A:601:G:H2'	1:2A:602:C:C6	2.52	0.44
13:2N:121:LYS:O	13:2N:123:LEU:HD12	2.18	0.44
1:2A:2889:C:O3'	15:2P:90:ARG:NH1	2.51	0.44
16:2Q:26:LEU:HD22	16:2Q:87:PHE:CD1	2.53	0.44
18:2S:85:LYS:HA	18:2S:85:LYS:HD3	1.82	0.44
19:2T:43:GLU:N	19:2T:43:GLU:OE2	2.50	0.44
19:2T:65:GLY:HA3	19:2T:91:TYR:CZ	2.53	0.44
23:2X:42:VAL:O	23:2X:46:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2478:C:H4'	14:1O:123:HIS:CD2	2.51	0.44
1:1A:385:U:O2'	1:1A:386:G:H5''	2.18	0.44
6:1F:20:LEU:HD22	6:1F:21:ALA:H	1.82	0.44
7:1G:103:LEU:HD23	7:1G:106:LEU:HD23	2.00	0.44
12:1M:47:ILE:HB	12:1M:48:PRO:HD2	2.00	0.44
25:1Z:86:SER:OG	25:1Z:89:GLU:HG2	2.18	0.44
1:2A:1784:C:OP1	17:2R:96:ARG:NH1	2.39	0.44
1:2A:2123:U:H2'	1:2A:2124:C:C6	2.52	0.44
1:2A:2218:U:H1'	1:2A:2219:A:C8	2.52	0.44
1:2A:2448:U:H2'	1:2A:2449:U:C6	2.53	0.44
1:2A:2901:G:H5''	1:2A:2902:G:O4'	2.17	0.44
1:2A:345:A:H5'	1:2A:363:A:H1'	1.99	0.44
23:2X:91:LEU:HD12	23:2X:91:LEU:HA	1.80	0.44
26:10:39:ALA:HB2	26:10:44:LEU:HD23	1.99	0.44
1:1A:1440:A:H1'	63:1A:3989:HOH:O	2.18	0.44
1:1A:2783:C:H2'	1:1A:2784:C:C6	2.53	0.44
1:1A:731:A:H5'	1:1A:820:A:H61	1.81	0.44
4:1D:108:PRO:HD2	4:1D:111:LEU:HG	2.00	0.44
16:1Q:14:VAL:HG21	16:1Q:90:GLY:O	2.17	0.44
22:1W:8:LYS:HG2	22:1W:9:LYS:O	2.18	0.44
1:2A:1155:G:O2'	1:2A:1156:A:H8	2.00	0.44
1:2A:1187:A:C4	1:2A:1189:G:C8	3.06	0.44
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.18	0.44
1:2A:1417:U:C2'	1:2A:1418:A:H5'	2.48	0.44
1:2A:1549:C:H2'	1:2A:1550:C:C6	2.52	0.44
1:2A:610:U:H2'	1:2A:611:C:C6	2.52	0.44
8:2H:113:VAL:HG11	8:2H:151:ILE:HD13	1.99	0.44
15:2P:30:THR:O	15:2P:78:LYS:NZ	2.51	0.44
15:2P:38:VAL:HB	15:2P:39:PRO:HD3	2.00	0.44
23:2X:75:ASN:HB2	23:2X:85:HIS:HB3	2.00	0.44
1:1A:1556:A:H2'	1:1A:1557:G:O4'	2.18	0.44
1:1A:1881:U:H2'	1:1A:1882:C:O4'	2.17	0.44
1:1A:608:A:H5'	6:1F:89:VAL:HG21	2.00	0.44
1:1A:714:G:H5'	1:1A:715:G:OP2	2.17	0.44
8:1H:55:PRO:HG2	8:1H:61:HIS:CE1	2.53	0.44
12:1M:77:ILE:HB	17:1R:74:ARG:HD3	1.99	0.44
1:2A:1383:G:N7	21:2V:62:LYS:NZ	2.53	0.44
1:2A:1406:G:H2'	1:2A:1407:C:C6	3.06	0.44
1:2A:1549:C:H2'	1:2A:1550:C:H6	1.83	0.44
1:2A:2706:C:H2'	1:2A:2707:U:C6	2.53	0.44
1:2A:548:U:H2'	1:2A:549:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:14:U:HO2'	2:2B:15:A:H8	1.64	0.44
4:2D:146:GLU:HB2	4:2D:189:CYS:HB3	1.99	0.44
6:2F:114:VAL:HG21	6:2F:202:PHE:CZ	2.53	0.44
8:2H:154:PRO:HB3	8:2H:163:TYR:CE2	2.52	0.44
21:2V:35:THR:O	21:2V:39:ILE:HG13	2.17	0.44
25:2Z:7:ILE:HD12	25:2Z:98:LEU:HD21	2.00	0.44
1:1A:614:G:O2'	32:16:4:MET:HG3	2.18	0.43
1:1A:1111:U:H2'	1:1A:1111:U:O2	2.17	0.43
1:1A:353:A:H2	1:1A:1254:A:H2'	1.82	0.43
1:1A:1562:G:H2'	1:1A:1563:C:C6	2.52	0.43
1:1A:1612:A:OP1	4:1D:211:ARG:NH1	2.51	0.43
1:1A:1994:G:H2'	1:1A:1995:C:H6	1.83	0.43
1:1A:2388:A:H2'	1:1A:2389:A:C8	2.53	0.43
5:1E:54:GLN:HE21	5:1E:76:ARG:HG2	1.83	0.43
1:1A:2695:U:O2'	12:1M:68:GLU:OE1	2.23	0.43
1:2A:1056:G:C6	1:2A:1196:G:C6	3.06	0.43
1:2A:1116:G:H1	1:2A:1145:C:H41	1.66	0.43
1:2A:1319:A:N3	1:2A:1342:C:H1'	2.32	0.43
1:2A:2341:G:H2'	1:2A:2342:G:O4'	2.17	0.43
1:2A:321:G:H5''	1:2A:322:A:OP1	2.18	0.43
4:2D:245:PRO:HA	4:2D:246:PRO:HD3	1.86	0.43
5:2E:144:ARG:HB3	5:2E:145:LYS:H	1.44	0.43
21:2V:1:MET:O	21:2V:2:LYS:HB3	2.18	0.43
22:2W:38:ILE:HD13	22:2W:66:PRO:HA	2.00	0.43
1:2A:508:A:O2'	22:2W:49:VAL:O	2.23	0.43
28:12:41:PRO:HG3	28:12:49:PHE:CE2	2.53	0.43
28:12:68:ARG:HH21	28:12:68:ARG:HA	1.81	0.43
30:14:11:LEU:HB3	30:14:49:HIS:HB3	2.01	0.43
1:1A:1111:U:H1'	1:1A:1113:G:N7	2.33	0.43
1:1A:1275:C:H2'	1:1A:1276:G:C8	2.52	0.43
1:1A:2171:U:H2'	1:1A:2172:G:C8	2.54	0.43
3:1C:42:GLU:HB2	3:1C:44:HIS:HE2	1.83	0.43
1:2A:982:G:OP1	32:26:52:LYS:HD2	2.18	0.43
1:2A:1194:G:H2'	1:2A:1195:C:H6	1.83	0.43
1:2A:13:A:N6	1:2A:14:G:C2	2.86	0.43
1:2A:2197:A:H2'	1:2A:2198:C:C6	2.53	0.43
1:2A:267:G:O2'	1:2A:268:G:H8	2.01	0.43
1:2A:2861:G:H2'	1:2A:2862:C:C6	2.54	0.43
2:2B:106:G:H5'	23:2X:31:ARG:HG2	2.01	0.43
2:2B:117:G:H2'	2:2B:118:G:O4'	2.18	0.43
7:2G:118:ARG:O	7:2G:181:ARG:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2N:100:LEU:HD12	13:2N:112:LEU:HD11	2.00	0.43
1:1A:1050:C:O2'	11:1L:28:THR:HG21	2.18	0.43
1:1A:1786:G:H4'	1:1A:1788:G:O4'	2.18	0.43
1:1A:2203:G:H2'	1:1A:2204:C:C6	2.52	0.43
1:1A:2206:C:H2'	1:1A:2207:G:H8	1.83	0.43
1:1A:2317:C:N4	7:1G:42:GLY:HA3	2.34	0.43
1:1A:319:C:H2'	1:1A:320:C:H6	1.83	0.43
1:1A:437:G:H3'	63:1A:4696:HOH:O	2.19	0.43
7:1G:64:THR:HB	7:1G:94:LEU:HD21	2.00	0.43
8:1H:11:VAL:HG21	8:1H:50:VAL:HG23	2.00	0.43
10:1K:106:GLU:H	10:1K:106:GLU:HG3	1.67	0.43
1:2A:1039:C:O2'	1:2A:1041:A:OP1	2.17	0.43
1:2A:1207:G:C4	1:2A:1208:G:C8	3.05	0.43
1:2A:1925:G:N2	1:2A:1926:C:H1'	2.33	0.43
1:2A:2155:A:H2	1:2A:2180:G:H4'	1.84	0.43
1:2A:2406:C:O2'	25:2Z:30:VAL:HG13	2.17	0.43
1:2A:2224:U:O4'	4:2D:151:LYS:HE2	2.18	0.43
12:2M:97:ARG:HD3	12:2M:99:PHE:CE2	2.53	0.43
16:2Q:7:TYR:CZ	16:2Q:91:PRO:HG3	2.53	0.43
17:2R:73:GLU:OE2	17:2R:103:ARG:NH2	2.51	0.43
23:2X:156:LYS:HE3	23:2X:158:PRO:HD3	1.99	0.43
1:1A:1245:C:H2'	1:1A:1246:C:C6	2.81	0.43
1:1A:2180:G:H2'	1:1A:2181:G:O4'	2.19	0.43
1:1A:228:G:H1'	1:1A:258:A:N1	40.19	0.43
1:1A:2864:C:H2'	1:1A:2865:C:H6	1.84	0.43
1:1A:29:G:H2'	1:1A:30:C:C6	2.53	0.43
1:1A:488:G:N2	1:1A:491:A:OP2	2.48	0.43
1:1A:483:G:O2'	1:1A:494:G:O6	2.29	0.43
1:1A:504:A:H4'	1:1A:505:A:OP1	2.19	0.43
1:1A:553:A:OP2	11:1L:114:ARG:NH2	2.50	0.43
1:1A:967:U:H2'	1:1A:968:C:C6	2.53	0.43
3:1C:46:LYS:HD3	3:1C:210:ARG:HG2	2.01	0.43
7:1G:139:LEU:HD12	7:1G:139:LEU:H	1.84	0.43
1:1A:2404:A:H5'	13:1N:63:PRO:HB3	1.99	0.43
1:2A:1064:U:O2'	1:2A:1066:A:H2	2.00	0.43
1:2A:1115:A:O2'	1:2A:1116:G:OP1	2.26	0.43
1:2A:1446:G:H2'	1:2A:1447:C:C6	2.54	0.43
1:2A:1519:G:H2'	1:2A:1520:C:O4'	2.18	0.43
1:2A:1614:G:H5''	4:2D:61:LEU:HD22	2.01	0.43
1:2A:2176:G:C6	1:2A:2177:G:H1'	2.52	0.43
1:2A:2812:G:H2'	1:2A:2813:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:323:A:P	22:2W:86:ARG:HH21	2.41	0.43
1:2A:875:A:N7	1:2A:2258:A:O2'	2.47	0.43
1:2A:710:C:H4'	1:2A:985:A:OP1	2.18	0.43
3:2C:44:HIS:ND1	3:2C:172:HIS:HA	2.33	0.43
4:2D:37:LEU:HA	4:2D:37:LEU:HD12	1.85	0.43
16:2Q:87:PHE:CZ	16:2Q:98:VAL:HG12	2.52	0.43
23:2X:102:LEU:N	23:2X:122:ARG:O	2.47	0.43
23:2X:156:LYS:HE2	23:2X:156:LYS:HB3	1.78	0.43
25:2Z:8:SER:HB3	25:2Z:66:HIS:CD2	2.54	0.43
28:12:56:VAL:HG23	28:12:57:GLU:H	1.82	0.43
1:1A:137:G:H2'	1:1A:138:A:C8	9.29	0.43
1:1A:1808:U:H2'	1:1A:1814:A:N6	2.33	0.43
1:1A:2375:C:H2'	1:1A:2376:G:O4'	2.19	0.43
1:1A:514:G:H8	1:1A:514:G:OP1	2.01	0.43
4:1D:146:GLU:HB2	4:1D:189:CYS:HB3	2.01	0.43
5:1E:111:ARG:HG3	5:1E:160:TYR:CD2	2.53	0.43
7:1G:66:GLN:NE2	7:1G:93:THR:O	2.46	0.43
10:1K:84:LEU:HD11	10:1K:96:VAL:HB	2.00	0.43
11:1L:28:THR:HG22	11:1L:29:LYS:N	2.32	0.43
21:1V:53:LYS:HB3	21:1V:82:GLN:HB3	2.01	0.43
1:2A:1018:G:OP1	1:2A:1231:G:O2'	2.23	0.43
1:2A:1960:U:OP1	1:2A:2615:U:O2'	2.29	0.43
1:2A:2088:G:O2'	1:2A:2090:G:H5'	2.18	0.43
3:2C:29:VAL:HB	3:2C:41:VAL:HG21	2.01	0.43
5:2E:9:VAL:HB	17:2R:3:ARG:HG2	2.00	0.43
23:2X:30:ASN:HA	23:2X:89:PHE:HE1	1.84	0.43
28:12:28:LYS:HB2	28:12:31:ILE:HD11	2.01	0.43
1:1A:353:A:H2	1:1A:1254:A:O2'	2.00	0.43
1:1A:1403:G:OP2	63:1A:3889:HOH:O	2.21	0.43
1:1A:1475:C:H2'	1:1A:1476:U:C6	2.52	0.43
1:1A:2206:C:H2'	1:1A:2207:G:C8	2.53	0.43
1:1A:639:A:C4	6:1F:180:GLY:HA3	2.54	0.43
1:1A:778:C:N4	1:1A:779:G:C6	2.87	0.43
3:1C:11:LEU:HA	3:1C:11:LEU:HD12	1.86	0.43
10:1K:80:LYS:HB3	10:1K:80:LYS:HE2	1.79	0.43
17:1R:94:ALA:HB1	17:1R:99:LEU:HD21	2.00	0.43
22:1W:30:VAL:O	22:1W:32:PRO:HD3	2.19	0.43
1:2A:2151:U:H4'	1:2A:2154:G:H4'	2.01	0.43
1:2A:2366:C:H1'	24:2Y:39:ARG:HH21	1.83	0.43
5:2E:199:ARG:NH1	5:2E:202:LYS:HE3	2.33	0.43
5:2E:56:PRO:HG3	5:2E:74:PRO:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2H:10:PRO:HA	8:2H:49:VAL:HG22	2.00	0.43
12:2M:100:GLY:O	12:2M:119:PRO:HD2	2.19	0.43
15:2P:44:LEU:HD22	15:2P:48:VAL:HG23	2.01	0.43
23:2X:155:LEU:HD23	23:2X:157:LEU:HD21	2.01	0.43
1:1A:2151:U:H4'	1:1A:2154:G:C5'	2.49	0.43
4:1D:68:LYS:HD3	4:1D:70:TRP:CZ2	2.54	0.43
8:1H:23:ARG:HD2	8:1H:34:GLU:OE2	2.18	0.43
1:1A:857:U:H2'	13:1N:21:ARG:HA	2.01	0.43
14:1O:41:TRP:CD1	14:1O:96:VAL:HG22	2.54	0.43
20:1U:94:ASP:O	20:1U:95:ILE:HD13	2.19	0.43
21:1V:84:ALA:O	21:1V:87:GLN:HB2	2.19	0.43
1:2A:1138:G:H1'	1:2A:1144:G:N2	2.34	0.43
1:2A:1369:G:C2	1:2A:1370:G:C8	13.56	0.43
1:2A:2333:A:H2'	1:2A:2334:G:O4'	2.19	0.43
1:2A:2358:C:H2'	1:2A:2359:U:C6	2.54	0.43
1:2A:825:U:H6	1:2A:825:U:P	3.63	0.43
1:2A:903:C:H4'	24:2Y:23:VAL:HG21	2.01	0.43
2:2B:3:C:H2'	2:2B:4:C:C6	2.53	0.43
3:2C:50:ASP:HB3	3:2C:56:GLN:CD	2.39	0.43
10:2K:131:ALA:HB1	10:2K:137:GLU:HA	2.01	0.43
11:2L:4:TYR:O	18:2S:64:ARG:NH2	2.38	0.43
13:2N:101:VAL:HG23	13:2N:106:LEU:HB3	2.01	0.43
19:2T:89:GLN:HA	19:2T:90:PRO:HD3	1.93	0.43
1:2A:1409:G:OP2	25:2Z:3:LYS:HG3	2.18	0.43
1:1A:1008:C:N4	1:1A:1009:C:H41	3.03	0.43
1:1A:2284:A:H2'	1:1A:2285:A:C8	2.53	0.43
1:1A:2818:A:C6	1:1A:2900:A:C8	3.07	0.43
1:1A:915:G:C4	1:1A:916:A:C8	3.07	0.43
1:1A:933:A:OP1	1:1A:934:C:N4	2.47	0.43
3:1C:62:VAL:HG22	3:1C:63:SER:O	2.18	0.43
4:1D:97:TYR:CE1	4:1D:103:ARG:HG3	2.54	0.43
17:1R:108:ARG:NH2	17:1R:112:ARG:HH21	2.16	0.43
17:1R:18:ASP:OD2	17:1R:18:ASP:N	2.30	0.43
1:2A:1017:A:OP2	63:2A:4936:HOH:O	2.21	0.43
1:2A:1479:A:H61	1:2A:1604:A:H62	1.65	0.43
1:2A:1840:A:H2'	1:2A:1841:G:O4'	2.19	0.43
1:2A:2133:G:N7	1:2A:2134:U:H1'	2.34	0.43
1:2A:2227:G:H3'	1:2A:2228:A:H5''	2.01	0.43
1:2A:2796:C:H1'	5:2E:37:ARG:HH12	1.83	0.43
1:2A:2817:U:H5'	1:2A:2899:G:O6	2.18	0.43
1:2A:931:C:H2'	1:2A:932:C:H4'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2C:200:LYS:HG3	3:2C:204:ALA:HB3	2.01	0.43
3:2C:205:LYS:HB3	3:2C:205:LYS:HE2	1.90	0.43
3:2C:26:ALA:O	3:2C:185:LEU:HD13	2.19	0.43
4:2D:70:TRP:CE2	4:2D:150:LYS:HD3	2.53	0.43
6:2F:78:ILE:HA	6:2F:83:PHE:CD2	2.53	0.43
16:2Q:15:ARG:NE	16:2Q:88:ASP:OD2	2.46	0.43
23:2X:70:LEU:HD21	23:2X:98:MET:HE2	1.99	0.43
28:12:46:GLN:O	28:12:48:ARG:HG2	2.19	0.43
1:1A:11:U:H2'	1:1A:11:U:O2	2.19	0.43
1:1A:2417:U:OP2	1:1A:2417:U:H2'	2.19	0.43
1:1A:2661:U:H2'	1:1A:2662:C:H6	1.84	0.43
1:1A:42:A:O2'	1:1A:43:G:H5'	2.19	0.43
2:1B:29:A:H2'	2:1B:30:C:C6	2.54	0.43
3:1C:19:VAL:HG22	3:1C:223:ARG:CD	2.47	0.43
1:1A:1856:G:H4'	4:1D:242:ARG:CZ	2.48	0.43
6:1F:129:PHE:HB3	6:1F:132:VAL:HG11	2.00	0.43
8:1H:24:VAL:HG22	8:1H:35:VAL:HB	2.00	0.43
8:1H:80:SER:OG	8:1H:81:GLU:N	2.52	0.43
1:1A:2573:U:O2'	12:1M:23:ARG:HD3	2.19	0.43
32:26:11:LYS:HE3	32:26:65:GLU:OE2	2.19	0.43
1:2A:1275:C:H2'	1:2A:1276:G:C8	2.54	0.43
1:2A:1439:U:H4'	1:2A:1648:A:H4'	2.00	0.43
1:2A:2058:G:H2'	1:2A:2059:G:C8	2.54	0.43
1:2A:274:C:H2'	1:2A:275:C:C6	2.54	0.43
1:2A:926:G:C2	1:2A:927:G:C8	3.06	0.43
6:2F:29:ASN:OD1	6:2F:32:LEU:N	2.39	0.43
8:2H:40:GLU:O	8:2H:55:PRO:HG2	2.19	0.43
1:2A:1108:G:H1'	10:2K:91:PRO:HG3	2.01	0.43
13:2N:50:ARG:O	13:2N:52:GLU:HG3	2.19	0.43
1:1A:1324:G:H4'	15:1P:31:HIS:CD2	2.54	0.43
1:1A:1512:G:H2'	1:1A:1593:C:N4	2.34	0.43
1:1A:309:C:H2'	1:1A:310:C:H6	1.83	0.43
1:1A:628:U:H4'	1:1A:704:C:H4'	2.00	0.43
1:1A:767:C:H2'	1:1A:768:A:C8	2.54	0.43
1:1A:930:C:N4	1:1A:937:G:H1	2.15	0.43
2:1B:86:G:H1	2:1B:91:C:N4	2.16	0.43
3:1C:8:ARG:HA	3:1C:11:LEU:HB2	2.00	0.43
4:1D:148:GLU:HB2	4:1D:151:LYS:HD2	1.99	0.43
6:1F:197:ASP:O	6:1F:201:VAL:HG12	2.19	0.43
8:1H:4:ILE:O	8:1H:69:ARG:HG2	2.19	0.43
1:2A:1138:G:H21	1:2A:1143:A:H62	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:124:A:H5''	1:2A:125:C:O4'	2.19	0.43
1:2A:1492:C:H42	1:2A:1511:G:H1	1.66	0.43
1:2A:1564:G:H2'	1:2A:1565:U:O4'	2.18	0.43
1:2A:1618:A:H2'	1:2A:1619:G:O4'	2.18	0.43
1:2A:1763:G:C6	1:2A:1764:U:C4	3.06	0.43
1:2A:2176:G:H3'	1:2A:2177:G:C8	2.54	0.43
1:2A:2637:C:H2'	1:2A:2638:G:C8	2.54	0.43
1:2A:303:C:H2'	1:2A:304:G:O4'	2.19	0.43
1:2A:591:U:C4	1:2A:592:G:C6	3.07	0.43
1:2A:872:U:H2'	1:2A:874:U:O4'	2.18	0.43
5:2E:12:THR:HG22	5:2E:13:ARG:H	1.84	0.43
5:2E:59:VAL:HG21	5:2E:74:PRO:HB3	2.01	0.43
7:2G:131:TYR:HB3	7:2G:159:VAL:HG13	2.00	0.43
26:10:61:LEU:HD23	26:10:61:LEU:HA	1.85	0.42
1:1A:1064:U:O2'	1:1A:1066:A:H2	1.83	0.42
1:1A:1443:C:H2'	1:1A:1444:C:O4'	2.81	0.42
1:1A:1472:A:H4'	1:1A:1473:C:O4'	2.19	0.42
1:1A:2220:A:H3'	1:1A:2221:C:H6	1.83	0.42
1:1A:2020:C:H5''	1:1A:2735:C:O2'	2.19	0.42
2:1B:33:G:C2	2:1B:50:G:C2	3.07	0.42
4:1D:5:LYS:HB3	4:1D:5:LYS:HE3	1.82	0.42
22:1W:38:ILE:HD11	22:1W:66:PRO:HG3	2.01	0.42
27:21:18:ASP:N	27:21:18:ASP:OD1	2.43	0.42
28:22:1:MET:HG3	28:22:6:HIS:CD2	2.54	0.42
30:24:7:ILE:CG2	30:24:27:LYS:HD3	2.49	0.42
1:2A:1107:G:OP1	1:2A:1115:A:H4'	2.19	0.42
1:2A:1247:G:H2'	1:2A:1248:A:C2	2.54	0.42
1:2A:1518:A:H2'	1:2A:1519:G:O4'	2.19	0.42
1:2A:1716:C:O2	5:2E:129:HIS:NE2	2.42	0.42
1:2A:2121:G:H2'	1:2A:2122:G:C8	2.54	0.42
1:2A:2187:G:H3'	1:2A:2188:U:C5'	2.47	0.42
1:2A:624:G:O2'	1:2A:701:A:N6	2.51	0.42
6:2F:110:LEU:HD22	6:2F:183:VAL:HG12	1.99	0.42
8:2H:149:ARG:NH1	8:2H:167:GLU:OE2	2.52	0.42
11:2L:96:GLU:O	11:2L:100:GLU:HB2	2.18	0.42
1:2A:909:A:P	14:2O:22:LYS:HG3	2.59	0.42
1:2A:2345:G:C6	24:2Y:75:LEU:HD21	2.54	0.42
28:12:57:GLU:HA	28:12:58:ARG:HA	1.70	0.42
1:1A:1039:C:OP1	18:1S:53:ARG:NH2	2.51	0.42
1:1A:1107:G:N3	1:1A:1107:G:H2'	2.35	0.42
1:1A:1116:G:C6	1:1A:1117:C:N4	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2514:A:OP1	63:1A:3888:HOH:O	2.21	0.42
1:1A:2672:G:OP1	63:1A:3890:HOH:O	2.22	0.42
1:1A:2839:G:N7	63:1A:3991:HOH:O	2.37	0.42
1:1A:765:C:H2'	1:1A:766:C:C6	2.55	0.42
1:1A:767:C:H2'	1:1A:768:A:H8	1.84	0.42
1:1A:830:A:O4'	4:1D:227:ASN:ND2	2.52	0.42
8:1H:3:ARG:HA	8:1H:3:ARG:NE	2.33	0.42
14:1O:1:MET:H1	14:1O:1:MET:HE3	1.84	0.42
17:1R:16:ARG:NH1	17:1R:19:LEU:HD21	2.34	0.42
1:1A:2342:G:O2'	24:1Y:43:THR:HG22	2.18	0.42
26:20:2:LYS:H	26:20:2:LYS:HG2	1.48	0.42
32:26:6:THR:HG22	32:26:63:PRO:HD2	2.01	0.42
1:2A:1280:G:C6	1:2A:1281:G:N1	2.87	0.42
1:2A:1493:G:H1'	1:2A:1591:A:H1'	2.00	0.42
1:2A:232:A:C2	1:2A:243:A:C4	3.07	0.42
1:2A:2549:C:H2'	1:2A:2550:C:H6	1.84	0.42
1:2A:830:A:C8	1:2A:838:G:C5	3.07	0.42
3:2C:20:TYR:CD1	3:2C:222:VAL:HG13	2.53	0.42
1:2A:2198:C:O2'	3:2C:46:LYS:HG3	2.20	0.42
9:2J:117:LEU:HA	9:2J:122:VAL:HA	2.01	0.42
13:2N:95:VAL:HA	13:2N:99:LEU:HD21	2.01	0.42
23:2X:18:LEU:H	23:2X:18:LEU:HD12	4.47	0.42
1:1A:1122:A:H2'	1:1A:1123:U:O4'	2.19	0.42
1:1A:2220:A:H3'	1:1A:2221:C:C6	2.54	0.42
1:1A:280:G:H2'	1:1A:281:G:H8	2.24	0.42
1:1A:385:U:H2'	1:1A:385:U:H6	1.52	0.42
1:1A:872:U:H2'	1:1A:874:U:O4'	2.19	0.42
14:1O:76:LYS:HB3	14:1O:91:GLU:HG3	2.01	0.42
23:1X:152:ALA:HA	23:1X:155:LEU:HD13	2.00	0.42
27:21:29:ARG:HB3	27:21:30:ARG:NH1	2.35	0.42
33:27:25:VAL:HB	33:27:34:GLN:HB2	2.00	0.42
1:2A:2609:A:OP1	63:2A:4948:HOH:O	2.21	0.42
1:2A:1683:A:H4'	1:2A:2722:A:O2'	2.19	0.42
1:2A:378:G:H2'	1:2A:379:G:H8	1.84	0.42
1:2A:387:A:H2'	1:2A:388:G:O4'	2.19	0.42
1:2A:630:A:H2'	1:2A:631:A:C8	2.54	0.42
1:2A:838:G:H5''	1:2A:839:A:H5'	2.01	0.42
5:2E:181:LEU:HD21	17:2R:6:LEU:HD12	2.01	0.42
11:2L:94:HIS:HB3	11:2L:97:ARG:HD3	2.02	0.42
1:2A:1711:A:H1'	12:2M:1:MET:HG3	2.02	0.42
17:2R:80:SER:HA	17:2R:81:PRO:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:126:C:H2'	1:1A:127:C:H6	1.85	0.42
1:1A:1302:C:H2'	1:1A:1303:C:O4'	2.83	0.42
1:1A:1469:G:H2'	1:1A:1470:G:O4'	2.19	0.42
1:1A:1748:G:H2'	1:1A:1749:G:O4'	2.20	0.42
1:1A:2095:U:H2'	1:1A:2096:U:C6	2.54	0.42
1:1A:2290:G:O6	24:1Y:14:ARG:HD2	2.19	0.42
1:1A:2309:A:H2'	1:1A:2310:G:O4'	2.19	0.42
4:1D:142:VAL:HG23	4:1D:193:VAL:HA	2.01	0.42
5:1E:93:VAL:HG21	5:1E:180:ASN:HA	2.02	0.42
6:1F:89:VAL:O	63:1F:5002:HOH:O	2.21	0.42
18:1S:17:ILE:HG23	18:1S:39:LEU:HD12	2.01	0.42
32:26:62:LEU:HB3	32:26:65:GLU:HG2	2.02	0.42
1:2A:1322:G:H2'	1:2A:1323:A:O4'	2.19	0.42
1:2A:1729:C:H2'	1:2A:1730:C:C6	2.54	0.42
1:2A:2768:U:H1'	1:2A:2769:A:H5''	2.00	0.42
1:2A:842:C:H2'	1:2A:843:C:C6	2.54	0.42
1:2A:885:U:H2'	1:2A:886:C:C6	2.54	0.42
4:2D:121:PRO:HB3	4:2D:135:PHE:CE2	2.54	0.42
6:2F:149:ASP:OD1	6:2F:149:ASP:N	2.46	0.42
18:2S:20:LEU:O	18:2S:39:LEU:HD21	2.20	0.42
23:2X:179:ASP:O	23:2X:182:LYS:HB3	2.19	0.42
1:2A:2288:G:P	24:2Y:12:ASN:HD22	2.42	0.42
1:1A:2593:G:C2	1:1A:2594:G:C8	3.08	0.42
1:1A:2734:G:H2'	1:1A:2735:C:C6	2.55	0.42
1:1A:353:A:HO2'	1:1A:354:A:H8	1.64	0.42
2:1B:42:C:OP1	7:1G:67:LYS:NZ	2.53	0.42
3:1C:182:PRO:C	3:1C:184:LYS:H	2.22	0.42
5:1E:181:LEU:HD12	5:1E:181:LEU:HA	1.82	0.42
6:1F:117:ARG:NH2	6:1F:189:THR:O	2.51	0.42
6:1F:18:ARG:HG2	6:1F:19:GLU:H	1.83	0.42
9:1J:77:PRO:O	9:1J:79:ALA:N	2.52	0.42
15:1P:44:LEU:HD22	15:1P:48:VAL:HG23	2.01	0.42
23:1X:145:GLU:O	23:1X:148:ASP:N	2.52	0.42
27:21:6:VAL:HG13	27:21:54:VAL:CG1	2.49	0.42
1:2A:1107:G:H1	1:2A:1121:C:H42	1.68	0.42
1:2A:1191:C:H2'	1:2A:1192:C:C6	2.54	0.42
1:2A:164:G:O2'	1:2A:165:G:H5'	2.20	0.42
1:2A:172:C:H1'	1:2A:205:G:H1'	2.01	0.42
1:2A:241:C:H2'	1:2A:242:G:O4'	2.19	0.42
1:2A:2858:U:H4'	1:2A:2877:A:C2	2.54	0.42
1:2A:557:G:H5'	18:2S:24:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:57:U:H2'	1:2A:58:G:C8	5.24	0.42
1:2A:65:U:H2'	1:2A:66:G:C8	2.54	0.42
1:2A:966:G:H4'	1:2A:2280:A:C5	2.54	0.42
7:2G:41:GLN:NE2	7:2G:154:GLY:O	2.36	0.42
15:2P:57:ARG:NE	15:2P:59:ASP:OD1	2.52	0.42
16:2Q:10:ARG:HG2	16:2Q:91:PRO:HA	2.01	0.42
32:16:63:PRO:HG2	32:16:64:TYR:CE2	2.55	0.42
1:1A:1361:U:H2'	1:1A:1362:A:C8	2.55	0.42
1:1A:1410:A:OP2	25:1Z:3:LYS:HG3	2.20	0.42
1:1A:171:C:H2'	1:1A:172:C:C6	3.71	0.42
1:1A:172:C:H2'	1:1A:173:U:H6	1.84	0.42
1:1A:173:U:H4'	1:1A:206:A:H4'	2.02	0.42
1:1A:1910:A:O2'	1:1A:2108:G:H5'	2.20	0.42
1:1A:2214:G:H2'	1:1A:2215:G:C8	2.55	0.42
1:1A:2611:A:H2'	1:1A:2612:C:C6	2.55	0.42
1:1A:552:A:H2	1:1A:2064:C:H5'	1.84	0.42
1:1A:63:C:H2'	1:1A:64:C:C6	2.55	0.42
2:1B:66:A:H61	2:1B:108:U:H2'	1.85	0.42
1:1A:1828:U:H5''	4:1D:260:ARG:HB3	2.00	0.42
6:1F:53:THR:CG2	6:1F:55:GLY:H	2.33	0.42
9:1J:4:LYS:HA	9:1J:5:ARG:HA	1.83	0.42
11:1L:104:LYS:HG3	11:1L:117:PHE:CD1	2.54	0.42
11:1L:33:LEU:HA	11:1L:33:LEU:HD12	1.91	0.42
12:1M:105:GLU:HG2	12:1M:105:GLU:H	1.48	0.42
15:1P:36:THR:HG22	15:1P:37:THR:N	2.34	0.42
15:1P:56:LYS:NZ	15:1P:90:ARG:O	2.53	0.42
17:1R:127:ALA:C	17:1R:129:ARG:H	2.21	0.42
20:1U:51:LEU:HD23	20:1U:51:LEU:HA	1.88	0.42
30:24:13:CYS:SG	30:24:47:THR:HG21	2.60	0.42
1:2A:1010:G:N3	1:2A:1012:G:C8	7.67	0.42
1:2A:107:G:C2	1:2A:108:A:C8	3.08	0.42
1:2A:186:C:H5'	1:2A:2255:U:OP1	2.19	0.42
1:2A:2128:C:H2'	1:2A:2129:C:O4'	2.20	0.42
1:2A:2183:G:H4'	1:2A:2193:U:O2'	2.20	0.42
1:2A:2210:U:H2'	1:2A:2211:G:H8	1.83	0.42
1:2A:320:C:H2'	1:2A:321:G:O4'	2.20	0.42
1:2A:612:A:H2'	1:2A:613:C:C6	2.55	0.42
3:2C:29:VAL:HG11	3:2C:214:VAL:HG12	2.02	0.42
3:2C:223:ARG:HB2	3:2C:223:ARG:NH1	2.35	0.42
6:2F:178:PRO:HB2	6:2F:201:VAL:CG2	2.49	0.42
8:2H:2:SER:O	8:2H:3:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2P:98:LEU:HB2	15:2P:113:LEU:HD11	2.02	0.42
16:2Q:84:GLN:HA	16:2Q:111:GLU:O	2.19	0.42
16:2Q:19:LYS:HG2	16:2Q:19:LYS:H	1.59	0.42
21:2V:41:ASN:O	21:2V:45:THR:HG23	2.19	0.42
1:1A:396:G:H4'	1:1A:397:A:OP2	2.19	0.42
9:1J:53:VAL:O	9:1J:85:ASP:HA	2.20	0.42
1:2A:673:G:C4'	32:26:46:ARG:HH12	2.32	0.42
1:2A:1270:G:C2	1:2A:1271:A:C2	3.08	0.42
1:2A:1494:G:H5''	1:2A:1588:A:OP2	2.19	0.42
1:2A:1346:A:H2	1:2A:1671:G:N3	2.17	0.42
1:2A:1816:A:C4	1:2A:1959:A:C6	3.08	0.42
1:2A:1834:C:O5'	1:2A:1834:C:H6	2.03	0.42
1:2A:333:A:H1'	1:2A:334:A:H2'	2.02	0.42
4:2D:13:ARG:HA	4:2D:13:ARG:HD2	1.88	0.42
5:2E:112:GLY:O	5:2E:159:HIS:HA	2.19	0.42
1:2A:1701:A:H4'	5:2E:115:GLY:N	2.35	0.42
9:2J:105:PRO:O	9:2J:107:VAL:N	2.53	0.42
10:2K:84:LEU:H	10:2K:84:LEU:HG	1.72	0.42
1:2A:2415:C:O3'	13:2N:77:ARG:NH2	2.52	0.42
16:2Q:25:ARG:NH1	16:2Q:42:ASP:OD1	2.53	0.42
20:2U:13:SER:HA	20:2U:14:PRO:HD3	1.89	0.42
23:2X:159:PRO:HA	23:2X:160:GLY:HA2	1.60	0.42
27:11:23:LEU:HD13	27:11:50:VAL:HG11	2.02	0.42
27:11:3:ARG:HH11	27:11:60:GLU:CD	2.22	0.42
1:1A:1889:A:N6	1:1A:1904:G:O2'	2.49	0.42
1:1A:2151:U:O2'	1:1A:2152:G:H5''	2.20	0.42
1:1A:2332:G:H5''	1:1A:2333:A:OP2	2.20	0.42
1:1A:265:C:H2'	1:1A:266:C:C6	2.55	0.42
6:1F:101:LEU:HD12	6:1F:102:PRO:HD2	2.01	0.42
6:1F:106:ARG:HG2	6:1F:106:ARG:H	1.53	0.42
13:1N:38:GLN:O	13:1N:44:GLY:HA2	2.19	0.42
21:1V:61:GLY:HA3	21:1V:73:ARG:O	2.19	0.42
26:20:53:LEU:HD23	26:20:53:LEU:HA	1.81	0.42
31:25:26:GLY:O	31:25:30:VAL:HG23	2.20	0.42
1:2A:1104:G:C6	1:2A:1105:U:C4	3.07	0.42
1:2A:1526:G:C6	1:2A:1527:U:C4	3.08	0.42
1:2A:1776:G:H2'	1:2A:1777:G:H8	1.85	0.42
1:2A:2185:C:C5	1:2A:2186:G:H1'	2.55	0.42
1:2A:792:A:HO2'	1:2A:2622:U:HO2'	1.66	0.42
1:2A:396:G:OP2	63:2A:4945:HOH:O	2.21	0.42
1:2A:895:A:H3'	1:2A:896:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2C:180:PHE:HA	3:2C:181:PRO:HD2	1.72	0.42
3:2C:46:LYS:HE2	3:2C:210:ARG:CZ	2.49	0.42
13:2N:6:LEU:HA	13:2N:6:LEU:HD23	1.84	0.42
16:2Q:110:LEU:HD12	16:2Q:110:LEU:HA	1.86	0.42
20:2U:73:ALA:HB3	20:2U:106:ILE:HD12	2.02	0.42
22:2W:23:ARG:HG3	22:2W:24:VAL:N	2.35	0.42
22:2W:35:TYR:CE2	22:2W:69:ALA:HB3	2.55	0.42
23:2X:122:ARG:H	23:2X:122:ARG:HG2	1.77	0.42
1:1A:1109:C:H4'	10:1K:86:LYS:HB2	2.00	0.42
1:1A:1440:A:N3	63:1A:3989:HOH:O	2.36	0.42
5:1E:126:PRO:HB2	5:1E:131:ALA:HB2	2.02	0.42
7:1G:144:ILE:HA	7:1G:148:MET:HE1	2.02	0.42
13:1N:135:LEU:HD23	13:1N:135:LEU:HA	1.75	0.42
16:1Q:61:ASN:O	16:1Q:65:VAL:HG23	2.19	0.42
21:1V:35:THR:O	21:1V:39:ILE:HG13	2.20	0.42
1:2A:1364:G:C6	1:2A:1365:C:N4	2.87	0.42
1:2A:1364:G:H1	1:2A:1378:C:H42	1.68	0.42
1:2A:28:U:H2'	1:2A:29:G:C8	2.55	0.42
3:2C:23:ASP:HB2	3:2C:190:ARG:NH2	2.35	0.42
6:2F:9:ILE:HA	6:2F:10:PRO:HD3	1.85	0.42
7:2G:36:LYS:HD3	7:2G:95:ARG:NH2	2.34	0.42
1:2A:24:U:H5'	20:2U:78:GLU:O	2.20	0.42
1:1A:59:G:P	26:10:51:ARG:HH21	2.43	0.42
1:1A:126:C:H2'	1:1A:127:C:C6	2.54	0.42
1:1A:177:G:O6	1:1A:193:G:O2'	2.34	0.42
1:1A:2239:G:C6	1:1A:2240:C:C4	3.08	0.42
1:1A:2341:G:H2'	1:1A:2342:G:O4'	2.20	0.42
3:1C:6:ARG:O	3:1C:10:LEU:HG	2.19	0.42
5:1E:101:ARG:NH2	5:1E:171:GLU:HB2	2.35	0.42
6:1F:8:GLN:HE22	6:1F:21:ALA:HB2	1.85	0.42
8:1H:22:GLY:HA2	8:1H:37:VAL:O	2.20	0.42
8:1H:87:LEU:HD23	8:1H:87:LEU:HA	1.87	0.42
10:1K:98:ARG:HD2	10:1K:137:GLU:OE2	2.19	0.42
12:1M:116:SER:OG	12:1M:117:LEU:N	2.53	0.42
1:2A:1100:G:H5'	9:2J:33:PRO:HA	2.02	0.42
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.85	0.42
1:2A:1571:G:C6	1:2A:1572:G:C2	3.07	0.42
1:2A:2641:G:H2'	1:2A:2642:G:C8	2.54	0.42
1:2A:2645:G:H4'	5:2E:63:LEU:HD21	2.02	0.42
1:2A:554:G:C6	1:2A:2043:U:H5''	2.55	0.42
1:2A:623:C:O2'	1:2A:627:C:OP1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:732:G:N2	1:2A:834:A:H61	2.18	0.42
7:2G:45:GLU:H	7:2G:45:GLU:HG2	1.45	0.42
11:2L:12:ARG:NH1	11:2L:50:ASP:OD2	2.53	0.42
11:2L:20:GLY:HA2	11:2L:61:ARG:HD3	2.01	0.42
15:2P:36:THR:HG22	15:2P:37:THR:N	2.34	0.42
20:2U:33:ARG:NH2	20:2U:52:GLU:OE1	2.47	0.42
23:2X:125:LEU:HB3	23:2X:165:VAL:HG13	2.01	0.42
27:11:31:LEU:HD23	27:11:31:LEU:HA	1.77	0.41
1:1A:1152:G:H4'	9:1J:81:VAL:HA	2.01	0.41
1:1A:1049:C:N3	1:1A:1173:A:N6	48.41	0.41
1:1A:865:A:C4	1:1A:1233:A:C2	3.08	0.41
1:1A:1268:G:O6	19:1T:69:LYS:NZ	2.51	0.41
1:1A:1474:G:H2'	1:1A:1475:C:C6	2.55	0.41
1:1A:1528:G:C6	1:1A:1552:A:C6	3.08	0.41
1:1A:2022:A:H2'	1:1A:2023:G:C8	2.54	0.41
1:1A:2819:A:N6	1:1A:2899:G:O2'	2.39	0.41
3:1C:22:ILE:HG21	3:1C:190:ARG:HG3	2.01	0.41
6:1F:122:LYS:O	6:1F:191:ARG:HG3	2.20	0.41
7:1G:181:ARG:HG3	7:1G:182:LYS:N	2.35	0.41
23:1X:146:ILE:HA	23:1X:147:GLY:HA2	1.65	0.41
27:21:8:LEU:O	27:21:32:GLN:N	2.46	0.41
1:2A:1510:C:H2'	1:2A:1511:G:C8	2.55	0.41
1:2A:2431:C:H5'	30:24:54:ILE:HD11	2.02	0.41
1:2A:2540:G:O6	33:27:31:LYS:NZ	2.53	0.41
1:2A:2622:U:H3'	1:2A:2622:U:OP2	2.20	0.41
4:2D:102:LYS:C	4:2D:103:ARG:HG2	2.41	0.41
5:2E:97:LYS:N	5:2E:100:GLU:OE1	2.34	0.41
1:2A:2691:C:H5'	5:2E:189:PRO:HA	2.02	0.41
13:2N:46:LYS:HE3	13:2N:46:LYS:HB3	1.87	0.41
15:2P:37:THR:HA	15:2P:111:LEU:HD12	2.02	0.41
23:2X:45:ASP:OD1	23:2X:49:ARG:HD2	2.19	0.41
24:2Y:53:MET:HG3	24:2Y:59:LEU:HD23	2.01	0.41
1:1A:1040:C:O2	11:1L:3:THR:OG1	2.37	0.41
1:1A:1117:C:H42	1:1A:1137:C:N4	2.18	0.41
1:1A:1140:A:H5''	1:1A:1141:A:OP2	2.20	0.41
1:1A:2459:A:OP1	63:1A:3804:HOH:O	2.22	0.41
1:1A:342:C:H2'	1:1A:343:A:O4'	2.19	0.41
2:1B:29:A:H2'	2:1B:30:C:O4'	2.20	0.41
3:1C:3:HIS:HA	3:1C:7:TYR:HD2	1.86	0.41
4:1D:273:ARG:NH1	4:1D:273:ARG:HB3	2.34	0.41
1:2A:1510:C:H2'	1:2A:1511:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1673:G:H2'	1:2A:1674:U:C6	2.55	0.41
1:2A:1986:C:H2'	1:2A:1987:A:C8	2.55	0.41
1:2A:2813:C:H2'	1:2A:2814:C:C6	2.54	0.41
1:2A:717:C:H2'	1:2A:718:C:C6	2.55	0.41
1:2A:954:A:C6	1:2A:957:C:C2	3.08	0.41
2:2B:32:C:H42	2:2B:50:G:H1	1.68	0.41
3:2C:163:PHE:CD2	3:2C:196:LEU:HD21	2.55	0.41
3:2C:21:THR:HG22	3:2C:22:ILE:H	1.85	0.41
4:2D:4:LYS:HB3	4:2D:4:LYS:HE2	1.84	0.41
5:2E:115:GLY:O	5:2E:119:ARG:HB2	2.20	0.41
7:2G:11:TYR:HA	7:2G:15:VAL:HB	2.02	0.41
1:2A:1127:U:OP1	10:2K:125:ARG:HD2	2.20	0.41
16:2Q:68:GLN:HE21	16:2Q:68:GLN:HB3	1.71	0.41
23:2X:8:TYR:CD2	23:2X:8:TYR:N	2.87	0.41
25:2Z:64:ALA:HA	25:2Z:67:ILE:HG13	2.02	0.41
25:2Z:94:LEU:O	25:2Z:97:LEU:HB2	2.19	0.41
31:15:16:HIS:HB2	31:15:44:PRO:HG2	2.01	0.41
1:1A:1113:G:H21	1:1A:1140:A:HO2'	1.63	0.41
1:1A:1992:A:OP1	63:1A:3886:HOH:O	2.21	0.41
1:1A:2339:A:H2'	1:1A:2340:G:H8	1.82	0.41
1:1A:2744:G:H3'	1:1A:2745:A:O4'	2.21	0.41
3:1C:195:ALA:O	3:1C:196:LEU:HB3	2.19	0.41
14:1O:85:LYS:N	14:1O:85:LYS:HD2	2.35	0.41
23:1X:180:VAL:O	23:1X:183:LEU:HB2	2.20	0.41
23:1X:183:LEU:HD23	23:1X:183:LEU:HA	1.85	0.41
28:22:40:HIS:HA	28:22:41:PRO:HD2	1.73	0.41
13:2N:52:GLU:CG	32:26:57:ARG:HH22	2.32	0.41
1:2A:1756:C:H2'	1:2A:1757:C:H6	1.84	0.41
1:2A:1846:G:O6	4:2D:35:LYS:NZ	2.46	0.41
1:2A:2187:G:O6	1:2A:2189:G:N2	2.52	0.41
1:2A:275:C:H2'	1:2A:276:G:O4'	2.20	0.41
1:2A:480:C:N3	1:2A:497:A:H2'	2.35	0.41
1:2A:651:A:C6	1:2A:661:A:C8	3.09	0.41
2:2B:31:C:H4'	7:2G:29:TRP:CZ2	2.55	0.41
2:2B:66:A:H61	2:2B:108:U:H2'	1.85	0.41
7:2G:96:ARG:HB3	7:2G:97:ASP:H	1.49	0.41
10:2K:100:THR:HB	10:2K:101:TRP:H	1.63	0.41
12:2M:104:ARG:NH2	12:2M:121:VAL:O	2.54	0.41
13:2N:135:LEU:HA	13:2N:135:LEU:HD23	1.75	0.41
13:2N:62:LEU:O	32:26:13:ARG:NH1	2.53	0.41
14:2O:66:ILE:HG12	14:2O:104:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2U:73:ALA:HB3	20:2U:106:ILE:HB	2.02	0.41
1:1A:1021:C:O5'	1:1A:1021:C:H6	2.36	0.41
1:1A:1099:A:H2'	1:1A:1100:G:O4'	2.21	0.41
1:1A:1169:C:H2'	1:1A:1170:G:O4'	2.20	0.41
1:1A:1222:C:H2'	1:1A:1223:C:H6	1.85	0.41
1:1A:1302:C:H4'	6:1F:83:PHE:CD1	2.56	0.41
1:1A:1332:A:H2'	1:1A:1333:U:O4'	3.05	0.41
1:1A:1533:G:OP2	63:1A:3892:HOH:O	2.22	0.41
1:1A:2033:G:OP1	20:1U:11:ARG:NH2	2.53	0.41
1:1A:1910:A:N1	1:1A:2245:G:H1'	2.35	0.41
1:1A:353:A:H2	1:1A:1254:A:C2'	2.33	0.41
1:1A:597:A:OP2	1:1A:2076:C:N4	2.46	0.41
4:1D:68:LYS:HD3	4:1D:70:TRP:CH2	2.56	0.41
1:2A:1107:G:P	1:2A:1115:A:H4'	2.61	0.41
1:2A:1252:C:C4	1:2A:1253:G:N7	2.88	0.41
1:2A:1541:A:N3	1:2A:1623:C:O2'	2.42	0.41
1:2A:2701:C:H6	1:2A:2701:C:OP2	2.03	0.41
1:2A:399:U:H1'	1:2A:449:A:N3	2.35	0.41
1:2A:754:C:H42	1:2A:769:G:H1	1.66	0.41
1:2A:979:C:H2'	1:2A:980:C:H6	1.86	0.41
2:2B:46:A:H2'	2:2B:47:C:H6	1.83	0.41
4:2D:124:PRO:O	4:2D:126:GLN:N	2.53	0.41
4:2D:88:ARG:NH1	63:2D:405:HOH:O	2.52	0.41
16:2Q:83:LYS:O	16:2Q:84:GLN:HB2	2.21	0.41
1:1A:1153:U:H1'	1:1A:1154:C:OP1	2.20	0.41
1:1A:2161:C:H2'	1:1A:2172:G:H22	1.86	0.41
1:1A:2198:C:H5'	3:1C:44:HIS:HB2	2.03	0.41
1:1A:251:C:H2'	1:1A:252:C:O4'	2.20	0.41
1:1A:2527:G:O2'	1:1A:2528:C:H5'	2.20	0.41
1:1A:25:G:C6	1:1A:26:G:N1	2.88	0.41
1:1A:2533:U:O2'	1:1A:2658:U:OP1	2.28	0.41
1:1A:323:A:C5	1:1A:357:C:H4'	2.56	0.41
1:1A:2583:A:N7	5:1E:145:LYS:HB2	2.35	0.41
6:1F:129:PHE:HB3	6:1F:132:VAL:CG1	2.51	0.41
8:1H:154:PRO:HB3	8:1H:163:TYR:CZ	2.55	0.41
9:1J:18:GLU:O	9:1J:20:ALA:N	2.52	0.41
16:1Q:94:TYR:CZ	16:1Q:99:LYS:HG3	2.55	0.41
1:1A:69:A:N7	21:1V:31:HIS:HE1	2.19	0.41
26:20:29:LYS:HG2	26:20:57:ILE:HD13	2.03	0.41
29:23:50:GLY:HA2	29:23:58:LEU:HD23	2.02	0.41
31:25:8:ASN:HB3	31:25:11:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:865:A:C4	1:2A:1233:A:C2	3.08	0.41
1:2A:13:A:N1	1:2A:2065:C:O2'	2.46	0.41
1:2A:1466:G:C2	1:2A:1467:G:C8	3.09	0.41
1:2A:1525:G:H5''	1:2A:1606:G:H4'	2.03	0.41
1:2A:1614:G:H5'	4:2D:60:ARG:HA	2.03	0.41
1:2A:427:A:H2'	1:2A:428:A:O4'	2.22	0.41
1:2A:673:G:H4'	32:26:46:ARG:HH12	1.85	0.41
1:2A:949:C:H2'	1:2A:950:U:C6	2.55	0.41
3:2C:196:LEU:HA	3:2C:196:LEU:HD23	1.85	0.41
7:2G:111:LEU:HD23	7:2G:117:PHE:CZ	2.56	0.41
10:2K:98:ARG:C	10:2K:99:ILE:HG12	2.41	0.41
1:2A:917:U:OP1	14:2O:5:ARG:HD2	2.19	0.41
18:2S:104:GLN:CD	18:2S:104:GLN:H	2.24	0.41
23:2X:24:LEU:HA	23:2X:25:PRO:HD3	1.95	0.41
24:2Y:14:ARG:HB2	24:2Y:14:ARG:HE	1.26	0.41
1:1A:1073:A:N3	1:1A:2497:G:O2'	2.48	0.41
1:1A:966:G:H4'	1:1A:2280:A:C5	2.56	0.41
4:1D:102:LYS:C	4:1D:103:ARG:HG2	2.41	0.41
7:1G:96:ARG:O	7:1G:99:MET:HB3	2.21	0.41
10:1K:99:ILE:HG12	10:1K:103:GLN:HE21	1.84	0.41
13:1N:21:ARG:HA	13:1N:21:ARG:HD3	1.92	0.41
24:1Y:75:LEU:O	24:1Y:78:TYR:HE1	2.03	0.41
1:2A:2523:C:H2'	1:2A:2524:G:O4'	2.21	0.41
1:2A:2822:A:C6	1:2A:2823:C:C4	3.08	0.41
1:2A:641:G:C2	1:2A:642:C:C2	3.09	0.41
1:2A:821:G:H2'	1:2A:822:G:C8	6.61	0.41
21:2V:11:PRO:HB3	21:2V:92:LEU:HD21	2.03	0.41
22:2W:94:LYS:NZ	22:2W:94:LYS:HA	2.35	0.41
25:2Z:26:ARG:HB3	25:2Z:26:ARG:HE	1.67	0.41
27:11:17:LYS:HB2	27:11:17:LYS:HE3	1.95	0.41
1:1A:733:C:H1'	31:15:4:THR:HG22	2.03	0.41
1:1A:1559:U:H2'	1:1A:1560:C:H6	1.85	0.41
1:1A:1828:U:H5'	4:1D:259:THR:CG2	2.35	0.41
1:1A:2127:G:C2	1:1A:2128:C:C2	3.09	0.41
1:1A:2258:A:H2'	1:1A:2259:C:C6	2.56	0.41
1:1A:2297:A:C6	30:14:34:LEU:HD11	2.55	0.41
1:1A:2316:A:H5''	7:1G:134:GLY:HA3	2.02	0.41
1:1A:26:G:O2'	1:1A:536:G:N2	2.53	0.41
1:1A:554:G:N3	1:1A:554:G:O4'	2.54	0.41
1:1A:927:G:C2	1:1A:942:C:C2	3.09	0.41
1:1A:905:G:O2'	1:1A:961:G:O6	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:47:LEU:HD23	3:1C:47:LEU:HA	2.47	0.41
20:1U:13:SER:HA	20:1U:14:PRO:HD3	1.89	0.41
24:1Y:11:ARG:O	24:1Y:14:ARG:NH2	2.54	0.41
26:20:8:LYS:HD2	26:20:8:LYS:HA	1.82	0.41
1:2A:1144:G:C6	1:2A:1145:C:C5	3.09	0.41
1:2A:1198:C:H2'	1:2A:1199:G:C8	2.56	0.41
1:2A:2127:G:N1	1:2A:2204:C:C2	2.86	0.41
1:2A:2760:A:C6	1:2A:2761:A:C5	3.08	0.41
1:2A:2859:A:H2'	1:2A:2860:A:C8	2.55	0.41
1:2A:638:G:H5''	1:2A:639:A:OP1	2.19	0.41
3:2C:8:ARG:HB2	3:2C:8:ARG:HE	1.65	0.41
4:2D:75:ILE:HA	4:2D:76:PRO:HD3	1.78	0.41
6:2F:32:LEU:O	6:2F:36:VAL:HG23	2.20	0.41
7:2G:46:ALA:HB2	7:2G:53:LEU:HD12	2.02	0.41
11:2L:62:VAL:CG1	11:2L:66:LYS:HB2	2.51	0.41
14:2O:32:TYR:CE1	14:2O:133:ARG:HG3	2.56	0.41
15:2P:1:MET:HB2	15:2P:2:ARG:H	1.70	0.41
29:13:16:ARG:NH1	29:13:17:ASP:OD1	2.46	0.41
1:1A:1920:G:N3	1:1A:1920:G:H2'	2.36	0.41
1:1A:2239:G:C5	1:1A:2240:C:C4	3.08	0.41
1:1A:2326:G:H2'	1:1A:2327:C:C6	2.56	0.41
1:1A:553:A:H62	1:1A:2062:U:H3	1.68	0.41
3:1C:68:LEU:HB3	3:1C:69:GLY:H	1.59	0.41
4:1D:16:MET:HG3	4:1D:206:LEU:O	2.21	0.41
4:1D:275:LYS:HB3	4:1D:276:LYS:H	1.46	0.41
5:1E:101:ARG:NH1	5:1E:169:ASN:O	2.52	0.41
7:1G:53:LEU:HA	7:1G:53:LEU:HD23	1.81	0.41
13:1N:3:LEU:HD12	13:1N:3:LEU:HA	1.81	0.41
13:1N:55:ARG:HG2	13:1N:56:SER:N	2.35	0.41
14:1O:1:MET:HB2	14:1O:2:LEU:H	1.66	0.41
15:1P:22:ARG:O	15:1P:26:LYS:HG3	2.20	0.41
24:1Y:27:GLU:HG3	24:1Y:68:GLU:HA	2.03	0.41
1:2A:1132:G:C6	1:2A:1134:G:C2	3.09	0.41
1:2A:1245:C:H2'	1:2A:1246:C:C6	2.76	0.41
1:2A:1348:G:H2'	1:2A:1349:C:O4'	2.80	0.41
1:2A:165:G:H3'	1:2A:166:G:C8	2.55	0.41
1:2A:2197:A:H4'	3:2C:44:HIS:CG	2.56	0.41
1:2A:2706:C:H2'	1:2A:2707:U:H6	1.84	0.41
1:2A:323:A:H8	22:2W:84:ARG:NH1	2.17	0.41
1:2A:473:U:C4	1:2A:605:G:H1'	2.56	0.41
1:2A:483:G:O2'	31:25:39:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:548:U:H4'	1:2A:577:U:H4'	2.03	0.41
1:2A:552:A:H2	1:2A:2064:C:C5'	2.34	0.41
4:2D:249:PRO:HD2	4:2D:250:TRP:CZ3	2.56	0.41
8:2H:103:LEU:HB3	8:2H:115:VAL:HG23	2.03	0.41
12:2M:118:ALA:HA	12:2M:119:PRO:HD3	1.95	0.41
14:2O:128:LYS:H	14:2O:128:LYS:HG2	1.73	0.41
16:2Q:28:VAL:HG11	16:2Q:98:VAL:HG13	2.02	0.41
23:2X:7:ALA:HA	23:2X:39:VAL:HG12	2.03	0.41
1:1A:2325:C:H2'	1:1A:2326:G:C8	2.55	0.41
1:1A:2661:U:H2'	1:1A:2662:C:C6	2.56	0.41
1:1A:366:C:H2'	1:1A:367:G:C8	3.19	0.41
1:1A:506:G:C4	1:1A:531:A:C2	3.09	0.41
2:1B:103:G:O2'	23:1X:73:GLN:NE2	2.53	0.41
14:1O:39:PRO:HA	14:1O:97:VAL:O	2.20	0.41
1:2A:150:C:H2'	1:2A:151:G:C8	2.55	0.41
1:2A:1935:C:H2'	1:2A:1936:U:C6	2.56	0.41
1:2A:1934:A:H4'	1:2A:1935:C:O5'	2.20	0.41
1:2A:2496:G:H5''	14:2O:46:GLN:HE21	1.86	0.41
1:2A:2639:C:H1'	1:2A:2793:A:H2'	2.03	0.41
1:2A:2690:A:H4'	5:2E:165:VAL:HG11	2.03	0.41
1:2A:2845:U:H2'	1:2A:2846:G:H8	1.84	0.41
1:2A:604:G:H2'	1:2A:605:G:C8	2.56	0.41
1:2A:871:C:H2'	1:2A:872:U:O4'	2.21	0.41
5:2E:78:LEU:O	5:2E:79:ARG:HG2	2.21	0.41
8:2H:40:GLU:OE1	8:2H:61:HIS:NE2	2.53	0.41
10:2K:103:GLN:HA	10:2K:106:GLU:CD	2.42	0.41
14:2O:30:GLY:HA2	14:2O:107:ALA:HB2	2.03	0.41
16:2Q:15:ARG:C	16:2Q:19:LYS:HE2	2.41	0.41
1:1A:1354:G:P	31:15:9:ARG:HD3	2.61	0.41
1:1A:1095:A:H2'	1:1A:1096:G:C8	2.56	0.41
1:1A:1764:U:H2'	1:1A:1765:G:O4'	2.21	0.41
1:1A:1824:U:H2'	1:1A:1825:C:C6	2.55	0.41
1:1A:2258:A:H2'	1:1A:2259:C:H6	1.85	0.41
1:1A:2353:C:O2'	1:1A:2385:C:H5''	2.20	0.41
1:1A:2864:C:H2'	1:1A:2865:C:C6	2.55	0.41
1:1A:2797:C:OP1	5:1E:41:LYS:HE3	2.21	0.41
6:1F:195:ASP:HB3	6:1F:198:ALA:H	1.85	0.41
15:1P:21:TYR:OH	15:1P:43:GLU:HG2	2.21	0.41
23:1X:30:ASN:HA	23:1X:89:PHE:HE1	1.85	0.41
1:2A:1015:C:H2'	1:2A:1016:G:O4'	2.21	0.41
1:2A:1187:A:C5	1:2A:1189:G:C5	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1328:G:N2	1:2A:1330:G:H3'	2.36	0.41
1:2A:1426:G:C2	17:2R:119:LYS:HB2	91.17	0.41
1:2A:722:A:H1'	1:2A:2454:C:H1'	2.03	0.41
1:2A:2564:G:C2	1:2A:2594:G:H1'	2.56	0.41
1:2A:2848:G:H5'	15:2P:46:GLY:CA	2.47	0.41
1:2A:2849:C:O3'	15:2P:53:HIS:NE2	2.54	0.41
1:2A:2878:G:H2'	1:2A:2879:C:O4'	2.21	0.41
1:2A:299:A:O5'	1:2A:299:A:H8	2.04	0.41
1:2A:673:G:C5	1:2A:674:C:C4	3.09	0.41
1:2A:898:G:H2'	1:2A:899:G:H8	1.86	0.41
1:2A:7:A:H2'	1:2A:8:U:O4'	2.21	0.41
1:2A:924:A:OP1	1:2A:924:A:H4'	2.21	0.41
1:2A:977:A:OP1	27:21:24:LYS:NZ	2.45	0.41
3:2C:68:LEU:HB3	3:2C:69:GLY:H	1.58	0.41
7:2G:151:ALA:HB3	7:2G:153:ARG:NH1	2.36	0.41
17:2R:26:ASP:O	17:2R:49:VAL:HG12	2.21	0.41
25:2Z:75:GLU:O	25:2Z:78:LYS:HB2	2.21	0.41
1:1A:1450:U:H2'	1:1A:1451:U:H6	1.85	0.41
1:1A:1722:A:H2'	1:1A:1723:A:O4'	2.21	0.41
1:1A:1934:A:H4'	1:1A:1935:C:H5''	2.02	0.41
1:1A:2214:G:H2'	1:1A:2215:G:H8	1.86	0.41
1:1A:2242:C:OP1	25:1Z:42:GLN:HA	2.20	0.41
1:1A:2347:A:H61	24:1Y:43:THR:HG22	1.86	0.41
1:1A:2573:U:H1'	12:1M:23:ARG:HH11	1.84	0.41
1:1A:517:G:H2'	1:1A:518:G:O4'	2.20	0.41
1:1A:831:G:C6	1:1A:832:C:C4	3.09	0.41
1:1A:864:G:H4'	1:1A:884:C:O3'	2.20	0.41
14:1O:52:VAL:HA	14:1O:55:VAL:HG13	2.03	0.41
16:1Q:48:LEU:HD23	16:1Q:82:ILE:HD11	2.02	0.41
17:1R:128:GLU:HG2	17:1R:129:ARG:N	2.36	0.41
17:1R:27:THR:HB	17:1R:90:GLN:HB3	2.03	0.41
1:2A:162:C:H2'	1:2A:163:G:O4'	2.21	0.41
1:2A:2046:C:H2'	1:2A:2047:C:C6	2.56	0.41
1:2A:2121:G:C2	1:2A:2211:G:C5	3.09	0.41
1:2A:2122:G:C6	1:2A:2123:U:C2	3.09	0.41
1:2A:2200:C:H6	1:2A:2200:C:O5'	2.03	0.41
1:2A:2896:U:H2'	1:2A:2897:C:H6	1.86	0.41
3:2C:27:ARG:HG2	3:2C:182:PRO:HB3	2.03	0.41
7:2G:126:ASP:HB2	7:2G:130:ASN:O	2.21	0.41
1:2A:2314:G:O2'	7:2G:132:ASN:HB2	2.21	0.41
7:2G:9:ARG:NH1	7:2G:13:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2H:125:VAL:HG22	8:2H:131:VAL:HG22	2.03	0.41
14:2O:66:ILE:HG12	14:2O:104:PHE:HD1	1.84	0.41
26:10:32:LEU:O	26:10:36:ARG:HG3	2.21	0.40
28:12:40:HIS:HA	28:12:41:PRO:HD2	1.66	0.40
1:1A:1687:A:H2'	1:1A:1688:G:O4'	2.20	0.40
1:1A:1972:U:O2	1:1A:1974:A:H8	2.03	0.40
1:1A:280:G:H2'	1:1A:281:G:C8	3.07	0.40
1:1A:319:C:H2'	1:1A:320:C:C6	2.56	0.40
1:1A:809:G:O2'	1:1A:811:G:H5'	2.21	0.40
6:1F:24:LEU:HB3	6:1F:115:ALA:HB2	2.03	0.40
7:1G:68:PRO:HB3	7:1G:92:VAL:HB	2.03	0.40
8:1H:88:LEU:HD13	8:1H:88:LEU:HA	1.83	0.40
1:1A:1133:A:H61	10:1K:130:SER:HA	1.87	0.40
11:1L:62:VAL:HG11	11:1L:66:LYS:HB2	2.03	0.40
13:1N:88:LEU:HD11	13:1N:114:ILE:HD12	2.03	0.40
19:1T:21:ARG:HD2	19:1T:91:TYR:CE1	2.55	0.40
26:20:63:VAL:HA	26:20:66:GLU:HB3	2.02	0.40
1:2A:1098:C:C4	1:2A:1099:A:C8	3.09	0.40
1:2A:1325:G:N2	1:2A:1336:C:C2	2.89	0.40
1:2A:1934:A:H4'	1:2A:1935:C:C5'	2.52	0.40
1:2A:2155:A:H3'	1:2A:2156:A:C8	2.55	0.40
3:2C:22:ILE:HG21	3:2C:190:ARG:CG	2.51	0.40
4:2D:118:VAL:N	4:2D:129:ASN:OD1	2.45	0.40
4:2D:108:PRO:HB3	4:2D:143:HIS:HE1	1.85	0.40
4:2D:221:VAL:HG22	4:2D:226:MET:HE3	2.01	0.40
6:2F:64:ILE:HD11	6:2F:75:HIS:HB2	2.02	0.40
16:2Q:87:PHE:HZ	16:2Q:98:VAL:HG12	1.86	0.40
17:2R:6:LEU:HA	17:2R:6:LEU:HD13	1.98	0.40
21:2V:5:TYR:HD1	26:20:33:MET:SD	2.43	0.40
25:2Z:3:LYS:HB2	25:2Z:61:ARG:NH1	2.35	0.40
1:1A:1714:A:H4'	1:1A:1715:A:O5'	2.20	0.40
1:1A:2845:U:H2'	1:1A:2846:G:C8	2.56	0.40
1:1A:76:A:H2'	1:1A:77:G:C8	2.56	0.40
5:1E:4:ILE:HD12	5:1E:91:VAL:HG12	2.03	0.40
8:1H:102:ALA:HB2	8:1H:116:GLU:HG3	2.03	0.40
8:1H:56:SER:OG	8:1H:58:GLU:OE1	2.39	0.40
8:1H:94:TYR:N	8:1H:94:TYR:CD1	2.89	0.40
13:1N:71:VAL:HG22	13:1N:72:PRO:HA	2.03	0.40
20:1U:78:GLU:OE2	20:1U:99:ARG:NH1	2.54	0.40
1:2A:1050:C:H2'	1:2A:1051:C:C6	2.57	0.40
1:2A:1107:G:N2	1:2A:1122:A:H1'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1185:U:H4'	1:2A:1187:A:O4'	2.21	0.40
1:2A:1196:G:H4'	18:2S:81:HIS:CG	2.57	0.40
1:2A:174:G:H2'	1:2A:175:G:C8	2.56	0.40
1:2A:299:A:H5''	1:2A:300:C:H5'	2.03	0.40
1:2A:501:G:N1	1:2A:504:A:OP2	2.49	0.40
1:2A:545:G:H2'	1:2A:546:G:C8	2.56	0.40
1:2A:765:C:H2'	1:2A:766:C:H6	1.86	0.40
2:2B:33:G:C2	2:2B:50:G:C2	3.09	0.40
2:2B:75:G:N1	2:2B:103:G:N2	2.69	0.40
1:2A:2769:A:N1	8:2H:67:LEU:HD22	2.36	0.40
22:2W:14:LEU:HB2	22:2W:75:ILE:HD11	2.02	0.40
23:2X:72:ARG:HD3	23:2X:72:ARG:HA	1.63	0.40
25:2Z:52:ARG:NH2	25:2Z:57:GLU:HB2	2.36	0.40
1:1A:2297:A:H4'	1:1A:2298:A:O4'	2.22	0.40
1:1A:2454:C:H2'	1:1A:2455:G:H8	1.86	0.40
1:1A:2572:A:H2'	1:1A:2573:U:O4'	2.21	0.40
3:1C:161:ILE:HD12	3:1C:174:PRO:O	2.21	0.40
6:1F:32:LEU:HD22	6:1F:112:MET:HE2	2.04	0.40
1:1A:2873:G:OP1	17:1R:119:LYS:HD2	2.21	0.40
21:2V:9:LEU:HA	26:20:36:ARG:HH21	1.87	0.40
29:23:16:ARG:NH1	29:23:17:ASP:OD1	2.51	0.40
1:2A:1109:C:H5'	10:2K:89:HIS:CD2	2.47	0.40
1:2A:1169:C:H2'	1:2A:1170:G:O4'	2.21	0.40
1:2A:1222:C:H2'	1:2A:1223:C:C6	2.57	0.40
1:2A:1784:C:H2'	1:2A:1785:A:O4'	2.21	0.40
1:2A:2568:G:H2'	1:2A:2569:C:C6	2.56	0.40
1:2A:1813:A:H5''	1:2A:2619:G:H4'	2.02	0.40
1:2A:384:G:O2'	1:2A:385:U:H5'	2.20	0.40
1:2A:894:G:C4	1:2A:977:A:C8	3.07	0.40
4:2D:96:HIS:HD2	4:2D:102:LYS:HG2	1.85	0.40
6:2F:13:SER:OG	6:2F:18:ARG:HG3	2.21	0.40
7:2G:20:ILE:O	7:2G:24:GLY:N	2.51	0.40
8:2H:126:PRO:HB2	8:2H:127:GLU:OE2	2.21	0.40
10:2K:105:LEU:O	10:2K:108:ALA:HB3	2.21	0.40
10:2K:117:THR:HB	10:2K:126:MET:SD	2.61	0.40
11:2L:43:THR:HA	11:2L:44:PRO:HD3	1.93	0.40
11:2L:86:PRO:HG2	11:2L:89:LYS:HB2	2.03	0.40
12:2M:2:ILE:HG13	12:2M:8:LEU:HD11	2.03	0.40
14:2O:39:PRO:HA	14:2O:97:VAL:O	2.21	0.40
14:2O:108:GLY:HA3	23:2X:116:VAL:HG13	2.03	0.40
1:1A:1603:C:H5''	1:1A:1604:A:OP2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2117:U:H2'	1:1A:2118:C:C6	2.56	0.40
1:1A:2139:U:H4'	1:1A:2140:A:OP1	2.21	0.40
1:1A:568:G:H8	1:1A:568:G:O5'	2.05	0.40
1:1A:622:G:H2'	1:1A:623:C:O4'	2.22	0.40
1:1A:800:C:H2'	1:1A:801:C:C6	2.57	0.40
1:1A:841:C:H2'	1:1A:842:C:C6	2.57	0.40
1:1A:988:G:H5''	1:1A:989:A:O5'	2.21	0.40
2:1B:88:C:H2'	2:1B:89:G:O4'	2.20	0.40
2:1B:94:C:H2'	2:1B:95:C:H6	1.86	0.40
4:1D:111:LEU:HA	4:1D:111:LEU:HD23	1.85	0.40
6:1F:32:LEU:O	6:1F:36:VAL:HG23	2.22	0.40
23:1X:180:VAL:HG13	23:1X:183:LEU:HD12	2.03	0.40
23:1X:16:SER:O	23:1X:20:ARG:HG3	2.22	0.40
23:1X:30:ASN:HD22	23:1X:90:VAL:HB	1.86	0.40
25:1Z:35:THR:OG1	25:1Z:35:THR:O	2.40	0.40
25:1Z:3:LYS:O	25:1Z:12:PRO:HD3	2.22	0.40
28:22:58:ARG:C	28:22:60:GLN:HB2	2.42	0.40
1:2A:1252:C:H2'	1:2A:1253:G:C8	3.51	0.40
1:2A:1703:C:H2'	1:2A:1704:C:C6	2.56	0.40
1:2A:2044:G:H4'	1:2A:2628:C:O3'	2.21	0.40
1:2A:508:A:H3'	1:2A:509:C:C6	2.57	0.40
4:2D:75:ILE:HG21	4:2D:99:ASP:HB3	2.04	0.40
6:2F:196:LEU:HD23	6:2F:196:LEU:HA	1.78	0.40
7:2G:148:MET:HG3	7:2G:148:MET:H	1.40	0.40
17:2R:120:ARG:HA	17:2R:123:GLN:HG3	2.04	0.40
14:2O:59:ARG:HA	23:2X:180:VAL:HG23	2.03	0.40
1:1A:672:G:O2'	1:1A:2362:G:OP1	2.37	0.40
1:1A:591:U:C4	1:1A:592:G:C6	3.10	0.40
1:1A:636:U:H4'	1:1A:639:A:C6	2.56	0.40
4:1D:89:SER:HB2	4:1D:201:HIS:CD2	2.57	0.40
7:1G:38:VAL:HG22	7:1G:93:THR:HG23	2.03	0.40
7:1G:39:ILE:HB	7:1G:92:VAL:HG12	2.02	0.40
20:1U:24:ILE:HA	20:1U:27:LYS:HG3	2.03	0.40
1:2A:1069:G:C6	1:2A:1070:G:C6	3.10	0.40
1:2A:1104:G:H2'	10:2K:130:SER:HB2	2.04	0.40
1:2A:184:A:N3	1:2A:184:A:H2'	2.36	0.40
1:2A:2103:A:H3'	1:2A:2104:G:H8	1.85	0.40
1:2A:2297:A:H4'	1:2A:2298:A:O4'	2.21	0.40
1:2A:377:G:H2'	1:2A:378:G:O4'	2.21	0.40
1:2A:629:U:OP1	6:2F:103:LYS:HG3	2.21	0.40
1:2A:6:G:H2'	1:2A:7:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:814:G:C6	1:2A:815:G:C5	3.10	0.40
3:2C:174:PRO:HA	3:2C:175:VAL:HA	1.95	0.40
5:2E:14:ILE:HG13	5:2E:21:VAL:HG13	2.03	0.40
8:2H:11:VAL:HG21	8:2H:50:VAL:HG23	2.04	0.40
14:2O:54:MET:HG3	14:2O:121:ALA:HB2	2.04	0.40
15:2P:51:LEU:HD22	15:2P:66:VAL:HG13	2.03	0.40
21:2V:31:HIS:CD2	21:2V:33:LYS:HB2	2.56	0.40
24:2Y:18:ALA:HB3	24:2Y:20:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1C	129/229 (56%)	96 (74%)	25 (19%)	8 (6%)	2	10
3	2C	129/229 (56%)	96 (74%)	26 (20%)	7 (5%)	2	13
4	1D	273/276 (99%)	258 (94%)	12 (4%)	3 (1%)	17	56
4	2D	273/276 (99%)	253 (93%)	16 (6%)	4 (2%)	12	48
5	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	32	74
5	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	32	74
6	1F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	32	74
6	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	32	74
7	1G	179/182 (98%)	162 (90%)	16 (9%)	1 (1%)	28	70
7	2G	179/182 (98%)	160 (89%)	16 (9%)	3 (2%)	11	44
8	1H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	28	70
8	2H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	28	70
9	1J	128/173 (74%)	71 (56%)	37 (29%)	20 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	2J	128/173 (74%)	81 (63%)	26 (20%)	21 (16%)	0	1
10	1K	65/147 (44%)	52 (80%)	11 (17%)	2 (3%)	5	26
10	2K	64/147 (44%)	45 (70%)	17 (27%)	2 (3%)	5	26
11	1L	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
11	2L	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	25	67
12	1M	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
12	2M	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
13	1N	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	13	49
13	2N	147/150 (98%)	139 (95%)	5 (3%)	3 (2%)	9	39
14	1O	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	25	67
14	2O	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	13	49
15	1P	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
15	2P	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
16	1Q	108/112 (96%)	97 (90%)	9 (8%)	2 (2%)	9	41
16	2Q	108/112 (96%)	98 (91%)	8 (7%)	2 (2%)	9	41
17	1R	129/146 (88%)	118 (92%)	9 (7%)	2 (2%)	11	46
17	2R	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
18	1S	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
18	2S	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
19	1T	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	18	59
19	2T	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	9	39
20	1U	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
20	2U	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
21	1V	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	17	56
21	2V	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	17	56
22	1W	105/110 (96%)	92 (88%)	12 (11%)	1 (1%)	18	59
22	2W	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
23	1X	184/206 (89%)	164 (89%)	17 (9%)	3 (2%)	11	46
23	2X	184/206 (89%)	161 (88%)	20 (11%)	3 (2%)	11	46
24	1Y	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
24	2Y	73/85 (86%)	70 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	1Z	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	17	56
25	2Z	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	17	56
26	10	68/72 (94%)	64 (94%)	3 (4%)	1 (2%)	12	48
26	20	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
27	11	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	21	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	12	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	3	17
28	22	67/71 (94%)	49 (73%)	12 (18%)	6 (9%)	1	4
29	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
29	23	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
30	14	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
30	24	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
31	15	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
31	25	46/49 (94%)	44 (96%)	0	2 (4%)	3	18
32	16	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
32	26	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
33	17	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	27	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
35	1b	229/256 (90%)	193 (84%)	27 (12%)	9 (4%)	3	20
35	2b	229/256 (90%)	193 (84%)	28 (12%)	8 (4%)	4	23
36	1c	204/239 (85%)	181 (89%)	20 (10%)	3 (2%)	12	48
36	2c	204/239 (85%)	185 (91%)	14 (7%)	5 (2%)	6	32
37	1d	206/209 (99%)	184 (89%)	22 (11%)	0	100	100
37	2d	206/209 (99%)	182 (88%)	24 (12%)	0	100	100
38	1e	146/162 (90%)	133 (91%)	13 (9%)	0	100	100
38	2e	146/162 (90%)	134 (92%)	11 (8%)	1 (1%)	25	67
39	1f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	18	59
39	2f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	18	59
40	1g	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	25	67
40	2g	153/156 (98%)	140 (92%)	9 (6%)	4 (3%)	6	31
41	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	2h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	25	67
42	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	22	64
42	2i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	22	64
43	1j	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	2	13
43	2j	94/105 (90%)	83 (88%)	8 (8%)	3 (3%)	5	26
44	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	20	62
44	2k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	20	62
45	1l	120/132 (91%)	114 (95%)	6 (5%)	0	100	100
45	2l	120/132 (91%)	112 (93%)	7 (6%)	1 (1%)	22	64
46	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	11	44
46	2m	120/126 (95%)	106 (88%)	13 (11%)	1 (1%)	22	64
47	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
47	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
48	1o	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	7	35
48	2o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	7	35
49	1p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
49	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
50	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
50	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
51	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
51	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
52	1s	82/93 (88%)	70 (85%)	12 (15%)	0	100	100
52	2s	81/93 (87%)	70 (86%)	8 (10%)	3 (4%)	4	22
53	1t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	3	18
53	2t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	8	38
54	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
54	2u	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	1	3
55	1z	726/758 (96%)	610 (84%)	92 (13%)	24 (3%)	4	25
55	2z	726/758 (96%)	609 (84%)	95 (13%)	22 (3%)	5	27
58	1x	17/35 (49%)	16 (94%)	0	1 (6%)	2	11
58	2x	17/35 (49%)	13 (76%)	1 (6%)	3 (18%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	13263/14516 (91%)	11963 (90%)	1067 (8%)	233 (2%)	10	43

