



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 02:21 PM EST

PDB ID : 6UCQ  
Title : Crystal structure of the Thermus thermophilus 70S ribosome recycling complex  
Authors : Zhou, D.; Tanzawa, T.; Gagnon, M.G.; Lin, J.  
Deposited on : 2019-09-17  
Resolution : 3.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

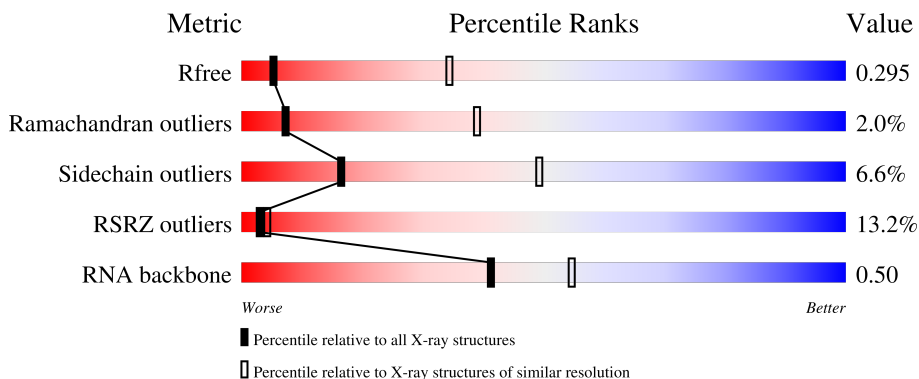
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

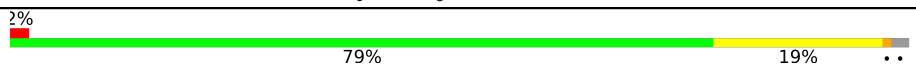


The reported resolution of this entry is 3.50 Å.

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))
$R_{free}$	130704	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	 2% 79% 19% ..
1	2A	2915	 4% 78% 17% .
2	1B	121	 86% 13% .
2	2B	121	 % 78% 21% .
3	1D	276	 6% 92% 8%

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Mol	Chain	Length	Quality of chain
3	2D	276	11% 93% 7%
4	1E	206	29% 89% 10%
4	2E	206	3% 93% 6%
5	1F	210	4% 90% 7%
5	2F	210	8% 94% ..
6	1G	182	% 93% 6%
6	2G	182	34% 93% 6%
7	1H	180	92% ..
7	2H	180	21% 93% ..
8	1N	140	3% 91% 9%
8	2N	140	19% 94% 6%
9	1O	122	53% 93% 7%
9	2O	122	49% 98% .
10	1P	150	3% 93% 7%
10	2P	150	26% 95% 5%
11	1Q	141	95% 5%
11	2Q	141	32% 95% 5%
12	1R	118	3% 84% 15%
12	2R	118	2% 95% 5%
13	1S	112	90% 8%
13	2S	112	2% 91% 7%
14	1T	146	32% 84% 6% 10%
14	2T	146	15% 86% 10%
15	1U	118	2% 94% ..
15	2U	118	6% 96% ..

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Mol	Chain	Length	Quality of chain
16	1V	101	90% 10%
16	2V	101	12% 97%
17	1W	113	7% 93% 6%
17	2W	113	89% 10%
18	1X	96	2% 93% 6%
18	2X	96	94% 5%
19	1Y	110	88% 9%
19	2Y	110	11% 92% 5%
20	1Z	206	86% 13%
20	2Z	206	20% 86% 12%
21	10	85	87% 12%
21	20	85	29% 85% 12%
22	11	98	15% 94% 5%
22	21	98	42% 93% 6%
23	12	72	89% 6%
23	22	72	96%
24	13	60	3% 87% 12%
24	23	60	17% 93% 5%
25	14	71	79% 17%
25	24	71	20% 83% 14%
26	15	60	13% 93% 5%
26	25	60	93% 5%
27	16	54	2% 93% 6%
27	26	54	74% 94%
28	17	49	4% 90% 8%

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Mol	Chain	Length	Quality of chain
28	27	49	4% 86% 12%
29	18	65	6% 91% 8%
29	28	65	60% 98%
30	19	37	97%
30	29	37	22% 92% 8%
31	1a	1521	6% 82% 16%
31	2a	1521	7% 82% 17%
32	1b	256	4% 84% 6% 10%
32	2b	256	4% 84% 6% 10%
33	1c	239	54% 83% 14%
33	2c	239	47% 83% 14%
34	1d	209	9% 93% 6%
34	2d	209	11% 96%
35	1e	162	14% 88% 9%
35	2e	162	31% 87% 9%
36	1f	101	98%
36	2f	101	95%
37	1g	156	44% 94% 6%
37	2g	156	73% 96%
38	1h	138	4% 96%
38	2h	138	7% 94% 5%
39	1i	128	24% 95%
39	2i	128	26% 95% 5%
40	1j	105	41% 87% 6% 8%
40	2j	105	23% 88% 9%

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Mol	Chain	Length	Quality of chain
41	1k	129	35% 85% 12%
41	2k	129	47% 87% 12%
42	1l	132	13% 87% 5% 8%
42	2l	132	40% 88% 5% 8%
43	1m	126	10% 91% 6%
43	2m	126	23% 92% 5%
44	1n	61	52% 93% 5%
44	2n	61	51% 93% 5%
45	1o	89	96% ..
45	2o	89	6% 88% 11%
46	1p	88	6% 85% 8% 7%
46	2p	88	2% 86% 7% 7%
47	1q	105	% 91% 6%
47	2q	105	46% 90% 6%
48	1r	88	% 74% 23%
48	2r	88	9% 74% 23%
49	1s	93	12% 81% 9% 11%
49	2s	93	24% 84% 5% 11%
50	1t	106	3% 83% 8% 9%
50	2t	106	3% 87% 9%
51	1u	27	85% 15%
51	2u	27	19% 85% 15%
52	1v	758	11% 81% 14%
52	2v	758	31% 82% 13%
53	1w	185	8% 83% 17%

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Mol	Chain	Length	Quality of chain
53	2w	185	
54	1x	76	
54	1y	76	
54	2x	76	
54	2y	76	
55	1z	21	
55	2z	21	

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
54	PSU	1y	32	-	-	-	X
54	PSU	2x	32	-	-	-	X
54	MIA	2x	37	-	-	-	X
54	7MG	2x	46	-	-	-	X
54	5MU	2x	54	-	-	-	X
54	PSU	2x	55	-	-	-	X
54	4SU	2x	8	-	-	-	X
54	PSU	2y	39	-	-	-	X
54	5MU	2y	54	-	-	-	X
54	PSU	2y	55	-	-	-	X
56	MG	10	101	-	-	-	X
56	MG	10	104	-	-	-	X
56	MG	12	101	-	-	-	X
56	MG	13	301	-	-	-	X
56	MG	1A	4009	-	-	-	X
56	MG	1A	4012	-	-	-	X
56	MG	1A	4027	-	-	-	X
56	MG	1A	4036	-	-	-	X
56	MG	1A	4038	-	-	-	X
56	MG	1A	4047	-	-	-	X
56	MG	1A	4048	-	-	-	X
56	MG	1A	4052	-	-	-	X
56	MG	1A	4054	-	-	-	X
56	MG	1A	4060	-	-	-	X
56	MG	1A	4068	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	4075	-	-	-	X
56	MG	1A	4121	-	-	-	X
56	MG	1A	4134	-	-	-	X
56	MG	1A	4197	-	-	-	X
56	MG	1A	4202	-	-	-	X
56	MG	1A	4259	-	-	-	X
56	MG	1A	4282	-	-	-	X
56	MG	1A	4285	-	-	-	X
56	MG	1A	4288	-	-	-	X
56	MG	1A	4291	-	-	-	X
56	MG	1A	4301	-	-	-	X
56	MG	1A	4304	-	-	-	X
56	MG	1A	4307	-	-	-	X
56	MG	1A	4323	-	-	-	X
56	MG	1A	4354	-	-	-	X
56	MG	1A	4373	-	-	-	X
56	MG	1A	4404	-	-	-	X
56	MG	1A	4428	-	-	-	X
56	MG	1A	4464	-	-	-	X
56	MG	1A	4503	-	-	-	X
56	MG	1A	4516	-	-	-	X
56	MG	1A	4518	-	-	-	X
56	MG	1A	4519	-	-	-	X
56	MG	1A	4521	-	-	-	X
56	MG	1A	4535	-	-	-	X
56	MG	1A	4538	-	-	-	X
56	MG	1A	4546	-	-	-	X
56	MG	1A	4549	-	-	-	X
56	MG	1A	4550	-	-	-	X
56	MG	1A	4600	-	-	-	X
56	MG	1A	4633	-	-	-	X
56	MG	1A	4639	-	-	-	X
56	MG	1A	4662	-	-	-	X
56	MG	1A	4677	-	-	-	X
56	MG	1A	4678	-	-	-	X
56	MG	1A	4699	-	-	-	X
56	MG	1A	4706	-	-	-	X
56	MG	1A	4714	-	-	-	X
56	MG	1A	4747	-	-	-	X
56	MG	1A	4756	-	-	-	X
56	MG	1A	4762	-	-	-	X
56	MG	1A	4764	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	4765	-	-	-	X
56	MG	1A	4772	-	-	-	X
56	MG	1A	4788	-	-	-	X
56	MG	1A	4790	-	-	-	X
56	MG	1A	4809	-	-	-	X
56	MG	1A	4861	-	-	-	X
56	MG	1A	4884	-	-	-	X
56	MG	1A	4888	-	-	-	X
56	MG	1A	4889	-	-	-	X
56	MG	1A	4895	-	-	-	X
56	MG	1A	4927	-	-	-	X
56	MG	1A	4933	-	-	-	X
56	MG	1A	4948	-	-	-	X
56	MG	1A	4960	-	-	-	X
56	MG	1A	4966	-	-	-	X
56	MG	1A	4973	-	-	-	X
56	MG	1A	4985	-	-	-	X
56	MG	1A	5006	-	-	-	X
56	MG	1A	5014	-	-	-	X
56	MG	1A	5033	-	-	-	X
56	MG	1A	5035	-	-	-	X
56	MG	1B	205	-	-	-	X
56	MG	1B	212	-	-	-	X
56	MG	1B	214	-	-	-	X
56	MG	1B	223	-	-	-	X
56	MG	1D	306	-	-	-	X
56	MG	1D	308	-	-	-	X
56	MG	1O	204	-	-	-	X
56	MG	1P	202	-	-	-	X
56	MG	1Q	201	-	-	-	X
56	MG	1a	1615	-	-	-	X
56	MG	1a	1621	-	-	-	X
56	MG	1a	1622	-	-	-	X
56	MG	1a	1629	-	-	-	X
56	MG	1a	1634	-	-	-	X
56	MG	1a	1642	-	-	-	X
56	MG	1a	1649	-	-	-	X
56	MG	1a	1669	-	-	-	X
56	MG	1a	1670	-	-	-	X
56	MG	1a	1682	-	-	-	X
56	MG	1a	1684	-	-	-	X
56	MG	1a	1685	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	1688	-	-	-	X
56	MG	1a	1704	-	-	-	X
56	MG	1a	1706	-	-	-	X
56	MG	1a	1730	-	-	-	X
56	MG	1a	1738	-	-	-	X
56	MG	1a	1742	-	-	-	X
56	MG	1a	1745	-	-	-	X
56	MG	1a	1752	-	-	-	X
56	MG	1a	1763	-	-	-	X
56	MG	1a	1765	-	-	-	X
56	MG	1a	1768	-	-	-	X
56	MG	1a	1776	-	-	-	X
56	MG	1a	1777	-	-	-	X
56	MG	1a	1780	-	-	-	X
56	MG	1a	1792	-	-	-	X
56	MG	1a	1794	-	-	-	X
56	MG	1a	1803	-	-	-	X
56	MG	1a	1805	-	-	-	X
56	MG	1a	1810	-	-	-	X
56	MG	1a	1843	-	-	-	X
56	MG	1a	1845	-	-	-	X
56	MG	1a	1850	-	-	-	X
56	MG	1a	1852	-	-	-	X
56	MG	1a	1854	-	-	-	X
56	MG	1a	1856	-	-	-	X
56	MG	1a	1863	-	-	-	X
56	MG	1a	1875	-	-	-	X
56	MG	1a	1898	-	-	-	X
56	MG	1a	1906	-	-	-	X
56	MG	1a	1908	-	-	-	X
56	MG	1a	1909	-	-	-	X
56	MG	1a	1910	-	-	-	X
56	MG	1a	1911	-	-	-	X
56	MG	1a	1912	-	-	-	X
56	MG	1b	304	-	-	-	X
56	MG	1b	305	-	-	-	X
56	MG	1d	301	-	-	-	X
56	MG	1m	201	-	-	-	X
56	MG	1q	201	-	-	-	X
56	MG	23	101	-	-	-	X
56	MG	23	103	-	-	-	X
56	MG	27	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	28	101	-	-	-	X
56	MG	2A	3016	-	-	-	X
56	MG	2A	3018	-	-	-	X
56	MG	2A	3019	-	-	-	X
56	MG	2A	3020	-	-	-	X
56	MG	2A	3021	-	-	-	X
56	MG	2A	3022	-	-	-	X
56	MG	2A	3025	-	-	-	X
56	MG	2A	3027	-	-	-	X
56	MG	2A	3028	-	-	-	X
56	MG	2A	3030	-	-	-	X
56	MG	2A	3034	-	-	-	X
56	MG	2A	3057	-	-	-	X
56	MG	2A	3071	-	-	-	X
56	MG	2A	3076	-	-	-	X
56	MG	2A	3077	-	-	-	X
56	MG	2A	3083	-	-	-	X
56	MG	2A	3084	-	-	-	X
56	MG	2A	3091	-	-	-	X
56	MG	2A	3094	-	-	-	X
56	MG	2A	3097	-	-	-	X
56	MG	2A	3105	-	-	-	X
56	MG	2A	3107	-	-	-	X
56	MG	2A	3111	-	-	-	X
56	MG	2A	3112	-	-	-	X
56	MG	2A	3116	-	-	-	X
56	MG	2A	3122	-	-	-	X
56	MG	2A	3131	-	-	-	X
56	MG	2A	3133	-	-	-	X
56	MG	2A	3136	-	-	-	X
56	MG	2A	3137	-	-	-	X
56	MG	2A	3142	-	-	-	X
56	MG	2A	3146	-	-	-	X
56	MG	2A	3151	-	-	-	X
56	MG	2A	3155	-	-	-	X
56	MG	2A	3160	-	-	-	X
56	MG	2A	3161	-	-	-	X
56	MG	2A	3176	-	-	-	X
56	MG	2A	3184	-	-	-	X
56	MG	2A	3191	-	-	-	X
56	MG	2A	3193	-	-	-	X
56	MG	2A	3204	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3206	-	-	-	X
56	MG	2A	3245	-	-	-	X
56	MG	2A	3246	-	-	-	X
56	MG	2A	3248	-	-	-	X
56	MG	2A	3252	-	-	-	X
56	MG	2A	3257	-	-	-	X
56	MG	2A	3263	-	-	-	X
56	MG	2A	3272	-	-	-	X
56	MG	2A	3283	-	-	-	X
56	MG	2A	3284	-	-	-	X
56	MG	2A	3299	-	-	-	X
56	MG	2A	3302	-	-	-	X
56	MG	2A	3305	-	-	-	X
56	MG	2A	3307	-	-	-	X
56	MG	2A	3319	-	-	-	X
56	MG	2A	3327	-	-	-	X
56	MG	2A	3329	-	-	-	X
56	MG	2A	3337	-	-	-	X
56	MG	2A	3350	-	-	-	X
56	MG	2A	3351	-	-	-	X
56	MG	2A	3383	-	-	-	X
56	MG	2A	3389	-	-	-	X
56	MG	2A	3397	-	-	-	X
56	MG	2A	3398	-	-	-	X
56	MG	2A	3402	-	-	-	X
56	MG	2A	3403	-	-	-	X
56	MG	2A	3431	-	-	-	X
56	MG	2A	3440	-	-	-	X
56	MG	2A	3449	-	-	-	X
56	MG	2A	3451	-	-	-	X
56	MG	2A	3461	-	-	-	X
56	MG	2A	3464	-	-	-	X
56	MG	2A	3465	-	-	-	X
56	MG	2A	3470	-	-	-	X
56	MG	2A	3472	-	-	-	X
56	MG	2A	3476	-	-	-	X
56	MG	2A	3477	-	-	-	X
56	MG	2A	3482	-	-	-	X
56	MG	2A	3486	-	-	-	X
56	MG	2A	3502	-	-	-	X
56	MG	2A	3512	-	-	-	X
56	MG	2A	3517	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3521	-	-	-	X
56	MG	2A	3529	-	-	-	X
56	MG	2A	3536	-	-	-	X
56	MG	2A	3546	-	-	-	X
56	MG	2A	3552	-	-	-	X
56	MG	2A	3555	-	-	-	X
56	MG	2A	3556	-	-	-	X
56	MG	2A	3572	-	-	-	X
56	MG	2A	3574	-	-	-	X
56	MG	2A	3579	-	-	-	X
56	MG	2A	3582	-	-	-	X
56	MG	2A	3583	-	-	-	X
56	MG	2A	3591	-	-	-	X
56	MG	2A	3612	-	-	-	X
56	MG	2A	3615	-	-	-	X
56	MG	2A	3624	-	-	-	X
56	MG	2A	3629	-	-	-	X
56	MG	2A	3637	-	-	-	X
56	MG	2A	3639	-	-	-	X
56	MG	2A	3647	-	-	-	X
56	MG	2A	3675	-	-	-	X
56	MG	2A	3681	-	-	-	X
56	MG	2A	3692	-	-	-	X
56	MG	2A	3695	-	-	-	X
56	MG	2A	3719	-	-	-	X
56	MG	2A	3724	-	-	-	X
56	MG	2A	3735	-	-	-	X
56	MG	2A	3739	-	-	-	X
56	MG	2A	3770	-	-	-	X
56	MG	2A	3783	-	-	-	X
56	MG	2A	3789	-	-	-	X
56	MG	2A	3798	-	-	-	X
56	MG	2A	3800	-	-	-	X
56	MG	2A	3808	-	-	-	X
56	MG	2A	3826	-	-	-	X
56	MG	2A	3828	-	-	-	X
56	MG	2A	3830	-	-	-	X
56	MG	2B	203	-	-	-	X
56	MG	2B	208	-	-	-	X
56	MG	2B	216	-	-	-	X
56	MG	2B	218	-	-	-	X
56	MG	2B	221	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2B	230	-	-	-	X
56	MG	2B	232	-	-	-	X
56	MG	2F	303	-	-	-	X
56	MG	2P	203	-	-	-	X
56	MG	2Q	202	-	-	-	X
56	MG	2Q	206	-	-	-	X
56	MG	2Z	401	-	-	-	X
56	MG	2Z	403	-	-	-	X
56	MG	2a	1602	-	-	-	X
56	MG	2a	1606	-	-	-	X
56	MG	2a	1607	-	-	-	X
56	MG	2a	1608	-	-	-	X
56	MG	2a	1609	-	-	-	X
56	MG	2a	1617	-	-	-	X
56	MG	2a	1620	-	-	-	X
56	MG	2a	1622	-	-	-	X
56	MG	2a	1625	-	-	-	X
56	MG	2a	1627	-	-	-	X
56	MG	2a	1628	-	-	-	X
56	MG	2a	1634	-	-	-	X
56	MG	2a	1648	-	-	-	X
56	MG	2a	1663	-	-	-	X
56	MG	2a	1664	-	-	-	X
56	MG	2a	1666	-	-	-	X
56	MG	2a	1668	-	-	-	X
56	MG	2a	1669	-	-	-	X
56	MG	2a	1671	-	-	-	X
56	MG	2a	1673	-	-	-	X
56	MG	2a	1674	-	-	-	X
56	MG	2a	1676	-	-	-	X
56	MG	2a	1678	-	-	-	X
56	MG	2a	1682	-	-	-	X
56	MG	2a	1683	-	-	-	X
56	MG	2a	1684	-	-	-	X
56	MG	2a	1688	-	-	-	X
56	MG	2a	1700	-	-	-	X
56	MG	2a	1706	-	-	-	X
56	MG	2a	1709	-	-	-	X
56	MG	2a	1710	-	-	-	X
56	MG	2a	1713	-	-	-	X
56	MG	2a	1714	-	-	-	X
56	MG	2a	1716	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2a	1718	-	-	-	X
56	MG	2a	1722	-	-	-	X
56	MG	2a	1732	-	-	-	X
56	MG	2a	1735	-	-	-	X
56	MG	2a	1748	-	-	-	X
56	MG	2a	1753	-	-	-	X
56	MG	2a	1754	-	-	-	X
56	MG	2a	1758	-	-	-	X
56	MG	2a	1766	-	-	-	X
56	MG	2a	1768	-	-	-	X
56	MG	2a	1776	-	-	-	X
56	MG	2a	1780	-	-	-	X
56	MG	2a	1785	-	-	-	X
56	MG	2a	1786	-	-	-	X
56	MG	2a	1791	-	-	-	X
56	MG	2a	1794	-	-	-	X
56	MG	2a	1805	-	-	-	X
56	MG	2a	1826	-	-	-	X
56	MG	2a	1828	-	-	-	X
56	MG	2a	1860	-	-	-	X
56	MG	2a	1887	-	-	-	X
56	MG	2a	1893	-	-	-	X
56	MG	2a	1899	-	-	-	X
56	MG	2a	1901	-	-	-	X
56	MG	2a	1905	-	-	-	X
56	MG	2a	1912	-	-	-	X
56	MG	2a	1918	-	-	-	X
56	MG	2a	1921	-	-	-	X
56	MG	2d	301	-	-	-	X
56	MG	2e	201	-	-	-	X
56	MG	2g	202	-	-	-	X
56	MG	2g	206	-	-	-	X
56	MG	2h	203	-	-	-	X
56	MG	2i	204	-	-	-	X
56	MG	2l	204	-	-	-	X
56	MG	2l	206	-	-	-	X
56	MG	2m	201	-	-	-	X
56	MG	2m	202	-	-	-	X
56	MG	2o	301	-	-	-	X
56	MG	2p	102	-	-	-	X
56	MG	2q	201	-	-	-	X
56	MG	2r	301	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
56	MG	2s	102	-	-	-	X
56	MG	2u	101	-	-	-	X
56	MG	2v	701	-	-	-	X
56	MG	2w	202	-	-	-	X
56	MG	2x	102	-	-	-	X
56	MG	2x	103	-	-	-	X
56	MG	2x	104	-	-	-	X
56	MG	2x	105	-	-	-	X
56	MG	2x	107	-	-	-	X
56	MG	2x	108	-	-	-	X
56	MG	2y	101	-	-	-	X
56	MG	2y	103	-	-	-	X
56	MG	2y	106	-	-	-	X
56	MG	2z	103	-	-	-	X



## 2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 305259 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
			Total	C	N	O	P			
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	1F	203	Total 1584	C 1009	N 298	O 275	S 2	0	0	1
5	2F	203	Total 1580	C 1007	N 297	O 274	S 2	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	1G	181	Total 1451	C 930	N 261	O 256	S 4	0	0	0
6	2G	181	Total 1453	C 930	N 263	O 256	S 4	0	0	0

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

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

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	1N	140	Total 1117	C 719	N 207	O 187	S 4	0	0	0
8	2N	140	Total 1117	C 719	N 207	O 187	S 4	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	1O	122	Total 933	C 588	N 171	O 170	S 4	0	0	0
9	2O	122	Total 933	C 588	N 171	O 170	S 4	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1P	149	Total 1135	C 706	N 230	O 196	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	2P	149	1135	706	230	196	3	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	1Q	141	1122	715	212	188	7	0	0	0
11	2Q	141	1122	715	212	188	7	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	1R	118	968	604	203	160	1	0	0	0
12	2R	118	968	604	203	160	1	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	1S	110	873	550	174	149	0	0	0
13	2S	110	870	549	173	148	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	1T	131	1091	680	225	185	1	0	0	0
14	2T	131	1083	675	224	183	1	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	1U	116	959	608	201	149	1	0	0	0
15	2U	116	959	608	201	149	1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	1V	101	Total 771	C 495	N 140	O 135	S 1	0	0	0
16	2V	101	Total 771	C 495	N 140	O 135	S 1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	1W	112	Total 886	C 557	N 174	O 153	S 2	0	0	0
17	2W	112	Total 886	C 557	N 174	O 153	S 2	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	1X	95	Total 750	C 488	N 135	O 126	S 1	0	0	0
18	2X	95	Total 750	C 488	N 135	O 126	S 1	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	1Y	107	Total 806	C 517	N 152	O 131	S 6	0	0	0
19	2Y	107	Total 806	C 517	N 152	O 131	S 6	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	1Z	204	Total 1582	C 1007	N 278	O 295	S 2	0	0	0
20	2Z	204	Total 1582	C 1007	N 278	O 295	S 2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	10	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			
21	20	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
22	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
23	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
24	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
25	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	15	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
27	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
28	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
29	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
30	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 31 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	1a	1499	Total	C	N	O	P	0	0	0
			32224	14348	5970	10407	1499			
31	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
32	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
33	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
34	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
35	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
36	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
37	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
38	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
39	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
40	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			
41	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	2l	122	932	586	185	159	2	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	1m	118	919	566	190	161	2	0	0	0
43	2m	122	950	586	197	165	2	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1n	60	492	312	104	72	4	0	0	0
44	2n	60	492	312	104	72	4	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1o	88	728	456	144	126	2	0	0	0
45	2o	88	728	456	144	126	2	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	1p	82	681	433	134	113	1	0	0	0
46	2p	82	677	430	133	113	1	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	1q	99	823	528	151	142	2	0	0	0
47	2q	99	823	528	151	142	2	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
48	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
48	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
49	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
50	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
51	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
51	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 52 is a protein called 50S ribosomal protein L9,Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	1v	728	Total	C	N	O	S	0	0	0
			5664	3599	974	1072	19			
52	2v	728	Total	C	N	O	S	0	0	0
			5664	3599	974	1072	19			

- Molecule 53 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1w	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
53	2w	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 54 is a RNA chain called P-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1x	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
54	2x	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
54	2y	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1z	10	Total	C	N	O	P	0	0	0
			212	96	39	67	10			
55	2z	10	Total	C	N	O	P	0	0	0
			212	96	39	67	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1063	Total	Mg	0	0
			1063	1063		
56	1B	26	Total	Mg	0	0
			26	26		
56	1D	8	Total	Mg	0	0
			8	8		
56	1E	8	Total	Mg	0	0
			8	8		
56	1F	1	Total	Mg	0	0
			1	1		
56	1H	2	Total	Mg	0	0
			2	2		
56	1N	1	Total	Mg	0	0
			1	1		
56	1O	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1P	5	Total Mg 5 5	0	0
56	1Q	3	Total Mg 3 3	0	0
56	1R	3	Total Mg 3 3	0	0
56	1S	2	Total Mg 2 2	0	0
56	1T	5	Total Mg 5 5	0	0
56	1U	3	Total Mg 3 3	0	0
56	1V	1	Total Mg 1 1	0	0
56	1W	2	Total Mg 2 2	0	0
56	1Y	1	Total Mg 1 1	0	0
56	1Z	5	Total Mg 5 5	0	0
56	10	4	Total Mg 4 4	0	0
56	11	1	Total Mg 1 1	0	0
56	12	1	Total Mg 1 1	0	0
56	13	1	Total Mg 1 1	0	0
56	15	2	Total Mg 2 2	0	0
56	16	1	Total Mg 1 1	0	0
56	17	3	Total Mg 3 3	0	0
56	18	3	Total Mg 3 3	0	0
56	19	1	Total Mg 1 1	0	0
56	1a	319	Total Mg 319 319	0	0
56	1b	9	Total Mg 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1d	4	Total Mg 4 4	0	0
56	1e	2	Total Mg 2 2	0	0
56	1g	2	Total Mg 2 2	0	0
56	1i	1	Total Mg 1 1	0	0
56	1l	1	Total Mg 1 1	0	0
56	1m	2	Total Mg 2 2	0	0
56	1n	2	Total Mg 2 2	0	0
56	1o	1	Total Mg 1 1	0	0
56	1p	1	Total Mg 1 1	0	0
56	1q	1	Total Mg 1 1	0	0
56	1s	3	Total Mg 3 3	0	0
56	1t	1	Total Mg 1 1	0	0
56	1u	1	Total Mg 1 1	0	0
56	1v	3	Total Mg 3 3	0	0
56	1x	2	Total Mg 2 2	0	0
56	1y	6	Total Mg 6 6	0	0
56	1z	1	Total Mg 1 1	0	0
56	2A	852	Total Mg 852 852	0	0
56	2B	32	Total Mg 32 32	0	0
56	2D	6	Total Mg 6 6	0	0
56	2E	5	Total Mg 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2F	4	Total Mg 4 4	0	0
56	2N	2	Total Mg 2 2	0	0
56	2O	1	Total Mg 1 1	0	0
56	2P	3	Total Mg 3 3	0	0
56	2Q	6	Total Mg 6 6	0	0
56	2S	1	Total Mg 1 1	0	0
56	2T	2	Total Mg 2 2	0	0
56	2V	1	Total Mg 1 1	0	0
56	2X	1	Total Mg 1 1	0	0
56	2Y	2	Total Mg 2 2	0	0
56	2Z	4	Total Mg 4 4	0	0
56	20	6	Total Mg 6 6	0	0
56	21	1	Total Mg 1 1	0	0
56	23	3	Total Mg 3 3	0	0
56	24	1	Total Mg 1 1	0	0
56	25	1	Total Mg 1 1	0	0
56	26	2	Total Mg 2 2	0	0
56	27	3	Total Mg 3 3	0	0
56	28	6	Total Mg 6 6	0	0
56	29	2	Total Mg 2 2	0	0
56	2a	321	Total Mg 321 321	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2b	3	Total Mg 3 3	0	0
56	2c	1	Total Mg 1 1	0	0
56	2d	3	Total Mg 3 3	0	0
56	2e	2	Total Mg 2 2	0	0
56	2f	4	Total Mg 4 4	0	0
56	2g	6	Total Mg 6 6	0	0
56	2h	5	Total Mg 5 5	0	0
56	2i	4	Total Mg 4 4	0	0
56	2k	2	Total Mg 2 2	0	0
56	2l	6	Total Mg 6 6	0	0
56	2m	3	Total Mg 3 3	0	0
56	2o	1	Total Mg 1 1	0	0
56	2p	3	Total Mg 3 3	0	0
56	2q	4	Total Mg 4 4	0	0
56	2r	2	Total Mg 2 2	0	0
56	2s	3	Total Mg 3 3	0	0
56	2t	1	Total Mg 1 1	0	0
56	2u	3	Total Mg 3 3	0	0
56	2v	3	Total Mg 3 3	0	0
56	2w	2	Total Mg 2 2	0	0
56	2x	8	Total Mg 8 8	0	0

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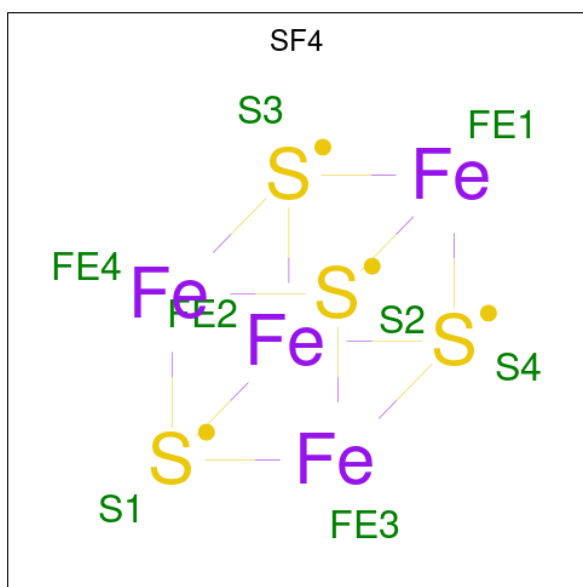
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2y	10	Total 10	Mg 10	0	0
56	2z	3	Total 3	Mg 3	0	0

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

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

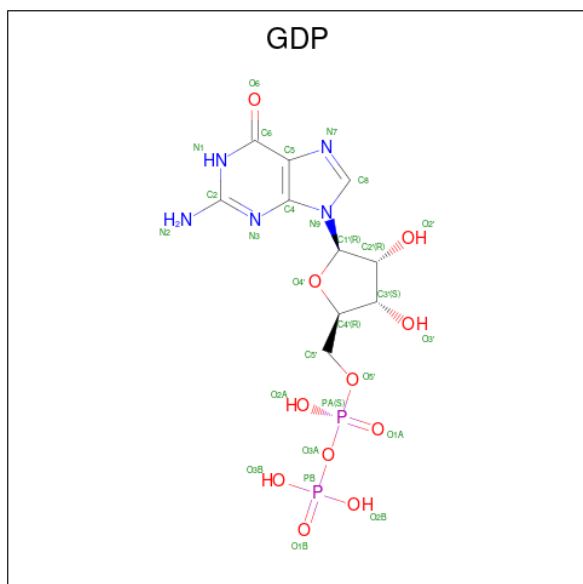
- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





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

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1v	1	Total C N O P 28 10 5 11 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
59	2v	1	28	10	5	11	2	0	0

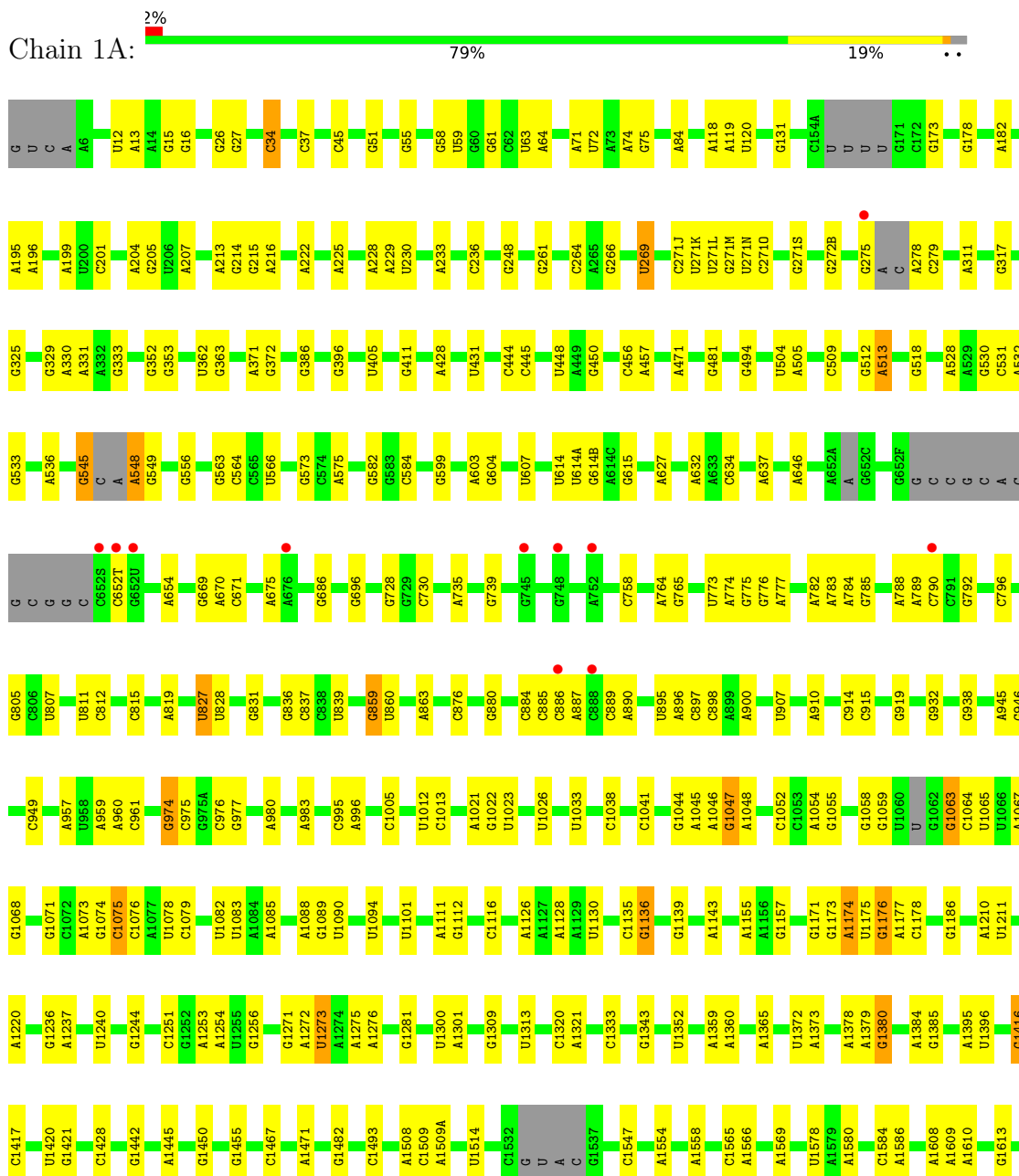
- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total	K	0	0
			1	1		

### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 2: 5S Ribosomal RNA

Chain 1B:  86% 13%



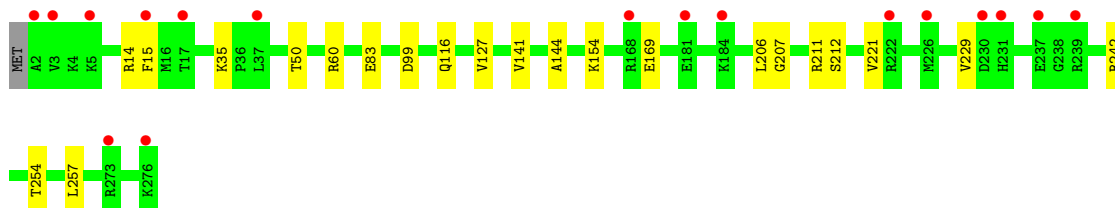
- Molecule 2: 5S Ribosomal RNA

Chain 2B:  78% 21%



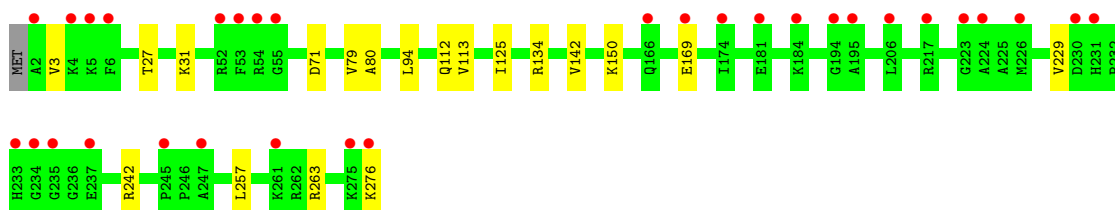
- Molecule 3: 50S ribosomal protein L2

Chain 1D:  92% 6% 8%




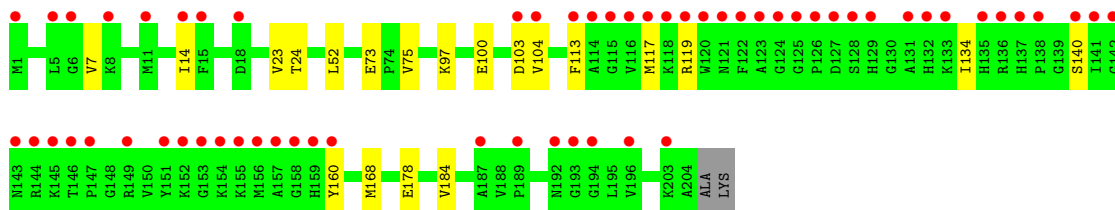
- Molecule 3: 50S ribosomal protein L2

Chain 2D:  93% 11% 7%

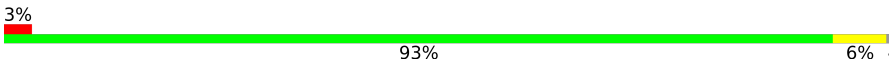


- Molecule 4: 50S ribosomal protein L3

Chain 1E:  89% 29% 10%

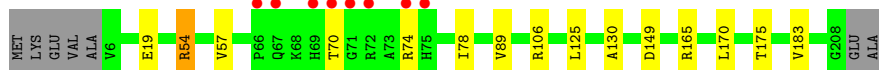
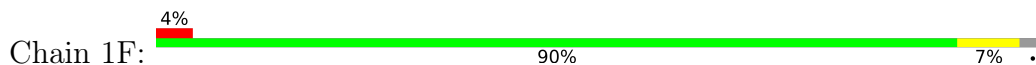


- Molecule 4: 50S ribosomal protein L3

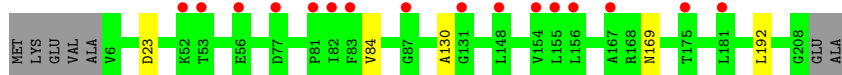
Chain 2E:  93% 3% 6%



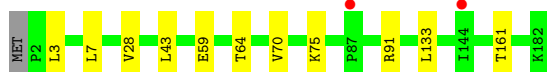
- Molecule 5: 50S ribosomal protein L4



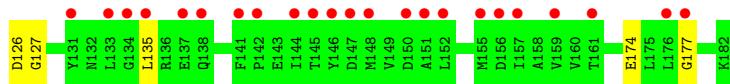
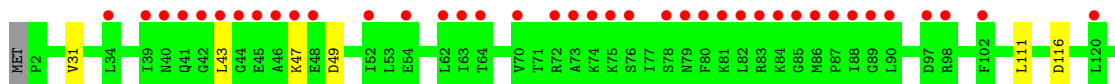
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5