All (233) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1C	175	VAL
3	1C	224	ILE
6	1F	130	ALA
7	1G	51	ARG
8	1H	126	PRO
9	1J	29	TYR
9	1J	74	LEU
9	1J	77	PRO
9	1J	80	VAL
9	1J	104	ILE
9	1J	105	PRO
9	1J	125	LEU
10	1K	87	GLY
10	1K	89	HIS
16	1Q	59	LYS
28	12	49	PHE
28	12	53	GLU
35	1b	9	GLU
35	1b	16	HIS
35	1b	17	PHE
35	1b	125	PRO
35	1b	231	GLU
35	1b	232	PRO
42	1i	54	ASP
43	1j	55	LYS
43	1j	56	HIS
46	1m	3	ARG
55	1z	-25	SER
55	1z	172	ASP
55	1z	400	GLU
55	1z	402	ILE
55	1z	404	VAL
55	1z	472	VAL
55	1z	473	ASP
55	1z	617	MET
3	2C	51	PRO
3	2C	52	ARG

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Mol	Chain	Res	Type
3	2C	224	ILE
4	2D	275	LYS
6	2F	21	ALA
7	2G	51	ARG
7	2G	81	LYS
7	2G	181	ARG
8	2H	126	PRO
9	2J	33	PRO
9	2J	39	ALA
9	2J	53	VAL
9	2J	71	LEU
9	2J	74	LEU
9	2J	77	PRO
9	2J	106	GLN
10	2K	89	HIS
28	22	46	GLN
28	22	62	ARG
31	25	46	VAL
35	2b	121	LEU
35	2b	125	PRO
36	2c	101	LEU
40	2g	4	ARG
40	2g	33	ASP
40	2g	79	ARG
42	2i	54	ASP
44	2k	106	LYS
46	2m	107	ALA
52	2s	30	LEU
54	2u	3	LYS
55	2z	92	ILE
55	2z	153	MET
55	2z	402	ILE
55	2z	472	VAL
55	2z	617	MET
3	1C	196	LEU
9	1J	20	ALA
9	1J	31	GLY
9	1J	33	PRO
9	1J	66	LEU
9	1J	78	SER
9	1J	91	LYS
9	1J	93	LEU

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Mol	Chain	Res	Type
9	1J	101	PRO
9	1J	107	VAL
9	1J	132	ASP
14	1O	59	ARG
21	1V	94	GLY
23	1X	152	ALA
23	1X	172	ALA
35	1b	37	ASN
39	1f	40	VAL
40	1g	79	ARG
43	1j	31	GLY
43	1j	75	ILE
43	1j	80	LYS
46	1m	118	ALA
53	1t	47	GLY
53	1t	96	GLY
53	1t	100	ILE
55	1z	88	VAL
55	1z	269	VAL
55	1z	446	THR
55	1z	447	GLY
55	1z	555	LEU
3	2C	68	LEU
4	2D	3	VAL
4	2D	239	ARG
9	2J	69	PRO
9	2J	80	VAL
9	2J	84	GLU
9	2J	93	LEU
9	2J	94	VAL
9	2J	107	VAL
9	2J	113	GLN
19	2T	79	VAL
21	2V	94	GLY
23	2X	175	VAL
28	22	45	GLY
35	2b	9	GLU
35	2b	10	LEU
36	2c	107	GLN
36	2c	181	ASN
43	2j	78	ASN
45	2l	28	LYS

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Mol	Chain	Res	Type
48	2o	19	PRO
53	2t	47	GLY
55	2z	-25	SER
55	2z	88	VAL
55	2z	93	GLU
55	2z	380	LEU
55	2z	671	MET
58	2x	14	ARG
3	1C	68	LEU
3	1C	172	HIS
3	1C	183	GLU
9	1J	56	ASN
13	1N	122	PRO
36	1c	65	ALA
48	1o	19	PRO
55	1z	-4	ALA
55	1z	39	ILE
55	1z	85	PRO
55	1z	171	GLU
55	1z	554	PRO
55	1z	671	MET
9	2J	91	LYS
9	2J	126	ALA
10	2K	113	PRO
13	2N	29	LYS
16	2Q	84	GLN
19	2T	53	GLU
23	2X	114	GLY
25	2Z	3	LYS
28	22	60	GLN
31	25	45	ALA
38	2e	37	ARG
43	2j	75	ILE
48	2o	23	GLY
54	2u	4	GLY
55	2z	-1	GLU
55	2z	85	PRO
55	2z	170	ARG
55	2z	404	VAL
4	1D	275	LYS
5	1E	52	LEU
9	1J	124	ALA

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Mol	Chain	Res	Type
13	1N	29	LYS
17	1R	128	GLU
19	1T	79	VAL
23	1X	157	LEU
48	1o	23	GLY
53	1t	102	GLY
55	1z	521	SER
58	1x	18	LEU
3	2C	172	HIS
5	2E	52	LEU
9	2J	30	GLN
13	2N	122	PRO
14	2O	27	VAL
14	2O	59	ARG
35	2b	20	GLU
36	2c	70	VAL
36	2c	108	ASN
52	2s	25	LYS
55	2z	-65	LYS
55	2z	460	GLU
58	2x	4	ARG
3	1C	178	ALA
9	1J	114	GLY
16	1Q	60	GLY
22	1W	54	LYS
26	10	69	ARG
35	1b	121	LEU
36	1c	66	VAL
55	1z	403	GLU
55	1z	471	LYS
9	2J	54	ALA
9	2J	68	LEU
11	2L	2	LYS
13	2N	45	LEU
23	2X	157	LEU
28	22	44	THR
28	22	68	ARG
35	2b	120	ALA
39	2f	40	VAL
41	2h	73	ASP
52	2s	13	ASP
55	2z	-4	ALA

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Mol	Chain	Res	Type
3	1C	62	VAL
4	1D	125	ILE
4	1D	156	ALA
17	1R	129	ARG
25	1Z	81	LYS
35	1b	20	GLU
55	1z	520	GLY
55	1z	598	ASP
35	2b	232	PRO
53	2t	100	ILE
55	2z	506	GLN
55	2z	531	GLY
44	1k	105	VAL
3	2C	171	ILE
4	2D	125	ILE
9	2J	59	ILE
35	2b	227	GLY
55	2z	533	VAL
16	2Q	85	VAL
9	2J	73	GLY
55	2z	444	PRO
55	2z	598	ASP
58	2x	10	LEU
28	12	54	GLY
36	1c	70	VAL
40	2g	55	GLY
43	2j	77	PRO
3	2C	65	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1C	103/181 (57%)	89 (86%)	14 (14%)	4 19
3	2C	103/181 (57%)	88 (85%)	15 (15%)	3 17
4	1D	215/218 (99%)	195 (91%)	20 (9%)	10 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2D	216/218 (99%)	200 (93%)	16 (7%)	16	49
5	1E	164/166 (99%)	151 (92%)	13 (8%)	14	46
5	2E	164/166 (99%)	147 (90%)	17 (10%)	8	31
6	1F	160/166 (96%)	141 (88%)	19 (12%)	6	25
6	2F	159/166 (96%)	143 (90%)	16 (10%)	9	33
7	1G	143/156 (92%)	123 (86%)	20 (14%)	4	18
7	2G	142/156 (91%)	119 (84%)	23 (16%)	3	14
8	1H	144/148 (97%)	136 (94%)	8 (6%)	25	62
8	2H	144/148 (97%)	127 (88%)	17 (12%)	6	25
10	1K	50/111 (45%)	40 (80%)	10 (20%)	1	8
10	2K	50/111 (45%)	38 (76%)	12 (24%)	1	4
11	1L	118/119 (99%)	108 (92%)	10 (8%)	12	43
11	2L	118/119 (99%)	107 (91%)	11 (9%)	10	38
12	1M	100/100 (100%)	94 (94%)	6 (6%)	22	60
12	2M	100/100 (100%)	89 (89%)	11 (11%)	7	28
13	1N	116/116 (100%)	104 (90%)	12 (10%)	8	31
13	2N	115/116 (99%)	106 (92%)	9 (8%)	15	47
14	1O	111/111 (100%)	102 (92%)	9 (8%)	14	45
14	2O	111/111 (100%)	101 (91%)	10 (9%)	11	40
15	1P	101/101 (100%)	83 (82%)	18 (18%)	2	11
15	2P	101/101 (100%)	85 (84%)	16 (16%)	3	14
16	1Q	87/88 (99%)	80 (92%)	7 (8%)	14	45
16	2Q	85/88 (97%)	75 (88%)	10 (12%)	6	25
17	1R	115/127 (91%)	103 (90%)	12 (10%)	8	31
17	2R	113/127 (89%)	102 (90%)	11 (10%)	9	35
18	1S	93/94 (99%)	83 (89%)	10 (11%)	7	29
18	2S	93/94 (99%)	87 (94%)	6 (6%)	20	56
19	1T	80/82 (98%)	70 (88%)	10 (12%)	5	23
19	2T	80/82 (98%)	73 (91%)	7 (9%)	12	41
20	1U	90/92 (98%)	83 (92%)	7 (8%)	15	47
20	2U	90/92 (98%)	83 (92%)	7 (8%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1V	77/78 (99%)	71 (92%)	6 (8%)	15	47
21	2V	77/78 (99%)	75 (97%)	2 (3%)	51	83
22	1W	85/91 (93%)	80 (94%)	5 (6%)	23	60
22	2W	85/91 (93%)	76 (89%)	9 (11%)	8	30
23	1X	157/179 (88%)	140 (89%)	17 (11%)	7	29
23	2X	156/179 (87%)	139 (89%)	17 (11%)	7	29
24	1Y	61/67 (91%)	55 (90%)	6 (10%)	9	34
24	2Y	60/67 (90%)	56 (93%)	4 (7%)	19	54
25	1Z	80/83 (96%)	73 (91%)	7 (9%)	12	41
25	2Z	80/83 (96%)	72 (90%)	8 (10%)	9	33
26	10	65/67 (97%)	60 (92%)	5 (8%)	15	48
26	20	65/67 (97%)	56 (86%)	9 (14%)	4	19
27	11	51/52 (98%)	46 (90%)	5 (10%)	9	34
27	21	50/52 (96%)	45 (90%)	5 (10%)	9	33
28	12	60/63 (95%)	48 (80%)	12 (20%)	1	8
28	22	53/63 (84%)	42 (79%)	11 (21%)	1	6
29	13	50/52 (96%)	45 (90%)	5 (10%)	9	33
29	23	50/52 (96%)	44 (88%)	6 (12%)	6	25
30	14	51/52 (98%)	46 (90%)	5 (10%)	9	34
30	24	50/52 (96%)	45 (90%)	5 (10%)	9	33
31	15	41/42 (98%)	39 (95%)	2 (5%)	29	68
31	25	41/42 (98%)	39 (95%)	2 (5%)	29	68
32	16	54/55 (98%)	49 (91%)	5 (9%)	10	38
32	26	54/55 (98%)	49 (91%)	5 (9%)	10	38
33	17	34/34 (100%)	34 (100%)	0	100	100
33	27	34/34 (100%)	33 (97%)	1 (3%)	48	82
35	1b	192/220 (87%)	170 (88%)	22 (12%)	6	27
35	2b	187/220 (85%)	171 (91%)	16 (9%)	12	42
36	1c	143/188 (76%)	135 (94%)	8 (6%)	25	62
36	2c	141/188 (75%)	128 (91%)	13 (9%)	11	38
37	1d	170/181 (94%)	153 (90%)	17 (10%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2d	174/181 (96%)	158 (91%)	16 (9%)	11	38
38	1e	113/123 (92%)	101 (89%)	12 (11%)	8	30
38	2e	114/123 (93%)	106 (93%)	8 (7%)	18	53
39	1f	84/90 (93%)	76 (90%)	8 (10%)	10	36
39	2f	86/90 (96%)	80 (93%)	6 (7%)	18	53
40	1g	119/127 (94%)	110 (92%)	9 (8%)	15	48
40	2g	120/127 (94%)	110 (92%)	10 (8%)	13	44
41	1h	114/119 (96%)	99 (87%)	15 (13%)	5	20
41	2h	114/119 (96%)	96 (84%)	18 (16%)	3	14
42	1i	91/99 (92%)	79 (87%)	12 (13%)	5	20
42	2i	89/99 (90%)	74 (83%)	15 (17%)	2	12
43	1j	66/92 (72%)	61 (92%)	5 (8%)	15	48
43	2j	69/92 (75%)	67 (97%)	2 (3%)	48	82
44	1k	83/99 (84%)	77 (93%)	6 (7%)	17	51
44	2k	83/99 (84%)	80 (96%)	3 (4%)	40	77
45	1l	97/109 (89%)	90 (93%)	7 (7%)	17	51
45	2l	97/109 (89%)	89 (92%)	8 (8%)	13	44
46	1m	95/101 (94%)	84 (88%)	11 (12%)	6	26
46	2m	92/101 (91%)	82 (89%)	10 (11%)	7	29
47	1n	49/50 (98%)	42 (86%)	7 (14%)	4	18
47	2n	49/50 (98%)	42 (86%)	7 (14%)	4	18
48	1o	78/80 (98%)	73 (94%)	5 (6%)	20	57
48	2o	78/80 (98%)	70 (90%)	8 (10%)	8	31
49	1p	69/74 (93%)	62 (90%)	7 (10%)	9	33
49	2p	68/74 (92%)	59 (87%)	9 (13%)	5	20
50	1q	94/97 (97%)	89 (95%)	5 (5%)	26	65
50	2q	94/97 (97%)	87 (93%)	7 (7%)	16	49
51	1r	59/77 (77%)	55 (93%)	4 (7%)	18	54
51	2r	59/77 (77%)	55 (93%)	4 (7%)	18	54
52	1s	70/80 (88%)	61 (87%)	9 (13%)	5	22
52	2s	67/80 (84%)	62 (92%)	5 (8%)	16	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	1t	70/82 (85%)	62 (89%)	8 (11%)	7	27
53	2t	71/82 (87%)	65 (92%)	6 (8%)	12	43
54	1u	18/22 (82%)	17 (94%)	1 (6%)	25	62
54	2u	18/22 (82%)	18 (100%)	0	100	100
55	1z	609/636 (96%)	538 (88%)	71 (12%)	6	25
55	2z	609/636 (96%)	534 (88%)	75 (12%)	5	24
58	1x	19/34 (56%)	17 (90%)	2 (10%)	8	30
58	2x	19/34 (56%)	18 (95%)	1 (5%)	26	65
All	All	10695/11742 (91%)	9614 (90%)	1081 (10%)	9	33

All (1081) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1C	6	ARG
3	1C	37	PHE
3	1C	46	LYS
3	1C	49	ILE
3	1C	55	ASP
3	1C	59	ARG
3	1C	68	LEU
3	1C	164	ARG
3	1C	183	GLU
3	1C	196	LEU
3	1C	209	LEU
3	1C	210	ARG
3	1C	211	SER
3	1C	215	THR
4	1D	27	THR
4	1D	61	LEU
4	1D	94	LEU
4	1D	103	ARG
4	1D	111	LEU
4	1D	113	VAL
4	1D	122	ASP
4	1D	126	GLN
4	1D	134	ARG
4	1D	142	VAL
4	1D	157	ARG
4	1D	200	ASP

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Mol	Chain	Res	Type
4	1D	211	ARG
4	1D	221	VAL
4	1D	229	VAL
4	1D	242	ARG
4	1D	257	LEU
4	1D	259	THR
4	1D	260	ARG
4	1D	273	ARG
5	1E	21	VAL
5	1E	34	VAL
5	1E	64	LYS
5	1E	75	VAL
5	1E	82	ARG
5	1E	116	VAL
5	1E	119	ARG
5	1E	144	ARG
5	1E	154	LYS
5	1E	163	GLU
5	1E	170	LEU
5	1E	175	VAL
5	1E	181	LEU
6	1F	20	LEU
6	1F	23	ASP
6	1F	24	LEU
6	1F	33	LEU
6	1F	53	THR
6	1F	57	VAL
6	1F	74	ARG
6	1F	106	ARG
6	1F	125	LEU
6	1F	132	VAL
6	1F	140	LEU
6	1F	170	LEU
6	1F	175	THR
6	1F	176	LEU
6	1F	191	ARG
6	1F	192	LEU
6	1F	197	ASP
6	1F	200	GLU
6	1F	201	VAL
7	1G	3	LEU
7	1G	4	ASP

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Mol	Chain	Res	Type
7	1G	7	LEU
7	1G	28	VAL
7	1G	31	VAL
7	1G	45	GLU
7	1G	49	ASP
7	1G	60	LEU
7	1G	79	ASN
7	1G	81	LYS
7	1G	82	LEU
7	1G	91	ARG
7	1G	139	LEU
7	1G	140	ILE
7	1G	143	GLU
7	1G	159	VAL
7	1G	161	THR
7	1G	162	THR
7	1G	170	ARG
7	1G	175	LEU
8	1H	3	ARG
8	1H	15	VAL
8	1H	69	ARG
8	1H	71	LEU
8	1H	98	LEU
8	1H	105	LEU
8	1H	107	VAL
8	1H	124	GLU
10	1K	79	ARG
10	1K	84	LEU
10	1K	95	LYS
10	1K	99	ILE
10	1K	106	GLU
10	1K	115	LEU
10	1K	121	GLU
10	1K	133	SER
10	1K	134	MET
10	1K	137	GLU
11	1L	28	THR
11	1L	33	LEU
11	1L	34	LEU
11	1L	48	MET
11	1L	61	ARG
11	1L	73	THR

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Mol	Chain	Res	Type
11	1L	84	LYS
11	1L	87	LEU
11	1L	120	LEU
11	1L	133	GLN
12	1M	23	ARG
12	1M	24	VAL
12	1M	94	ARG
12	1M	98	VAL
12	1M	105	GLU
12	1M	113	LYS
13	1N	42	SER
13	1N	55	ARG
13	1N	59	LEU
13	1N	65	ARG
13	1N	70	GLN
13	1N	95	VAL
13	1N	98	GLU
13	1N	99	LEU
13	1N	106	LEU
13	1N	112	LEU
13	1N	137	LYS
13	1N	149	GLU
14	1O	1	MET
14	1O	21	THR
14	1O	35	VAL
14	1O	45	GLN
14	1O	55	VAL
14	1O	56	ARG
14	1O	59	ARG
14	1O	75	THR
14	1O	98	LYS
15	1P	1	MET
15	1P	18	LEU
15	1P	24	GLN
15	1P	28	LEU
15	1P	29	LEU
15	1P	33	ARG
15	1P	44	LEU
15	1P	54	LEU
15	1P	60	LEU
15	1P	65	LEU
15	1P	67	LEU

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Mol	Chain	Res	Type
15	1P	75	LEU
15	1P	79	LEU
15	1P	91	GLN
15	1P	100	LEU
15	1P	111	LEU
15	1P	114	VAL
15	1P	117	VAL
16	1Q	3	ARG
16	1Q	19	LYS
16	1Q	20	ARG
16	1Q	48	LEU
16	1Q	50	SER
16	1Q	78	LEU
16	1Q	103	GLU
17	1R	16	ARG
17	1R	28	VAL
17	1R	42	ILE
17	1R	49	VAL
17	1R	65	LYS
17	1R	74	ARG
17	1R	78	LEU
17	1R	89	VAL
17	1R	96	ARG
17	1R	109	GLU
17	1R	118	ARG
17	1R	128	GLU
18	1S	8	VAL
18	1S	36	ARG
18	1S	60	LEU
18	1S	74	LEU
18	1S	84	LYS
18	1S	92	ARG
18	1S	95	LEU
18	1S	104	GLN
18	1S	108	GLU
18	1S	111	GLU
19	1T	1	MET
19	1T	18	LEU
19	1T	21	ARG
19	1T	43	GLU
19	1T	46	VAL
19	1T	52	VAL

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Mol	Chain	Res	Type
19	1T	61	VAL
19	1T	62	LEU
19	1T	79	VAL
19	1T	95	LEU
20	1U	11	ARG
20	1U	17	VAL
20	1U	23	LEU
20	1U	51	LEU
20	1U	60	ASN
20	1U	100	THR
20	1U	107	LEU
21	1V	33	LYS
21	1V	35	THR
21	1V	52	VAL
21	1V	57	LEU
21	1V	66	LEU
21	1V	88	LYS
22	1W	7	VAL
22	1W	23	ARG
22	1W	43	ASN
22	1W	90	LEU
22	1W	91	GLU
23	1X	5	LEU
23	1X	11	GLU
23	1X	18	LEU
23	1X	19	ARG
23	1X	31	ARG
23	1X	33	LEU
23	1X	58	VAL
23	1X	72	ARG
23	1X	73	GLN
23	1X	76	LEU
23	1X	86	VAL
23	1X	87	ASP
23	1X	91	LEU
23	1X	107	THR
23	1X	126	VAL
23	1X	136	PHE
23	1X	150	LEU
24	1Y	10	THR
24	1Y	11	ARG
24	1Y	19	LYS

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Mol	Chain	Res	Type
24	1Y	20	ARG
24	1Y	55	ARG
24	1Y	74	ARG
25	1Z	11	ARG
25	1Z	35	THR
25	1Z	40	ARG
25	1Z	59	THR
25	1Z	65	SER
25	1Z	75	GLU
25	1Z	95	LEU
26	10	30	ARG
26	10	32	LEU
26	10	53	LEU
26	10	64	LEU
26	10	70	GLN
27	11	8	LEU
27	11	23	LEU
27	11	29	ARG
27	11	48	GLU
27	11	55	ARG
28	12	1	MET
28	12	34	GLU
28	12	46	GLN
28	12	47	GLN
28	12	49	PHE
28	12	50	VAL
28	12	55	ARG
28	12	58	ARG
28	12	63	TYR
28	12	66	SER
28	12	67	TYR
28	12	69	LYS
29	13	6	VAL
29	13	16	ARG
29	13	26	THR
29	13	40	LYS
29	13	58	LEU
30	14	4	GLU
30	14	6	ARG
30	14	34	LEU
30	14	35	GLU
30	14	48	VAL

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Mol	Chain	Res	Type
31	15	1	MET
31	15	24	THR
32	16	14	VAL
32	16	31	HIS
32	16	32	LEU
32	16	37	SER
32	16	46	ARG
35	1b	8	LYS
35	1b	11	LEU
35	1b	15	VAL
35	1b	17	PHE
35	1b	20	GLU
35	1b	21	ARG
35	1b	76	GLN
35	1b	80	ILE
35	1b	94	ASN
35	1b	121	LEU
35	1b	137	ARG
35	1b	145	LEU
35	1b	153	ARG
35	1b	169	LYS
35	1b	170	GLU
35	1b	178	ARG
35	1b	179	LYS
35	1b	185	ILE
35	1b	187	LEU
35	1b	209	ARG
35	1b	217	ARG
35	1b	221	LEU
36	1c	15	THR
36	1c	28	GLN
36	1c	29	TYR
36	1c	45	LYS
36	1c	124	ILE
36	1c	127	ARG
36	1c	181	ASN
36	1c	191	THR
37	1d	5	ILE
37	1d	8	VAL
37	1d	24	GLU
37	1d	28	SER
37	1d	47	ARG

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Mol	Chain	Res	Type
37	1d	49	ARG
37	1d	57	ARG
37	1d	58	LEU
37	1d	127	THR
37	1d	135	LEU
37	1d	137	SER
37	1d	155	LEU
37	1d	168	ARG
37	1d	173	TRP
37	1d	182	LYS
37	1d	196	LEU
37	1d	202	LEU
38	1e	13	ILE
38	1e	38	GLN
38	1e	40	ARG
38	1e	41	VAL
38	1e	47	LYS
38	1e	56	GLN
38	1e	73	ASN
38	1e	79	GLU
38	1e	91	LEU
38	1e	137	GLU
38	1e	144	THR
38	1e	147	ASP
39	1f	25	ILE
39	1f	28	ARG
39	1f	43	LEU
39	1f	61	LEU
39	1f	70	ASP
39	1f	74	ASP
39	1f	82	ARG
39	1f	92	LYS
40	1g	8	GLU
40	1g	16	LEU
40	1g	51	GLN
40	1g	75	VAL
40	1g	97	GLN
40	1g	104	LEU
40	1g	113	GLU
40	1g	129	GLU
40	1g	140	ASP
41	1h	3	THR

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Mol	Chain	Res	Type
41	1h	18	ARG
41	1h	21	LYS
41	1h	26	VAL
41	1h	37	ARG
41	1h	39	LEU
41	1h	51	VAL
41	1h	52	ASP
41	1h	91	ARG
41	1h	112	LEU
41	1h	120	THR
41	1h	122	ARG
41	1h	127	LEU
41	1h	129	VAL
41	1h	133	LEU
42	1i	23	ASN
42	1i	47	LEU
42	1i	53	VAL
42	1i	54	ASP
42	1i	81	ILE
42	1i	86	VAL
42	1i	93	ARG
42	1i	102	LEU
42	1i	104	ARG
42	1i	108	VAL
42	1i	121	ARG
42	1i	128	ARG
43	1j	16	LEU
43	1j	17	ASP
43	1j	21	GLN
43	1j	92	THR
43	1j	98	ILE
44	1k	14	VAL
44	1k	48	ILE
44	1k	77	MET
44	1k	79	SER
44	1k	106	LYS
44	1k	114	VAL
45	1l	23	LYS
45	1l	27	LEU
45	1l	36	VAL
45	1l	55	VAL
45	1l	67	THR

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Mol	Chain	Res	Type
45	1l	83	VAL
45	1l	116	SER
46	1m	3	ARG
46	1m	4	ILE
46	1m	27	LYS
46	1m	64	TRP
46	1m	70	LEU
46	1m	84	ILE
46	1m	99	ARG
46	1m	106	ASN
46	1m	110	ARG
46	1m	117	VAL
46	1m	121	LYS
47	1n	18	VAL
47	1n	22	THR
47	1n	23	ARG
47	1n	31	ARG
47	1n	33	VAL
47	1n	41	ARG
47	1n	57	ARG
48	1o	5	LYS
48	1o	26	GLU
48	1o	39	LEU
48	1o	57	LEU
48	1o	66	LEU
49	1p	19	ILE
49	1p	20	VAL
49	1p	25	ARG
49	1p	45	THR
49	1p	60	LEU
49	1p	69	THR
49	1p	72	ARG
50	1q	35	VAL
50	1q	45	HIS
50	1q	49	GLU
50	1q	89	LEU
50	1q	92	ARG
51	1r	28	GLU
51	1r	32	ARG
51	1r	38	GLU
51	1r	47	THR
52	1s	12	ASP

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Mol	Chain	Res	Type
52	1s	22	LEU
52	1s	28	LYS
52	1s	37	ARG
52	1s	65	ASN
52	1s	66	MET
52	1s	78	ARG
52	1s	83	HIS
52	1s	85	LYS
53	1t	9	ASN
53	1t	10	LEU
53	1t	13	LEU
53	1t	24	LEU
53	1t	56	MET
53	1t	62	LEU
53	1t	75	ASN
53	1t	84	LEU
54	1u	15	ARG
55	1z	-29	LEU
55	1z	-27	THR
55	1z	-10	ARG
55	1z	-6	ARG
55	1z	-3	GLU
55	1z	1	LEU
55	1z	13	ARG
55	1z	21	ILE
55	1z	30	GLU
55	1z	31	ARG
55	1z	39	ILE
55	1z	88	VAL
55	1z	92	ILE
55	1z	98	MET
55	1z	100	VAL
55	1z	106	VAL
55	1z	130	VAL
55	1z	132	ARG
55	1z	142	THR
55	1z	152	THR
55	1z	156	ARG
55	1z	160	ARG
55	1z	172	ASP
55	1z	197	ARG
55	1z	207	ASP

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Mol	Chain	Res	Type
55	1z	208	GLN
55	1z	215	LYS
55	1z	225	GLU
55	1z	236	GLU
55	1z	264	LEU
55	1z	286	ILE
55	1z	299	VAL
55	1z	309	LEU
55	1z	328	ILE
55	1z	336	THR
55	1z	339	SER
55	1z	352	VAL
55	1z	355	LEU
55	1z	356	LEU
55	1z	363	ARG
55	1z	385	THR
55	1z	389	LEU
55	1z	422	GLU
55	1z	428	LEU
55	1z	437	THR
55	1z	442	THR
55	1z	473	ASP
55	1z	481	VAL
55	1z	484	ARG
55	1z	500	GLN
55	1z	512	ILE
55	1z	515	GLU
55	1z	526	VAL
55	1z	530	VAL
55	1z	546	ILE
55	1z	569	ASP
55	1z	590	ILE
55	1z	598	ASP
55	1z	605	ILE
55	1z	614	GLU
55	1z	624	LEU
55	1z	630	GLN
55	1z	641	GLN
55	1z	647	VAL
55	1z	649	LEU
55	1z	651	GLU
55	1z	660	ARG

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Mol	Chain	Res	Type
55	1z	669	PHE
55	1z	670	VAL
55	1z	678	GLU
55	1z	679	VAL
58	1x	9	ARG
58	1x	18	LEU
3	2C	6	ARG
3	2C	24	GLU
3	2C	37	PHE
3	2C	46	LYS
3	2C	49	ILE
3	2C	52	ARG
3	2C	62	VAL
3	2C	68	LEU
3	2C	172	HIS
3	2C	175	VAL
3	2C	188	ASN
3	2C	199	HIS
3	2C	207	THR
3	2C	208	PHE
3	2C	209	LEU
4	2D	54	ARG
4	2D	61	LEU
4	2D	94	LEU
4	2D	99	ASP
4	2D	103	ARG
4	2D	134	ARG
4	2D	142	VAL
4	2D	157	ARG
4	2D	211	ARG
4	2D	221	VAL
4	2D	229	VAL
4	2D	242	ARG
4	2D	257	LEU
4	2D	259	THR
4	2D	260	ARG
4	2D	276	LYS
5	2E	21	VAL
5	2E	38	THR
5	2E	40	GLU
5	2E	52	LEU
5	2E	58	ARG

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Mol	Chain	Res	Type
5	2E	75	VAL
5	2E	76	ARG
5	2E	79	ARG
5	2E	82	ARG
5	2E	119	ARG
5	2E	144	ARG
5	2E	154	LYS
5	2E	167	VAL
5	2E	175	VAL
5	2E	181	LEU
5	2E	195	LEU
5	2E	202	LYS
6	2F	20	LEU
6	2F	33	LEU
6	2F	53	THR
6	2F	57	VAL
6	2F	74	ARG
6	2F	110	LEU
6	2F	140	LEU
6	2F	158	THR
6	2F	170	LEU
6	2F	175	THR
6	2F	176	LEU
6	2F	191	ARG
6	2F	192	LEU
6	2F	197	ASP
6	2F	200	GLU
6	2F	201	VAL
7	2G	3	LEU
7	2G	4	ASP
7	2G	16	ARG
7	2G	21	ARG
7	2G	45	GLU
7	2G	49	ASP
7	2G	51	ARG
7	2G	60	LEU
7	2G	79	ASN
7	2G	91	ARG
7	2G	96	ARG
7	2G	98	ARG
7	2G	113	ARG
7	2G	115	ARG

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Mol	Chain	Res	Type
7	2G	136	ARG
7	2G	139	LEU
7	2G	140	ILE
7	2G	143	GLU
7	2G	148	MET
7	2G	152	LEU
7	2G	159	VAL
7	2G	162	THR
7	2G	170	ARG
8	2H	3	ARG
8	2H	16	SER
8	2H	19	VAL
8	2H	27	LYS
8	2H	33	LEU
8	2H	43	VAL
8	2H	44	VAL
8	2H	69	ARG
8	2H	71	LEU
8	2H	88	LEU
8	2H	107	VAL
8	2H	114	VAL
8	2H	116	GLU
8	2H	122	THR
8	2H	130	ARG
8	2H	139	GLN
8	2H	175	LYS
10	2K	80	LYS
10	2K	84	LEU
10	2K	86	LYS
10	2K	90	LYS
10	2K	95	LYS
10	2K	99	ILE
10	2K	105	LEU
10	2K	106	GLU
10	2K	115	LEU
10	2K	119	ASP
10	2K	133	SER
10	2K	136	VAL
11	2L	10	GLU
11	2L	33	LEU
11	2L	34	LEU
11	2L	38	HIS

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Mol	Chain	Res	Type
11	2L	48	MET
11	2L	87	LEU
11	2L	115	ARG
11	2L	120	LEU
11	2L	121	LYS
11	2L	133	GLN
11	2L	138	LEU
12	2M	10	VAL
12	2M	23	ARG
12	2M	24	VAL
12	2M	53	LYS
12	2M	78	ARG
12	2M	80	ASP
12	2M	92	GLU
12	2M	94	ARG
12	2M	98	VAL
12	2M	108	GLU
12	2M	113	LYS
13	2N	42	SER
13	2N	55	ARG
13	2N	59	LEU
13	2N	65	ARG
13	2N	71	VAL
13	2N	98	GLU
13	2N	106	LEU
13	2N	112	LEU
13	2N	125	VAL
14	2O	1	MET
14	2O	21	THR
14	2O	45	GLN
14	2O	56	ARG
14	2O	59	ARG
14	2O	60	ARG
14	2O	75	THR
14	2O	109	VAL
14	2O	110	THR
14	2O	128	LYS
15	2P	1	MET
15	2P	18	LEU
15	2P	24	GLN
15	2P	28	LEU
15	2P	29	LEU

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Mol	Chain	Res	Type
15	2P	33	ARG
15	2P	44	LEU
15	2P	54	LEU
15	2P	60	LEU
15	2P	65	LEU
15	2P	67	LEU
15	2P	75	LEU
15	2P	79	LEU
15	2P	111	LEU
15	2P	114	VAL
15	2P	118	GLU
16	2Q	19	LYS
16	2Q	20	ARG
16	2Q	44	LYS
16	2Q	48	LEU
16	2Q	50	SER
16	2Q	58	LEU
16	2Q	67	ARG
16	2Q	78	LEU
16	2Q	83	LYS
16	2Q	103	GLU
17	2R	9	LEU
17	2R	17	THR
17	2R	28	VAL
17	2R	42	ILE
17	2R	53	ARG
17	2R	78	LEU
17	2R	85	LYS
17	2R	87	ASP
17	2R	96	ARG
17	2R	118	ARG
17	2R	123	GLN
18	2S	52	ARG
18	2S	60	LEU
18	2S	74	LEU
18	2S	92	ARG
18	2S	95	LEU
18	2S	104	GLN
19	2T	1	MET
19	2T	18	LEU
19	2T	33	VAL
19	2T	46	VAL

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Mol	Chain	Res	Type
19	2T	52	VAL
19	2T	79	VAL
19	2T	95	LEU
20	2U	11	ARG
20	2U	17	VAL
20	2U	23	LEU
20	2U	51	LEU
20	2U	67	ASP
20	2U	100	THR
20	2U	107	LEU
21	2V	57	LEU
21	2V	92	LEU
22	2W	6	HIS
22	2W	7	VAL
22	2W	23	ARG
22	2W	43	ASN
22	2W	49	VAL
22	2W	70	SER
22	2W	72	VAL
22	2W	94	LYS
22	2W	107	ASP
23	2X	5	LEU
23	2X	11	GLU
23	2X	33	LEU
23	2X	42	VAL
23	2X	72	ARG
23	2X	73	GLN
23	2X	86	VAL
23	2X	91	LEU
23	2X	98	MET
23	2X	120	ILE
23	2X	122	ARG
23	2X	129	SER
23	2X	136	PHE
23	2X	150	LEU
23	2X	156	LYS
23	2X	170	THR
23	2X	183	LEU
24	2Y	10	THR
24	2Y	14	ARG
24	2Y	19	LYS
24	2Y	20	ARG

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Mol	Chain	Res	Type
25	2Z	4	VAL
25	2Z	14	VAL
25	2Z	21	ARG
25	2Z	26	ARG
25	2Z	40	ARG
25	2Z	59	THR
25	2Z	65	SER
25	2Z	85	LEU
26	20	2	LYS
26	20	19	VAL
26	20	30	ARG
26	20	32	LEU
26	20	41	ILE
26	20	45	SER
26	20	51	ARG
26	20	53	LEU
26	20	65	ASN
27	21	8	LEU
27	21	23	LEU
27	21	30	ARG
27	21	44	ARG
27	21	48	GLU
28	22	1	MET
28	22	3	GLU
28	22	5	ILE
28	22	34	GLU
28	22	50	VAL
28	22	53	GLU
28	22	58	ARG
28	22	61	ARG
28	22	62	ARG
28	22	67	TYR
28	22	68	ARG
29	23	6	VAL
29	23	16	ARG
29	23	29	THR
29	23	35	GLU
29	23	57	VAL
29	23	58	LEU
30	24	5	VAL
30	24	6	ARG
30	24	34	LEU

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Mol	Chain	Res	Type
30	24	38	LYS
30	24	48	VAL
31	25	1	MET
31	25	32	LYS
32	26	6	THR
32	26	14	VAL
32	26	26	LYS
32	26	31	HIS
32	26	37	SER
33	27	8	LYS
35	2b	8	LYS
35	2b	15	VAL
35	2b	45	GLN
35	2b	51	LEU
35	2b	80	ILE
35	2b	94	ASN
35	2b	97	TRP
35	2b	114	ARG
35	2b	137	ARG
35	2b	154	LEU
35	2b	157	ARG
35	2b	185	ILE
35	2b	187	LEU
35	2b	208	ILE
35	2b	217	ARG
35	2b	224	GLN
36	2c	3	ASN
36	2c	49	SER
36	2c	52	LEU
36	2c	72	LYS
36	2c	98	ASN
36	2c	102	ASN
36	2c	104	GLN
36	2c	105	GLU
36	2c	125	GLU
36	2c	127	ARG
36	2c	136	GLN
36	2c	152	ILE
36	2c	191	THR
37	2d	3	ARG
37	2d	8	VAL
37	2d	34	GLU

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Mol	Chain	Res	Type
37	2d	47	ARG
37	2d	61	LYS
37	2d	65	ARG
37	2d	73	ARG
37	2d	127	THR
37	2d	135	LEU
37	2d	141	ARG
37	2d	150	GLU
37	2d	155	LEU
37	2d	157	LEU
37	2d	187	ARG
37	2d	194	LEU
37	2d	196	LEU
38	2e	38	GLN
38	2e	41	VAL
38	2e	47	LYS
38	2e	71	LEU
38	2e	72	GLN
38	2e	78	HIS
38	2e	144	THR
38	2e	147	ASP
39	2f	61	LEU
39	2f	63	TYR
39	2f	70	ASP
39	2f	74	ASP
39	2f	81	ILE
39	2f	87	ARG
40	2g	12	LEU
40	2g	16	LEU
40	2g	72	ARG
40	2g	75	VAL
40	2g	90	GLU
40	2g	97	GLN
40	2g	104	LEU
40	2g	139	GLU
40	2g	153	HIS
40	2g	155	ARG
41	2h	2	LEU
41	2h	21	LYS
41	2h	34	GLU
41	2h	37	ARG
41	2h	52	ASP

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Mol	Chain	Res	Type
41	2h	78	GLN
41	2h	84	ARG
41	2h	91	ARG
41	2h	98	LYS
41	2h	99	GLU
41	2h	107	LEU
41	2h	111	ILE
41	2h	112	LEU
41	2h	114	THR
41	2h	120	THR
41	2h	125	ARG
41	2h	129	VAL
41	2h	133	LEU
42	2i	7	THR
42	2i	12	GLU
42	2i	14	VAL
42	2i	23	ASN
42	2i	31	GLN
42	2i	64	THR
42	2i	81	ILE
42	2i	83	ARG
42	2i	93	ARG
42	2i	102	LEU
42	2i	104	ARG
42	2i	108	VAL
42	2i	111	ARG
42	2i	114	TYR
42	2i	128	ARG
43	2j	67	THR
43	2j	85	LEU
44	2k	14	VAL
44	2k	18	ARG
44	2k	105	VAL
45	2l	10	LEU
45	2l	23	LYS
45	2l	33	ARG
45	2l	52	LEU
45	2l	53	ARG
45	2l	55	VAL
45	2l	83	VAL
45	2l	114	LYS
46	2m	3	ARG

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Mol	Chain	Res	Type
46	2m	8	GLU
46	2m	19	LEU
46	2m	27	LYS
46	2m	56	LEU
46	2m	66	LEU
46	2m	70	LEU
46	2m	77	ASN
46	2m	106	ASN
46	2m	110	ARG
47	2n	3	ARG
47	2n	15	LYS
47	2n	18	VAL
47	2n	22	THR
47	2n	23	ARG
47	2n	33	VAL
47	2n	41	ARG
48	2o	3	ILE
48	2o	4	THR
48	2o	38	ARG
48	2o	39	LEU
48	2o	48	LYS
48	2o	66	LEU
48	2o	68	ARG
48	2o	83	GLU
49	2p	6	LEU
49	2p	20	VAL
49	2p	28	ARG
49	2p	45	THR
49	2p	57	ARG
49	2p	60	LEU
49	2p	62	VAL
49	2p	67	THR
49	2p	74	LEU
50	2q	4	LYS
50	2q	6	LEU
50	2q	14	LYS
50	2q	49	GLU
50	2q	63	ARG
50	2q	76	LEU
50	2q	91	ARG
51	2r	31	LEU
51	2r	32	ARG

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Mol	Chain	Res	Type
51	2r	38	GLU
51	2r	41	LYS
52	2s	22	LEU
52	2s	33	THR
52	2s	37	ARG
52	2s	65	ASN
52	2s	78	ARG
53	2t	24	LEU
53	2t	45	GLN
53	2t	56	MET
53	2t	62	LEU
53	2t	75	ASN
53	2t	84	LEU
55	2z	-62	LEU
55	2z	-47	ASP
55	2z	-27	THR
55	2z	-20	LEU
55	2z	-10	ARG
55	2z	-6	ARG
55	2z	-1	GLU
55	2z	6	GLU
55	2z	9	LEU
55	2z	14	ASN
55	2z	15	ILE
55	2z	26	THR
55	2z	30	GLU
55	2z	91	THR
55	2z	92	ILE
55	2z	96	ARG
55	2z	123	ARG
55	2z	130	VAL
55	2z	132	ARG
55	2z	152	THR
55	2z	156	ARG
55	2z	157	LEU
55	2z	160	ARG
55	2z	170	ARG
55	2z	187	THR
55	2z	197	ARG
55	2z	198	GLU
55	2z	207	ASP
55	2z	215	LYS

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Mol	Chain	Res	Type
55	2z	219	VAL
55	2z	225	GLU
55	2z	228	MET
55	2z	232	LEU
55	2z	260	LEU
55	2z	299	VAL
55	2z	315	LYS
55	2z	328	ILE
55	2z	336	THR
55	2z	337	SER
55	2z	352	VAL
55	2z	355	LEU
55	2z	363	ARG
55	2z	377	VAL
55	2z	378	VAL
55	2z	385	THR
55	2z	396	ARG
55	2z	418	LYS
55	2z	440	VAL
55	2z	471	LYS
55	2z	473	ASP
55	2z	478	LYS
55	2z	484	ARG
55	2z	485	GLU
55	2z	497	PHE
55	2z	507	TYR
55	2z	512	ILE
55	2z	515	GLU
55	2z	555	LEU
55	2z	569	ASP
55	2z	573	HIS
55	2z	574	GLU
55	2z	575	VAL
55	2z	590	ILE
55	2z	598	ASP
55	2z	603	GLU
55	2z	614	GLU
55	2z	623	ASP
55	2z	624	LEU
55	2z	630	GLN
55	2z	634	MET
55	2z	647	VAL

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Mol	Chain	Res	Type
55	2z	657	THR
55	2z	662	LYS
55	2z	669	PHE
55	2z	688	ILE
58	2x	18	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (160) such sidechains are listed below:

Mol	Chain	Res	Type
4	1D	87	ASN
4	1D	201	HIS
4	1D	253	GLN
6	1F	169	ASN
6	1F	203	GLN
7	1G	40	ASN
10	1K	103	GLN
11	1L	69	GLN
11	1L	133	GLN
13	1N	27	HIS
13	1N	38	GLN
14	1O	57	HIS
14	1O	123	HIS
17	1R	58	ASN
17	1R	123	GLN
18	1S	94	ASN
18	1S	104	GLN
18	1S	117	GLN
21	1V	31	HIS
21	1V	82	GLN
22	1W	6	HIS
22	1W	43	ASN
23	1X	55	HIS
23	1X	73	GLN
23	1X	151	HIS
26	10	9	GLN
26	10	70	GLN
28	12	46	GLN
29	13	23	HIS
32	16	35	GLN
33	17	36	GLN
35	1b	94	ASN
35	1b	95	GLN

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Mol	Chain	Res	Type
36	1c	28	GLN
36	1c	123	GLN
36	1c	136	GLN
36	1c	162	GLN
36	1c	181	ASN
37	1d	45	GLN
37	1d	123	HIS
38	1e	38	GLN
38	1e	56	GLN
38	1e	73	ASN
38	1e	141	GLN
39	1f	7	ASN
40	1g	28	ASN
40	1g	64	GLN
40	1g	96	GLN
40	1g	97	GLN
42	1i	23	ASN
42	1i	31	GLN
42	1i	34	ASN
42	1i	73	GLN
42	1i	89	ASN
42	1i	124	GLN
43	1j	56	HIS
44	1k	104	GLN
45	1l	78	GLN
48	1o	28	GLN
50	1q	16	GLN
50	1q	94	ASN
52	1s	65	ASN
52	1s	69	HIS
52	1s	83	HIS
53	1t	26	ASN
53	1t	45	GLN
55	1z	-50	GLN
55	1z	-13	GLN
55	1z	7	ASN
55	1z	77	HIS
55	1z	124	GLN
55	1z	154	GLN
55	1z	165	GLN
55	1z	359	HIS
55	1z	426	GLN

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Mol	Chain	Res	Type
55	1z	458	HIS
55	1z	500	GLN
55	1z	543	GLN
55	1z	573	HIS
55	1z	641	GLN
55	1z	664	GLN
55	1z	675	HIS
55	1z	677	GLN
4	2D	253	GLN
6	2F	75	HIS
6	2F	169	ASN
6	2F	203	GLN
7	2G	40	ASN
7	2G	132	ASN
8	2H	147	ASN
10	2K	89	HIS
10	2K	103	GLN
10	2K	116	ASN
11	2L	8	GLN
11	2L	69	GLN
11	2L	133	GLN
13	2N	35	HIS
13	2N	38	GLN
14	2O	57	HIS
16	2Q	68	GLN
17	2R	58	ASN
18	2S	104	GLN
20	2U	60	ASN
21	2V	31	HIS
21	2V	82	GLN
22	2W	43	ASN
23	2X	121	HIS
23	2X	151	HIS
29	23	23	HIS
32	26	35	GLN
33	27	20	HIS
33	27	36	GLN
35	2b	16	HIS
35	2b	40	HIS
35	2b	45	GLN
35	2b	94	ASN
35	2b	95	GLN

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Mol	Chain	Res	Type
35	2b	104	ASN
35	2b	224	GLN
36	2c	3	ASN
36	2c	6	HIS
36	2c	37	GLN
36	2c	123	GLN
36	2c	162	GLN
37	2d	45	GLN
37	2d	123	HIS
37	2d	129	ASN
37	2d	160	GLN
37	2d	161	ASN
38	2e	72	GLN
38	2e	130	ASN
39	2f	7	ASN
39	2f	27	GLN
39	2f	94	GLN
40	2g	28	ASN
40	2g	97	GLN
40	2g	110	GLN
42	2i	31	GLN
42	2i	73	GLN
43	2j	62	HIS
43	2j	68	HIS
45	2l	49	ASN
45	2l	75	HIS
45	2l	78	GLN
45	2l	99	HIS
48	2o	28	GLN
50	2q	16	GLN
52	2s	83	HIS
55	2z	-50	GLN
55	2z	14	ASN
55	2z	77	HIS
55	2z	165	GLN
55	2z	426	GLN
55	2z	509	HIS
55	2z	543	GLN
55	2z	573	HIS
55	2z	595	GLN
55	2z	641	GLN
55	2z	675	HIS

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Mol	Chain	Res	Type
55	2z	677	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	434 (15%)	24 (0%)
1	2A	2860/2915 (98%)	515 (18%)	22 (0%)
2	1B	119/121 (98%)	10 (8%)	1 (0%)
2	2B	119/121 (98%)	17 (14%)	0
34	1a	1491/1521 (98%)	266 (17%)	0
34	2a	1498/1521 (98%)	258 (17%)	0
56	1y	5/24 (20%)	0	0
56	2y	4/24 (16%)	0	0
57	1w	75/77 (97%)	19 (25%)	0
57	2w	75/77 (97%)	18 (24%)	0
All	All	9111/9316 (97%)	1537 (16%)	47 (0%)

All (1537) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	14	G
1	1A	28	U
1	1A	33	C
1	1A	44	C
1	1A	53	G
1	1A	61	U
1	1A	62	A
1	1A	69	A
1	1A	72	A
1	1A	73	G
1	1A	115	A
1	1A	116	A
1	1A	117	U
1	1A	122	G
1	1A	148	A
1	1A	169	A
1	1A	176	G
1	1A	184	A
1	1A	185	A
1	1A	187	A

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Mol	Chain	Res	Type
1	1A	193	G
1	1A	203	G
1	1A	204	A
1	1A	209	A
1	1A	210	A
1	1A	213	A
1	1A	216	A
1	1A	217	A
1	1A	221	A
1	1A	236	G
1	1A	238	G
1	1A	249	G
1	1A	254	G
1	1A	268	G
1	1A	270	U
1	1A	271	U
1	1A	272	G
1	1A	273	U
1	1A	287	U
1	1A	288	G
1	1A	294	C
1	1A	296	C
1	1A	298	G
1	1A	302	C
1	1A	334	A
1	1A	352	G
1	1A	353	A
1	1A	365	G
1	1A	375	G
1	1A	386	G
1	1A	412	G
1	1A	422	G
1	1A	433	G
1	1A	437	G
1	1A	438	A
1	1A	454	A
1	1A	468	A
1	1A	469	C
1	1A	473	U
1	1A	480	C
1	1A	482	A
1	1A	495	A

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Mol	Chain	Res	Type
1	1A	506	G
1	1A	518	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	585	G
1	1A	595	G
1	1A	597	A
1	1A	615	G
1	1A	625	A
1	1A	626	G
1	1A	629	U
1	1A	632	G
1	1A	637	U
1	1A	638	G
1	1A	640	G
1	1A	661	A
1	1A	669	C
1	1A	670	A
1	1A	681	G
1	1A	696	C
1	1A	700	A
1	1A	715	G
1	1A	731	A
1	1A	732	G
1	1A	763	G
1	1A	776	C
1	1A	797	A
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	838	G
1	1A	851	G
1	1A	858	C
1	1A	873	U

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Mol	Chain	Res	Type
1	1A	874	U
1	1A	876	G
1	1A	878	G
1	1A	901	G
1	1A	905	G
1	1A	926	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	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	997	A
1	1A	1002	U
1	1A	1003	A
1	1A	1005	C
1	1A	1018	G
1	1A	1019	C
1	1A	1028	A
1	1A	1041	A
1	1A	1057	U
1	1A	1058	C
1	1A	1067	G
1	1A	1071	U
1	1A	1078	U
1	1A	1083	C
1	1A	1085	C
1	1A	1091	A
1	1A	1092	G
1	1A	1095	A
1	1A	1098	C
1	1A	1099	A

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Mol	Chain	Res	Type
1	1A	1103	G
1	1A	1104	G
1	1A	1105	U
1	1A	1106	U
1	1A	1110	U
1	1A	1111	U
1	1A	1115	A
1	1A	1116	G
1	1A	1117	C
1	1A	1118	A
1	1A	1120	C
1	1A	1121	C
1	1A	1124	C
1	1A	1125	C
1	1A	1128	U
1	1A	1133	A
1	1A	1135	U
1	1A	1140	A
1	1A	1142	U
1	1A	1153	U
1	1A	1154	C
1	1A	1155	G
1	1A	1156	A
1	1A	1157	G
1	1A	1174	A
1	1A	1175	U
1	1A	1179	C
1	1A	1180	G
1	1A	1183	G
1	1A	1185	U
1	1A	1216	G
1	1A	1217	G
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1221	A
1	1A	1254	A
1	1A	1255	U
1	1A	1264	A
1	1A	1269	C
1	1A	1295	G
1	1A	1298	A

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Mol	Chain	Res	Type
1	1A	1301	G
1	1A	1316	G
1	1A	1317	A
1	1A	1320	A
1	1A	1345	U
1	1A	1346	A
1	1A	1387	A
1	1A	1397	U
1	1A	1404	A
1	1A	1405	A
1	1A	1410	A
1	1A	1425	G
1	1A	1429	A
1	1A	1430	G
1	1A	1440	A
1	1A	1461	G
1	1A	1462	C
1	1A	1465	U
1	1A	1466	G
1	1A	1472	A
1	1A	1473	C
1	1A	1490	A
1	1A	1495	A
1	1A	1496	G
1	1A	1501	G
1	1A	1513	C
1	1A	1517	A
1	1A	1528	G
1	1A	1535	A
1	1A	1538	C
1	1A	1553	A
1	1A	1554	C
1	1A	1555	A
1	1A	1570	G
1	1A	1578	C
1	1A	1588	A
1	1A	1589	C
1	1A	1604	A
1	1A	1612	A
1	1A	1615	A
1	1A	1624	U
1	1A	1626	A

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Mol	Chain	Res	Type
1	1A	1627	G
1	1A	1630	C
1	1A	1631	A
1	1A	1653	A
1	1A	1654	A
1	1A	1658	G
1	1A	1685	U
1	1A	1694	C
1	1A	1710	A
1	1A	1720	G
1	1A	1721	C
1	1A	1742	G
1	1A	1746	A
1	1A	1747	A
1	1A	1765	G
1	1A	1766	A
1	1A	1775	G
1	1A	1792	A
1	1A	1793	G
1	1A	1794	G
1	1A	1803	A
1	1A	1810	A
1	1A	1812	C
1	1A	1821	A
1	1A	1830	C
1	1A	1831	G
1	1A	1838	U
1	1A	1846	G
1	1A	1869	G
1	1A	1877	A
1	1A	1890	G
1	1A	1899	G
1	1A	1910	A
1	1A	1921	A
1	1A	1926	C
1	1A	1927	G
1	1A	1934	A
1	1A	1950	G
1	1A	1951	G
1	1A	1952	U
1	1A	1958	A
1	1A	1959	A

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Mol	Chain	Res	Type
1	1A	1976	U
1	1A	1984	U
1	1A	1988	C
1	1A	1991	A
1	1A	1992	A
1	1A	1993	A
1	1A	2014	U
1	1A	2018	G
1	1A	2042	C
1	1A	2044	G
1	1A	2052	A
1	1A	2053	G
1	1A	2054	A
1	1A	2064	C
1	1A	2072	A
1	1A	2076	C
1	1A	2077	G
1	1A	2078	A
1	1A	2081	A
1	1A	2082	G
1	1A	2083	A
1	1A	2090	G
1	1A	2091	G
1	1A	2120	U
1	1A	2122	G
1	1A	2129	C
1	1A	2132	C
1	1A	2133	G
1	1A	2139	U
1	1A	2140	A
1	1A	2144	G
1	1A	2147	A
1	1A	2148	G
1	1A	2153	U
1	1A	2154	G
1	1A	2155	A
1	1A	2157	C
1	1A	2158	C
1	1A	2159	C
1	1A	2161	C
1	1A	2162	G
1	1A	2163	C

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Mol	Chain	Res	Type
1	1A	2166	C
1	1A	2167	C
1	1A	2178	G
1	1A	2179	A
1	1A	2180	G
1	1A	2185	C
1	1A	2187	G
1	1A	2188	U
1	1A	2189	G
1	1A	2190	A
1	1A	2191	A
1	1A	2193	U
1	1A	2194	A
1	1A	2195	C
1	1A	2196	C
1	1A	2203	G
1	1A	2204	C
1	1A	2205	G
1	1A	2206	C
1	1A	2209	C
1	1A	2210	U
1	1A	2213	G
1	1A	2219	A
1	1A	2220	A
1	1A	2221	C
1	1A	2226	G
1	1A	2227	G
1	1A	2228	A
1	1A	2229	U
1	1A	2230	G
1	1A	2236	A
1	1A	2237	C
1	1A	2249	G
1	1A	2253	G
1	1A	2279	A
1	1A	2280	A
1	1A	2284	A
1	1A	2286	C
1	1A	2291	G
1	1A	2294	C
1	1A	2298	A
1	1A	2316	A

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Mol	Chain	Res	Type
1	1A	2319	G
1	1A	2320	A
1	1A	2323	U
1	1A	2331	A
1	1A	2332	G
1	1A	2335	C
1	1A	2336	G
1	1A	2345	G
1	1A	2347	A
1	1A	2354	C
1	1A	2358	C
1	1A	2361	C
1	1A	2383	G
1	1A	2390	G
1	1A	2394	G
1	1A	2396	C
1	1A	2417	U
1	1A	2433	A
1	1A	2436	A
1	1A	2440	G
1	1A	2441	A
1	1A	2446	A
1	1A	2450	A
1	1A	2452	C
1	1A	2458	G
1	1A	2459	A
1	1A	2487	A
1	1A	2489	A
1	1A	2498	G
1	1A	2509	C
1	1A	2513	G
1	1A	2516	G
1	1A	2517	U
1	1A	2529	A
1	1A	2536	G
1	1A	2540	G
1	1A	2565	U
1	1A	2577	A
1	1A	2578	G
1	1A	2590	C
1	1A	2593	G
1	1A	2597	C

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Mol	Chain	Res	Type
1	1A	2613	A
1	1A	2615	U
1	1A	2620	U
1	1A	2622	U
1	1A	2623	C
1	1A	2640	A
1	1A	2641	G
1	1A	2665	A
1	1A	2700	U
1	1A	2701	C
1	1A	2713	U
1	1A	2724	A
1	1A	2725	A
1	1A	2726	G
1	1A	2732	U
1	1A	2738	U
1	1A	2745	A
1	1A	2760	A
1	1A	2769	A
1	1A	2770	A
1	1A	2777	A
1	1A	2778	G
1	1A	2790	A
1	1A	2793	A
1	1A	2802	A
1	1A	2812	G
1	1A	2829	A
1	1A	2830	A
1	1A	2842	G
1	1A	2848	G
1	1A	2881	G
1	1A	2882	A
1	1A	2889	C
1	1A	2900	A
1	1A	2902	G
2	1B	2	C
2	1B	13	A
2	1B	47	C
2	1B	52	A
2	1B	53	A
2	1B	56	G
2	1B	73	A

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Mol	Chain	Res	Type
2	1B	85	G
2	1B	106	G
2	1B	110	G
34	1a	6	U
34	1a	10	G
34	1a	14	U
34	1a	23	G
34	1a	33	A
34	1a	40	G
34	1a	43	G
34	1a	48	C
34	1a	49	C
34	1a	51	A
34	1a	52	A
34	1a	55	C
34	1a	62	G
34	1a	75	C
34	1a	77	G
34	1a	91	G
34	1a	94	C
34	1a	95	A
34	1a	110	A
34	1a	115	C
34	1a	116	G
34	1a	126	C
34	1a	137	G
34	1a	138	A
34	1a	151	G
34	1a	158	C
34	1a	169	C
34	1a	177	U
34	1a	189	U
34	1a	202	A
34	1a	204	A
34	1a	208	C
34	1a	209	U
34	1a	210	U
34	1a	211	U
34	1a	212	G
34	1a	243	G
34	1a	247	G
34	1a	262	G

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Mol	Chain	Res	Type
34	1a	263	C
34	1a	285	G
34	1a	297	G
34	1a	301	G
34	1a	317	A
34	1a	324	C
34	1a	325	A
34	1a	328	G
34	1a	338	C
34	1a	342	G
34	1a	344	G
34	1a	347	G
34	1a	348	C
34	1a	349	A
34	1a	350	G
34	1a	351	C
34	1a	363	U
34	1a	368	C
34	1a	380	G
34	1a	393	A
34	1a	394	C
34	1a	402	G
34	1a	408	A
34	1a	409	G
34	1a	419	G
34	1a	420	G
34	1a	425	U
34	1a	426	A
34	1a	435	A
34	1a	437	C
34	1a	447	A
34	1a	456	C
34	1a	461	G
34	1a	469	G
34	1a	470	G
34	1a	481	A
34	1a	482	U
34	1a	489	G
34	1a	493	A
34	1a	494	A
34	1a	495	C
34	1a	502	C