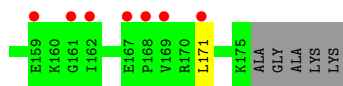


- Molecule 7: 50S ribosomal protein L6

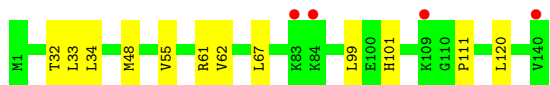


- Molecule 7: 50S ribosomal protein L6

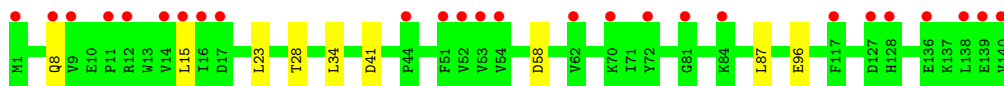




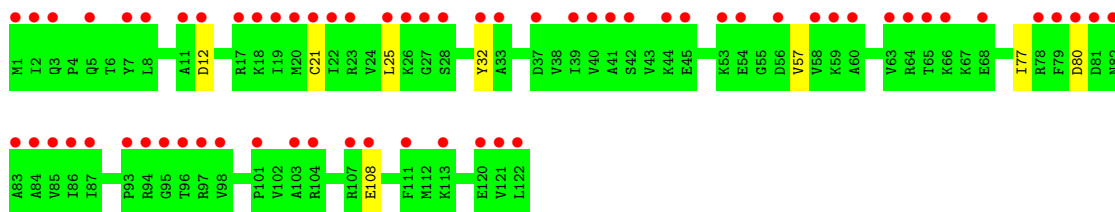
• Molecule 8: 50S ribosomal protein L13



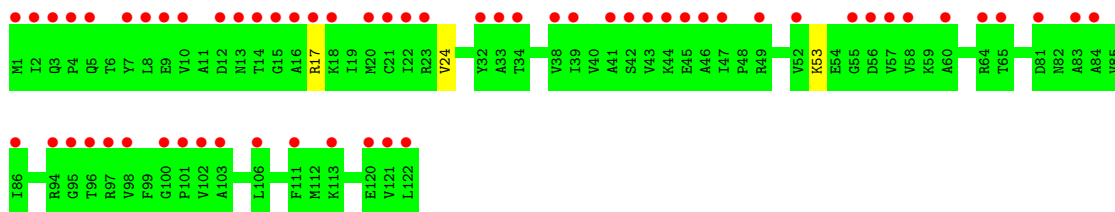
• Molecule 8: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L14



• Molecule 9: 50S ribosomal protein L14

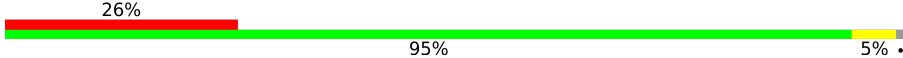


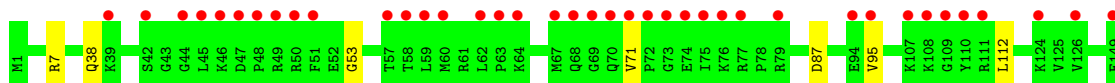
• Molecule 10: 50S ribosomal protein L15



• Molecule 10: 50S ribosomal protein L15



Chain 2P:  26% 95% 5%



ALA

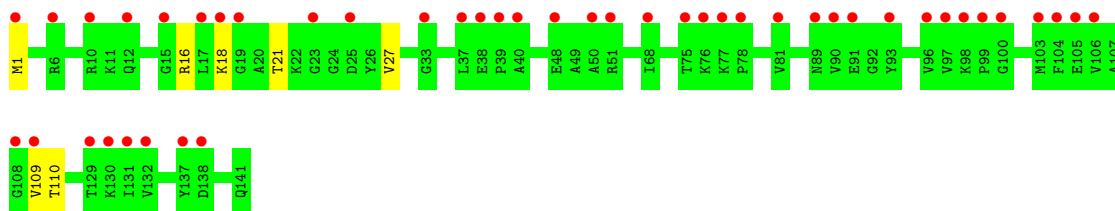
- Molecule 11: 50S ribosomal protein L16

Chain 1Q:  95% 5%




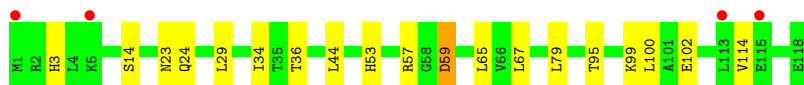
- Molecule 11: 50S ribosomal protein L16

Chain 2Q:  32% 95% 5%



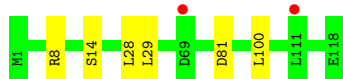
- Molecule 12: 50S ribosomal protein L17

Chain 1R:  3% 84% 15%




- Molecule 12: 50S ribosomal protein L17

Chain 2R:  2% 95% 5%

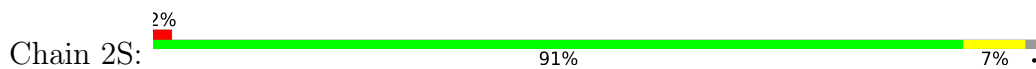


- Molecule 13: 50S ribosomal protein L18

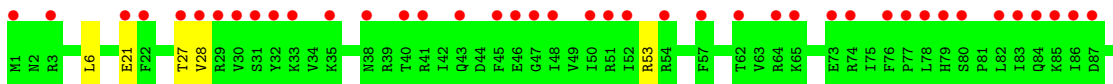
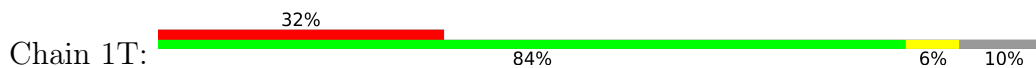
Chain 1S:  90% 8%



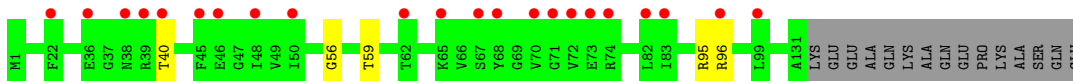
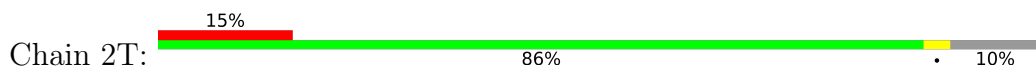
- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19



- Molecule 14: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L20



- Molecule 15: 50S ribosomal protein L20

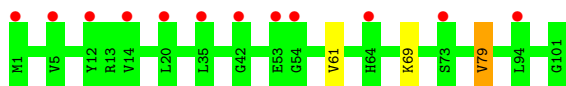


- Molecule 16: 50S ribosomal protein L21

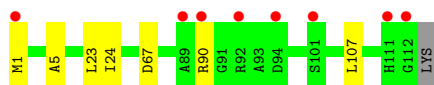


- Molecule 16: 50S ribosomal protein L21





- Molecule 17: 50S ribosomal protein L22



- Molecule 17: 50S ribosomal protein L22



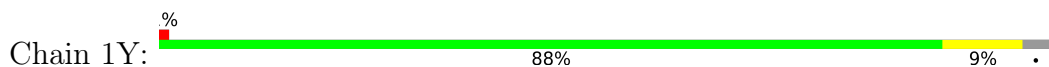
- Molecule 18: 50S ribosomal protein L23



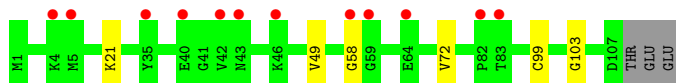
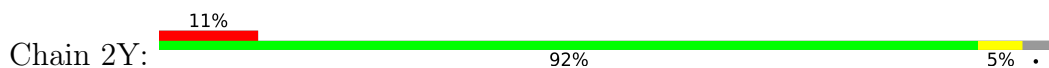
- Molecule 18: 50S ribosomal protein L23




- Molecule 19: 50S ribosomal protein L24



- Molecule 19: 50S ribosomal protein L24




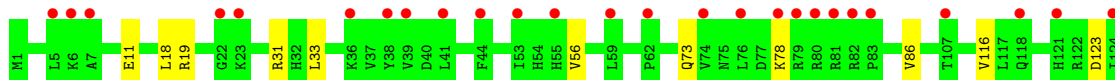
- Molecule 20: 50S ribosomal protein L25

Chain 1Z:  86% 13%




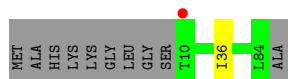
• Molecule 20: 50S ribosomal protein L25

Chain 2Z:  20% 86% 12%




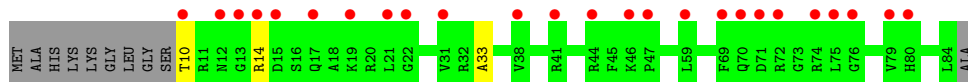
• Molecule 21: 50S ribosomal protein L27

Chain 10:  87% 12%



• Molecule 21: 50S ribosomal protein L27

Chain 20:  29% 85% 12%

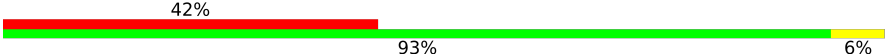


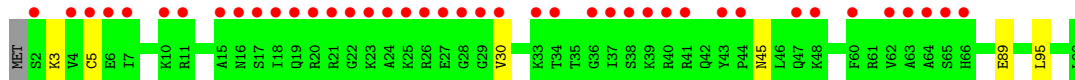
• Molecule 22: 50S ribosomal protein L28

Chain 11:  15% 94% 5%




• Molecule 22: 50S ribosomal protein L28

Chain 21:  42% 93% 6%

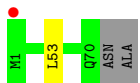


• Molecule 23: 50S ribosomal protein L29

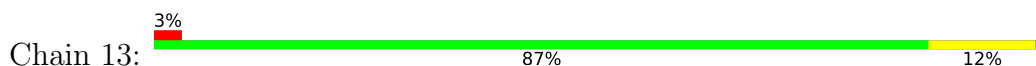
Chain 12:  89% 6%



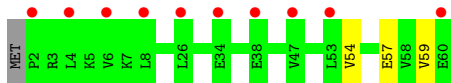
- Molecule 23: 50S ribosomal protein L29



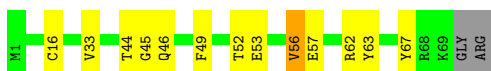
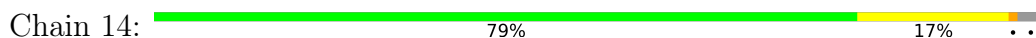
- Molecule 24: 50S ribosomal protein L30



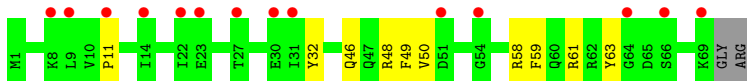
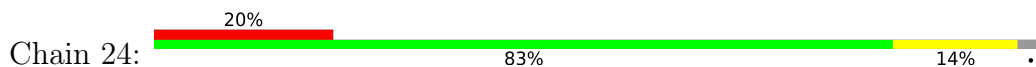
- Molecule 24: 50S ribosomal protein L30



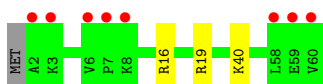
- Molecule 25: 50S ribosomal protein L31



- Molecule 25: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L32

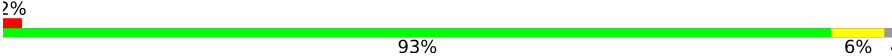


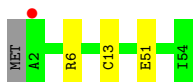
- Molecule 26: 50S ribosomal protein L32

Chain 25:  93% 5%

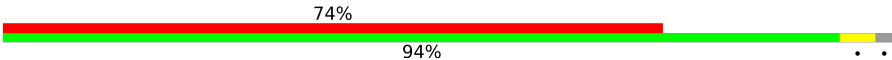


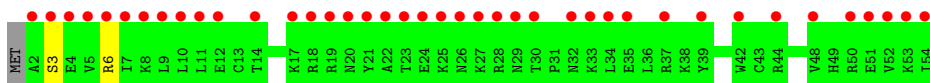
• Molecule 27: 50S ribosomal protein L33

Chain 16:  93% 6% 2%




• Molecule 27: 50S ribosomal protein L33

Chain 26:  94% 74% 6%




• Molecule 28: 50S ribosomal protein L34

Chain 17:  90% 8% 4%

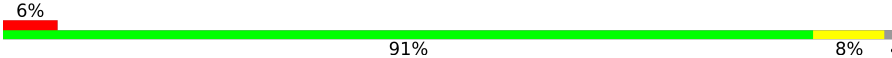


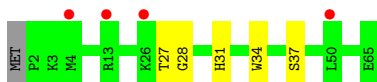
• Molecule 28: 50S ribosomal protein L34

Chain 27:  86% 12% 4%



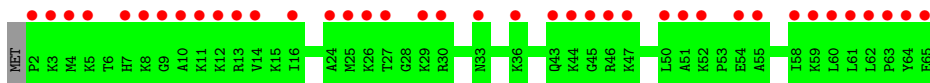
• Molecule 29: 50S ribosomal protein L35

Chain 18:  91% 8% 6%



• Molecule 29: 50S ribosomal protein L35

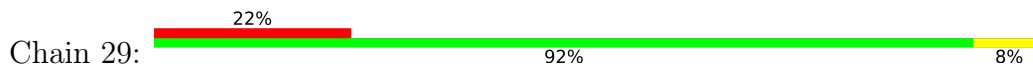
Chain 28:  98% 60%



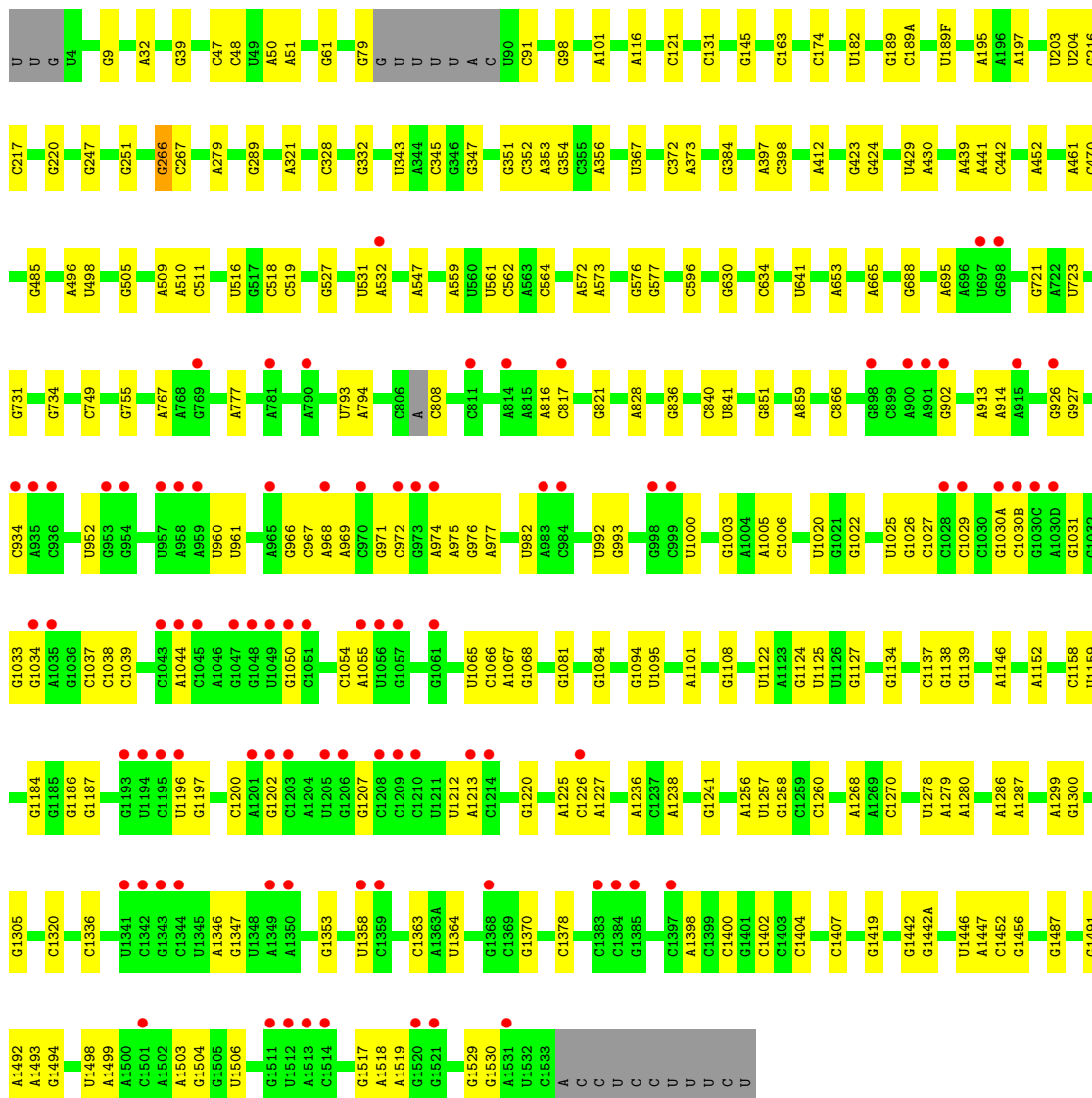
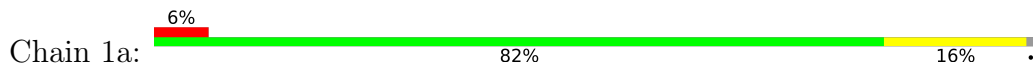
• Molecule 30: 50S ribosomal protein L36



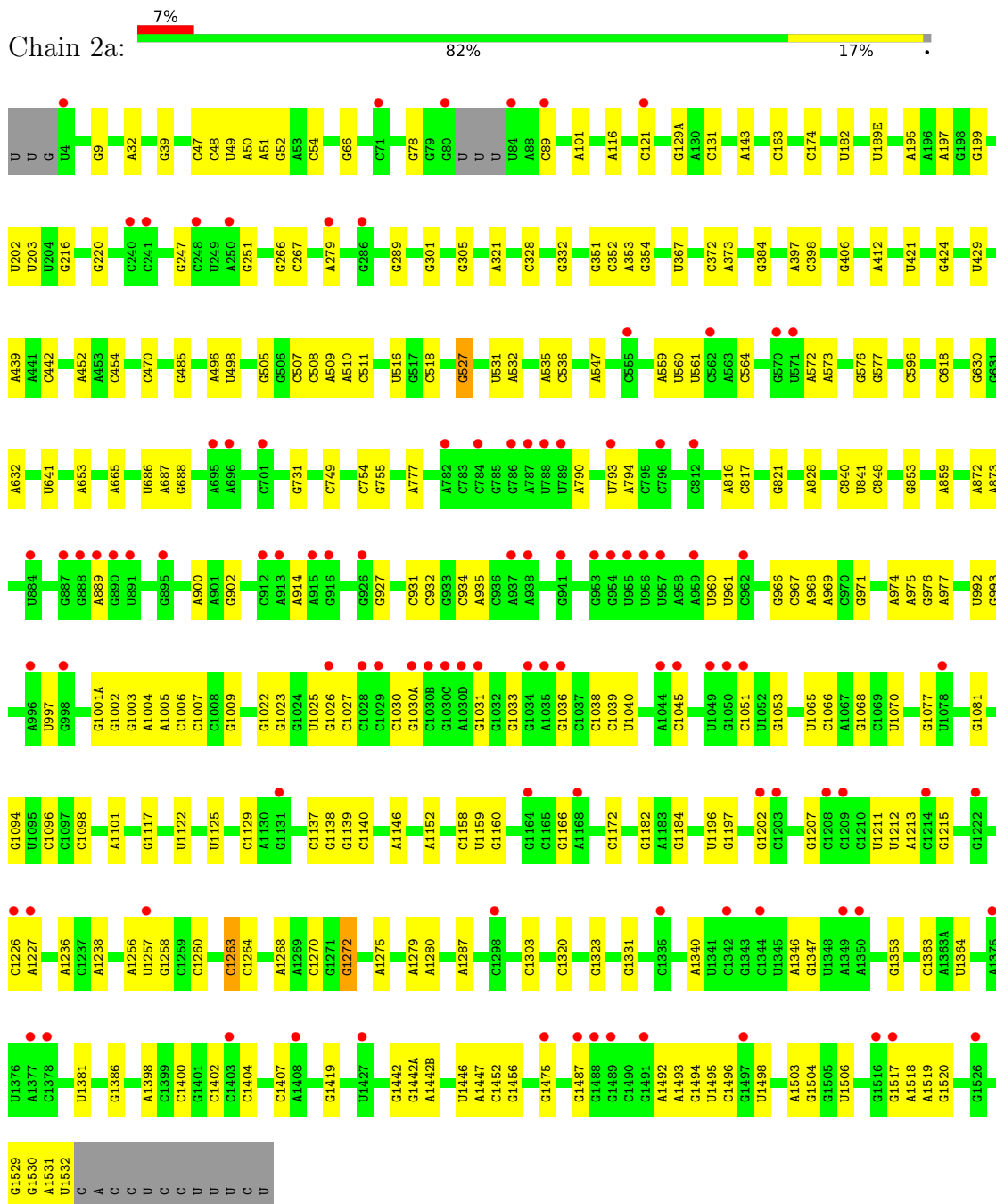
• Molecule 30: 50S ribosomal protein L36



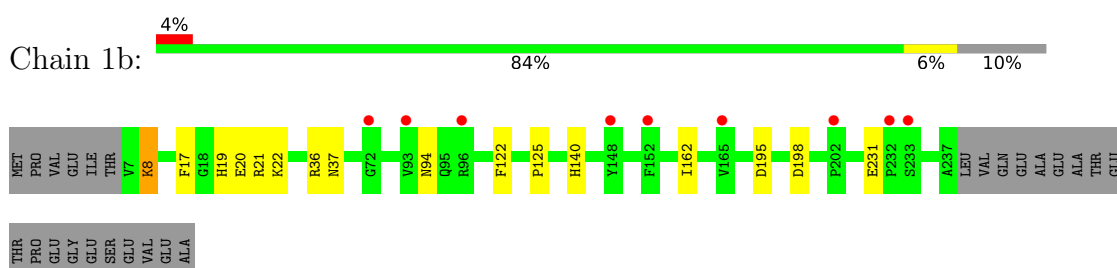
• Molecule 31: 16S Ribosomal RNA



• Molecule 31: 16S Ribosomal RNA



• Molecule 32: 30S ribosomal protein S2

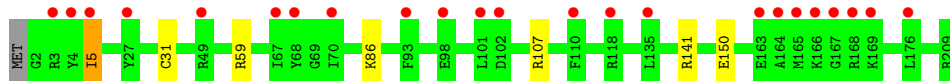




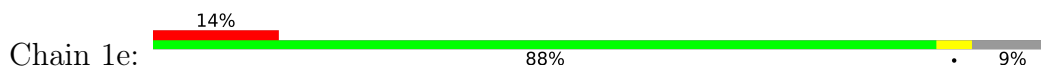




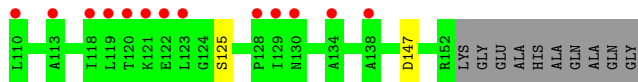
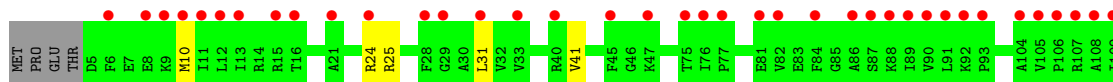
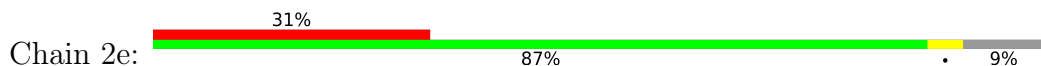
- Molecule 34: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S5



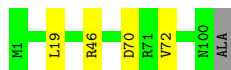
- Molecule 35: 30S ribosomal protein S5



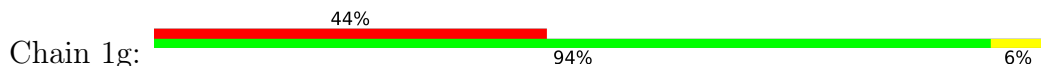
- Molecule 36: 30S ribosomal protein S6

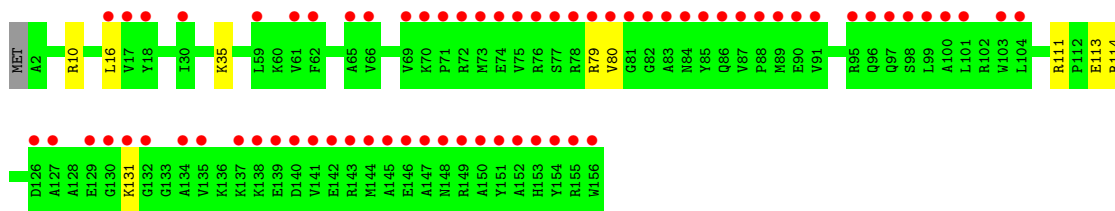


- Molecule 36: 30S ribosomal protein S6

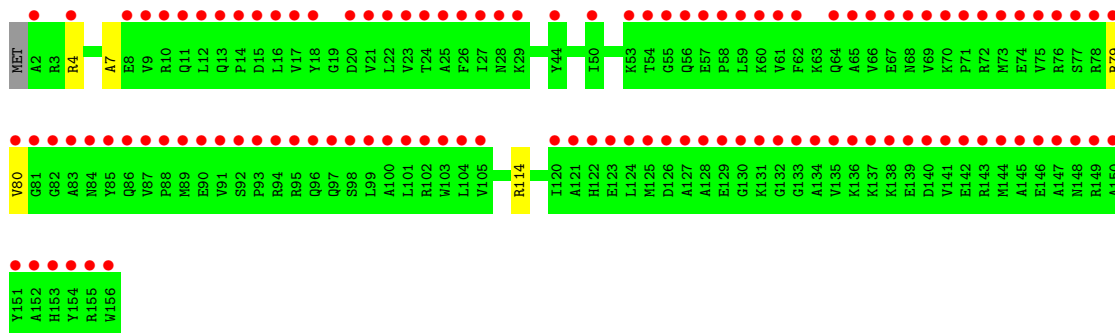
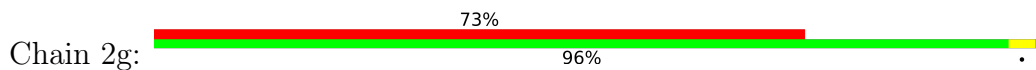


- Molecule 37: 30S ribosomal protein S7

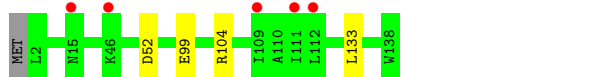




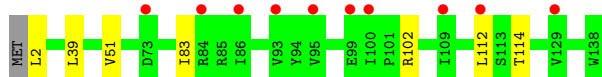
- Molecule 37: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S8



- Molecule 38: 30S ribosomal protein S8

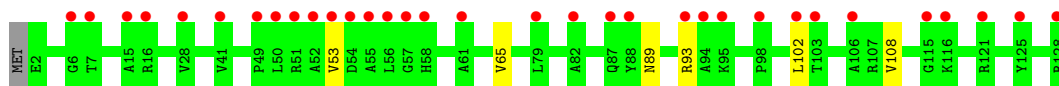


- Molecule 39: 30S ribosomal protein S9

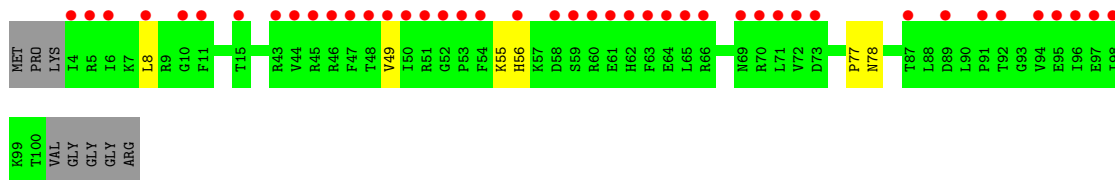
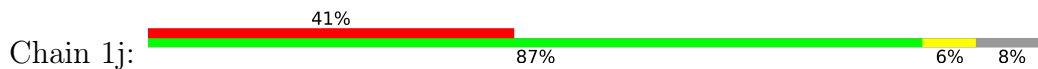


- Molecule 39: 30S ribosomal protein S9

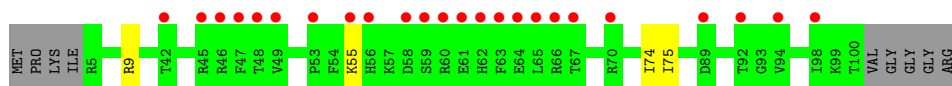
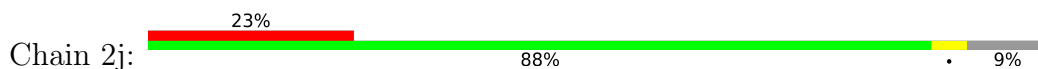




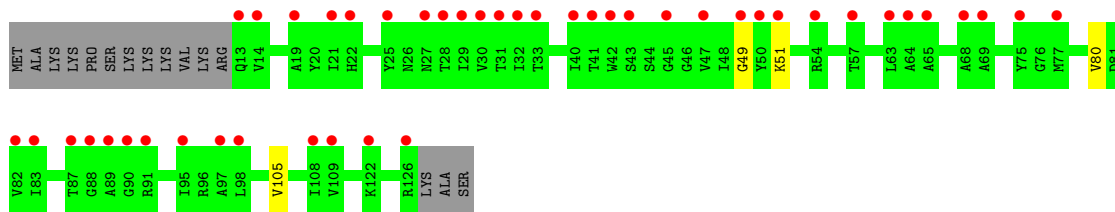
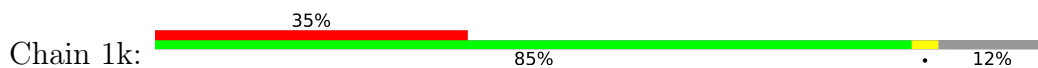
• Molecule 40: 30S ribosomal protein S10



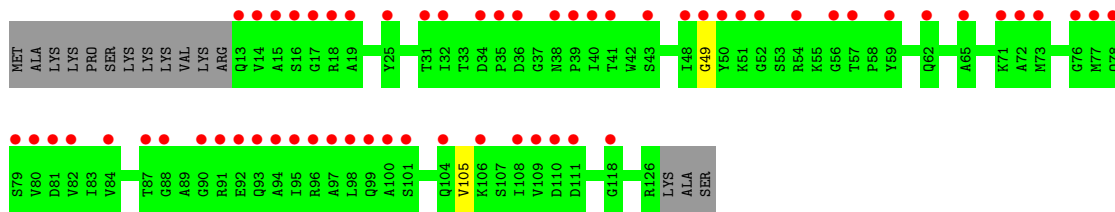
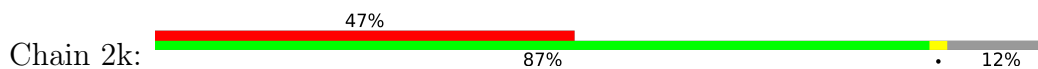
• Molecule 40: 30S ribosomal protein S10



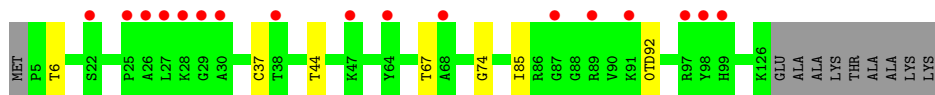
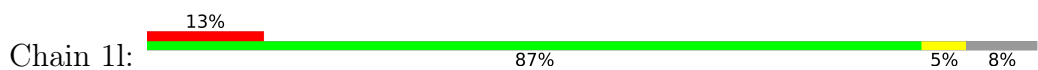
• Molecule 41: 30S ribosomal protein S11



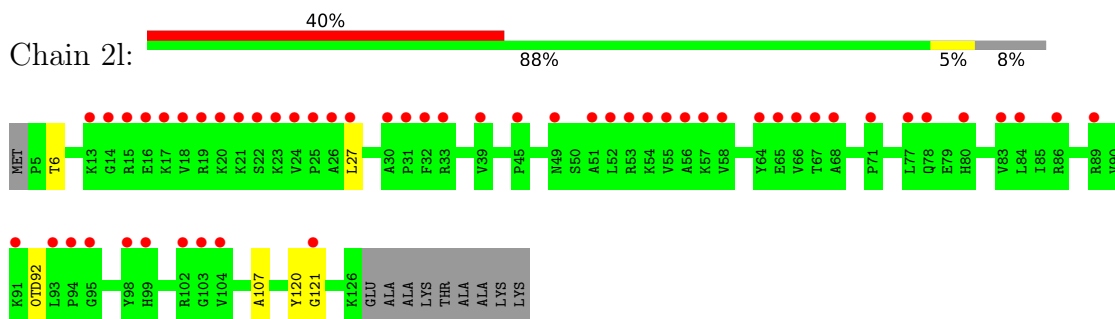
• Molecule 41: 30S ribosomal protein S11



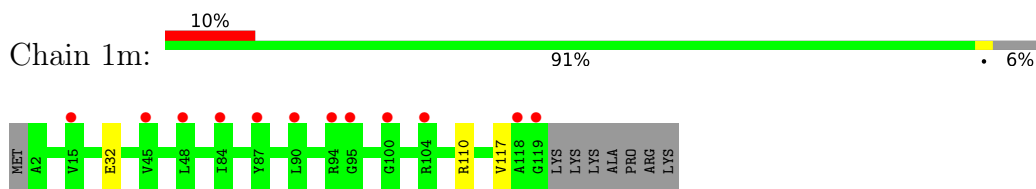
• Molecule 42: 30S ribosomal protein S12



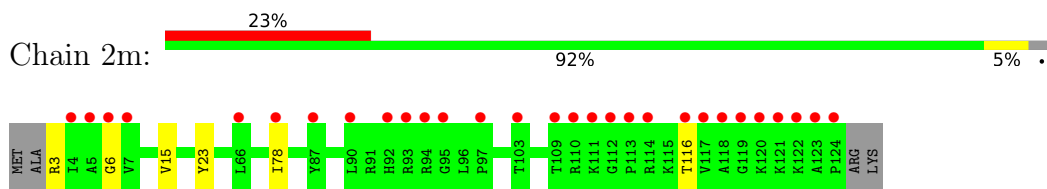
- Molecule 42: 30S ribosomal protein S12



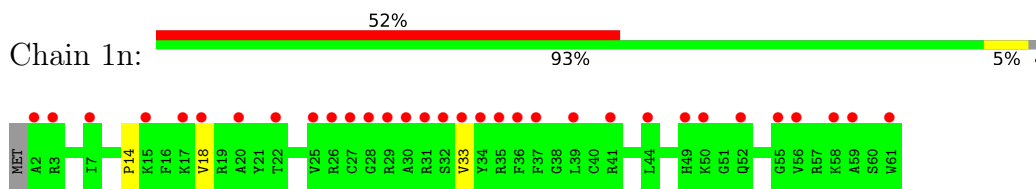
- Molecule 43: 30S ribosomal protein S13



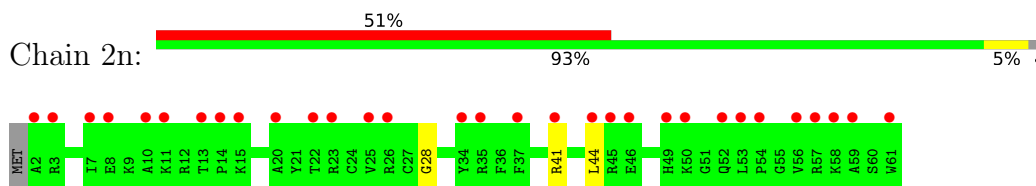
- Molecule 43: 30S ribosomal protein S13



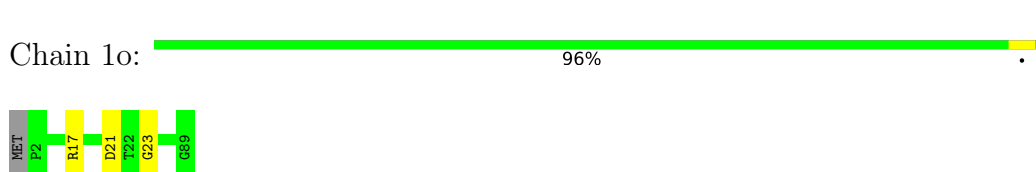
- Molecule 44: 30S ribosomal protein S14 type Z



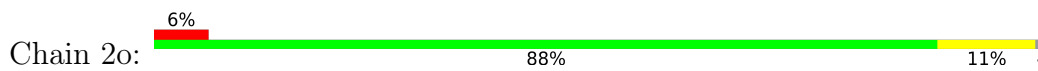
- Molecule 44: 30S ribosomal protein S14 type Z



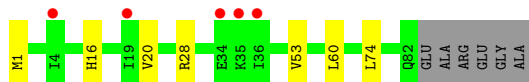
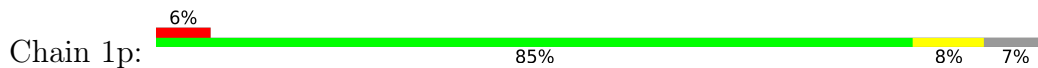
- Molecule 45: 30S ribosomal protein S15



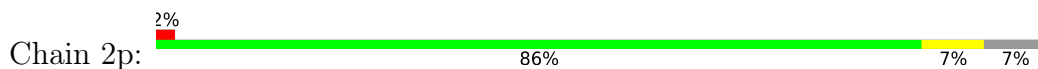
- Molecule 45: 30S ribosomal protein S15



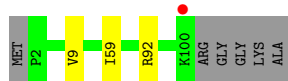
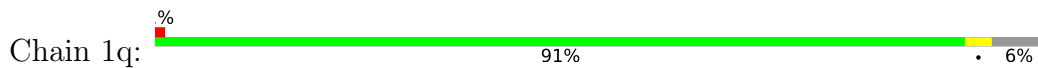
• Molecule 46: 30S ribosomal protein S16



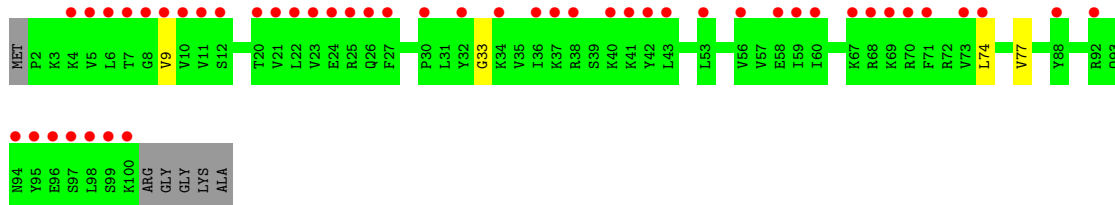
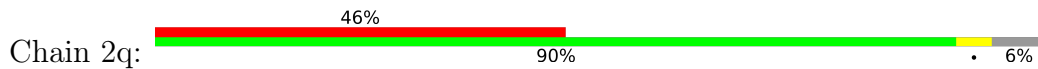
• Molecule 46: 30S ribosomal protein S16



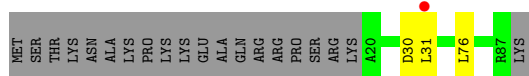
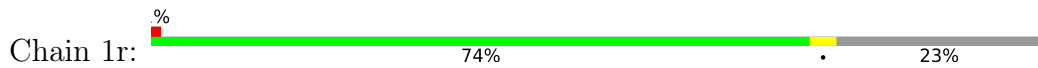
• Molecule 47: 30S ribosomal protein S17



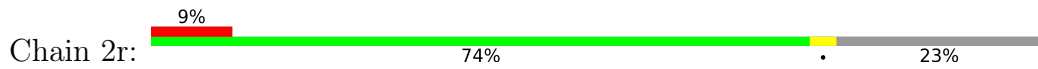
• Molecule 47: 30S ribosomal protein S17

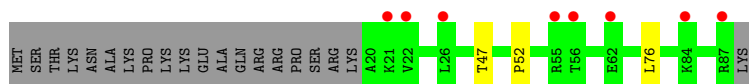


• Molecule 48: 30S ribosomal protein S18

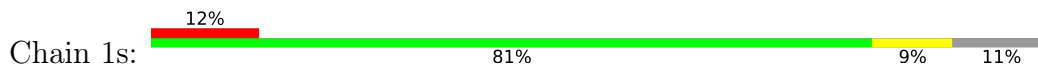


• Molecule 48: 30S ribosomal protein S18

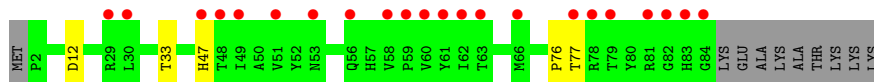
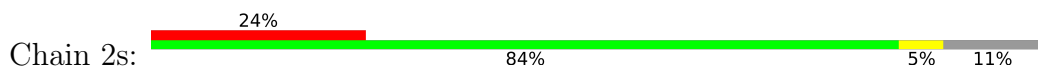




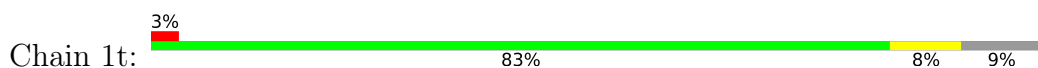
• Molecule 49: 30S ribosomal protein S19



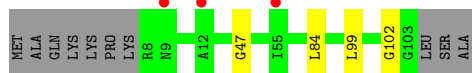
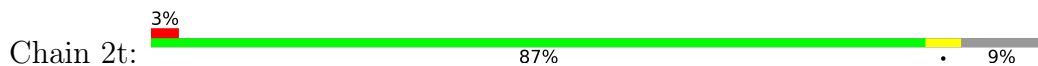
• Molecule 49: 30S ribosomal protein S19



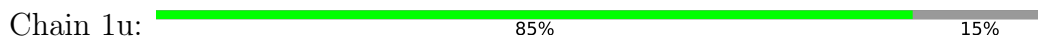
• Molecule 50: 30S ribosomal protein S20



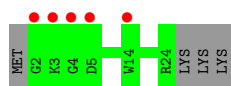
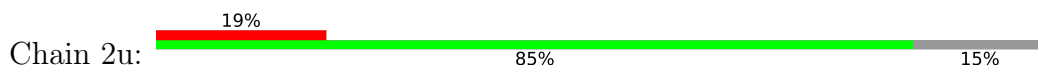
• Molecule 50: 30S ribosomal protein S20