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Mol	Chain	Res	Type
34	1a	505	G
34	1a	511	G
34	1a	515	U
34	1a	516	A
34	1a	517	A
34	1a	531	A
34	1a	543	A
34	1a	544	U
34	1a	545	U
34	1a	548	C
34	1a	556	A
34	1a	557	A
34	1a	560	G
34	1a	561	G
34	1a	591	A
34	1a	599	C
34	1a	602	C
34	1a	611	G
34	1a	612	G
34	1a	614	G
34	1a	615	G
34	1a	616	A
34	1a	630	U
34	1a	634	G
34	1a	637	A
34	1a	649	A
34	1a	655	G
34	1a	671	A
34	1a	672	G
34	1a	701	C
34	1a	707	U
34	1a	715	G
34	1a	733	C
34	1a	736	G
34	1a	739	G
34	1a	750	A
34	1a	758	G
34	1a	761	A
34	1a	776	A
34	1a	777	U
34	1a	778	A
34	1a	786	A

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Mol	Chain	Res	Type
34	1a	801	C
34	1a	805	G
34	1a	811	U
34	1a	812	A
34	1a	813	G
34	1a	824	C
34	1a	825	U
34	1a	826	C
34	1a	829	G
34	1a	837	A
34	1a	850	A
34	1a	851	A
34	1a	869	U
34	1a	880	G
34	1a	890	C
34	1a	900	G
34	1a	904	G
34	1a	905	G
34	1a	912	C
34	1a	913	A
34	1a	936	A
34	1a	938	U
34	1a	939	U
34	1a	946	A
34	1a	947	A
34	1a	949	G
34	1a	950	C
34	1a	952	A
34	1a	953	A
34	1a	954	G
34	1a	955	A
34	1a	967	C
34	1a	970	U
34	1a	971	G
34	1a	976	G
34	1a	977	C
34	1a	982	G
34	1a	983	A
34	1a	984	A
34	1a	985	C
34	1a	988	G
34	1a	995	A

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Mol	Chain	Res	Type
34	1a	998	C
34	1a	1000	G
34	1a	1001	G
34	1a	1002	G
34	1a	1003	G
34	1a	1004	U
34	1a	1005	G
34	1a	1006	C
34	1a	1007	C
34	1a	1008	C
34	1a	1009	C
34	1a	1010	G
34	1a	1037	C
34	1a	1038	A
34	1a	1048	U
34	1a	1049	C
34	1a	1051	G
34	1a	1064	G
34	1a	1072	G
34	1a	1077	G
34	1a	1078	U
34	1a	1084	A
34	1a	1105	U
34	1a	1106	A
34	1a	1107	G
34	1a	1109	U
34	1a	1113	A
34	1a	1119	U
34	1a	1120	C
34	1a	1121	G
34	1a	1122	G
34	1a	1123	C
34	1a	1129	A
34	1a	1134	A
34	1a	1135	A
34	1a	1142	U
34	1a	1149	G
34	1a	1163	G
34	1a	1165	A
34	1a	1166	G
34	1a	1178	U
34	1a	1179	G

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Mol	Chain	Res	Type
34	1a	1183	A
34	1a	1184	G
34	1a	1194	U
34	1a	1195	A
34	1a	1196	C
34	1a	1209	A
34	1a	1210	C
34	1a	1218	A
34	1a	1220	A
34	1a	1222	U
34	1a	1235	G
34	1a	1238	A
34	1a	1239	U
34	1a	1240	G
34	1a	1242	C
34	1a	1244	C
34	1a	1252	C
34	1a	1260	U
34	1a	1261	A
34	1a	1262	A
34	1a	1263	U
34	1a	1264	C
34	1a	1268	A
34	1a	1269	A
34	1a	1281	A
34	1a	1282	G
34	1a	1284	U
34	1a	1287	G
34	1a	1294	G
34	1a	1299	C
34	1a	1304	C
34	1a	1306	A
34	1a	1320	G
34	1a	1322	A
34	1a	1329	G
34	1a	1335	G
34	1a	1340	U
34	1a	1342	A
34	1a	1345	C
34	1a	1351	G
34	1a	1353	G
34	1a	1380	C

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Mol	Chain	Res	Type
34	1a	1381	A
34	1a	1402	G
34	1a	1426	G
34	1a	1430	C
34	1a	1431	U
34	1a	1432	A
34	1a	1433	C
34	1a	1434	G
34	1a	1465	G
34	1a	1475	G
34	1a	1482	G
34	1a	1484	U
34	1a	1495	G
34	1a	1497	A
34	1a	1507	G
34	1a	1508	G
34	1a	1509	A
57	1w	6	G
57	1w	9	G
57	1w	13	C
57	1w	16	C
57	1w	17	C
57	1w	20	U
57	1w	21	A
57	1w	31	G
57	1w	43	A
57	1w	47	U
57	1w	52	G
57	1w	53	G
57	1w	54	5MU
57	1w	61	C
57	1w	65	C
57	1w	66	C
57	1w	67	C
57	1w	73	A
57	1w	76	A
1	2A	10	G
1	2A	11	U
1	2A	33	C
1	2A	35	G
1	2A	44	C
1	2A	59	G

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Mol	Chain	Res	Type
1	2A	69	A
1	2A	72	A
1	2A	73	G
1	2A	81	G
1	2A	82	A
1	2A	88	U
1	2A	91	C
1	2A	93	G
1	2A	96	G
1	2A	98	G
1	2A	99	G
1	2A	100	A
1	2A	115	A
1	2A	116	A
1	2A	117	U
1	2A	138	A
1	2A	154	C
1	2A	155	U
1	2A	170	A
1	2A	184	A
1	2A	193	G
1	2A	202	G
1	2A	203	G
1	2A	204	A
1	2A	209	A
1	2A	210	A
1	2A	216	A
1	2A	217	A
1	2A	218	U
1	2A	221	A
1	2A	236	G
1	2A	240	G
1	2A	252	C
1	2A	254	G
1	2A	268	G
1	2A	269	C
1	2A	271	U
1	2A	272	G
1	2A	273	U
1	2A	287	U
1	2A	288	G
1	2A	300	C

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Mol	Chain	Res	Type
1	2A	301	A
1	2A	325	C
1	2A	334	A
1	2A	335	G
1	2A	352	G
1	2A	353	A
1	2A	356	G
1	2A	361	G
1	2A	375	G
1	2A	385	U
1	2A	386	G
1	2A	388	G
1	2A	406	U
1	2A	412	G
1	2A	422	G
1	2A	437	G
1	2A	438	A
1	2A	454	A
1	2A	468	A
1	2A	469	C
1	2A	471	G
1	2A	479	A
1	2A	480	C
1	2A	495	A
1	2A	506	G
1	2A	507	A
1	2A	528	U
1	2A	529	A
1	2A	533	C
1	2A	552	A
1	2A	553	A
1	2A	554	G
1	2A	555	C
1	2A	556	A
1	2A	557	G
1	2A	568	G
1	2A	573	G
1	2A	585	G
1	2A	595	G
1	2A	597	A
1	2A	608	A
1	2A	610	U

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Mol	Chain	Res	Type
1	2A	625	A
1	2A	626	G
1	2A	629	U
1	2A	635	G
1	2A	638	G
1	2A	640	G
1	2A	641	G
1	2A	642	C
1	2A	644	G
1	2A	651	A
1	2A	661	A
1	2A	669	C
1	2A	670	A
1	2A	674	C
1	2A	678	A
1	2A	679	G
1	2A	680	C
1	2A	697	G
1	2A	713	U
1	2A	715	G
1	2A	732	G
1	2A	763	G
1	2A	776	C
1	2A	807	A
1	2A	808	U
1	2A	810	A
1	2A	811	G
1	2A	817	G
1	2A	820	A
1	2A	821	G
1	2A	822	G
1	2A	828	A
1	2A	830	A
1	2A	831	G
1	2A	835	A
1	2A	838	G
1	2A	851	G
1	2A	858	C
1	2A	865	A
1	2A	873	U
1	2A	874	U
1	2A	877	G

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Mol	Chain	Res	Type
1	2A	905	G
1	2A	912	A
1	2A	915	G
1	2A	918	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	935	C
1	2A	936	A
1	2A	938	C
1	2A	941	A
1	2A	942	C
1	2A	943	C
1	2A	945	A
1	2A	946	A
1	2A	955	A
1	2A	959	C
1	2A	962	A
1	2A	975	G
1	2A	976	G
1	2A	982	G
1	2A	985	A
1	2A	989	A
1	2A	990	G
1	2A	997	A
1	2A	1002	U
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	1053	C
1	2A	1057	U
1	2A	1058	C
1	2A	1067	G
1	2A	1070	G
1	2A	1075	G

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Mol	Chain	Res	Type
1	2A	1078	U
1	2A	1083	C
1	2A	1084	G
1	2A	1087	G
1	2A	1088	C
1	2A	1090	A
1	2A	1092	G
1	2A	1093	A
1	2A	1099	A
1	2A	1103	G
1	2A	1105	U
1	2A	1106	U
1	2A	1107	G
1	2A	1108	G
1	2A	1109	C
1	2A	1114	A
1	2A	1115	A
1	2A	1117	C
1	2A	1121	C
1	2A	1124	C
1	2A	1127	U
1	2A	1128	U
1	2A	1132	G
1	2A	1133	A
1	2A	1134	G
1	2A	1135	U
1	2A	1142	U
1	2A	1143	A
1	2A	1145	C
1	2A	1151	G
1	2A	1152	G
1	2A	1154	C
1	2A	1155	G
1	2A	1156	A
1	2A	1157	G
1	2A	1158	U
1	2A	1164	C
1	2A	1167	G
1	2A	1173	A
1	2A	1174	A
1	2A	1175	U
1	2A	1179	C

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Mol	Chain	Res	Type
1	2A	1180	G
1	2A	1183	G
1	2A	1200	A
1	2A	1216	G
1	2A	1249	U
1	2A	1250	G
1	2A	1256	G
1	2A	1264	A
1	2A	1293	G
1	2A	1298	A
1	2A	1301	G
1	2A	1316	G
1	2A	1317	A
1	2A	1329	A
1	2A	1345	U
1	2A	1346	A
1	2A	1350	C
1	2A	1359	C
1	2A	1366	A
1	2A	1372	C
1	2A	1374	U
1	2A	1397	U
1	2A	1404	A
1	2A	1405	A
1	2A	1410	A
1	2A	1413	G
1	2A	1415	C
1	2A	1417	U
1	2A	1418	A
1	2A	1425	G
1	2A	1429	A
1	2A	1430	G
1	2A	1431	C
1	2A	1461	G
1	2A	1462	C
1	2A	1465	U
1	2A	1466	G
1	2A	1473	C
1	2A	1490	A
1	2A	1495	A
1	2A	1496	G
1	2A	1501	G

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Mol	Chain	Res	Type
1	2A	1505	G
1	2A	1506	A
1	2A	1513	C
1	2A	1517	A
1	2A	1528	G
1	2A	1534	U
1	2A	1535	A
1	2A	1538	C
1	2A	1542	U
1	2A	1553	A
1	2A	1554	C
1	2A	1555	A
1	2A	1579	G
1	2A	1588	A
1	2A	1591	A
1	2A	1594	C
1	2A	1604	A
1	2A	1605	G
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	1661	A
1	2A	1662	C
1	2A	1676	C
1	2A	1677	A
1	2A	1686	C
1	2A	1692	C
1	2A	1694	C
1	2A	1697	G
1	2A	1700	A
1	2A	1720	G
1	2A	1742	G
1	2A	1746	A
1	2A	1747	A
1	2A	1749	G
1	2A	1765	G
1	2A	1766	A

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Mol	Chain	Res	Type
1	2A	1768	G
1	2A	1786	G
1	2A	1788	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	1813	A
1	2A	1821	A
1	2A	1828	U
1	2A	1830	C
1	2A	1831	G
1	2A	1846	G
1	2A	1865	G
1	2A	1869	G
1	2A	1877	A
1	2A	1898	A
1	2A	1899	G
1	2A	1910	A
1	2A	1921	A
1	2A	1927	G
1	2A	1934	A
1	2A	1935	C
1	2A	1950	G
1	2A	1951	G
1	2A	1957	A
1	2A	1959	A
1	2A	1965	U
1	2A	1973	A
1	2A	1976	U
1	2A	1984	U
1	2A	1986	C
1	2A	1988	C
1	2A	1991	A
1	2A	1992	A
1	2A	1993	A
1	2A	2013	G
1	2A	2014	U
1	2A	2018	G
1	2A	2041	A

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Mol	Chain	Res	Type
1	2A	2042	C
1	2A	2044	G
1	2A	2052	A
1	2A	2054	A
1	2A	2064	C
1	2A	2076	C
1	2A	2077	G
1	2A	2081	A
1	2A	2082	G
1	2A	2083	A
1	2A	2090	G
1	2A	2103	A
1	2A	2114	G
1	2A	2120	U
1	2A	2123	U
1	2A	2124	C
1	2A	2126	C
1	2A	2127	G
1	2A	2128	C
1	2A	2131	G
1	2A	2132	C
1	2A	2134	U
1	2A	2136	G
1	2A	2137	G
1	2A	2140	A
1	2A	2143	U
1	2A	2147	A
1	2A	2148	G
1	2A	2149	C
1	2A	2150	C
1	2A	2152	G
1	2A	2153	U
1	2A	2154	G
1	2A	2155	A
1	2A	2157	C
1	2A	2158	C
1	2A	2161	C
1	2A	2163	C
1	2A	2165	U
1	2A	2167	C
1	2A	2169	G
1	2A	2171	U

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Mol	Chain	Res	Type
1	2A	2174	G
1	2A	2175	G
1	2A	2178	G
1	2A	2179	A
1	2A	2183	G
1	2A	2185	C
1	2A	2186	G
1	2A	2188	U
1	2A	2189	G
1	2A	2193	U
1	2A	2194	A
1	2A	2195	C
1	2A	2198	C
1	2A	2202	G
1	2A	2203	G
1	2A	2209	C
1	2A	2210	U
1	2A	2211	G
1	2A	2219	A
1	2A	2226	G
1	2A	2227	G
1	2A	2228	A
1	2A	2229	U
1	2A	2230	G
1	2A	2236	A
1	2A	2249	G
1	2A	2250	G
1	2A	2279	A
1	2A	2280	A
1	2A	2286	C
1	2A	2289	A
1	2A	2291	G
1	2A	2294	C
1	2A	2297	A
1	2A	2298	A
1	2A	2300	G
1	2A	2316	A
1	2A	2319	G
1	2A	2320	A
1	2A	2329	G
1	2A	2330	G
1	2A	2331	A

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Mol	Chain	Res	Type
1	2A	2332	G
1	2A	2336	G
1	2A	2337	C
1	2A	2338	A
1	2A	2345	G
1	2A	2347	A
1	2A	2354	C
1	2A	2358	C
1	2A	2361	C
1	2A	2365	G
1	2A	2387	A
1	2A	2390	G
1	2A	2394	G
1	2A	2396	C
1	2A	2402	G
1	2A	2412	U
1	2A	2417	U
1	2A	2421	G
1	2A	2433	A
1	2A	2434	U
1	2A	2436	A
1	2A	2439	G
1	2A	2440	G
1	2A	2441	A
1	2A	2446	A
1	2A	2450	A
1	2A	2451	C
1	2A	2452	C
1	2A	2459	A
1	2A	2480	A
1	2A	2485	C
1	2A	2487	A
1	2A	2502	U
1	2A	2513	G
1	2A	2516	G
1	2A	2517	U
1	2A	2529	A
1	2A	2531	C
1	2A	2565	U
1	2A	2573	U
1	2A	2577	A
1	2A	2578	G

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Mol	Chain	Res	Type
1	2A	2584	C
1	2A	2597	C
1	2A	2613	A
1	2A	2615	U
1	2A	2620	U
1	2A	2622	U
1	2A	2623	C
1	2A	2632	A
1	2A	2640	A
1	2A	2641	G
1	2A	2665	A
1	2A	2674	G
1	2A	2700	U
1	2A	2701	C
1	2A	2702	C
1	2A	2714	C
1	2A	2724	A
1	2A	2725	A
1	2A	2726	G
1	2A	2738	U
1	2A	2745	A
1	2A	2765	A
1	2A	2769	A
1	2A	2770	A
1	2A	2773	G
1	2A	2776	A
1	2A	2777	A
1	2A	2782	G
1	2A	2789	G
1	2A	2790	A
1	2A	2793	A
1	2A	2794	G
1	2A	2801	C
1	2A	2812	G
1	2A	2813	C
1	2A	2817	U
1	2A	2827	G
1	2A	2829	A
1	2A	2830	A
1	2A	2844	A
1	2A	2848	G
1	2A	2881	G

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Mol	Chain	Res	Type
1	2A	2885	G
1	2A	2889	C
1	2A	2900	A
1	2A	2901	G
1	2A	2902	G
2	2B	7	G
2	2B	8	U
2	2B	13	A
2	2B	23	G
2	2B	25	A
2	2B	32	C
2	2B	42	C
2	2B	51	G
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	73	A
2	2B	85	G
2	2B	89	G
2	2B	98	G
2	2B	106	G
2	2B	110	G
34	2a	6	U
34	2a	10	G
34	2a	14	U
34	2a	23	G
34	2a	33	A
34	2a	40	G
34	2a	43	G
34	2a	48	C
34	2a	49	C
34	2a	51	A
34	2a	52	A
34	2a	53	G
34	2a	55	C
34	2a	67	G
34	2a	77	G
34	2a	84	A
34	2a	85	C
34	2a	91	G
34	2a	94	C
34	2a	95	A

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Mol	Chain	Res	Type
34	2a	110	A
34	2a	115	C
34	2a	126	C
34	2a	137	G
34	2a	138	A
34	2a	158	C
34	2a	169	C
34	2a	177	U
34	2a	189	U
34	2a	202	A
34	2a	204	A
34	2a	208	C
34	2a	210	U
34	2a	211	U
34	2a	212	G
34	2a	243	G
34	2a	247	G
34	2a	262	G
34	2a	263	C
34	2a	285	G
34	2a	297	G
34	2a	301	G
34	2a	317	A
34	2a	324	C
34	2a	325	A
34	2a	328	G
34	2a	338	C
34	2a	340	A
34	2a	342	G
34	2a	347	G
34	2a	348	C
34	2a	349	A
34	2a	350	G
34	2a	351	C
34	2a	363	U
34	2a	368	C
34	2a	380	G
34	2a	394	C
34	2a	402	G
34	2a	408	A
34	2a	409	G
34	2a	419	G

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Mol	Chain	Res	Type
34	2a	420	G
34	2a	425	U
34	2a	426	A
34	2a	435	A
34	2a	437	C
34	2a	447	A
34	2a	456	C
34	2a	469	G
34	2a	470	G
34	2a	481	A
34	2a	482	U
34	2a	489	G
34	2a	493	A
34	2a	494	A
34	2a	495	C
34	2a	502	C
34	2a	505	G
34	2a	511	G
34	2a	515	U
34	2a	516	A
34	2a	517	A
34	2a	531	A
34	2a	543	A
34	2a	545	U
34	2a	548	C
34	2a	556	A
34	2a	557	A
34	2a	560	G
34	2a	561	G
34	2a	591	A
34	2a	599	C
34	2a	602	C
34	2a	611	G
34	2a	612	G
34	2a	614	G
34	2a	616	A
34	2a	630	U
34	2a	634	G
34	2a	637	A
34	2a	649	A
34	2a	655	G
34	2a	671	A

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Mol	Chain	Res	Type
34	2a	672	G
34	2a	701	C
34	2a	707	U
34	2a	715	G
34	2a	733	C
34	2a	736	G
34	2a	739	G
34	2a	750	A
34	2a	758	G
34	2a	761	A
34	2a	776	A
34	2a	777	U
34	2a	778	A
34	2a	786	A
34	2a	801	C
34	2a	805	G
34	2a	811	U
34	2a	812	A
34	2a	813	G
34	2a	824	C
34	2a	825	U
34	2a	826	C
34	2a	829	G
34	2a	837	A
34	2a	850	A
34	2a	851	A
34	2a	869	U
34	2a	880	G
34	2a	890	C
34	2a	892	A
34	2a	900	G
34	2a	904	G
34	2a	905	G
34	2a	912	C
34	2a	913	A
34	2a	936	A
34	2a	938	U
34	2a	939	U
34	2a	946	A
34	2a	947	A
34	2a	949	G
34	2a	950	C

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Mol	Chain	Res	Type
34	2a	952	A
34	2a	953	A
34	2a	954	G
34	2a	955	A
34	2a	967	C
34	2a	969	U
34	2a	970	U
34	2a	971	G
34	2a	981	G
34	2a	982	G
34	2a	984	A
34	2a	985	C
34	2a	995	A
34	2a	998	C
34	2a	1000	G
34	2a	1001	G
34	2a	1003	G
34	2a	1004	U
34	2a	1005	G
34	2a	1006	C
34	2a	1007	C
34	2a	1009	C
34	2a	1010	G
34	2a	1016	G
34	2a	1024	A
34	2a	1033	G
34	2a	1048	U
34	2a	1049	C
34	2a	1051	G
34	2a	1064	G
34	2a	1072	G
34	2a	1077	G
34	2a	1078	U
34	2a	1084	A
34	2a	1100	G
34	2a	1107	G
34	2a	1109	U
34	2a	1112	C
34	2a	1113	A
34	2a	1119	U
34	2a	1120	C
34	2a	1121	G

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Mol	Chain	Res	Type
34	2a	1122	G
34	2a	1123	C
34	2a	1129	A
34	2a	1134	A
34	2a	1135	A
34	2a	1142	U
34	2a	1149	G
34	2a	1163	G
34	2a	1165	A
34	2a	1166	G
34	2a	1178	U
34	2a	1179	G
34	2a	1183	A
34	2a	1184	G
34	2a	1194	U
34	2a	1195	A
34	2a	1196	C
34	2a	1202	G
34	2a	1207	A
34	2a	1209	A
34	2a	1210	C
34	2a	1218	A
34	2a	1220	A
34	2a	1222	U
34	2a	1235	G
34	2a	1238	A
34	2a	1239	U
34	2a	1240	G
34	2a	1242	C
34	2a	1244	C
34	2a	1260	U
34	2a	1261	A
34	2a	1262	A
34	2a	1263	U
34	2a	1268	A
34	2a	1269	A
34	2a	1281	A
34	2a	1282	G
34	2a	1287	G
34	2a	1299	C
34	2a	1304	C
34	2a	1306	A

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Mol	Chain	Res	Type
34	2a	1320	G
34	2a	1322	A
34	2a	1329	G
34	2a	1335	G
34	2a	1340	U
34	2a	1342	A
34	2a	1345	C
34	2a	1351	G
34	2a	1353	G
34	2a	1380	C
34	2a	1381	A
34	2a	1402	G
34	2a	1426	G
34	2a	1430	C
34	2a	1431	U
34	2a	1432	A
34	2a	1433	C
34	2a	1434	G
34	2a	1475	G
34	2a	1482	G
34	2a	1484	U
34	2a	1495	G
34	2a	1497	A
34	2a	1498	G
34	2a	1507	G
34	2a	1508	G
34	2a	1509	A
34	2a	1510	U
57	2w	6	G
57	2w	9	G
57	2w	13	C
57	2w	16	C
57	2w	17	C
57	2w	20	U
57	2w	21	A
57	2w	31	G
57	2w	43	A
57	2w	47	U
57	2w	50	U
57	2w	52	G
57	2w	61	C
57	2w	65	C

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Mol	Chain	Res	Type
57	2w	66	C
57	2w	67	C
57	2w	73	A
57	2w	76	A

All (47) 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	792	A
1	1A	1097	C
1	1A	1134	G
1	1A	1153	U
1	1A	1187	A
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1238	A
1	1A	1254	A
1	1A	1425	G
1	1A	1653	A
1	1A	2013	G
1	1A	2204	C
1	1A	2208	G
1	1A	2433	A
1	1A	2450	A
1	1A	2700	U
1	1A	2768	U
1	1A	2901	G
2	1B	52	A
1	2A	183	A
1	2A	272	G
1	2A	300	C
1	2A	552	A
1	2A	810	A
1	2A	945	A
1	2A	1047	G
1	2A	1087	G
1	2A	1238	A

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Mol	Chain	Res	Type
1	2A	1424	A
1	2A	1425	G
1	2A	1604	A
1	2A	1699	G
1	2A	1934	A
1	2A	1964	U
1	2A	2013	G
1	2A	2131	G
1	2A	2329	G
1	2A	2417	U
1	2A	2433	A
1	2A	2700	U
1	2A	2768	U

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	$\# Z > 2$
57	5MC	1w	32	57	15,22,23	1.50	1 (6%)	17,32,35	1.14	2 (11%)
57	5MU	1w	54	57	14,22,23	0.78	0	16,32,35	2.56	3 (18%)
57	PSU	1w	55	57	16,21,22	1.51	1 (6%)	20,30,33	3.70	6 (30%)
57	4SU	1w	8	57	14,21,22	1.43	2 (14%)	15,30,33	2.68	2 (13%)
57	5MC	2w	32	57	15,22,23	1.53	1 (6%)	17,32,35	1.07	1 (5%)
57	5MU	2w	54	57	14,22,23	0.73	0	16,32,35	2.16	3 (18%)
57	PSU	2w	55	57	16,21,22	1.55	1 (6%)	20,30,33	3.49	7 (35%)
57	4SU	2w	8	57	14,21,22	1.31	2 (14%)	15,30,33	2.72	2 (13%)

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
57	5MC	1w	32	57	-	0/3/25/26	0/2/2/2
57	5MU	1w	54	57	-	0/3/25/26	0/2/2/2
57	PSU	1w	55	57	-	0/7/25/26	0/2/2/2
57	4SU	1w	8	57	-	0/3/25/26	0/2/2/2
57	5MC	2w	32	57	-	0/3/25/26	0/2/2/2
57	5MU	2w	54	57	-	0/3/25/26	0/2/2/2
57	PSU	2w	55	57	-	0/7/25/26	0/2/2/2
57	4SU	2w	8	57	-	0/3/25/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1w	55	PSU	C5-C1'	-4.88	1.48	1.52
57	2w	55	PSU	C5-C1'	-4.71	1.48	1.52
57	1w	8	4SU	C4-S4	-3.55	1.60	1.67
57	1w	8	4SU	C2-N3	-3.39	1.31	1.38
57	2w	8	4SU	C4-S4	-3.34	1.61	1.67
57	2w	8	4SU	C2-N3	-2.91	1.32	1.38
57	1w	32	5MC	C5-C4	5.22	1.49	1.41
57	2w	32	5MC	C5-C4	5.45	1.49	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1w	55	PSU	N1-C2-N3	-9.74	121.40	128.40
57	2w	55	PSU	C5-C4-N3	-8.71	118.29	125.43
57	1w	55	PSU	C5-C4-N3	-8.42	118.52	125.43
57	2w	55	PSU	N1-C2-N3	-8.41	122.35	128.40
57	1w	54	5MU	C5-C4-N3	-6.29	118.30	125.24
57	2w	54	5MU	C5-C4-N3	-5.37	119.32	125.24
57	2w	8	4SU	C5-C4-N3	-5.27	117.07	123.73
57	1w	8	4SU	C5-C4-N3	-4.85	117.60	123.73
57	2w	55	PSU	C5-C6-N1	-4.77	118.21	124.39
57	1w	55	PSU	C5-C6-N1	-4.44	118.63	124.39
57	1w	55	PSU	C5-C1'-C2'	-4.14	108.42	115.55
57	2w	54	5MU	C5-C6-N1	-2.83	119.09	122.15
57	1w	32	5MC	C5-C6-N1	-2.49	119.46	122.15
57	2w	32	5MC	C5-C6-N1	-2.47	119.48	122.15
57	2w	55	PSU	C5-C1'-C2'	-2.08	111.95	115.55
57	1w	54	5MU	C5-C6-N1	-2.08	119.90	122.15
57	2w	55	PSU	O4'-C1'-C2'	2.15	107.91	104.45
57	1w	32	5MC	N4-C4-N3	2.50	120.70	117.00
57	2w	55	PSU	C6-N1-C2	4.29	122.23	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1w	55	PSU	C6-N1-C2	4.39	122.39	115.36
57	2w	54	5MU	C4-N3-C2	5.81	120.24	115.16
57	2w	55	PSU	C4-N3-C2	5.95	120.36	115.16
57	1w	55	PSU	C4-N3-C2	6.36	120.72	115.16
57	1w	54	5MU	C4-N3-C2	7.52	121.73	115.16
57	2w	8	4SU	C2-N3-C4	8.73	128.00	115.11
57	1w	8	4SU	C2-N3-C4	8.78	128.06	115.11

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 1945 ligands modelled in this entry, 1941 are monoatomic - leaving 4 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	$\# Z > 2$
61	SF4	1d	501	37	0,12,12	0.00	-	0,24,24	0.00	-
62	GDP	1z	701	59	25,30,30	1.09	2 (8%)	26,47,47	1.90	6 (23%)
61	SF4	2d	501	37	0,12,12	0.00	-	0,24,24	0.00	-
62	GDP	2z	702	59	25,30,30	1.13	2 (8%)	26,47,47	1.98	6 (23%)

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
61	SF4	1d	501	37	-	0/0/48/48	0/6/5/5
62	GDP	1z	701	59	-	0/12/32/32	0/3/3/3
61	SF4	2d	501	37	-	0/0/48/48	0/6/5/5
62	GDP	2z	702	59	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	1z	701	GDP	C5-C4	3.01	1.47	1.40
62	2z	702	GDP	C5-C4	3.04	1.47	1.40
62	1z	701	GDP	C6-C5	3.62	1.48	1.41
62	2z	702	GDP	C6-C5	3.67	1.48	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	2z	702	GDP	C5-C6-N1	-4.31	117.35	123.48
62	1z	701	GDP	C5-C6-N1	-3.80	118.08	123.48
62	2z	702	GDP	C6-C5-C4	-3.44	117.42	120.84
62	1z	701	GDP	C6-C5-C4	-3.28	117.58	120.84
62	2z	702	GDP	N3-C2-N1	-3.27	122.68	127.46
62	1z	701	GDP	C4-C5-N7	-2.99	106.53	109.41
62	1z	701	GDP	N3-C2-N1	-2.96	123.14	127.46
62	2z	702	GDP	C4-C5-N7	-2.73	106.77	109.41
62	1z	701	GDP	C6-N1-C2	4.13	122.00	116.06
62	2z	702	GDP	C2-N3-C4	4.63	120.56	115.16
62	2z	702	GDP	C6-N1-C2	4.76	122.91	116.06
62	1z	701	GDP	C2-N3-C4	4.94	120.93	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1A	2872/2915 (98%)	-0.11	87 (3%)	51	23	20, 43, 93, 111	0
1	2A	2868/2915 (98%)	-0.28	91 (3%)	48	21	22, 46, 97, 112	0
2	1B	120/121 (99%)	-0.36	0	100	100	37, 57, 71, 82	0
2	2B	120/121 (99%)	-0.40	0	100	100	43, 62, 74, 83	0
3	1C	135/229 (58%)	3.52	102 (75%)	0	0	82, 99, 105, 108	2 (1%)
3	2C	135/229 (58%)	3.83	111 (82%)	0	0	82, 100, 104, 108	2 (1%)
4	1D	275/276 (99%)	-0.50	0	100	100	23, 41, 57, 85	0
4	2D	275/276 (99%)	-0.58	0	100	100	24, 42, 58, 84	0
5	1E	204/206 (99%)	-0.44	0	100	100	23, 44, 63, 75	0
5	2E	204/206 (99%)	-0.48	0	100	100	22, 48, 65, 77	0
6	1F	203/210 (96%)	-0.38	0	100	100	22, 51, 72, 89	0
6	2F	203/210 (96%)	-0.42	0	100	100	25, 54, 73, 88	0
7	1G	181/182 (99%)	-0.40	1 (0%)	89	71	50, 66, 81, 88	0
7	2G	181/182 (99%)	-0.19	0	100	100	55, 69, 82, 90	0
8	1H	174/180 (96%)	-0.32	1 (0%)	89	71	45, 62, 75, 81	0
8	2H	174/180 (96%)	0.27	1 (0%)	89	71	50, 66, 78, 83	0
9	1J	130/173 (75%)	0.46	12 (9%)	10	4	65, 82, 95, 100	0
9	2J	130/173 (75%)	1.04	20 (15%)	2	1	70, 88, 100, 104	0
10	1K	67/147 (45%)	1.68	21 (31%)	0	0	79, 94, 100, 102	0
10	2K	66/147 (44%)	2.52	38 (57%)	0	0	87, 95, 101, 104	0
11	1L	140/140 (100%)	-0.43	0	100	100	31, 44, 65, 82	0
11	2L	140/140 (100%)	-0.37	0	100	100	33, 49, 67, 81	0
12	1M	122/122 (100%)	-0.43	0	100	100	27, 46, 64, 71	0
12	2M	122/122 (100%)	-0.49	0	100	100	30, 47, 66, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1N	149/150 (99%)	-0.32	0 100 100	24, 53, 76, 84	0
13	2N	149/150 (99%)	-0.13	1 (0%) 87 67	27, 56, 77, 88	0
14	1O	141/141 (100%)	-0.37	0 100 100	32, 48, 61, 74	0
14	2O	141/141 (100%)	-0.60	0 100 100	35, 51, 65, 76	0
15	1P	118/118 (100%)	-0.40	0 100 100	27, 40, 54, 66	0
15	2P	118/118 (100%)	-0.45	0 100 100	29, 43, 58, 68	0
16	1Q	110/112 (98%)	-0.31	0 100 100	44, 56, 71, 76	0
16	2Q	110/112 (98%)	-0.17	0 100 100	47, 60, 73, 78	0
17	1R	131/146 (89%)	-0.41	1 (0%) 86 64	33, 50, 72, 84	0
17	2R	131/146 (89%)	-0.53	0 100 100	34, 52, 73, 82	0
18	1S	116/118 (98%)	-0.65	1 (0%) 84 61	15, 31, 47, 71	0
18	2S	116/118 (98%)	-0.43	0 100 100	37, 56, 70, 74	0
19	1T	101/101 (100%)	-0.58	0 100 100	21, 35, 57, 72	0
19	2T	101/101 (100%)	-0.26	0 100 100	33, 65, 78, 83	0
20	1U	112/113 (99%)	-0.57	0 100 100	19, 32, 54, 85	0
20	2U	112/113 (99%)	-0.39	0 100 100	35, 49, 65, 82	0
21	1V	95/96 (98%)	-0.52	0 100 100	23, 39, 60, 84	0
21	2V	95/96 (98%)	-0.20	2 (2%) 64 34	40, 59, 76, 84	0
22	1W	107/110 (97%)	-0.27	1 (0%) 84 61	39, 57, 74, 81	0
22	2W	107/110 (97%)	0.23	2 (1%) 67 37	44, 61, 76, 85	0
23	1X	186/206 (90%)	-0.39	0 100 100	44, 65, 77, 85	0
23	2X	186/206 (90%)	-0.01	3 (1%) 72 44	50, 68, 80, 88	0
24	1Y	76/85 (89%)	-0.51	1 (1%) 77 51	20, 36, 58, 67	0
24	2Y	76/85 (89%)	-0.11	1 (1%) 77 51	38, 56, 69, 79	0
25	1Z	97/98 (98%)	-0.31	1 (1%) 82 58	25, 44, 67, 75	0
25	2Z	97/98 (98%)	-0.25	1 (1%) 82 58	31, 56, 77, 81	0
26	10	70/72 (97%)	-0.31	0 100 100	44, 57, 69, 81	0
26	20	70/72 (97%)	-0.34	0 100 100	46, 60, 70, 81	0
27	11	59/60 (98%)	-0.23	1 (1%) 70 42	30, 45, 63, 76	0
27	21	59/60 (98%)	0.05	0 100 100	34, 49, 68, 79	0
28	12	69/71 (97%)	0.12	3 (4%) 36 15	61, 81, 93, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	22	69/71 (97%)	0.18	5 (7%) 16 6	66, 82, 95, 99	0
29	13	59/60 (98%)	-0.47	0 100 100	25, 40, 57, 63	0
29	23	59/60 (98%)	-0.52	0 100 100	27, 42, 62, 68	0
30	14	53/54 (98%)	-0.39	0 100 100	37, 47, 59, 64	0
30	24	53/54 (98%)	-0.38	0 100 100	40, 49, 61, 65	0
31	15	48/49 (97%)	-0.33	0 100 100	23, 29, 58, 72	0
31	25	48/49 (97%)	-0.37	0 100 100	30, 40, 66, 78	0
32	16	64/65 (98%)	-0.55	0 100 100	20, 33, 44, 61	0
32	26	64/65 (98%)	-0.34	0 100 100	37, 50, 60, 72	0
33	17	37/37 (100%)	-0.05	0 100 100	36, 49, 59, 65	0
33	27	37/37 (100%)	-0.19	1 (2%) 55 26	39, 53, 63, 68	0
34	1a	1495/1521 (98%)	-0.12	35 (2%) 61 31	40, 72, 96, 109	0
34	2a	1501/1521 (98%)	-0.12	34 (2%) 61 31	42, 73, 96, 109	0
35	1b	231/256 (90%)	0.01	3 (1%) 77 51	67, 82, 91, 100	0
35	2b	231/256 (90%)	0.17	12 (5%) 28 11	68, 83, 93, 103	0
36	1c	206/239 (86%)	0.05	1 (0%) 90 74	68, 80, 90, 95	0
36	2c	206/239 (86%)	0.24	4 (1%) 67 37	71, 81, 90, 95	0
37	1d	208/209 (99%)	-0.24	0 100 100	56, 73, 83, 92	0
37	2d	208/209 (99%)	-0.25	0 100 100	58, 73, 82, 92	0
38	1e	148/162 (91%)	-0.33	0 100 100	54, 68, 77, 83	0
38	2e	148/162 (91%)	-0.19	0 100 100	56, 70, 78, 85	0
39	1f	100/101 (99%)	-0.43	0 100 100	54, 70, 79, 85	0
39	2f	100/101 (99%)	-0.23	0 100 100	56, 71, 81, 84	0
40	1g	155/156 (99%)	0.12	10 (6%) 20 7	70, 78, 89, 94	0
40	2g	155/156 (99%)	0.36	15 (9%) 8 3	69, 79, 91, 96	0
41	1h	137/138 (99%)	-0.18	0 100 100	58, 71, 79, 85	0
41	2h	137/138 (99%)	-0.16	0 100 100	60, 71, 79, 85	0
42	1i	127/128 (99%)	0.16	0 100 100	62, 82, 89, 94	0
42	2i	127/128 (99%)	0.63	7 (5%) 26 10	66, 83, 90, 95	0
43	1j	97/105 (92%)	0.28	2 (2%) 64 34	66, 84, 92, 94	0
43	2j	96/105 (91%)	0.77	11 (11%) 5 2	68, 85, 93, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1k	114/129 (88%)	-0.25	0 100 100	53, 69, 80, 84	0
44	2k	114/129 (88%)	-0.05	0 100 100	54, 71, 82, 85	0
45	1l	122/132 (92%)	-0.34	0 100 100	50, 60, 70, 75	0
45	2l	122/132 (92%)	-0.31	0 100 100	49, 61, 70, 75	0
46	1m	123/126 (97%)	0.27	7 (5%) 24 9	65, 78, 90, 105	0
46	2m	122/126 (96%)	0.58	9 (7%) 15 6	70, 83, 94, 105	0
47	1n	60/61 (98%)	-0.07	1 (1%) 70 42	69, 79, 84, 86	0
47	2n	60/61 (98%)	0.35	2 (3%) 47 21	70, 81, 85, 89	0
48	1o	88/89 (98%)	-0.16	0 100 100	52, 67, 79, 87	0
48	2o	88/89 (98%)	-0.05	0 100 100	51, 68, 78, 87	0
49	1p	82/88 (93%)	0.01	1 (1%) 79 53	54, 69, 79, 85	0
49	2p	82/88 (93%)	0.04	0 100 100	55, 69, 79, 84	0
50	1q	99/105 (94%)	-0.21	0 100 100	54, 67, 76, 83	0
50	2q	99/105 (94%)	-0.04	1 (1%) 82 58	55, 67, 77, 85	0
51	1r	68/88 (77%)	0.19	3 (4%) 35 14	57, 69, 82, 90	0
51	2r	68/88 (77%)	0.14	1 (1%) 74 47	60, 70, 81, 90	0
52	1s	84/93 (90%)	0.66	3 (3%) 43 18	76, 84, 92, 95	0
52	2s	83/93 (89%)	0.85	5 (6%) 23 9	75, 85, 92, 94	0
53	1t	96/106 (90%)	0.05	1 (1%) 82 58	60, 70, 80, 85	0
53	2t	96/106 (90%)	-0.04	0 100 100	59, 70, 81, 84	0
54	1u	23/27 (85%)	0.50	0 100 100	70, 77, 81, 82	0
54	2u	23/27 (85%)	1.00	2 (8%) 11 4	70, 78, 82, 84	0
55	1z	730/758 (96%)	0.38	82 (11%) 6 2	52, 79, 96, 105	0
55	2z	730/758 (96%)	0.56	108 (14%) 3 1	47, 81, 99, 108	0
56	1y	6/24 (25%)	0.59	0 100 100	61, 67, 93, 95	0
56	2y	5/24 (20%)	0.88	1 (20%) 1 1	64, 66, 89, 96	0
57	1w	72/77 (93%)	-0.20	0 100 100	32, 64, 78, 97	0
57	2w	72/77 (93%)	-0.09	0 100 100	33, 66, 79, 98	0
58	1x	19/35 (54%)	-0.31	0 100 100	35, 42, 64, 65	0
58	2x	19/35 (54%)	-0.14	0 100 100	36, 45, 65, 65	0
All	All	22619/23832 (94%)	-0.06	871 (3%) 40 16	15, 63, 94, 112	4 (0%)

All (871) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	2m	124	PRO	13.8
3	2C	165	ASN	11.9
46	1m	123	ALA	11.7
3	1C	165	ASN	11.3
3	1C	56	GLN	10.9
3	1C	170	ALA	10.9
46	2m	123	ALA	10.8
3	2C	174	PRO	10.6
46	2m	122	LYS	10.5
3	1C	166	ASP	10.2
3	2C	63	SER	9.9
46	2m	119	GLY	9.7
3	1C	58	VAL	9.7
55	2z	576	ASP	9.4
46	2m	121	LYS	9.4
3	2C	57	ASN	9.1
3	1C	225	ASN	8.8
3	2C	4	GLY	8.7
3	1C	158	ALA	8.7
3	1C	65	PRO	8.3
3	2C	58	VAL	8.1
3	2C	179	SER	8.1
55	2z	575	VAL	8.0
1	2A	2144	G	7.9
3	1C	24	GLU	7.8
1	1A	2166	C	7.7
3	2C	186	ALA	7.6
1	1A	2136	G	7.6
1	1A	2200	C	7.5
3	2C	170	ALA	7.5
3	2C	51	PRO	7.4
1	2A	2145	G	7.4
3	2C	34	THR	7.3
10	2K	107	ILE	7.3
1	2A	1110	U	7.3
1	2A	2167	C	7.3
3	1C	176	GLY	7.3
3	2C	203	GLY	7.1
3	2C	180	PHE	7.1
3	1C	163	PHE	7.0
1	2A	2136	G	6.8
3	2C	188	ASN	6.7

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Mol	Chain	Res	Type	RSRZ
1	1A	2187	G	6.7
3	1C	168	THR	6.7
55	2z	425	SER	6.6
10	2K	123	ALA	6.5
1	1A	2164	C	6.5
55	2z	569	ASP	6.5
3	2C	164	ARG	6.4
3	2C	166	ASP	6.4
46	2m	120	LYS	6.4
3	1C	51	PRO	6.4
3	2C	226	PRO	6.4
55	2z	463	VAL	6.4
3	1C	171	ILE	6.4
3	2C	211	SER	6.4
3	2C	175	VAL	6.4
3	2C	21	THR	6.3
1	2A	2180	G	6.3
1	2A	2195	C	6.3
3	1C	63	SER	6.3
46	1m	119	GLY	6.3
55	2z	507	TYR	6.3
1	2A	1111	U	6.2
3	2C	56	GLN	6.2
1	2A	2132	C	6.1
3	2C	26	ALA	6.1
1	1A	2167	C	6.1
1	1A	2165	U	6.1
9	1J	88	ALA	6.1
1	1A	2138	A	6.0
3	1C	57	ASN	6.0
1	2A	2131	G	6.0
1	2A	2133	G	5.9
3	1C	196	LEU	5.9
55	1z	89	ASP	5.9
46	1m	120	LYS	5.9
3	2C	67	GLY	5.9
1	2A	2200	C	5.9
1	1A	2133	G	5.9
1	1A	2181	G	5.9
1	1A	2202	G	5.9
3	1C	164	ARG	5.8
46	1m	124	PRO	5.8