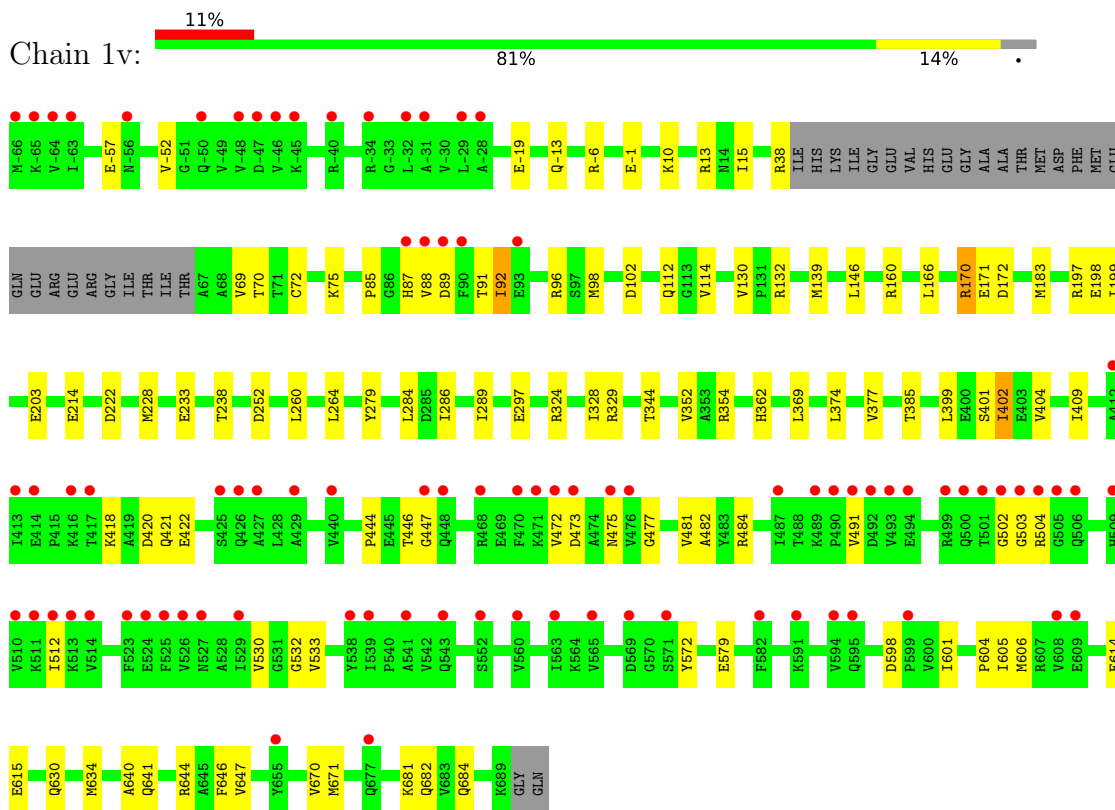
• Molecule 51: 30S ribosomal protein Thx



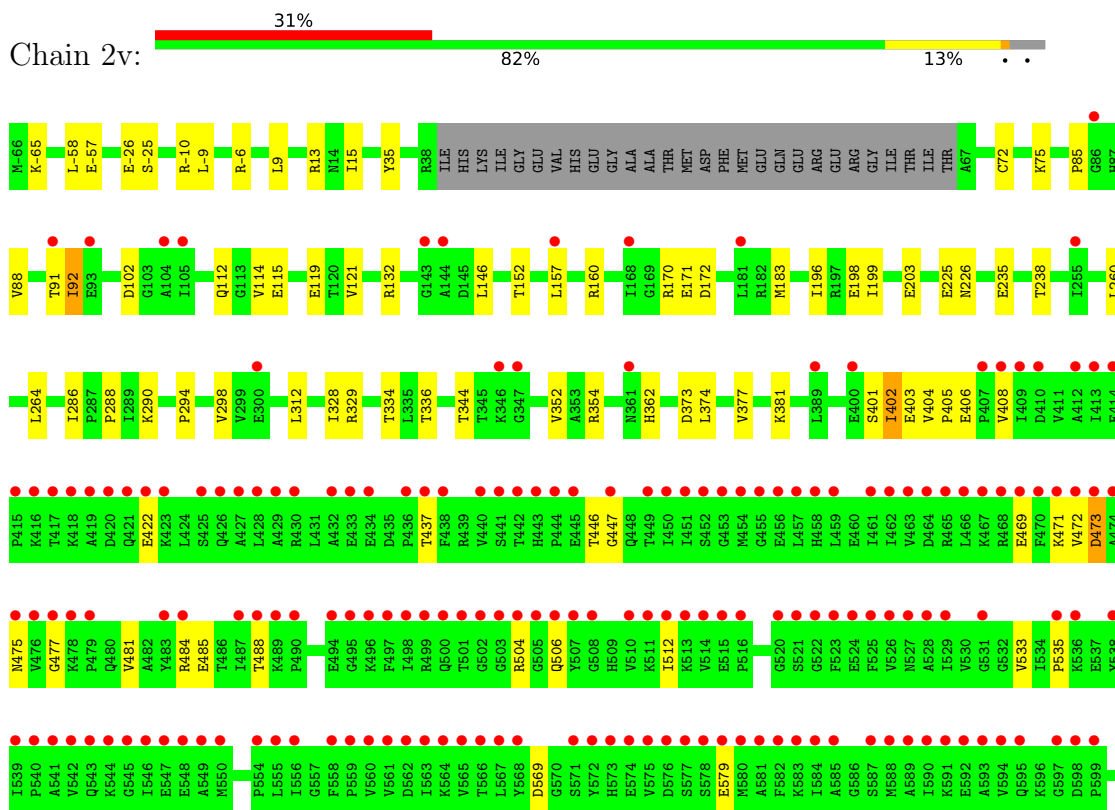
• Molecule 51: 30S ribosomal protein Thx



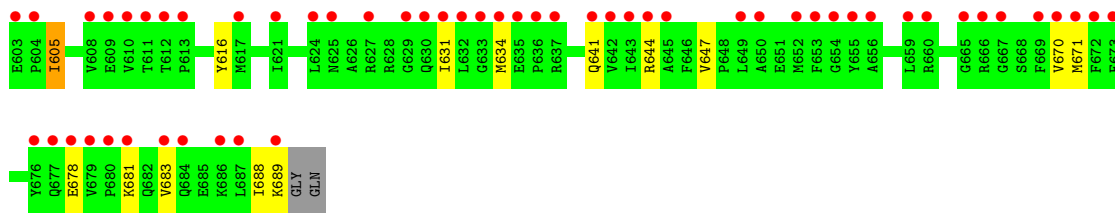
• Molecule 52: 50S ribosomal protein L9, Elongation factor G



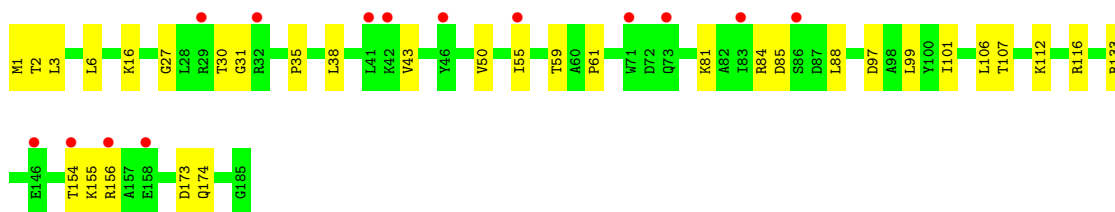
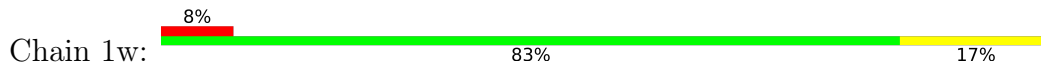
• Molecule 52: 50S ribosomal protein L9, Elongation factor G



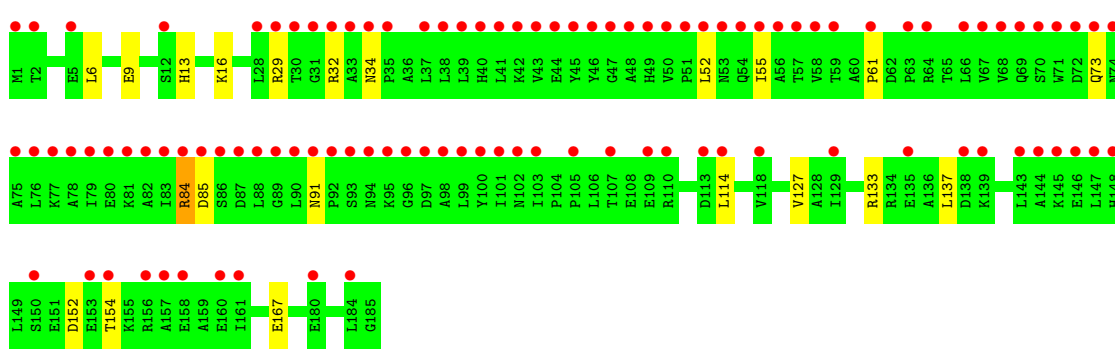
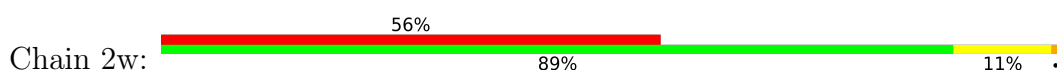




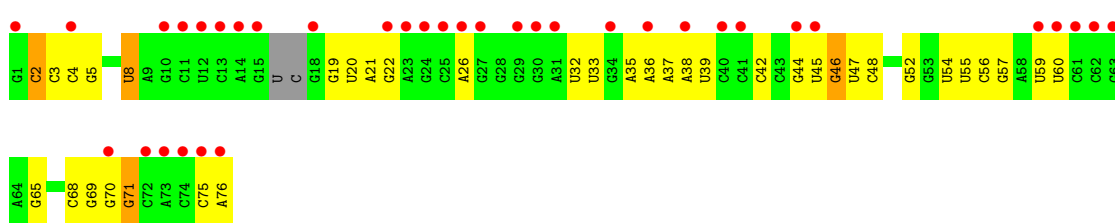
• Molecule 53: Ribosome-recycling factor



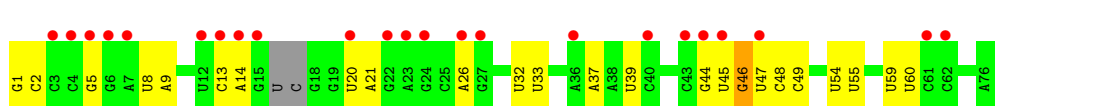
• Molecule 53: Ribosome-recycling factor



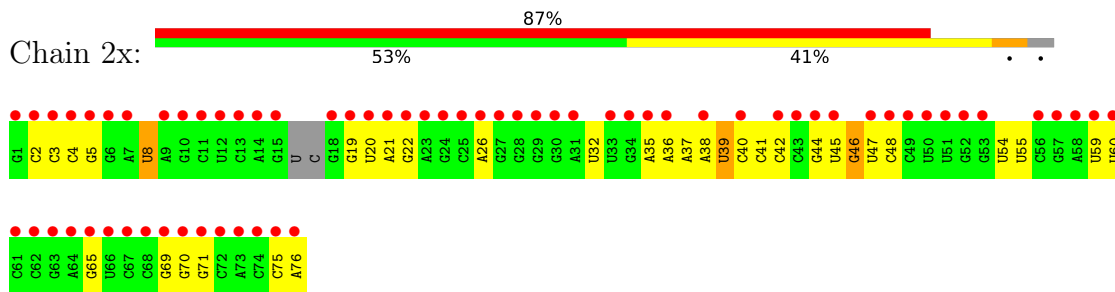
• Molecule 54: P-site and E-site tRNAs



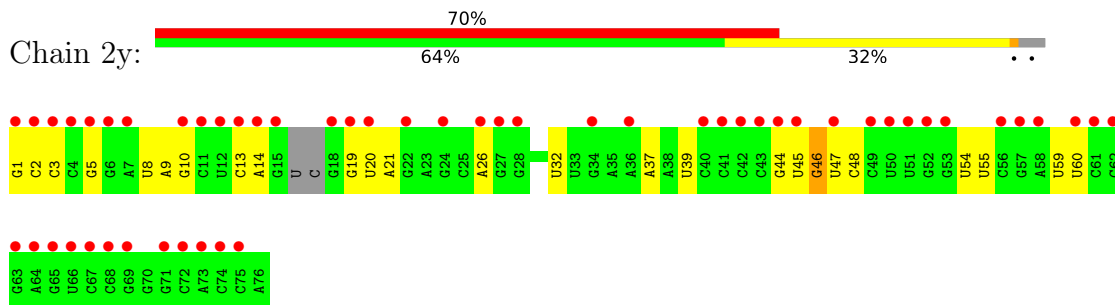
• Molecule 54: P-site and E-site tRNAs



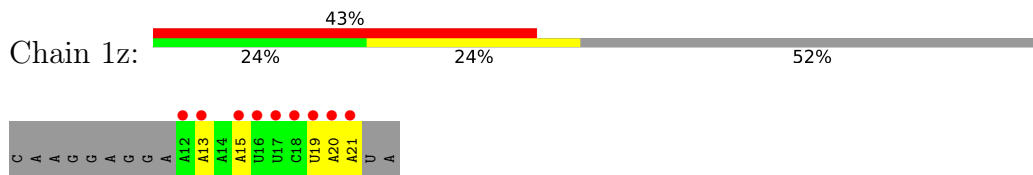
• Molecule 54: P-site and E-site tRNAs



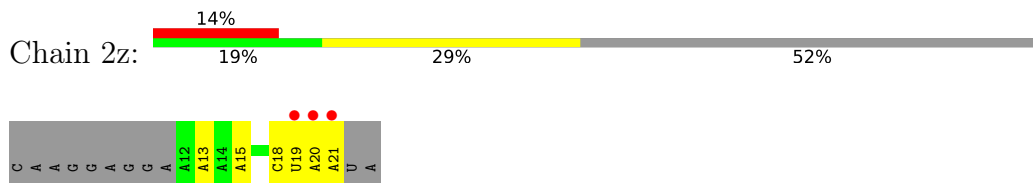
• Molecule 54: P-site and E-site tRNAs



• Molecule 55: mRNA



• Molecule 55: mRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.66Å 448.74Å 623.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.89 – 3.50 188.71 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.89-3.50) 98.3 (188.71-3.50)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 3.49Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.244 , 0.294 0.245 , 0.295	Depositor DCC
$R_{free}$ test set	36340 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.7	Xtrriage
Anisotropy	0.257	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 93.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	305259	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 2MG, PSU, MIA, UR3, GDP, 0TD, M2G, 4SU, 5MU, 7MG, MG, 5MC, K, OMC, 2MA, 4OC, MA6, SF4, OMG, 2MU

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	0.62	0/69010	1.08	104/107716 (0.1%)
1	2A	0.41	2/67294 (0.0%)	0.87	15/105038 (0.0%)
2	1B	0.56	1/2882 (0.0%)	0.94	0/4494
2	2B	0.35	1/2879 (0.0%)	0.80	1/4487 (0.0%)
3	1D	0.41	0/2186	0.58	0/2944
3	2D	0.34	0/2186	0.51	0/2944
4	1E	0.42	0/1592	0.57	0/2149
4	2E	0.31	0/1592	0.51	0/2149
5	1F	0.42	0/1619	0.55	0/2193
5	2F	0.31	0/1615	0.48	0/2188
6	1G	0.31	0/1476	0.49	0/1989
6	2G	0.26	0/1478	0.45	0/1992
7	1H	0.38	0/1356	0.52	0/1834
7	2H	0.28	0/1356	0.46	0/1834
8	1N	0.41	0/1144	0.54	0/1543
8	2N	0.29	0/1144	0.47	0/1543
9	1O	0.38	0/943	0.54	0/1269
9	2O	0.32	0/943	0.50	0/1269
10	1P	0.38	0/1152	0.61	0/1533
10	2P	0.31	0/1152	0.51	0/1533
11	1Q	0.43	0/1143	0.58	0/1527
11	2Q	0.30	0/1143	0.48	0/1527
12	1R	0.39	0/982	0.58	0/1312
12	2R	0.30	0/982	0.47	0/1312
13	1S	0.36	0/883	0.52	0/1176
13	2S	0.28	0/880	0.45	0/1172
14	1T	0.37	0/1105	0.53	0/1477
14	2T	0.30	0/1097	0.46	0/1468
15	1U	0.47	0/977	0.57	0/1301
15	2U	0.29	0/977	0.42	0/1301
16	1V	0.43	0/782	0.59	0/1049

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2V	0.31	0/782	0.49	0/1049
17	1W	0.45	0/897	0.60	0/1205
17	2W	0.33	0/897	0.50	0/1205
18	1X	0.46	0/764	0.58	0/1025
18	2X	0.35	0/764	0.49	0/1025
19	1Y	0.46	0/819	0.58	0/1095
19	2Y	0.32	0/819	0.48	0/1095
20	1Z	0.40	0/1615	0.57	0/2197
20	2Z	0.28	0/1615	0.50	0/2197
21	10	0.40	0/606	0.56	0/808
21	20	0.30	0/606	0.48	0/808
22	11	0.39	0/762	0.55	0/1014
22	21	0.31	0/762	0.49	0/1014
23	12	0.41	0/590	0.55	0/781
23	22	0.30	0/590	0.41	0/781
24	13	0.45	0/474	0.58	0/635
24	23	0.34	0/469	0.50	0/630
25	14	0.32	0/565	0.54	0/761
25	24	0.26	0/545	0.46	0/737
26	15	0.47	0/469	0.63	0/635
26	25	0.34	0/469	0.52	0/635
27	16	0.44	0/460	0.57	0/613
27	26	0.30	0/456	0.48	0/608
28	17	0.45	0/426	0.59	0/561
28	27	0.35	0/426	0.53	0/561
29	18	0.45	0/525	0.59	0/691
29	28	0.33	0/525	0.48	0/691
30	19	0.38	0/310	0.55	0/407
30	29	0.29	0/310	0.52	0/407
31	1a	0.34	0/35769	0.83	14/55821 (0.0%)
31	2a	0.31	0/35886	0.82	11/56005 (0.0%)
32	1b	0.28	0/1881	0.46	0/2542
32	2b	0.26	0/1860	0.44	0/2518
33	1c	0.25	0/1572	0.43	0/2126
33	2c	0.25	0/1566	0.44	0/2119
34	1d	0.28	0/1685	0.44	0/2262
34	2d	0.27	0/1704	0.43	0/2284
35	1e	0.29	0/1145	0.46	0/1543
35	2e	0.29	0/1149	0.47	0/1548
36	1f	0.28	0/823	0.45	0/1115
36	2f	0.28	0/829	0.46	0/1123
37	1g	0.25	0/1250	0.40	0/1679
37	2g	0.25	0/1254	0.41	0/1683

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1h	0.29	0/1108	0.45	0/1494
38	2h	0.28	0/1108	0.46	0/1494
39	1i	0.26	0/1002	0.44	0/1346
39	2i	0.26	0/997	0.43	0/1343
40	1j	0.24	0/722	0.46	0/982
40	2j	0.24	0/727	0.44	0/988
41	1k	0.29	0/844	0.47	0/1145
41	2k	0.28	0/848	0.46	0/1149
42	1l	0.30	0/937	0.47	0/1260
42	2l	0.29	0/937	0.50	0/1260
43	1m	0.25	0/929	0.44	0/1250
43	2m	0.25	0/961	0.45	0/1291
44	1n	0.25	0/501	0.42	0/664
44	2n	0.26	0/501	0.46	0/664
45	1o	0.29	0/739	0.43	0/985
45	2o	0.26	0/739	0.43	0/985
46	1p	0.29	0/697	0.44	0/939
46	2p	0.28	0/693	0.46	0/935
47	1q	0.34	0/836	0.49	0/1117
47	2q	0.29	0/836	0.44	0/1117
48	1r	0.28	0/560	0.46	0/746
48	2r	0.27	0/560	0.43	0/746
49	1s	0.26	0/667	0.48	0/900
49	2s	0.25	0/661	0.48	0/893
50	1t	0.28	0/730	0.42	0/965
50	2t	0.26	0/729	0.40	0/965
51	1u	0.26	0/203	0.44	0/266
51	2u	0.22	0/203	0.40	0/266
52	1v	0.32	1/5765 (0.0%)	0.51	0/7809
52	2v	0.29	0/5765	0.49	0/7809
53	1w	0.35	0/1497	0.51	0/2017
53	2w	0.30	0/1497	0.45	0/2017
54	1x	0.39	0/1602	1.06	6/2493 (0.2%)
54	1y	0.36	0/1602	0.98	3/2493 (0.1%)
54	2x	0.32	0/1602	0.96	2/2493 (0.1%)
54	2y	0.32	0/1602	0.92	1/2493 (0.0%)
55	1z	0.36	0/237	0.74	0/366
55	2z	0.30	0/237	0.73	0/366
All	All	0.43	5/326021 (0.0%)	0.83	157/486013 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2426	A	O3'-P	-10.56	1.48	1.61
2	1B	1	U	OP3-P	-10.13	1.49	1.61
2	2B	1	U	OP3-P	-10.12	1.49	1.61
52	1v	199	ILE	C-N	8.10	1.49	1.34
1	2A	2440	C	O3'-P	6.55	1.69	1.61

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2a	1272	G	C5-C6-O6	11.42	135.45	128.60
31	1a	1030(B)	C	C2-N1-C1'	8.79	128.47	118.80
1	1A	1075	C	N1-C2-O2	8.70	124.12	118.90
31	2a	1272	G	N3-C2-N2	8.58	125.91	119.90
31	1a	1030(B)	C	N1-C2-O2	8.46	123.98	118.90
31	2a	1272	G	N1-C6-O6	-8.31	114.92	119.90
31	2a	1272	G	N1-C2-N2	-8.17	108.85	116.20
1	1A	1979	C	C6-N1-C2	-8.01	117.10	120.30
1	1A	974	G	C8-N9-C4	-7.83	103.27	106.40
31	1a	1158	C	C2-N1-C1'	7.59	127.15	118.80
1	1A	2167	U	C2-N1-C1'	7.56	126.77	117.70
1	1A	1380	G	O5'-P-OP2	-7.50	98.95	105.70
1	1A	1075	C	C2-N3-C4	7.40	123.60	119.90
1	1A	2167	U	N1-C2-O2	7.25	127.88	122.80
1	1A	2167	U	N3-C2-O2	-7.02	117.28	122.20
31	1a	1030(B)	C	N3-C2-O2	-6.96	117.03	121.90
31	1a	808	C	C6-N1-C2	-6.91	117.53	120.30
31	2a	754	C	C2-N1-C1'	6.83	126.31	118.80
1	1A	977	G	O5'-P-OP1	-6.82	99.56	105.70
31	1a	266	G	P-O3'-C3'	6.81	127.87	119.70
54	1x	56	C	C2-N3-C4	6.78	123.29	119.90
1	1A	1653	G	P-O3'-C3'	6.72	127.76	119.70
1	1A	1665	A	O5'-P-OP1	-6.70	99.67	105.70
1	1A	859	G	N3-C4-C5	6.66	131.93	128.60
1	1A	512	G	O4'-C1'-N9	6.64	113.52	108.20
2	2B	80	U	O4'-C1'-N1	6.64	113.51	108.20
54	1x	2	C	C2-N3-C4	6.63	123.21	119.90
1	1A	513	A	N1-C6-N6	-6.62	114.63	118.60
1	1A	837	C	C6-N1-C2	-6.56	117.68	120.30
1	1A	1629	U	C5-C6-N1	6.55	125.97	122.70
31	1a	1030(B)	C	C6-N1-C2	-6.51	117.69	120.30
1	2A	529	A	O5'-P-OP1	-6.48	99.87	105.70
1	2A	1380	G	O5'-P-OP2	-6.41	99.93	105.70
54	2x	2	C	N1-C2-O2	6.34	122.70	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1653	G	N3-C4-C5	-6.33	125.43	128.60
54	1x	56	C	C5-C4-N4	6.31	124.61	120.20
1	2A	1983	C	C6-N1-C2	-6.25	117.80	120.30
1	1A	59	U	C5-C6-N1	6.23	125.82	122.70
1	1A	450	G	C8-N9-C4	-6.23	103.91	106.40
1	1A	445	C	C6-N1-C2	-6.22	117.81	120.30
1	1A	1653	G	C4-N9-C1'	6.21	134.58	126.50
1	1A	2423	U	C6-N1-C2	6.20	124.72	121.00
1	1A	2006	C	C2-N1-C1'	6.06	125.47	118.80
31	1a	1158	C	C6-N1-C2	-6.05	117.88	120.30
1	1A	269	U	P-O3'-C3'	6.04	126.95	119.70
1	1A	582	G	C8-N9-C4	6.04	108.81	106.40
1	1A	518	G	N3-C4-C5	-6.04	125.58	128.60
1	1A	859	G	C8-N9-C4	6.03	108.81	106.40
1	2A	1779	U	C2-N1-C1'	6.02	124.93	117.70
54	1y	33	U	C2-N1-C1'	6.01	124.91	117.70
1	1A	2501	C	C6-N1-C2	5.99	122.70	120.30
1	1A	548	A	P-O3'-C3'	5.99	126.88	119.70
1	2A	228	A	OP1-P-O3'	5.98	118.35	105.20
1	1A	26	G	N3-C4-C5	-5.95	125.62	128.60
1	1A	614	U	N3-C2-O2	-5.95	118.04	122.20
31	1a	1158	C	N1-C2-O2	5.95	122.47	118.90
31	1a	1030(B)	C	C6-N1-C1'	-5.89	113.73	120.80
1	2A	1610	A	C8-N9-C4	-5.83	103.47	105.80
1	2A	2136	C	N1-C2-O2	5.81	122.39	118.90
54	1x	2	C	N1-C2-O2	5.80	122.38	118.90
1	1A	1174	A	P-O3'-C3'	5.79	126.65	119.70
1	1A	739	G	N3-C4-C5	-5.79	125.71	128.60
1	1A	2044	C	C6-N1-C2	-5.71	118.01	120.30
31	2a	754	C	N1-C2-O2	5.71	122.33	118.90
54	1y	1	G	P-O3'-C3'	5.71	126.56	119.70
1	1A	1640	C	O4'-C1'-N1	5.71	112.77	108.20
1	1A	1176	G	OP1-P-O3'	5.70	117.74	105.20
1	1A	1251	C	C5-C6-N1	-5.68	118.16	121.00
54	2x	2	C	C2-N3-C4	5.66	122.73	119.90
1	1A	728	G	N3-C4-N9	5.65	129.39	126.00
1	1A	774	A	O5'-P-OP2	-5.65	100.62	105.70
1	1A	1136	G	N3-C4-C5	-5.64	125.78	128.60
1	2A	2848	G	O4'-C1'-N9	5.63	112.71	108.20
1	1A	2515	C	N3-C2-O2	-5.63	117.96	121.90
1	1A	333	G	C4-N9-C1'	5.63	133.81	126.50
1	1A	1658	C	C6-N1-C2	-5.62	118.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2589	A	C8-N9-C4	5.60	108.04	105.80
1	1A	1653	G	N3-C4-N9	5.59	129.35	126.00
1	1A	827	U	C6-N1-C2	5.59	124.35	121.00
1	1A	1372	U	C5-C4-O4	-5.59	122.55	125.90
1	1A	1174	A	OP1-P-O3'	5.57	117.45	105.20
1	1A	178	G	C8-N9-C4	5.55	108.62	106.40
1	1A	2432	A	N1-C6-N6	5.55	121.93	118.60
31	2a	1263	C	N1-C2-O2	5.55	122.23	118.90
54	1x	71	G	N3-C2-N2	5.53	123.77	119.90
1	1A	2271	G	N3-C4-N9	5.52	129.31	126.00
1	1A	2320	A	C8-N9-C4	-5.50	103.60	105.80
1	1A	545	G	C8-N9-C4	-5.48	104.21	106.40
1	1A	2271	G	N3-C4-C5	-5.48	125.86	128.60
1	1A	1082	U	N3-C4-O4	-5.47	115.57	119.40
31	1a	1034	G	C6-N1-C2	5.47	128.38	125.10
1	1A	1251	C	C6-N1-C2	5.46	122.48	120.30
1	1A	1416	G	O4'-C1'-N9	5.46	112.56	108.20
1	1A	34	C	C6-N1-C2	5.45	122.48	120.30
1	1A	2335	A	O4'-C1'-N9	5.45	112.56	108.20
1	1A	807	U	C5-C4-O4	-5.44	122.63	125.90
31	1a	1067	A	P-O3'-C3'	5.43	126.22	119.70
1	1A	2423	U	C5-C6-N1	-5.38	120.01	122.70
1	1A	1186	G	N1-C6-O6	-5.38	116.67	119.90
1	1A	1157	G	C4-N9-C1'	5.38	133.49	126.50
31	2a	1158	C	C2-N1-C1'	5.38	124.72	118.80
1	2A	2579	C	C5-C6-N1	5.37	123.68	121.00
1	1A	859	G	N1-C6-O6	5.36	123.11	119.90
1	1A	59	U	C6-N1-C2	-5.35	117.79	121.00
1	1A	518	G	N3-C4-N9	5.35	129.21	126.00
1	1A	1784	A	N1-C6-N6	-5.35	115.39	118.60
1	1A	2319	G	O4'-C1'-N9	5.35	112.48	108.20
1	1A	735	A	C8-N9-C4	5.34	107.94	105.80
1	1A	773	U	C5-C6-N1	-5.34	120.03	122.70
54	1x	68	C	N1-C2-O2	5.34	122.10	118.90
1	1A	207	A	C8-N9-C4	5.34	107.94	105.80
1	1A	431	U	C5-C6-N1	5.34	125.37	122.70
1	1A	236	C	C6-N1-C2	5.33	122.43	120.30
1	1A	1047	G	C8-N9-C4	-5.33	104.27	106.40
1	2A	1350	C	C6-N1-C2	5.32	122.43	120.30
1	1A	2689	U	P-O3'-C3'	5.32	126.08	119.70
1	1A	16	G	N1-C6-O6	5.32	123.09	119.90
1	1A	2446	G	O5'-P-OP2	-5.30	100.93	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	26	G	N3-C4-N9	5.30	129.18	126.00
1	1A	333	G	C8-N9-C1'	-5.30	120.11	127.00
1	2A	752	A	P-O3'-C3'	5.30	126.06	119.70
1	1A	783	A	C4-C5-C6	5.28	119.64	117.00
1	1A	1273	U	N1-C2-N3	5.28	118.07	114.90
31	1a	1030(B)	C	C5-C6-N1	5.28	123.64	121.00
1	1A	2006	C	C5-C4-N4	-5.27	116.51	120.20
1	1A	974	G	N7-C8-N9	5.23	115.72	113.10
1	1A	976	C	C6-N1-C2	-5.23	118.21	120.30
1	1A	863	A	O5'-P-OP2	-5.21	101.01	105.70
1	1A	1653	G	C8-N9-C1'	-5.20	120.24	127.00
54	2y	1	G	P-O3'-C3'	5.20	125.94	119.70
1	2A	1905	C	N1-C2-O2	5.19	122.02	118.90
1	1A	1333	C	N3-C4-C5	5.19	123.98	121.90
1	1A	1781	C	C6-N1-C2	5.18	122.37	120.30
1	1A	836	G	C8-N9-C4	-5.18	104.33	106.40
1	2A	528	A	OP1-P-O3'	5.17	116.58	105.20
1	1A	783	A	N3-C4-C5	-5.16	123.19	126.80
1	1A	1885	A	C8-N9-C4	5.15	107.86	105.80
54	1y	33	U	N1-C2-O2	5.15	126.40	122.80
1	1A	599	G	N3-C4-N9	5.14	129.09	126.00
1	1A	2069	G	N3-C4-C5	-5.13	126.03	128.60
1	2A	228	A	P-O3'-C3'	5.12	125.85	119.70
31	2a	1263	C	C2-N3-C4	5.12	122.46	119.90
31	2a	1158	C	N1-C2-O2	5.12	121.97	118.90
1	1A	671	C	C6-N1-C2	-5.11	118.25	120.30
31	2a	1272	G	C4-N9-C1'	5.10	133.13	126.50
1	1A	1063	G	C5-C6-O6	5.09	131.66	128.60
1	1A	2553	G	N3-C4-N9	5.08	129.05	126.00
1	1A	790	C	N1-C2-O2	5.08	121.95	118.90
31	1a	913	A	P-O3'-C3'	5.07	125.79	119.70
1	1A	815	C	OP2-P-O3'	5.06	116.34	105.20
1	1A	2028	U	N3-C4-C5	-5.05	111.57	114.60
1	1A	1157	G	C8-N9-C1'	-5.05	120.44	127.00
1	1A	949	C	C6-N1-C2	5.04	122.32	120.30
1	2A	1963	U	N1-C2-N3	-5.04	111.88	114.90
1	1A	2032	G	C5-N7-C8	-5.01	101.80	104.30
1	1A	2432	A	C6-C5-N7	-5.01	128.79	132.30
1	1A	859	G	C4-N9-C1'	-5.01	119.99	126.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	241 (88%)	26 (10%)	6 (2%)	6	37
3	2D	273/276 (99%)	234 (86%)	33 (12%)	6 (2%)	6	37
4	1E	202/206 (98%)	179 (89%)	19 (9%)	4 (2%)	7	39
4	2E	202/206 (98%)	174 (86%)	26 (13%)	2 (1%)	15	54
5	1F	201/210 (96%)	182 (90%)	17 (8%)	2 (1%)	15	54
5	2F	201/210 (96%)	183 (91%)	15 (8%)	3 (2%)	10	45
6	1G	179/182 (98%)	155 (87%)	23 (13%)	1 (1%)	25	64
6	2G	179/182 (98%)	147 (82%)	27 (15%)	5 (3%)	5	32
7	1H	172/180 (96%)	152 (88%)	18 (10%)	2 (1%)	13	50
7	2H	172/180 (96%)	151 (88%)	19 (11%)	2 (1%)	13	50
8	1N	138/140 (99%)	121 (88%)	16 (12%)	1 (1%)	22	61
8	2N	138/140 (99%)	127 (92%)	8 (6%)	3 (2%)	6	37
9	1O	120/122 (98%)	105 (88%)	13 (11%)	2 (2%)	9	42
9	2O	120/122 (98%)	103 (86%)	16 (13%)	1 (1%)	19	58
10	1P	147/150 (98%)	134 (91%)	11 (8%)	2 (1%)	11	46
10	2P	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	11	46
11	1Q	139/141 (99%)	123 (88%)	14 (10%)	2 (1%)	11	46
11	2Q	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	22	61
12	1R	116/118 (98%)	91 (78%)	21 (18%)	4 (3%)	3	28
12	2R	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	56
13	1S	108/112 (96%)	96 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	2S	108/112 (96%)	96 (89%)	10 (9%)	2 (2%)	8	40
14	1T	129/146 (88%)	117 (91%)	12 (9%)	0	100	100
14	2T	129/146 (88%)	115 (89%)	13 (10%)	1 (1%)	19	58
15	1U	114/118 (97%)	104 (91%)	8 (7%)	2 (2%)	8	41
15	2U	114/118 (97%)	109 (96%)	4 (4%)	1 (1%)	17	56
16	1V	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	7	39
16	2V	99/101 (98%)	86 (87%)	12 (12%)	1 (1%)	15	54
17	1W	110/113 (97%)	98 (89%)	10 (9%)	2 (2%)	8	41
17	2W	110/113 (97%)	102 (93%)	7 (6%)	1 (1%)	17	56
18	1X	93/96 (97%)	84 (90%)	6 (6%)	3 (3%)	4	29
18	2X	93/96 (97%)	81 (87%)	11 (12%)	1 (1%)	14	52
19	1Y	105/110 (96%)	88 (84%)	15 (14%)	2 (2%)	8	40
19	2Y	105/110 (96%)	92 (88%)	10 (10%)	3 (3%)	4	31
20	1Z	202/206 (98%)	159 (79%)	34 (17%)	9 (4%)	2	21
20	2Z	202/206 (98%)	161 (80%)	28 (14%)	13 (6%)	1	14
21	10	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
21	20	73/85 (86%)	67 (92%)	5 (7%)	1 (1%)	11	46
22	11	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
22	21	95/98 (97%)	89 (94%)	4 (4%)	2 (2%)	7	38
23	12	68/72 (94%)	60 (88%)	5 (7%)	3 (4%)	2	21
23	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
24	13	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	8	41
24	23	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	8	41
25	14	67/71 (94%)	51 (76%)	10 (15%)	6 (9%)	1	8
25	24	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	15
26	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	25	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	16	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
27	26	51/54 (94%)	48 (94%)	2 (4%)	1 (2%)	7	39
28	17	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
28	27	46/49 (94%)	40 (87%)	5 (11%)	1 (2%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	18	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	9	43
29	28	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
30	19	35/37 (95%)	30 (86%)	5 (14%)	0	100	100
30	29	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
32	1b	229/256 (90%)	190 (83%)	32 (14%)	7 (3%)	4	30
32	2b	229/256 (90%)	199 (87%)	22 (10%)	8 (4%)	3	27
33	1c	204/239 (85%)	183 (90%)	17 (8%)	4 (2%)	7	39
33	2c	204/239 (85%)	172 (84%)	30 (15%)	2 (1%)	15	54
34	1d	206/209 (99%)	181 (88%)	21 (10%)	4 (2%)	8	40
34	2d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	29	68
35	1e	146/162 (90%)	127 (87%)	17 (12%)	2 (1%)	11	46
35	2e	146/162 (90%)	127 (87%)	19 (13%)	0	100	100
36	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
36	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	1g	153/156 (98%)	135 (88%)	14 (9%)	4 (3%)	5	33
37	2g	153/156 (98%)	135 (88%)	14 (9%)	4 (3%)	5	33
38	1h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
38	2h	135/138 (98%)	118 (87%)	16 (12%)	1 (1%)	22	61
39	1i	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
39	2i	125/128 (98%)	104 (83%)	21 (17%)	0	100	100
40	1j	95/105 (90%)	82 (86%)	9 (10%)	4 (4%)	3	23
40	2j	94/105 (90%)	78 (83%)	15 (16%)	1 (1%)	14	52
41	1k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	41
41	2k	112/129 (87%)	98 (88%)	12 (11%)	2 (2%)	8	41
42	1l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	19	58
42	2l	119/132 (90%)	97 (82%)	19 (16%)	3 (2%)	5	34
43	1m	116/126 (92%)	100 (86%)	16 (14%)	0	100	100
43	2m	120/126 (95%)	104 (87%)	14 (12%)	2 (2%)	9	42
44	1n	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	42
44	2n	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	42
45	1o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	2o	86/89 (97%)	78 (91%)	4 (5%)	4 (5%)	2	20
46	1p	80/88 (91%)	66 (82%)	12 (15%)	2 (2%)	5	34
46	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	12	48
47	1q	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
47	2q	97/105 (92%)	84 (87%)	11 (11%)	2 (2%)	7	38
48	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
48	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10	45
49	1s	81/93 (87%)	68 (84%)	9 (11%)	4 (5%)	2	19
49	2s	81/93 (87%)	65 (80%)	14 (17%)	2 (2%)	5	34
50	1t	94/106 (89%)	82 (87%)	7 (7%)	5 (5%)	2	17
50	2t	94/106 (89%)	81 (86%)	10 (11%)	3 (3%)	4	29
51	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
51	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	1v	724/758 (96%)	593 (82%)	105 (14%)	26 (4%)	3	26
52	2v	724/758 (96%)	602 (83%)	97 (13%)	25 (4%)	3	27
53	1w	183/185 (99%)	159 (87%)	16 (9%)	8 (4%)	2	21
53	2w	183/185 (99%)	165 (90%)	13 (7%)	5 (3%)	5	33
All	All	12975/13718 (95%)	11321 (87%)	1394 (11%)	260 (2%)	7	39

All (260) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
10	1P	53	GLY
11	1Q	16	ARG
16	1V	97	LYS
20	1Z	177	PRO
20	1Z	184	ALA
20	1Z	198	LYS
35	1e	21	ALA
40	1j	55	LYS
52	1v	-57	GLU
52	1v	85	PRO
52	1v	92	ILE
52	1v	183	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	1v	401	SER
52	1v	472	VAL
53	1w	61	PRO
5	2F	130	ALA
7	2H	29	PRO
7	2H	126	PRO
19	2Y	21	LYS
20	2Z	182	LYS
20	2Z	183	LEU
28	27	46	VAL
42	2l	121	GLY
52	2v	-57	GLU
52	2v	85	PRO
52	2v	92	ILE
52	2v	183	MET
52	2v	472	VAL
3	1D	169	GLU
4	1E	113	PHE
5	1F	54	ARG
12	1R	3	HIS
12	1R	23	ASN
16	1V	79	VAL
20	1Z	119	GLU
23	12	69	ARG
25	14	44	THR
25	14	45	GLY
25	14	53	GLU
32	1b	22	LYS
37	1g	79	ARG
45	1o	17	ARG
46	1p	53	VAL
49	1s	63	THR
52	1v	402	ILE
52	1v	444	PRO
52	1v	447	GLY
53	1w	30	THR
53	1w	84	ARG
53	1w	97	ASP
3	2D	3	VAL
6	2G	126	ASP
8	2N	8	GLN
10	2P	38	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	2Q	27	VAL
13	2S	94	TYR
14	2T	56	GLY
16	2V	79	VAL
17	2W	98	LYS
20	2Z	154	ASP
25	24	46	GLN
34	2d	5	ILE
37	2g	114	ARG
41	2k	105	VAL
43	2m	23	TYR
52	2v	88	VAL
52	2v	401	SER
52	2v	605	ILE
53	2w	85	ASP
3	1D	144	ALA
3	1D	206	LEU
4	1E	52	LEU
10	1P	58	THR
17	1W	90	ARG
18	1X	93	GLU
19	1Y	54	LYS
25	14	57	GLU
32	1b	8	LYS
32	1b	36	ARG
32	1b	231	GLU
33	1c	98	ASN
40	1j	78	ASN
45	1o	23	GLY
49	1s	35	SER
49	1s	65	ASN
50	1t	9	ASN
50	1t	95	ALA
52	1v	87	HIS
52	1v	88	VAL
52	1v	171	GLU
52	1v	482	ALA
3	2D	79	VAL
3	2D	125	ILE
3	2D	257	LEU
12	2R	14	SER
15	2U	5	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	2Z	135	GLU
22	21	3	LYS
25	24	61	ARG
32	2b	8	LYS
32	2b	16	HIS
32	2b	17	PHE
32	2b	95	GLN
32	2b	150	SER
37	2g	7	ALA
43	2m	6	GLY
44	2n	28	GLY
45	2o	6	GLU
50	2t	47	GLY
52	2v	171	GLU
52	2v	469	GLU
52	2v	471	LYS
52	2v	473	ASP
52	2v	688	ILE
3	1D	99	ASP
6	1G	75	LYS
9	1O	25	LEU
12	1R	53	HIS
15	1U	9	VAL
15	1U	24	TYR
19	1Y	53	PRO
20	1Z	155	LEU
32	1b	20	GLU
32	1b	125	PRO
34	1d	5	ILE
37	1g	114	ARG
46	1p	28	ARG
50	1t	10	LEU
50	1t	100	ILE
52	1v	404	VAL
52	1v	473	ASP
53	1w	2	THR
3	2D	31	LYS
3	2D	80	ALA
4	2E	52	LEU
5	2F	169	ASN
6	2G	47	LYS
6	2G	116	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	2N	23	LEU
8	2N	41	ASP
18	2X	2	LYS
20	2Z	155	LEU
20	2Z	184	ALA
20	2Z	198	LYS
22	21	45	ASN
32	2b	125	PRO
32	2b	231	GLU
33	2c	71	ALA
37	2g	4	ARG
41	2k	49	GLY
42	2l	107	ALA
45	2o	17	ARG
45	2o	88	ARG
49	2s	12	ASP
50	2t	102	GLY
52	2v	-25	SER
53	2w	167	GLU
3	1D	127	VAL
4	1E	134	ILE
11	1Q	13	GLN
12	1R	59	ASP
17	1W	5	ALA
20	1Z	161	VAL
20	1Z	197	ILE
23	12	32	LEU
23	12	68	ARG
24	13	16	PRO
25	14	56	VAL
33	1c	66	VAL
37	1g	80	VAL
37	1g	131	LYS
40	1j	56	HIS
40	1j	77	PRO
42	1l	74	GLY
49	1s	66	MET
52	1v	170	ARG
52	1v	604	PRO
52	1v	671	MET
4	2E	41	LYS
5	2F	23	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	2O	17	ARG
10	2P	53	GLY
19	2Y	58	GLY
20	2Z	11	GLU
20	2Z	157	LEU
20	2Z	179	ASP
20	2Z	197	ILE
21	20	33	ALA
27	26	3	SER
33	2c	3	ASN
37	2g	80	VAL
38	2h	102	ARG
42	2l	120	TYR
48	2r	52	PRO
52	2v	404	VAL
52	2v	671	MET
4	1E	100	GLU
18	1X	45	THR
20	1Z	191	VAL
25	14	62	ARG
32	1b	17	PHE
33	1c	3	ASN
33	1c	99	VAL
34	1d	73	ARG
44	1n	14	PRO
52	1v	324	ARG
52	1v	640	ALA
52	1v	684	GLN
13	2S	84	GLN
19	2Y	103	GLY
24	23	59	VAL
25	24	11	PRO
25	24	48	ARG
32	2b	131	PRO
45	2o	23	GLY
49	2s	76	PRO
50	2t	99	LEU
52	2v	447	GLY
52	2v	481	VAL
53	2w	55	ILE
53	2w	84	ARG
34	1d	90	GLY

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Mol	Chain	Res	Type
41	1k	49	GLY
41	1k	105	VAL
52	1v	477	GLY
20	2Z	161	VAL
47	2q	33	GLY
52	2v	288	PRO
20	1Z	157	LEU
52	1v	598	ASP
53	1w	31	GLY
6	2G	177	GLY
52	2v	402	ILE
52	2v	477	GLY
7	1H	55	PRO
18	1X	94	GLY
29	18	28	GLY
34	1d	69	GLY
35	1e	85	GLY
50	1t	47	GLY
52	1v	502	GLY
52	1v	503	GLY
6	2G	127	GLY
20	2Z	180	VAL
40	2j	75	ILE
47	2q	77	VAL
52	2v	294	PRO
52	2v	405	PRO
53	2w	61	PRO
3	1D	207	GLY
8	1N	111	PRO
52	1v	532	GLY
53	1w	35	PRO
46	2p	53	VAL
52	2v	115	GLU
52	2v	535	PRO
9	1O	77	ILE
53	1w	27	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	199 (93%)	16 (7%)	13	44
3	2D	215/218 (99%)	202 (94%)	13 (6%)	19	52
4	1E	164/166 (99%)	148 (90%)	16 (10%)	8	33
4	2E	164/166 (99%)	152 (93%)	12 (7%)	14	45
5	1F	160/166 (96%)	146 (91%)	14 (9%)	10	38
5	2F	159/166 (96%)	157 (99%)	2 (1%)	69	86
6	1G	150/156 (96%)	140 (93%)	10 (7%)	16	48
6	2G	150/156 (96%)	144 (96%)	6 (4%)	31	64
7	1H	144/148 (97%)	138 (96%)	6 (4%)	30	63
7	2H	144/148 (97%)	139 (96%)	5 (4%)	36	67
8	1N	118/119 (99%)	107 (91%)	11 (9%)	9	35
8	2N	118/119 (99%)	112 (95%)	6 (5%)	24	57
9	1O	100/100 (100%)	94 (94%)	6 (6%)	19	52
9	2O	100/100 (100%)	98 (98%)	2 (2%)	55	79
10	1P	115/116 (99%)	107 (93%)	8 (7%)	15	46
10	2P	115/116 (99%)	110 (96%)	5 (4%)	29	62
11	1Q	111/111 (100%)	106 (96%)	5 (4%)	27	61
11	2Q	111/111 (100%)	105 (95%)	6 (5%)	22	55
12	1R	101/101 (100%)	85 (84%)	16 (16%)	2	15
12	2R	101/101 (100%)	96 (95%)	5 (5%)	24	58
13	1S	86/88 (98%)	77 (90%)	9 (10%)	7	31
13	2S	85/88 (97%)	79 (93%)	6 (7%)	14	46
14	1T	115/127 (91%)	106 (92%)	9 (8%)	12	42
14	2T	113/127 (89%)	109 (96%)	4 (4%)	36	67
15	1U	93/94 (99%)	90 (97%)	3 (3%)	39	69
15	2U	93/94 (99%)	91 (98%)	2 (2%)	52	78
16	1V	80/82 (98%)	72 (90%)	8 (10%)	7	32
16	2V	80/82 (98%)	77 (96%)	3 (4%)	33	65
17	1W	90/92 (98%)	85 (94%)	5 (6%)	21	54
17	2W	90/92 (98%)	80 (89%)	10 (11%)	6	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1X	77/78 (99%)	74 (96%)	3 (4%)	32	64
18	2X	77/78 (99%)	73 (95%)	4 (5%)	23	56
19	1Y	85/91 (93%)	77 (91%)	8 (9%)	8	35
19	2Y	85/91 (93%)	82 (96%)	3 (4%)	36	67
20	1Z	167/179 (93%)	150 (90%)	17 (10%)	7	32
20	2Z	167/179 (93%)	151 (90%)	16 (10%)	8	34
21	10	60/67 (90%)	59 (98%)	1 (2%)	60	82
21	20	60/67 (90%)	58 (97%)	2 (3%)	38	68
22	11	80/83 (96%)	75 (94%)	5 (6%)	18	51
22	21	80/83 (96%)	76 (95%)	4 (5%)	24	58
23	12	65/67 (97%)	60 (92%)	5 (8%)	13	42
23	22	65/67 (97%)	64 (98%)	1 (2%)	65	84
24	13	51/52 (98%)	45 (88%)	6 (12%)	5	25
24	23	50/52 (96%)	48 (96%)	2 (4%)	31	64
25	14	59/63 (94%)	51 (86%)	8 (14%)	3	20
25	24	53/63 (84%)	47 (89%)	6 (11%)	6	27
26	15	50/52 (96%)	47 (94%)	3 (6%)	19	52
26	25	50/52 (96%)	47 (94%)	3 (6%)	19	52
27	16	51/52 (98%)	48 (94%)	3 (6%)	19	53
27	26	50/52 (96%)	49 (98%)	1 (2%)	55	79
28	17	41/42 (98%)	37 (90%)	4 (10%)	8	33
28	27	41/42 (98%)	36 (88%)	5 (12%)	5	23
29	18	54/55 (98%)	50 (93%)	4 (7%)	13	44
29	28	54/55 (98%)	54 (100%)	0	100	100
30	19	34/34 (100%)	33 (97%)	1 (3%)	42	71
30	29	34/34 (100%)	31 (91%)	3 (9%)	10	38
32	1b	192/220 (87%)	182 (95%)	10 (5%)	23	56
32	2b	187/220 (85%)	180 (96%)	7 (4%)	34	65
33	1c	142/188 (76%)	138 (97%)	4 (3%)	43	72
33	2c	140/188 (74%)	133 (95%)	7 (5%)	24	58
34	1d	169/181 (93%)	160 (95%)	9 (5%)	22	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	2d	173/181 (96%)	166 (96%)	7 (4%)	31	64
35	1e	113/123 (92%)	109 (96%)	4 (4%)	36	67
35	2e	114/123 (93%)	107 (94%)	7 (6%)	18	51
36	1f	84/90 (93%)	83 (99%)	1 (1%)	71	87
36	2f	85/90 (94%)	81 (95%)	4 (5%)	26	60
37	1g	119/127 (94%)	114 (96%)	5 (4%)	30	63
37	2g	120/127 (94%)	119 (99%)	1 (1%)	81	91
38	1h	114/119 (96%)	110 (96%)	4 (4%)	36	67
38	2h	114/119 (96%)	108 (95%)	6 (5%)	22	55
39	1i	90/99 (91%)	85 (94%)	5 (6%)	21	54
39	2i	89/99 (90%)	83 (93%)	6 (7%)	16	48
40	1j	66/92 (72%)	64 (97%)	2 (3%)	41	71
40	2j	69/92 (75%)	66 (96%)	3 (4%)	29	62
41	1k	82/99 (83%)	80 (98%)	2 (2%)	49	76
41	2k	83/99 (84%)	83 (100%)	0	100	100
42	1l	96/108 (89%)	91 (95%)	5 (5%)	23	56
42	2l	96/108 (89%)	94 (98%)	2 (2%)	53	79
43	1m	89/101 (88%)	86 (97%)	3 (3%)	37	68
43	2m	92/101 (91%)	88 (96%)	4 (4%)	29	62
44	1n	49/50 (98%)	47 (96%)	2 (4%)	30	63
44	2n	49/50 (98%)	47 (96%)	2 (4%)	30	63
45	1o	78/80 (98%)	77 (99%)	1 (1%)	69	86
45	2o	78/80 (98%)	72 (92%)	6 (8%)	13	42
46	1p	69/74 (93%)	64 (93%)	5 (7%)	14	45
46	2p	68/74 (92%)	63 (93%)	5 (7%)	13	44
47	1q	94/97 (97%)	91 (97%)	3 (3%)	39	69
47	2q	94/97 (97%)	92 (98%)	2 (2%)	53	79
48	1r	59/77 (77%)	56 (95%)	3 (5%)	24	57
48	2r	59/77 (77%)	57 (97%)	2 (3%)	37	68
49	1s	69/80 (86%)	65 (94%)	4 (6%)	20	53
49	2s	67/80 (84%)	64 (96%)	3 (4%)	27	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	1t	70/82 (85%)	67 (96%)	3 (4%)	29	62
50	2t	70/82 (85%)	69 (99%)	1 (1%)	67	85
51	1u	18/22 (82%)	18 (100%)	0	100	100
51	2u	18/22 (82%)	18 (100%)	0	100	100
52	1v	605/636 (95%)	518 (86%)	87 (14%)	3	18
52	2v	605/636 (95%)	523 (86%)	82 (14%)	3	20
53	1w	157/157 (100%)	133 (85%)	24 (15%)	2	17
53	2w	157/157 (100%)	140 (89%)	17 (11%)	6	30
All	All	10671/11402 (94%)	9964 (93%)	707 (7%)	16	49

All (707) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	14	ARG
3	1D	15	PHE
3	1D	35	LYS
3	1D	50	THR
3	1D	60	ARG
3	1D	83	GLU
3	1D	116	GLN
3	1D	141	VAL
3	1D	154	LYS
3	1D	211	ARG
3	1D	212	SER
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	254	THR
3	1D	257	LEU
4	1E	7	VAL
4	1E	14	ILE
4	1E	23	VAL
4	1E	24	THR
4	1E	73	GLU
4	1E	75	VAL
4	1E	97	LYS
4	1E	103	ASP
4	1E	104	VAL
4	1E	117	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	1E	119	ARG
4	1E	140	SER
4	1E	160	TYR
4	1E	168	MET
4	1E	178	GLU
4	1E	184	VAL
5	1F	19	GLU
5	1F	54	ARG
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	78	ILE
5	1F	89	VAL
5	1F	106	ARG
5	1F	125	LEU
5	1F	149	ASP
5	1F	165	ARG
5	1F	170	LEU
5	1F	175	THR
5	1F	183	VAL
6	1G	3	LEU
6	1G	7	LEU
6	1G	28	VAL
6	1G	43	LEU
6	1G	59	GLU
6	1G	64	THR
6	1G	70	VAL
6	1G	91	ARG
6	1G	133	LEU
6	1G	161	THR
7	1H	2	SER
7	1H	15	VAL
7	1H	45	VAL
7	1H	69	ARG
7	1H	71	LEU
7	1H	155	SER
8	1N	32	THR
8	1N	33	LEU
8	1N	34	LEU
8	1N	48	MET
8	1N	55	VAL
8	1N	61	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	1N	62	VAL
8	1N	67	LEU
8	1N	99	LEU
8	1N	101	HIS
8	1N	120	LEU
9	1O	12	ASP
9	1O	21	CYS
9	1O	32	TYR
9	1O	57	VAL
9	1O	80	ASP
9	1O	108	GLU
10	1P	46	LYS
10	1P	71	VAL
10	1P	95	VAL
10	1P	96	THR
10	1P	98	GLU
10	1P	112	LEU
10	1P	133	SER
10	1P	148	LEU
11	1Q	14	ARG
11	1Q	79	LEU
11	1Q	85	LYS
11	1Q	109	VAL
11	1Q	110	THR
12	1R	14	SER
12	1R	24	GLN
12	1R	29	LEU
12	1R	34	ILE
12	1R	36	THR
12	1R	44	LEU
12	1R	57	ARG
12	1R	59	ASP
12	1R	65	LEU
12	1R	67	LEU
12	1R	79	LEU
12	1R	95	THR
12	1R	99	LYS
12	1R	100	LEU
12	1R	102	GLU
12	1R	114	VAL
13	1S	8	GLU
13	1S	19	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	1S	25	ARG
13	1S	31	SER
13	1S	36	TYR
13	1S	49	VAL
13	1S	50	SER
13	1S	85	VAL
13	1S	98	VAL
14	1T	6	LEU
14	1T	21	GLU
14	1T	27	THR
14	1T	28	VAL
14	1T	53	ARG
14	1T	96	ARG
14	1T	106	SER
14	1T	114	LEU
14	1T	128	GLU
15	1U	74	LEU
15	1U	77	SER
15	1U	97	ASP
16	1V	13	ARG
16	1V	33	VAL
16	1V	52	VAL
16	1V	62	LEU
16	1V	72	VAL
16	1V	82	ARG
16	1V	95	LEU
16	1V	98	GLU
17	1W	1	MET
17	1W	23	LEU
17	1W	24	ILE
17	1W	67	ASP
17	1W	107	LEU
18	1X	3	THR
18	1X	35	THR
18	1X	57	LEU
19	1Y	12	THR
19	1Y	31	LEU
19	1Y	43	ASN
19	1Y	55	TYR
19	1Y	60	PHE
19	1Y	72	VAL
19	1Y	98	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	1Y	99	CYS
20	1Z	33	LEU
20	1Z	34	ASN
20	1Z	41	LEU
20	1Z	49	ARG
20	1Z	56	VAL
20	1Z	63	ASP
20	1Z	78	LYS
20	1Z	81	ARG
20	1Z	87	ASP
20	1Z	91	LEU
20	1Z	123	ASP
20	1Z	126	VAL
20	1Z	136	PHE
20	1Z	154	ASP
20	1Z	156	LYS
20	1Z	178	GLU
20	1Z	180	VAL
21	10	36	ILE
22	11	14	VAL
22	11	30	VAL
22	11	35	THR
22	11	40	ARG
22	11	56	GLN
23	12	3	LEU
23	12	4	SER
23	12	32	LEU
23	12	33	MET
23	12	69	ARG
24	13	17	LYS
24	13	29	ARG
24	13	31	LEU
24	13	40	THR
24	13	56	VAL
24	13	60	GLU
25	14	16	CYS
25	14	33	VAL
25	14	46	GLN
25	14	49	PHE
25	14	52	THR
25	14	56	VAL
25	14	63	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	14	67	TYR
26	15	16	ARG
26	15	19	ARG
26	15	40	LYS
27	16	6	ARG
27	16	13	CYS
27	16	51	GLU
28	17	1	MET
28	17	4	THR
28	17	41	ARG
28	17	43	THR
29	18	27	THR
29	18	31	HIS
29	18	34	TRP
29	18	37	SER
30	19	12	ASP
32	1b	8	LYS
32	1b	19	HIS
32	1b	21	ARG
32	1b	37	ASN
32	1b	94	ASN
32	1b	122	PHE
32	1b	140	HIS
32	1b	162	ILE
32	1b	195	ASP
32	1b	198	ASP
33	1c	17	ASP
33	1c	57	ILE
33	1c	115	LEU
33	1c	124	ILE
34	1d	28	SER
34	1d	59	ARG
34	1d	108	LEU
34	1d	134	ASP
34	1d	135	LEU
34	1d	170	VAL
34	1d	188	LEU
34	1d	190	ASP
34	1d	204	ILE
35	1e	10	MET
35	1e	41	VAL
35	1e	67	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	1e	81	GLU
36	1f	15	ASP
37	1g	10	ARG
37	1g	16	LEU
37	1g	35	LYS
37	1g	111	ARG
37	1g	113	GLU
38	1h	52	ASP
38	1h	99	GLU
38	1h	104	ARG
38	1h	133	LEU
39	1i	17	VAL
39	1i	31	GLN
39	1i	65	VAL
39	1i	92	TYR
39	1i	128	ARG
40	1j	8	LEU
40	1j	49	VAL
41	1k	51	LYS
41	1k	80	VAL
42	1l	6	THR
42	1l	37	CYS
42	1l	44	THR
42	1l	67	THR
42	1l	85	ILE
43	1m	32	GLU
43	1m	110	ARG
43	1m	117	VAL
44	1n	18	VAL
44	1n	33	VAL
45	1o	21	ASP
46	1p	1	MET
46	1p	16	HIS
46	1p	20	VAL
46	1p	60	LEU
46	1p	74	LEU
47	1q	9	VAL
47	1q	59	ILE
47	1q	92	ARG
48	1r	30	ASP
48	1r	31	LEU
48	1r	76	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	1s	7	LYS
49	1s	16	LEU
49	1s	28	LYS
49	1s	81	ARG
50	1t	13	LEU
50	1t	15	ARG
50	1t	84	LEU
52	1v	-52	VAL
52	1v	-19	GLU
52	1v	-13	GLN
52	1v	-6	ARG
52	1v	-1	GLU
52	1v	10	LYS
52	1v	13	ARG
52	1v	15	ILE
52	1v	38	ARG
52	1v	69	VAL
52	1v	70	THR
52	1v	72	CYS
52	1v	75	LYS
52	1v	89	ASP
52	1v	91	THR
52	1v	92	ILE
52	1v	96	ARG
52	1v	98	MET
52	1v	102	ASP
52	1v	112	GLN
52	1v	114	VAL
52	1v	130	VAL
52	1v	132	ARG
52	1v	139	MET
52	1v	146	LEU
52	1v	160	ARG
52	1v	166	LEU
52	1v	170	ARG
52	1v	172	ASP
52	1v	197	ARG
52	1v	198	GLU
52	1v	203	GLU
52	1v	214	GLU
52	1v	222	ASP
52	1v	228	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	1v	233	GLU
52	1v	238	THR
52	1v	252	ASP
52	1v	260	LEU
52	1v	264	LEU
52	1v	279	TYR
52	1v	284	LEU
52	1v	286	ILE
52	1v	289	ILE
52	1v	297	GLU
52	1v	328	ILE
52	1v	329	ARG
52	1v	344	THR
52	1v	352	VAL
52	1v	354	ARG
52	1v	362	HIS
52	1v	369	LEU
52	1v	374	LEU
52	1v	377	VAL
52	1v	385	THR
52	1v	399	LEU
52	1v	402	ILE
52	1v	409	ILE
52	1v	418	LYS
52	1v	420	ASP
52	1v	421	GLN
52	1v	422	GLU
52	1v	446	THR
52	1v	475	ASN
52	1v	481	VAL
52	1v	484	ARG
52	1v	491	VAL
52	1v	504	ARG
52	1v	512	ILE
52	1v	530	VAL
52	1v	533	VAL
52	1v	572	TYR
52	1v	579	GLU
52	1v	601	ILE
52	1v	605	ILE
52	1v	606	MET
52	1v	614	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	1v	615	GLU
52	1v	630	GLN
52	1v	634	MET
52	1v	641	GLN
52	1v	644	ARG
52	1v	646	PHE
52	1v	647	VAL
52	1v	670	VAL
52	1v	681	LYS
52	1v	682	GLN
53	1w	1	MET
53	1w	3	LEU
53	1w	6	LEU
53	1w	16	LYS
53	1w	38	LEU
53	1w	43	VAL
53	1w	50	VAL
53	1w	55	ILE
53	1w	59	THR
53	1w	81	LYS
53	1w	85	ASP
53	1w	88	LEU
53	1w	99	LEU
53	1w	101	ILE
53	1w	106	LEU
53	1w	107	THR
53	1w	112	LYS
53	1w	116	ARG
53	1w	133	ARG
53	1w	154	THR
53	1w	155	LYS
53	1w	156	ARG
53	1w	173	ASP
53	1w	174	GLN
3	2D	27	THR
3	2D	71	ASP
3	2D	94	LEU
3	2D	112	GLN
3	2D	113	VAL
3	2D	134	ARG
3	2D	142	VAL
3	2D	150	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	2D	169	GLU
3	2D	229	VAL
3	2D	242	ARG
3	2D	263	ARG
3	2D	276	LYS
4	2E	7	VAL
4	2E	19	ARG
4	2E	21	VAL
4	2E	24	THR
4	2E	33	VAL
4	2E	52	LEU
4	2E	75	VAL
4	2E	107	THR
4	2E	119	ARG
4	2E	184	VAL
4	2E	195	LEU
4	2E	201	THR
5	2F	84	VAL
5	2F	192	LEU
6	2G	31	VAL
6	2G	43	LEU
6	2G	49	ASP
6	2G	111	LEU
6	2G	135	LEU
6	2G	174	GLU
7	2H	68	THR
7	2H	69	ARG
7	2H	71	LEU
7	2H	129	THR
7	2H	171	LEU
8	2N	15	LEU
8	2N	28	THR
8	2N	34	LEU
8	2N	58	ASP
8	2N	87	LEU
8	2N	96	GLU
9	2O	24	VAL
9	2O	53	LYS
10	2P	7	ARG
10	2P	71	VAL
10	2P	87	ASP
10	2P	95	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	2P	112	LEU
11	2Q	1	MET
11	2Q	16	ARG
11	2Q	18	LYS
11	2Q	21	THR
11	2Q	109	VAL
11	2Q	110	THR
12	2R	8	ARG
12	2R	28	LEU
12	2R	29	LEU
12	2R	81	ASP
12	2R	100	LEU
13	2S	8	GLU
13	2S	25	ARG
13	2S	58	LEU
13	2S	69	VAL
13	2S	85	VAL
13	2S	110	LEU
14	2T	40	THR
14	2T	59	THR
14	2T	95	ARG
14	2T	96	ARG
15	2U	45	TYR
15	2U	78	THR
16	2V	61	VAL
16	2V	69	LYS
16	2V	79	VAL
17	2W	11	ARG
17	2W	19	LEU
17	2W	23	LEU
17	2W	28	SER
17	2W	60	ASN
17	2W	63	ASP
17	2W	94	ASP
17	2W	100	THR
17	2W	102	HIS
17	2W	107	LEU
18	2X	27	THR
18	2X	35	THR
18	2X	66	LEU
18	2X	70	LEU
19	2Y	49	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	2Y	72	VAL
19	2Y	99	CYS
20	2Z	18	LEU
20	2Z	19	ARG
20	2Z	31	ARG
20	2Z	33	LEU
20	2Z	56	VAL
20	2Z	73	GLN
20	2Z	78	LYS
20	2Z	86	VAL
20	2Z	116	VAL
20	2Z	123	ASP
20	2Z	139	VAL
20	2Z	154	ASP
20	2Z	156	LYS
20	2Z	170	THR
20	2Z	175	VAL
20	2Z	179	ASP
21	20	10	THR
21	20	14	ARG
22	21	5	CYS
22	21	30	VAL
22	21	89	GLU
22	21	95	LEU
23	22	53	LEU
24	23	54	VAL
24	23	57	GLU
25	24	32	TYR
25	24	49	PHE
25	24	50	VAL
25	24	58	ARG
25	24	59	PHE
25	24	63	TYR
26	25	6	VAL
26	25	16	ARG
26	25	44	THR
27	26	6	ARG
28	27	4	THR
28	27	39	ARG
28	27	42	LEU
28	27	43	THR
28	27	47	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
30	29	7	VAL
30	29	11	CYS
30	29	14	CYS
32	2b	7	VAL
32	2b	11	LEU
32	2b	76	GLN
32	2b	94	ASN
32	2b	126	GLU
32	2b	127	ILE
32	2b	189	ASP
33	2c	3	ASN
33	2c	36	ASP
33	2c	98	ASN
33	2c	124	ILE
33	2c	152	ILE
33	2c	166	GLU
33	2c	191	THR
34	2d	5	ILE
34	2d	31	CYS
34	2d	59	ARG
34	2d	86	LYS
34	2d	107	ARG
34	2d	141	ARG
34	2d	150	GLU
35	2e	10	MET
35	2e	24	ARG
35	2e	25	ARG
35	2e	31	LEU
35	2e	41	VAL
35	2e	125	SER
35	2e	147	ASP
36	2f	19	LEU
36	2f	46	ARG
36	2f	70	ASP
36	2f	72	VAL
37	2g	79	ARG
38	2h	2	LEU
38	2h	39	LEU
38	2h	51	VAL
38	2h	83	ILE
38	2h	112	LEU
38	2h	114	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	2i	53	VAL
39	2i	65	VAL
39	2i	89	ASN
39	2i	93	ARG
39	2i	102	LEU
39	2i	108	VAL
40	2j	9	ARG
40	2j	55	LYS
40	2j	74	ILE
42	2l	6	THR
42	2l	27	LEU
43	2m	3	ARG
43	2m	15	VAL
43	2m	78	ILE
43	2m	116	THR
44	2n	41	ARG
44	2n	44	LEU
45	2o	7	GLU
45	2o	28	GLN
45	2o	39	LEU
45	2o	70	LEU
45	2o	72	ARG
45	2o	83	GLU
46	2p	2	VAL
46	2p	20	VAL
46	2p	25	ARG
46	2p	52	ASP
46	2p	67	THR
47	2q	9	VAL
47	2q	74	LEU
48	2r	47	THR
48	2r	76	LEU
49	2s	33	THR
49	2s	47	HIS
49	2s	77	THR
50	2t	84	LEU
52	2v	-65	LYS
52	2v	-58	LEU
52	2v	-26	GLU
52	2v	-10	ARG
52	2v	-9	LEU
52	2v	-6	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2v	9	LEU
52	2v	13	ARG
52	2v	15	ILE
52	2v	35	TYR
52	2v	72	CYS
52	2v	75	LYS
52	2v	91	THR
52	2v	92	ILE
52	2v	102	ASP
52	2v	112	GLN
52	2v	114	VAL
52	2v	119	GLU
52	2v	121	VAL
52	2v	132	ARG
52	2v	146	LEU
52	2v	152	THR
52	2v	157	LEU
52	2v	160	ARG
52	2v	170	ARG
52	2v	172	ASP
52	2v	196	ILE
52	2v	198	GLU
52	2v	199	ILE
52	2v	203	GLU
52	2v	225	GLU
52	2v	226	ASN
52	2v	235	GLU
52	2v	238	THR
52	2v	260	LEU
52	2v	264	LEU
52	2v	286	ILE
52	2v	290	LYS
52	2v	298	VAL
52	2v	312	LEU
52	2v	328	ILE
52	2v	329	ARG
52	2v	334	THR
52	2v	336	THR
52	2v	344	THR
52	2v	352	VAL
52	2v	354	ARG
52	2v	362	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2v	373	ASP
52	2v	374	LEU
52	2v	377	VAL
52	2v	381	LYS
52	2v	402	ILE
52	2v	403	GLU
52	2v	406	GLU
52	2v	408	VAL
52	2v	422	GLU
52	2v	437	THR
52	2v	446	THR
52	2v	473	ASP
52	2v	475	ASN
52	2v	484	ARG
52	2v	485	GLU
52	2v	488	THR
52	2v	504	ARG
52	2v	506	GLN
52	2v	512	ILE
52	2v	533	VAL
52	2v	569	ASP
52	2v	579	GLU
52	2v	605	ILE
52	2v	616	TYR
52	2v	631	ILE
52	2v	634	MET
52	2v	641	GLN
52	2v	644	ARG
52	2v	647	VAL
52	2v	670	VAL
52	2v	678	GLU
52	2v	681	LYS
52	2v	683	VAL
52	2v	689	LYS
53	2w	6	LEU
53	2w	9	GLU
53	2w	13	HIS
53	2w	16	LYS
53	2w	29	ARG
53	2w	32	ARG
53	2w	34	ASN
53	2w	52	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	2w	73	GLN
53	2w	84	ARG
53	2w	91	ASN
53	2w	114	LEU
53	2w	127	VAL
53	2w	133	ARG
53	2w	137	LEU
53	2w	152	ASP
53	2w	154	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	1D	87	ASN
3	1D	96	HIS
3	1D	116	GLN
3	1D	126	GLN
3	1D	220	HIS
3	1D	231	HIS
4	1E	48	GLN
4	1E	137	HIS
5	1F	8	GLN
5	1F	69	HIS
5	1F	75	HIS
10	1P	27	HIS
11	1Q	12	GLN
11	1Q	57	HIS
11	1Q	123	HIS
13	1S	61	ASN
14	1T	43	GLN
16	1V	80	GLN
18	1X	31	HIS
20	1Z	73	GLN
20	1Z	121	HIS
22	11	56	GLN
24	13	32	GLN
26	15	23	HIS
33	1c	170	GLN
34	1d	160	GLN
34	1d	161	ASN
35	1e	78	HIS
37	1g	13	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
37	1g	28	ASN
38	1h	78	GLN
39	1i	73	GLN
39	1i	124	GLN
41	1k	26	ASN
42	1l	99	HIS
45	1o	62	GLN
46	1p	65	GLN
47	1q	26	GLN
49	1s	23	ASN
49	1s	47	HIS
52	1v	-50	GLN
52	1v	154	GLN
52	1v	165	GLN
52	1v	208	GLN
52	1v	421	GLN
52	1v	475	ASN
52	1v	625	ASN
52	1v	641	GLN
52	1v	675	HIS
52	1v	677	GLN
52	1v	684	GLN
53	1w	69	GLN
53	1w	74	ASN
53	1w	174	GLN
3	2D	203	ASN
4	2E	48	GLN
4	2E	159	HIS
6	2G	123	ASN
7	2H	143	GLN
9	2O	5	GLN
11	2Q	57	HIS
11	2Q	89	ASN
12	2R	3	HIS
12	2R	24	GLN
12	2R	71	GLN
12	2R	91	GLN
13	2S	38	GLN
14	2T	43	GLN
14	2T	55	ASN
14	2T	58	ASN
15	2U	94	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	2W	60	ASN
20	2Z	34	ASN
20	2Z	73	GLN
22	21	47	GLN
22	21	56	GLN
23	22	47	ASN
24	23	19	GLN
24	23	32	GLN
26	25	22	HIS
28	27	6	GLN
30	29	20	HIS
32	2b	94	ASN
32	2b	140	HIS
32	2b	212	GLN
33	2c	6	HIS
33	2c	102	ASN
34	2d	116	GLN
34	2d	125	HIS
35	2e	73	ASN
35	2e	78	HIS
36	2f	32	ASN
37	2g	28	ASN
37	2g	37	ASN
37	2g	64	GLN
37	2g	68	ASN
37	2g	106	GLN
37	2g	109	ASN
39	2i	89	ASN
40	2j	62	HIS
43	2m	12	ASN
43	2m	106	ASN
45	2o	28	GLN
45	2o	46	HIS
46	2p	76	GLN
49	2s	47	HIS
52	2v	-50	GLN
52	2v	-13	GLN
52	2v	7	ASN
52	2v	77	HIS
52	2v	208	GLN
52	2v	426	GLN
52	2v	448	GLN

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Mol	Chain	Res	Type
52	2v	506	GLN
52	2v	527	ASN
52	2v	641	GLN
52	2v	675	HIS
52	2v	684	GLN
53	2w	15	GLN
53	2w	23	HIS
53	2w	34	ASN
53	2w	49	HIS
53	2w	120	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	486 (16%)	28 (0%)
1	2A	2789/2915 (95%)	495 (17%)	21 (0%)
2	1B	119/121 (98%)	15 (12%)	0
2	2B	118/121 (97%)	24 (20%)	0
31	1a	1492/1521 (98%)	230 (15%)	0
31	2a	1498/1521 (98%)	245 (16%)	0
54	1x	71/76 (93%)	30 (42%)	0
54	1y	71/76 (93%)	16 (22%)	0
54	2x	71/76 (93%)	29 (40%)	0
54	2y	71/76 (93%)	18 (25%)	0
55	1z	9/21 (42%)	5 (55%)	0
55	2z	9/21 (42%)	6 (66%)	0
All	All	9180/9460 (97%)	1599 (17%)	49 (0%)