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Mol	Chain	Res	Type	RSRZ
1	1A	2162	G	5.8
34	2a	1239	U	5.8
55	2z	532	GLY	5.8
1	2A	2166	C	5.8
55	2z	423	LYS	5.8
3	2C	187	ASP	5.7
3	1C	21	THR	5.7
24	2Y	8	GLY	5.7
46	2m	6	GLY	5.7
55	2z	89	ASP	5.7
1	1A	2134	U	5.7
55	2z	574	GLU	5.7
1	2A	2181	G	5.6
10	2K	99	ILE	5.6
1	1A	2150	C	5.6
1	1A	2199	C	5.6
3	2C	181	PRO	5.6
3	2C	25	ALA	5.6
40	2g	83	ALA	5.6
55	1z	492	ASP	5.6
3	2C	183	GLU	5.6
55	2z	419	ALA	5.5
9	2J	125	LEU	5.5
55	2z	422	GLU	5.5
3	2C	185	LEU	5.5
55	2z	436	PRO	5.5
55	2z	435	ASP	5.5
1	2A	2165	U	5.5
3	2C	59	ARG	5.5
1	1A	1113	G	5.5
9	2J	85	ASP	5.4
3	1C	66	HIS	5.4
55	2z	506	GLN	5.4
1	1A	2151	U	5.4
3	1C	162	GLU	5.4
1	2A	2141	G	5.4
10	2K	97	GLY	5.4
3	2C	182	PRO	5.4
55	2z	461	ILE	5.4
3	1C	197	GLU	5.4
1	2A	2154	G	5.3
3	1C	179	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2189	G	5.3
55	2z	410	ASP	5.3
3	2C	60	GLY	5.3
1	2A	2149	C	5.3
9	1J	89	ALA	5.3
1	2A	2135	A	5.2
46	1m	121	LYS	5.2
40	1g	156	TRP	5.2
3	1C	50	ASP	5.2
46	1m	122	LYS	5.2
1	2A	2163	C	5.1
34	2a	981	G	5.1
3	2C	208	PHE	5.1
55	1z	411	VAL	5.1
3	2C	69	GLY	5.1
3	1C	34	THR	5.1
1	1A	2188	U	5.1
3	1C	55	ASP	5.1
3	1C	62	VAL	5.0
1	2A	2142	G	5.0
3	2C	173	ALA	5.0
9	1J	53	VAL	5.0
40	2g	80	VAL	5.0
1	1A	2180	G	5.0
34	1a	1011	C	5.0
1	1A	2131	G	5.0
1	1A	2142	G	5.0
3	1C	20	TYR	5.0
1	2A	2190	A	5.0
1	1A	2168	G	5.0
1	2A	2138	A	5.0
9	2J	49	ALA	4.9
55	2z	418	LYS	4.9
1	2A	2199	C	4.9
55	2z	437	THR	4.9
3	1C	67	GLY	4.9
34	2a	1011	C	4.9
1	1A	2141	G	4.9
10	2K	85	GLU	4.9
10	2K	108	ALA	4.9
3	2C	66	HIS	4.9
3	1C	188	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	2A	2201	U	4.8
40	2g	78	ARG	4.8
55	2z	462	ILE	4.8
34	2a	979	A	4.8
1	2A	2175	G	4.8
35	2b	233	SER	4.8
55	2z	573	HIS	4.8
3	2C	17	ASN	4.8
10	2K	98	ARG	4.8
1	1A	2153	U	4.8
1	2A	1123	U	4.8
1	2A	2143	U	4.8
1	1A	2130	U	4.7
1	2A	2164	C	4.7
1	2A	2168	G	4.7
1	1A	2132	C	4.7
40	2g	82	GLY	4.7
55	2z	420	ASP	4.7
3	1C	68	LEU	4.7
1	1A	2137	G	4.7
1	1A	2135	A	4.7
34	2a	980	G	4.7
55	2z	530	VAL	4.7
1	1A	2175	G	4.6
55	2z	492	ASP	4.6
9	1J	49	ALA	4.6
3	2C	22	ILE	4.6
3	2C	193	ILE	4.6
3	1C	198	ALA	4.6
3	2C	28	LEU	4.6
3	2C	68	LEU	4.6
1	1A	2157	C	4.6
55	1z	461	ILE	4.6
3	1C	25	ALA	4.6
3	2C	161	ILE	4.5
3	1C	187	ASP	4.5
1	2A	2130	U	4.5
34	1a	981	G	4.5
3	2C	65	PRO	4.5
40	1g	85	TYR	4.5
1	2A	2159	C	4.5
10	2K	127	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
34	2a	1010	G	4.5
3	2C	55	ASP	4.4
55	1z	427	ALA	4.4
3	1C	193	ILE	4.4
55	2z	472	VAL	4.4
3	2C	35	ALA	4.4
9	2J	133	GLU	4.4
1	1A	1112	A	4.4
10	2K	105	LEU	4.4
34	2a	1012	G	4.4
55	2z	494	GLU	4.4
3	1C	49	ILE	4.4
3	1C	161	ILE	4.4
3	1C	199	HIS	4.4
3	1C	4	GLY	4.4
10	1K	135	GLY	4.4
1	2A	2137	G	4.4
34	1a	1019	G	4.4
10	2K	76	TYR	4.4
34	1a	982	G	4.3
55	2z	421	GLN	4.3
3	2C	9	ALA	4.3
1	2A	2150	C	4.3
3	1C	173	ALA	4.3
3	1C	178	ALA	4.3
10	1K	136	VAL	4.3
1	1A	1220	G	4.3
55	1z	458	HIS	4.3
55	1z	466	LEU	4.3
55	2z	570	GLY	4.3
9	1J	50	ARG	4.3
1	2A	2179	A	4.3
3	2C	30	LYS	4.3
10	2K	129	GLY	4.3
3	1C	64	LEU	4.3
10	2K	136	VAL	4.3
1	2A	2146	G	4.2
1	1A	2170	G	4.2
1	1A	2144	G	4.2
1	2A	2169	G	4.2
1	2A	2176	G	4.2
55	2z	527	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
3	2C	46	LYS	4.2
55	2z	415	PRO	4.2
3	1C	195	ALA	4.2
55	2z	441	SER	4.2
3	2C	11	LEU	4.2
1	2A	2189	G	4.1
1	1A	2152	G	4.1
9	2J	50	ARG	4.1
34	1a	980	G	4.1
3	2C	27	ARG	4.1
10	2K	138	VAL	4.1
1	1A	2201	U	4.1
1	1A	2195	C	4.1
3	1C	9	ALA	4.1
3	2C	33	ALA	4.1
10	2K	130	SER	4.1
1	1A	2163	C	4.1
3	2C	163	PHE	4.1
3	2C	204	ALA	4.1
55	2z	601	ILE	4.1
34	2a	1016	G	4.1
1	2A	2187	G	4.1
55	2z	490	PRO	4.1
40	2g	154	TYR	4.1
55	2z	491	VAL	4.1
1	1A	2182	C	4.1
3	2C	184	LYS	4.0
3	2C	31	GLU	4.0
3	1C	60	GLY	4.0
3	1C	182	PRO	4.0
3	2C	168	THR	4.0
1	1A	2143	U	4.0
3	2C	54	SER	4.0
10	2K	137	GLU	4.0
3	2C	167	LYS	4.0
55	2z	538	TYR	4.0
3	1C	59	ARG	4.0
3	1C	159	GLY	4.0
1	1A	2183	G	4.0
55	1z	433	GLU	4.0
1	2A	2178	G	4.0
55	2z	475	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	1A	2190	A	4.0
3	2C	198	ALA	4.0
10	2K	83	GLY	3.9
3	2C	162	GLU	3.9
55	1z	570	GLY	3.9
3	1C	191	ALA	3.9
1	2A	2198	C	3.9
55	2z	411	VAL	3.9
36	2c	87	LEU	3.9
55	1z	457	LEU	3.9
1	2A	2160	C	3.9
1	2A	934	C	3.9
1	2A	2134	U	3.9
3	2C	189	ILE	3.9
1	2A	1112	A	3.9
1	2A	2202	G	3.9
55	2z	427	ALA	3.9
55	2z	408	VAL	3.9
3	1C	169	GLY	3.9
3	2C	199	HIS	3.9
55	2z	432	ALA	3.9
3	2C	43	VAL	3.8
3	2C	24	GLU	3.8
3	1C	204	ALA	3.8
10	2K	104	VAL	3.8
55	1z	463	VAL	3.8
55	2z	501	THR	3.8
1	1A	2125	G	3.8
3	2C	171	ILE	3.8
3	1C	175	VAL	3.8
10	2K	135	GLY	3.8
1	1A	2129	C	3.8
3	2C	10	LEU	3.8
55	1z	530	VAL	3.8
3	2C	3	HIS	3.8
1	1A	2169	G	3.7
34	2a	1019	G	3.7
55	1z	528	ALA	3.7
22	2W	1	MET	3.7
34	2a	1509	A	3.7
1	1A	2172	G	3.7
34	2a	1510	U	3.7

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Mol	Chain	Res	Type	RSRZ
55	1z	456	GLU	3.7
55	2z	234	GLY	3.7
9	2J	89	ALA	3.7
10	1K	124	ALA	3.7
55	1z	462	ILE	3.7
55	2z	581	ALA	3.7
10	1K	134	MET	3.7
55	2z	514	VAL	3.7
3	2C	16	PRO	3.7
3	2C	191	ALA	3.7
1	1A	2186	G	3.7
3	2C	207	THR	3.7
10	2K	113	PRO	3.6
34	1a	1010	G	3.6
3	2C	177	LYS	3.6
3	2C	47	LEU	3.6
1	1A	2176	G	3.6
3	1C	26	ALA	3.6
55	1z	437	THR	3.6
3	2C	169	GLY	3.6
55	1z	476	VAL	3.6
42	2i	30	GLY	3.6
1	1A	2161	C	3.6
55	1z	464	ASP	3.6
1	2A	2188	U	3.6
3	2C	197	GLU	3.6
10	2K	94	GLU	3.6
3	1C	33	ALA	3.6
54	2u	24	ARG	3.6
55	1z	642	VAL	3.6
3	1C	200	LYS	3.5
55	2z	599	PRO	3.5
55	2z	457	LEU	3.5
34	1a	1013	A	3.5
3	2C	29	VAL	3.5
10	2K	122	ALA	3.5
55	1z	546	ILE	3.5
10	1K	118	THR	3.5
55	1z	451	ILE	3.5
55	1z	563	ILE	3.5
1	2A	2127	G	3.5
34	1a	1008	C	3.5

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Mol	Chain	Res	Type	RSRZ
34	1a	1018	A	3.5
3	2C	176	GLY	3.5
3	2C	52	ARG	3.5
55	2z	474	ALA	3.5
1	1A	1554	C	3.5
34	1a	1003	G	3.5
34	2a	1000	G	3.5
55	1z	514	VAL	3.5
1	1A	2159	C	3.5
3	1C	22	ILE	3.5
55	2z	539	ILE	3.5
1	2A	1554	C	3.4
10	2K	79	ARG	3.4
3	2C	206	GLY	3.4
55	2z	434	GLU	3.4
3	2C	210	ARG	3.4
9	1J	52	PHE	3.4
3	1C	180	PHE	3.4
9	1J	51	LEU	3.4
9	2J	116	ILE	3.4
40	1g	84	ASN	3.4
1	2A	1121	C	3.4
43	2j	10	GLY	3.4
1	2A	2153	U	3.4
1	2A	2148	G	3.4
10	1K	86	LYS	3.4
55	2z	464	ASP	3.4
1	2A	2157	C	3.4
55	1z	422	GLU	3.4
3	1C	40	THR	3.4
10	1K	90	LYS	3.4
55	1z	509	HIS	3.3
55	2z	424	LEU	3.3
1	1A	697	G	3.3
1	1A	2154	G	3.3
10	2K	96	VAL	3.3
3	1C	189	ILE	3.3
9	2J	62	ALA	3.3
1	1A	2191	A	3.3
3	1C	61	THR	3.3
55	2z	629	GLY	3.3
55	2z	499	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	1A	934	C	3.3
1	2A	2186	G	3.3
10	1K	120	LEU	3.3
3	1C	226	PRO	3.3
3	1C	69	GLY	3.3
43	2j	26	ALA	3.3
10	2K	80	LYS	3.3
55	1z	541	ALA	3.2
3	1C	192	PHE	3.2
13	2N	93	GLY	3.2
1	1A	2148	G	3.2
1	2A	2203	G	3.2
10	2K	133	SER	3.2
1	2A	2191	A	3.2
55	2z	525	PHE	3.2
34	2a	1020	C	3.2
55	2z	444	PRO	3.2
1	2A	217	A	3.2
34	2a	1013	A	3.2
55	2z	500	GLN	3.2
55	2z	429	ALA	3.2
1	2A	2126	C	3.2
3	1C	19	VAL	3.2
9	1J	99	SER	3.2
1	2A	2155	A	3.2
40	2g	156	TRP	3.2
55	2z	493	VAL	3.2
3	2C	61	THR	3.2
9	2J	97	ALA	3.2
55	1z	405	PRO	3.2
3	1C	27	ARG	3.2
34	1a	1005	G	3.2
40	2g	155	ARG	3.2
28	12	53	GLU	3.2
10	1K	89	HIS	3.2
34	1a	1009	C	3.1
34	2a	1023	U	3.1
34	2a	1017	G	3.1
3	2C	38	ASP	3.1
43	1j	10	GLY	3.1
1	1A	2198	C	3.1
1	1A	2203	G	3.1