All (1599) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	27	G
1	1A	34	C
1	1A	37	C
1	1A	45	C
1	1A	51	G
1	1A	55	G
1	1A	58	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	61	G
1	1A	63	U
1	1A	64	A
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	131	G
1	1A	173	G
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	201	C
1	1A	204	A
1	1A	205	G
1	1A	213	A
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	230	U
1	1A	233	A
1	1A	248	G
1	1A	261	G
1	1A	264	C
1	1A	266	G
1	1A	269	U
1	1A	271(J)	C
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	275	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	279	C
1	1A	311	A
1	1A	317	G
1	1A	325	G
1	1A	329	G
1	1A	330	A
1	1A	331	A
1	1A	352	G
1	1A	353	G
1	1A	362	U
1	1A	363	G
1	1A	371	A
1	1A	372	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	471	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	513	A
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	536	A
1	1A	545	G
1	1A	549	G
1	1A	556	G
1	1A	563	G
1	1A	564	C
1	1A	566	U
1	1A	573	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	575	A
1	1A	584	C
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	632	A
1	1A	634	C
1	1A	637	A
1	1A	646	A
1	1A	652(T)	C
1	1A	654	A
1	1A	669	G
1	1A	670	A
1	1A	675	A
1	1A	686	G
1	1A	696	G
1	1A	730	C
1	1A	758	C
1	1A	764	A
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	777	A
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	788	A
1	1A	789	A
1	1A	792	G
1	1A	796	C
1	1A	805	G
1	1A	811	U
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	831	G
1	1A	839	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	859	G
1	1A	860	U
1	1A	876	C
1	1A	880	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	900	A
1	1A	907	U
1	1A	910	A
1	1A	914	C
1	1A	915	C
1	1A	919	G
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	957	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	980	A
1	1A	983	A
1	1A	995	C
1	1A	996	A
1	1A	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1021	A
1	1A	1022	G
1	1A	1023	U
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1052	C
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1064	C
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1083	U
1	1A	1085	A
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1094	U
1	1A	1101	U
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1126	A
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1139	G
1	1A	1143	A
1	1A	1155	A
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1210	A
1	1A	1211	U
1	1A	1220	A
1	1A	1236	G
1	1A	1237	A
1	1A	1240	U
1	1A	1244	G
1	1A	1253	A
1	1A	1254	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1276	A
1	1A	1281	G
1	1A	1300	U
1	1A	1301	A
1	1A	1309	G
1	1A	1313	U
1	1A	1320	C
1	1A	1321	A
1	1A	1343	G
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1373	A
1	1A	1378	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1514	U
1	1A	1547	C
1	1A	1554	A
1	1A	1558	A
1	1A	1565	C
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1613	G
1	1A	1616	A
1	1A	1639	U
1	1A	1646	C
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1763	G
1	1A	1764	G
1	1A	1769	G
1	1A	1773	A
1	1A	1780	A
1	1A	1791	A
1	1A	1800	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1816	G
1	1A	1821	A
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1897	G
1	1A	1900	A
1	1A	1906	G
1	1A	1912	A
1	1A	1913	A
1	1A	1914	C
1	1A	1918	A
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1940	U
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2013	A
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2078	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2093	G
1	1A	2111	C
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2121	G
1	1A	2122	U
1	1A	2125	G
1	1A	2126	A
1	1A	2127	G
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2140	C
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2150	U
1	1A	2151	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2168	G
1	1A	2169	A
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2185	C
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2278	A
1	1A	2279	G
1	1A	2283	C
1	1A	2287	A
1	1A	2288	A
1	1A	2299	G
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2341	G
1	1A	2347	C
1	1A	2350	C
1	1A	2358	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2391	G
1	1A	2406	U
1	1A	2410	G
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2434	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2470	G
1	1A	2474	C
1	1A	2476	A
1	1A	2482	G
1	1A	2484	G
1	1A	2490	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2491	U
1	1A	2495	G
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2529	G
1	1A	2554	U
1	1A	2562	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2581	G
1	1A	2585	U
1	1A	2586	C
1	1A	2601	C
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2615	U
1	1A	2628	C
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2663	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2726	U
1	1A	2730	C
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2764	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2805	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2834	G
1	1A	2872	G
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	5	C
2	1B	13	A
2	1B	33	G
2	1B	35	U
2	1B	42	C
2	1B	44	G
2	1B	45	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	85	G
2	1B	106	G
2	1B	110	G
2	1B	120	A
31	1a	9	G
31	1a	32	A
31	1a	39	G
31	1a	47	C
31	1a	48	C
31	1a	50	A
31	1a	51	A
31	1a	61	G
31	1a	79	G
31	1a	91	C
31	1a	98	G
31	1a	101	A
31	1a	116	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	1a	121	C
31	1a	131	C
31	1a	145	G
31	1a	163	C
31	1a	174	C
31	1a	182	U
31	1a	189	G
31	1a	189(A)	C
31	1a	189(F)	U
31	1a	195	A
31	1a	197	A
31	1a	203	U
31	1a	204	U
31	1a	216	G
31	1a	217	C
31	1a	220	G
31	1a	247	G
31	1a	251	G
31	1a	266	G
31	1a	267	C
31	1a	279	A
31	1a	289	G
31	1a	321	A
31	1a	328	C
31	1a	332	G
31	1a	343	U
31	1a	345	C
31	1a	347	G
31	1a	351	G
31	1a	352	C
31	1a	353	A
31	1a	354	G
31	1a	356	A
31	1a	367	U
31	1a	372	C
31	1a	373	A
31	1a	384	G
31	1a	397	A
31	1a	398	C
31	1a	412	A
31	1a	423	G
31	1a	424	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	1a	429	U
31	1a	430	A
31	1a	439	A
31	1a	441	A
31	1a	442	C
31	1a	452	A
31	1a	461	A
31	1a	470	C
31	1a	485	G
31	1a	496	A
31	1a	498	U
31	1a	505	G
31	1a	509	A
31	1a	510	A
31	1a	511	C
31	1a	518	C
31	1a	519	C
31	1a	531	U
31	1a	532	A
31	1a	547	A
31	1a	559	A
31	1a	561	U
31	1a	562	C
31	1a	564	C
31	1a	572	A
31	1a	573	A
31	1a	576	G
31	1a	577	G
31	1a	596	C
31	1a	630	G
31	1a	634	C
31	1a	641	U
31	1a	653	A
31	1a	665	A
31	1a	688	G
31	1a	695	A
31	1a	721	G
31	1a	723	U
31	1a	731	G
31	1a	734	G
31	1a	749	C
31	1a	755	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	1a	767	A
31	1a	777	A
31	1a	793	U
31	1a	794	A
31	1a	816	A
31	1a	817	C
31	1a	821	G
31	1a	828	A
31	1a	836	G
31	1a	840	C
31	1a	841	U
31	1a	851	G
31	1a	859	A
31	1a	866	C
31	1a	902	G
31	1a	914	A
31	1a	926	G
31	1a	927	G
31	1a	934	C
31	1a	952	U
31	1a	960	U
31	1a	961	U
31	1a	968	A
31	1a	969	A
31	1a	971	G
31	1a	972	C
31	1a	974	A
31	1a	975	A
31	1a	976	G
31	1a	977	A
31	1a	982	U
31	1a	992	U
31	1a	993	G
31	1a	1000	U
31	1a	1003	G
31	1a	1005	A
31	1a	1006	C
31	1a	1020	U
31	1a	1022	G
31	1a	1025	U
31	1a	1026	G
31	1a	1027	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	1a	1029	C
31	1a	1030(A)	G
31	1a	1031	G
31	1a	1033	G
31	1a	1037	C
31	1a	1038	C
31	1a	1039	C
31	1a	1044	A
31	1a	1050	G
31	1a	1054	C
31	1a	1055	A
31	1a	1065	U
31	1a	1066	C
31	1a	1068	G
31	1a	1081	G
31	1a	1084	G
31	1a	1094	G
31	1a	1095	U
31	1a	1101	A
31	1a	1108	G
31	1a	1122	U
31	1a	1124	G
31	1a	1125	U
31	1a	1127	G
31	1a	1134	G
31	1a	1137	C
31	1a	1138	G
31	1a	1139	G
31	1a	1146	A
31	1a	1152	A
31	1a	1159	U
31	1a	1184	G
31	1a	1186	G
31	1a	1187	G
31	1a	1196	U
31	1a	1197	G
31	1a	1200	C
31	1a	1202	G
31	1a	1212	U
31	1a	1213	A
31	1a	1220	G
31	1a	1225	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	1a	1226	C
31	1a	1227	A
31	1a	1236	A
31	1a	1238	A
31	1a	1241	G
31	1a	1256	A
31	1a	1257	U
31	1a	1258	G
31	1a	1260	C
31	1a	1268	A
31	1a	1270	C
31	1a	1278	U
31	1a	1279	A
31	1a	1280	A
31	1a	1286	A
31	1a	1287	A
31	1a	1299	A
31	1a	1300	G
31	1a	1305	G
31	1a	1320	C
31	1a	1336	C
31	1a	1346	A
31	1a	1347	G
31	1a	1353	G
31	1a	1358	U
31	1a	1363	C
31	1a	1364	U
31	1a	1370	G
31	1a	1378	C
31	1a	1398	A
31	1a	1419	G
31	1a	1442	G
31	1a	1442(A)	G
31	1a	1446	U
31	1a	1447	A
31	1a	1452	C
31	1a	1456	G
31	1a	1487	G
31	1a	1491	G
31	1a	1492	A
31	1a	1493	A
31	1a	1494	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	1a	1499	A
31	1a	1503	A
31	1a	1504	G
31	1a	1506	U
31	1a	1517	G
31	1a	1529	G
31	1a	1530	G
54	1x	2	C
54	1x	3	C
54	1x	4	C
54	1x	5	G
54	1x	8	4SU
54	1x	19	G
54	1x	20	U
54	1x	21	A
54	1x	22	G
54	1x	26	A
54	1x	33	U
54	1x	35	A
54	1x	36	A
54	1x	38	A
54	1x	42	C
54	1x	44	G
54	1x	45	U
54	1x	46	7MG
54	1x	47	U
54	1x	48	C
54	1x	52	G
54	1x	57	G
54	1x	59	U
54	1x	60	U
54	1x	65	G
54	1x	69	G
54	1x	70	G
54	1x	71	G
54	1x	75	C
54	1x	76	A
54	1y	2	C
54	1y	5	G
54	1y	9	A
54	1y	13	C
54	1y	14	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1y	20	U
54	1y	21	A
54	1y	26	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	59	U
54	1y	60	U
55	1z	13	A
55	1z	15	A
55	1z	19	U
55	1z	20	A
55	1z	21	A
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	27	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	49	A
1	2A	50	U
1	2A	51	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	98	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	125	G
1	2A	139(A)	G
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	196	A
1	2A	199	A
1	2A	201	C
1	2A	204	A
1	2A	205	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	266	G
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	302	C
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	372	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	406	G
1	2A	411	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	422	A
1	2A	435	C
1	2A	444	C
1	2A	448	U
1	2A	449	A
1	2A	454	A
1	2A	457	A
1	2A	480	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	610	G
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	632	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	668	G
1	2A	669	G
1	2A	675	A
1	2A	686	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	783	A
1	2A	784	A
1	2A	785	G
1	2A	789	A
1	2A	792	G
1	2A	793	A
1	2A	801	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	825	C
1	2A	827	U
1	2A	829	A
1	2A	831	G
1	2A	843	G
1	2A	846	C
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	874	G
1	2A	875	G
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	895	U
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	907	U
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	957	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	973	A
1	2A	974	G
1	2A	975	C
1	2A	975(A)	G
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1125	G
1	2A	1129	A
1	2A	1130	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1132	A
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1143	A
1	2A	1144	G
1	2A	1169	G
1	2A	1171	G
1	2A	1187	G
1	2A	1188	U
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1237	A
1	2A	1250	G
1	2A	1252	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1313	U
1	2A	1314	C
1	2A	1321	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1378	A
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1411	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1427	A
1	2A	1428	C
1	2A	1435	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1507	A
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1543	C
1	2A	1546	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1602	U
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1646	C
1	2A	1648	C
1	2A	1654	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1674	G
1	2A	1696	G
1	2A	1698	A
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1745(A)	C
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G
1	2A	1773	A
1	2A	1778	U
1	2A	1780	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1809	A
1	2A	1813	G
1	2A	1816	G
1	2A	1827	C
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1902	C
1	2A	1912	A
1	2A	1914	C
1	2A	1915	5MU
1	2A	1916	A
1	2A	1917	PSU
1	2A	1918	A
1	2A	1919	A
1	2A	1920	OMC
1	2A	1929	G
1	2A	1930	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1934	C
1	2A	1936	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2027	G
1	2A	2030	A
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2034	U
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2093	G
1	2A	2096	U
1	2A	2105	C
1	2A	2108	C
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2156	G
1	2A	2157	G
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2291	U
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2352	A
1	2A	2371	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2425	A
1	2A	2427	C
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2447	G
1	2A	2448	A
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2490	G
1	2A	2491	U
1	2A	2492	U
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2507	C
1	2A	2518	A
1	2A	2519	U
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2538	C
1	2A	2554	U
1	2A	2564	A
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2579	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2582	G
1	2A	2585	U
1	2A	2586	C
1	2A	2601	C
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2626	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2646	C
1	2A	2654	A
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2739	U
1	2A	2748	A
1	2A	2751	G
1	2A	2752	C
1	2A	2757	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2789	C
1	2A	2802	G
1	2A	2807	G
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2823	A
1	2A	2833	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2835	A
1	2A	2836	U
1	2A	2872	G
1	2A	2876	G
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	13	A
2	2B	16	G
2	2B	20	C
2	2B	24	G
2	2B	30	C
2	2B	42	C
2	2B	53	A
2	2B	63	G
2	2B	66	A
2	2B	67	G
2	2B	72	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	89	G
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	112	U
2	2B	114	C
31	2a	9	G
31	2a	32	A
31	2a	39	G
31	2a	47	C
31	2a	48	C
31	2a	49	U
31	2a	50	A
31	2a	51	A
31	2a	52	G
31	2a	54	C
31	2a	66	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	2a	78	G
31	2a	89	C
31	2a	101	A
31	2a	116	A
31	2a	121	C
31	2a	129(A)	G
31	2a	131	C
31	2a	143	A
31	2a	163	C
31	2a	174	C
31	2a	182	U
31	2a	189(E)	U
31	2a	195	A
31	2a	197	A
31	2a	199	G
31	2a	202	U
31	2a	203	U
31	2a	216	G
31	2a	220	G
31	2a	247	G
31	2a	251	G
31	2a	266	G
31	2a	267	C
31	2a	279	A
31	2a	289	G
31	2a	301	G
31	2a	305	G
31	2a	321	A
31	2a	328	C
31	2a	332	G
31	2a	351	G
31	2a	352	C
31	2a	353	A
31	2a	354	G
31	2a	367	U
31	2a	372	C
31	2a	373	A
31	2a	384	G
31	2a	397	A
31	2a	398	C
31	2a	406	G
31	2a	412	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	2a	421	U
31	2a	424	G
31	2a	429	U
31	2a	439	A
31	2a	442	C
31	2a	452	A
31	2a	454	C
31	2a	470	C
31	2a	485	G
31	2a	496	A
31	2a	498	U
31	2a	505	G
31	2a	507	C
31	2a	508	C
31	2a	509	A
31	2a	510	A
31	2a	511	C
31	2a	518	C
31	2a	527	7MG
31	2a	531	U
31	2a	532	A
31	2a	535	A
31	2a	536	C
31	2a	547	A
31	2a	559	A
31	2a	560	U
31	2a	561	U
31	2a	564	C
31	2a	572	A
31	2a	573	A
31	2a	576	G
31	2a	577	G
31	2a	596	C
31	2a	618	C
31	2a	630	G
31	2a	632	A
31	2a	641	U
31	2a	653	A
31	2a	665	A
31	2a	686	U
31	2a	687	A
31	2a	688	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	2a	731	G
31	2a	749	C
31	2a	755	G
31	2a	777	A
31	2a	790	A
31	2a	793	U
31	2a	794	A
31	2a	816	A
31	2a	817	C
31	2a	821	G
31	2a	828	A
31	2a	840	C
31	2a	841	U
31	2a	848	C
31	2a	853	G
31	2a	859	A
31	2a	872	A
31	2a	873	A
31	2a	889	A
31	2a	900	A
31	2a	902	G
31	2a	914	A
31	2a	927	G
31	2a	931	C
31	2a	932	C
31	2a	934	C
31	2a	935	A
31	2a	960	U
31	2a	961	U
31	2a	968	A
31	2a	969	A
31	2a	971	G
31	2a	974	A
31	2a	975	A
31	2a	976	G
31	2a	977	A
31	2a	992	U
31	2a	993	G
31	2a	997	U
31	2a	1001(A)	G
31	2a	1002	G
31	2a	1003	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	2a	1004	A
31	2a	1005	A
31	2a	1006	C
31	2a	1007	C
31	2a	1009	G
31	2a	1022	G
31	2a	1023	G
31	2a	1025	U
31	2a	1026	G
31	2a	1027	C
31	2a	1030	C
31	2a	1030(A)	G
31	2a	1031	G
31	2a	1033	G
31	2a	1036	G
31	2a	1038	C
31	2a	1039	C
31	2a	1040	U
31	2a	1045	C
31	2a	1051	C
31	2a	1053	G
31	2a	1065	U
31	2a	1066	C
31	2a	1068	G
31	2a	1070	U
31	2a	1077	G
31	2a	1081	G
31	2a	1094	G
31	2a	1096	C
31	2a	1098	C
31	2a	1101	A
31	2a	1117	G
31	2a	1122	U
31	2a	1125	U
31	2a	1129	C
31	2a	1137	C
31	2a	1138	G
31	2a	1139	G
31	2a	1140	C
31	2a	1146	A
31	2a	1152	A
31	2a	1159	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	2a	1160	G
31	2a	1166	G
31	2a	1172	C
31	2a	1182	G
31	2a	1184	G
31	2a	1196	U
31	2a	1197	G
31	2a	1202	G
31	2a	1211	U
31	2a	1212	U
31	2a	1213	A
31	2a	1215	G
31	2a	1226	C
31	2a	1227	A
31	2a	1236	A
31	2a	1238	A
31	2a	1256	A
31	2a	1257	U
31	2a	1258	G
31	2a	1260	C
31	2a	1263	C
31	2a	1264	C
31	2a	1268	A
31	2a	1270	C
31	2a	1272	G
31	2a	1275	A
31	2a	1279	A
31	2a	1280	A
31	2a	1287	A
31	2a	1303	C
31	2a	1320	C
31	2a	1323	G
31	2a	1331	G
31	2a	1340	A
31	2a	1346	A
31	2a	1347	G
31	2a	1353	G
31	2a	1363	C
31	2a	1364	U
31	2a	1381	U
31	2a	1386	G
31	2a	1398	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	2a	1419	G
31	2a	1442	G
31	2a	1442(A)	G
31	2a	1442(B)	A
31	2a	1446	U
31	2a	1447	A
31	2a	1452	C
31	2a	1456	G
31	2a	1475	G
31	2a	1487	G
31	2a	1492	A
31	2a	1493	A
31	2a	1494	G
31	2a	1495	U
31	2a	1496	C
31	2a	1503	A
31	2a	1504	G
31	2a	1506	U
31	2a	1517	G
31	2a	1520	G
31	2a	1529	G
31	2a	1530	G
31	2a	1531	A
31	2a	1532	U
54	2x	3	C
54	2x	4	C
54	2x	5	G
54	2x	8	4SU
54	2x	19	G
54	2x	20	U
54	2x	21	A
54	2x	22	G
54	2x	26	A
54	2x	35	A
54	2x	36	A
54	2x	38	A
54	2x	39	PSU
54	2x	40	C
54	2x	41	C
54	2x	42	C
54	2x	44	G
54	2x	45	U

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Mol	Chain	Res	Type
54	2x	46	7MG
54	2x	47	U
54	2x	48	C
54	2x	59	U
54	2x	60	U
54	2x	65	G
54	2x	69	G
54	2x	70	G
54	2x	71	G
54	2x	75	C
54	2x	76	A
54	2y	2	C
54	2y	3	C
54	2y	5	G
54	2y	9	A
54	2y	10	G
54	2y	13	C
54	2y	14	A
54	2y	19	G
54	2y	20	U
54	2y	21	A
54	2y	26	A
54	2y	44	G
54	2y	45	U
54	2y	46	7MG
54	2y	47	U
54	2y	48	C
54	2y	59	U
54	2y	60	U
55	2z	13	A
55	2z	15	A
55	2z	18	C
55	2z	19	U
55	2z	20	A
55	2z	21	A

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	214	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	764	A
1	1A	859	G
1	1A	895	U
1	1A	960	A
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1210	A
1	1A	1275	A
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1653	G
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2439	A
1	1A	2689	U
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	856	C
1	2A	900	A
1	2A	1187	G
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1911	PSU
1	2A	1992	G

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Mol	Chain	Res	Type
1	2A	2119	A
1	2A	2351	G
1	2A	2689	U
1	2A	2756	U

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

76 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	7MG	1y	46	54	22,26,27	1.28	4 (18%)	29,39,42	2.60	7 (24%)
1	5MC	1A	1962	1	18,22,23	0.94	2 (11%)	26,32,35	1.19	3 (11%)
31	PSU	1a	516	31,56	18,21,22	1.35	2 (11%)	22,30,33	1.79	5 (22%)
1	PSU	1A	1911	1	18,21,22	1.36	4 (22%)	22,30,33	1.74	4 (18%)
1	5MC	2A	1942	1	18,22,23	0.94	2 (11%)	26,32,35	1.17	3 (11%)
1	5MU	2A	1939	1	19,22,23	1.37	5 (26%)	28,32,35	2.19	6 (21%)
1	OMG	1A	2251	1,56	18,26,27	1.08	1 (5%)	19,38,41	1.18	3 (15%)
31	4OC	1a	1402	31	20,23,24	0.76	0	26,32,35	0.98	1 (3%)
54	4SU	1y	8	54	18,21,22	1.83	5 (27%)	26,30,33	2.21	5 (19%)
54	PSU	1y	55	54	18,21,22	1.31	2 (11%)	22,30,33	1.95	3 (13%)
54	MIA	2x	37	54	18,24,32	1.10	2 (11%)	18,35,47	1.31	2 (11%)
31	MA6	2a	1518	31,56	19,26,27	0.94	1 (5%)	18,38,41	1.80	6 (33%)
54	PSU	2x	39	54	18,21,22	1.29	2 (11%)	22,30,33	2.08	4 (18%)
1	5MC	1A	1942	1	18,22,23	0.93	2 (11%)	26,32,35	1.35	4 (15%)
54	5MU	2x	54	54	19,22,23	1.46	5 (26%)	28,32,35	1.94	5 (17%)
1	2MA	1A	2503	1,56	17,25,26	1.10	1 (5%)	17,37,40	1.21	3 (17%)
1	5MC	2A	1962	1	18,22,23	0.97	1 (5%)	26,32,35	1.11	3 (11%)
31	MA6	1a	1518	31	19,26,27	0.95	1 (5%)	18,38,41	1.62	4 (22%)
54	PSU	2y	32	54	18,21,22	1.33	2 (11%)	22,30,33	1.84	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MA	2A	2503	1,56	17,25,26	1.02	1 (5%)	17,37,40	1.04	2 (11%)
54	PSU	2y	39	54	18,21,22	1.33	2 (11%)	22,30,33	1.81	3 (13%)
1	PSU	2A	1911	1,56	18,21,22	1.40	3 (16%)	22,30,33	2.02	3 (13%)
1	PSU	1A	1917	1	18,21,22	1.40	2 (11%)	22,30,33	1.92	4 (18%)
31	M2G	2a	966	31	20,27,28	1.48	3 (15%)	22,40,43	0.92	2 (9%)
1	5MU	1A	1915	1	19,22,23	1.41	5 (26%)	28,32,35	2.11	6 (21%)
1	2MU	2A	2552	1	19,22,24	1.25	4 (21%)	26,31,36	1.82	5 (19%)
54	MIA	1y	37	31,54	18,24,32	1.10	2 (11%)	18,35,47	1.26	2 (11%)
1	2MU	1A	2552	1,56	19,22,24	1.30	3 (15%)	26,31,36	1.95	3 (11%)
31	UR3	2a	1498	31	19,22,23	1.03	2 (10%)	26,32,35	1.46	1 (3%)
31	MA6	2a	1519	31	19,26,27	1.00	1 (5%)	18,38,41	1.70	5 (27%)
54	PSU	1x	55	54	18,21,22	1.33	2 (11%)	22,30,33	1.95	4 (18%)
54	MIA	1x	37	54	18,24,32	1.16	2 (11%)	18,35,47	1.34	2 (11%)
54	7MG	1x	46	54	22,26,27	1.28	3 (13%)	29,39,42	2.60	7 (24%)
42	0TD	1l	92	42	7,9,10	4.64	1 (14%)	6,11,13	4.72	2 (33%)
54	5MU	1x	54	54	19,22,23	1.37	5 (26%)	28,32,35	2.23	6 (21%)
31	5MC	1a	1400	31	18,22,23	0.98	2 (11%)	26,32,35	1.15	2 (7%)
31	5MC	1a	1404	31	18,22,23	0.98	2 (11%)	26,32,35	1.23	4 (15%)
54	PSU	2x	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
31	5MC	1a	1407	31	18,22,23	0.94	1 (5%)	26,32,35	1.00	1 (3%)
1	5MU	2A	1915	1,56	19,22,23	1.53	4 (21%)	28,32,35	2.07	7 (25%)
54	4SU	2y	8	54	18,21,22	1.74	4 (22%)	26,30,33	2.07	4 (15%)
54	PSU	1x	32	54,56	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
54	PSU	1x	39	54	18,21,22	1.42	3 (16%)	22,30,33	1.86	4 (18%)
31	PSU	2a	516	31,56	18,21,22	1.32	2 (11%)	22,30,33	1.82	3 (13%)
54	7MG	2x	46	54	22,26,27	1.29	4 (18%)	29,39,42	2.65	8 (27%)
54	PSU	2y	55	54	18,21,22	1.32	2 (11%)	22,30,33	1.91	3 (13%)
31	5MC	2a	1404	31	18,22,23	0.94	2 (11%)	26,32,35	1.12	3 (11%)
54	4SU	2x	8	54	18,21,22	1.65	4 (22%)	26,30,33	2.21	4 (15%)
42	0TD	2l	92	42	7,9,10	4.63	1 (14%)	6,11,13	1.98	2 (33%)
1	OMC	1A	1920	1	19,22,23	0.83	0	26,31,34	1.16	3 (11%)
31	7MG	1a	527	31,56	22,26,27	1.31	3 (13%)	29,39,42	2.51	8 (27%)
31	2MG	1a	1207	31	18,26,27	0.89	1 (5%)	16,38,41	1.17	2 (12%)
1	PSU	2A	2605	1,56	18,21,22	1.37	2 (11%)	22,30,33	2.14	4 (18%)
54	7MG	2y	46	54	22,26,27	1.32	4 (18%)	29,39,42	2.56	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	MIA	2y	37	54	18,24,32	1.06	2 (11%)	18,35,47	1.33	2 (11%)
31	MA6	1a	1519	31	19,26,27	1.05	1 (5%)	18,38,41	1.59	4 (22%)
1	5MU	1A	1939	1	19,22,23	1.49	5 (26%)	28,32,35	2.11	7 (25%)
31	5MC	1a	967	31	18,22,23	0.97	1 (5%)	26,32,35	1.17	3 (11%)
31	7MG	2a	527	31	22,26,27	1.36	3 (13%)	29,39,42	2.48	7 (24%)
1	PSU	2A	1917	1,56	18,21,22	1.43	2 (11%)	22,30,33	1.74	4 (18%)
31	M2G	1a	966	31	20,27,28	1.51	3 (15%)	22,40,43	0.92	2 (9%)
1	OMG	2A	2251	1,56	18,26,27	0.98	1 (5%)	19,38,41	0.99	2 (10%)
31	2MG	2a	1207	31	18,26,27	0.88	1 (5%)	16,38,41	1.17	2 (12%)
31	4OC	2a	1402	31	20,23,24	0.79	0	26,32,35	1.03	1 (3%)
31	5MC	2a	1407	31,56	18,22,23	0.96	1 (5%)	26,32,35	1.05	2 (7%)
54	PSU	1y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.72	3 (13%)
54	PSU	2x	32	54,56	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
54	PSU	1y	39	54	18,21,22	1.33	2 (11%)	22,30,33	1.97	4 (18%)
54	5MU	1y	54	54	19,22,23	1.46	5 (26%)	28,32,35	2.10	7 (25%)
54	5MU	2y	54	54	19,22,23	1.44	5 (26%)	28,32,35	2.09	6 (21%)
31	UR3	1a	1498	31,56	19,22,23	1.04	2 (10%)	26,32,35	1.45	3 (11%)
31	5MC	2a	967	31	18,22,23	0.95	2 (11%)	26,32,35	1.15	3 (11%)
31	5MC	2a	1400	31	18,22,23	0.98	1 (5%)	26,32,35	1.11	3 (11%)
1	PSU	1A	2605	1	18,21,22	1.42	2 (11%)	22,30,33	1.96	4 (18%)
1	OMC	2A	1920	1	19,22,23	0.80	0	26,31,34	0.81	0
54	4SU	1x	8	54,56	18,21,22	1.61	4 (22%)	26,30,33	2.39	8 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
31	PSU	1a	516	31,56	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,56	-	0/5/27/28	0/3/3/3
31	4OC	1a	1402	31	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4SU	1y	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	MIA	2x	37	54	-	3/3/25/34	0/3/3/3
31	MA6	2a	1518	31,56	-	1/7/29/30	0/3/3/3
54	PSU	2x	39	54	-	2/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	1/7/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	2/3/25/26	0/3/3/3
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
31	MA6	1a	1518	31	-	3/7/29/30	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	2/3/25/26	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1,56	-	1/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
31	M2G	2a	966	31	-	0/7/29/30	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	2MU	2A	2552	1	-	0/9/27/28	0/2/2/2
54	MIA	1y	37	31,54	-	3/3/25/34	0/3/3/3
1	2MU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
31	UR3	2a	1498	31	-	0/7/25/26	0/2/2/2
31	MA6	2a	1519	31	-	4/7/29/30	0/3/3/3
54	PSU	1x	55	54	-	1/7/25/26	0/2/2/2
54	MIA	1x	37	54	-	2/3/25/34	0/3/3/3
54	7MG	1x	46	54	-	1/7/37/38	0/3/3/3
42	0TD	1l	92	42	-	3/7/12/14	-
54	5MU	1x	54	54	-	2/7/25/26	0/2/2/2
31	5MC	1a	1400	31	-	0/7/25/26	0/2/2/2
31	5MC	1a	1404	31	-	0/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	2/7/25/26	0/2/2/2
31	5MC	1a	1407	31	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1,56	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1x	32	54,56	-	2/7/25/26	0/2/2/2
54	PSU	1x	39	54	-	2/7/25/26	0/2/2/2
31	PSU	2a	516	31,56	-	0/7/25/26	0/2/2/2
54	7MG	2x	46	54	-	1/7/37/38	0/3/3/3
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
31	5MC	2a	1404	31	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4SU	2x	8	54	-	2/7/25/26	0/2/2/2
42	0TD	2l	92	42	-	2/7/12/14	-
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
31	7MG	1a	527	31,56	-	2/7/37/38	0/3/3/3
31	2MG	1a	1207	31	-	0/5/27/28	0/3/3/3
1	PSU	2A	2605	1,56	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	4/7/37/38	0/3/3/3
54	MIA	2y	37	54	-	3/3/25/34	0/3/3/3
31	MA6	1a	1519	31	-	3/7/29/30	0/3/3/3
1	5MU	1A	1939	1	-	1/7/25/26	0/2/2/2
31	5MC	1a	967	31	-	0/7/25/26	0/2/2/2
31	7MG	2a	527	31	-	2/7/37/38	0/3/3/3
1	PSU	2A	1917	1,56	-	5/7/25/26	0/2/2/2
31	M2G	1a	966	31	-	0/7/29/30	0/3/3/3
1	OMG	2A	2251	1,56	-	0/5/27/28	0/3/3/3
31	2MG	2a	1207	31	-	1/5/27/28	0/3/3/3
31	4OC	2a	1402	31	-	2/9/29/30	0/2/2/2
31	5MC	2a	1407	31,56	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	PSU	2x	32	54,56	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
31	UR3	1a	1498	31,56	-	0/7/25/26	0/2/2/2
31	5MC	2a	967	31	-	1/7/25/26	0/2/2/2
31	5MC	2a	1400	31	-	4/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
54	4SU	1x	8	54,56	-	4/7/25/26	0/2/2/2

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1l	92	0TD	CB-SB	-11.95	1.70	1.82
42	2l	92	0TD	CB-SB	-11.94	1.70	1.82
31	1a	966	M2G	C2-N3	4.83	1.36	1.30
31	2a	966	M2G	C2-N3	4.74	1.36	1.30
54	1y	8	4SU	C4-S4	-4.64	1.59	1.68
54	2y	8	4SU	C4-S4	-4.49	1.59	1.68
54	2x	8	4SU	C4-S4	-4.29	1.60	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	8	4SU	C4-S4	-3.84	1.61	1.68
1	1A	2605	PSU	C6-C5	3.67	1.39	1.35
31	2a	527	7MG	C4-N9	-3.66	1.33	1.37
54	2y	32	PSU	C6-C5	3.63	1.39	1.35
54	2x	55	PSU	C6-C5	3.60	1.39	1.35
54	1y	8	4SU	C4-N3	-3.56	1.33	1.37
54	1y	32	PSU	C6-C5	3.55	1.39	1.35
1	2A	1917	PSU	C6-C5	3.45	1.39	1.35
54	1x	32	PSU	C6-C5	3.45	1.39	1.35
54	1x	39	PSU	C6-C5	3.42	1.39	1.35
54	1x	55	PSU	C6-C5	3.40	1.39	1.35
54	1x	46	7MG	C4-N9	-3.39	1.33	1.37
54	2y	39	PSU	C6-C5	3.39	1.39	1.35
54	2y	8	4SU	C4-N3	-3.38	1.34	1.37
31	1a	516	PSU	C6-C5	3.36	1.39	1.35
1	1A	1917	PSU	C6-C5	3.33	1.39	1.35
1	2A	1911	PSU	C6-C5	3.29	1.39	1.35
54	1y	39	PSU	C6-C5	3.25	1.39	1.35
1	1A	2251	OMG	C6-N1	-3.23	1.33	1.37
54	2x	32	PSU	C6-C5	3.22	1.39	1.35
54	2y	55	PSU	C6-C5	3.21	1.39	1.35
54	1y	55	PSU	C6-C5	3.13	1.39	1.35
1	2A	2605	PSU	C4-N3	-3.12	1.33	1.38
1	2A	1915	5MU	C2-N1	3.11	1.43	1.38
54	2x	39	PSU	C6-C5	3.10	1.38	1.35
54	2x	46	7MG	C4-N9	-3.06	1.34	1.37
31	2a	1400	5MC	C6-C5	3.05	1.39	1.34
54	1y	46	7MG	C5-C4	3.04	1.48	1.38
31	2a	516	PSU	C6-C5	3.02	1.38	1.35
54	2y	46	7MG	C5-C4	3.02	1.48	1.38
1	1A	1911	PSU	C6-C5	3.02	1.38	1.35
1	1A	1939	5MU	C6-C5	3.01	1.39	1.34
31	1a	527	7MG	C4-N9	-2.98	1.34	1.37
1	2A	1915	5MU	C6-C5	2.97	1.39	1.34
31	2a	1407	5MC	C6-C5	2.96	1.39	1.34
1	2A	1962	5MC	C6-C5	2.95	1.39	1.34
31	1a	966	M2G	C2-N2	2.92	1.40	1.35
31	1a	527	7MG	C5-C4	2.91	1.47	1.38
54	2x	46	7MG	C5-C4	2.91	1.47	1.38
1	1A	2552	2MU	C4-N3	-2.87	1.33	1.38
31	2a	527	7MG	C5-C4	2.86	1.47	1.38
54	2x	54	5MU	C6-C5	2.84	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	46	7MG	C5-C4	2.83	1.47	1.38
1	1A	1915	5MU	C6-C5	2.83	1.39	1.34
54	2x	8	4SU	C4-N3	-2.83	1.34	1.37
54	1x	37	MIA	C2-N3	2.82	1.36	1.32
1	2A	1939	5MU	C6-C5	2.81	1.39	1.34
31	1a	967	5MC	C6-C5	2.81	1.39	1.34
54	1y	54	5MU	C6-C5	2.80	1.39	1.34
54	2y	54	5MU	C6-C5	2.80	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.79	1.33	1.38
31	1a	1400	5MC	C6-C5	2.78	1.39	1.34
54	1x	54	5MU	C6-C5	2.77	1.39	1.34
31	2a	966	M2G	C2-N2	2.76	1.40	1.35
31	2a	1519	MA6	C5-C4	2.75	1.48	1.40
54	1y	54	5MU	C2-N1	2.74	1.42	1.38
54	1x	37	MIA	C5-C4	2.73	1.48	1.40
54	1x	8	4SU	C2-N1	2.72	1.42	1.38
31	1a	1404	5MC	C6-C5	2.72	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.71	1.33	1.38
1	2A	1911	PSU	C4-N3	-2.69	1.33	1.38
54	1y	8	4SU	C5-C4	-2.69	1.39	1.42
31	1a	1407	5MC	C6-C5	2.67	1.39	1.34
1	1A	1915	5MU	C4-N3	-2.67	1.33	1.38
54	2x	37	MIA	C5-C4	2.66	1.48	1.40
54	2y	46	7MG	C4-N9	-2.66	1.34	1.37
54	2y	54	5MU	C2-N1	2.66	1.42	1.38
1	1A	1917	PSU	C4-N3	-2.65	1.33	1.38
54	1x	55	PSU	C4-N3	-2.65	1.33	1.38
31	1a	1519	MA6	C5-C4	2.64	1.47	1.40
1	2A	1915	5MU	C4-C5	2.64	1.49	1.44
1	2A	2251	OMG	C6-N1	-2.64	1.33	1.37
1	2A	1939	5MU	C4-N3	-2.64	1.33	1.38
54	1x	8	4SU	C4-N3	-2.63	1.34	1.37
31	2a	967	5MC	C6-C5	2.63	1.38	1.34
54	1y	37	MIA	C5-C4	2.63	1.47	1.40
1	2A	1917	PSU	C4-N3	-2.63	1.34	1.38
54	2x	54	5MU	C4-N3	-2.63	1.34	1.38
1	1A	2552	2MU	C5-C4	2.61	1.49	1.43
54	2x	39	PSU	C4-N3	-2.61	1.34	1.38
54	1y	39	PSU	C4-N3	-2.60	1.34	1.38
54	2x	54	5MU	C2-N1	2.60	1.42	1.38
1	2A	2605	PSU	C6-C5	2.59	1.38	1.35
31	2a	516	PSU	C4-N3	-2.59	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	55	PSU	C4-N3	-2.57	1.34	1.38
54	1x	39	PSU	C4-N3	-2.56	1.34	1.38
54	1y	37	MIA	C2-N3	2.56	1.36	1.32
54	2x	32	PSU	C4-N3	-2.56	1.34	1.38
54	2x	37	MIA	C2-N3	2.55	1.36	1.32
54	2y	37	MIA	C5-C4	2.55	1.47	1.40
1	2A	1915	5MU	C4-N3	-2.54	1.34	1.38
54	1y	54	5MU	C4-N3	-2.53	1.34	1.38
31	2a	966	M2G	C6-N1	-2.53	1.34	1.37
54	1y	54	5MU	C4-C5	2.53	1.49	1.44
54	1x	32	PSU	C4-N3	-2.52	1.34	1.38
1	2A	2552	2MU	C4-N3	-2.52	1.34	1.38
1	2A	1942	5MC	C6-C5	2.52	1.38	1.34
1	1A	2605	PSU	C4-N3	-2.51	1.34	1.38
54	1x	54	5MU	C4-N3	-2.51	1.34	1.38
54	1y	55	PSU	C4-N3	-2.51	1.34	1.38
31	2a	1518	MA6	C5-C4	2.50	1.47	1.40
1	2A	1939	5MU	C6-N1	-2.49	1.33	1.38
54	2y	54	5MU	C4-C5	2.48	1.48	1.44
54	2y	37	MIA	C2-N3	2.48	1.36	1.32
54	1y	46	7MG	C4-N9	-2.48	1.34	1.37
1	1A	1962	5MC	C6-C5	2.47	1.38	1.34
31	1a	1518	MA6	C5-C4	2.46	1.47	1.40
31	2a	1404	5MC	C6-C5	2.44	1.38	1.34
54	1x	8	4SU	C5-C4	-2.43	1.39	1.42
31	1a	516	PSU	C4-N3	-2.43	1.34	1.38
54	2x	55	PSU	C4-N3	-2.43	1.34	1.38
1	2A	1939	5MU	C4-C5	2.43	1.48	1.44
54	2y	39	PSU	C4-N3	-2.42	1.34	1.38
54	2y	8	4SU	C5-C4	-2.41	1.39	1.42
1	1A	1942	5MC	C6-N1	-2.40	1.33	1.38
54	2y	54	5MU	C4-N3	-2.39	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.39	1.34	1.38
1	1A	1939	5MU	C2-N1	2.38	1.42	1.38
31	1a	1207	2MG	C6-N1	-2.38	1.34	1.37
31	1a	966	M2G	C6-N1	-2.37	1.34	1.37
1	1A	1942	5MC	C6-C5	2.36	1.38	1.34
54	1x	54	5MU	C4-C5	2.35	1.48	1.44
54	1y	32	PSU	C4-N3	-2.34	1.34	1.38
54	2y	32	PSU	C4-N3	-2.34	1.34	1.38
31	1a	1400	5MC	C6-N1	-2.34	1.34	1.38
1	1A	2503	2MA	C2-N3	2.34	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2x	54	5MU	C4-C5	2.32	1.48	1.44
31	1a	1404	5MC	C6-N1	-2.32	1.34	1.38
1	1A	1915	5MU	C4-C5	2.30	1.48	1.44
31	2a	967	5MC	C6-N1	-2.30	1.34	1.38
31	2a	1207	2MG	C6-N1	-2.30	1.34	1.37
54	2x	8	4SU	C5-C4	-2.30	1.39	1.42
54	1x	54	5MU	C2-N1	2.28	1.42	1.38
31	1a	527	7MG	C6-N1	-2.28	1.34	1.38
54	1y	8	4SU	C2-N3	-2.27	1.33	1.38
54	2y	46	7MG	C6-N1	-2.25	1.34	1.38
54	1x	54	5MU	C6-N1	-2.25	1.34	1.38
54	2x	8	4SU	C2-N1	2.24	1.42	1.38
54	2y	8	4SU	C2-N3	-2.23	1.34	1.38
1	1A	1939	5MU	C4-C5	2.23	1.48	1.44
31	2a	527	7MG	C6-N1	-2.23	1.34	1.38
1	2A	2552	2MU	C2-N3	-2.19	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.18	1.34	1.38
54	1y	54	5MU	C6-N1	-2.18	1.34	1.38
31	2a	1404	5MC	C6-N1	-2.18	1.34	1.38
54	2y	46	7MG	C8-N9	2.17	1.47	1.46
54	1y	8	4SU	C2-N1	2.17	1.41	1.38
1	2A	1939	5MU	C2-N3	-2.16	1.34	1.38
1	2A	2552	2MU	C5-C4	2.15	1.48	1.43
54	2y	54	5MU	C6-N1	-2.14	1.34	1.38
31	1a	1498	UR3	C6-C5	2.14	1.40	1.35
31	2a	1498	UR3	C2-N1	2.12	1.41	1.38
31	1a	1498	UR3	C2-N1	2.11	1.41	1.38
1	2A	2552	2MU	C2-N1	2.09	1.41	1.38
1	1A	1915	5MU	C2-N3	-2.08	1.34	1.38
54	2x	46	7MG	C6-N1	-2.08	1.35	1.38
1	2A	1911	PSU	C2-N1	-2.07	1.33	1.36
54	1y	46	7MG	C6-N1	-2.07	1.35	1.38
1	1A	1911	PSU	C2-N1	-2.06	1.33	1.36
54	2x	54	5MU	C6-N1	-2.06	1.34	1.38
1	1A	1911	PSU	C2-N3	-2.06	1.34	1.37
54	1x	46	7MG	C5-C6	2.05	1.48	1.43
54	1x	39	PSU	C4-C5	2.04	1.50	1.44
1	1A	2552	2MU	C6-C5	2.03	1.39	1.35
31	2a	1498	UR3	C6-C5	2.03	1.39	1.35
1	1A	1939	5MU	C6-N1	-2.02	1.34	1.38
1	2A	2503	2MA	C2-N3	2.02	1.35	1.31
1	1A	1962	5MC	C6-N1	-2.01	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2x	46	7MG	C5-C6	2.01	1.48	1.43
54	1y	46	7MG	C5-C6	2.01	1.48	1.43

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1l	92	0TD	CSB-SB-CB	-11.03	82.48	102.44
54	1y	46	7MG	N9-C4-N3	9.13	139.12	125.47
54	2y	46	7MG	N9-C4-N3	9.06	139.03	125.47
54	2x	46	7MG	N9-C4-N3	8.86	138.72	125.47
31	1a	527	7MG	N9-C4-N3	8.71	138.50	125.47
31	2a	527	7MG	N9-C4-N3	8.47	138.13	125.47
54	1x	46	7MG	N9-C4-N3	8.36	137.97	125.47
54	2x	8	4SU	C4-N3-C2	-6.94	120.60	127.34
54	1y	8	4SU	C4-N3-C2	-6.76	120.77	127.34
1	2A	2605	PSU	N1-C2-N3	6.69	122.71	115.13
1	1A	2552	2MU	N3-C2-N1	6.49	123.50	114.89
1	2A	1911	PSU	N1-C2-N3	6.44	122.43	115.13
54	2y	8	4SU	C4-N3-C2	-6.40	121.12	127.34
54	1y	39	PSU	N1-C2-N3	6.29	122.26	115.13
54	1x	8	4SU	C1'-N1-C2	6.23	128.85	117.57
54	1y	8	4SU	C5-C4-N3	6.21	120.44	114.69
54	1x	46	7MG	N9-C8-N7	-6.12	94.63	103.38
54	2x	32	PSU	N1-C2-N3	6.06	122.00	115.13
31	2a	1498	UR3	C4-N3-C2	-6.02	118.89	124.56
54	1x	55	PSU	N1-C2-N3	6.02	121.95	115.13
54	1y	55	PSU	N1-C2-N3	5.98	121.91	115.13
1	1A	1917	PSU	N1-C2-N3	5.98	121.91	115.13
54	2x	39	PSU	N1-C2-N3	5.95	121.87	115.13
54	2y	55	PSU	N1-C2-N3	5.95	121.87	115.13
54	1x	39	PSU	N1-C2-N3	5.86	121.77	115.13
54	2y	8	4SU	C5-C4-N3	5.83	120.10	114.69
31	1a	1498	UR3	C4-N3-C2	-5.83	119.07	124.56
54	2x	55	PSU	N1-C2-N3	5.81	121.72	115.13
54	2x	8	4SU	C5-C4-N3	5.80	120.07	114.69
54	1x	32	PSU	N1-C2-N3	5.76	121.65	115.13
31	2a	516	PSU	N1-C2-N3	5.71	121.60	115.13
54	2y	39	PSU	N1-C2-N3	5.68	121.57	115.13
54	1y	46	7MG	C5-C4-N3	-5.66	117.34	128.13
54	2x	46	7MG	C5-C4-N3	-5.65	117.36	128.13
54	1x	54	5MU	C4-N3-C2	-5.64	120.05	127.35
1	1A	2605	PSU	N1-C2-N3	5.62	121.50	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	8	4SU	C4-N3-C2	-5.61	121.89	127.34
1	2A	1917	PSU	N1-C2-N3	5.58	121.45	115.13
54	2y	32	PSU	N1-C2-N3	5.54	121.40	115.13
31	2a	527	7MG	N9-C8-N7	-5.50	95.52	103.38
1	2A	1939	5MU	C4-N3-C2	-5.48	120.26	127.35
54	1x	54	5MU	N3-C2-N1	5.44	122.11	114.89
54	2x	46	7MG	N9-C8-N7	-5.37	95.70	103.38
54	2y	46	7MG	C5-C4-N3	-5.37	117.90	128.13
54	1y	32	PSU	N1-C2-N3	5.36	121.20	115.13
1	1A	1915	5MU	C4-N3-C2	-5.33	120.44	127.35
54	1x	46	7MG	C5-C4-N3	-5.33	117.97	128.13
31	1a	527	7MG	C5-C4-N3	-5.30	118.03	128.13
1	2A	1939	5MU	N3-C2-N1	5.23	121.83	114.89
54	2y	46	7MG	N9-C8-N7	-5.22	95.91	103.38
54	2y	54	5MU	C4-N3-C2	-5.20	120.62	127.35
31	1a	516	PSU	N1-C2-N3	5.17	120.99	115.13
54	1y	54	5MU	C4-N3-C2	-5.16	120.67	127.35
31	1a	527	7MG	N9-C8-N7	-5.14	96.03	103.38
54	1y	46	7MG	N9-C8-N7	-5.14	96.03	103.38
31	2a	527	7MG	C5-C4-N3	-5.08	118.44	128.13
1	2A	1915	5MU	C4-N3-C2	-5.06	120.80	127.35
1	1A	1911	PSU	N1-C2-N3	5.06	120.86	115.13
1	2A	1915	5MU	N3-C2-N1	5.03	121.56	114.89
1	1A	1939	5MU	C4-N3-C2	-5.03	120.84	127.35
54	1y	54	5MU	N3-C2-N1	4.98	121.51	114.89
1	1A	1939	5MU	C5-C6-N1	-4.98	118.21	123.34
1	1A	1915	5MU	N3-C2-N1	4.95	121.46	114.89
1	1A	1939	5MU	N3-C2-N1	4.94	121.45	114.89
54	2y	54	5MU	N3-C2-N1	4.94	121.44	114.89
1	1A	1915	5MU	C5-C4-N3	4.89	119.48	115.31
54	2x	54	5MU	N3-C2-N1	4.73	121.17	114.89
54	2x	54	5MU	C4-N3-C2	-4.72	121.23	127.35
1	2A	2552	2MU	N3-C2-N1	4.67	121.09	114.89
1	2A	2605	PSU	C4-N3-C2	-4.59	119.73	126.34
54	2x	46	7MG	C2-N3-C4	4.58	120.45	112.30
1	1A	2552	2MU	C4-N3-C2	-4.55	120.57	126.58
54	1x	8	4SU	C5-C4-N3	4.51	118.87	114.69
54	1y	46	7MG	C2-N3-C4	4.50	120.31	112.30
54	1y	54	5MU	C5-C4-N3	4.45	119.11	115.31
1	2A	2552	2MU	C4-N3-C2	-4.44	120.73	126.58
54	2y	54	5MU	C5-C4-N3	4.41	119.08	115.31
1	2A	1915	5MU	C5-C4-N3	4.38	119.05	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1939	5MU	C5-C4-N3	4.34	119.01	115.31
1	2A	1939	5MU	C5-C6-N1	-4.29	118.92	123.34
31	1a	527	7MG	C2-N3-C4	4.27	119.91	112.30
54	1x	54	5MU	C5-C4-N3	4.27	118.95	115.31
54	2y	46	7MG	C2-N3-C4	4.24	119.84	112.30
54	1x	46	7MG	C2-N3-C4	4.23	119.83	112.30
54	1x	54	5MU	O4-C4-C5	-4.19	120.05	124.90
54	1y	39	PSU	C4-N3-C2	-4.17	120.33	126.34
54	1x	55	PSU	C4-N3-C2	-4.15	120.35	126.34
1	2A	1911	PSU	O2-C2-N1	-4.11	118.27	122.79
31	2a	527	7MG	C2-N3-C4	4.11	119.61	112.30
54	1x	8	4SU	N3-C2-N1	4.10	120.33	114.89
54	2x	8	4SU	N3-C2-N1	4.06	120.28	114.89
1	1A	1917	PSU	C4-N3-C2	-4.06	120.48	126.34
1	2A	1911	PSU	C4-N3-C2	-4.03	120.53	126.34
1	1A	1915	5MU	O4-C4-C5	-4.03	120.23	124.90
54	2x	54	5MU	C5-C4-N3	4.02	118.74	115.31
1	2A	2605	PSU	O2-C2-N1	-4.00	118.39	122.79
31	1a	1400	5MC	C5-C6-N1	-3.98	119.24	123.34
1	1A	2605	PSU	C4-N3-C2	-3.97	120.62	126.34
54	1y	55	PSU	O2-C2-N1	-3.97	118.42	122.79
54	2x	39	PSU	C4-N3-C2	-3.95	120.64	126.34
54	2y	54	5MU	O4-C4-C5	-3.94	120.34	124.90
54	2y	55	PSU	C4-N3-C2	-3.92	120.69	126.34
1	2A	1939	5MU	O2-C2-N1	-3.90	117.60	122.79
54	2x	55	PSU	C4-N3-C2	-3.89	120.74	126.34
54	1y	55	PSU	C4-N3-C2	-3.88	120.74	126.34
54	2y	8	4SU	N3-C2-N1	3.85	120.00	114.89
54	2x	32	PSU	C4-N3-C2	-3.84	120.81	126.34
1	1A	1915	5MU	C5-C6-N1	-3.83	119.40	123.34
54	2x	32	PSU	O2-C2-N1	-3.82	118.59	122.79
54	1y	8	4SU	N3-C2-N1	3.81	119.95	114.89
54	1x	54	5MU	C5-C6-N1	-3.80	119.42	123.34
31	2a	516	PSU	C4-N3-C2	-3.79	120.87	126.34
54	1y	54	5MU	O4-C4-C5	-3.76	120.55	124.90
54	2y	55	PSU	O2-C2-N1	-3.75	118.67	122.79
54	2y	32	PSU	C4-N3-C2	-3.74	120.94	126.34
54	2x	8	4SU	C5-C4-S4	-3.74	119.65	124.47
54	2y	39	PSU	C4-N3-C2	-3.73	120.96	126.34
1	2A	1915	5MU	O4-C4-C5	-3.73	120.58	124.90
31	1a	516	PSU	C4-N3-C2	-3.71	121.00	126.34
31	2a	1519	MA6	N1-C6-N6	3.69	120.94	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	5MU	C5-C4-N3	3.67	118.44	115.31
1	2A	1939	5MU	O4-C4-C5	-3.65	120.67	124.90
1	1A	1942	5MC	C5-C6-N1	-3.61	119.62	123.34
54	1x	32	PSU	O2-C2-N1	-3.61	118.81	122.79
54	1x	32	PSU	C4-N3-C2	-3.60	121.15	126.34
54	2x	55	PSU	O2-C2-N1	-3.56	118.87	122.79
54	1y	8	4SU	C5-C4-S4	-3.56	119.88	124.47
31	1a	1519	MA6	C4-C5-N7	-3.56	105.69	109.40
54	2x	54	5MU	C5-C6-N1	-3.56	119.68	123.34
31	1a	1404	5MC	C5-C6-N1	-3.55	119.68	123.34
54	2y	37	MIA	N3-C2-N1	-3.53	123.17	128.68
54	2x	54	5MU	O4-C4-C5	-3.52	120.82	124.90
54	2x	39	PSU	C3'-C2'-C1'	3.49	105.70	101.64
31	2a	1518	MA6	C9-N6-C6	-3.48	108.97	119.51
1	1A	2552	2MU	O2-C2-N1	-3.48	118.16	122.79
54	2x	37	MIA	N3-C2-N1	-3.47	123.25	128.68
1	1A	1962	5MC	C5-C6-N1	-3.47	119.77	123.34
1	2A	1917	PSU	O2-C2-N1	-3.46	118.98	122.79
54	1x	39	PSU	C4-N3-C2	-3.46	121.36	126.34
54	1y	39	PSU	O2-C2-N1	-3.45	118.99	122.79
54	1x	8	4SU	C1'-N1-C6	-3.44	113.33	120.84
1	2A	1915	5MU	C5-C6-N1	-3.44	119.80	123.34
1	1A	1939	5MU	O4-C4-C5	-3.43	120.93	124.90
54	2x	39	PSU	O2-C2-N1	-3.41	119.04	122.79
54	1y	32	PSU	C4-N3-C2	-3.39	121.45	126.34
31	1a	1518	MA6	N3-C2-N1	-3.38	123.39	128.68
54	1x	39	PSU	O2-C2-N1	-3.37	119.08	122.79
54	1y	37	MIA	N3-C2-N1	-3.36	123.42	128.68
1	1A	1939	5MU	O2-C2-N1	-3.36	118.32	122.79
54	1x	54	5MU	O2-C2-N1	-3.36	118.32	122.79
31	2a	516	PSU	O2-C2-N1	-3.35	119.10	122.79
1	1A	1911	PSU	C4-N3-C2	-3.32	121.55	126.34
54	2y	54	5MU	C5-C6-N1	-3.31	119.93	123.34
54	1y	54	5MU	C5-C6-N1	-3.31	119.94	123.34
54	1x	8	4SU	C5-C4-S4	-3.30	120.22	124.47
31	1a	1518	MA6	C9-N6-C6	-3.29	109.55	119.51
31	2a	1400	5MC	C5-C6-N1	-3.28	119.97	123.34
1	1A	2605	PSU	C6-C5-C4	-3.20	115.96	118.20
31	2a	1518	MA6	C4-C5-N7	-3.16	106.10	109.40
31	2a	1404	5MC	C5-C6-N1	-3.16	120.09	123.34
54	2x	46	7MG	C5-C6-N1	3.14	116.53	110.99
54	1x	37	MIA	N3-C2-N1	-3.14	123.77	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	55	PSU	O2-C2-N1	-3.12	119.35	122.79
1	1A	1911	PSU	O2-C2-N1	-3.11	119.37	122.79
31	1a	1518	MA6	C4-C5-N7	-3.10	106.17	109.40
31	2a	1519	MA6	C9-N6-C6	-3.08	110.17	119.51
54	2y	32	PSU	O2-C2-N1	-3.07	119.41	122.79
54	2y	8	4SU	C5-C4-S4	-3.06	120.52	124.47
42	2l	92	0TD	CSB-SB-CB	-3.05	96.92	102.44
1	2A	2552	2MU	C5-C4-N3	3.04	119.39	114.84
31	2a	1518	MA6	C10-N6-C6	-3.03	110.33	119.51
31	2a	1519	MA6	C4-C5-N7	-3.03	106.24	109.40
31	1a	967	5MC	C5-C6-N1	-3.03	120.22	123.34
54	2y	39	PSU	O2-C2-N1	-3.01	119.48	122.79
1	1A	2605	PSU	O2-C2-N1	-3.00	119.49	122.79
1	1A	1911	PSU	C6-C5-C4	-2.99	116.10	118.20
54	1y	32	PSU	O2-C2-N1	-2.99	119.50	122.79
31	2a	1518	MA6	N3-C2-N1	-2.99	124.01	128.68
31	1a	1519	MA6	N3-C2-N1	-2.98	124.02	128.68
1	1A	1917	PSU	O2-C2-N1	-2.98	119.51	122.79
31	2a	967	5MC	C5-C6-N1	-2.97	120.28	123.34
1	2A	1962	5MC	C5-C6-N1	-2.96	120.29	123.34
1	2A	2552	2MU	O4-C4-C5	-2.95	119.98	125.16
1	1A	1915	5MU	O2-C2-N1	-2.92	118.90	122.79
54	1x	37	MIA	C4-C5-N7	-2.92	106.36	109.40
1	1A	1920	OMC	C1'-N1-C2	2.92	124.94	118.42
1	2A	1942	5MC	C5-C6-N1	-2.92	120.34	123.34
1	2A	1917	PSU	C4-N3-C2	-2.90	122.16	126.34
31	2a	1518	MA6	N1-C6-N6	2.89	120.10	117.06
54	1y	46	7MG	C5-C6-N1	2.87	116.04	110.99
31	2a	967	5MC	C5-C4-N3	-2.87	118.58	121.67
31	1a	1519	MA6	C9-N6-C6	-2.81	111.00	119.51
42	2l	92	0TD	OD2-CG-CB	2.78	119.16	113.15
54	1x	8	4SU	O2-C2-N3	-2.77	116.34	121.50
31	1a	527	7MG	C5-C6-N1	2.75	115.84	110.99
31	2a	1400	5MC	C5-C4-N3	-2.73	118.73	121.67
31	2a	1407	5MC	C5-C6-N1	-2.70	120.56	123.34
1	1A	2503	2MA	C3'-C2'-C1'	2.70	105.05	100.98
31	1a	516	PSU	O2-C2-N1	-2.70	119.82	122.79
31	1a	1407	5MC	C5-C4-N3	-2.68	118.78	121.67
54	1x	46	7MG	N2-C2-N3	-2.67	114.54	119.73
54	2y	46	7MG	C5-C6-N1	2.66	115.69	110.99
1	1A	1942	5MC	C5-C4-N3	-2.66	118.80	121.67
1	2A	2503	2MA	C5-C6-N1	2.66	118.62	114.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1942	5MC	CM5-C5-C6	-2.66	119.30	122.85
31	2a	1407	5MC	C5-C4-N3	-2.65	118.82	121.67
31	2a	1404	5MC	C5-C4-N3	-2.62	118.85	121.67
31	2a	527	7MG	C5-C6-N1	2.62	115.60	110.99
31	2a	1518	MA6	C10-N6-C9	-2.61	107.72	116.12
54	1x	46	7MG	C5-C6-N1	2.60	115.57	110.99
54	2y	37	MIA	C4-C5-N7	-2.60	106.69	109.40
1	1A	1942	5MC	O2-C2-N3	-2.59	118.12	122.33
54	1x	39	PSU	C6-C5-C4	-2.59	116.39	118.20
42	1l	92	0TD	OD2-CG-CB	2.57	118.70	113.15
1	1A	2251	OMG	C5-C6-N1	2.57	118.48	113.95
31	2a	1519	MA6	C10-N6-C6	-2.56	111.77	119.51
54	1y	37	MIA	C4-C5-N7	-2.54	106.75	109.40
31	1a	1207	2MG	C8-N7-C5	2.54	107.83	102.99
1	2A	2503	2MA	C8-N7-C5	2.53	107.81	102.99
54	2y	46	7MG	C5-C4-N9	-2.53	103.06	106.35
1	2A	2605	PSU	C5-C6-N1	-2.53	118.32	122.11
54	1x	8	4SU	C6-N1-C2	-2.52	117.77	120.99
1	2A	2552	2MU	C2'-C1'-N1	-2.52	109.34	114.22
31	1a	1400	5MC	C5-C4-N3	-2.47	119.00	121.67
1	2A	1942	5MC	C5-C4-N3	-2.46	119.02	121.67
31	1a	516	PSU	C6-C5-C4	-2.46	116.48	118.20
54	2x	37	MIA	C4-C5-N7	-2.44	106.86	109.40
31	1a	1402	4OC	CM4-N4-C4	-2.42	117.72	122.45
31	1a	967	5MC	O2-C2-N3	-2.42	118.39	122.33
31	2a	1519	MA6	N3-C2-N1	-2.41	124.92	128.68
31	1a	1519	MA6	N1-C6-N6	2.40	119.58	117.06
31	1a	967	5MC	C5-C4-N3	-2.40	119.09	121.67
1	1A	1939	5MU	C6-C5-C4	2.37	120.02	118.03
31	2a	1207	2MG	C8-N7-C5	2.37	107.51	102.99
31	1a	1207	2MG	C5-C6-N1	2.36	118.13	113.95
54	1y	54	5MU	C1'-N1-C2	2.36	121.84	117.57
1	1A	2503	2MA	C8-N7-C5	2.33	107.43	102.99
31	1a	1404	5MC	O2-C2-N3	-2.33	118.54	122.33
31	1a	1518	MA6	C10-N6-C9	-2.32	108.64	116.12
31	2a	1207	2MG	C5-C6-N1	2.32	118.05	113.95
54	2x	46	7MG	O6-C6-C5	-2.32	121.86	127.54
31	1a	1498	UR3	C6-N1-C2	-2.32	119.72	121.79
1	1A	1920	OMC	O2-C2-N3	-2.30	118.59	122.33
31	2a	527	7MG	O6-C6-C5	-2.29	121.91	127.54
54	2y	54	5MU	C1'-N1-C2	2.29	121.71	117.57
1	2A	1962	5MC	O2-C2-N3	-2.28	118.63	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	32	PSU	C6-C5-C4	-2.27	116.61	118.20
1	1A	2503	2MA	C5-C6-N1	2.27	117.94	114.02
31	2a	527	7MG	C5-C4-N9	-2.26	103.41	106.35
31	1a	966	M2G	C8-N7-C5	2.26	107.29	102.99
54	1y	46	7MG	O6-C6-C5	-2.25	122.01	127.54
1	2A	1942	5MC	O2-C2-N3	-2.25	118.67	122.33
31	2a	1402	4OC	C6-C5-C4	2.25	119.71	116.96
31	1a	1498	UR3	C3U-N3-C2	2.23	121.23	117.31
31	1a	527	7MG	C5-C4-N9	-2.23	103.45	106.35
31	1a	527	7MG	O6-C6-C5	-2.23	122.08	127.54
31	2a	1404	5MC	CM5-C5-C6	-2.23	119.88	122.85
31	1a	516	PSU	O4'-C1'-C2'	2.22	108.28	105.14
31	1a	966	M2G	C5-C6-N1	2.22	117.88	113.95
1	1A	1917	PSU	O4'-C1'-C2'	2.22	108.27	105.14
1	1A	2251	OMG	C2-N1-C6	-2.21	121.03	125.10
1	1A	1962	5MC	O2-C2-N3	-2.19	118.77	122.33
54	2x	32	PSU	O4'-C1'-C2'	2.18	108.22	105.14
1	2A	1915	5MU	O2-C2-N3	-2.18	117.45	121.50
54	1y	46	7MG	C5-C4-N9	-2.17	103.54	106.35
54	1x	46	7MG	O6-C6-C5	-2.16	122.25	127.54
54	2x	46	7MG	C2-N1-C6	-2.15	121.17	125.10
31	1a	1404	5MC	C5-C4-N3	-2.15	119.35	121.67
1	1A	1920	OMC	N4-C4-N3	2.14	121.73	117.97
1	2A	1962	5MC	C5-C4-N3	-2.13	119.37	121.67
54	2y	46	7MG	O6-C6-C5	-2.13	122.33	127.54
31	1a	527	7MG	CM7-N7-C5	2.12	131.87	126.40
31	2a	967	5MC	C1'-N1-C6	-2.11	117.61	121.12
31	2a	966	M2G	C8-N7-C5	2.11	107.01	102.99
31	1a	1404	5MC	CM5-C5-C6	-2.09	120.05	122.85
1	1A	2251	OMG	CM2-O2'-C2'	-2.08	109.07	114.52
1	2A	2251	OMG	C5-C6-N1	2.07	117.62	113.95
1	2A	2251	OMG	C8-N7-C5	2.07	106.94	102.99
31	2a	1400	5MC	O2-C2-N3	-2.06	118.98	122.33
54	1y	8	4SU	C1'-N1-C2	2.05	121.29	117.57
1	2A	1915	5MU	C1'-N1-C2	2.05	121.28	117.57
31	2a	966	M2G	C5-C6-N1	2.05	117.57	113.95
54	1y	54	5MU	C5M-C5-C4	2.04	121.01	118.77
54	1x	55	PSU	O4'-C1'-C2'	2.04	108.02	105.14
54	2x	46	7MG	CM7-N7-C5	2.04	131.66	126.40
54	1y	39	PSU	C5-C6-N1	-2.03	119.06	122.11
54	2x	55	PSU	C6-C5-C4	-2.03	116.78	118.20
1	2A	1917	PSU	O4'-C1'-C2'	2.02	108.00	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1962	5MC	C5-C4-N3	-2.02	119.50	121.67

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	1l	92	0TD	CA-CB-SB-CSB
42	1l	92	0TD	CG-CB-SB-CSB
1	2A	1917	PSU	C2'-C1'-C5-C4
1	2A	1917	PSU	C2'-C1'-C5-C6
31	2a	527	7MG	C3'-C4'-C5'-O5'
31	2a	1207	2MG	N3-C2-N2-CM2
31	1a	1402	4OC	O4'-C4'-C5'-O5'
31	2a	1402	4OC	O4'-C4'-C5'-O5'
31	1a	1518	MA6	C5-C6-N6-C9
31	1a	1518	MA6	C5-C6-N6-C10
31	1a	1519	MA6	C5-C6-N6-C10
31	2a	1519	MA6	O4'-C4'-C5'-O5'
31	2a	1519	MA6	C3'-C4'-C5'-O5'
54	1x	37	MIA	C3'-C4'-C5'-O5'
54	1y	37	MIA	C3'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	1x	39	PSU	C2'-C1'-C5-C4
54	1x	39	PSU	C2'-C1'-C5-C6
54	2x	39	PSU	C3'-C4'-C5'-O5'
54	1y	46	7MG	C4'-C5'-O5'-P
54	1y	46	7MG	C3'-C4'-C5'-O5'
54	2y	46	7MG	C4'-C5'-O5'-P
54	2y	46	7MG	C3'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C8
54	2x	55	PSU	C2'-C1'-C5-C6
54	2x	55	PSU	O4'-C1'-C5-C6
54	1x	8	4SU	C2'-C1'-N1-C6
54	1x	8	4SU	C2'-C1'-N1-C2
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C3'-C4'-C5'-O5'
31	1a	1402	4OC	C3'-C4'-C5'-O5'
31	2a	1402	4OC	C3'-C4'-C5'-O5'
54	1x	37	MIA	O4'-C4'-C5'-O5'
54	2x	37	MIA	O4'-C4'-C5'-O5'
54	2x	37	MIA	C3'-C4'-C5'-O5'
31	2a	527	7MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	1y	37	MIA	O4'-C4'-C5'-O5'
31	1a	1518	MA6	N1-C6-N6-C9
31	2a	1400	5MC	C2'-C1'-N1-C6
31	1a	1519	MA6	O4'-C4'-C5'-O5'
1	2A	1917	PSU	C3'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
54	2x	37	MIA	C4'-C5'-O5'-P
54	1x	46	7MG	C4'-C5'-O5'-P
31	1a	527	7MG	C3'-C4'-C5'-O5'
54	2x	39	PSU	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C4'-C5'-O5'
54	1x	54	5MU	C3'-C4'-C5'-O5'
1	1A	1915	5MU	C3'-C4'-C5'-O5'
54	2x	8	4SU	O4'-C4'-C5'-O5'
31	2a	1400	5MC	C2'-C1'-N1-C2
31	2a	1400	5MC	O4'-C1'-N1-C6
54	1y	46	7MG	C2'-C1'-N9-C8
1	2A	1917	PSU	O4'-C4'-C5'-O5'
54	2x	8	4SU	C3'-C4'-C5'-O5'
42	2l	92	0TD	CG-CB-SB-CSB
54	1x	54	5MU	O4'-C4'-C5'-O5'
42	2l	92	0TD	SB-CB-CG-OD1
1	2A	2503	2MA	O4'-C4'-C5'-O5'
31	1a	527	7MG	O4'-C4'-C5'-O5'
1	2A	1917	PSU	C4'-C5'-O5'-P
31	2a	1400	5MC	O4'-C1'-N1-C2
31	2a	1518	MA6	C5-C6-N6-C10
31	2a	1519	MA6	C5-C6-N6-C10
54	1y	37	MIA	C4'-C5'-O5'-P
54	2x	46	7MG	C4'-C5'-O5'-P
1	2A	2503	2MA	C4'-C5'-O5'-P
54	2y	37	MIA	C4'-C5'-O5'-P
31	1a	1519	MA6	C3'-C4'-C5'-O5'
54	2x	54	5MU	C3'-C4'-C5'-O5'
54	1x	8	4SU	C3'-C4'-C5'-O5'
31	2a	1519	MA6	C4'-C5'-O5'-P
54	1x	32	PSU	O4'-C1'-C5-C4
54	1x	55	PSU	O4'-C1'-C5-C4
31	2a	967	5MC	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C1'-N9-C8
1	1A	1920	OMC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C4'-C5'-O5'
1	1A	1939	5MU	O4'-C4'-C5'-O5'
54	1x	8	4SU	O4'-C4'-C5'-O5'
1	2A	1911	PSU	O4'-C1'-C5-C6
54	1x	32	PSU	O4'-C1'-C5-C6
42	1l	92	0TD	SB-CB-CG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

Of 2890 ligands modelled in this entry, 2886 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
58	SF4	1d	304	34	0,12,12	-	-	-		
58	SF4	2d	303	34	0,12,12	-	-	-		
59	GDP	1v	704	56	24,30,30	1.00	1 (4%)	30,47,47	1.38	3 (10%)
59	GDP	2v	704	-	24,30,30	0.98	1 (4%)	30,47,47	1.35	4 (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
58	SF4	1d	304	34	-	-	0/6/5/5
58	SF4	2d	303	34	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GDP	1v	704	56	-	0/12/32/32	0/3/3/3
59	GDP	2v	704	-	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1v	704	GDP	C6-N1	-2.48	1.34	1.37
59	2v	704	GDP	C6-N1	-2.34	1.34	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1v	704	GDP	PA-O3A-PB	-4.50	117.38	132.83
59	2v	704	GDP	PA-O3A-PB	-4.37	117.83	132.83
59	1v	704	GDP	C3'-C2'-C1'	3.23	105.84	100.98
59	2v	704	GDP	C3'-C2'-C1'	2.86	105.28	100.98
59	1v	704	GDP	C8-N7-C5	2.48	107.71	102.99
59	2v	704	GDP	C8-N7-C5	2.34	107.45	102.99
59	2v	704	GDP	C5-C6-N1	2.03	117.54	113.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

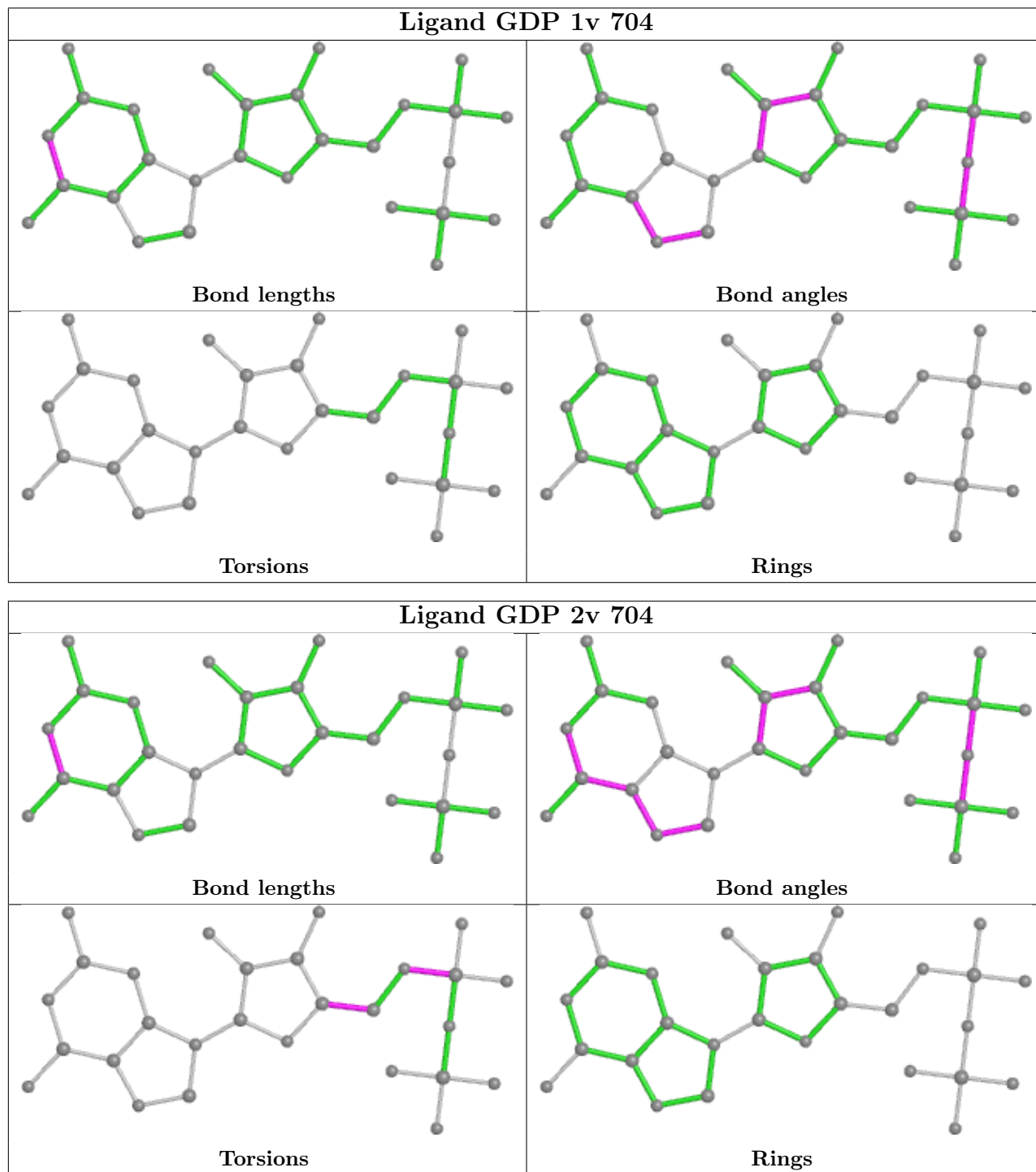
Mol	Chain	Res	Type	Atoms
59	2v	704	GDP	C5'-O5'-PA-O1A
59	2v	704	GDP	O4'-C4'-C5'-O5'
59	2v	704	GDP	C3'-C4'-C5'-O5'
59	2v	704	GDP	C5'-O5'-PA-O3A
59	2v	704	GDP	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

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 i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	0.13	44 (1%) 73 68	54, 75, 190, 283	0
1	2A	2789/2915 (95%)	0.15	130 (4%) 31 28	84, 119, 191, 306	0
2	1B	120/121 (99%)	-0.11	0 100 100	71, 95, 113, 126	0
2	2B	120/121 (99%)	-0.59	1 (0%) 86 81	132, 165, 184, 198	0
3	1D	275/276 (99%)	0.62	17 (6%) 20 18	62, 80, 92, 98	0
3	2D	275/276 (99%)	0.64	31 (11%) 5 6	89, 102, 117, 121	0
4	1E	204/206 (99%)	1.16	60 (29%) 0 0	60, 81, 94, 100	0
4	2E	204/206 (99%)	0.08	7 (3%) 45 40	96, 125, 137, 142	0
5	1F	203/210 (96%)	0.03	8 (3%) 39 35	55, 82, 100, 109	0
5	2F	203/210 (96%)	0.43	16 (7%) 12 13	94, 141, 155, 160	0
6	1G	181/182 (99%)	-0.34	2 (1%) 80 75	105, 135, 158, 175	0
6	2G	181/182 (99%)	1.76	62 (34%) 0 0	175, 205, 219, 227	0
7	1H	174/180 (96%)	-0.18	0 100 100	80, 88, 97, 101	0
7	2H	174/180 (96%)	1.16	38 (21%) 0 0	150, 166, 181, 184	0
8	1N	140/140 (100%)	0.25	4 (2%) 51 45	64, 73, 84, 90	0
8	2N	140/140 (100%)	1.05	26 (18%) 1 1	113, 128, 139, 141	0
9	1O	122/122 (100%)	2.10	65 (53%) 0 0	74, 85, 96, 100	0
9	2O	122/122 (100%)	2.04	60 (49%) 0 0	108, 121, 131, 132	0
10	1P	149/150 (99%)	0.04	4 (2%) 54 48	55, 82, 104, 111	0
10	2P	149/150 (99%)	1.18	39 (26%) 0 0	102, 134, 149, 151	0
11	1Q	141/141 (100%)	0.03	0 100 100	64, 79, 89, 101	0
11	2Q	141/141 (100%)	1.50	45 (31%) 0 0	108, 134, 150, 153	0
12	1R	118/118 (100%)	0.56	4 (3%) 45 40	64, 72, 81, 84	0
12	2R	118/118 (100%)	0.03	2 (1%) 70 64	96, 112, 122, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1S	110/112 (98%)	-0.44	0 100 100	83, 90, 97, 100	0
13	2S	110/112 (98%)	-0.02	2 (1%) 68 62	147, 159, 166, 168	0
14	1T	131/146 (89%)	1.52	47 (35%) 0 0	79, 89, 111, 118	0
14	2T	131/146 (89%)	0.70	22 (16%) 1 2	120, 128, 143, 148	0
15	1U	116/118 (98%)	0.30	2 (1%) 70 64	58, 65, 73, 75	0
15	2U	116/118 (98%)	0.44	7 (6%) 21 19	105, 125, 137, 139	0
16	1V	101/101 (100%)	0.06	1 (0%) 82 77	55, 74, 81, 83	0
16	2V	101/101 (100%)	0.67	12 (11%) 4 5	106, 138, 144, 148	0
17	1W	112/113 (99%)	0.95	8 (7%) 16 15	60, 65, 81, 91	0
17	2W	112/113 (99%)	0.16	0 100 100	88, 99, 107, 117	0
18	1X	95/96 (98%)	0.04	2 (2%) 63 58	71, 76, 84, 88	0
18	2X	95/96 (98%)	-0.44	0 100 100	102, 110, 118, 129	0
19	1Y	107/110 (97%)	-0.15	1 (0%) 84 79	78, 83, 90, 101	0
19	2Y	107/110 (97%)	0.69	12 (11%) 5 6	118, 137, 145, 147	0
20	1Z	204/206 (99%)	-0.22	1 (0%) 91 88	83, 99, 113, 123	0
20	2Z	204/206 (99%)	1.05	41 (20%) 1 1	127, 157, 174, 179	0
21	10	75/85 (88%)	-0.01	1 (1%) 77 71	68, 74, 81, 85	0
21	20	75/85 (88%)	1.34	25 (33%) 0 0	118, 129, 139, 144	0
22	11	97/98 (98%)	0.82	15 (15%) 2 2	67, 82, 107, 111	0
22	21	97/98 (98%)	1.73	41 (42%) 0 0	106, 124, 149, 156	0
23	12	70/72 (97%)	-0.04	0 100 100	82, 87, 97, 104	0
23	22	70/72 (97%)	-0.23	1 (1%) 75 69	119, 132, 140, 141	0
24	13	59/60 (98%)	0.47	2 (3%) 45 40	63, 71, 83, 90	0
24	23	59/60 (98%)	1.08	10 (16%) 1 2	122, 130, 133, 135	0
25	14	69/71 (97%)	-0.77	0 100 100	123, 162, 237, 238	0
25	24	69/71 (97%)	0.80	14 (20%) 1 1	195, 221, 254, 255	0
26	15	59/60 (98%)	0.96	8 (13%) 3 4	57, 73, 77, 79	0
26	25	59/60 (98%)	-0.11	0 100 100	92, 114, 120, 121	0
27	16	53/54 (98%)	0.12	1 (1%) 66 61	74, 80, 83, 85	0
27	26	53/54 (98%)	3.26	40 (75%) 0 0	123, 130, 134, 147	0
28	17	48/49 (97%)	0.70	2 (4%) 36 32	60, 63, 71, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	27	48/49 (97%)	0.31	2 (4%) 36 32	85, 96, 100, 101	0
29	18	64/65 (98%)	0.77	4 (6%) 20 18	63, 70, 76, 78	0
29	28	64/65 (98%)	2.62	39 (60%) 0 0	114, 119, 128, 133	0
30	19	37/37 (100%)	0.01	0 100 100	77, 79, 81, 83	0
30	29	37/37 (100%)	1.11	8 (21%) 0 1	133, 141, 149, 152	0
31	1a	1487/1521 (97%)	-0.04	89 (5%) 21 19	90, 142, 235, 306	0
31	2a	1491/1521 (98%)	0.13	102 (6%) 17 16	117, 163, 259, 294	0
32	1b	231/256 (90%)	0.07	9 (3%) 39 35	157, 172, 189, 196	0
32	2b	231/256 (90%)	0.04	9 (3%) 39 35	185, 199, 223, 234	0
33	1c	206/239 (86%)	3.16	130 (63%) 0 0	185, 200, 218, 220	0
33	2c	206/239 (86%)	2.58	112 (54%) 0 0	216, 231, 246, 248	0
34	1d	208/209 (99%)	0.47	19 (9%) 9 9	137, 149, 154, 155	0
34	2d	208/209 (99%)	0.34	23 (11%) 5 6	140, 164, 167, 169	0
35	1e	148/162 (91%)	0.78	23 (15%) 2 2	127, 141, 148, 153	0
35	2e	148/162 (91%)	1.65	51 (34%) 0 0	157, 171, 185, 190	0
36	1f	100/101 (99%)	0.04	0 100 100	132, 138, 147, 153	0
36	2f	100/101 (99%)	-0.20	0 100 100	143, 148, 155, 160	0
37	1g	155/156 (99%)	2.48	69 (44%) 0 0	175, 205, 212, 215	0
37	2g	155/156 (99%)	5.37	114 (73%) 0 0	201, 227, 234, 238	0
38	1h	137/138 (99%)	0.35	5 (3%) 42 38	125, 138, 147, 157	0
38	2h	137/138 (99%)	0.28	10 (7%) 15 15	153, 163, 173, 185	0
39	1i	127/128 (99%)	1.06	31 (24%) 0 0	182, 221, 226, 229	0
39	2i	127/128 (99%)	1.12	33 (25%) 0 0	213, 246, 251, 252	0
40	1j	97/105 (92%)	2.31	43 (44%) 0 0	199, 222, 226, 227	0
40	2j	96/105 (91%)	0.87	24 (25%) 0 0	229, 244, 251, 252	0
41	1k	114/129 (88%)	1.75	45 (39%) 0 0	116, 144, 150, 157	0
41	2k	114/129 (88%)	2.40	61 (53%) 0 0	134, 161, 170, 176	0
42	1l	121/132 (91%)	0.75	17 (14%) 2 3	116, 130, 138, 140	0
42	2l	121/132 (91%)	2.09	53 (43%) 0 0	144, 153, 162, 166	0
43	1m	118/126 (93%)	0.26	12 (10%) 6 7	201, 226, 227, 229	0
43	2m	122/126 (96%)	1.52	29 (23%) 0 0	222, 242, 245, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1n	60/61 (98%)	2.59	32 (53%) 0 0	207, 215, 227, 228	0
44	2n	60/61 (98%)	2.32	31 (51%) 0 0	234, 239, 249, 250	0
45	1o	88/89 (98%)	-0.30	0 100 100	116, 128, 133, 135	0
45	2o	88/89 (98%)	0.28	5 (5%) 23 21	136, 148, 153, 154	0
46	1p	82/88 (93%)	0.28	5 (6%) 21 19	135, 146, 154, 159	0
46	2p	82/88 (93%)	0.37	2 (2%) 59 53	152, 160, 168, 176	0
47	1q	99/105 (94%)	-0.12	1 (1%) 82 77	116, 125, 131, 134	0
47	2q	99/105 (94%)	2.08	48 (48%) 0 0	138, 151, 155, 156	0
48	1r	68/88 (77%)	0.24	1 (1%) 73 68	133, 139, 143, 147	0
48	2r	68/88 (77%)	0.45	8 (11%) 4 5	147, 154, 159, 160	0
49	1s	83/93 (89%)	0.18	11 (13%) 3 4	213, 234, 238, 239	0
49	2s	83/93 (89%)	1.29	22 (26%) 0 0	235, 252, 255, 255	0
50	1t	96/106 (90%)	-0.01	3 (3%) 49 43	136, 144, 148, 149	0
50	2t	96/106 (90%)	0.11	3 (3%) 49 43	152, 157, 163, 165	0
51	1u	23/27 (85%)	-0.38	0 100 100	217, 220, 226, 227	0
51	2u	23/27 (85%)	0.39	5 (21%) 0 0	239, 242, 244, 244	0
52	1v	728/758 (96%)	0.35	86 (11%) 4 5	30, 144, 211, 217	0
52	2v	728/758 (96%)	1.46	232 (31%) 0 0	30, 197, 259, 264	0
53	1w	185/185 (100%)	0.59	14 (7%) 13 14	87, 118, 158, 166	0
53	2w	185/185 (100%)	3.44	103 (55%) 0 0	123, 157, 206, 217	0
54	1x	67/76 (88%)	2.28	36 (53%) 0 0	91, 195, 204, 206	0
54	1y	67/76 (88%)	1.57	23 (34%) 0 0	74, 212, 238, 247	0
54	2x	67/76 (88%)	10.21	66 (98%) 0 0	124, 232, 243, 245	0
54	2y	67/76 (88%)	4.02	53 (79%) 0 0	118, 252, 277, 282	0
55	1z	10/21 (47%)	3.36	9 (90%) 0 0	150, 157, 164, 164	0
55	2z	10/21 (47%)	2.57	3 (30%) 0 0	181, 185, 203, 204	0
All	All	22334/23178 (96%)	0.60	2951 (13%) 3 4	30, 134, 241, 306	0