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Mol	Chain	Res	Type	RSRZ
55	2z	417	THR	3.1
55	2z	454	MET	3.1
55	2z	455	GLY	3.1
3	1C	207	THR	3.1
40	1g	83	ALA	3.1
3	2C	50	ASP	3.1
3	2C	18	LYS	3.1
36	2c	81	GLY	3.1
34	1a	1509	A	3.1
55	1z	426	GLN	3.1
34	2a	1025	G	3.1
55	1z	472	VAL	3.1
1	1A	2149	C	3.1
10	2K	93	ARG	3.1
1	1A	2179	A	3.1
55	1z	599	PRO	3.1
55	1z	408	VAL	3.1
1	1A	2140	A	3.1
3	1C	28	LEU	3.1
40	2g	79	ARG	3.1
3	1C	70	LYS	3.0
43	2j	36	GLY	3.0
55	1z	531	GLY	3.0
1	2A	2162	G	3.0
40	2g	81	GLY	3.0
3	2C	70	LYS	3.0
3	1C	208	PHE	3.0
1	2A	2196	C	3.0
40	1g	78	ARG	3.0
3	1C	23	ASP	3.0
24	1Y	9	SER	3.0
55	2z	577	SER	3.0
3	2C	19	VAL	3.0
3	1C	3	HIS	3.0
28	22	68	ARG	3.0
35	2b	232	PRO	3.0
55	2z	540	PRO	3.0
1	1A	682	G	3.0
3	2C	160	ARG	3.0
46	2m	93	ARG	3.0
3	1C	177	LYS	3.0
43	2j	73	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
8	1H	2	SER	3.0
1	1A	1109	C	3.0
3	2C	64	LEU	3.0
34	1a	1020	C	3.0
1	1A	2155	A	3.0
55	2z	433	GLU	3.0
3	2C	23	ASP	2.9
1	1A	2185	C	2.9
9	2J	56	ASN	2.9
40	1g	79	ARG	2.9
1	2A	1136	G	2.9
1	1A	695	C	2.9
40	1g	82	GLY	2.9
55	1z	500	GLN	2.9
3	1C	209	LEU	2.9
1	2A	2170	G	2.9
55	2z	476	VAL	2.9
1	2A	2156	A	2.9
3	1C	52	ARG	2.9
3	2C	209	LEU	2.9
10	2K	116	ASN	2.9
55	2z	40	HIS	2.9
55	2z	430	ARG	2.9
40	2g	84	ASN	2.9
52	2s	59	PRO	2.9
28	12	57	GLU	2.9
42	2i	87	GLN	2.9
9	2J	129	PRO	2.9
1	1A	2126	C	2.9
1	1A	2158	C	2.9
1	2A	2158	C	2.9
1	2A	2182	C	2.9
1	2A	2177	G	2.9
10	2K	89	HIS	2.9
34	2a	976	G	2.9
34	1a	209	U	2.9
55	1z	404	VAL	2.9
3	1C	194	ARG	2.9
55	1z	467	LYS	2.9
3	1C	181	PRO	2.9
55	2z	582	PHE	2.9
9	1J	90	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
34	2a	1002	G	2.9
34	2a	1018	A	2.9
34	2a	982	G	2.8
34	2a	211	U	2.8
55	1z	496	LYS	2.8
10	1K	107	ILE	2.8
55	1z	495	GLY	2.8
3	1C	15	ASP	2.8
10	1K	85	GLU	2.8
55	2z	456	GLU	2.8
3	1C	186	ALA	2.8
1	1A	2156	A	2.8
28	22	49	PHE	2.8
34	1a	1015	G	2.8
1	1A	2160	C	2.8
3	1C	53	ARG	2.8
55	1z	465	ARG	2.8
55	1z	428	LEU	2.8
3	1C	17	ASN	2.8
55	1z	634	MET	2.8
55	1z	529	ILE	2.8
51	1r	23	LYS	2.8
55	1z	538	TYR	2.8
3	2C	12	GLU	2.8
51	2r	58	LEU	2.8
51	1r	24	ALA	2.8
3	1C	160	ARG	2.8
55	1z	575	VAL	2.8
10	1K	138	VAL	2.7
55	1z	507	TYR	2.7
1	2A	2125	G	2.7
1	2A	2152	G	2.7
55	1z	410	ASP	2.7
55	2z	600	VAL	2.7
25	2Z	2	SER	2.7
34	1a	1004	U	2.7
55	2z	571	SER	2.7
10	2K	82	ALA	2.7
47	1n	2	ALA	2.7
3	2C	217	THR	2.7
35	1b	136	VAL	2.7
55	1z	572	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
55	2z	533	VAL	2.7
55	2z	568	TYR	2.7
55	2z	681	LYS	2.7
34	1a	211	U	2.7
3	2C	15	ASP	2.7
55	2z	682	GLN	2.7
34	1a	707	U	2.7
1	2A	678	A	2.7
1	2A	2151	U	2.7
55	1z	539	ILE	2.7
9	2J	48	GLY	2.7
28	22	52	THR	2.7
1	2A	679	G	2.7
3	1C	45	ALA	2.7
3	2C	62	VAL	2.6
40	1g	80	VAL	2.6
55	2z	595	GLN	2.6
34	2a	1026	C	2.6
1	2A	2174	G	2.6
55	2z	578	SER	2.6
1	2A	1126	U	2.6
27	11	60	GLU	2.6
55	2z	543	GLN	2.6
55	2z	534	ILE	2.6
35	2b	226	ARG	2.6
55	1z	569	ASP	2.6
1	1A	2123	U	2.6
55	2z	511	LYS	2.6
1	2A	1137	C	2.6
55	2z	688	ILE	2.6
55	2z	440	VAL	2.6
9	2J	99	SER	2.6
55	1z	536	LYS	2.6
55	1z	506	GLN	2.6
53	1t	9	ASN	2.6
34	2a	983	A	2.6
1	1A	696	C	2.6
34	1a	985	C	2.6
10	1K	141	ALA	2.6
3	1C	48	GLY	2.6
43	1j	72	VAL	2.6
47	2n	25	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
55	2z	405	PRO	2.6
3	2C	13	LYS	2.5
55	1z	412	ALA	2.5
55	2z	630	GLN	2.5
3	1C	32	LEU	2.5
1	2A	2139	U	2.5
3	2C	5	LYS	2.5
1	2A	933	A	2.5
34	1a	1002	G	2.5
34	1a	1017	G	2.5
55	1z	423	LYS	2.5
1	1A	2122	G	2.5
9	2J	53	VAL	2.5
10	1K	79	ARG	2.5
9	1J	48	GLY	2.5
3	1C	38	ASP	2.5
56	2y	14	A	2.5
9	2J	98	LYS	2.5
3	1C	224	ILE	2.5
43	2j	38	ILE	2.5
34	1a	1239	U	2.5
1	2A	1107	G	2.5
34	1a	1012	G	2.5
55	2z	438	PHE	2.5
3	1C	211	SER	2.5
9	2J	57	THR	2.5
1	1A	2177	G	2.5
10	1K	121	GLU	2.5
55	1z	592	GLU	2.5
1	1A	2194	A	2.4
1	2A	2140	A	2.4
3	1C	185	LEU	2.4
43	2j	40	LEU	2.4
3	1C	203	GLY	2.4
34	1a	77	G	2.4
42	2i	70	LYS	2.4
3	2C	6	ARG	2.4
55	2z	653	PHE	2.4
55	1z	601	ILE	2.4
55	2z	639	ASN	2.4
3	1C	174	PRO	2.4
9	2J	132	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
34	2a	1009	C	2.4
34	2a	1014	G	2.4
55	1z	234	GLY	2.4
40	1g	153	HIS	2.4
1	2A	2147	A	2.4
34	2a	1005	G	2.4
3	1C	12	GLU	2.4
9	2J	54	ALA	2.4
3	2C	159	GLY	2.4
55	2z	526	VAL	2.4
28	22	57	GLU	2.4
40	2g	85	TYR	2.4
55	2z	442	THR	2.4
1	1A	681	G	2.4
1	1A	2146	G	2.4
34	1a	1016	G	2.4
34	1a	825	U	2.4
43	2j	39	PRO	2.4
3	2C	7	TYR	2.4
10	1K	140	GLY	2.4
52	2s	43	GLU	2.4
3	2C	224	ILE	2.4
52	2s	45	VAL	2.3
42	2i	7	THR	2.3
1	1A	933	A	2.3
3	2C	196	LEU	2.3
55	2z	529	ILE	2.3
55	2z	556	ILE	2.3
1	1A	2174	G	2.3
55	2z	86	GLY	2.3
1	2A	932	C	2.3
36	1c	193	TYR	2.3
52	2s	71	LEU	2.3
3	1C	206	GLY	2.3
10	2K	87	GLY	2.3
23	2X	156	LYS	2.3
21	2V	68	ARG	2.3
3	2C	20	TYR	2.3
3	1C	30	LYS	2.3
10	1K	81	ALA	2.3
46	2m	42	ALA	2.3
9	1J	105	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
35	1b	122	PHE	2.3
1	1A	2139	U	2.3
55	1z	505	GLY	2.3
55	2z	426	GLN	2.3
3	1C	213	TYR	2.3
55	1z	429	ALA	2.3
3	2C	225	ASN	2.3
3	1C	217	THR	2.3
17	1R	37	GLY	2.3
35	2b	227	GLY	2.3
55	1z	635	GLU	2.3
34	1a	208	C	2.3
28	12	59	PHE	2.3
55	1z	455	GLY	2.3
34	1a	1268	A	2.3
35	2b	122	PHE	2.3
55	1z	491	VAL	2.3
21	2V	67	GLY	2.3
10	1K	77	LEU	2.3
35	2b	101	MET	2.3
55	1z	443	HIS	2.3
10	1K	114	ASP	2.3
52	1s	48	THR	2.3
55	2z	90	PHE	2.3
7	1G	49	ASP	2.2
34	2a	1021	C	2.2
55	2z	404	VAL	2.2
1	2A	2183	G	2.2
35	2b	48	MET	2.2
10	2K	110	GLN	2.2
55	1z	585	ALA	2.2
55	1z	540	PRO	2.2
1	2A	2172	G	2.2
3	1C	31	GLU	2.2
34	1a	1022	C	2.2
55	1z	533	VAL	2.2
55	2z	428	LEU	2.2
55	1z	441	SER	2.2
9	1J	116	ILE	2.2
55	1z	231	TYR	2.2
55	1z	434	GLU	2.2
55	1z	475	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
10	2K	126	MET	2.2
10	2K	134	MET	2.2
1	1A	2209	C	2.2
34	1a	1006	C	2.2
34	1a	1007	C	2.2
52	2s	38	SER	2.2
55	1z	469	GLU	2.2
47	2n	2	ALA	2.2
1	1A	2196	C	2.2
1	2A	669	C	2.2
3	2C	32	LEU	2.2
35	1b	135	GLN	2.2
43	2j	72	VAL	2.2
55	2z	458	HIS	2.2
3	2C	42	GLU	2.2
40	1g	155	ARG	2.2
3	2C	40	THR	2.2
28	22	56	VAL	2.2
55	2z	235	GLU	2.2
1	1A	2171	U	2.2
9	2J	117	LEU	2.2
35	2b	136	VAL	2.2
3	1C	205	LYS	2.2
42	2i	62	TYR	2.2
55	1z	223	PHE	2.2
22	1W	1	MET	2.2
35	2b	231	GLU	2.2
42	2i	64	THR	2.2
51	1r	25	THR	2.2
52	1s	33	THR	2.2
52	1s	47	HIS	2.2
46	1m	87	TYR	2.1
34	1a	1026	C	2.1
3	1C	54	SER	2.1
34	1a	978	U	2.1
34	2a	86	U	2.1
3	1C	222	VAL	2.1
55	1z	542	VAL	2.1
55	1z	597	GLY	2.1
22	2W	91	GLU	2.1
55	1z	578	SER	2.1
55	2z	536	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
9	2J	90	ALA	2.1
10	2K	118	THR	2.1
1	2A	1103	G	2.1
55	1z	494	GLU	2.1
23	2X	159	PRO	2.1
1	2A	2129	C	2.1
55	2z	502	GLY	2.1
10	2K	115	LEU	2.1
42	2i	56	LEU	2.1
54	2u	5	ASP	2.1
35	2b	165	VAL	2.1
43	2j	74	ILE	2.1
55	1z	227	ILE	2.1
55	2z	685	GLU	2.1
1	2A	2173	G	2.1
34	2a	1238	A	2.1
43	2j	65	LEU	2.1
55	1z	490	PRO	2.1
55	2z	471	LYS	2.1
55	2z	523	PHE	2.1
40	2g	42	ILE	2.1
3	2C	53	ARG	2.1
3	2C	218	MET	2.1
55	2z	489	LYS	2.1
25	1Z	2	SER	2.1
55	2z	598	ASP	2.1
55	1z	600	VAL	2.1
36	2c	159	GLY	2.1
49	1p	57	ARG	2.1
55	2z	495	GLY	2.1
3	2C	45	ALA	2.1
10	2K	75	SER	2.1
55	1z	474	ALA	2.1
3	2C	205	LYS	2.1
35	2b	228	GLY	2.1
36	2c	158	GLY	2.1
1	2A	1105	U	2.1
34	2a	984	A	2.1
34	2a	1024	A	2.1
8	2H	96	ALA	2.1
55	1z	588	MET	2.1
3	2C	158	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	1C	221	SER	2.1
50	2q	8	GLY	2.1
55	2z	580	MET	2.1
10	2K	111	LYS	2.1
40	2g	52	GLU	2.1
3	1C	212	VAL	2.1
43	2j	32	ALA	2.1
18	1S	117	GLN	2.0
34	2a	1006	C	2.1
23	2X	132	ASN	2.0
3	2C	200	LYS	2.0
34	2a	1432	A	2.0
1	1A	2184	C	2.0
1	1A	2206	C	2.0
40	2g	112	PRO	2.0
55	1z	556	ILE	2.0
1	2A	681	G	2.0
55	1z	682	GLN	2.0
3	2C	8	ARG	2.0
55	2z	504	ARG	2.0
10	2K	112	MET	2.0
1	1A	679	G	2.0
10	1K	93	ARG	2.0
35	2b	133	LYS	2.0
3	1C	8	ARG	2.0
40	2g	4	ARG	2.0
1	2A	1132	G	2.0
33	27	37	GLY	2.0
55	1z	633	GLY	2.0
10	1K	116	ASN	2.0
34	1a	72	C	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	4SU	1w	8	20/21	0.95	0.14	-	43,61,72,73	0
57	5MC	1w	32	21/22	0.96	0.20	-	48,64,75,79	0
57	5MU	2w	54	21/22	0.94	0.17	-	61,67,79,97	0
57	5MC	2w	32	21/22	0.95	0.22	-	52,75,83,85	0
57	PSU	1w	55	20/21	0.92	0.16	-	53,63,72,82	0
57	PSU	2w	55	20/21	0.93	0.12	-	53,63,80,86	0
57	4SU	2w	8	20/21	0.94	0.16	-	51,68,81,83	0
57	5MU	1w	54	21/22	0.96	0.13	-	22,55,66,75	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3125	1/1	0.93	0.66	81.31	39,39,39,39	0
59	MG	1A	3029	1/1	0.95	0.61	74.93	40,40,40,40	0
59	MG	1A	3236	1/1	0.96	0.69	72.21	52,52,52,52	0
59	MG	1A	3658	1/1	0.95	0.60	56.93	38,38,38,38	0
59	MG	1A	3705	1/1	0.93	0.68	53.34	56,56,56,56	0
59	MG	2A	3239	1/1	0.95	0.67	47.01	50,50,50,50	0
59	MG	2A	3549	1/1	0.98	0.36	46.99	31,31,31,31	0
59	MG	1A	3032	1/1	0.97	0.68	39.72	46,46,46,46	0
59	MG	1A	3580	1/1	0.83	0.31	33.32	54,54,54,54	0
59	MG	1Y	103	1/1	0.90	0.84	31.88	73,73,73,73	0
59	MG	1A	3713	1/1	0.96	0.63	30.97	42,42,42,42	0
59	MG	2a	1693	1/1	0.97	0.37	30.61	51,51,51,51	0
59	MG	2A	3539	1/1	0.96	0.41	30.20	41,41,41,41	0
59	MG	1A	3018	1/1	0.80	0.45	28.59	43,43,43,43	0
59	MG	1A	3525	1/1	0.97	0.57	26.87	61,61,61,61	0
59	MG	11	8001	1/1	0.95	0.67	26.84	44,44,44,44	0
59	MG	2a	1669	1/1	0.94	0.59	26.42	55,55,55,55	0
59	MG	1S	3003	1/1	0.96	0.58	25.49	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3211	1/1	0.88	0.29	25.01	48,48,48,48	0
59	MG	2A	3031	1/1	0.91	0.43	23.90	52,52,52,52	0
59	MG	2A	3252	1/1	0.71	0.23	23.70	55,55,55,55	0
59	MG	1A	3215	1/1	0.85	0.43	22.92	37,37,37,37	0
59	MG	1A	3119	1/1	0.95	0.45	22.64	41,41,41,41	0
59	MG	2A	3185	1/1	0.87	0.35	21.94	33,33,33,33	0
59	MG	2a	1684	1/1	0.96	0.45	20.88	55,55,55,55	0
59	MG	1A	3440	1/1	0.93	0.32	20.09	50,50,50,50	0
59	MG	1A	3033	1/1	0.95	0.43	20.03	49,49,49,49	0
59	MG	1D	301	1/1	0.89	0.39	19.96	32,32,32,32	0
59	MG	2A	3199	1/1	0.95	0.41	19.68	41,41,41,41	0
59	MG	1A	3761	1/1	0.97	0.35	19.65	27,27,27,27	0
59	MG	2A	3077	1/1	0.98	0.32	19.25	40,40,40,40	0
59	MG	1A	3202	1/1	0.96	0.37	17.91	38,38,38,38	0
59	MG	1D	302	1/1	0.93	0.43	17.66	39,39,39,39	0
59	MG	1S	3001	1/1	0.93	0.44	17.38	40,40,40,40	0
59	MG	1A	3066	1/1	0.97	0.63	17.35	43,43,43,43	0
59	MG	1A	3175	1/1	0.97	0.35	16.90	46,46,46,46	0
59	MG	2A	3198	1/1	0.98	0.40	16.81	20,20,20,20	0
59	MG	1A	3085	1/1	0.96	0.44	16.53	55,55,55,55	0
59	MG	1A	3210	1/1	0.96	0.33	16.09	38,38,38,38	0
59	MG	2A	3020	1/1	0.97	0.33	15.84	37,37,37,37	0
59	MG	1S	3002	1/1	0.94	0.55	15.81	32,32,32,32	0
59	MG	1A	3088	1/1	0.97	0.37	15.76	39,39,39,39	0
59	MG	1A	3181	1/1	0.92	0.27	14.83	52,52,52,52	0
59	MG	13	104	1/1	0.89	0.42	14.74	48,48,48,48	0
59	MG	2B	208	1/1	0.94	0.24	14.73	58,58,58,58	0
59	MG	1N	202	1/1	0.95	0.41	14.72	29,29,29,29	0
59	MG	2A	3236	1/1	0.81	0.38	14.69	48,48,48,48	0
59	MG	1A	3208	1/1	0.98	0.32	14.65	33,33,33,33	0
59	MG	2n	502	1/1	0.90	0.65	14.32	76,76,76,76	0
59	MG	2A	3080	1/1	0.92	0.34	14.27	36,36,36,36	0
59	MG	1a	1657	1/1	0.89	0.28	14.24	48,48,48,48	0
59	MG	2A	3369	1/1	0.95	0.30	14.14	29,29,29,29	0
59	MG	2A	3559	1/1	0.99	0.33	13.89	48,48,48,48	0
59	MG	1F	302	1/1	0.93	0.49	13.81	40,40,40,40	0
59	MG	2A	3064	1/1	0.95	0.30	13.80	28,28,28,28	0
59	MG	2A	3161	1/1	0.92	0.30	13.56	47,47,47,47	0
59	MG	2A	3117	1/1	0.98	0.30	13.37	35,35,35,35	0
59	MG	2A	3128	1/1	0.95	0.25	13.33	29,29,29,29	0
59	MG	1A	3178	1/1	0.94	0.31	13.32	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3159	1/1	0.94	0.34	13.16	53,53,53,53	0
60	ZN	13	103	1/1	0.48	0.52	12.76	278,278,278,278	0
59	MG	1A	3576	1/1	0.65	0.30	12.64	51,51,51,51	0
59	MG	1A	3115	1/1	0.83	0.29	12.55	36,36,36,36	0
59	MG	2A	3186	1/1	0.83	0.22	12.55	38,38,38,38	0
59	MG	2E	303	1/1	0.88	0.28	12.30	31,31,31,31	0
59	MG	1A	3028	1/1	0.95	0.57	12.12	40,40,40,40	0
59	MG	1A	3452	1/1	0.91	0.27	12.04	46,46,46,46	0
59	MG	2A	3029	1/1	0.95	0.25	11.66	24,24,24,24	0
59	MG	2A	3326	1/1	0.72	0.27	11.65	49,49,49,49	0
59	MG	1A	3105	1/1	0.99	0.22	11.62	22,22,22,22	0
59	MG	1A	3040	1/1	0.80	0.31	11.44	31,31,31,31	0
59	MG	2A	3202	1/1	0.92	0.24	11.43	35,35,35,35	0
59	MG	2a	1628	1/1	0.93	0.32	11.36	62,62,62,62	0
59	MG	1A	3078	1/1	0.94	0.31	11.31	45,45,45,45	0
59	MG	1a	1704	1/1	0.93	0.39	11.20	54,54,54,54	0
59	MG	1A	3764	1/1	0.81	0.29	10.88	33,33,33,33	0
59	MG	2A	3258	1/1	0.89	0.39	10.87	55,55,55,55	0
59	MG	2A	3542	1/1	0.98	0.32	10.86	36,36,36,36	0
59	MG	2A	3322	1/1	0.94	0.24	10.77	28,28,28,28	0
59	MG	1a	1748	1/1	0.90	0.44	10.76	82,82,82,82	0
59	MG	2A	3159	1/1	0.94	0.43	10.71	49,49,49,49	0
59	MG	1A	3144	1/1	0.98	0.32	10.68	44,44,44,44	0
59	MG	2A	3065	1/1	0.97	0.27	10.65	51,51,51,51	0
59	MG	1a	1720	1/1	0.82	0.32	10.45	54,54,54,54	0
59	MG	1A	3226	1/1	0.74	0.28	10.44	50,50,50,50	0
59	MG	2a	1742	1/1	0.83	0.34	10.31	82,82,82,82	0
59	MG	2B	207	1/1	0.93	0.26	10.15	40,40,40,40	0
59	MG	2A	3157	1/1	0.96	0.36	10.06	35,35,35,35	0
59	MG	1A	3023	1/1	0.74	0.81	9.91	37,37,37,37	0
59	MG	1a	1779	1/1	0.94	0.41	9.89	54,54,54,54	0
59	MG	2A	3092	1/1	0.89	0.20	9.84	40,40,40,40	0
59	MG	1A	3759	1/1	0.87	0.41	9.76	46,46,46,46	0
59	MG	2A	3162	1/1	0.96	0.24	9.76	30,30,30,30	0
59	MG	1a	1679	1/1	0.93	0.42	9.57	60,60,60,60	0
59	MG	2A	3411	1/1	0.96	0.26	9.48	43,43,43,43	0
59	MG	1A	3760	1/1	0.81	0.39	9.42	44,44,44,44	0
59	MG	2A	3216	1/1	0.97	0.25	9.29	42,42,42,42	0
59	MG	1A	3780	1/1	0.98	0.47	9.22	31,31,31,31	0
59	MG	1A	3517	1/1	0.96	0.26	9.20	27,27,27,27	0
59	MG	2A	3001	1/1	0.94	0.28	9.11	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3098	1/1	0.87	0.28	8.96	49,49,49,49	0
59	MG	2a	1744	1/1	0.85	0.28	8.95	65,65,65,65	0
59	MG	1a	1695	1/1	0.82	0.28	8.91	49,49,49,49	0
59	MG	2A	3393	1/1	0.81	0.23	8.91	45,45,45,45	0
59	MG	2A	3548	1/1	0.98	0.24	8.87	32,32,32,32	0
59	MG	1A	3273	1/1	0.97	0.27	8.79	37,37,37,37	0
59	MG	2A	3118	1/1	0.98	0.27	8.61	35,35,35,35	0
59	MG	2A	3518	1/1	0.98	0.26	8.61	40,40,40,40	0
59	MG	2A	3528	1/1	0.91	0.25	8.59	30,30,30,30	0
59	MG	2A	3143	1/1	0.96	0.31	8.40	47,47,47,47	0
59	MG	2A	3269	1/1	0.90	0.28	8.31	48,48,48,48	0
59	MG	1A	3048	1/1	0.91	0.27	8.24	32,32,32,32	0
59	MG	1A	3071	1/1	0.98	0.30	8.15	31,31,31,31	0
59	MG	2A	3366	1/1	0.96	0.23	8.07	40,40,40,40	0
59	MG	1A	3729	1/1	0.85	0.32	8.04	54,54,54,54	0
59	MG	1a	1672	1/1	0.95	0.30	8.03	43,43,43,43	0
59	MG	1A	3774	1/1	0.96	0.40	7.94	49,49,49,49	0
59	MG	2A	3013	1/1	0.88	0.22	7.94	55,55,55,55	0
59	MG	1a	1616	1/1	0.84	0.38	7.73	55,55,55,55	0
59	MG	2A	3110	1/1	0.88	0.24	7.63	38,38,38,38	0
59	MG	2A	3201	1/1	0.95	0.35	7.45	38,38,38,38	0
59	MG	1A	3433	1/1	0.88	0.25	7.41	34,34,34,34	0
59	MG	2A	3403	1/1	0.86	0.20	7.40	28,28,28,28	0
59	MG	1A	3130	1/1	0.92	0.25	7.31	34,34,34,34	0
59	MG	2A	3354	1/1	0.85	0.23	7.25	33,33,33,33	0
59	MG	2A	3267	1/1	0.99	0.22	7.23	23,23,23,23	0
59	MG	2a	1664	1/1	0.91	0.32	7.17	59,59,59,59	0
59	MG	2A	3026	1/1	0.92	0.21	7.13	44,44,44,44	0
59	MG	2a	1653	1/1	0.90	0.21	7.11	43,43,43,43	0
59	MG	1A	3778	1/1	0.98	0.31	7.05	33,33,33,33	0
59	MG	2A	3335	1/1	0.99	0.22	7.04	25,25,25,25	0
59	MG	2A	3526	1/1	0.96	0.27	6.99	56,56,56,56	0
59	MG	2A	3619	1/1	0.95	0.23	6.97	43,43,43,43	0
59	MG	2A	3008	1/1	0.97	0.20	6.97	33,33,33,33	0
59	MG	1A	3552	1/1	0.90	0.24	6.95	47,47,47,47	0
59	MG	1F	301	1/1	0.98	0.25	6.78	27,27,27,27	0
59	MG	1a	1691	1/1	0.93	0.30	6.76	54,54,54,54	0
59	MG	1A	3271	1/1	0.93	0.25	6.66	40,40,40,40	0
59	MG	2A	3423	1/1	0.96	0.24	6.60	34,34,34,34	0
59	MG	1A	3382	1/1	0.94	0.22	6.60	46,46,46,46	0
59	MG	1A	3090	1/1	0.94	0.23	6.58	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3127	1/1	0.84	0.28	6.57	31,31,31,31	0
59	MG	2A	3130	1/1	0.93	0.21	6.48	34,34,34,34	0
59	MG	1a	1741	1/1	0.84	0.26	6.28	71,71,71,71	0
59	MG	2A	3608	1/1	0.95	0.22	6.18	35,35,35,35	0
59	MG	2A	3420	1/1	0.94	0.19	6.01	36,36,36,36	0
59	MG	1A	3731	1/1	0.97	0.24	5.99	16,16,16,16	0
59	MG	1A	3217	1/1	0.90	0.24	5.91	45,45,45,45	0
59	MG	2A	3251	1/1	0.92	0.26	5.87	28,28,28,28	0
59	MG	2S	201	1/1	0.94	0.25	5.86	52,52,52,52	0
59	MG	2A	3396	1/1	0.87	0.22	5.85	24,24,24,24	0
59	MG	1A	3742	1/1	0.94	0.29	5.82	47,47,47,47	0
59	MG	1A	3030	1/1	0.94	0.22	5.66	50,50,50,50	0
59	MG	1a	1740	1/1	0.95	0.33	5.65	39,39,39,39	0
59	MG	1A	3355	1/1	0.95	0.21	5.58	27,27,27,27	0
59	MG	1U	203	1/1	0.94	0.39	5.44	39,39,39,39	0
59	MG	2a	1711	1/1	0.81	0.25	5.39	76,76,76,76	0
59	MG	1A	3291	1/1	0.98	0.20	5.35	60,60,60,60	0
59	MG	2A	3341	1/1	0.96	0.26	5.33	24,24,24,24	0
59	MG	1A	3227	1/1	0.94	0.32	5.29	45,45,45,45	0
59	MG	1A	3276	1/1	0.96	0.23	5.16	18,18,18,18	0
59	MG	2A	3103	1/1	0.93	0.23	5.15	46,46,46,46	0
59	MG	2A	3096	1/1	0.91	0.25	5.09	55,55,55,55	0
59	MG	1A	3043	1/1	0.97	0.23	5.06	23,23,23,23	0
59	MG	1A	3462	1/1	0.99	0.26	5.06	42,42,42,42	0
59	MG	2A	3337	1/1	0.85	0.20	4.95	41,41,41,41	0
59	MG	2A	3616	1/1	0.97	0.36	4.94	51,51,51,51	0
59	MG	1A	3730	1/1	0.94	0.27	4.87	25,25,25,25	0
59	MG	2A	3024	1/1	0.91	0.22	4.86	45,45,45,45	0
59	MG	2A	3419	1/1	0.83	0.20	4.80	30,30,30,30	0
59	MG	2A	3214	1/1	0.97	0.21	4.75	41,41,41,41	0
59	MG	2A	3558	1/1	0.97	0.29	4.71	30,30,30,30	0
59	MG	1A	3190	1/1	0.94	0.21	4.71	28,28,28,28	0
59	MG	2w	3004	1/1	0.96	0.28	4.64	52,52,52,52	0
59	MG	1A	3350	1/1	0.95	0.25	4.60	29,29,29,29	0
59	MG	1a	1784	1/1	0.98	0.23	4.48	37,37,37,37	0
59	MG	1O	3001	1/1	0.97	0.26	4.45	35,35,35,35	0
59	MG	1A	3387	1/1	0.96	0.23	4.40	17,17,17,17	0
59	MG	2a	1649	1/1	0.81	0.22	4.37	69,69,69,69	0
59	MG	2a	1729	1/1	0.96	0.21	4.35	54,54,54,54	0
59	MG	1A	3349	1/1	0.91	0.24	4.25	18,18,18,18	0
59	MG	2A	3300	1/1	0.83	0.19	4.19	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3348	1/1	0.97	0.19	4.13	28,28,28,28	0
59	MG	16	102	1/1	0.94	0.24	4.05	47,47,47,47	0
59	MG	2A	3015	1/1	0.97	0.17	4.03	36,36,36,36	0
59	MG	1A	3451	1/1	0.98	0.27	3.99	51,51,51,51	0
59	MG	2A	3086	1/1	0.97	0.19	3.98	25,25,25,25	0
59	MG	2D	303	1/1	0.95	0.23	3.96	24,24,24,24	0
59	MG	2A	3187	1/1	0.89	0.21	3.93	55,55,55,55	0
59	MG	1A	3150	1/1	0.96	0.21	3.93	31,31,31,31	0
59	MG	2A	3524	1/1	0.93	0.22	3.85	78,78,78,78	0
59	MG	1A	3779	1/1	0.88	0.40	3.82	39,39,39,39	0
59	MG	1A	3093	1/1	0.86	0.24	3.79	41,41,41,41	0
59	MG	1A	3669	1/1	0.89	0.25	3.79	52,52,52,52	0
59	MG	1A	3499	1/1	0.97	0.21	3.78	39,39,39,39	0
59	MG	1D	304	1/1	0.87	0.34	3.77	40,40,40,40	0
59	MG	1a	1793	1/1	0.94	0.24	3.74	53,53,53,53	0
59	MG	2A	3246	1/1	0.86	0.22	3.70	47,47,47,47	0
59	MG	2A	3188	1/1	0.88	0.21	3.70	41,41,41,41	0
59	MG	2A	3192	1/1	0.88	0.20	3.68	47,47,47,47	0
59	MG	2A	3465	1/1	0.86	0.17	3.67	22,22,22,22	0
59	MG	2a	1690	1/1	0.90	0.22	3.65	63,63,63,63	0
59	MG	1a	1803	1/1	0.97	0.25	3.65	53,53,53,53	0
59	MG	2A	3330	1/1	0.75	0.19	3.63	28,28,28,28	0
59	MG	2A	3331	1/1	0.86	0.20	3.59	39,39,39,39	0
59	MG	1S	3004	1/1	0.97	0.27	3.54	36,36,36,36	0
59	MG	2A	3327	1/1	0.95	0.22	3.48	59,59,59,59	0
59	MG	1A	3699	1/1	0.96	0.22	3.46	51,51,51,51	0
59	MG	1A	3456	1/1	0.94	0.21	3.41	32,32,32,32	0
59	MG	2a	1635	1/1	0.91	0.20	3.39	40,40,40,40	0
59	MG	2Y	8001	1/1	0.95	0.18	3.39	59,59,59,59	0
59	MG	2A	3390	1/1	0.98	0.25	3.35	36,36,36,36	0
59	MG	2A	3507	1/1	0.83	0.20	3.30	39,39,39,39	0
59	MG	1A	3503	1/1	0.97	0.23	3.27	19,19,19,19	0
59	MG	2A	3076	1/1	0.83	0.18	3.23	45,45,45,45	0
59	MG	2a	1655	1/1	0.91	0.23	3.22	63,63,63,63	0
59	MG	1A	3037	1/1	0.93	0.20	3.20	41,41,41,41	0
59	MG	2A	3333	1/1	0.97	0.18	3.16	35,35,35,35	0
59	MG	2A	3129	1/1	0.98	0.21	3.08	39,39,39,39	0
59	MG	1a	1689	1/1	0.92	0.21	3.05	22,22,22,22	0
59	MG	2A	3290	1/1	0.95	0.24	3.03	25,25,25,25	0
59	MG	1A	3435	1/1	0.89	0.21	3.03	45,45,45,45	0
59	MG	1a	1630	1/1	0.69	0.23	3.02	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3212	1/1	0.85	0.19	3.01	40,40,40,40	0
59	MG	1A	3139	1/1	0.83	0.15	3.01	67,67,67,67	0
59	MG	2A	3594	1/1	0.92	0.14	3.01	56,56,56,56	0
59	MG	2A	3304	1/1	0.94	0.17	2.97	38,38,38,38	0
59	MG	1A	3204	1/1	0.90	0.26	2.95	42,42,42,42	0
59	MG	1A	3492	1/1	0.94	0.21	2.92	48,48,48,48	0
59	MG	2A	3455	1/1	0.95	0.16	2.88	47,47,47,47	0
59	MG	1A	3195	1/1	0.95	0.24	2.87	21,21,21,21	0
59	MG	1A	3537	1/1	0.96	0.20	2.84	46,46,46,46	0
59	MG	1A	3020	1/1	0.99	0.19	2.81	25,25,25,25	0
59	MG	1a	1760	1/1	0.87	0.17	2.81	65,65,65,65	0
59	MG	1a	1638	1/1	0.94	0.21	2.80	46,46,46,46	0
59	MG	2A	3592	1/1	0.84	0.17	2.78	63,63,63,63	0
59	MG	1a	1739	1/1	0.85	0.20	2.78	44,44,44,44	0
59	MG	1a	1798	1/1	0.87	0.34	2.75	55,55,55,55	0
59	MG	2t	3001	1/1	0.96	0.35	2.74	45,45,45,45	0
59	MG	2A	3177	1/1	0.95	0.22	2.67	15,15,15,15	0
59	MG	1A	3478	1/1	0.94	0.21	2.65	28,28,28,28	0
59	MG	1A	3468	1/1	0.90	0.20	2.62	37,37,37,37	0
59	MG	2A	3223	1/1	0.97	0.17	2.62	39,39,39,39	0
59	MG	2A	3315	1/1	0.97	0.16	2.62	38,38,38,38	0
59	MG	1a	1627	1/1	0.94	0.20	2.61	50,50,50,50	0
59	MG	1A	3260	1/1	0.91	0.17	2.58	48,48,48,48	0
59	MG	2A	3093	1/1	0.93	0.17	2.55	28,28,28,28	0
59	MG	1A	3148	1/1	0.94	0.19	2.55	30,30,30,30	0
59	MG	1A	3389	1/1	0.83	0.20	2.54	37,37,37,37	0
59	MG	2A	3394	1/1	0.95	0.18	2.49	34,34,34,34	0
59	MG	1A	3739	1/1	0.92	0.22	2.43	50,50,50,50	0
59	MG	1a	1767	1/1	0.93	0.22	2.38	60,60,60,60	0
59	MG	2A	3073	1/1	0.94	0.18	2.36	28,28,28,28	0
59	MG	1A	3337	1/1	0.94	0.22	2.36	30,30,30,30	0
59	MG	15	101	1/1	0.93	0.21	2.35	54,54,54,54	0
59	MG	2a	1738	1/1	0.93	0.26	2.33	52,52,52,52	0
59	MG	2A	3207	1/1	0.91	0.24	2.33	51,51,51,51	0
59	MG	1A	3012	1/1	0.96	0.19	2.28	40,40,40,40	0
59	MG	1A	3411	1/1	0.98	0.18	2.19	21,21,21,21	0
59	MG	1A	3716	1/1	0.89	0.16	2.17	56,56,56,56	0
59	MG	1A	3126	1/1	0.96	0.18	2.16	34,34,34,34	0
59	MG	1A	3019	1/1	0.86	0.24	2.13	50,50,50,50	0
59	MG	1t	3001	1/1	0.83	0.32	2.08	54,54,54,54	0
59	MG	1A	3434	1/1	0.93	0.23	2.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3197	1/1	0.98	0.21	2.03	41,41,41,41	0
59	MG	1A	3124	1/1	0.91	0.22	1.99	46,46,46,46	0
59	MG	1A	3177	1/1	0.97	0.19	1.99	21,21,21,21	0
59	MG	1a	1747	1/1	0.97	0.15	1.98	47,47,47,47	0
59	MG	1A	3295	1/1	0.95	0.21	1.94	36,36,36,36	0
59	MG	1a	1612	1/1	0.83	0.18	1.92	41,41,41,41	0
59	MG	2A	3412	1/1	0.95	0.16	1.91	39,39,39,39	0
59	MG	1A	3415	1/1	0.97	0.20	1.90	42,42,42,42	0
59	MG	1a	1731	1/1	0.95	0.20	1.83	47,47,47,47	0
59	MG	1A	3545	1/1	0.98	0.20	1.83	46,46,46,46	0
59	MG	2A	3183	1/1	0.97	0.18	1.82	45,45,45,45	0
59	MG	1a	1665	1/1	0.94	0.20	1.81	41,41,41,41	0
59	MG	1A	3244	1/1	0.95	0.17	1.78	41,41,41,41	0
59	MG	1B	207	1/1	0.96	0.18	1.71	50,50,50,50	0
59	MG	1A	3453	1/1	0.92	0.19	1.63	36,36,36,36	0
59	MG	1A	3520	1/1	0.92	0.20	1.61	70,70,70,70	0
59	MG	2A	3595	1/1	0.89	0.17	1.57	51,51,51,51	0
59	MG	1A	3267	1/1	0.98	0.19	1.57	45,45,45,45	0
59	MG	1A	3354	1/1	0.96	0.18	1.56	31,31,31,31	0
59	MG	2B	202	1/1	0.89	0.19	1.52	56,56,56,56	0
59	MG	1A	3174	1/1	0.88	0.18	1.47	38,38,38,38	0
59	MG	2A	3492	1/1	0.91	0.29	1.45	48,48,48,48	0
59	MG	1A	3756	1/1	0.88	0.22	1.43	30,30,30,30	0
59	MG	1A	3463	1/1	0.92	0.20	1.43	26,26,26,26	0
59	MG	2A	3329	1/1	0.95	0.17	1.41	46,46,46,46	0
59	MG	2A	3147	1/1	0.98	0.23	1.41	33,33,33,33	0
59	MG	2A	3277	1/1	0.87	0.14	1.41	69,69,69,69	0
59	MG	2A	3174	1/1	0.87	0.18	1.40	34,34,34,34	0
59	MG	1a	1733	1/1	0.94	0.16	1.39	61,61,61,61	0
59	MG	1A	3201	1/1	0.95	0.20	1.38	36,36,36,36	0
59	MG	2A	3618	1/1	0.88	0.23	1.37	43,43,43,43	0
59	MG	2A	3261	1/1	0.95	0.17	1.33	27,27,27,27	0
59	MG	1a	1659	1/1	0.87	0.22	1.30	63,63,63,63	0
59	MG	1A	3173	1/1	0.96	0.22	1.25	48,48,48,48	0
59	MG	2A	3151	1/1	0.97	0.17	1.25	29,29,29,29	0
59	MG	1A	3512	1/1	0.96	0.18	1.24	19,19,19,19	0
59	MG	2a	1615	1/1	0.95	0.18	1.23	43,43,43,43	0
59	MG	2A	3288	1/1	0.97	0.20	1.22	34,34,34,34	0
59	MG	1a	1650	1/1	0.92	0.16	1.17	48,48,48,48	0
59	MG	1A	3469	1/1	0.98	0.21	1.14	36,36,36,36	0
59	MG	2A	3485	1/1	0.86	0.15	1.13	38,38,38,38	0
59	MG	2A	3055	1/1	0.84	0.17	1.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3353	1/1	0.91	0.20	1.12	26,26,26,26	0
59	MG	1A	3135	1/1	0.95	0.19	1.07	36,36,36,36	0
59	MG	2a	1698	1/1	0.94	0.18	1.02	29,29,29,29	0
59	MG	1a	1700	1/1	0.96	0.16	1.02	50,50,50,50	0
60	ZN	17	102	1/1	0.84	0.32	0.97	120,120,120,120	0
59	MG	1A	3199	1/1	0.90	0.17	0.90	34,34,34,34	0
59	MG	1A	3146	1/1	0.84	0.17	0.86	56,56,56,56	0
59	MG	2E	302	1/1	0.96	0.14	0.86	27,27,27,27	0
59	MG	1A	3502	1/1	0.93	0.19	0.75	20,20,20,20	0
59	MG	1A	3151	1/1	0.95	0.18	0.73	36,36,36,36	0
59	MG	1A	3473	1/1	0.98	0.18	0.72	46,46,46,46	0
59	MG	1A	3021	1/1	0.97	0.18	0.70	40,40,40,40	0
59	MG	2A	3613	1/1	0.97	0.18	0.69	21,21,21,21	0
59	MG	1A	3306	1/1	0.91	0.21	0.67	23,23,23,23	0
59	MG	1A	3188	1/1	0.94	0.28	0.65	56,56,56,56	0
59	MG	1a	1732	1/1	0.94	0.17	0.62	54,54,54,54	0
59	MG	1A	3718	1/1	0.94	0.22	0.57	53,53,53,53	0
59	MG	2A	3530	1/1	0.92	0.17	0.54	40,40,40,40	0
59	MG	2A	3302	1/1	0.97	0.14	0.52	35,35,35,35	0
59	MG	1A	3609	1/1	0.95	0.18	0.46	26,26,26,26	0
59	MG	2A	3615	1/1	0.96	0.21	0.45	53,53,53,53	0
59	MG	1A	3361	1/1	0.94	0.18	0.44	30,30,30,30	0
59	MG	2a	1604	1/1	0.86	0.15	0.41	51,51,51,51	0
59	MG	1a	1608	1/1	0.83	0.19	0.40	65,65,65,65	0
59	MG	2a	1769	1/1	0.95	0.22	0.40	54,54,54,54	0
59	MG	1A	3479	1/1	0.90	0.17	0.39	50,50,50,50	0
59	MG	1A	3039	1/1	0.94	0.18	0.37	36,36,36,36	0
59	MG	2A	3508	1/1	0.98	0.17	0.36	32,32,32,32	0
59	MG	1A	3368	1/1	0.93	0.18	0.34	26,26,26,26	0
59	MG	1A	3369	1/1	0.93	0.18	0.28	53,53,53,53	0
59	MG	2A	3498	1/1	0.95	0.16	0.27	36,36,36,36	0
59	MG	1B	209	1/1	0.91	0.15	0.18	45,45,45,45	0
59	MG	2A	3007	1/1	0.89	0.14	0.18	28,28,28,28	0
59	MG	2A	3444	1/1	0.93	0.15	0.17	45,45,45,45	0
59	MG	1A	3007	1/1	0.96	0.16	0.16	18,18,18,18	0
59	MG	2A	3398	1/1	0.93	0.16	0.15	32,32,32,32	0
59	MG	2A	3493	1/1	0.98	0.15	0.14	23,23,23,23	0
59	MG	1A	3675	1/1	0.94	0.23	0.13	32,32,32,32	0
59	MG	2a	1715	1/1	0.97	0.14	0.13	68,68,68,68	0
59	MG	1A	3471	1/1	0.96	0.17	0.11	23,23,23,23	0
59	MG	1a	1684	1/1	0.79	0.17	0.09	78,78,78,78	0
59	MG	2B	204	1/1	0.95	0.17	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3472	1/1	0.96	0.16	0.06	47,47,47,47	0
59	MG	2a	1704	1/1	0.92	0.16	0.05	39,39,39,39	0
59	MG	2A	3011	1/1	0.94	0.15	0.04	40,40,40,40	0
59	MG	1A	3318	1/1	0.97	0.16	0.04	22,22,22,22	0
59	MG	1a	1617	1/1	0.93	0.18	0.02	72,72,72,72	0
59	MG	1A	3386	1/1	0.91	0.20	0.01	32,32,32,32	0
59	MG	1A	3163	1/1	0.97	0.15	0.00	43,43,43,43	0
59	MG	1b	3001	1/1	0.84	0.16	-0.00	70,70,70,70	0
59	MG	1A	3229	1/1	0.94	0.17	-0.02	51,51,51,51	0
59	MG	2A	3468	1/1	0.96	0.15	-0.04	55,55,55,55	0
59	MG	1E	302	1/1	0.97	0.17	-0.07	51,51,51,51	0
59	MG	1A	3156	1/1	0.94	0.15	-0.10	54,54,54,54	0
59	MG	1A	3775	1/1	0.91	0.17	-0.11	41,41,41,41	0
59	MG	1A	3518	1/1	0.92	0.17	-0.11	59,59,59,59	0
59	MG	1A	3004	1/1	0.90	0.17	-0.12	30,30,30,30	0
59	MG	1Y	105	1/1	0.97	0.17	-0.15	57,57,57,57	0
59	MG	1A	3300	1/1	0.92	0.17	-0.15	47,47,47,47	0
59	MG	2A	3042	1/1	0.89	0.12	-0.17	39,39,39,39	0
59	MG	1A	3358	1/1	0.96	0.16	-0.18	30,30,30,30	0
59	MG	1A	3539	1/1	0.97	0.16	-0.21	31,31,31,31	0
60	ZN	23	501	1/1	0.97	0.15	-0.22	85,85,85,85	0
59	MG	1a	1769	1/1	0.94	0.19	-0.22	68,68,68,68	0
59	MG	17	101	1/1	0.97	0.18	-0.23	45,45,45,45	0
59	MG	2A	3215	1/1	0.89	0.13	-0.23	51,51,51,51	0
60	ZN	24	501	1/1	0.96	0.18	-0.24	72,72,72,72	0
59	MG	1A	3164	1/1	0.92	0.15	-0.26	46,46,46,46	0
59	MG	1A	3620	1/1	0.90	0.17	-0.29	26,26,26,26	0
59	MG	1A	3343	1/1	0.99	0.16	-0.34	46,46,46,46	0
59	MG	2a	1748	1/1	0.97	0.13	-0.34	39,39,39,39	0
60	ZN	1W	202	1/1	0.99	0.12	-0.34	68,68,68,68	0
59	MG	1a	1802	1/1	0.90	0.16	-0.35	45,45,45,45	0
59	MG	2A	3134	1/1	0.92	0.12	-0.39	36,36,36,36	0
59	MG	1A	3364	1/1	0.96	0.17	-0.44	27,27,27,27	0
59	MG	2A	3410	1/1	0.91	0.15	-0.46	27,27,27,27	0
59	MG	2A	3332	1/1	0.94	0.14	-0.48	25,25,25,25	0
59	MG	1A	3248	1/1	0.95	0.17	-0.48	36,36,36,36	0
59	MG	1B	204	1/1	0.86	0.15	-0.49	51,51,51,51	0
59	MG	1a	1671	1/1	0.92	0.14	-0.49	53,53,53,53	0
60	ZN	14	102	1/1	0.99	0.15	-0.50	48,48,48,48	0
59	MG	2A	3037	1/1	0.93	0.15	-0.51	37,37,37,37	0
59	MG	1a	1677	1/1	0.97	0.17	-0.56	36,36,36,36	0
59	MG	1A	3772	1/1	0.97	0.17	-0.57	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3318	1/1	0.91	0.14	-0.58	42,42,42,42	0
59	MG	2A	3233	1/1	0.94	0.13	-0.60	41,41,41,41	0
59	MG	1A	3423	1/1	0.98	0.17	-0.62	17,17,17,17	0
59	MG	1A	3741	1/1	0.91	0.16	-0.63	50,50,50,50	0
59	MG	2A	3292	1/1	0.87	0.14	-0.63	46,46,46,46	0
59	MG	2a	1679	1/1	0.91	0.13	-0.66	50,50,50,50	0
59	MG	2A	3150	1/1	0.93	0.13	-0.68	37,37,37,37	0
59	MG	1Y	101	1/1	0.89	0.16	-0.70	51,51,51,51	0
59	MG	2G	3001	1/1	0.92	0.17	-0.72	34,34,34,34	0
59	MG	1A	3356	1/1	0.97	0.17	-0.72	26,26,26,26	0
59	MG	1a	1628	1/1	0.96	0.16	-0.75	53,53,53,53	0
59	MG	2A	3021	1/1	0.99	0.13	-0.75	25,25,25,25	0
59	MG	1A	3683	1/1	0.94	0.16	-0.82	62,62,62,62	0
59	MG	1A	3327	1/1	0.97	0.14	-0.84	36,36,36,36	0
59	MG	2A	3365	1/1	0.88	0.13	-0.87	22,22,22,22	0
59	MG	2a	1642	1/1	0.95	0.15	-0.87	29,29,29,29	0
59	MG	1a	1727	1/1	0.93	0.15	-0.87	39,39,39,39	0
59	MG	2A	3422	1/1	0.83	0.15	-0.87	37,37,37,37	0
59	MG	2A	3614	1/1	0.95	0.13	-0.89	53,53,53,53	0
59	MG	1A	3691	1/1	0.82	0.15	-0.92	53,53,53,53	0
59	MG	1A	3773	1/1	0.95	0.14	-0.95	25,25,25,25	0
59	MG	1A	3450	1/1	0.94	0.14	-0.96	53,53,53,53	0
59	MG	2A	3132	1/1	0.90	0.10	-0.99	46,46,46,46	0
59	MG	1l	201	1/1	0.93	0.15	-0.99	50,50,50,50	0
62	GDP	2z	702	28/28	0.96	0.14	-1.01	50,62,73,81	0
59	MG	1A	3067	1/1	0.97	0.12	-1.04	43,43,43,43	0
59	MG	1A	3765	1/1	0.94	0.15	-1.05	58,58,58,58	0
59	MG	1a	1724	1/1	0.98	0.15	-1.08	18,18,18,18	0
59	MG	1A	3307	1/1	0.96	0.16	-1.09	18,18,18,18	0
59	MG	1X	3002	1/1	0.99	0.12	-1.09	53,53,53,53	0
61	SF4	2d	501	8/8	0.99	0.12	-1.09	63,67,88,88	0
59	MG	2F	303	1/1	0.97	0.14	-1.12	40,40,40,40	0
60	ZN	1n	501	1/1	0.99	0.13	-1.14	77,77,77,77	0
62	GDP	1z	701	28/28	0.97	0.14	-1.14	30,50,64,75	0
59	MG	2A	3384	1/1	0.96	0.14	-1.15	25,25,25,25	0
59	MG	1A	3519	1/1	0.98	0.14	-1.15	21,21,21,21	0
59	MG	2A	3339	1/1	0.88	0.15	-1.15	46,46,46,46	0
59	MG	1A	3233	1/1	0.96	0.16	-1.15	51,51,51,51	0
61	SF4	1d	501	8/8	0.99	0.13	-1.17	61,67,75,78	0
59	MG	1A	3509	1/1	0.63	0.15	-1.19	50,50,50,50	0
59	MG	1A	3008	1/1	0.91	0.15	-1.21	31,31,31,31	0
60	ZN	27	101	1/1	0.97	0.11	-1.22	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2a	1607	1/1	0.86	0.13	-1.23	68,68,68,68	0
60	ZN	2n	501	1/1	0.92	0.10	-1.24	102,102,102,102	0
59	MG	2a	1618	1/1	0.92	0.13	-1.27	47,47,47,47	0
59	MG	1F	304	1/1	0.90	0.13	-1.29	33,33,33,33	0
59	MG	2A	3346	1/1	0.97	0.11	-1.33	64,64,64,64	0
59	MG	1E	306	1/1	0.99	0.16	-1.36	39,39,39,39	0
59	MG	2A	3072	1/1	0.86	0.09	-1.41	65,65,65,65	0
59	MG	1A	3484	1/1	0.96	0.14	-1.42	42,42,42,42	0
60	ZN	12	501	1/1	0.94	0.09	-1.43	100,100,100,100	0
59	MG	1A	3757	1/1	0.94	0.15	-1.45	26,26,26,26	0
59	MG	2A	3022	1/1	0.88	0.09	-1.51	54,54,54,54	0
59	MG	2A	3003	1/1	0.95	0.14	-1.51	40,40,40,40	0
59	MG	1A	3371	1/1	0.87	0.16	-1.52	30,30,30,30	0
59	MG	2a	1640	1/1	0.81	0.11	-1.53	65,65,65,65	0
60	ZN	22	501	1/1	0.90	0.04	-1.58	118,118,118,118	0
59	MG	1A	3414	1/1	0.95	0.13	-1.59	53,53,53,53	0
59	MG	1a	1604	1/1	0.78	0.12	-1.60	51,51,51,51	0
59	MG	1A	3554	1/1	0.94	0.14	-1.61	43,43,43,43	0
59	MG	2a	1701	1/1	0.96	0.13	-1.62	63,63,63,63	0
59	MG	1d	503	1/1	0.92	0.09	-1.63	80,80,80,80	0
59	MG	2A	3314	1/1	0.96	0.14	-1.63	54,54,54,54	0
59	MG	1A	3663	1/1	0.96	0.13	-1.67	32,32,32,32	0
59	MG	1a	1673	1/1	0.94	0.12	-1.68	43,43,43,43	0
59	MG	1F	305	1/1	0.96	0.14	-1.71	36,36,36,36	0
59	MG	2A	3603	1/1	0.99	0.12	-1.73	50,50,50,50	0
59	MG	1A	3589	1/1	0.90	0.15	-1.74	29,29,29,29	0
59	MG	1A	3141	1/1	0.80	0.14	-1.77	46,46,46,46	0
59	MG	1A	3393	1/1	0.90	0.15	-1.78	28,28,28,28	0
59	MG	1A	3232	1/1	0.93	0.17	-1.78	47,47,47,47	0
59	MG	1A	3317	1/1	0.98	0.15	-1.79	33,33,33,33	0
59	MG	2A	3294	1/1	0.93	0.11	-1.82	21,21,21,21	0
59	MG	1A	3347	1/1	0.90	0.15	-1.83	27,27,27,27	0
59	MG	1a	1801	1/1	0.95	0.17	-1.85	55,55,55,55	0
59	MG	1A	3377	1/1	0.89	0.13	-1.85	27,27,27,27	0
59	MG	1A	3388	1/1	0.98	0.15	-1.87	21,21,21,21	0
59	MG	2A	3152	1/1	0.94	0.12	-1.88	27,27,27,27	0
59	MG	2A	3324	1/1	0.98	0.11	-1.89	43,43,43,43	0
59	MG	2A	3610	1/1	0.96	0.09	-1.91	52,52,52,52	0
59	MG	1A	3459	1/1	0.93	0.16	-1.91	30,30,30,30	0
59	MG	1A	3770	1/1	0.85	0.13	-1.92	68,68,68,68	0
59	MG	1A	3056	1/1	0.96	0.11	-1.95	30,30,30,30	0
59	MG	1A	3160	1/1	0.96	0.13	-1.99	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2a	1667	1/1	0.88	0.11	-2.04	65,65,65,65	0
59	MG	1a	1804	1/1	0.97	0.10	-2.05	60,60,60,60	0
59	MG	2A	3579	1/1	0.98	0.10	-2.06	42,42,42,42	0
59	MG	2A	3352	1/1	0.82	0.12	-2.07	31,31,31,31	0
59	MG	1E	305	1/1	0.94	0.11	-2.09	30,30,30,30	0
59	MG	2A	3596	1/1	0.93	0.13	-2.10	64,64,64,64	0
59	MG	2a	1633	1/1	0.96	0.14	-2.12	36,36,36,36	0
59	MG	2A	3375	1/1	0.96	0.12	-2.13	28,28,28,28	0
59	MG	2A	3523	1/1	0.97	0.09	-2.17	38,38,38,38	0
59	MG	1A	3754	1/1	0.98	0.12	-2.19	28,28,28,28	0
59	MG	2A	3309	1/1	0.95	0.12	-2.21	27,27,27,27	0
59	MG	2A	3345	1/1	0.95	0.11	-2.24	25,25,25,25	0
59	MG	1a	1721	1/1	0.98	0.09	-2.30	46,46,46,46	0
60	ZN	2W	501	1/1	0.97	0.05	-2.30	79,79,79,79	0
59	MG	1a	1678	1/1	0.96	0.11	-2.31	48,48,48,48	0
59	MG	1A	3047	1/1	0.96	0.12	-2.33	37,37,37,37	0
59	MG	2A	3413	1/1	0.96	0.11	-2.34	30,30,30,30	0
59	MG	1A	3269	1/1	0.93	0.13	-2.38	21,21,21,21	0
59	MG	1B	221	1/1	0.82	0.12	-2.39	42,42,42,42	0
59	MG	1A	3345	1/1	0.96	0.14	-2.41	38,38,38,38	0
59	MG	1a	1668	1/1	0.99	0.13	-2.44	41,41,41,41	0
59	MG	2A	3566	1/1	0.98	0.10	-2.45	54,54,54,54	0
59	MG	1D	303	1/1	0.95	0.11	-2.46	33,33,33,33	0
59	MG	2A	3451	1/1	0.96	0.11	-2.52	56,56,56,56	0
59	MG	1A	3101	1/1	0.98	0.11	-2.57	38,38,38,38	0
59	MG	1A	3284	1/1	0.98	0.14	-2.61	48,48,48,48	0
59	MG	1A	3406	1/1	0.97	0.13	-2.65	56,56,56,56	0
59	MG	1A	3602	1/1	0.95	0.15	-2.65	53,53,53,53	0
59	MG	2A	3016	1/1	0.96	0.11	-2.69	48,48,48,48	0
59	MG	1G	3001	1/1	0.92	0.11	-2.70	31,31,31,31	0
59	MG	2A	3010	1/1	0.97	0.11	-2.75	34,34,34,34	0
59	MG	1A	3031	1/1	0.98	0.13	-2.76	28,28,28,28	0
59	MG	1A	3001	1/1	0.97	0.11	-2.78	30,30,30,30	0