All (2951) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	2g	91	VAL	20.4
37	2g	85	TYR	18.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	2x	62	C	18.2
37	2g	84	ASN	18.2
52	2v	501	THR	17.2
54	2x	48	C	17.1
37	2g	86	GLN	16.9
37	2g	78	ARG	16.8
37	2g	83	ALA	16.4
43	2m	123	ALA	16.3
37	2g	90	GLU	16.3
53	2w	32	ARG	16.1
40	1j	62	HIS	15.9
37	2g	89	MET	15.7
37	2g	76	ARG	15.6
37	2g	74	GLU	15.4
1	2A	2140	C	15.4
43	2m	119	GLY	15.3
54	2x	49	C	15.1
37	2g	77	SER	14.9
54	2x	22	G	14.7
54	2x	61	C	14.7
54	2x	72	C	14.7
43	2m	120	LYS	14.6
37	2g	152	ALA	14.5
54	2x	59	U	14.5
49	2s	84	GLY	14.5
43	2m	124	PRO	14.5
54	2x	44	G	14.4
54	2x	69	G	14.4
54	2x	21	A	14.3
54	2x	47	U	14.0
54	2x	19	G	14.0
52	2v	413	ILE	13.9
54	2x	12	U	13.9
54	2x	13	C	13.6
54	2x	7	A	13.6
54	2x	70	G	13.5
54	2x	11	C	13.3
37	2g	148	ASN	13.2
37	2g	153	HIS	13.1
54	2x	3	C	13.1
37	2g	156	TRP	12.9
54	2x	64	A	12.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	2x	74	C	12.9
54	2x	65	G	12.9
54	2x	5	G	12.7
54	2x	57	G	12.7
33	1c	156	ARG	12.6
54	2x	71	G	12.6
52	1v	502	GLY	12.5
31	2a	1030(B)	C	12.5
37	2g	82	GLY	12.5
37	2g	88	PRO	12.4
37	1g	74	GLU	12.2
54	2x	20	U	12.2
54	2y	62	C	12.2
54	2x	27	G	12.1
33	2c	79	ARG	12.1
54	2x	56	C	12.0
54	2y	61	C	12.0
37	1g	77	SER	11.9
39	2i	56	LEU	11.8
53	2w	45	TYR	11.8
53	2w	40	HIS	11.7
54	2x	63	G	11.7
54	2x	52	G	11.7
54	2x	24	G	11.6
53	2w	71	TRP	11.5
37	2g	144	MET	11.2
37	2g	71	PRO	11.2
37	1g	85	TYR	11.2
37	2g	72	ARG	11.0
40	1j	47	PHE	11.0
53	2w	70	SER	10.9
20	2Z	204	GLU	10.8
52	2v	414	GLU	10.7
54	2x	58	A	10.6
54	2x	51	U	10.4
53	2w	41	LEU	10.3
37	2g	70	LYS	10.3
37	2g	87	VAL	10.3
37	2g	81	GLY	10.3
54	2x	28	G	10.3
39	1i	121	ARG	10.2
54	2x	75	C	10.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
53	2w	93	SER	10.1
33	2c	81	GLY	10.1
52	1v	501	THR	10.1
43	2m	122	LYS	10.1
53	2w	44	GLU	10.1
37	2g	73	MET	10.1
37	2g	145	ALA	10.0
52	2v	471	LYS	10.0
54	2x	43	C	10.0
37	2g	149	ARG	10.0
53	2w	74	ASN	9.9
33	1c	190	ARG	9.9
37	1g	78	ARG	9.9
33	1c	155	GLY	9.9
52	2v	454	MET	9.9
52	2v	500	GLN	9.9
54	2x	50	U	9.9
54	2y	1	G	9.8
40	2j	47	PHE	9.8
52	2v	442	THR	9.8
1	2A	2132	U	9.7
53	2w	100	TYR	9.7
53	2w	72	ASP	9.7
54	2x	73	A	9.7
27	26	54	ILE	9.7
33	2c	103	VAL	9.7
54	2x	6	G	9.6
37	2g	75	VAL	9.6
1	2A	2139	C	9.6
42	2l	68	ALA	9.6
22	2l	2	SER	9.6
54	2x	9	A	9.6
54	2x	23	A	9.6
33	2c	80	GLY	9.6
37	2g	101	LEU	9.5
54	2x	45	U	9.5
54	2x	53	G	9.5
37	2g	139	GLU	9.4
37	1g	144	MET	9.4
37	2g	155	ARG	9.4
54	2x	1	G	9.4
6	2G	87	PRO	9.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
37	2g	154	TYR	9.3
55	2z	21	A	9.3
53	2w	87	ASP	9.3
53	2w	73	GLN	9.2
53	2w	97	ASP	9.2
53	2w	43	VAL	9.2
1	2A	2153	G	9.2
54	2x	60	U	9.1
1	2A	2154	G	9.1
37	2g	80	VAL	9.1
37	1g	153	HIS	9.0
52	2v	453	GLY	9.0
40	1j	60	ARG	9.0
37	2g	151	TYR	8.9
53	2w	46	TYR	8.9
53	2w	90	LEU	8.9
33	1c	161	GLU	8.9
37	2g	103	TRP	8.9
6	2G	88	ILE	8.8
33	2c	78	GLY	8.7
1	2A	888	C	8.7
35	2e	9	LYS	8.6
52	2v	452	SER	8.6
6	2G	138	GLN	8.6
37	2g	54	THR	8.6
54	2x	66	U	8.5
20	2Z	203	GLU	8.5
37	1g	86	GLN	8.5
43	2m	118	ALA	8.4
39	1i	128	ARG	8.4
54	2x	18	G	8.4
43	2m	121	LYS	8.4
44	1n	34	TYR	8.4
1	2A	2152	G	8.4
53	2w	38	LEU	8.4
54	2x	76	A	8.3
37	2g	137	LYS	8.3
52	2v	427	ALA	8.3
53	2w	99	LEU	8.3
53	2w	58	VAL	8.2
6	2G	41	GLN	8.2
52	2v	522	GLY	8.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	2c	76	VAL	8.2
52	2v	597	GLY	8.2
37	2g	104	LEU	8.2
40	1j	61	GLU	8.2
54	2y	6	G	8.2
52	2v	467	LYS	8.1
52	2v	598	ASP	8.0
37	2g	97	GLN	8.0
43	2m	94	ARG	8.0
40	1j	96	ILE	8.0
1	2A	2141	G	8.0
37	1g	76	ARG	8.0
47	2q	24	GLU	8.0
52	2v	477	GLY	7.9
52	2v	578	SER	7.9
27	26	25	LYS	7.9
52	2v	472	VAL	7.9
37	1g	73	MET	7.8
49	2s	81	ARG	7.8
54	2x	68	C	7.8
40	2j	61	GLU	7.8
33	1c	66	VAL	7.8
1	2A	2156	G	7.7
33	1c	157	ILE	7.7
37	1g	82	GLY	7.7
33	2c	188	LEU	7.7
52	2v	466	LEU	7.7
37	2g	79	ARG	7.7
52	2v	456	GLU	7.6
43	2m	117	VAL	7.6
54	1x	44	G	7.6
53	2w	83	ILE	7.6
52	2v	475	ASN	7.6
53	2w	42	LYS	7.6
53	2w	102	ASN	7.6
25	24	54	GLY	7.5
54	2x	4	C	7.5
41	2k	49	GLY	7.5
7	2H	24	VAL	7.5
52	2v	426	GLN	7.5
37	2g	96	GLN	7.5
53	2w	56	ALA	7.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
37	2g	69	VAL	7.5
33	1c	131	ARG	7.4
33	2c	71	ALA	7.4
35	2e	10	MET	7.4
54	2x	2	C	7.4
33	1c	59	ARG	7.4
20	2Z	201	LYS	7.4
54	2x	25	C	7.4
53	2w	91	ASN	7.3
52	2v	561	VAL	7.3
40	1j	63	PHE	7.3
52	2v	609	GLU	7.3
33	2c	72	LYS	7.2
33	2c	89	GLU	7.2
54	2x	29	G	7.2
7	2H	25	LYS	7.2
54	2x	10	G	7.2
37	2g	140	ASP	7.2
37	1g	156	TRP	7.2
52	2v	687	LEU	7.1
37	1g	89	MET	7.1
53	2w	89	GLY	7.1
1	2A	2115	G	7.1
53	2w	86	SER	7.1
37	2g	146	GLU	7.1
53	2w	1	MET	7.1
42	2l	94	PRO	7.1
33	2c	86	VAL	7.1
37	2g	141	VAL	7.0
22	11	2	SER	7.0
52	2v	656	ALA	7.0
54	2x	67	C	7.0
37	1g	84	ASN	7.0
29	28	12	LYS	7.0
39	1i	127	LYS	7.0
54	2y	63	G	7.0
33	1c	58	GLU	7.0
35	2e	8	GLU	7.0
41	2k	77	MET	7.0
41	2k	16	SER	6.9
47	2q	9	VAL	6.9
54	2x	26	A	6.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	2x	36	A	6.9
52	2v	595	GLN	6.9
33	1c	201	TYR	6.9
52	2v	441	SER	6.9
37	1g	88	PRO	6.9
52	2v	556	ILE	6.9
53	2w	98	ALA	6.9
6	2G	155	MET	6.9
1	2A	2146	C	6.9
27	26	23	THR	6.9
52	2v	428	LEU	6.8
54	2x	38	A	6.8
47	2q	59	ILE	6.8
37	2g	129	GLU	6.8
42	2l	67	THR	6.8
33	1c	56	ASP	6.8
52	2v	488	THR	6.8
44	2n	44	LEU	6.8
52	2v	409	ILE	6.8
33	2c	44	GLU	6.7
52	2v	502	GLY	6.7
33	1c	103	VAL	6.7
1	2A	2131	G	6.7
52	1v	503	GLY	6.7
52	2v	653	PHE	6.7
37	2g	16	LEU	6.7
20	2Z	191	VAL	6.7
6	2G	81	LYS	6.7
37	2g	142	GLU	6.7
42	2l	33	ARG	6.7
6	2G	45	GLU	6.6
52	2v	567	LEU	6.6
33	2c	45	LYS	6.6
37	2g	68	ASN	6.6
53	2w	47	GLY	6.6
27	26	53	LYS	6.6
52	2v	412	ALA	6.6
33	1c	170	GLN	6.6
54	2y	41	C	6.6
53	2w	96	GLY	6.6
33	1c	164	ARG	6.6
37	1g	90	GLU	6.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	2v	469	GLU	6.6
54	2y	5	G	6.6
37	2g	132	GLY	6.6
33	1c	57	ILE	6.6
33	1c	55	VAL	6.6
53	2w	146	GLU	6.6
54	2x	15	G	6.6
53	2w	69	GLN	6.6
54	2y	3	C	6.6
40	1j	46	ARG	6.5
52	2v	594	VAL	6.5
33	1c	54	ARG	6.5
52	2v	670	VAL	6.5
53	2w	39	LEU	6.5
54	2y	64	A	6.5
6	2G	135	LEU	6.5
52	2v	444	PRO	6.5
53	2w	55	ILE	6.5
47	2q	23	VAL	6.5
52	2v	417	THR	6.5
47	2q	25	ARG	6.5
54	2y	18	G	6.5
6	2G	72	ARG	6.4
6	2G	43	LEU	6.4
33	2c	75	VAL	6.4
30	29	15	LYS	6.4
33	1c	162	GLN	6.4
33	2c	85	ARG	6.4
6	2G	157	ILE	6.4
20	2Z	79	ARG	6.4
44	2n	26	ARG	6.4
53	2w	143	LEU	6.4
1	2A	2138	C	6.4
52	2v	474	ALA	6.4
53	2w	79	ILE	6.4
37	1g	142	GLU	6.3
40	1j	53	PRO	6.3
53	2w	76	LEU	6.3
52	1v	417	THR	6.3
53	2w	101	ILE	6.3
35	2e	120	THR	6.3
37	2g	26	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
10	2P	50	ARG	6.3
33	1c	191	THR	6.3
40	2j	63	PHE	6.3
52	2v	455	GLY	6.3
33	1c	130	VAL	6.3
37	1g	154	TYR	6.3
33	1c	154	SER	6.3
39	1i	122	ALA	6.2
1	2A	2175	C	6.2
25	24	8	LYS	6.2
16	2V	1	MET	6.2
37	1g	75	VAL	6.2
37	2g	130	GLY	6.2
37	2g	58	PRO	6.2
49	2s	59	PRO	6.1
1	2A	2157	G	6.1
1	2A	2155	G	6.1
29	28	4	MET	6.1
33	2c	77	ILE	6.1
33	1c	189	ALA	6.1
44	2n	58	LYS	6.1
37	2g	143	ARG	6.1
37	2g	133	GLY	6.1
37	1g	79	ARG	6.1
52	2v	599	PRO	6.1
9	2O	1	MET	6.0
33	2c	87	LEU	6.0
52	2v	548	GLU	6.0
52	2v	425	SER	6.0
52	2v	503	GLY	6.0
1	1A	2141	G	6.0
52	2v	465	ARG	6.0
41	1k	88	GLY	6.0
44	1n	58	LYS	6.0
53	2w	57	THR	6.0
33	1c	4	LYS	6.0
27	26	27	LYS	6.0
41	2k	13	GLN	6.0
52	2v	580	MET	6.0
52	2v	612	THR	6.0
39	2i	57	GLY	5.9
39	2i	115	GLY	5.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	1v	512	ILE	5.9
20	2Z	78	LYS	5.9
52	2v	496	LYS	5.9
34	2d	168	ARG	5.9
33	1c	68	VAL	5.9
52	2v	632	LEU	5.9
29	28	13	ARG	5.9
40	2j	56	HIS	5.9
54	2x	14	A	5.9
33	1c	166	GLU	5.9
37	2g	93	PRO	5.9
8	2N	140	VAL	5.9
33	2c	90	GLU	5.8
39	2i	52	ALA	5.8
44	1n	26	ARG	5.8
53	2w	92	PRO	5.8
52	2v	415	PRO	5.8
54	2y	60	U	5.8
53	2w	33	ALA	5.8
33	1c	183	ASP	5.8
33	1c	160	ALA	5.8
37	2g	138	LYS	5.8
38	2h	129	VAL	5.8
1	2A	2151	G	5.8
54	2y	4	C	5.8
54	2y	65	G	5.8
37	1g	83	ALA	5.7
52	2v	430	ARG	5.7
33	2c	49	SER	5.7
33	2c	28	GLN	5.7
52	2v	610	VAL	5.7
37	2g	61	VAL	5.7
47	2q	100	LYS	5.7
31	1a	1030(B)	C	5.7
6	2G	86	MET	5.7
53	2w	110	ARG	5.7
37	1g	148	ASN	5.7
33	1c	52	LEU	5.7
52	1v	505	GLY	5.7
47	2q	26	GLN	5.7
41	2k	14	VAL	5.7
37	2g	150	ALA	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
39	1i	116	LYS	5.6
41	2k	90	GLY	5.6
33	2c	82	GLU	5.6
37	1g	101	LEU	5.6
33	1c	85	ARG	5.6
51	2u	2	GLY	5.6
52	1v	510	VAL	5.6
33	1c	159	GLY	5.6
33	2c	156	ARG	5.6
1	2A	2106	G	5.6
52	2v	585	ALA	5.6
1	2A	2133	G	5.6
10	2P	76	LYS	5.6
52	2v	449	THR	5.6
33	1c	65	ALA	5.6
44	2n	22	THR	5.6
54	1y	47	U	5.6
52	2v	630	GLN	5.6
52	2v	554	PRO	5.6
41	1k	89	ALA	5.6
52	2v	489	LYS	5.6
52	2v	576	ASP	5.6
53	2w	85	ASP	5.6
1	2A	2104	G	5.5
33	1c	127	ARG	5.5
40	1j	48	THR	5.5
49	1s	82	GLY	5.5
53	2w	113	ASP	5.5
37	1g	141	VAL	5.5
43	1m	94	ARG	5.5
35	2e	89	ILE	5.5
1	2A	2105	C	5.5
37	2g	65	ALA	5.5
52	1v	499	ARG	5.5
54	2y	53	G	5.5
35	2e	118	ILE	5.5
52	2v	525	PHE	5.5
41	2k	15	ALA	5.5
14	2T	39	ARG	5.5
41	2k	98	LEU	5.5
52	2v	665	GLY	5.5
6	2G	90	LEU	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
27	26	26	ASN	5.5
54	2y	42	C	5.5
43	2m	116	THR	5.4
41	1k	50	TYR	5.4
31	2a	1030(A)	G	5.4
33	1c	165	THR	5.4
42	2l	18	VAL	5.4
43	2m	110	ARG	5.4
52	2v	544	LYS	5.4
40	1j	59	SER	5.4
10	2P	46	LYS	5.4
33	2c	41	GLY	5.4
37	2g	136	LYS	5.4
31	1a	901	A	5.4
6	2G	39	ILE	5.4
33	1c	15	THR	5.4
9	1O	41	ALA	5.4
33	1c	105	GLU	5.4
22	2l	36	GLY	5.4
41	2k	79	SER	5.4
33	1c	138	VAL	5.4
33	1c	153	VAL	5.4
33	1c	195	VAL	5.4
53	2w	34	ASN	5.4
33	1c	67	THR	5.4
52	2v	589	ALA	5.4
42	2l	66	VAL	5.4
54	2y	72	C	5.4
29	28	10	ALA	5.3
41	2k	17	GLY	5.3
22	2l	38	SER	5.3
52	2v	543	GLN	5.3
33	2c	91	LEU	5.3
35	2e	109	ILE	5.3
52	1v	594	VAL	5.3
9	2O	84	ALA	5.3
37	2g	134	ALA	5.3
53	2w	52	LEU	5.3
1	2A	2145	C	5.3
52	1v	509	HIS	5.3
53	2w	37	LEU	5.3
52	2v	642	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
52	2v	510	VAL	5.3
52	2v	635	GLU	5.3
37	1g	18	TYR	5.3
31	2a	956	U	5.3
40	1j	72	VAL	5.3
37	2g	100	ALA	5.3
33	1c	102	ASN	5.3
54	1x	24	G	5.3
52	2v	499	ARG	5.3
22	2l	66	HIS	5.3
1	1A	2152	G	5.3
54	2y	15	G	5.3
54	2y	27	G	5.3
44	1n	37	PHE	5.3
10	2P	59	LEU	5.2
52	2v	673	PHE	5.2
21	10	10	THR	5.2
52	2v	408	VAL	5.2
39	2i	51	ARG	5.2
10	2P	108	LYS	5.2
1	2A	887	A	5.2
32	1b	233	SER	5.2
35	2e	88	LYS	5.2
9	2O	20	MET	5.2
33	2c	37	GLN	5.2
37	1g	69	VAL	5.2
5	2F	87	GLY	5.2
43	2m	113	PRO	5.2
35	2e	130	ASN	5.2
55	2z	19	U	5.1
42	2l	23	LYS	5.1
42	2l	56	ALA	5.1
10	2P	72	PRO	5.1
54	2y	19	G	5.1
20	2Z	200	GLY	5.1
53	2w	109	GLU	5.1
9	2O	101	PRO	5.1
43	1m	118	ALA	5.1
55	1z	19	U	5.1
53	2w	95	LYS	5.1
37	2g	24	THR	5.1
1	2A	229	A	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2129	C	5.1
33	1c	101	LEU	5.1
1	1A	2602	A	5.1
37	1g	143	ARG	5.1
54	2y	40	C	5.1
1	2A	2119	A	5.1
33	2c	31	HIS	5.1
33	1c	7	PRO	5.1
37	1g	72	ARG	5.1
33	2c	189	ALA	5.1
40	1j	50	ILE	5.1
39	2i	53	VAL	5.1
44	1n	25	VAL	5.1
33	1c	158	GLY	5.1
33	2c	84	ILE	5.1
42	2l	14	GLY	5.1
6	2G	73	ALA	5.0
7	2H	89	ILE	5.0
52	1v	413	ILE	5.0
40	1j	8	LEU	5.0
42	2l	22	SER	5.0
33	2c	55	VAL	5.0
54	2y	7	A	5.0
54	1x	1	G	5.0
35	2e	81	GLU	5.0
55	2z	20	A	5.0
9	2O	22	ILE	5.0
1	2A	2174	C	5.0
47	2q	71	PHE	5.0
40	2j	46	ARG	5.0
33	2c	68	VAL	5.0
53	2w	50	VAL	5.0
37	2g	99	LEU	5.0
37	2g	123	GLU	5.0
33	1c	8	ILE	5.0
37	1g	145	ALA	5.0
41	2k	97	ALA	5.0
52	2v	562	ASP	5.0
6	2G	52	ILE	5.0
33	1c	150	LYS	5.0
31	1a	1030(C)	G	5.0
14	1T	45	PHE	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
27	26	28	ARG	5.0
54	2y	43	C	5.0
52	1v	506	GLN	5.0
49	2s	82	GLY	5.0
52	2v	463	VAL	5.0
31	2a	1488	G	5.0
54	1x	74	C	5.0
33	2c	66	VAL	4.9
33	2c	74	GLY	4.9
40	1j	64	GLU	4.9
44	1n	49	HIS	4.9
9	2O	64	ARG	4.9
37	1g	97	GLN	4.9
47	2q	58	GLU	4.9
27	26	52	VAL	4.9
53	2w	153	GLU	4.9
37	1g	100	ALA	4.9
22	11	22	GLY	4.9
37	1g	87	VAL	4.9
53	2w	48	ALA	4.9
6	2G	74	LYS	4.9
54	2y	2	C	4.9
33	1c	75	VAL	4.9
52	1v	87	HIS	4.9
33	1c	202	ILE	4.9
24	13	60	GLU	4.9
44	1n	30	ALA	4.9
53	2w	78	ALA	4.9
17	1W	112	GLY	4.9
37	1g	149	ARG	4.9
54	2y	44	G	4.9
8	2N	16	ILE	4.9
4	1E	143	ASN	4.9
31	1a	1397	C	4.9
54	2x	42	C	4.9
48	2r	22	VAL	4.9
53	2w	82	ALA	4.8
14	1T	46	GLU	4.8
33	2c	101	LEU	4.8
22	21	6	GLU	4.8
37	2g	126	ASP	4.8
1	2A	2107	C	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	1913	A	4.8
1	1A	2132	U	4.8
44	1n	29	ARG	4.8
41	2k	36	ASP	4.8
54	1y	13	C	4.8
55	1z	21	A	4.8
53	2w	59	THR	4.8
33	1c	53	ALA	4.8
53	2w	63	PRO	4.8
6	2G	152	LEU	4.8
20	2Z	23	LYS	4.8
27	26	34	LEU	4.8
6	2G	80	PHE	4.8
37	2g	53	LYS	4.8
52	2v	464	ASP	4.8
22	21	37	ILE	4.8
54	2y	73	A	4.8
40	1j	49	VAL	4.8
40	1j	58	ASP	4.8
47	2q	21	VAL	4.8
1	1A	2151	G	4.8
14	2T	46	GLU	4.8
33	1c	129	ALA	4.8
37	2g	147	ALA	4.8
39	1i	110	GLU	4.8
49	2s	61	TYR	4.7
1	2A	2117	A	4.7
45	2o	89	GLY	4.7
52	2v	470	PHE	4.7
33	2c	39	ILE	4.7
33	2c	131	ARG	4.7
37	2g	18	TYR	4.7
49	1s	81	ARG	4.7
6	2G	159	VAL	4.7
52	2v	542	VAL	4.7
11	2Q	17	LEU	4.7
47	2q	43	LEU	4.7
6	2G	134	GLY	4.7
27	26	8	LYS	4.7
29	28	9	GLY	4.7
49	2s	58	VAL	4.7
52	1v	524	GLU	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2123	G	4.7
6	2G	144	ILE	4.7
14	1T	84	GLN	4.7
33	1c	128	PHE	4.7
27	26	50	ARG	4.7
33	2c	88	ARG	4.7
52	2v	650	ALA	4.7
53	2w	88	LEU	4.7
24	23	60	GLU	4.7
37	2g	10	ARG	4.7
44	1n	39	LEU	4.7
14	2T	45	PHE	4.7
35	2e	106	PRO	4.7
54	2x	33	U	4.7
21	20	10	THR	4.7
54	1y	44	G	4.7
37	1g	99	LEU	4.7
6	2G	82	LEU	4.6
9	1O	120	GLU	4.6
52	2v	457	LEU	4.6
52	2v	689	LYS	4.6
20	2Z	5	LEU	4.6
37	2g	20	ASP	4.6
42	2l	20	LYS	4.6
37	2g	64	GLN	4.6
47	2q	98	LEU	4.6
6	2G	147	ASP	4.6
29	28	29	LYS	4.6
22	21	27	GLU	4.6
7	2H	26	VAL	4.6
27	26	22	ALA	4.6
37	2g	57	GLU	4.6
7	2H	105	LEU	4.6
10	2P	45	LEU	4.6
37	2g	17	VAL	4.6
52	2v	579	GLU	4.6
7	2H	162	ILE	4.6
33	1c	39	ILE	4.6
33	1c	142	MET	4.6
39	2i	95	LYS	4.6
42	1l	89	ARG	4.6
52	2v	547	GLU	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	2G	83	ARG	4.6
9	2O	102	VAL	4.6
10	2P	149	GLU	4.6
52	2v	93	GLU	4.6
29	28	61	LEU	4.6
3	2D	5	LYS	4.6
52	1v	523	PHE	4.6
54	2x	30	G	4.6
44	1n	55	GLY	4.6
31	1a	935	A	4.6
52	2v	592	GLU	4.6
33	1c	188	LEU	4.6
6	2G	63	ILE	4.6
37	2g	21	VAL	4.6
39	1i	115	GLY	4.6
37	2g	27	ILE	4.5
22	11	23	LYS	4.5
39	2i	54	ASP	4.5
29	28	3	LYS	4.5
52	1v	471	LYS	4.5
9	1O	26	LYS	4.5
15	2U	72	HIS	4.5
41	2k	40	ILE	4.5
41	1k	51	LYS	4.5
11	2Q	97	VAL	4.5
37	2g	105	VAL	4.5
42	2l	31	PRO	4.5
31	1a	1035	A	4.5
53	2w	81	LYS	4.5
43	2m	93	ARG	4.5
49	1s	83	HIS	4.5
9	2O	83	ALA	4.5
54	2y	49	C	4.5
26	15	60	VAL	4.5
1	2A	1118	C	4.5
7	2H	33	LEU	4.5
22	21	22	GLY	4.5
37	2g	62	PHE	4.5
37	1g	146	GLU	4.5
42	2l	93	LEU	4.5
52	2v	484	ARG	4.5
6	2G	47	LYS	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
41	2k	50	TYR	4.5
47	2q	22	LEU	4.5
4	1E	142	GLY	4.5
43	2m	111	LYS	4.5
33	2c	157	ILE	4.5
6	2G	141	PHE	4.5
9	1O	59	LYS	4.5
37	2g	131	LYS	4.5
34	2d	68	TYR	4.4
33	1c	5	ILE	4.4
47	2q	38	ARG	4.4
1	2A	2179	C	4.4
1	2A	2185	C	4.4
33	1c	28	GLN	4.4
33	1c	38	ARG	4.4
39	1i	125	TYR	4.4
3	2D	231	HIS	4.4
34	2d	102	ASP	4.4
33	2c	155	GLY	4.4
54	1y	14	A	4.4
19	2Y	64	GLU	4.4
37	1g	134	ALA	4.4
4	2E	126	PRO	4.4
37	1g	155	ARG	4.4
44	1n	35	ARG	4.4
47	2q	37	LYS	4.4
27	26	20	ASN	4.4
1	2A	2142	C	4.4
40	1j	89	ASP	4.4
41	2k	99	GLN	4.4
6	2G	75	LYS	4.4
11	2Q	98	LYS	4.4
22	2I	25	LYS	4.4
37	2g	29	LYS	4.4
7	2H	169	VAL	4.4
33	1c	64	VAL	4.4
37	1g	91	VAL	4.4
41	2k	35	PRO	4.4
39	1i	95	LYS	4.4
52	1v	-50	GLN	4.4
11	2Q	10	ARG	4.4
33	1c	199	LYS	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
53	2w	53	ASN	4.4
47	2q	36	ILE	4.4
52	1v	487	ILE	4.4
52	2v	669	PHE	4.4
41	2k	92	GLU	4.4
44	2n	25	VAL	4.4
39	1i	111	ARG	4.4
22	2l	16	ASN	4.4
40	1j	44	VAL	4.4
53	2w	35	PRO	4.4
54	2y	67	C	4.4
42	2l	26	ALA	4.4
52	2v	429	ALA	4.4
10	2P	60	MET	4.4
52	2v	590	ILE	4.4
33	1c	76	VAL	4.4
54	1x	76	A	4.4
10	2P	51	PHE	4.4
31	1a	1056	U	4.4
35	2e	91	LEU	4.4
42	2l	95	GLY	4.4
33	2c	64	VAL	4.4
52	1v	89	ASP	4.4
1	2A	2181	G	4.4
54	2y	57	G	4.4
54	2y	58	A	4.3
1	2A	1924	C	4.3
52	2v	591	LYS	4.3
1	1A	2153	G	4.3
31	2a	1030(C)	G	4.3
52	2v	649	LEU	4.3
33	2c	164	ARG	4.3
35	1e	18	ARG	4.3
31	2a	1349	A	4.3
9	2O	65	THR	4.3
49	2s	49	ILE	4.3
6	2G	142	PRO	4.3
24	23	2	PRO	4.3
33	2c	152	ILE	4.3
47	2q	7	THR	4.3
1	2A	1914	C	4.3
39	2i	103	THR	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	1j	10	GLY	4.3
52	2v	584	ILE	4.3
42	2l	16	GLU	4.3
37	1g	140	ASP	4.3
33	1c	89	GLU	4.3
40	1j	97	GLU	4.3
33	1c	91	LEU	4.3
42	2l	21	LYS	4.3
52	2v	583	LYS	4.3
52	2v	636	PRO	4.3
53	2w	94	ASN	4.3
1	2A	1925	C	4.3
31	1a	1384	C	4.3
3	2D	276	LYS	4.3
47	2q	42	TYR	4.3
10	2P	67	MET	4.3
31	2a	957	U	4.3
52	1v	563	ILE	4.3
43	1m	119	GLY	4.3
21	20	70	GLN	4.2
7	2H	103	LEU	4.2
6	2G	145	THR	4.2
42	2l	65	GLU	4.2
33	1c	167	TRP	4.2
27	26	5	VAL	4.2
54	2x	31	A	4.2
49	2s	56	GLN	4.2
54	2y	74	C	4.2
14	2T	50	ILE	4.2
40	2j	62	HIS	4.2
52	2v	573	HIS	4.2
55	1z	13	A	4.2
55	1z	20	A	4.2
33	1c	104	GLN	4.2
33	2c	40	ARG	4.2
33	1c	99	VAL	4.2
7	2H	17	VAL	4.2
53	2w	68	VAL	4.2
37	2g	28	ASN	4.2
54	2y	75	C	4.2
41	2k	91	ARG	4.2
37	1g	71	PRO	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
41	2k	32	ILE	4.2
33	2c	83	ARG	4.2
31	1a	1209	C	4.2
33	1c	163	ALA	4.2
6	2G	62	LEU	4.2
14	1T	85	LYS	4.2
10	2P	47	ASP	4.2
42	2l	15	ARG	4.2
52	2v	528	ALA	4.2
54	1x	13	C	4.2
54	1y	12	U	4.2
6	2G	44	GLY	4.2
31	2a	1168	A	4.2
54	1x	15	G	4.2
49	1s	56	GLN	4.2
41	1k	31	THR	4.2
27	26	24	GLU	4.2
29	28	8	LYS	4.2
52	2v	686	LYS	4.2
35	1e	24	ARG	4.2
31	1a	1050	G	4.1
9	2O	45	GLU	4.1
33	2c	73	PRO	4.1
14	2T	67	SER	4.1
6	2G	70	VAL	4.1
52	2v	604	PRO	4.1
54	1x	22	G	4.1
14	1T	22	PHE	4.1
8	2N	51	PHE	4.1
35	1e	25	ARG	4.1
54	2y	47	U	4.1
27	26	2	ALA	4.1
52	1v	476	VAL	4.1
50	2t	9	ASN	4.1
24	23	53	LEU	4.1
27	26	9	LEU	4.1
41	1k	87	THR	4.1
52	1v	-32	LEU	4.1
52	2v	683	VAL	4.1
54	1x	75	C	4.1
9	1O	17	ARG	4.1
33	2c	153	VAL	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
41	2k	104	GLN	4.1
53	2w	5	GLU	4.1
1	2A	2112	G	4.1
31	1a	811	C	4.1
4	1E	157	ALA	4.1
35	2e	104	ALA	4.1
53	2w	138	ASP	4.1
6	2G	84	LYS	4.1
29	28	14	VAL	4.1
34	1d	181	MET	4.1
35	2e	33	VAL	4.1
44	1n	50	LYS	4.1
11	2Q	40	ALA	4.1
1	2A	2113	U	4.1
31	2a	955	U	4.1
34	1d	7	PRO	4.1
8	2N	52	VAL	4.1
44	2n	45	ARG	4.1
11	2Q	75	THR	4.1
44	1n	61	TRP	4.1
54	2y	26	A	4.1
35	2e	75	THR	4.1
10	2P	68	GLN	4.0
14	1T	29	ARG	4.0
37	1g	138	LYS	4.0
9	2O	41	ALA	4.0
35	2e	108	ALA	4.0
41	2k	101	SER	4.0
53	2w	49	HIS	4.0
52	2v	476	VAL	4.0
31	2a	1203	C	4.0
37	1g	151	TYR	4.0
35	2e	6	PHE	4.0
41	1k	13	GLN	4.0
22	21	39	LYS	4.0
29	28	26	LYS	4.0
37	2g	22	LEU	4.0
49	1s	59	PRO	4.0
41	2k	94	ALA	4.0
31	1a	1028	C	4.0
33	1c	49	SER	4.0
35	2e	76	ILE	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
49	2s	47	HIS	4.0
53	2w	80	GLU	4.0
44	1n	36	PHE	4.0
1	2A	2159	G	4.0
27	26	6	ARG	4.0
33	1c	141	VAL	4.0
37	1g	80	VAL	4.0
52	2v	684	GLN	4.0
53	2w	147	LEU	4.0
44	2n	54	PRO	4.0
40	1j	71	LEU	4.0
54	1y	23	A	4.0
54	1y	20	U	4.0
1	2A	2186	G	4.0
53	2w	84	ARG	4.0
9	2O	5	GLN	4.0
37	1g	131	LYS	4.0
37	1g	135	VAL	4.0
53	2w	114	LEU	4.0
33	2c	63	ASN	4.0
33	2c	108	ASN	4.0
4	1E	158	GLY	4.0
31	2a	890	G	4.0
27	26	4	GLU	4.0
33	2c	104	GLN	4.0
31	1a	1045	C	4.0
35	2e	87	SER	4.0
9	2O	9	GLU	4.0
37	2g	128	ALA	4.0
4	1E	6	GLY	4.0
33	2c	102	ASN	4.0
1	2A	2184	G	3.9
16	2V	53	GLU	3.9
41	2k	19	ALA	4.0
31	1a	1049	U	3.9
41	2k	78	GLN	3.9
37	2g	135	VAL	3.9
31	1a	1044	A	3.9
43	2m	95	GLY	3.9
29	28	11	LYS	3.9
42	2l	91	LYS	3.9
52	2v	678	GLU	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	1y	27	G	3.9
41	1k	90	GLY	3.9
51	2u	3	LYS	3.9
31	2a	1028	C	3.9
42	2l	64	TYR	3.9
29	28	25	MET	3.9
1	2A	2147	G	3.9
7	2H	36	PRO	3.9
9	1O	68	GLU	3.9
9	2O	33	ALA	3.9
33	1c	29	TYR	3.9
42	1l	64	TYR	3.9
52	2v	655	TYR	3.9
52	2v	681	LYS	3.9
14	1T	86	ILE	3.9
54	1x	72	C	3.9
31	2a	1517	G	3.9
6	2G	64	THR	3.9
37	2g	23	VAL	3.9
33	1c	193	TYR	3.9
33	2c	54	ARG	3.9
7	2H	35	VAL	3.9
33	1c	196	LEU	3.9
44	2n	11	LYS	3.9
10	2P	49	ARG	3.9
31	2a	787	A	3.9
6	2G	146	TYR	3.9
48	2r	87	ARG	3.9
39	2i	94	ALA	3.9
52	2v	421	GLN	3.9
9	1O	95	GLY	3.9
25	24	31	ILE	3.9
34	1d	110	PHE	3.9
6	2G	40	ASN	3.9
52	2v	495	GLY	3.9
54	1x	11	C	3.9
6	1G	87	PRO	3.9
9	1O	19	ILE	3.9
1	2A	2585	U	3.9
40	2j	64	GLU	3.9
31	1a	1202	G	3.9
42	2l	24	VAL	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	2v	555	LEU	3.9
4	1E	115	GLY	3.8
33	1c	184	TYR	3.8
53	2w	30	THR	3.8
44	1n	2	ALA	3.8
54	1y	24	G	3.8
29	28	2	PRO	3.8
7	2H	130	ARG	3.8
22	11	21	ARG	3.8
29	28	7	HIS	3.8
4	2E	124	GLY	3.8
27	26	7	ILE	3.8
52	2v	459	LEU	3.8
22	21	60	PHE	3.8
33	2c	65	ALA	3.8
40	1j	66	ARG	3.8
1	2A	2143	C	3.8
54	2y	52	G	3.8
37	1g	16	LEU	3.8
52	1v	565	VAL	3.8
9	2O	42	SER	3.8
47	2q	99	SER	3.8
11	2Q	6	ARG	3.8
41	2k	54	ARG	3.8
29	28	50	LEU	3.8
38	2h	112	LEU	3.8
52	2v	624	LEU	3.8
54	2y	20	U	3.8
33	2c	207	VAL	3.8
44	1n	44	LEU	3.8
6	2G	133	LEU	3.8
10	2P	62	LEU	3.8
35	2e	128	PRO	3.8
10	2P	79	ARG	3.8
44	2n	2	ALA	3.8
33	1c	32	LEU	3.8
31	2a	1029	C	3.8
40	1j	73	ASP	3.8
7	2H	104	GLU	3.8
52	1v	489	LYS	3.8
53	2w	139	LYS	3.8
7	2H	90	LYS	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	2v	524	GLU	3.8
9	2O	15	GLY	3.8
17	1W	92	ARG	3.8
4	1E	124	GLY	3.8
14	1T	38	ASN	3.8
10	2P	77	ARG	3.8
37	2g	67	GLU	3.8
1	2A	384	U	3.8
20	2Z	7	ALA	3.8
35	2e	122	GLU	3.8
37	2g	66	VAL	3.7
52	1v	470	PHE	3.7
31	2a	1257	U	3.7
7	2H	82	GLY	3.7
14	1T	47	GLY	3.7
52	2v	526	VAL	3.7
52	2v	574	GLU	3.7
43	2m	6	GLY	3.7
20	2Z	80	ARG	3.7
33	2c	120	VAL	3.7
47	2q	11	VAL	3.7
33	2c	21	ARG	3.7
47	2q	74	LEU	3.7
9	2O	46	ALA	3.7
33	2c	60	ALA	3.7
39	2i	15	ALA	3.7
35	2e	121	LYS	3.7
9	1O	63	VAL	3.7
42	1l	98	TYR	3.7
3	2D	226	MET	3.7
4	1E	151	TYR	3.7
22	21	28	GLY	3.7
52	2v	577	SER	3.7
1	2A	2158	A	3.7
10	2P	64	LYS	3.7
33	2c	56	ASP	3.7
1	1A	2140	C	3.7
39	2i	7	THR	3.7
42	2l	19	ARG	3.7
52	2v	676	TYR	3.7
9	1O	22	ILE	3.7
33	1c	168	ALA	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
44	1n	17	LYS	3.7
19	2Y	42	VAL	3.7
44	1n	31	ARG	3.7
52	2v	407	PRO	3.7
31	2a	912	C	3.7
33	1c	144	SER	3.7
44	2n	50	LYS	3.7
37	1g	150	ALA	3.7
54	2y	24	G	3.7
39	1i	81	ILE	3.7
9	1O	5	GLN	3.7
42	1l	26	ALA	3.7
27	26	51	GLU	3.7
40	1j	95	GLU	3.7
52	1v	468	ARG	3.7
54	1x	25	C	3.7
1	2A	250	G	3.7
54	2y	28	G	3.7
3	1D	2	ALA	3.7
44	2n	10	ALA	3.7
37	1g	132	GLY	3.7
4	1E	138	PRO	3.7
50	1t	55	ILE	3.7
33	1c	198	VAL	3.7
11	2Q	104	PHE	3.7
31	1a	1383	C	3.7
33	1c	200	ALA	3.7
39	2i	121	ARG	3.7
52	2v	523	PHE	3.7
52	2v	634	MET	3.6
5	2F	131	GLY	3.6
37	1g	96	GLN	3.6
33	1c	98	ASN	3.6
42	2l	57	LYS	3.6
49	2s	63	THR	3.6
33	1c	126	ARG	3.6
52	2v	416	LYS	3.6
39	2i	58	HIS	3.6
9	1O	21	CYS	3.6
49	2s	29	ARG	3.6
39	2i	93	ARG	3.6
54	1x	70	G	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	2v	566	THR	3.6
8	1N	83	LYS	3.6
14	1T	105	LEU	3.6
52	2v	575	VAL	3.6
1	2A	2180	U	3.6
1	2A	2602	A	3.6
31	1a	1043	C	3.6
53	2w	54	GLN	3.6
9	1O	82	ASN	3.6
49	2s	60	VAL	3.6
52	1v	514	VAL	3.6
9	1O	1	MET	3.6
37	2g	8	GLU	3.6
37	2g	92	SER	3.6
52	2v	611	THR	3.6
20	2Z	6	LYS	3.6
26	15	2	ALA	3.6
37	2g	25	ALA	3.6
33	2c	38	ARG	3.6
40	1j	70	ARG	3.6
22	21	30	VAL	3.6
33	2c	158	GLY	3.6
33	1c	87	LEU	3.6
40	1j	11	PHE	3.6
52	2v	420	ASP	3.6
52	2v	652	MET	3.6
8	2N	53	VAL	3.6
52	2v	447	GLY	3.6
31	1a	1195	C	3.6
52	1v	504	ARG	3.6
41	2k	80	VAL	3.6
52	2v	478	LYS	3.6
52	2v	521	SER	3.6
37	2g	127	ALA	3.6
53	2w	75	ALA	3.6
39	1i	7	THR	3.6
52	2v	490	PRO	3.6
37	2g	11	GLN	3.6
44	2n	20	ALA	3.6
33	1c	6	HIS	3.6
37	2g	98	SER	3.6
49	2s	83	HIS	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2110	G	3.6
43	2m	114	ARG	3.6
50	1t	9	ASN	3.6
8	2N	128	HIS	3.6
52	2v	571	SER	3.6
43	2m	7	VAL	3.6
33	2c	13	GLY	3.6
40	1j	65	LEU	3.6
52	2v	473	ASP	3.6
5	1F	69	HIS	3.5
9	1O	18	LYS	3.5
52	1v	571	SER	3.5
54	2y	68	C	3.5
52	2v	514	VAL	3.5
9	1O	64	ARG	3.5
34	2d	164	ALA	3.5
37	1g	127	ALA	3.5
8	2N	8	GLN	3.5
26	15	59	GLU	3.5
33	1c	33	LEU	3.5
52	1v	426	GLN	3.5
1	2A	2286	A	3.5
29	28	30	ARG	3.5
42	2l	71	PRO	3.5
52	1v	-28	ALA	3.5
42	2l	98	TYR	3.5
47	2q	60	ILE	3.5
29	28	62	LEU	3.5
35	2e	119	LEU	3.5
52	1v	527	ASN	3.5
20	2Z	202	GLU	3.5
22	21	21	ARG	3.5
33	1c	44	GLU	3.5
54	1y	6	G	3.5
7	2H	88	LEU	3.5
17	1W	94	ASP	3.5
37	2g	12	LEU	3.5
8	2N	12	ARG	3.5
33	1c	151	VAL	3.5
37	2g	59	LEU	3.5
9	1O	104	ARG	3.5
15	2U	88	ILE	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
29	28	47	LYS	3.5
41	1k	25	TYR	3.5
53	1w	29	ARG	3.5