59	MG	2A	3125	1/1	0.96	0.10	-2.79	30,30,30,30	0
59	MG	1A	3655	1/1	0.97	0.12	-2.80	31,31,31,31	0
59	MG	1A	3482	1/1	0.89	0.15	-2.80	27,27,27,27	0
59	MG	1A	3009	1/1	0.96	0.09	-2.83	20,20,20,20	0
59	MG	1a	1625	1/1	0.95	0.09	-2.84	53,53,53,53	0
59	MG	2a	1678	1/1	0.87	0.12	-2.85	51,51,51,51	0
59	MG	1B	217	1/1	0.97	0.11	-2.85	24,24,24,24	0
59	MG	1A	3767	1/1	0.97	0.06	-2.90	44,44,44,44	0
59	MG	2A	3028	1/1	0.95	0.11	-2.92	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3562	1/1	0.95	0.06	-2.93	34,34,34,34	0
59	MG	1A	3555	1/1	0.92	0.11	-3.03	56,56,56,56	0
59	MG	2a	1672	1/1	0.94	0.12	-3.05	57,57,57,57	0
59	MG	1A	3402	1/1	0.94	0.13	-3.10	22,22,22,22	0
59	MG	2A	3097	1/1	0.96	0.08	-3.20	56,56,56,56	0
59	MG	1A	3631	1/1	0.96	0.11	-3.29	48,48,48,48	0
59	MG	1A	3280	1/1	0.94	0.09	-3.30	40,40,40,40	0
59	MG	1A	3220	1/1	0.94	0.11	-3.37	33,33,33,33	0
59	MG	2A	3359	1/1	0.87	0.12	-3.40	33,33,33,33	0
59	MG	1A	3651	1/1	0.93	0.11	-3.43	28,28,28,28	0
59	MG	1a	1621	1/1	0.99	0.10	-3.50	66,66,66,66	0
59	MG	1a	1696	1/1	0.89	0.06	-3.61	54,54,54,54	0
59	MG	1F	303	1/1	0.98	0.12	-3.66	45,45,45,45	0
59	MG	1A	3644	1/1	0.97	0.11	-3.70	26,26,26,26	0
59	MG	1A	3550	1/1	0.95	0.12	-3.75	36,36,36,36	0
59	MG	1a	1667	1/1	0.82	0.10	-3.84	67,67,67,67	0
59	MG	1A	3632	1/1	0.97	0.12	-3.85	14,14,14,14	0
59	MG	1A	3011	1/1	0.96	0.12	-3.87	28,28,28,28	0
59	MG	1A	3282	1/1	0.94	0.13	-3.89	21,21,21,21	0
59	MG	2A	3487	1/1	0.96	0.06	-3.92	41,41,41,41	0
59	MG	1A	3363	1/1	0.92	0.11	-3.99	45,45,45,45	0
59	MG	1A	3272	1/1	0.99	0.11	-4.01	33,33,33,33	0
59	MG	1A	3332	1/1	0.88	0.11	-4.10	44,44,44,44	0
59	MG	2A	3050	1/1	0.96	0.05	-4.16	42,42,42,42	0
59	MG	2a	1646	1/1	0.96	0.08	-4.18	55,55,55,55	0
59	MG	1A	3441	1/1	0.99	0.14	-4.19	34,34,34,34	0
59	MG	1A	3549	1/1	0.98	0.11	-4.20	27,27,27,27	0
59	MG	1A	3076	1/1	0.86	0.09	-4.22	50,50,50,50	0
59	MG	2A	3470	1/1	0.97	0.10	-4.25	26,26,26,26	0
59	MG	1A	3661	1/1	0.96	0.11	-4.28	40,40,40,40	0
59	MG	1A	3289	1/1	0.95	0.12	-4.29	46,46,46,46	0
59	MG	1A	3278	1/1	0.98	0.11	-4.31	37,37,37,37	0
59	MG	1A	3339	1/1	0.96	0.10	-4.35	30,30,30,30	0
59	MG	1a	1644	1/1	0.99	0.11	-4.36	33,33,33,33	0
59	MG	1A	3613	1/1	0.98	0.06	-4.37	53,53,53,53	0
59	MG	1A	3532	1/1	0.94	0.10	-4.39	25,25,25,25	0
59	MG	2a	1623	1/1	0.90	0.12	-4.53	37,37,37,37	0
59	MG	1A	3488	1/1	0.94	0.09	-4.57	45,45,45,45	0
59	MG	1A	3496	1/1	0.96	0.11	-4.99	36,36,36,36	0
59	MG	2a	1694	1/1	0.96	0.08	-5.21	41,41,41,41	0
59	MG	1A	3422	1/1	0.98	0.13	-5.71	21,21,21,21	0
59	MG	1A	3017	1/1	0.81	0.09	-5.97	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1a	1697	1/1	0.98	0.07	-6.00	61,61,61,61	0
59	MG	2A	3481	1/1	0.96	0.09	-6.03	51,51,51,51	0
59	MG	1a	1641	1/1	0.98	0.08	-6.28	49,49,49,49	0
59	MG	1A	3409	1/1	0.95	0.11	-6.42	29,29,29,29	0
59	MG	1A	3481	1/1	0.94	0.14	-6.43	27,27,27,27	0
59	MG	2R	8001	1/1	0.98	0.05	-6.47	41,41,41,41	0
59	MG	1A	3622	1/1	0.98	0.10	-6.56	21,21,21,21	0
59	MG	1A	3617	1/1	0.95	0.12	-6.89	25,25,25,25	0
59	MG	2a	1613	1/1	0.93	0.08	-6.91	43,43,43,43	0
59	MG	1A	3334	1/1	0.97	0.11	-6.94	29,29,29,29	0
59	MG	1A	3445	1/1	0.96	0.12	-7.26	46,46,46,46	0
59	MG	2A	3432	1/1	0.80	0.08	-7.36	55,55,55,55	0
59	MG	1A	3370	1/1	0.98	0.07	-7.45	21,21,21,21	0
59	MG	2A	3479	1/1	0.95	0.09	-7.61	34,34,34,34	0
59	MG	1A	3600	1/1	0.92	0.10	-7.85	33,33,33,33	0
59	MG	1A	3059	1/1	0.96	0.06	-7.89	36,36,36,36	0
59	MG	1A	3022	1/1	0.99	0.11	-7.94	36,36,36,36	0
59	MG	2f	3002	1/1	0.99	0.07	-7.97	69,69,69,69	0
59	MG	2A	3071	1/1	0.98	0.05	-11.75	35,35,35,35	0
59	MG	2A	3456	1/1	0.92	0.07	-21.95	65,65,65,65	0
59	MG	2a	1688	1/1	0.93	0.15	-	35,35,35,35	0
59	MG	1a	1714	1/1	0.97	0.11	-	48,48,48,48	0
59	MG	1A	3366	1/1	0.90	0.12	-	51,51,51,51	0
59	MG	2a	1718	1/1	0.95	0.10	-	50,50,50,50	0
59	MG	2a	1755	1/1	0.87	0.33	-	77,77,77,77	0
59	MG	2A	3285	1/1	0.94	0.09	-	53,53,53,53	0
59	MG	2A	3262	1/1	0.89	0.24	-	51,51,51,51	0
59	MG	2A	3293	1/1	0.93	0.31	-	44,44,44,44	0
59	MG	1a	1656	1/1	0.89	0.54	-	51,51,51,51	0
59	MG	1A	3647	1/1	0.95	0.13	-	39,39,39,39	0
59	MG	2A	3138	1/1	0.95	0.47	-	58,58,58,58	0
59	MG	1A	3566	1/1	0.97	0.13	-	49,49,49,49	0
59	MG	2A	3074	1/1	0.96	0.19	-	39,39,39,39	0
59	MG	13	101	1/1	0.97	0.18	-	38,38,38,38	0
59	MG	1A	3421	1/1	0.97	0.14	-	41,41,41,41	0
59	MG	2A	3401	1/1	0.95	0.17	-	25,25,25,25	0
59	MG	1A	3738	1/1	0.95	0.49	-	88,88,88,88	0
59	MG	2A	3598	1/1	0.97	0.14	-	46,46,46,46	0
59	MG	1A	3584	1/1	0.92	0.12	-	62,62,62,62	0
59	MG	2M	201	1/1	0.96	0.09	-	54,54,54,54	0
59	MG	1a	1726	1/1	0.91	0.16	-	60,60,60,60	0
59	MG	1A	3758	1/1	0.87	0.21	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3526	1/1	0.93	0.17	-	47,47,47,47	0
59	MG	2A	3056	1/1	0.97	0.13	-	27,27,27,27	0
59	MG	2A	3457	1/1	0.97	0.07	-	48,48,48,48	0
59	MG	2a	1671	1/1	0.92	0.14	-	38,38,38,38	0
59	MG	2A	3449	1/1	0.98	0.11	-	27,27,27,27	0
59	MG	1A	3732	1/1	0.86	0.29	-	75,75,75,75	0
59	MG	1a	1613	1/1	0.86	0.14	-	66,66,66,66	0
59	MG	2A	3536	1/1	0.96	0.16	-	50,50,50,50	0
59	MG	1A	3383	1/1	0.91	0.17	-	47,47,47,47	0
59	MG	2A	3568	1/1	0.92	0.14	-	72,72,72,72	0
59	MG	1A	3112	1/1	0.92	0.12	-	44,44,44,44	0
59	MG	2z	704	1/1	0.85	0.23	-	55,55,55,55	0
59	MG	1A	3657	1/1	0.97	0.10	-	43,43,43,43	0
59	MG	2A	3018	1/1	0.94	0.18	-	39,39,39,39	0
59	MG	2B	209	1/1	0.99	0.18	-	71,71,71,71	0
59	MG	1A	3477	1/1	0.96	0.13	-	18,18,18,18	0
59	MG	2a	1645	1/1	0.91	0.18	-	58,58,58,58	0
59	MG	1A	3748	1/1	0.92	0.35	-	67,67,67,67	0
59	MG	2A	3224	1/1	0.85	0.30	-	62,62,62,62	0
59	MG	1A	3490	1/1	0.96	0.09	-	64,64,64,64	0
59	MG	1A	3679	1/1	0.94	0.18	-	55,55,55,55	0
59	MG	26	101	1/1	0.94	0.27	-	33,33,33,33	0
59	MG	1A	3762	1/1	0.90	0.34	-	25,25,25,25	0
59	MG	1A	3329	1/1	0.94	0.25	-	33,33,33,33	0
59	MG	1A	3314	1/1	0.98	0.13	-	36,36,36,36	0
59	MG	2a	1723	1/1	0.98	0.12	-	65,65,65,65	0
59	MG	2A	3509	1/1	0.95	0.11	-	49,49,49,49	0
59	MG	1E	301	1/1	0.94	0.13	-	18,18,18,18	0
59	MG	1A	3123	1/1	0.95	0.23	-	38,38,38,38	0
59	MG	2A	3370	1/1	0.96	0.14	-	46,46,46,46	0
59	MG	1A	3752	1/1	0.95	0.20	-	42,42,42,42	0
59	MG	2a	1612	1/1	0.88	0.24	-	48,48,48,48	0
59	MG	2a	1621	1/1	0.79	0.29	-	66,66,66,66	0
59	MG	1A	3500	1/1	0.98	0.12	-	63,63,63,63	0
59	MG	1a	1749	1/1	0.84	0.12	-	68,68,68,68	0
59	MG	1A	3582	1/1	0.93	0.19	-	17,17,17,17	0
59	MG	1A	3454	1/1	0.95	0.11	-	52,52,52,52	0
59	MG	2a	1762	1/1	0.65	0.26	-	65,65,65,65	0
59	MG	1a	1754	1/1	0.97	0.07	-	42,42,42,42	0
59	MG	2A	3023	1/1	0.89	0.31	-	34,34,34,34	0
59	MG	2d	502	1/1	0.97	0.21	-	35,35,35,35	0
59	MG	1a	1710	1/1	0.90	0.42	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3446	1/1	0.96	0.05	-	31,31,31,31	0
59	MG	2A	3500	1/1	0.80	0.26	-	56,56,56,56	0
59	MG	2A	3052	1/1	0.87	0.17	-	47,47,47,47	0
59	MG	1A	3103	1/1	0.99	0.06	-	40,40,40,40	0
59	MG	1A	3724	1/1	0.87	0.19	-	47,47,47,47	0
59	MG	2A	3534	1/1	0.96	0.28	-	58,58,58,58	0
59	MG	2A	3513	1/1	0.97	0.10	-	54,54,54,54	0
59	MG	2A	3391	1/1	0.96	0.13	-	47,47,47,47	0
59	MG	2A	3158	1/1	0.97	0.14	-	33,33,33,33	0
59	MG	1A	3010	1/1	0.86	0.29	-	45,45,45,45	0
59	MG	2S	202	1/1	0.83	0.18	-	58,58,58,58	0
59	MG	1A	3219	1/1	0.93	0.32	-	55,55,55,55	0
59	MG	2A	3474	1/1	0.93	0.20	-	41,41,41,41	0
59	MG	1a	1713	1/1	0.82	0.16	-	62,62,62,62	0
59	MG	1A	3230	1/1	0.92	0.23	-	56,56,56,56	0
59	MG	1A	3439	1/1	0.95	0.28	-	26,26,26,26	0
59	MG	1a	1709	1/1	0.90	0.50	-	50,50,50,50	0
59	MG	2A	3379	1/1	0.94	0.14	-	48,48,48,48	0
59	MG	2A	3167	1/1	0.91	0.12	-	52,52,52,52	0
59	MG	2A	3441	1/1	0.87	0.38	-	45,45,45,45	0
59	MG	1Y	104	1/1	0.87	0.20	-	50,50,50,50	0
59	MG	1A	3346	1/1	0.93	0.20	-	26,26,26,26	0
59	MG	1a	1624	1/1	0.95	0.13	-	38,38,38,38	0
59	MG	1A	3628	1/1	0.94	0.22	-	13,13,13,13	0
59	MG	2A	3512	1/1	0.95	0.07	-	63,63,63,63	0
59	MG	2a	1626	1/1	0.84	0.34	-	57,57,57,57	0
59	MG	1A	3109	1/1	0.98	0.10	-	36,36,36,36	0
59	MG	1A	3209	1/1	0.98	0.27	-	41,41,41,41	0
59	MG	1A	3322	1/1	0.93	0.26	-	42,42,42,42	0
59	MG	1A	3191	1/1	0.97	0.25	-	31,31,31,31	0
59	MG	1A	3595	1/1	0.91	0.12	-	49,49,49,49	0
59	MG	2a	1689	1/1	0.79	0.16	-	69,69,69,69	0
59	MG	2A	3280	1/1	0.85	0.29	-	68,68,68,68	0
59	MG	2A	3255	1/1	0.95	0.19	-	37,37,37,37	0
59	MG	1B	215	1/1	0.97	0.10	-	37,37,37,37	0
59	MG	1A	3328	1/1	0.90	0.24	-	50,50,50,50	0
59	MG	2A	3095	1/1	0.92	0.16	-	37,37,37,37	0
59	MG	1A	3702	1/1	0.95	0.10	-	51,51,51,51	0
59	MG	2A	3428	1/1	0.96	0.16	-	28,28,28,28	0
59	MG	1B	210	1/1	0.93	0.23	-	49,49,49,49	0
59	MG	1l	202	1/1	0.93	0.16	-	47,47,47,47	0
59	MG	2a	1750	1/1	0.93	0.20	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3013	1/1	0.82	0.28	-	35,35,35,35	0
59	MG	1A	3122	1/1	0.84	0.18	-	60,60,60,60	0
59	MG	2A	3342	1/1	0.98	0.20	-	48,48,48,48	0
59	MG	1A	3069	1/1	0.92	0.24	-	39,39,39,39	0
59	MG	2A	3160	1/1	0.93	0.22	-	41,41,41,41	0
59	MG	1A	3167	1/1	0.89	0.63	-	50,50,50,50	0
59	MG	2a	1647	1/1	0.89	0.14	-	61,61,61,61	0
59	MG	1a	1619	1/1	0.88	0.10	-	51,51,51,51	0
59	MG	1a	1786	1/1	0.93	0.27	-	48,48,48,48	0
59	MG	1U	202	1/1	0.83	0.27	-	37,37,37,37	0
59	MG	1A	3055	1/1	0.81	0.25	-	49,49,49,49	0
59	MG	1A	3527	1/1	0.89	0.15	-	38,38,38,38	0
59	MG	1A	3583	1/1	0.96	0.29	-	39,39,39,39	0
59	MG	2A	3399	1/1	0.90	0.25	-	39,39,39,39	0
59	MG	2a	1638	1/1	0.98	0.38	-	54,54,54,54	0
59	MG	1a	1607	1/1	0.88	0.33	-	69,69,69,69	0
59	MG	1a	1631	1/1	0.97	0.06	-	41,41,41,41	0
59	MG	1A	3523	1/1	0.97	0.14	-	35,35,35,35	0
59	MG	2A	3503	1/1	0.95	0.15	-	32,32,32,32	0
59	MG	1a	1688	1/1	0.84	0.14	-	60,60,60,60	0
59	MG	2a	1699	1/1	0.95	0.10	-	47,47,47,47	0
59	MG	1A	3676	1/1	0.97	0.13	-	51,51,51,51	0
59	MG	1A	3416	1/1	0.94	0.08	-	49,49,49,49	0
59	MG	2A	3070	1/1	0.90	0.26	-	36,36,36,36	0
59	MG	1A	3068	1/1	0.87	0.43	-	33,33,33,33	0
59	MG	1A	3569	1/1	0.98	0.14	-	41,41,41,41	0
59	MG	1A	3157	1/1	0.88	0.18	-	34,34,34,34	0
59	MG	1A	3050	1/1	0.87	0.22	-	42,42,42,42	0
59	MG	2A	3108	1/1	0.93	0.21	-	44,44,44,44	0
59	MG	1A	3193	1/1	0.88	0.17	-	47,47,47,47	0
59	MG	1a	1745	1/1	0.96	0.11	-	47,47,47,47	0
59	MG	2A	3106	1/1	0.98	0.20	-	39,39,39,39	0
59	MG	2A	3386	1/1	0.93	0.27	-	43,43,43,43	0
59	MG	1A	3571	1/1	0.95	0.14	-	45,45,45,45	0
59	MG	1A	3455	1/1	0.94	0.18	-	50,50,50,50	0
59	MG	1A	3121	1/1	0.87	0.66	-	49,49,49,49	0
59	MG	2a	1658	1/1	0.82	0.23	-	58,58,58,58	0
59	MG	1A	3776	1/1	0.90	0.31	-	46,46,46,46	0
59	MG	1A	3709	1/1	0.98	0.15	-	41,41,41,41	0
59	MG	1A	3769	1/1	0.98	0.14	-	35,35,35,35	0
59	MG	2a	1768	1/1	0.91	0.14	-	64,64,64,64	0
59	MG	1A	3419	1/1	0.97	0.14	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3243	1/1	0.94	0.12	-	51,51,51,51	0
59	MG	1A	3170	1/1	0.86	0.10	-	61,61,61,61	0
59	MG	1A	3685	1/1	0.98	0.16	-	60,60,60,60	0
59	MG	1A	3664	1/1	0.99	0.17	-	39,39,39,39	0
59	MG	1A	3659	1/1	0.98	0.36	-	31,31,31,31	0
59	MG	1A	3194	1/1	0.97	0.35	-	43,43,43,43	0
59	MG	1a	1670	1/1	0.95	0.19	-	54,54,54,54	0
59	MG	1A	3648	1/1	0.99	0.14	-	40,40,40,40	0
59	MG	1A	3091	1/1	0.91	0.16	-	54,54,54,54	0
59	MG	2A	3112	1/1	0.97	0.24	-	20,20,20,20	0
59	MG	2A	3325	1/1	0.94	0.18	-	30,30,30,30	0
59	MG	2A	3502	1/1	0.94	0.22	-	47,47,47,47	0
59	MG	1A	3521	1/1	0.95	0.09	-	45,45,45,45	0
59	MG	1A	3285	1/1	0.97	0.27	-	51,51,51,51	0
59	MG	2A	3153	1/1	0.90	0.10	-	43,43,43,43	0
59	MG	1B	216	1/1	0.97	0.07	-	34,34,34,34	0
59	MG	1A	3712	1/1	0.87	0.24	-	80,80,80,80	0
59	MG	1A	3263	1/1	0.90	0.19	-	33,33,33,33	0
59	MG	2A	3257	1/1	0.97	0.08	-	49,49,49,49	0
59	MG	1A	3265	1/1	0.91	0.13	-	36,36,36,36	0
59	MG	2A	3069	1/1	0.91	0.14	-	50,50,50,50	0
59	MG	2A	3105	1/1	0.96	0.09	-	33,33,33,33	0
59	MG	2A	3436	1/1	0.92	0.12	-	50,50,50,50	0
59	MG	2A	3494	1/1	0.95	0.11	-	44,44,44,44	0
59	MG	2A	3581	1/1	0.86	0.19	-	71,71,71,71	0
59	MG	2A	3009	1/1	0.82	0.16	-	50,50,50,50	0
59	MG	1F	307	1/1	0.98	0.10	-	19,19,19,19	0
59	MG	1a	1687	1/1	0.86	0.22	-	55,55,55,55	0
59	MG	2a	1773	1/1	0.98	0.09	-	50,50,50,50	0
59	MG	1A	3470	1/1	0.90	0.25	-	28,28,28,28	0
59	MG	1w	3004	1/1	0.85	0.24	-	49,49,49,49	0
59	MG	2A	3540	1/1	0.95	0.40	-	31,31,31,31	0
59	MG	2A	3497	1/1	0.96	0.08	-	41,41,41,41	0
59	MG	2a	1650	1/1	0.92	0.18	-	43,43,43,43	0
59	MG	1a	1792	1/1	0.97	0.11	-	55,55,55,55	0
59	MG	1A	3086	1/1	0.94	0.12	-	31,31,31,31	0
59	MG	1a	1686	1/1	0.77	0.32	-	75,75,75,75	0
59	MG	1A	3176	1/1	0.92	0.16	-	33,33,33,33	0
59	MG	2a	1732	1/1	0.88	0.25	-	55,55,55,55	0
59	MG	1a	1675	1/1	0.94	0.17	-	38,38,38,38	0
59	MG	2A	3347	1/1	0.97	0.09	-	51,51,51,51	0
59	MG	2a	1700	1/1	0.97	0.15	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3289	1/1	0.96	0.15	-	45,45,45,45	0
59	MG	1A	3171	1/1	0.95	0.32	-	50,50,50,50	0
59	MG	1A	3585	1/1	0.92	0.12	-	52,52,52,52	0
59	MG	1A	3715	1/1	0.96	0.27	-	42,42,42,42	0
59	MG	2A	3172	1/1	0.94	0.14	-	49,49,49,49	0
59	MG	1A	3299	1/1	0.95	0.12	-	44,44,44,44	0
59	MG	2a	1617	1/1	0.81	0.12	-	65,65,65,65	0
59	MG	1a	1778	1/1	0.84	0.07	-	81,81,81,81	0
59	MG	2A	3589	1/1	0.94	0.29	-	50,50,50,50	0
59	MG	1A	3614	1/1	0.96	0.47	-	43,43,43,43	0
59	MG	1A	3524	1/1	0.98	0.14	-	30,30,30,30	0
59	MG	1A	3147	1/1	0.96	0.18	-	32,32,32,32	0
59	MG	1A	3516	1/1	0.94	0.10	-	27,27,27,27	0
59	MG	1A	3567	1/1	0.94	0.09	-	63,63,63,63	0
59	MG	1A	3588	1/1	0.96	0.11	-	51,51,51,51	0
59	MG	1A	3401	1/1	0.88	0.08	-	44,44,44,44	0
59	MG	1a	1773	1/1	0.96	0.27	-	55,55,55,55	0
59	MG	2A	3222	1/1	0.93	0.18	-	40,40,40,40	0
59	MG	1A	3330	1/1	0.93	0.11	-	41,41,41,41	0
59	MG	2a	1752	1/1	0.95	0.19	-	64,64,64,64	0
59	MG	2A	3374	1/1	0.99	0.07	-	26,26,26,26	0
59	MG	2A	3605	1/1	0.98	0.12	-	35,35,35,35	0
59	MG	1A	3196	1/1	0.79	0.34	-	49,49,49,49	0
59	MG	2A	3476	1/1	0.96	0.17	-	61,61,61,61	0
59	MG	2A	3062	1/1	0.87	0.11	-	41,41,41,41	0
59	MG	1A	3677	1/1	0.96	0.29	-	58,58,58,58	0
59	MG	1a	1708	1/1	0.96	0.22	-	37,37,37,37	0
59	MG	1A	3319	1/1	0.93	0.20	-	42,42,42,42	0
59	MG	2A	3447	1/1	0.89	0.20	-	41,41,41,41	0
59	MG	1A	3489	1/1	0.98	0.04	-	48,48,48,48	0
59	MG	1A	3603	1/1	0.85	0.22	-	65,65,65,65	0
59	MG	1A	3494	1/1	0.98	0.22	-	46,46,46,46	0
59	MG	1A	3396	1/1	0.95	0.14	-	51,51,51,51	0
59	MG	1A	3114	1/1	0.79	0.11	-	43,43,43,43	0
59	MG	1a	1685	1/1	0.91	0.29	-	51,51,51,51	0
59	MG	2A	3574	1/1	0.97	0.34	-	62,62,62,62	0
59	MG	1A	3556	1/1	0.97	0.13	-	57,57,57,57	0
59	MG	2A	3541	1/1	0.95	0.14	-	49,49,49,49	0
59	MG	2a	1721	1/1	0.92	0.38	-	62,62,62,62	0
59	MG	2A	3472	1/1	0.94	0.21	-	21,21,21,21	0
59	MG	1A	3185	1/1	0.94	0.19	-	60,60,60,60	0
59	MG	1A	3654	1/1	0.98	0.20	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2a	1691	1/1	0.84	0.51	-	64,64,64,64	0
59	MG	1A	3626	1/1	0.98	0.16	-	31,31,31,31	0
59	MG	2A	3126	1/1	0.87	0.10	-	45,45,45,45	0
59	MG	1A	3026	1/1	0.94	0.26	-	42,42,42,42	0
59	MG	1A	3073	1/1	0.95	0.10	-	35,35,35,35	0
59	MG	2A	3587	1/1	0.99	0.29	-	29,29,29,29	0
59	MG	1A	3084	1/1	0.97	0.24	-	29,29,29,29	0
59	MG	2A	3046	1/1	0.88	0.26	-	51,51,51,51	0
59	MG	2A	3443	1/1	0.95	0.21	-	52,52,52,52	0
59	MG	2A	3226	1/1	0.96	0.27	-	34,34,34,34	0
59	MG	2a	1629	1/1	0.91	0.09	-	57,57,57,57	0
59	MG	2a	1697	1/1	0.94	0.25	-	55,55,55,55	0
59	MG	1a	1632	1/1	0.92	0.17	-	63,63,63,63	0
59	MG	2A	3328	1/1	0.94	0.19	-	30,30,30,30	0
59	MG	1a	1753	1/1	0.93	0.12	-	65,65,65,65	0
59	MG	1A	3587	1/1	0.89	0.18	-	18,18,18,18	0
59	MG	2a	1666	1/1	0.93	0.37	-	48,48,48,48	0
59	MG	2A	3584	1/1	0.96	0.16	-	40,40,40,40	0
59	MG	1A	3546	1/1	0.87	0.12	-	54,54,54,54	0
59	MG	1A	3274	1/1	0.91	0.18	-	25,25,25,25	0
59	MG	1A	3766	1/1	0.96	0.09	-	28,28,28,28	0
59	MG	2a	1686	1/1	0.88	0.16	-	40,40,40,40	0
59	MG	1A	3140	1/1	0.97	0.17	-	42,42,42,42	0
59	MG	1A	3038	1/1	0.97	0.09	-	40,40,40,40	0
59	MG	1A	3313	1/1	0.94	0.07	-	43,43,43,43	0
59	MG	2A	3407	1/1	0.94	0.30	-	32,32,32,32	0
59	MG	1A	3522	1/1	0.96	0.12	-	42,42,42,42	0
59	MG	1A	3436	1/1	0.96	0.05	-	46,46,46,46	0
59	MG	1A	3258	1/1	0.96	0.13	-	24,24,24,24	0
59	MG	2A	3298	1/1	0.96	0.19	-	42,42,42,42	0
59	MG	1A	3137	1/1	0.93	0.08	-	55,55,55,55	0
59	MG	2A	3256	1/1	0.90	0.23	-	48,48,48,48	0
59	MG	2A	3611	1/1	0.86	0.17	-	59,59,59,59	0
59	MG	1a	1690	1/1	0.97	0.30	-	58,58,58,58	0
59	MG	1A	3621	1/1	0.88	0.15	-	21,21,21,21	0
59	MG	2a	1726	1/1	0.97	0.17	-	62,62,62,62	0
59	MG	1A	3551	1/1	0.86	0.16	-	48,48,48,48	0
59	MG	1a	1703	1/1	0.95	0.21	-	52,52,52,52	0
59	MG	2a	1760	1/1	0.83	0.19	-	44,44,44,44	0
59	MG	1A	3070	1/1	0.97	0.13	-	37,37,37,37	0
59	MG	1a	1636	1/1	0.84	0.26	-	62,62,62,62	0
59	MG	2A	3320	1/1	0.92	0.19	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3488	1/1	0.97	0.26	-	51,51,51,51	0
59	MG	1A	3692	1/1	0.95	0.19	-	45,45,45,45	0
59	MG	1A	3304	1/1	0.95	0.16	-	39,39,39,39	0
59	MG	1A	3604	1/1	0.96	0.15	-	52,52,52,52	0
59	MG	2A	3043	1/1	0.96	0.12	-	43,43,43,43	0
59	MG	2A	3306	1/1	0.87	0.15	-	45,45,45,45	0
59	MG	2A	3453	1/1	0.98	0.15	-	21,21,21,21	0
59	MG	2A	3265	1/1	0.85	0.57	-	62,62,62,62	0
59	MG	2A	3514	1/1	0.93	0.22	-	58,58,58,58	0
59	MG	2A	3355	1/1	0.97	0.24	-	27,27,27,27	0
59	MG	1w	3005	1/1	0.95	0.13	-	78,78,78,78	0
59	MG	1a	1765	1/1	0.98	0.07	-	44,44,44,44	0
59	MG	1A	3616	1/1	0.97	0.09	-	63,63,63,63	0
59	MG	1A	3543	1/1	0.98	0.07	-	61,61,61,61	0
59	MG	1a	1653	1/1	0.87	0.30	-	60,60,60,60	0
59	MG	2A	3175	1/1	0.90	0.15	-	44,44,44,44	0
59	MG	1A	3184	1/1	0.94	0.19	-	39,39,39,39	0
59	MG	1a	1626	1/1	0.90	0.31	-	54,54,54,54	0
59	MG	1A	3275	1/1	0.97	0.18	-	51,51,51,51	0
59	MG	2a	1675	1/1	0.94	0.21	-	43,43,43,43	0
59	MG	1a	1615	1/1	0.88	0.31	-	54,54,54,54	0
59	MG	1A	3129	1/1	0.97	0.13	-	29,29,29,29	0
59	MG	1a	1771	1/1	0.33	0.79	-	94,94,94,94	0
59	MG	2A	3480	1/1	0.95	0.07	-	59,59,59,59	0
59	MG	2A	3090	1/1	0.92	0.18	-	40,40,40,40	0
59	MG	2A	3606	1/1	0.88	0.17	-	29,29,29,29	0
59	MG	1A	3315	1/1	0.98	0.09	-	34,34,34,34	0
59	MG	2A	3067	1/1	0.97	0.24	-	42,42,42,42	0
59	MG	1l	203	1/1	0.95	0.18	-	56,56,56,56	0
59	MG	1a	1680	1/1	0.91	0.22	-	65,65,65,65	0
59	MG	2a	1708	1/1	0.91	0.13	-	64,64,64,64	0
59	MG	2a	1651	1/1	0.83	0.18	-	67,67,67,67	0
59	MG	1A	3694	1/1	0.86	0.17	-	47,47,47,47	0
59	MG	1A	3507	1/1	0.96	0.20	-	21,21,21,21	0
59	MG	2A	3237	1/1	0.84	0.14	-	54,54,54,54	0
59	MG	1a	1676	1/1	0.95	0.15	-	42,42,42,42	0
59	MG	2a	1674	1/1	0.95	0.23	-	60,60,60,60	0
59	MG	1A	3336	1/1	0.94	0.19	-	20,20,20,20	0
59	MG	1A	3120	1/1	0.97	0.17	-	31,31,31,31	0
59	MG	1A	3365	1/1	0.96	0.24	-	39,39,39,39	0
59	MG	2A	3244	1/1	0.98	0.35	-	49,49,49,49	0
59	MG	1a	1658	1/1	0.90	0.11	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3504	1/1	0.99	0.09	-	33,33,33,33	0
59	MG	2A	3417	1/1	0.92	0.15	-	53,53,53,53	0
59	MG	2A	3478	1/1	0.91	0.34	-	58,58,58,58	0
59	MG	1A	3241	1/1	0.95	0.35	-	40,40,40,40	0
59	MG	1A	3074	1/1	0.97	0.28	-	28,28,28,28	0
59	MG	2A	3362	1/1	0.94	0.17	-	35,35,35,35	0
59	MG	2A	3484	1/1	0.96	0.08	-	38,38,38,38	0
59	MG	2A	3079	1/1	0.92	0.09	-	33,33,33,33	0
59	MG	2A	3543	1/1	0.98	0.24	-	28,28,28,28	0
59	MG	1a	1736	1/1	0.97	0.22	-	32,32,32,32	0
59	MG	2E	304	1/1	0.88	0.46	-	56,56,56,56	0
59	MG	2A	3019	1/1	0.97	0.13	-	41,41,41,41	0
59	MG	1a	1795	1/1	0.93	0.07	-	45,45,45,45	0
59	MG	2A	3461	1/1	0.96	0.07	-	54,54,54,54	0
59	MG	2A	3319	1/1	0.96	0.29	-	29,29,29,29	0
59	MG	1A	3635	1/1	0.85	0.18	-	72,72,72,72	0
59	MG	1A	3573	1/1	0.98	0.11	-	50,50,50,50	0
59	MG	1A	3309	1/1	0.97	0.12	-	37,37,37,37	0
59	MG	1A	3727	1/1	0.94	0.19	-	38,38,38,38	0
59	MG	1A	3746	1/1	0.90	0.24	-	53,53,53,53	0
59	MG	2a	1743	1/1	0.88	0.14	-	68,68,68,68	0
59	MG	1A	3442	1/1	0.96	0.09	-	50,50,50,50	0
59	MG	1A	3262	1/1	0.95	0.11	-	53,53,53,53	0
59	MG	1A	3559	1/1	0.97	0.14	-	44,44,44,44	0
59	MG	1A	3380	1/1	0.91	0.18	-	44,44,44,44	0
59	MG	2A	3058	1/1	0.96	0.13	-	48,48,48,48	0
59	MG	1A	3561	1/1	0.91	0.10	-	35,35,35,35	0
59	MG	1A	3303	1/1	0.87	0.24	-	48,48,48,48	0
59	MG	2a	1709	1/1	0.93	0.24	-	68,68,68,68	0
59	MG	2A	3259	1/1	0.85	0.91	-	72,72,72,72	0
59	MG	2a	1687	1/1	0.79	0.35	-	48,48,48,48	0
59	MG	1a	1705	1/1	0.89	0.24	-	64,64,64,64	0
59	MG	2A	3454	1/1	0.95	0.08	-	66,66,66,66	0
59	MG	2A	3590	1/1	0.97	0.09	-	38,38,38,38	0
59	MG	2A	3344	1/1	0.96	0.13	-	49,49,49,49	0
59	MG	1A	3095	1/1	0.91	0.56	-	40,40,40,40	0
59	MG	1a	1661	1/1	0.92	0.18	-	47,47,47,47	0
59	MG	2B	212	1/1	0.94	0.14	-	47,47,47,47	0
59	MG	2A	3102	1/1	0.94	0.05	-	48,48,48,48	0
59	MG	2A	3085	1/1	0.94	0.54	-	58,58,58,58	0
59	MG	1A	3052	1/1	0.92	0.28	-	40,40,40,40	0
59	MG	2A	3272	1/1	0.82	0.25	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2B	210	1/1	0.86	0.15	-	55,55,55,55	0
59	MG	2A	3119	1/1	0.91	0.21	-	39,39,39,39	0
59	MG	2A	3113	1/1	0.97	0.23	-	33,33,33,33	0
59	MG	2A	3429	1/1	0.88	0.12	-	56,56,56,56	0
59	MG	23	502	1/1	0.93	0.49	-	49,49,49,49	0
59	MG	2f	3001	1/1	0.99	0.07	-	40,40,40,40	0
59	MG	2A	3017	1/1	0.98	0.12	-	47,47,47,47	0
59	MG	1a	1715	1/1	0.97	0.19	-	28,28,28,28	0
59	MG	1a	1633	1/1	0.94	0.10	-	46,46,46,46	0
59	MG	2A	3350	1/1	0.86	0.19	-	71,71,71,71	0
59	MG	1A	3075	1/1	0.92	0.20	-	44,44,44,44	0
59	MG	1A	3514	1/1	0.91	0.07	-	43,43,43,43	0
59	MG	1a	1649	1/1	0.96	0.23	-	52,52,52,52	0
59	MG	1A	3310	1/1	0.99	0.07	-	39,39,39,39	0
59	MG	1a	1800	1/1	0.86	0.44	-	68,68,68,68	0
59	MG	1A	3089	1/1	0.97	0.10	-	42,42,42,42	0
59	MG	2A	3213	1/1	0.88	0.20	-	48,48,48,48	0
59	MG	2A	3358	1/1	0.93	0.10	-	56,56,56,56	0
59	MG	1A	3508	1/1	0.89	0.19	-	47,47,47,47	0
59	MG	2A	3121	1/1	0.90	0.15	-	57,57,57,57	0
59	MG	2A	3501	1/1	0.92	0.20	-	50,50,50,50	0
59	MG	2A	3274	1/1	0.84	0.22	-	56,56,56,56	0
59	MG	2A	3124	1/1	0.94	0.28	-	44,44,44,44	0
59	MG	1A	3321	1/1	0.78	0.17	-	74,74,74,74	0
59	MG	2A	3414	1/1	0.86	0.12	-	42,42,42,42	0
59	MG	2A	3027	1/1	0.96	0.39	-	44,44,44,44	0
59	MG	1A	3053	1/1	0.94	0.21	-	46,46,46,46	0
59	MG	2a	1637	1/1	0.96	0.23	-	54,54,54,54	0
59	MG	1A	3394	1/1	0.97	0.21	-	50,50,50,50	0
59	MG	2A	3060	1/1	0.92	0.11	-	36,36,36,36	0
59	MG	1A	3643	1/1	0.94	0.09	-	23,23,23,23	0
59	MG	2a	1767	1/1	0.95	0.14	-	45,45,45,45	0
59	MG	2A	3238	1/1	0.54	0.42	-	60,60,60,60	0
59	MG	1A	3338	1/1	0.93	0.20	-	38,38,38,38	0
59	MG	2A	3372	1/1	0.96	0.09	-	36,36,36,36	0
59	MG	2A	3220	1/1	0.79	0.46	-	60,60,60,60	0
59	MG	1U	201	1/1	0.91	0.14	-	48,48,48,48	0
59	MG	2a	1641	1/1	0.89	0.13	-	51,51,51,51	0
59	MG	2a	1712	1/1	0.98	0.23	-	62,62,62,62	0
59	MG	1A	3649	1/1	0.98	0.15	-	35,35,35,35	0
59	MG	1A	3082	1/1	0.88	0.21	-	39,39,39,39	0
59	MG	1A	3034	1/1	0.94	0.10	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3688	1/1	0.93	0.09	-	89,89,89,89	0
59	MG	1a	1666	1/1	0.80	0.16	-	49,49,49,49	0
59	MG	1A	3290	1/1	0.89	0.21	-	34,34,34,34	0
59	MG	1A	3398	1/1	0.97	0.15	-	26,26,26,26	0
59	MG	2a	1682	1/1	0.94	0.15	-	42,42,42,42	0
59	MG	1A	3634	1/1	0.99	0.07	-	20,20,20,20	0
59	MG	1a	1787	1/1	0.96	0.14	-	70,70,70,70	0
59	MG	2A	3291	1/1	0.90	0.09	-	34,34,34,34	0
59	MG	1A	3187	1/1	0.91	0.15	-	48,48,48,48	0
59	MG	2a	1606	1/1	0.97	0.19	-	24,24,24,24	0
59	MG	2a	1733	1/1	0.98	0.12	-	62,62,62,62	0
59	MG	2A	3586	1/1	0.92	0.23	-	45,45,45,45	0
59	MG	1A	3493	1/1	0.94	0.13	-	41,41,41,41	0
59	MG	2A	3307	1/1	0.97	0.11	-	27,27,27,27	0
59	MG	2A	3268	1/1	0.87	0.37	-	56,56,56,56	0
59	MG	2A	3200	1/1	0.98	0.25	-	34,34,34,34	0
59	MG	1A	3138	1/1	0.96	0.06	-	43,43,43,43	0
59	MG	1A	3568	1/1	0.82	0.36	-	54,54,54,54	0
59	MG	1B	205	1/1	0.53	0.37	-	72,72,72,72	0
59	MG	1A	3256	1/1	0.97	0.09	-	49,49,49,49	0
59	MG	1A	3292	1/1	0.92	0.10	-	39,39,39,39	0
59	MG	1A	3182	1/1	0.96	0.10	-	37,37,37,37	0
59	MG	2a	1731	1/1	0.95	0.19	-	48,48,48,48	0
59	MG	2A	3348	1/1	0.98	0.10	-	36,36,36,36	0
59	MG	1w	3002	1/1	0.93	0.07	-	51,51,51,51	0
59	MG	1A	3360	1/1	0.88	0.31	-	36,36,36,36	0
59	MG	1A	3057	1/1	0.95	0.10	-	38,38,38,38	0
59	MG	1A	3495	1/1	0.98	0.17	-	53,53,53,53	0
59	MG	1A	3044	1/1	0.96	0.18	-	33,33,33,33	0
59	MG	2A	3165	1/1	0.90	0.37	-	44,44,44,44	0
59	MG	1A	3596	1/1	0.86	0.14	-	52,52,52,52	0
59	MG	2A	3570	1/1	0.93	0.34	-	48,48,48,48	0
59	MG	1A	3553	1/1	0.90	0.12	-	47,47,47,47	0
59	MG	1A	3438	1/1	0.96	0.13	-	49,49,49,49	0
59	MG	2a	1758	1/1	0.89	0.25	-	65,65,65,65	0
59	MG	2A	3048	1/1	0.97	0.21	-	40,40,40,40	0
59	MG	2A	3156	1/1	0.93	0.11	-	53,53,53,53	0
59	MG	1A	3444	1/1	0.97	0.09	-	35,35,35,35	0
59	MG	1a	1642	1/1	0.85	0.42	-	43,43,43,43	0
59	MG	1G	3002	1/1	0.84	0.09	-	64,64,64,64	0
59	MG	2a	1696	1/1	0.94	0.34	-	40,40,40,40	0
59	MG	2A	3473	1/1	0.92	0.30	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3457	1/1	0.93	0.20	-	47,47,47,47	0
59	MG	1A	3239	1/1	0.97	0.09	-	49,49,49,49	0
59	MG	1A	3733	1/1	0.93	0.31	-	59,59,59,59	0
59	MG	1A	3671	1/1	0.97	0.20	-	36,36,36,36	0
59	MG	2a	1624	1/1	0.88	0.14	-	56,56,56,56	0
59	MG	2a	1673	1/1	0.82	0.34	-	55,55,55,55	0
59	MG	2A	3435	1/1	0.97	0.17	-	38,38,38,38	0
59	MG	1A	3437	1/1	0.87	0.09	-	49,49,49,49	0
59	MG	2A	3477	1/1	0.94	0.10	-	54,54,54,54	0
59	MG	2a	1719	1/1	0.98	0.12	-	56,56,56,56	0
59	MG	1P	202	1/1	0.94	0.18	-	36,36,36,36	0
59	MG	1A	3449	1/1	0.98	0.15	-	47,47,47,47	0
59	MG	2A	3295	1/1	0.95	0.20	-	52,52,52,52	0
59	MG	2A	3448	1/1	0.93	0.14	-	37,37,37,37	0
59	MG	1A	3639	1/1	0.99	0.10	-	54,54,54,54	0
59	MG	2A	3312	1/1	0.98	0.20	-	60,60,60,60	0
59	MG	2A	3081	1/1	0.85	0.13	-	63,63,63,63	0
59	MG	2F	302	1/1	0.88	0.16	-	46,46,46,46	0
59	MG	2A	3088	1/1	0.80	0.19	-	41,41,41,41	0
59	MG	1A	3072	1/1	0.81	0.39	-	61,61,61,61	0
59	MG	1A	3172	1/1	0.97	0.19	-	53,53,53,53	0
59	MG	1A	3100	1/1	0.94	0.25	-	38,38,38,38	0
59	MG	2a	1616	1/1	0.81	0.26	-	57,57,57,57	0
59	MG	1A	3333	1/1	0.91	0.15	-	45,45,45,45	0
59	MG	1A	3412	1/1	0.89	0.17	-	54,54,54,54	0
59	MG	2A	3004	1/1	0.96	0.12	-	53,53,53,53	0
59	MG	2A	3044	1/1	0.93	0.15	-	47,47,47,47	0
59	MG	2A	3446	1/1	0.97	0.06	-	45,45,45,45	0
59	MG	1B	212	1/1	0.93	0.06	-	49,49,49,49	0
59	MG	2A	3316	1/1	0.87	0.16	-	65,65,65,65	0
59	MG	1A	3234	1/1	0.83	0.23	-	50,50,50,50	0
59	MG	1A	3116	1/1	0.98	0.20	-	40,40,40,40	0
59	MG	1A	3297	1/1	0.95	0.10	-	45,45,45,45	0
59	MG	1a	1799	1/1	0.79	0.29	-	80,80,80,80	0
59	MG	2a	1676	1/1	0.96	0.49	-	47,47,47,47	0
59	MG	2A	3353	1/1	0.98	0.12	-	44,44,44,44	0
59	MG	2A	3464	1/1	0.97	0.09	-	60,60,60,60	0
59	MG	1A	3060	1/1	0.91	0.19	-	45,45,45,45	0
59	MG	2A	3053	1/1	0.95	0.28	-	44,44,44,44	0
59	MG	1A	3410	1/1	0.95	0.10	-	52,52,52,52	0
59	MG	1A	3534	1/1	0.97	0.08	-	38,38,38,38	0
59	MG	1a	1614	1/1	0.93	0.09	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3458	1/1	0.92	0.15	-	52,52,52,52	0
59	MG	2A	3368	1/1	0.88	0.16	-	56,56,56,56	0
59	MG	1A	3379	1/1	0.98	0.16	-	38,38,38,38	0
59	MG	2A	3521	1/1	0.93	0.19	-	69,69,69,69	0
59	MG	1A	3696	1/1	0.90	0.13	-	70,70,70,70	0
59	MG	2A	3427	1/1	0.97	0.20	-	44,44,44,44	0
59	MG	1A	3254	1/1	0.97	0.30	-	43,43,43,43	0
59	MG	1A	3128	1/1	0.88	0.19	-	28,28,28,28	0
59	MG	1a	1757	1/1	0.84	0.12	-	56,56,56,56	0
59	MG	1A	3474	1/1	0.97	0.09	-	42,42,42,42	0
59	MG	2A	3197	1/1	0.91	0.53	-	55,55,55,55	0
59	MG	2A	3578	1/1	0.92	0.12	-	46,46,46,46	0
59	MG	2A	3377	1/1	0.92	0.22	-	44,44,44,44	0
59	MG	2A	3098	1/1	0.97	0.28	-	50,50,50,50	0
59	MG	1A	3223	1/1	0.79	0.41	-	59,59,59,59	0
59	MG	2A	3263	1/1	0.60	0.38	-	69,69,69,69	0
59	MG	1A	3352	1/1	0.96	0.14	-	33,33,33,33	0
59	MG	2A	3434	1/1	0.96	0.27	-	54,54,54,54	0
59	MG	1A	3640	1/1	0.98	0.17	-	41,41,41,41	0
59	MG	2a	1605	1/1	0.95	0.13	-	40,40,40,40	0
59	MG	1A	3548	1/1	0.90	0.09	-	61,61,61,61	0
59	MG	1A	3466	1/1	0.89	0.23	-	26,26,26,26	0
59	MG	1A	3633	1/1	0.95	0.14	-	23,23,23,23	0
59	MG	2a	1722	1/1	0.98	0.21	-	45,45,45,45	0
59	MG	1A	3575	1/1	0.95	0.12	-	52,52,52,52	0
59	MG	1A	3771	1/1	0.74	0.37	-	68,68,68,68	0
59	MG	1A	3430	1/1	0.95	0.08	-	63,63,63,63	0
59	MG	2A	3620	1/1	0.93	0.14	-	58,58,58,58	0
59	MG	1A	3714	1/1	0.93	0.12	-	72,72,72,72	0
59	MG	1A	3344	1/1	0.89	0.10	-	42,42,42,42	0
59	MG	2a	1602	1/1	0.91	0.12	-	47,47,47,47	0
59	MG	2a	1710	1/1	0.98	0.16	-	46,46,46,46	0
59	MG	1A	3298	1/1	0.87	0.23	-	43,43,43,43	0
59	MG	2A	3111	1/1	0.91	0.37	-	47,47,47,47	0
59	MG	1A	3697	1/1	0.98	0.33	-	43,43,43,43	0
59	MG	1A	3698	1/1	0.93	0.16	-	33,33,33,33	0
59	MG	1a	1711	1/1	0.93	0.19	-	52,52,52,52	0
59	MG	2A	3154	1/1	0.94	0.22	-	59,59,59,59	0
59	MG	2A	3275	1/1	0.93	0.09	-	58,58,58,58	0
59	MG	2A	3083	1/1	0.91	0.24	-	55,55,55,55	0
59	MG	1A	3581	1/1	0.96	0.12	-	61,61,61,61	0
59	MG	2A	3525	1/1	0.97	0.25	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3556	1/1	0.97	0.12	-	37,37,37,37	0
59	MG	1A	3652	1/1	0.92	0.27	-	39,39,39,39	0
59	MG	1A	3417	1/1	0.98	0.06	-	51,51,51,51	0
59	MG	1A	3268	1/1	0.96	0.08	-	48,48,48,48	0
59	MG	1A	3316	1/1	0.95	0.07	-	48,48,48,48	0
59	MG	1A	3249	1/1	0.96	0.19	-	40,40,40,40	0
59	MG	1A	3118	1/1	0.83	0.30	-	42,42,42,42	0
59	MG	2A	3361	1/1	0.95	0.10	-	26,26,26,26	0
59	MG	2A	3575	1/1	0.97	0.18	-	36,36,36,36	0
59	MG	1A	3143	1/1	0.95	0.09	-	46,46,46,46	0
59	MG	1A	3081	1/1	0.87	0.20	-	56,56,56,56	0
59	MG	1A	3168	1/1	0.94	0.31	-	60,60,60,60	0
59	MG	1A	3092	1/1	0.97	0.19	-	48,48,48,48	0
59	MG	2A	3561	1/1	0.94	0.25	-	46,46,46,46	0
59	MG	2A	3552	1/1	0.95	0.30	-	39,39,39,39	0
59	MG	1A	3564	1/1	0.99	0.08	-	30,30,30,30	0
59	MG	1A	3598	1/1	0.95	0.21	-	48,48,48,48	0
59	MG	2A	3577	1/1	0.92	0.18	-	56,56,56,56	0
59	MG	1a	1761	1/1	0.98	0.18	-	41,41,41,41	0
59	MG	2A	3486	1/1	0.96	0.17	-	49,49,49,49	0
59	MG	2a	1739	1/1	0.92	0.11	-	51,51,51,51	0
59	MG	2A	3146	1/1	0.92	0.37	-	60,60,60,60	0
59	MG	1a	1652	1/1	0.89	0.11	-	48,48,48,48	0
59	MG	1a	1770	1/1	0.91	0.11	-	67,67,67,67	0
59	MG	1A	3264	1/1	0.97	0.07	-	47,47,47,47	0
59	MG	1B	203	1/1	0.94	0.17	-	43,43,43,43	0
59	MG	2a	1741	1/1	0.96	0.12	-	43,43,43,43	0
59	MG	1A	3296	1/1	0.96	0.21	-	17,17,17,17	0
59	MG	2A	3243	1/1	0.94	0.26	-	39,39,39,39	0
59	MG	2A	3107	1/1	0.97	0.21	-	38,38,38,38	0
59	MG	2A	3068	1/1	0.84	0.29	-	43,43,43,43	0
59	MG	2A	3094	1/1	0.80	0.26	-	53,53,53,53	0
59	MG	2A	3078	1/1	0.90	0.19	-	47,47,47,47	0
59	MG	2a	1692	1/1	0.92	0.31	-	45,45,45,45	0
59	MG	1A	3533	1/1	0.94	0.17	-	53,53,53,53	0
59	MG	1A	3266	1/1	0.89	0.13	-	28,28,28,28	0
59	MG	1A	3305	1/1	0.81	0.13	-	42,42,42,42	0
59	MG	1A	3723	1/1	0.98	0.16	-	36,36,36,36	0
59	MG	2a	1665	1/1	0.92	0.24	-	65,65,65,65	0
59	MG	1A	3531	1/1	0.94	0.17	-	61,61,61,61	0
59	MG	1a	1790	1/1	0.96	0.16	-	51,51,51,51	0
59	MG	1a	1629	1/1	0.86	0.41	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3650	1/1	0.92	0.17	-	49,49,49,49	0
59	MG	2A	3515	1/1	0.91	0.23	-	48,48,48,48	0
59	MG	1A	3186	1/1	0.95	0.23	-	45,45,45,45	0
59	MG	2A	3286	1/1	0.99	0.19	-	30,30,30,30	0
59	MG	2A	3351	1/1	0.85	0.13	-	43,43,43,43	0
59	MG	1a	1764	1/1	0.86	0.11	-	67,67,67,67	0
59	MG	1A	3408	1/1	0.93	0.12	-	55,55,55,55	0
59	MG	1a	1756	1/1	0.89	0.34	-	67,67,67,67	0
59	MG	1a	1634	1/1	0.85	0.12	-	48,48,48,48	0
59	MG	1A	3505	1/1	0.82	0.18	-	55,55,55,55	0
59	MG	1A	3283	1/1	0.96	0.14	-	33,33,33,33	0
59	MG	2A	3025	1/1	0.93	0.12	-	42,42,42,42	0
59	MG	2a	1725	1/1	0.87	0.12	-	64,64,64,64	0
59	MG	1A	3653	1/1	0.90	0.17	-	62,62,62,62	0
59	MG	1A	3763	1/1	0.87	0.35	-	38,38,38,38	0
59	MG	2a	1713	1/1	0.97	0.11	-	43,43,43,43	0
59	MG	1a	1783	1/1	0.96	0.23	-	44,44,44,44	0
59	MG	1A	3041	1/1	0.93	0.18	-	52,52,52,52	0
59	MG	2A	3599	1/1	0.99	0.18	-	46,46,46,46	0
59	MG	2A	3012	1/1	0.95	0.24	-	39,39,39,39	0
59	MG	1A	3165	1/1	0.96	0.08	-	40,40,40,40	0
59	MG	2z	701	1/1	0.94	0.19	-	76,76,76,76	0
59	MG	1A	3288	1/1	0.97	0.17	-	45,45,45,45	0
59	MG	1A	3607	1/1	0.97	0.33	-	27,27,27,27	0
59	MG	2B	211	1/1	0.94	0.23	-	56,56,56,56	0
59	MG	15	102	1/1	0.95	0.12	-	40,40,40,40	0
59	MG	1A	3689	1/1	0.94	0.26	-	57,57,57,57	0
59	MG	1A	3080	1/1	0.97	0.11	-	43,43,43,43	0
59	MG	1A	3420	1/1	0.98	0.14	-	38,38,38,38	0
59	MG	1a	1662	1/1	0.94	0.20	-	58,58,58,58	0
59	MG	1a	1782	1/1	0.94	0.10	-	48,48,48,48	0
59	MG	2a	1609	1/1	0.92	0.27	-	53,53,53,53	0
59	MG	1A	3375	1/1	0.96	0.16	-	12,12,12,12	0
59	MG	1A	3362	1/1	0.89	0.27	-	40,40,40,40	0
59	MG	1a	1728	1/1	0.94	0.13	-	44,44,44,44	0
59	MG	1a	1776	1/1	0.94	0.18	-	66,66,66,66	0
59	MG	2A	3221	1/1	0.88	0.22	-	41,41,41,41	0
59	MG	1a	1681	1/1	0.80	0.19	-	60,60,60,60	0
59	MG	2A	3580	1/1	0.96	0.07	-	53,53,53,53	0
59	MG	1L	3001	1/1	0.97	0.13	-	38,38,38,38	0
59	MG	1A	3222	1/1	0.84	0.23	-	49,49,49,49	0
59	MG	1B	213	1/1	0.91	0.14	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3656	1/1	0.94	0.17	-	45,45,45,45	0
59	MG	2D	301	1/1	0.87	0.30	-	48,48,48,48	0
59	MG	1A	3625	1/1	0.95	0.14	-	58,58,58,58	0
59	MG	1a	1647	1/1	0.86	0.20	-	73,73,73,73	0
59	MG	1A	3425	1/1	0.91	0.14	-	68,68,68,68	0
59	MG	2A	3131	1/1	0.97	0.36	-	40,40,40,40	0
59	MG	1a	1651	1/1	0.97	0.26	-	54,54,54,54	0
59	MG	2A	3104	1/1	0.92	0.15	-	53,53,53,53	0
59	MG	1A	3530	1/1	0.94	0.22	-	34,34,34,34	0
59	MG	1A	3427	1/1	0.96	0.06	-	30,30,30,30	0
59	MG	1A	3378	1/1	0.94	0.19	-	24,24,24,24	0
59	MG	1A	3189	1/1	0.96	0.05	-	44,44,44,44	0
59	MG	1A	3755	1/1	0.95	0.19	-	53,53,53,53	0
59	MG	1a	1759	1/1	0.88	0.17	-	65,65,65,65	0
59	MG	1A	3721	1/1	0.96	0.10	-	31,31,31,31	0
59	MG	1A	3706	1/1	0.93	0.14	-	46,46,46,46	0
59	MG	2A	3145	1/1	0.78	0.24	-	55,55,55,55	0
59	MG	2A	3547	1/1	0.99	0.25	-	42,42,42,42	0
59	MG	2A	3460	1/1	0.85	0.18	-	59,59,59,59	0
59	MG	2A	3532	1/1	0.98	0.37	-	35,35,35,35	0
59	MG	2A	3564	1/1	0.91	0.33	-	72,72,72,72	0
59	MG	2A	3496	1/1	0.98	0.36	-	41,41,41,41	0
59	MG	2A	3297	1/1	0.97	0.09	-	29,29,29,29	0
59	MG	2A	3440	1/1	0.94	0.14	-	51,51,51,51	0
59	MG	1A	3372	1/1	0.98	0.11	-	19,19,19,19	0
59	MG	2P	8001	1/1	0.95	0.09	-	30,30,30,30	0
59	MG	1a	1788	1/1	0.98	0.19	-	45,45,45,45	0
59	MG	1A	3670	1/1	0.88	0.16	-	60,60,60,60	0
59	MG	2A	3404	1/1	0.88	0.22	-	30,30,30,30	0
59	MG	2A	3385	1/1	0.95	0.10	-	45,45,45,45	0
59	MG	1a	1699	1/1	0.91	0.22	-	60,60,60,60	0
59	MG	2A	3550	1/1	0.88	0.23	-	50,50,50,50	0
59	MG	1O	3002	1/1	0.95	0.22	-	27,27,27,27	0
59	MG	1A	3432	1/1	0.97	0.22	-	47,47,47,47	0
59	MG	2A	3136	1/1	0.78	0.32	-	52,52,52,52	0
59	MG	1A	3162	1/1	0.86	0.34	-	46,46,46,46	0
59	MG	1A	3107	1/1	0.94	0.20	-	37,37,37,37	0
59	MG	1A	3132	1/1	0.97	0.14	-	36,36,36,36	0
59	MG	1A	3611	1/1	0.83	0.14	-	46,46,46,46	0
59	MG	2A	3588	1/1	0.97	0.24	-	32,32,32,32	0
59	MG	1A	3734	1/1	0.95	0.24	-	45,45,45,45	0
59	MG	1a	1674	1/1	0.94	0.12	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2B	203	1/1	0.97	0.07	-	62,62,62,62	0
59	MG	1A	3108	1/1	0.94	0.36	-	38,38,38,38	0
59	MG	1A	3221	1/1	0.94	0.29	-	38,38,38,38	0
59	MG	1A	3311	1/1	0.86	0.16	-	40,40,40,40	0
59	MG	2a	1608	1/1	0.96	0.26	-	56,56,56,56	0
59	MG	1A	3467	1/1	0.88	0.21	-	27,27,27,27	0
59	MG	2A	3510	1/1	0.91	0.18	-	35,35,35,35	0
59	MG	1a	1729	1/1	0.88	0.41	-	83,83,83,83	0
59	MG	10	102	1/1	0.90	0.19	-	44,44,44,44	0
59	MG	1A	3749	1/1	0.90	0.26	-	54,54,54,54	0
59	MG	1A	3198	1/1	0.92	0.09	-	60,60,60,60	0
59	MG	1A	3641	1/1	0.94	0.30	-	49,49,49,49	0
59	MG	2D	304	1/1	0.93	0.25	-	51,51,51,51	0
59	MG	1A	3036	1/1	0.86	0.28	-	38,38,38,38	0
59	MG	1w	3003	1/1	0.89	0.12	-	54,54,54,54	0
59	MG	1A	3431	1/1	0.96	0.05	-	44,44,44,44	0
59	MG	2A	3120	1/1	0.95	0.19	-	53,53,53,53	0
59	MG	1a	1701	1/1	0.78	0.24	-	65,65,65,65	0
59	MG	2a	1754	1/1	0.70	0.63	-	61,61,61,61	0
59	MG	1a	1646	1/1	0.95	0.32	-	43,43,43,43	0
59	MG	2a	1730	1/1	0.92	0.11	-	47,47,47,47	0
59	MG	1a	1618	1/1	0.89	0.29	-	42,42,42,42	0
59	MG	1A	3024	1/1	0.94	0.07	-	47,47,47,47	0
59	MG	1a	1719	1/1	0.94	0.24	-	59,59,59,59	0
59	MG	1A	3747	1/1	0.95	0.11	-	42,42,42,42	0
59	MG	1A	3511	1/1	0.94	0.13	-	37,37,37,37	0
59	MG	2A	3264	1/1	0.88	0.24	-	49,49,49,49	0
59	MG	2A	3569	1/1	0.93	0.12	-	60,60,60,60	0
59	MG	1A	3111	1/1	0.97	0.39	-	39,39,39,39	0
59	MG	2a	1761	1/1	0.94	0.12	-	39,39,39,39	0
59	MG	2a	1652	1/1	0.92	0.16	-	36,36,36,36	0
59	MG	2A	3389	1/1	0.95	0.20	-	39,39,39,39	0
59	MG	1A	3014	1/1	0.94	0.11	-	41,41,41,41	0
59	MG	1a	1645	1/1	0.94	0.21	-	45,45,45,45	0
59	MG	1A	3751	1/1	0.90	0.13	-	43,43,43,43	0
59	MG	1A	3016	1/1	0.96	0.27	-	37,37,37,37	0
59	MG	2a	1759	1/1	0.86	0.31	-	62,62,62,62	0
59	MG	1A	3680	1/1	0.86	0.30	-	46,46,46,46	0
59	MG	2q	201	1/1	0.92	0.17	-	52,52,52,52	0
59	MG	2a	1751	1/1	0.86	0.36	-	104,104,104,104	0
59	MG	1A	3461	1/1	0.83	0.17	-	31,31,31,31	0
59	MG	1a	1796	1/1	0.94	0.22	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3720	1/1	0.95	0.14	-	64,64,64,64	0
59	MG	1a	1664	1/1	0.94	0.11	-	48,48,48,48	0
59	MG	2a	1707	1/1	0.92	0.20	-	49,49,49,49	0
59	MG	1A	3046	1/1	0.88	0.27	-	57,57,57,57	0
59	MG	1A	3113	1/1	0.90	0.28	-	27,27,27,27	0
59	MG	1W	201	1/1	0.94	0.20	-	32,32,32,32	0
59	MG	2a	1740	1/1	0.95	0.31	-	53,53,53,53	0
59	MG	2A	3014	1/1	0.98	0.16	-	34,34,34,34	0
59	MG	2A	3173	1/1	0.92	0.12	-	52,52,52,52	0
59	MG	1A	3646	1/1	0.90	0.18	-	48,48,48,48	0
59	MG	1A	3577	1/1	0.94	0.14	-	60,60,60,60	0
59	MG	2A	3505	1/1	0.94	0.14	-	46,46,46,46	0
59	MG	2A	3181	1/1	0.90	0.20	-	37,37,37,37	0
59	MG	1A	3083	1/1	0.90	0.38	-	55,55,55,55	0
59	MG	2A	3208	1/1	0.93	0.31	-	47,47,47,47	0
59	MG	2A	3313	1/1	0.96	0.22	-	30,30,30,30	0
59	MG	1a	1643	1/1	0.73	0.12	-	50,50,50,50	0
59	MG	1A	3606	1/1	0.88	0.34	-	60,60,60,60	0
59	MG	1A	3259	1/1	0.77	0.14	-	45,45,45,45	0
59	MG	1A	3326	1/1	0.97	0.14	-	34,34,34,34	0
59	MG	1A	3390	1/1	0.89	0.21	-	53,53,53,53	0
59	MG	1A	3572	1/1	0.97	0.13	-	43,43,43,43	0
59	MG	1A	3717	1/1	0.83	0.35	-	89,89,89,89	0
59	MG	2a	1716	1/1	0.95	0.18	-	62,62,62,62	0
59	MG	2A	3063	1/1	0.81	0.28	-	52,52,52,52	0
59	MG	1A	3597	1/1	0.95	0.11	-	50,50,50,50	0
59	MG	2a	1772	1/1	0.97	0.17	-	64,64,64,64	0
59	MG	1a	1750	1/1	0.97	0.11	-	86,86,86,86	0
59	MG	1A	3027	1/1	0.84	0.53	-	34,34,34,34	0
59	MG	1A	3666	1/1	0.98	0.17	-	32,32,32,32	0
59	MG	2A	3463	1/1	0.96	0.10	-	45,45,45,45	0
59	MG	2A	3563	1/1	0.98	0.20	-	41,41,41,41	0
59	MG	1A	3424	1/1	0.99	0.19	-	34,34,34,34	0
59	MG	1A	3255	1/1	0.90	0.23	-	63,63,63,63	0
59	MG	1w	3001	1/1	0.96	0.07	-	55,55,55,55	0
59	MG	1A	3058	1/1	0.97	0.48	-	34,34,34,34	0
59	MG	2a	1745	1/1	0.96	0.21	-	60,60,60,60	0
59	MG	2A	3445	1/1	0.93	0.12	-	52,52,52,52	0
59	MG	1A	3662	1/1	0.97	0.08	-	31,31,31,31	0
59	MG	1A	3630	1/1	0.90	0.11	-	51,51,51,51	0
59	MG	1a	1725	1/1	0.98	0.15	-	50,50,50,50	0
59	MG	1A	3458	1/1	0.97	0.09	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	10	101	1/1	0.91	0.18	-	38,38,38,38	0
59	MG	1A	3302	1/1	0.95	0.20	-	29,29,29,29	0
59	MG	1A	3242	1/1	0.97	0.73	-	51,51,51,51	0
59	MG	1A	3750	1/1	0.92	0.21	-	53,53,53,53	0
59	MG	2A	3115	1/1	0.89	0.31	-	42,42,42,42	0
59	MG	1a	1609	1/1	0.97	0.23	-	37,37,37,37	0
59	MG	2a	1771	1/1	0.98	0.17	-	72,72,72,72	0
59	MG	2A	3051	1/1	0.96	0.15	-	35,35,35,35	0
59	MG	1A	3200	1/1	0.94	0.15	-	40,40,40,40	0
59	MG	1A	3728	1/1	0.98	0.21	-	35,35,35,35	0
59	MG	1A	3476	1/1	0.90	0.19	-	29,29,29,29	0
59	MG	2A	3554	1/1	0.96	0.16	-	47,47,47,47	0
59	MG	2a	1753	1/1	0.95	0.09	-	39,39,39,39	0
59	MG	1A	3506	1/1	0.86	0.26	-	33,33,33,33	0
59	MG	1A	3599	1/1	0.93	0.21	-	51,51,51,51	0
59	MG	2A	3408	1/1	0.95	0.14	-	33,33,33,33	0
59	MG	1A	3214	1/1	0.95	0.84	-	61,61,61,61	0
59	MG	1A	3486	1/1	0.93	0.07	-	65,65,65,65	0
59	MG	1B	222	1/1	0.96	0.09	-	41,41,41,41	0
59	MG	2M	202	1/1	0.90	0.17	-	55,55,55,55	0
59	MG	1a	1762	1/1	0.90	0.32	-	62,62,62,62	0
59	MG	2A	3049	1/1	0.93	0.19	-	38,38,38,38	0
59	MG	1A	3161	1/1	0.91	0.27	-	54,54,54,54	0
59	MG	2a	1627	1/1	0.88	0.39	-	44,44,44,44	0
59	MG	1B	211	1/1	0.95	0.10	-	32,32,32,32	0
59	MG	1a	1755	1/1	0.98	0.11	-	42,42,42,42	0
59	MG	2a	1611	1/1	0.94	0.43	-	70,70,70,70	0
59	MG	1A	3704	1/1	0.85	0.38	-	71,71,71,71	0
59	MG	2A	3040	1/1	0.90	0.23	-	45,45,45,45	0
59	MG	2A	3469	1/1	0.92	0.17	-	60,60,60,60	0
59	MG	2w	3002	1/1	0.94	0.07	-	52,52,52,52	0
59	MG	1A	3106	1/1	0.93	0.21	-	48,48,48,48	0
59	MG	2A	3438	1/1	0.89	0.23	-	54,54,54,54	0
59	MG	1A	3245	1/1	0.92	0.46	-	31,31,31,31	0
59	MG	1A	3180	1/1	0.86	0.23	-	50,50,50,50	0
59	MG	2A	3462	1/1	0.96	0.28	-	40,40,40,40	0
59	MG	1A	3247	1/1	0.93	0.42	-	35,35,35,35	0
59	MG	2A	3054	1/1	0.89	0.29	-	48,48,48,48	0
59	MG	1A	3578	1/1	0.96	0.19	-	40,40,40,40	0
59	MG	2A	3099	1/1	0.95	0.18	-	58,58,58,58	0
59	MG	2a	1659	1/1	0.84	0.22	-	46,46,46,46	0
59	MG	1B	214	1/1	0.99	0.15	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3418	1/1	0.98	0.13	-	46,46,46,46	0
59	MG	2a	1643	1/1	0.93	0.29	-	39,39,39,39	0
59	MG	1A	3726	1/1	0.92	0.28	-	34,34,34,34	0
59	MG	1A	3145	1/1	0.93	0.16	-	47,47,47,47	0
59	MG	1a	1735	1/1	0.97	0.12	-	69,69,69,69	0
59	MG	2A	3437	1/1	0.94	0.12	-	37,37,37,37	0
59	MG	2A	3036	1/1	0.87	0.14	-	53,53,53,53	0
59	MG	1a	1768	1/1	0.98	0.17	-	56,56,56,56	0
59	MG	1a	1738	1/1	0.96	0.18	-	66,66,66,66	0
59	MG	2A	3254	1/1	0.94	0.26	-	35,35,35,35	0
59	MG	1A	3312	1/1	0.97	0.14	-	30,30,30,30	0
59	MG	2A	3431	1/1	0.95	0.22	-	46,46,46,46	0
59	MG	1A	3097	1/1	0.90	0.17	-	55,55,55,55	0
59	MG	2A	3607	1/1	0.93	0.20	-	32,32,32,32	0
59	MG	1A	3627	1/1	0.98	0.07	-	34,34,34,34	0
59	MG	2A	3032	1/1	0.79	0.33	-	57,57,57,57	0
59	MG	2a	1736	1/1	0.89	0.11	-	42,42,42,42	0
59	MG	2A	3516	1/1	0.81	0.08	-	78,78,78,78	0
59	MG	2A	3116	1/1	0.94	0.12	-	34,34,34,34	0
59	MG	1A	3428	1/1	0.98	0.18	-	64,64,64,64	0
59	MG	1B	206	1/1	0.96	0.08	-	33,33,33,33	0
59	MG	2A	3506	1/1	0.97	0.11	-	56,56,56,56	0
59	MG	1Y	102	1/1	0.97	0.07	-	31,31,31,31	0
59	MG	1A	3154	1/1	0.94	0.09	-	64,64,64,64	0
59	MG	2A	3380	1/1	0.97	0.10	-	36,36,36,36	0
59	MG	2A	3123	1/1	0.97	0.20	-	39,39,39,39	0
59	MG	1A	3063	1/1	0.95	0.09	-	47,47,47,47	0
59	MG	2a	1683	1/1	0.91	0.36	-	59,59,59,59	0
59	MG	2A	3576	1/1	0.91	0.15	-	40,40,40,40	0
59	MG	2A	3089	1/1	0.92	0.15	-	51,51,51,51	0
59	MG	1a	1777	1/1	0.93	0.18	-	53,53,53,53	0
59	MG	1A	3104	1/1	0.52	0.48	-	52,52,52,52	0
59	MG	2w	3001	1/1	0.84	0.15	-	64,64,64,64	0
59	MG	1A	3385	1/1	0.96	0.14	-	43,43,43,43	0
59	MG	1z	702	1/1	0.97	0.33	-	39,39,39,39	0
59	MG	2a	1728	1/1	0.93	0.15	-	60,60,60,60	0
59	MG	2a	1720	1/1	0.91	0.13	-	63,63,63,63	0
59	MG	2A	3442	1/1	0.97	0.14	-	49,49,49,49	0
59	MG	2A	3340	1/1	0.96	0.17	-	44,44,44,44	0
59	MG	1A	3323	1/1	0.95	0.27	-	33,33,33,33	0
59	MG	2A	3005	1/1	0.99	0.09	-	27,27,27,27	0
59	MG	2a	1714	1/1	0.95	0.26	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3510	1/1	0.97	0.10	-	42,42,42,42	0
59	MG	1a	1794	1/1	0.96	0.08	-	71,71,71,71	0
59	MG	1A	3513	1/1	0.92	0.18	-	43,43,43,43	0
59	MG	2A	3235	1/1	0.90	0.24	-	39,39,39,39	0
59	MG	2A	3349	1/1	0.81	0.28	-	56,56,56,56	0
59	MG	2A	3038	1/1	0.83	0.22	-	43,43,43,43	0
59	MG	1A	3719	1/1	0.90	0.12	-	68,68,68,68	0
59	MG	1A	3134	1/1	0.93	0.15	-	54,54,54,54	0
59	MG	2A	3338	1/1	0.95	0.18	-	31,31,31,31	0
59	MG	1A	3237	1/1	0.91	0.14	-	55,55,55,55	0
59	MG	2a	1695	1/1	0.85	0.23	-	61,61,61,61	0
59	MG	1a	1683	1/1	0.86	0.15	-	75,75,75,75	0
59	MG	1A	3077	1/1	0.96	0.22	-	38,38,38,38	0
59	MG	2A	3218	1/1	0.88	0.18	-	50,50,50,50	0
59	MG	1A	3051	1/1	0.98	0.15	-	35,35,35,35	0
59	MG	1a	1775	1/1	0.99	0.34	-	46,46,46,46	0
59	MG	1A	3687	1/1	0.99	0.18	-	69,69,69,69	0
59	MG	1A	3205	1/1	0.91	0.39	-	56,56,56,56	0
59	MG	2A	3140	1/1	0.92	0.27	-	39,39,39,39	0
59	MG	1a	1639	1/1	0.82	0.18	-	67,67,67,67	0
59	MG	2a	1746	1/1	0.98	0.21	-	43,43,43,43	0
59	MG	1A	3540	1/1	0.97	0.19	-	47,47,47,47	0
59	MG	2A	3230	1/1	0.93	0.09	-	54,54,54,54	0
59	MG	1A	3528	1/1	0.96	0.18	-	49,49,49,49	0
59	MG	2A	3210	1/1	0.85	0.09	-	45,45,45,45	0
59	MG	1A	3293	1/1	0.91	0.08	-	41,41,41,41	0
59	MG	2l	201	1/1	0.85	0.16	-	64,64,64,64	0
59	MG	2A	3270	1/1	0.90	0.18	-	52,52,52,52	0
59	MG	2A	3545	1/1	0.97	0.17	-	38,38,38,38	0
59	MG	1A	3277	1/1	0.96	0.12	-	36,36,36,36	0
59	MG	1A	3557	1/1	0.96	0.14	-	44,44,44,44	0
59	MG	1B	219	1/1	0.90	0.21	-	71,71,71,71	0
59	MG	1A	3155	1/1	0.92	0.13	-	31,31,31,31	0
59	MG	2A	3149	1/1	0.96	0.30	-	46,46,46,46	0
59	MG	1A	3341	1/1	0.98	0.15	-	29,29,29,29	0
59	MG	1A	3745	1/1	0.88	0.17	-	87,87,87,87	0
59	MG	1A	3110	1/1	0.95	0.27	-	61,61,61,61	0
59	MG	1A	3672	1/1	0.95	0.06	-	47,47,47,47	0
59	MG	2a	1631	1/1	0.96	0.15	-	48,48,48,48	0
59	MG	2A	3522	1/1	0.94	0.11	-	38,38,38,38	0
59	MG	1A	3183	1/1	0.95	0.24	-	33,33,33,33	0
59	MG	1a	1723	1/1	0.98	0.16	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3395	1/1	0.92	0.09	-	53,53,53,53	0
59	MG	2A	3002	1/1	0.81	0.20	-	40,40,40,40	0
59	MG	1A	3061	1/1	0.96	0.35	-	21,21,21,21	0
59	MG	2a	1610	1/1	0.94	0.36	-	52,52,52,52	0
59	MG	1A	3686	1/1	0.93	0.12	-	62,62,62,62	0
59	MG	1A	3062	1/1	0.97	0.17	-	17,17,17,17	0
59	MG	2A	3560	1/1	0.94	0.35	-	32,32,32,32	0
59	MG	1a	1660	1/1	0.83	0.37	-	59,59,59,59	0
59	MG	2A	3034	1/1	0.92	0.18	-	47,47,47,47	0
59	MG	1H	3001	1/1	0.86	0.15	-	51,51,51,51	0
59	MG	2a	1656	1/1	0.91	0.24	-	61,61,61,61	0
59	MG	14	101	1/1	0.97	0.08	-	46,46,46,46	0
59	MG	16	101	1/1	0.98	0.15	-	24,24,24,24	0
59	MG	1E	304	1/1	0.94	0.21	-	58,58,58,58	0
59	MG	1A	3231	1/1	0.92	0.69	-	45,45,45,45	0
59	MG	1A	3538	1/1	0.91	0.13	-	63,63,63,63	0
59	MG	1A	3213	1/1	0.89	0.16	-	47,47,47,47	0
59	MG	2A	3544	1/1	0.88	0.33	-	53,53,53,53	0
59	MG	2A	3585	1/1	0.97	0.11	-	49,49,49,49	0
59	MG	2A	3311	1/1	0.77	0.31	-	63,63,63,63	0
59	MG	2A	3075	1/1	0.91	0.09	-	46,46,46,46	0
59	MG	2A	3101	1/1	0.84	0.21	-	50,50,50,50	0
59	MG	1A	3400	1/1	0.95	0.06	-	66,66,66,66	0
59	MG	2A	3604	1/1	0.93	0.16	-	40,40,40,40	0
59	MG	2A	3519	1/1	0.96	0.06	-	31,31,31,31	0
59	MG	1P	201	1/1	0.95	0.31	-	52,52,52,52	0
59	MG	2A	3612	1/1	0.91	0.21	-	46,46,46,46	0
59	MG	1A	3133	1/1	0.89	0.27	-	44,44,44,44	0
59	MG	1a	1751	1/1	0.96	0.42	-	48,48,48,48	0
59	MG	1B	220	1/1	0.93	0.09	-	38,38,38,38	0
59	MG	2A	3321	1/1	0.94	0.09	-	31,31,31,31	0
59	MG	2A	3305	1/1	0.97	0.09	-	46,46,46,46	0
59	MG	1A	3483	1/1	0.71	0.20	-	40,40,40,40	0
59	MG	2a	1705	1/1	0.86	0.17	-	52,52,52,52	0
59	MG	1A	3637	1/1	0.89	0.14	-	59,59,59,59	0
59	MG	1A	3610	1/1	0.95	0.31	-	46,46,46,46	0
59	MG	2A	3483	1/1	0.97	0.10	-	47,47,47,47	0
59	MG	2A	3137	1/1	0.96	0.23	-	40,40,40,40	0
59	MG	1A	3690	1/1	0.96	0.07	-	56,56,56,56	0
59	MG	1A	3294	1/1	0.90	0.18	-	18,18,18,18	0
59	MG	1A	3594	1/1	0.87	0.11	-	22,22,22,22	0
59	MG	1A	3054	1/1	0.97	0.37	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3171	1/1	0.90	0.23	-	54,54,54,54	0
59	MG	2A	3571	1/1	0.96	0.33	-	36,36,36,36	0
59	MG	2A	3066	1/1	0.88	0.23	-	45,45,45,45	0
59	MG	2A	3364	1/1	0.97	0.13	-	30,30,30,30	0
59	MG	1A	3096	1/1	0.94	0.18	-	47,47,47,47	0
59	MG	1A	3235	1/1	0.89	0.15	-	49,49,49,49	0
59	MG	2A	3308	1/1	0.95	0.23	-	29,29,29,29	0
59	MG	2j	8001	1/1	0.84	0.22	-	65,65,65,65	0
59	MG	1A	3668	1/1	0.92	0.11	-	48,48,48,48	0
59	MG	1A	3592	1/1	0.97	0.16	-	44,44,44,44	0
59	MG	2A	3206	1/1	0.95	0.31	-	39,39,39,39	0
59	MG	1A	3629	1/1	0.97	0.12	-	27,27,27,27	0
59	MG	2A	3135	1/1	0.89	0.16	-	45,45,45,45	0
59	MG	1a	1758	1/1	0.93	0.12	-	79,79,79,79	0
59	MG	2a	1703	1/1	0.86	0.16	-	50,50,50,50	0
59	MG	2A	3424	1/1	0.95	0.14	-	23,23,23,23	0
59	MG	2a	1681	1/1	0.93	0.56	-	58,58,58,58	0
59	MG	1A	3287	1/1	0.93	0.19	-	22,22,22,22	0
59	MG	1A	3695	1/1	0.91	0.18	-	38,38,38,38	0
59	MG	1A	3006	1/1	0.94	0.15	-	33,33,33,33	0
59	MG	2a	1622	1/1	0.94	0.24	-	33,33,33,33	0
59	MG	2A	3180	1/1	0.78	0.15	-	56,56,56,56	0
59	MG	2A	3163	1/1	0.92	0.21	-	47,47,47,47	0
59	MG	1A	3342	1/1	0.94	0.10	-	48,48,48,48	0
59	MG	1F	306	1/1	0.70	0.34	-	46,46,46,46	0
59	MG	1A	3673	1/1	0.77	0.20	-	70,70,70,70	0
59	MG	2W	502	1/1	0.94	0.13	-	45,45,45,45	0
59	MG	2A	3182	1/1	0.89	0.17	-	41,41,41,41	0
59	MG	1A	3541	1/1	0.95	0.10	-	53,53,53,53	0
59	MG	2a	1657	1/1	0.57	0.45	-	66,66,66,66	0
59	MG	1a	1785	1/1	0.95	0.32	-	41,41,41,41	0
59	MG	2A	3495	1/1	0.95	0.07	-	56,56,56,56	0
59	MG	1a	1734	1/1	0.96	0.15	-	36,36,36,36	0
59	MG	1A	3491	1/1	0.99	0.09	-	41,41,41,41	0
59	MG	2A	3168	1/1	0.96	0.22	-	45,45,45,45	0
59	MG	1A	3684	1/1	0.94	0.18	-	57,57,57,57	0
59	MG	2A	3381	1/1	0.95	0.16	-	42,42,42,42	0
59	MG	2A	3602	1/1	0.88	0.26	-	62,62,62,62	0
59	MG	1a	1752	1/1	0.92	0.28	-	75,75,75,75	0
59	MG	13	102	1/1	0.94	0.17	-	34,34,34,34	0
59	MG	1a	1654	1/1	0.83	0.14	-	42,42,42,42	0
59	MG	1A	3608	1/1	0.93	0.21	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3591	1/1	0.99	0.13	-	31,31,31,31	0
59	MG	1A	3025	1/1	0.94	0.17	-	42,42,42,42	0
59	MG	1A	3443	1/1	0.97	0.11	-	49,49,49,49	0
59	MG	2A	3367	1/1	0.89	0.16	-	45,45,45,45	0
59	MG	1a	1623	1/1	0.93	0.65	-	65,65,65,65	0
59	MG	2B	206	1/1	0.41	0.27	-	67,67,67,67	0
59	MG	1A	3725	1/1	0.94	0.12	-	43,43,43,43	0
59	MG	1A	3257	1/1	0.91	0.26	-	34,34,34,34	0
59	MG	2B	205	1/1	0.95	0.30	-	56,56,56,56	0
59	MG	2a	1644	1/1	0.94	0.28	-	50,50,50,50	0
59	MG	1A	3645	1/1	0.93	0.42	-	40,40,40,40	0
59	MG	2A	3582	1/1	0.94	0.13	-	62,62,62,62	0
59	MG	2a	1756	1/1	0.96	0.28	-	73,73,73,73	0
59	MG	1a	1712	1/1	0.92	0.21	-	69,69,69,69	0
59	MG	1A	3192	1/1	0.90	0.23	-	47,47,47,47	0
59	MG	1A	3708	1/1	0.96	0.18	-	51,51,51,51	0
59	MG	1A	3002	1/1	0.79	0.22	-	44,44,44,44	0
59	MG	2A	3531	1/1	0.97	0.29	-	38,38,38,38	0
59	MG	2A	3467	1/1	0.96	0.10	-	35,35,35,35	0
59	MG	2A	3176	1/1	0.86	0.15	-	38,38,38,38	0
59	MG	2A	3127	1/1	0.96	0.20	-	38,38,38,38	0
59	MG	2A	3114	1/1	0.95	0.46	-	37,37,37,37	0
59	MG	2A	3538	1/1	0.87	0.31	-	28,28,28,28	0
59	MG	2A	3196	1/1	0.97	0.22	-	51,51,51,51	0
59	MG	1A	3413	1/1	0.96	0.29	-	47,47,47,47	0
59	MG	1a	1622	1/1	0.70	0.41	-	64,64,64,64	0
59	MG	2A	3356	1/1	0.91	0.09	-	58,58,58,58	0
59	MG	2A	3387	1/1	0.98	0.12	-	46,46,46,46	0
59	MG	1A	3035	1/1	0.93	0.10	-	38,38,38,38	0
59	MG	1a	1694	1/1	0.95	0.14	-	39,39,39,39	0
59	MG	2A	3227	1/1	0.92	0.21	-	49,49,49,49	0
59	MG	1A	3665	1/1	0.91	0.10	-	70,70,70,70	0
59	MG	1d	502	1/1	0.95	0.36	-	39,39,39,39	0
59	MG	2A	3133	1/1	0.94	0.14	-	52,52,52,52	0
59	MG	2A	3376	1/1	0.94	0.12	-	41,41,41,41	0
59	MG	2a	1670	1/1	0.92	0.15	-	51,51,51,51	0
59	MG	2O	3001	1/1	0.95	0.24	-	42,42,42,42	0
59	MG	1a	1640	1/1	0.94	0.11	-	44,44,44,44	0
59	MG	1a	1730	1/1	0.97	0.15	-	49,49,49,49	0
59	MG	2A	3609	1/1	0.91	0.12	-	51,51,51,51	0
59	MG	17	103	1/1	0.94	0.18	-	34,34,34,34	0
59	MG	1X	3001	1/1	0.92	0.28	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3736	1/1	0.93	0.16	-	69,69,69,69	0
59	MG	1A	3542	1/1	0.96	0.23	-	67,67,67,67	0
59	MG	2a	1685	1/1	0.95	0.25	-	51,51,51,51	0
59	MG	2A	3573	1/1	0.95	0.26	-	43,43,43,43	0
59	MG	1A	3238	1/1	0.94	0.23	-	29,29,29,29	0
59	MG	2a	1619	1/1	0.95	0.51	-	46,46,46,46	0
59	MG	1A	3384	1/1	0.93	0.10	-	25,25,25,25	0
59	MG	1A	3335	1/1	0.92	0.12	-	46,46,46,46	0
59	MG	1a	1746	1/1	0.96	0.06	-	76,76,76,76	0
59	MG	2A	3459	1/1	0.98	0.08	-	48,48,48,48	0
59	MG	1A	3485	1/1	0.98	0.12	-	29,29,29,29	0
59	MG	1a	1707	1/1	0.85	0.20	-	60,60,60,60	0
59	MG	1A	3250	1/1	0.92	0.18	-	51,51,51,51	0
59	MG	1A	3281	1/1	0.94	0.15	-	42,42,42,42	0
59	MG	1A	3504	1/1	0.96	0.19	-	21,21,21,21	0
59	MG	2A	3363	1/1	0.88	0.12	-	53,53,53,53	0
59	MG	2A	3241	1/1	0.85	0.13	-	52,52,52,52	0
59	MG	1A	3094	1/1	0.95	0.23	-	43,43,43,43	0
59	MG	1A	3087	1/1	0.95	0.56	-	48,48,48,48	0
59	MG	1a	1637	1/1	0.97	0.39	-	42,42,42,42	0
59	MG	2a	1632	1/1	0.95	0.12	-	45,45,45,45	0
59	MG	1w	3006	1/1	0.95	0.19	-	72,72,72,72	0
59	MG	2A	3212	1/1	0.89	0.23	-	46,46,46,46	0
59	MG	2E	301	1/1	0.96	0.26	-	20,20,20,20	0
59	MG	2A	3284	1/1	0.95	0.15	-	53,53,53,53	0
59	MG	2A	3155	1/1	0.99	0.21	-	27,27,27,27	0
59	MG	1A	3395	1/1	0.96	0.22	-	42,42,42,42	0
59	MG	2A	3378	1/1	0.98	0.23	-	35,35,35,35	0
59	MG	1a	1742	1/1	0.89	0.17	-	43,43,43,43	0
59	MG	1a	1791	1/1	0.94	0.17	-	52,52,52,52	0
59	MG	1a	1772	1/1	0.96	0.20	-	59,59,59,59	0
59	MG	2a	1648	1/1	0.95	0.24	-	61,61,61,61	0
59	MG	1a	1766	1/1	0.87	0.37	-	67,67,67,67	0
59	MG	2A	3276	1/1	0.89	0.17	-	61,61,61,61	0
59	MG	1a	1655	1/1	0.89	0.25	-	53,53,53,53	0
59	MG	2a	1765	1/1	0.63	0.34	-	79,79,79,79	0
59	MG	2A	3109	1/1	0.94	0.26	-	47,47,47,47	0
59	MG	2A	3245	1/1	0.94	0.20	-	51,51,51,51	0
59	MG	2A	3334	1/1	0.89	0.19	-	54,54,54,54	0
59	MG	1B	223	1/1	0.96	0.16	-	46,46,46,46	0
59	MG	1B	208	1/1	0.90	0.23	-	38,38,38,38	0
59	MG	1A	3252	1/1	0.96	0.11	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3166	1/1	0.89	0.12	-	43,43,43,43	0
59	MG	2A	3415	1/1	0.95	0.30	-	34,34,34,34	0
59	MG	1A	3246	1/1	0.91	0.15	-	39,39,39,39	0
59	MG	2A	3260	1/1	0.95	0.09	-	49,49,49,49	0
59	MG	1A	3560	1/1	0.93	0.14	-	56,56,56,56	0
59	MG	2A	3084	1/1	0.97	0.09	-	33,33,33,33	0
59	MG	1A	3351	1/1	0.96	0.09	-	29,29,29,29	0
59	MG	2A	3061	1/1	0.87	0.23	-	31,31,31,31	0
59	MG	1A	3279	1/1	0.96	0.12	-	45,45,45,45	0
59	MG	1a	1610	1/1	0.82	0.17	-	50,50,50,50	0
59	MG	2a	1654	1/1	0.93	0.22	-	29,29,29,29	0
59	MG	2A	3433	1/1	0.98	0.10	-	35,35,35,35	0
59	MG	2A	3283	1/1	0.96	0.08	-	32,32,32,32	0
59	MG	2A	3597	1/1	0.96	0.21	-	43,43,43,43	0
59	MG	1A	3623	1/1	0.96	0.20	-	16,16,16,16	0
59	MG	1a	1663	1/1	0.91	0.20	-	79,79,79,79	0
59	MG	1A	3777	1/1	0.94	0.11	-	45,45,45,45	0
59	MG	1a	1601	1/1	0.93	0.12	-	30,30,30,30	0
59	MG	1a	1692	1/1	0.94	0.28	-	57,57,57,57	0
59	MG	2A	3600	1/1	0.92	0.25	-	47,47,47,47	0
59	MG	1A	3367	1/1	0.99	0.15	-	49,49,49,49	0
59	MG	2a	1639	1/1	0.91	0.26	-	43,43,43,43	0
59	MG	1a	1716	1/1	0.87	0.39	-	63,63,63,63	0
59	MG	2a	1603	1/1	0.79	0.74	-	65,65,65,65	0
59	MG	2a	1763	1/1	0.93	0.32	-	71,71,71,71	0
59	MG	2a	1662	1/1	0.71	0.38	-	62,62,62,62	0
59	MG	2A	3209	1/1	0.93	0.23	-	46,46,46,46	0
59	MG	2A	3336	1/1	0.95	0.13	-	30,30,30,30	0
59	MG	1a	1702	1/1	0.88	0.15	-	51,51,51,51	0
59	MG	2A	3271	1/1	0.95	0.17	-	58,58,58,58	0
59	MG	1a	1648	1/1	0.97	0.17	-	60,60,60,60	0
59	MG	1A	3003	1/1	0.98	0.09	-	29,29,29,29	0
59	MG	2A	3310	1/1	0.93	0.16	-	55,55,55,55	0
59	MG	1A	3225	1/1	0.95	0.17	-	39,39,39,39	0
59	MG	1f	3001	1/1	0.98	0.30	-	39,39,39,39	0
59	MG	2A	3499	1/1	0.95	0.12	-	53,53,53,53	0
59	MG	1A	3636	1/1	0.61	0.52	-	56,56,56,56	0
59	MG	2A	3317	1/1	0.99	0.28	-	37,37,37,37	0
59	MG	2A	3178	1/1	0.91	0.21	-	50,50,50,50	0
59	MG	2A	3529	1/1	0.99	0.14	-	28,28,28,28	0
59	MG	1A	3049	1/1	0.94	0.30	-	41,41,41,41	0
59	MG	1a	1603	1/1	0.91	0.24	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3452	1/1	0.94	0.34	-	52,52,52,52	0
59	MG	2A	3491	1/1	0.95	0.24	-	42,42,42,42	0
59	MG	2A	3204	1/1	0.98	0.14	-	26,26,26,26	0
59	MG	2a	1764	1/1	0.98	0.21	-	61,61,61,61	0
59	MG	1a	1780	1/1	0.96	0.26	-	33,33,33,33	0
59	MG	2A	3195	1/1	0.88	0.22	-	53,53,53,53	0
59	MG	2A	3409	1/1	0.96	0.06	-	48,48,48,48	0
59	MG	2A	3144	1/1	0.84	0.47	-	50,50,50,50	0
59	MG	1A	3357	1/1	0.87	0.14	-	22,22,22,22	0
59	MG	2A	3511	1/1	0.97	0.22	-	39,39,39,39	0
59	MG	2A	3169	1/1	0.89	0.36	-	54,54,54,54	0
59	MG	1A	3381	1/1	0.91	0.09	-	23,23,23,23	0
59	MG	2A	3357	1/1	0.86	0.17	-	27,27,27,27	0
59	MG	2A	3091	1/1	0.83	0.31	-	60,60,60,60	0
59	MG	1A	3624	1/1	0.94	0.20	-	48,48,48,48	0
59	MG	2a	1702	1/1	0.94	0.25	-	53,53,53,53	0
59	MG	1A	3117	1/1	0.99	0.15	-	38,38,38,38	0
59	MG	1A	3464	1/1	0.87	0.14	-	43,43,43,43	0
59	MG	1a	1763	1/1	0.88	0.27	-	55,55,55,55	0
59	MG	2A	3475	1/1	0.95	0.15	-	51,51,51,51	0
59	MG	2A	3179	1/1	0.83	0.40	-	50,50,50,50	0
59	MG	2a	1620	1/1	0.85	0.24	-	63,63,63,63	0
59	MG	1a	1611	1/1	0.87	0.26	-	84,84,84,84	0
59	MG	1A	3240	1/1	0.97	0.35	-	37,37,37,37	0
59	MG	2A	3142	1/1	0.88	0.20	-	48,48,48,48	0
59	MG	2A	3039	1/1	0.84	0.58	-	43,43,43,43	0
59	MG	2A	3217	1/1	0.92	0.13	-	45,45,45,45	0
59	MG	2a	1614	1/1	0.85	0.20	-	49,49,49,49	0
59	MG	1A	3562	1/1	0.98	0.06	-	38,38,38,38	0
59	MG	2A	3184	1/1	0.94	0.34	-	56,56,56,56	0
59	MG	1A	3308	1/1	0.92	0.13	-	52,52,52,52	0
59	MG	2A	3416	1/1	0.92	0.15	-	50,50,50,50	0
59	MG	2A	3122	1/1	0.77	0.24	-	42,42,42,42	0
59	MG	1A	3142	1/1	0.93	0.26	-	55,55,55,55	0
59	MG	2A	3248	1/1	0.94	0.17	-	49,49,49,49	0
59	MG	1A	3320	1/1	0.98	0.12	-	35,35,35,35	0
59	MG	2A	3100	1/1	0.95	0.21	-	32,32,32,32	0
59	MG	1a	1781	1/1	0.92	0.13	-	48,48,48,48	0
59	MG	1A	3403	1/1	0.81	0.19	-	57,57,57,57	0
59	MG	1A	3064	1/1	0.91	0.18	-	52,52,52,52	0
59	MG	1T	201	1/1	0.93	0.27	-	40,40,40,40	0
59	MG	2A	3249	1/1	0.91	0.19	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3557	1/1	0.97	0.18	-	60,60,60,60	0
59	MG	1a	1744	1/1	0.87	0.24	-	64,64,64,64	0
59	MG	2a	1625	1/1	0.84	0.43	-	60,60,60,60	0
59	MG	2A	3279	1/1	0.97	0.28	-	37,37,37,37	0
59	MG	2A	3601	1/1	0.96	0.25	-	53,53,53,53	0
59	MG	1A	3475	1/1	0.88	0.15	-	50,50,50,50	0
59	MG	2A	3273	1/1	0.79	0.18	-	63,63,63,63	0
59	MG	1A	3480	1/1	0.96	0.07	-	26,26,26,26	0
59	MG	2a	1724	1/1	0.97	0.27	-	52,52,52,52	0
59	MG	2A	3388	1/1	0.93	0.09	-	55,55,55,55	0
59	MG	2z	703	1/1	0.95	0.17	-	41,41,41,41	0
59	MG	1A	3079	1/1	0.94	0.19	-	22,22,22,22	0
59	MG	1a	1774	1/1	0.94	0.09	-	68,68,68,68	0
59	MG	2a	1660	1/1	0.98	0.39	-	36,36,36,36	0
59	MG	2A	3490	1/1	0.97	0.09	-	32,32,32,32	0
59	MG	1A	3501	1/1	0.93	0.08	-	49,49,49,49	0
59	MG	2A	3030	1/1	0.91	0.17	-	37,37,37,37	0
59	MG	1A	3536	1/1	0.97	0.27	-	31,31,31,31	0
59	MG	26	102	1/1	0.95	0.25	-	47,47,47,47	0
59	MG	1A	3042	1/1	0.97	0.23	-	19,19,19,19	0
59	MG	1A	3005	1/1	0.91	0.22	-	52,52,52,52	0
59	MG	2a	1757	1/1	0.84	0.11	-	64,64,64,64	0
59	MG	2A	3450	1/1	0.98	0.07	-	45,45,45,45	0
59	MG	1A	3253	1/1	0.96	0.13	-	40,40,40,40	0
59	MG	2A	3299	1/1	0.96	0.10	-	38,38,38,38	0
59	MG	2A	3287	1/1	0.95	0.22	-	55,55,55,55	0
59	MG	1A	3753	1/1	0.96	0.06	-	54,54,54,54	0
59	MG	1A	3593	1/1	0.95	0.17	-	53,53,53,53	0
59	MG	1A	3570	1/1	0.97	0.23	-	54,54,54,54	0
59	MG	1A	3166	1/1	0.98	0.24	-	45,45,45,45	0
59	MG	1A	3158	1/1	0.96	0.26	-	29,29,29,29	0
59	MG	1A	3768	1/1	0.92	0.25	-	50,50,50,50	0
59	MG	2w	3003	1/1	0.66	0.20	-	80,80,80,80	0
59	MG	1A	3618	1/1	0.98	0.09	-	33,33,33,33	0
59	MG	2A	3225	1/1	0.93	0.12	-	45,45,45,45	0
59	MG	1a	1698	1/1	0.95	0.16	-	45,45,45,45	0
59	MG	2A	3281	1/1	0.94	0.22	-	43,43,43,43	0
59	MG	2A	3194	1/1	0.93	0.28	-	35,35,35,35	0
59	MG	1A	3136	1/1	0.98	0.17	-	41,41,41,41	0
59	MG	1A	3579	1/1	0.95	0.12	-	44,44,44,44	0
59	MG	1A	3286	1/1	0.89	0.23	-	71,71,71,71	0
59	MG	2A	3232	1/1	0.92	0.10	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3547	1/1	0.96	0.10	-	42,42,42,42	0
59	MG	1a	1605	1/1	0.91	0.11	-	40,40,40,40	0
59	MG	2A	3229	1/1	0.94	0.19	-	44,44,44,44	0
59	MG	1A	3667	1/1	0.93	0.20	-	52,52,52,52	0
59	MG	1B	201	1/1	0.96	0.17	-	54,54,54,54	0
59	MG	2A	3439	1/1	0.90	0.18	-	52,52,52,52	0
59	MG	1A	3448	1/1	0.94	0.08	-	41,41,41,41	0
59	MG	2A	3205	1/1	0.90	0.33	-	58,58,58,58	0
59	MG	1A	3340	1/1	0.98	0.14	-	19,19,19,19	0
59	MG	1A	3565	1/1	0.93	0.12	-	46,46,46,46	0
59	MG	1a	1706	1/1	0.85	0.29	-	57,57,57,57	0
59	MG	2A	3520	1/1	0.88	0.17	-	54,54,54,54	0
59	MG	2A	3535	1/1	0.96	0.06	-	55,55,55,55	0
59	MG	2A	3148	1/1	0.92	0.18	-	40,40,40,40	0
59	MG	1A	3207	1/1	0.79	0.47	-	45,45,45,45	0
59	MG	1A	3426	1/1	0.97	0.11	-	57,57,57,57	0
59	MG	2a	1706	1/1	0.96	0.18	-	87,87,87,87	0
59	MG	1A	3700	1/1	0.98	0.06	-	66,66,66,66	0
59	MG	1A	3407	1/1	0.98	0.09	-	32,32,32,32	0
59	MG	2a	1677	1/1	0.88	0.69	-	52,52,52,52	0
59	MG	1A	3251	1/1	0.98	0.23	-	48,48,48,48	0
59	MG	2A	3189	1/1	0.96	0.37	-	29,29,29,29	0
59	MG	1B	202	1/1	0.91	0.28	-	59,59,59,59	0
59	MG	2a	1601	1/1	0.90	0.08	-	68,68,68,68	0
59	MG	2A	3296	1/1	0.95	0.11	-	45,45,45,45	0
59	MG	1A	3218	1/1	0.97	0.21	-	58,58,58,58	0
59	MG	1B	224	1/1	0.98	0.07	-	56,56,56,56	0
59	MG	2A	3572	1/1	0.87	0.19	-	61,61,61,61	0
59	MG	2A	3219	1/1	0.96	0.21	-	43,43,43,43	0
59	MG	1A	3586	1/1	0.90	0.11	-	56,56,56,56	0
59	MG	2a	1735	1/1	0.88	0.14	-	50,50,50,50	0
59	MG	2A	3190	1/1	0.93	0.39	-	34,34,34,34	0
59	MG	1A	3497	1/1	0.75	0.25	-	30,30,30,30	0
59	MG	1A	3391	1/1	0.94	0.22	-	55,55,55,55	0
59	MG	2a	1630	1/1	0.85	0.42	-	55,55,55,55	0
59	MG	1a	1693	1/1	0.86	0.11	-	57,57,57,57	0
59	MG	1A	3224	1/1	0.97	0.42	-	35,35,35,35	0
59	MG	1A	3612	1/1	0.93	0.25	-	48,48,48,48	0
59	MG	1A	3642	1/1	0.95	0.22	-	45,45,45,45	0
59	MG	2A	3406	1/1	0.93	0.16	-	43,43,43,43	0
59	MG	2A	3517	1/1	0.87	0.12	-	50,50,50,50	0
59	MG	2A	3343	1/1	0.95	0.14	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3425	1/1	0.95	0.28	-	50,50,50,50	0
59	MG	1a	1797	1/1	0.97	0.25	-	66,66,66,66	0
59	MG	2A	3593	1/1	0.88	0.10	-	73,73,73,73	0
59	MG	2A	3228	1/1	0.78	0.31	-	46,46,46,46	0
59	MG	1A	3711	1/1	0.97	0.17	-	41,41,41,41	0
59	MG	1A	3710	1/1	0.72	0.37	-	60,60,60,60	0
59	MG	1A	3152	1/1	0.89	0.14	-	24,24,24,24	0
59	MG	2A	3617	1/1	0.92	0.26	-	62,62,62,62	0
59	MG	1A	3301	1/1	0.78	0.19	-	65,65,65,65	0
59	MG	1L	3002	1/1	0.97	0.13	-	29,29,29,29	0
59	MG	1A	3153	1/1	0.92	0.34	-	33,33,33,33	0
59	MG	1a	1789	1/1	0.96	0.22	-	43,43,43,43	0
59	MG	2A	3383	1/1	0.98	0.10	-	39,39,39,39	0
59	MG	2A	3193	1/1	0.87	0.25	-	51,51,51,51	0
59	MG	1A	3535	1/1	0.86	0.27	-	54,54,54,54	0
59	MG	1A	3737	1/1	0.77	0.12	-	65,65,65,65	0
59	MG	1A	3743	1/1	0.97	0.09	-	53,53,53,53	0
59	MG	1A	3015	1/1	0.96	0.21	-	45,45,45,45	0
59	MG	2A	3041	1/1	0.95	0.23	-	22,22,22,22	0
59	MG	2A	3405	1/1	0.98	0.25	-	45,45,45,45	0
59	MG	1A	3615	1/1	0.98	0.05	-	59,59,59,59	0
59	MG	1A	3605	1/1	0.90	0.18	-	67,67,67,67	0
59	MG	2A	3006	1/1	0.94	0.19	-	29,29,29,29	0
59	MG	1A	3418	1/1	0.96	0.11	-	37,37,37,37	0
59	MG	1A	3270	1/1	0.95	0.16	-	47,47,47,47	0
59	MG	1A	3376	1/1	0.98	0.04	-	45,45,45,45	0
59	MG	2A	3035	1/1	0.79	0.25	-	45,45,45,45	0
59	MG	1A	3529	1/1	0.94	0.14	-	53,53,53,53	0
59	MG	1A	3707	1/1	0.98	0.12	-	51,51,51,51	0
59	MG	1a	1737	1/1	0.97	0.07	-	40,40,40,40	0
59	MG	1a	1717	1/1	0.96	0.12	-	56,56,56,56	0
59	MG	2A	3555	1/1	0.98	0.40	-	42,42,42,42	0
59	MG	2A	3141	1/1	0.97	0.44	-	49,49,49,49	0
59	MG	2A	3301	1/1	0.84	0.12	-	30,30,30,30	0
59	MG	2A	3164	1/1	0.93	0.18	-	48,48,48,48	0
59	MG	1A	3179	1/1	0.90	0.20	-	51,51,51,51	0
59	MG	1A	3498	1/1	0.97	0.11	-	70,70,70,70	0
59	MG	2a	1634	1/1	0.94	0.27	-	52,52,52,52	0
59	MG	1A	3465	1/1	0.98	0.16	-	33,33,33,33	0
59	MG	2A	3240	1/1	0.93	0.19	-	42,42,42,42	0
59	MG	2a	1663	1/1	0.94	0.14	-	51,51,51,51	0
59	MG	1A	3203	1/1	0.92	0.28	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	1A	3674	1/1	0.90	0.15	-	48,48,48,48	0
59	MG	1A	3131	1/1	0.90	0.18	-	47,47,47,47	0
59	MG	1A	3405	1/1	0.92	0.14	-	55,55,55,55	0
59	MG	2A	3402	1/1	0.90	0.17	-	45,45,45,45	0
59	MG	2B	213	1/1	0.92	0.13	-	64,64,64,64	0
59	MG	1A	3590	1/1	0.95	0.13	-	44,44,44,44	0
59	MG	2A	3400	1/1	0.95	0.06	-	46,46,46,46	0
59	MG	1A	3619	1/1	0.95	0.18	-	49,49,49,49	0
59	MG	1A	3206	1/1	0.97	0.18	-	34,34,34,34	0
59	MG	1A	3324	1/1	0.98	0.11	-	51,51,51,51	0
59	MG	2A	3047	1/1	0.90	0.23	-	48,48,48,48	0
59	MG	2A	3482	1/1	0.91	0.10	-	53,53,53,53	0
59	MG	2A	3553	1/1	0.97	0.26	-	40,40,40,40	0
59	MG	1A	3591	1/1	0.92	0.12	-	47,47,47,47	0
59	MG	2A	3278	1/1	0.93	0.26	-	44,44,44,44	0
59	MG	2A	3203	1/1	0.97	0.38	-	36,36,36,36	0
59	MG	1a	1606	1/1	0.87	0.12	-	63,63,63,63	0
59	MG	2A	3087	1/1	0.90	0.14	-	56,56,56,56	0
59	MG	2a	1661	1/1	0.72	0.15	-	67,67,67,67	0
59	MG	1A	3397	1/1	0.94	0.19	-	49,49,49,49	0
59	MG	2A	3397	1/1	0.89	0.15	-	46,46,46,46	0
59	MG	2A	3583	1/1	0.94	0.12	-	38,38,38,38	0
59	MG	2a	1680	1/1	0.86	0.27	-	52,52,52,52	0
59	MG	1A	3216	1/1	0.92	0.30	-	47,47,47,47	0
59	MG	2A	3266	1/1	0.91	0.18	-	38,38,38,38	0
59	MG	2B	201	1/1	0.75	0.32	-	62,62,62,62	0
59	MG	1A	3228	1/1	0.98	0.15	-	44,44,44,44	0
59	MG	1A	3099	1/1	0.92	0.18	-	63,63,63,63	0
59	MG	1A	3399	1/1	0.96	0.12	-	55,55,55,55	0
59	MG	2a	1727	1/1	0.93	0.10	-	63,63,63,63	0
59	MG	2A	3323	1/1	0.91	0.15	-	50,50,50,50	0
59	MG	1A	3211	1/1	0.78	0.40	-	59,59,59,59	0
59	MG	2A	3489	1/1	0.94	0.10	-	47,47,47,47	0
59	MG	1A	3693	1/1	0.96	0.14	-	48,48,48,48	0
59	MG	1A	3682	1/1	0.82	0.14	-	97,97,97,97	0
59	MG	1A	3487	1/1	0.96	0.18	-	47,47,47,47	0
59	MG	1a	1682	1/1	0.89	0.22	-	55,55,55,55	0
59	MG	2A	3466	1/1	0.96	0.09	-	51,51,51,51	0
59	MG	2A	3045	1/1	0.90	0.28	-	56,56,56,56	0
59	MG	1A	3735	1/1	0.92	0.30	-	32,32,32,32	0
59	MG	1A	3374	1/1	0.96	0.15	-	35,35,35,35	0
59	MG	2A	3242	1/1	0.94	0.20	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3533	1/1	0.99	0.36	-	23,23,23,23	0
59	MG	1A	3660	1/1	0.95	0.19	-	55,55,55,55	0
59	MG	2A	3231	1/1	0.84	0.21	-	56,56,56,56	0
59	MG	2N	201	1/1	0.89	0.21	-	42,42,42,42	0
59	MG	2A	3170	1/1	0.86	0.30	-	54,54,54,54	0
59	MG	2A	3392	1/1	0.96	0.15	-	39,39,39,39	0
59	MG	2A	3282	1/1	0.91	0.12	-	26,26,26,26	0
59	MG	2A	3382	1/1	0.96	0.18	-	34,34,34,34	0
59	MG	1A	3065	1/1	0.94	0.09	-	36,36,36,36	0
59	MG	1a	1718	1/1	0.97	0.13	-	39,39,39,39	0
59	MG	2a	1668	1/1	0.86	0.18	-	43,43,43,43	0
59	MG	2a	1737	1/1	0.96	0.24	-	63,63,63,63	0
59	MG	2A	3373	1/1	0.90	0.17	-	47,47,47,47	0
59	MG	2a	1747	1/1	0.97	0.21	-	39,39,39,39	0
59	MG	1a	1620	1/1	0.98	0.07	-	40,40,40,40	0
59	MG	1A	3703	1/1	0.93	0.34	-	42,42,42,42	0
59	MG	2A	3360	1/1	0.97	0.19	-	34,34,34,34	0
59	MG	2D	302	1/1	0.93	0.27	-	62,62,62,62	0
59	MG	1A	3373	1/1	0.97	0.13	-	37,37,37,37	0
59	MG	1a	1669	1/1	0.97	0.21	-	44,44,44,44	0
59	MG	2a	1717	1/1	0.92	0.22	-	52,52,52,52	0
59	MG	2a	1749	1/1	0.94	0.17	-	59,59,59,59	0
59	MG	1A	3601	1/1	0.95	0.11	-	33,33,33,33	0
59	MG	1A	3460	1/1	0.94	0.16	-	47,47,47,47	0
59	MG	2a	1734	1/1	0.96	0.19	-	70,70,70,70	0
59	MG	2a	1766	1/1	0.94	0.28	-	61,61,61,61	0
59	MG	1A	3149	1/1	0.98	0.10	-	36,36,36,36	0
59	MG	1A	3045	1/1	0.90	0.31	-	44,44,44,44	0
59	MG	1A	3563	1/1	0.89	0.23	-	53,53,53,53	0
59	MG	2A	3426	1/1	0.91	0.29	-	58,58,58,58	0
59	MG	1A	3558	1/1	0.97	0.14	-	42,42,42,42	0
59	MG	2A	3546	1/1	0.88	0.39	-	56,56,56,56	0
59	MG	2A	3527	1/1	0.94	0.26	-	32,32,32,32	0
59	MG	1N	201	1/1	0.92	0.17	-	40,40,40,40	0
59	MG	1A	3325	1/1	0.98	0.27	-	64,64,64,64	0
59	MG	2A	3139	1/1	0.95	0.21	-	42,42,42,42	0
59	MG	1A	3744	1/1	0.91	0.15	-	45,45,45,45	0
59	MG	2z	705	1/1	0.86	0.31	-	67,67,67,67	0
59	MG	2A	3253	1/1	0.90	0.27	-	53,53,53,53	0
59	MG	2A	3082	1/1	0.89	0.27	-	45,45,45,45	0
59	MG	2A	3057	1/1	0.96	0.16	-	41,41,41,41	0
59	MG	2A	3565	1/1	0.94	0.32	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3430	1/1	0.94	0.34	-	40,40,40,40	0
59	MG	1A	3544	1/1	0.88	0.22	-	43,43,43,43	0
59	MG	1A	3447	1/1	0.94	0.04	-	30,30,30,30	0
59	MG	1A	3515	1/1	0.69	0.12	-	48,48,48,48	0
59	MG	1A	3359	1/1	0.91	0.13	-	22,22,22,22	0
59	MG	1a	1602	1/1	0.91	0.13	-	49,49,49,49	0
59	MG	1A	3638	1/1	0.73	0.23	-	89,89,89,89	0
59	MG	2O	3002	1/1	0.90	0.27	-	59,59,59,59	0
59	MG	1A	3722	1/1	0.97	0.19	-	27,27,27,27	0
59	MG	1a	1635	1/1	0.91	0.24	-	55,55,55,55	0
59	MG	1A	3740	1/1	0.95	0.07	-	45,45,45,45	0
59	MG	1M	201	1/1	0.95	0.21	-	48,48,48,48	0
59	MG	2a	1636	1/1	0.94	0.16	-	42,42,42,42	0
59	MG	2A	3471	1/1	0.90	0.15	-	56,56,56,56	0
59	MG	1A	3392	1/1	0.94	0.14	-	31,31,31,31	0
59	MG	1a	1722	1/1	0.90	0.26	-	78,78,78,78	0
59	MG	2A	3191	1/1	0.97	0.22	-	44,44,44,44	0
59	MG	1A	3102	1/1	0.95	0.34	-	43,43,43,43	0
59	MG	1B	218	1/1	0.86	0.18	-	65,65,65,65	0
59	MG	1A	3678	1/1	0.99	0.08	-	16,16,16,16	0
59	MG	2A	3421	1/1	0.95	0.11	-	48,48,48,48	0
59	MG	2A	3551	1/1	0.94	0.14	-	58,58,58,58	0
59	MG	2A	3234	1/1	0.96	0.52	-	56,56,56,56	0
59	MG	1a	1743	1/1	0.97	0.14	-	64,64,64,64	0
59	MG	1A	3681	1/1	0.97	0.12	-	30,30,30,30	0
59	MG	1A	3429	1/1	0.98	0.12	-	44,44,44,44	0
59	MG	1A	3574	1/1	0.95	0.16	-	47,47,47,47	0
59	MG	1A	3169	1/1	0.95	0.15	-	55,55,55,55	0
59	MG	1A	3331	1/1	0.91	0.27	-	53,53,53,53	0
59	MG	1A	3404	1/1	0.97	0.11	-	40,40,40,40	0
59	MG	1E	303	1/1	0.92	0.33	-	41,41,41,41	0
59	MG	2A	3567	1/1	0.97	0.19	-	45,45,45,45	0
59	MG	1A	3701	1/1	0.96	0.13	-	47,47,47,47	0
59	MG	1A	3261	1/1	0.95	0.06	-	34,34,34,34	0
59	MG	2A	3250	1/1	0.92	0.21	-	45,45,45,45	0
59	MG	2A	3537	1/1	0.91	0.29	-	38,38,38,38	0
59	MG	2A	3371	1/1	0.99	0.14	-	26,26,26,26	0
59	MG	2A	3059	1/1	0.95	0.13	-	49,49,49,49	0
59	MG	2a	1770	1/1	0.98	0.10	-	59,59,59,59	0
59	MG	2A	3303	1/1	0.91	0.10	-	43,43,43,43	0
59	MG	2A	3033	1/1	0.89	0.13	-	50,50,50,50	0
59	MG	2F	301	1/1	0.71	0.31	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	2A	3247	1/1	0.94	0.19	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.