6	2G	85	GLY	3.5
52	2v	461	ILE	3.5
37	1g	139	GLU	3.5
40	1j	4	ILE	3.5
11	2Q	1	MET	3.5
39	2i	128	ARG	3.5
31	1a	1203	C	3.5
8	2N	15	LEU	3.5
4	1E	125	GLY	3.5
14	2T	62	THR	3.5
32	1b	148	TYR	3.5
16	2V	5	VAL	3.5
27	26	10	LEU	3.5
31	1a	1194	U	3.5
14	1T	32	TYR	3.5
29	28	44	LYS	3.5
33	2c	199	LYS	3.5
44	1n	33	VAL	3.5
44	1n	41	ARG	3.5
6	2G	89	GLY	3.5
35	2e	24	ARG	3.5
49	2s	30	LEU	3.5
54	1x	26	A	3.5
14	1T	43	GLN	3.5
52	1v	-47	ASP	3.5
9	2O	120	GLU	3.5
9	1O	107	ARG	3.5
37	1g	104	LEU	3.5
52	2v	644	ARG	3.5
1	2A	382	G	3.5
4	1E	123	ALA	3.5
54	1x	34	G	3.5
9	2O	38	VAL	3.5
33	2c	48	TYR	3.5
33	2c	201	TYR	3.5
49	1s	76	PRO	3.4
33	1c	37	GLN	3.4
4	1E	153	GLY	3.4
33	1c	69	HIS	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	2c	109	PRO	3.4
33	2c	151	VAL	3.4
39	1i	113	LYS	3.4
40	1j	52	GLY	3.4
35	2e	11	ILE	3.4
47	2q	68	ARG	3.4
29	28	51	ALA	3.4
22	2l	47	GLN	3.4
35	1e	14	ARG	3.4
42	2l	78	GLN	3.4
31	2a	913	A	3.4
1	2A	886	C	3.4
42	2l	25	PRO	3.4
52	2v	540	PRO	3.4
3	2D	230	ASP	3.4
52	2v	593	ALA	3.4
7	2H	18	GLU	3.4
1	1A	2062	A	3.4
9	2O	3	GLN	3.4
11	2Q	12	GLN	3.4
37	2g	50	ILE	3.4
1	2A	1922	G	3.4
1	2A	2188	C	3.4
31	1a	1512	U	3.4
3	2D	166	GLN	3.4
33	1c	152	ILE	3.4
39	1i	77	ILE	3.4
4	1E	155	LYS	3.4
41	2k	71	LYS	3.4
22	2l	17	SER	3.4
41	1k	42	TRP	3.4
31	2a	996	A	3.4
54	1x	40	C	3.4
54	1x	45	U	3.4
41	2k	57	THR	3.4
52	1v	-64	VAL	3.4
33	2c	22	TRP	3.4
9	1O	122	LEU	3.4
21	20	21	LEU	3.4
1	2A	226	G	3.4
22	2l	33	LYS	3.4
6	2G	46	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
6	2G	79	ASN	3.4
41	2k	52	GLY	3.4
20	2Z	176	PRO	3.4
25	24	11	PRO	3.4
37	2g	56	GLN	3.4
42	2l	83	VAL	3.4
53	2w	77	LYS	3.4
8	2N	54	VAL	3.4
43	2m	90	LEU	3.4
44	2n	52	GLN	3.4
52	2v	483	TYR	3.4
1	2A	2284	C	3.4
10	2P	111	ARG	3.4
40	2j	55	LYS	3.4
14	1T	109	GLU	3.4
43	2m	87	TYR	3.4
35	2e	15	ARG	3.4
22	2l	34	THR	3.4
52	2v	560	VAL	3.4
4	1E	154	LYS	3.4
35	2e	31	LEU	3.4
42	2l	13	LYS	3.4
52	2v	462	ILE	3.4
33	1c	79	ARG	3.4
52	2v	637	ARG	3.4
10	2P	109	GLY	3.3
22	1l	36	GLY	3.3
52	2v	468	ARG	3.3
14	1T	83	ILE	3.3
27	26	21	TYR	3.3
46	1p	4	ILE	3.3
14	1T	87	ASP	3.3
10	2P	44	GLY	3.3
44	2n	41	ARG	3.3
20	2Z	55	HIS	3.3
47	1q	100	LYS	3.3
31	1a	1214	C	3.3
6	2G	102	PHE	3.3
9	2O	14	THR	3.3
35	2e	29	GLY	3.3
53	2w	31	GLY	3.3
42	2l	52	LEU	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	21	10	LYS	3.3
26	15	3	LYS	3.3
31	2a	250	A	3.3
33	2c	70	VAL	3.3
9	2O	56	ASP	3.3
31	2a	84	U	3.3
37	2g	122	HIS	3.3
41	2k	43	SER	3.3
37	2g	94	ARG	3.3
40	1j	5	ARG	3.3
11	2Q	33	GLY	3.3
37	1g	81	GLY	3.3
37	2g	102	ARG	3.3
6	2G	131	TYR	3.3
11	2Q	25	ASP	3.3
33	1c	9	GLY	3.3
1	2A	1039	G	3.3
29	28	46	ARG	3.3
52	2v	588	MET	3.3
7	2H	168	PRO	3.3
48	2r	84	LYS	3.3
52	2v	613	PRO	3.3
4	1E	137	HIS	3.3
41	2k	118	GLY	3.3
1	2A	245	G	3.3
9	1O	86	ILE	3.3
4	1E	140	SER	3.3
41	2k	41	THR	3.3
17	1W	90	ARG	3.3
30	29	12	ASP	3.3
35	2e	77	PRO	3.3
35	2e	129	ILE	3.3
37	1g	17	VAL	3.3
53	2w	105	PRO	3.3
22	11	34	THR	3.3
29	28	65	GLU	3.3
33	2c	27	LYS	3.3
41	2k	96	ARG	3.3
1	2A	251	A	3.3
4	1E	129	HIS	3.3
17	1W	111	HIS	3.3
31	2a	1378	C	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	1c	204	LEU	3.3
33	2c	93	LYS	3.3
11	2Q	90	VAL	3.3
41	1k	30	VAL	3.3
21	20	76	GLY	3.2
41	2k	51	LYS	3.2
6	2G	78	SER	3.2
41	1k	32	ILE	3.2
1	1A	2586	C	3.2
33	2c	67	THR	3.2
9	2O	60	ALA	3.2
10	2P	39	LYS	3.2
22	21	40	ARG	3.2
44	1n	59	ALA	3.2
52	1v	599	PRO	3.2
53	2w	29	ARG	3.2
32	2b	197	VAL	3.2
1	2A	2144	U	3.2
9	2O	39	ILE	3.2
53	2w	156	ARG	3.2
6	2G	148	MET	3.2
41	2k	110	ASP	3.2
3	1D	184	LYS	3.2
37	2g	124	LEU	3.2
37	2g	95	ARG	3.2
44	1n	32	SER	3.2
22	21	64	ALA	3.2
52	2v	627	ARG	3.2
53	1w	46	TYR	3.2
33	1c	35	GLU	3.2
52	2v	181	LEU	3.2
6	2G	54	GLU	3.2
29	28	43	GLN	3.2
35	2e	45	PHE	3.2
37	2g	14	PRO	3.2
22	11	33	LYS	3.2
47	2q	40	LYS	3.2
52	2v	144	ALA	3.2
14	1T	76	PHE	3.2
31	2a	1350	A	3.2
41	2k	108	ILE	3.2
44	2n	3	ARG	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	1E	18	ASP	3.2
52	1v	569	ASP	3.2
52	2v	347	GLY	3.2
4	1E	141	ILE	3.2
41	1k	29	ILE	3.2
44	2n	7	ILE	3.2
54	2y	51	U	3.2
34	1d	115	ARG	3.2
52	2v	559	PRO	3.2
1	2A	2176	A	3.2
11	2Q	89	ASN	3.2
11	2Q	93	TYR	3.2
33	2c	25	GLY	3.2
10	2P	75	ILE	3.2
34	1d	5	ILE	3.2
42	2l	77	LEU	3.2
31	1a	1029	C	3.2
54	1y	3	C	3.2
21	20	31	VAL	3.2
9	1O	20	MET	3.2
9	2O	100	GLY	3.2
11	2Q	108	GLY	3.2
9	2O	97	ARG	3.2
52	2v	643	ILE	3.2
31	2a	941	G	3.2
53	2w	154	THR	3.2
5	2F	154	VAL	3.2
33	1c	71	ALA	3.2
30	29	26	ILE	3.2
31	2a	571	U	3.2
34	2d	49	ARG	3.2
40	1j	51	ARG	3.2
12	1R	5	LYS	3.2
53	2w	107	THR	3.2
7	2H	159	GLU	3.2
20	2Z	155	LEU	3.2
33	1c	77	ILE	3.2
29	28	24	ALA	3.2
37	1g	66	VAL	3.2
55	1z	16	U	3.2
5	1F	72	ARG	3.2
8	2N	117	PHE	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	1c	169	ALA	3.2
52	2v	536	LYS	3.2
25	24	27	THR	3.2
42	2l	99	HIS	3.2
53	2w	160	GLU	3.2
1	2A	246	C	3.2
25	24	66	SER	3.2
31	2a	562	C	3.2
3	2D	223	GLY	3.2
9	2O	17	ARG	3.2
35	1e	40	ARG	3.2
41	2k	62	GLN	3.1
11	2Q	19	GLY	3.1
1	2A	2182	G	3.1
27	26	35	GLU	3.1
31	2a	998	G	3.1
11	2Q	130	LYS	3.1
22	11	20	ARG	3.1
33	1c	50	ALA	3.1
26	15	7	PRO	3.1
39	1i	99	LEU	3.1
52	2v	516	PRO	3.1
4	1E	159	HIS	3.1
14	1T	28	VAL	3.1
44	1n	18	VAL	3.1
54	2y	66	U	3.1
33	1c	192	THR	3.1
52	1v	-29	LEU	3.1
31	2a	887	G	3.1
22	21	23	LYS	3.1
9	2O	57	VAL	3.1
40	1j	92	THR	3.1
44	2n	35	ARG	3.1
31	2a	1035	A	3.1
9	2O	10	VAL	3.1
16	2V	64	HIS	3.1
7	2H	27	LYS	3.1
34	2d	165	MET	3.1
9	1O	40	VAL	3.1
40	1j	54	PHE	3.1
27	26	3	SER	3.1
40	2j	49	VAL	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
44	1n	27	CYS	3.1
35	2e	21	ALA	3.1
55	1z	15	A	3.1
41	2k	31	THR	3.1
52	2v	617	MET	3.1
31	2a	4	U	3.1
33	1c	2	GLY	3.1
33	1c	19	GLU	3.1
34	2d	163	GLU	3.1
52	2v	641	GLN	3.1
41	1k	98	LEU	3.1
38	2h	86	ILE	3.1
46	1p	36	ILE	3.1
33	1c	70	VAL	3.1
9	1O	3	GLN	3.1
31	1a	1342	C	3.1
31	1a	1359	C	3.1
42	2l	49	ASN	3.1
52	2v	581	ALA	3.1
54	2y	71	G	3.1
15	2U	108	GLU	3.1
44	1n	3	ARG	3.1
37	1g	137	LYS	3.1
4	1E	122	PHE	3.1
4	1E	187	ALA	3.1
2	2B	91	C	3.1
54	2x	40	C	3.1
20	2Z	76	LEU	3.1
31	1a	1057	G	3.1
11	2Q	38	GLU	3.1
1	1A	888	C	3.1
31	2a	788	U	3.1
40	1j	6	ILE	3.1
14	2T	70	VAL	3.1
49	2s	79	THR	3.1
41	1k	49	GLY	3.1
52	1v	-46	VAL	3.1
52	2v	432	ALA	3.1
31	1a	898	G	3.1
9	1O	84	ALA	3.1
9	1O	96	THR	3.1
35	2e	105	VAL	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	1E	128	SER	3.1
25	24	30	GLU	3.1
31	1a	1205	U	3.1
53	1w	71	TRP	3.1
14	1T	30	VAL	3.1
27	26	17	LYS	3.1
9	1O	54	GLU	3.1
10	2P	58	THR	3.1
31	2a	959	A	3.1
41	1k	43	SER	3.1
9	2O	86	ILE	3.1
9	2O	16	ALA	3.0
52	2v	504	ARG	3.0
53	2w	157	ALA	3.0
55	1z	17	U	3.0
33	2c	110	ASN	3.0
52	2v	437	THR	3.0
49	1s	49	ILE	3.0
52	1v	541	ALA	3.0
9	1O	45	GLU	3.0
53	2w	66	LEU	3.0
54	1x	38	A	3.0
27	26	18	ARG	3.0
47	2q	27	PHE	3.0
14	1T	33	LYS	3.0
47	2q	95	TYR	3.0
10	2P	73	GLY	3.0
33	2c	107	GLN	3.0
12	2R	69	ASP	3.0
39	2i	28	VAL	3.0
41	2k	81	ASP	3.0
33	2c	182	ILE	3.0
1	2A	2137	C	3.0
31	2a	1209	C	3.0
52	2v	440	VAL	3.0
20	2Z	192	ALA	3.0
37	1g	98	SER	3.0
8	2N	138	LEU	3.0
41	2k	76	GLY	3.0
11	2Q	39	PRO	3.0
1	2A	1912	A	3.0
11	2Q	131	ILE	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	1a	1055	A	3.0
33	1c	20	SER	3.0
39	1i	19	LEU	3.0
21	20	17	GLN	3.0
52	1v	560	VAL	3.0
5	1F	70	THR	3.0
19	2Y	59	GLY	3.0
31	2a	793	U	3.0
25	24	14	ILE	3.0
31	2a	938	A	3.0
33	1c	82	GLU	3.0
35	1e	89	ILE	3.0
54	1y	7	A	3.0
39	1i	123	PRO	3.0
3	2D	2	ALA	3.0
6	2G	34	LEU	3.0
52	2v	451	ILE	3.0
1	2A	1032	A	3.0
3	1D	222	ARG	3.0
14	1T	64	ARG	3.0
34	1d	144	ASP	3.0
54	2x	35	A	3.0
29	28	36	LYS	3.0
52	2v	513	LYS	3.0
1	2A	2103	C	3.0
31	1a	1385	G	3.0
31	1a	1511	G	3.0
21	20	46	LYS	3.0
33	2c	130	VAL	3.0
1	2A	227	A	3.0
19	2Y	83	THR	3.0
31	1a	974	A	3.0
31	2a	1227	A	3.0
33	2c	43	LEU	3.0
47	2q	32	TYR	3.0
42	2l	89	ARG	3.0
9	2O	2	ILE	3.0
1	2A	2124	G	3.0
31	1a	769	G	3.0
10	2P	63	PRO	3.0
20	2Z	22	GLY	3.0
34	2d	3	ARG	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	2c	57	ILE	3.0
43	2m	4	ILE	3.0
5	2F	77	ASP	3.0
8	2N	17	ASP	3.0
52	2v	443	HIS	3.0
52	2v	671	MET	3.0
27	26	33	LYS	3.0
32	2b	196	LEU	3.0
35	2e	113	ALA	3.0
49	1s	79	THR	3.0
49	2s	48	THR	3.0
52	1v	429	ALA	3.0
52	1v	511	LYS	3.0
1	2A	1119	C	3.0
24	23	34	GLU	3.0
1	1A	275	G	3.0
41	1k	126	ARG	3.0
45	2o	88	ARG	3.0
29	28	27	THR	3.0
41	1k	47	VAL	3.0
41	2k	82	VAL	3.0
54	1y	26	A	3.0
1	2A	2109	U	3.0
33	1c	10	PHE	3.0
33	1c	21	ARG	3.0
1	1A	2551	C	2.9
31	2a	1403	C	2.9
47	2q	12	SER	2.9
40	1j	98	ILE	2.9
49	2s	62	ILE	2.9
53	2w	103	ILE	2.9
1	2A	242	G	2.9
1	2A	2125	G	2.9
40	2j	65	LEU	2.9
52	2v	418	LYS	2.9
4	1E	121	ASN	2.9
47	2q	94	ASN	2.9
3	1D	230	ASP	2.9
4	1E	194	GLY	2.9
33	1c	146	ALA	2.9
1	2A	2130	U	2.9
14	1T	1	MET	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	2Z	194	PRO	2.9
22	21	44	PRO	2.9
41	2k	106	LYS	2.9
1	2A	252	G	2.9
31	2a	1489	G	2.9
1	2A	383	U	2.9
21	20	79	VAL	2.9
9	1O	2	ILE	2.9
9	1O	44	LYS	2.9
42	1l	28	LYS	2.9
14	1T	21	GLU	2.9
52	2v	680	PRO	2.9
48	2r	56	THR	2.9
22	21	15	ALA	2.9
37	2g	2	ALA	2.9
52	2v	419	ALA	2.9
42	2l	102	ARG	2.9
54	1x	59	U	2.9
54	2y	69	G	2.9
34	2d	93	PHE	2.9
39	2i	49	PRO	2.9
22	21	63	ALA	2.9
29	28	45	GLY	2.9
35	2e	86	ALA	2.9
31	1a	934	C	2.9
31	2a	121	C	2.9
41	2k	93	GLN	2.9
37	1g	61	VAL	2.9
42	1l	25	PRO	2.9
31	1a	965	A	2.9
35	1e	17	ALA	2.9
1	2A	2121	G	2.9
33	2c	32	LEU	2.9
39	1i	120	ARG	2.9
47	2q	6	LEU	2.9
3	1D	181	GLU	2.9
52	2v	422	GLU	2.9
54	2y	22	G	2.9
52	2v	587	SER	2.9
4	1E	131	ALA	2.9
54	1y	40	C	2.9
11	2Q	48	GLU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	2E	127	ASP	2.9
27	26	29	ASN	2.9
11	2Q	50	ALA	2.9
1	2A	1907	G	2.9
22	2I	26	ARG	2.9
33	2c	183	ASP	2.9
43	2m	112	GLY	2.9
42	2l	32	PHE	2.9
8	2N	14	VAL	2.9
37	2g	9	VAL	2.9
47	2q	73	VAL	2.9
52	1v	-65	LYS	2.9
3	2D	174	ILE	2.9
22	2I	7	ILE	2.9
20	2Z	107	THR	2.9
44	1n	56	VAL	2.9
54	1x	31	A	2.9
38	2h	100	ILE	2.9
44	2n	23	ARG	2.9
31	2a	888	G	2.9
52	2v	361	ASN	2.9
1	1A	790	C	2.9
38	2h	99	GLU	2.9
52	2v	608	VAL	2.9
54	1y	45	U	2.9
1	2A	255	A	2.9
11	2Q	99	PRO	2.9
3	1D	226	MET	2.9
52	2v	445	GLU	2.9
40	2j	67	THR	2.9
9	2O	95	GLY	2.9
43	2m	5	ALA	2.9
52	2v	505	GLY	2.9
52	2v	300	GLU	2.9
37	2g	120	ILE	2.9
6	2G	42	GLY	2.9
42	1l	68	ALA	2.9
42	2l	53	ARG	2.9
31	2a	786	G	2.9
37	1g	147	ALA	2.9
52	2v	520	GLY	2.8
41	2k	109	VAL	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	1v	414	GLU	2.8
10	2P	70	GLN	2.8
52	2v	438	PHE	2.8
51	2u	4	GLY	2.8
5	2F	175	THR	2.8
54	2y	12	U	2.8
22	11	27	GLU	2.8
27	26	11	LEU	2.8
31	1a	1048	G	2.8
54	1y	43	C	2.8
42	2l	30	ALA	2.8
31	2a	696	A	2.8
20	2Z	193	GLU	2.8
4	1E	15	PHE	2.8
14	2T	99	LEU	2.8
31	2a	1427	U	2.8
42	1l	99	HIS	2.8
33	1c	181	ASN	2.8
54	1x	62	C	2.8
1	1A	748	G	2.8
54	1x	10	G	2.8
1	2A	2134	A	2.8
33	2c	146	ALA	2.8
33	1c	132	ARG	2.8
9	2O	21	CYS	2.8
34	2d	4	TYR	2.8
31	1a	984	C	2.8
31	2a	962	C	2.8
39	2i	55	ALA	2.8
42	2l	80	HIS	2.8
1	2A	247	G	2.8
1	2A	257	A	2.8
31	2a	570	G	2.8
35	2e	12	LEU	2.8
54	1y	22	G	2.8
54	2y	34	G	2.8
14	2T	38	ASN	2.8
9	2O	58	VAL	2.8
43	2m	109	THR	2.8
52	2v	538	TYR	2.8
4	1E	132	HIS	2.8
9	2O	44	LYS	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	1c	178	LEU	2.8
6	2G	150	ASP	2.8
37	1g	103	TRP	2.8
41	1k	40	ILE	2.8
41	2k	84	VAL	2.8
52	1v	412	ALA	2.8
1	2A	2114	A	2.8
4	1E	145	LYS	2.8
3	2D	6	PHE	2.8
7	2H	34	GLU	2.8
43	1m	90	LEU	2.8
3	2D	54	ARG	2.8
29	28	55	ALA	2.8
33	1c	73	PRO	2.8
43	1m	100	GLY	2.8
11	2Q	18	LYS	2.8
38	1h	109	ILE	2.8
35	2e	40	ARG	2.8
14	1T	35	LYS	2.8
52	1v	416	LYS	2.8
53	2w	51	PRO	2.8
1	2A	2148	G	2.8
31	2a	1050	G	2.8
33	1c	34	LEU	2.8
38	1h	15	ASN	2.8
53	2w	145	LYS	2.8
1	2A	2178	C	2.8
12	2R	111	LEU	2.8
4	1E	116	VAL	2.8
17	1W	1	MET	2.8
41	1k	83	ILE	2.8
52	2v	105	ILE	2.8
43	1m	87	TYR	2.8
35	2e	28	PHE	2.8
39	1i	37	PHE	2.8
9	1O	98	VAL	2.8
11	2Q	96	VAL	2.8
14	1T	62	THR	2.8
21	20	12	ASN	2.8
39	1i	17	VAL	2.8
49	1s	60	VAL	2.8
49	2s	51	VAL	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
53	1w	32	ARG	2.8
31	2a	89	C	2.8
35	2e	92	LYS	2.8
47	2q	41	LYS	2.8
41	1k	19	ALA	2.8
4	1E	189	PRO	2.8
22	21	41	ARG	2.8
29	28	5	LYS	2.8
44	1n	22	THR	2.8
5	2F	181	LEU	2.8
37	2g	121	ALA	2.8
52	2v	458	HIS	2.8
3	2D	52	ARG	2.8
10	2P	95	VAL	2.8
37	1g	70	LYS	2.8
31	1a	968	A	2.8
33	1c	47	LEU	2.8
7	2H	21	PRO	2.7
33	1c	140	ARG	2.7
35	1e	41	VAL	2.7
29	28	64	TYR	2.7
1	1A	1667	G	2.7
31	2a	1164	G	2.7
31	2a	891	U	2.7
1	1A	2142	C	2.7
3	2D	4	LYS	2.7
6	2G	48	GLU	2.7
31	2a	1344	C	2.7
52	1v	88	VAL	2.7
35	2e	93	PRO	2.7
31	2a	1377	A	2.7
13	2S	82	ILE	2.7
14	2T	40	THR	2.7
33	2c	26	LYS	2.7
11	2Q	103	MET	2.7
19	2Y	82	PRO	2.7
52	2v	479	PRO	2.7
31	2a	1222	G	2.7
14	1T	74	ARG	2.7
16	2V	14	VAL	2.7
31	2a	1335	C	2.7
38	2h	95	VAL	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	1x	61	C	2.7
20	2Z	38	TYR	2.7
29	28	63	PRO	2.7
39	1i	117	HIS	2.7
37	1g	130	GLY	2.7
9	2O	43	VAL	2.7
31	1a	1196	U	2.7
12	1R	1	MET	2.7
19	1Y	1	MET	2.7
40	1j	15	THR	2.7
1	2A	264	C	2.7
1	2A	2313	C	2.7
49	1s	74	PHE	2.7
9	1O	121	VAL	2.7
38	2h	84	ARG	2.7
52	2v	645	ALA	2.7
35	2e	110	LEU	2.7
3	2D	55	GLY	2.7
4	1E	149	ARG	2.7
7	2H	23	ARG	2.7
27	26	37	ARG	2.7
40	1j	45	ARG	2.7
43	2m	92	HIS	2.7
33	2c	50	ALA	2.7
33	2c	163	ALA	2.7
9	1O	39	ILE	2.7
10	2P	126	VAL	2.7
11	2Q	109	VAL	2.7
1	2A	2116	G	2.7
31	2a	954	G	2.7
31	2a	1026	G	2.7
20	2Z	74	VAL	2.7
44	2n	59	ALA	2.7
6	2G	176	LEU	2.7
34	1d	11	LEU	2.7
5	1F	66	PRO	2.7
53	2w	12	SER	2.7
31	2a	555	C	2.7
54	1x	4	C	2.7
31	1a	958	A	2.7
52	2v	507	TYR	2.7
21	20	13	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	2e	134	ALA	2.7
44	1n	7	ILE	2.7
47	2q	8	GLY	2.7
14	1T	77	PRO	2.7
52	2v	631	ILE	2.7
8	2N	70	LYS	2.7
9	2O	111	PHE	2.7
14	1T	27	THR	2.7
31	2a	889	A	2.7
54	2y	14	A	2.7
42	2l	58	VAL	2.7
3	2D	195	ALA	2.7
33	1c	81	GLY	2.7
46	1p	19	ILE	2.7
20	2Z	83	PRO	2.7
51	2u	14	TRP	2.7
21	20	41	ARG	2.7
35	2e	123	LEU	2.7
52	2v	91	THR	2.7
10	2P	71	VAL	2.7
52	2v	625	ASN	2.7
1	2A	254	G	2.7
37	1g	126	ASP	2.7
52	2v	558	PHE	2.7
12	1R	115	GLU	2.7
52	2v	660	ARG	2.7
53	1w	41	LEU	2.7
9	1O	83	ALA	2.7
29	28	58	ILE	2.7
31	1a	532	A	2.7
31	2a	937	A	2.7
1	1A	2513	G	2.7
5	2F	148	LEU	2.6
20	2Z	44	PHE	2.7
34	2d	118	ARG	2.6
54	2x	34	G	2.7
52	2v	436	PRO	2.6
6	2G	151	ALA	2.6
33	2c	53	ALA	2.6
52	1v	591	LYS	2.6
4	1E	119	ARG	2.6
35	1e	91	LEU	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
27	26	48	VAL	2.6
44	2n	8	GLU	2.6
30	29	1	MET	2.6
34	1d	102	ASP	2.6
42	1l	97	ARG	2.6
43	1m	48	LEU	2.6
52	1v	472	VAL	2.6
19	2Y	4	LYS	2.6
31	2a	1078	U	2.6
39	2i	98	PRO	2.6
52	2v	511	LYS	2.6
20	2Z	150	LEU	2.6
21	20	14	ARG	2.6
44	1n	28	GLY	2.6
31	1a	900	A	2.6
44	2n	57	ARG	2.6
8	2N	62	VAL	2.6
24	23	38	GLU	2.6
53	2w	67	VAL	2.6
6	2G	76	SER	2.6
24	23	8	LEU	2.6
34	2d	167	GLY	2.6
40	2j	66	ARG	2.6
22	21	62	VAL	2.6
34	1d	125	HIS	2.6
4	1E	133	LYS	2.6
11	2Q	137	TYR	2.6
27	26	12	GLU	2.6
52	2v	563	ILE	2.6
5	1F	67	GLN	2.6
33	2c	62	ASP	2.6
3	2D	237	GLU	2.6
4	1E	113	PHE	2.6
11	2Q	51	ARG	2.6
31	2a	1202	G	2.6
33	2c	52	LEU	2.6
33	2c	160	ALA	2.6
52	2v	535	PRO	2.6
14	1T	31	SER	2.6
31	1a	936	C	2.6
33	2c	195	VAL	2.6
15	2U	106	PHE	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	2Z	81	ARG	2.6
33	1c	145	GLY	2.6
7	2H	115	VAL	2.6
9	1O	85	VAL	2.6
13	2S	28	VAL	2.6
19	2Y	43	ASN	2.6
7	2H	119	GLU	2.6
9	1O	28	SER	2.6
9	1O	78	ARG	2.6
30	29	9	ARG	2.6
31	2a	916	G	2.6
31	2a	1036	G	2.6
35	2e	84	PHE	2.6
40	1j	87	THR	2.6
1	2A	2108	C	2.6
29	28	59	LYS	2.6
43	1m	45	VAL	2.6
31	2a	279	A	2.6
11	2Q	68	ILE	2.6
1	1A	2585	U	2.6
6	2G	156	ASP	2.6
7	2H	137	ASP	2.6
21	20	71	ASP	2.6
3	1D	276	LYS	2.6
34	1d	8	VAL	2.6
40	2j	53	PRO	2.6
10	2P	74	GLU	2.6
54	2y	11	C	2.6
4	1E	193	GLY	2.6
8	2N	84	LYS	2.6
9	2O	12	ASP	2.6
31	2a	1030(D)	A	2.6
33	1c	62	ASP	2.6
52	1v	513	LYS	2.6
41	2k	18	ARG	2.6
52	2v	677	GLN	2.6
33	1c	171	GLY	2.6
52	2v	423	LYS	2.6
1	2A	1765	C	2.6
31	2a	1487	G	2.6
1	2A	1690	A	2.6
14	2T	68	TYR	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	2E	133	LYS	2.6
31	1a	1030(D)	A	2.6
52	1v	677	GLN	2.6
6	2G	161	THR	2.6
22	11	37	ILE	2.6
35	1e	19	MET	2.6
21	20	22	GLY	2.6
31	2a	240	C	2.6
1	1A	652(U)	G	2.6
31	1a	1030(A)	G	2.6
31	2a	1034	G	2.6
31	2a	1408	A	2.6
3	2D	181	GLU	2.6
4	1E	8	LYS	2.6
14	2T	82	LEU	2.6
9	1O	58	VAL	2.6
33	2c	198	VAL	2.6
39	2i	16	ARG	2.6
39	2i	106	ALA	2.6
35	1e	26	PHE	2.6
9	2O	122	LEU	2.5
30	29	24	TYR	2.5
42	2l	84	LEU	2.5
27	26	30	THR	2.5
1	1A	1792	G	2.5
31	1a	1193	G	2.5
5	2F	82	ILE	2.5
24	23	26	LEU	2.5
41	2k	95	ILE	2.5
9	2O	32	TYR	2.5
47	2q	10	VAL	2.5
3	2D	234	GLY	2.5
41	1k	68	ALA	2.5
31	2a	71	C	2.5
52	1v	493	VAL	2.5
54	1y	4	C	2.5
25	24	51	ASP	2.5
9	1O	53	LYS	2.5
9	1O	111	PHE	2.5
14	2T	83	ILE	2.5
39	1i	118	LYS	2.5
46	1p	35	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
52	2v	512	ILE	2.5
7	2H	80	SER	2.5
52	2v	434	GLU	2.5
11	2Q	23	GLY	2.5
14	2T	71	GLY	2.5
15	1U	117	GLN	2.5
16	2V	54	GLY	2.5
21	20	47	PRO	2.5
28	17	48	LYS	2.5
32	2b	163	PHE	2.5
35	1e	92	LYS	2.5
53	1w	73	GLN	2.5
1	2A	393	C	2.5
14	1T	99	LEU	2.5
39	2i	50	LEU	2.5
47	2q	20	THR	2.5
31	1a	790	A	2.5
35	2e	90	VAL	2.5
4	1E	136	ARG	2.5
22	21	65	SER	2.5
39	2i	88	TYR	2.5
5	1F	75	HIS	2.5
33	1c	137	ALA	2.5
52	2v	541	ALA	2.5
41	1k	108	ILE	2.5
33	2c	106	VAL	2.5
52	1v	526	VAL	2.5
4	2E	125	GLY	2.5
5	2F	52	LYS	2.5
20	2Z	62	PRO	2.5
22	21	24	ALA	2.5
54	1y	61	C	2.5
34	1d	126	ILE	2.5
32	1b	96	ARG	2.5
1	2A	2127	G	2.5
3	2D	184	LYS	2.5
23	22	1	MET	2.5
16	2V	73	SER	2.5
54	1x	27	G	2.5
52	1v	539	ILE	2.5
5	2F	56	GLU	2.5
9	1O	94	ARG	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
25	24	23	GLU	2.5
9	2O	34	THR	2.5
22	21	48	LYS	2.5
40	2j	92	THR	2.5
47	2q	4	LYS	2.5
30	29	37	GLY	2.5
31	2a	695	A	2.5
43	1m	95	GLY	2.5
33	2c	34	LEU	2.5
3	1D	273	ARG	2.5
16	2V	12	TYR	2.5
1	2A	386	G	2.5
31	1a	698	G	2.5
4	1E	5	LEU	2.5
14	1T	80	SER	2.5
21	20	59	LEU	2.5
27	26	42	TRP	2.5
30	29	16	VAL	2.5
21	20	72	ARG	2.5
1	1A	2143	C	2.5
1	1A	2571	C	2.5
3	2D	233	HIS	2.5
52	2v	497	PHE	2.5
52	2v	568	TYR	2.5
53	1w	146	GLU	2.5
33	2c	175	LEU	2.5
41	1k	28	THR	2.5
41	1k	57	THR	2.5
41	1k	97	ALA	2.5
42	2l	121	GLY	2.5
52	1v	447	GLY	2.5
33	1c	134	ILE	2.5
52	2v	529	ILE	2.5
22	21	11	ARG	2.5
27	26	44	ARG	2.5
9	1O	81	ASP	2.5
33	2c	145	GLY	2.5
41	1k	22	HIS	2.5
9	2O	52	VAL	2.5
22	21	18	ILE	2.5
22	21	20	ARG	2.5
41	1k	14	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	1a	970	C	2.5
31	2a	1298	C	2.5
41	2k	87	THR	2.5
9	1O	42	SER	2.5
55	1z	12	A	2.5
15	2U	47	TYR	2.5
9	1O	33	ALA	2.5
42	2l	103	GLY	2.5
11	2Q	77	LYS	2.5
14	1T	65	LYS	2.5
33	2c	17	ASP	2.5
34	1d	118	ARG	2.5
41	2k	48	ILE	2.5
47	2q	5	VAL	2.5
1	2A	1117	G	2.5
8	2N	44	PRO	2.5
8	2N	139	GLU	2.5
1	2A	2586	C	2.5
54	1y	36	A	2.5
10	2P	124	LYS	2.5
35	1e	88	LYS	2.5
4	1E	147	PRO	2.5
37	1g	62	PHE	2.5
39	1i	114	TYR	2.5
29	28	60	LEU	2.5
10	2P	107	LYS	2.5
38	2h	109	ILE	2.5
39	2i	116	LYS	2.5
42	2l	17	LYS	2.5
52	1v	440	VAL	2.5
53	2w	118	VAL	2.5
21	20	69	PHE	2.5
52	2v	582	PHE	2.5
27	26	32	ASN	2.4
31	1a	972	C	2.4
31	2a	1051	C	2.4
41	1k	33	THR	2.4
41	2k	39	PRO	2.4
43	2m	66	LEU	2.4
49	2s	53	ASN	2.4
52	1v	448	GLN	2.4
7	2H	107	VAL	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
11	2Q	106	VAL	2.4
14	2T	72	VAL	2.4
20	2Z	82	ARG	2.4
33	1c	149	ALA	2.4
41	2k	72	ALA	2.4
52	2v	531	GLY	2.4
8	2N	72	TYR	2.4
52	2v	515	GLU	2.4
14	2T	48	ILE	2.4
26	15	6	VAL	2.4
52	1v	425	SER	2.4
1	2A	2111	C	2.4
31	1a	926	G	2.4
31	1a	1210	C	2.4
9	2O	8	LEU	2.4
33	1c	12	LEU	2.4
34	2d	67	ILE	2.4
53	1w	83	ILE	2.4
8	2N	9	VAL	2.4
14	1T	54	ARG	2.4
52	1v	609	GLU	2.4
1	2A	171	G	2.4
1	2A	194	G	2.4
31	2a	953	G	2.4
41	2k	38	ASN	2.4
5	2F	155	LEU	2.4
14	1T	73	GLU	2.4
22	11	26	ARG	2.4
41	1k	63	LEU	2.4
52	2v	157	LEU	2.4
33	1c	31	HIS	2.4
39	2i	41	VAL	2.4
37	1g	152	ALA	2.4
52	2v	654	GLY	2.4
37	2g	15	ASP	2.4
52	2v	410	ASP	2.4
11	2Q	91	GLU	2.4
22	21	43	TYR	2.4
31	2a	884	U	2.4
35	2e	107	ARG	2.4
37	1g	129	GLU	2.4
41	2k	59	TYR	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
47	2q	34	LYS	2.4
52	1v	491	VAL	2.4
5	1F	71	GLY	2.4
41	2k	56	GLY	2.4
52	2v	487	ILE	2.4
54	1x	41	C	2.4
31	2a	1131	G	2.4
52	1v	500	GLN	2.4
9	1O	8	LEU	2.4
35	1e	120	THR	2.4
51	2u	5	ASP	2.4
14	2T	96	ARG	2.4
27	26	19	ARG	2.4
40	1j	43	ARG	2.4
8	2N	81	GLY	2.4
29	18	4	MET	2.4
41	1k	21	ILE	2.4
40	1j	56	HIS	2.4
1	1A	2440	C	2.4
19	2Y	35	TYR	2.4
33	2c	127	ARG	2.4
38	1h	46	LYS	2.4
52	1v	655	TYR	2.4
18	1X	1	MET	2.4
33	2c	200	ALA	2.4
16	2V	20	LEU	2.4
34	2d	169	LYS	2.4
1	2A	2118	U	2.4
4	1E	14	ILE	2.4
20	2Z	169	GLU	2.4
43	1m	84	ILE	2.4
52	2v	168	ILE	2.4
53	1w	86	SER	2.4
33	2c	147	LYS	2.4
1	1A	1990	C	2.4
1	2A	896	A	2.4
22	21	19	GLN	2.4
24	23	6	VAL	2.4
31	1a	1344	C	2.4
33	2c	42	LEU	2.4
35	1e	141	GLN	2.4
54	1x	36	A	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	1x	73	A	2.4
6	2G	137	GLU	2.4
32	2b	97	TRP	2.4
52	2v	498	ILE	2.4
53	2w	161	ILE	2.4
42	2l	51	ALA	2.4
32	1b	232	PRO	2.4
39	2i	125	TYR	2.4
44	1n	52	GLN	2.4
11	2Q	105	GLU	2.4
14	1T	57	PHE	2.4
37	1g	30	ILE	2.4
1	1A	652(T)	C	2.4
1	1A	1656	C	2.4
25	24	64	GLY	2.4
9	2O	96	THR	2.4
31	1a	1201	A	2.4
52	2v	564	LYS	2.4
52	2v	633	GLY	2.4
20	2Z	195	GLU	2.4
33	2c	58	GLU	2.4
52	2v	494	GLU	2.4
29	28	52	LYS	2.4
31	1a	1521	G	2.4
31	2a	895	G	2.4
54	1x	63	G	2.4
15	1U	28	ARG	2.4
24	23	4	LEU	2.4
39	1i	93	ARG	2.4
40	2j	59	SER	2.4
41	1k	82	VAL	2.4
29	28	16	ILE	2.4
31	1a	915	A	2.4
31	1a	1208	C	2.4
31	2a	915	A	2.4
45	2o	46	HIS	2.4
47	2q	96	GLU	2.4
53	2w	135	GLU	2.4
43	1m	104	ARG	2.4
7	2H	131	VAL	2.4
3	2D	275	LYS	2.4
34	2d	70	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
25	24	9	LEU	2.4
33	2c	159	GLY	2.4
35	1e	43	LEU	2.4
39	2i	102	LEU	2.4
52	2v	143	GLY	2.4
41	1k	65	ALA	2.4
34	2d	166	LYS	2.4
52	1v	93	GLU	2.3
21	20	80	HIS	2.3
33	1c	78	GLY	2.3
42	1l	27	LEU	2.3
42	2l	27	LEU	2.3
53	2w	184	LEU	2.3
1	1A	2125	G	2.3
46	2p	36	ILE	2.3
9	1O	101	PRO	2.3
1	2A	412	A	2.3
6	2G	120	LEU	2.3
21	20	75	LEU	2.3
31	1a	1349	A	2.3
37	1g	65	ALA	2.3
1	2A	2128	C	2.3
17	1W	101	SER	2.3
31	1a	957	U	2.3
53	2w	180	GLU	2.3
9	1O	25	LEU	2.3
52	2v	539	ILE	2.3
54	1x	30	G	2.3
31	1a	1350	A	2.3
11	2Q	81	VAL	2.3
31	1a	817	C	2.3
31	2a	789	U	2.3
40	2j	42	THR	2.3
42	1l	87	GLY	2.3
52	2v	506	GLN	2.3
14	1T	78	LEU	2.3
4	1E	117	MET	2.3
3	1D	17	THR	2.3
5	2F	53	THR	2.3
20	2Z	118	GLN	2.3
21	20	19	LYS	2.3
42	2l	54	LYS	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
43	2m	103	THR	2.3
52	2v	104	ALA	2.3
1	2A	1764	G	2.3
3	2D	217	ARG	2.3
14	1T	52	ILE	2.3
31	1a	1061	G	2.3
31	1a	1343	G	2.3
31	2a	286	G	2.3
35	1e	143	ARG	2.3
52	1v	-63	ILE	2.3
54	1x	23	A	2.3
32	1b	165	VAL	2.3
53	1w	158	GLU	2.3
19	2Y	5	MET	2.3
6	2G	98	ARG	2.3
9	2O	81	ASP	2.3
10	2P	48	PRO	2.3
29	18	13	ARG	2.3
7	2H	161	GLY	2.3
9	2O	18	LYS	2.3
40	1j	69	ASN	2.3
52	2v	679	VAL	2.3
52	1v	-66	MET	2.3
52	2v	667	GLY	2.3
22	11	24	ALA	2.3
1	1A	2139	C	2.3
9	2O	47	ILE	2.3
15	2U	36	ARG	2.3
31	1a	902	G	2.3
31	2a	1375	A	2.3
33	1c	136	GLN	2.3
42	2l	86	ARG	2.3
52	1v	-40	ARG	2.3
53	2w	61	PRO	2.3
54	2y	36	A	2.3
54	1y	62	C	2.3
3	1D	5	LYS	2.3
14	2T	73	GLU	2.3
52	2v	346	LYS	2.3
52	2v	672	PHE	2.3
9	1O	87	ILE	2.3
14	1T	51	ARG	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
25	24	69	LYS	2.3
28	27	46	VAL	2.3
29	18	50	LEU	2.3
33	1c	175	LEU	2.3
42	1l	38	THR	2.3
42	1l	91	LYS	2.3
1	2A	2310	A	2.3
16	1V	101	GLY	2.3
1	1A	1657	C	2.3
4	1E	1	MET	2.3
31	1a	1520	G	2.3
31	2a	796	C	2.3
31	2a	1226	C	2.3
41	1k	91	ARG	2.3
47	2q	92	ARG	2.3
54	1y	15	G	2.3
54	2y	56	C	2.3
12	1R	113	LEU	2.3
34	2d	176	LEU	2.3
41	2k	34	ASP	2.3
42	2l	104	VAL	2.3
44	2n	34	TYR	2.3
8	2N	136	GLU	2.3
34	1d	156	GLU	2.3
52	1v	492	ASP	2.3
11	2Q	100	GLY	2.3
52	1v	-31	ALA	2.3
14	1T	50	ILE	2.3
8	1N	84	LYS	2.3
10	1P	59	LEU	2.3
20	2Z	41	LEU	2.3
31	1a	781	A	2.3
4	1E	103	ASP	2.3
31	2a	784	C	2.3
33	1c	74	GLY	2.3
41	1k	41	THR	2.3
3	2D	224	ALA	2.3
4	1E	135	HIS	2.3
14	1T	79	HIS	2.3
9	2O	113	LYS	2.3
11	2Q	78	PRO	2.3
33	2c	170	GLN	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
39	1i	85	LEU	2.3
44	2n	53	LEU	2.3
52	1v	595	GLN	2.3
4	1E	144	ARG	2.3
32	1b	152	PHE	2.3
39	1i	101	PHE	2.3
35	2e	138	ALA	2.3
1	2A	2388	A	2.3
31	1a	1213	A	2.3
47	2q	88	TYR	2.3
53	2w	28	LEU	2.3
31	1a	999	C	2.3
31	2a	241	C	2.3
31	2a	701	C	2.3
31	2a	1208	C	2.3
3	1D	15	PHE	2.3
40	2j	45	ARG	2.3
1	1A	2506	U	2.3
7	2H	151	ILE	2.3
52	2v	621	ILE	2.3
40	1j	94	VAL	2.3
54	2y	45	U	2.3
14	1T	3	ARG	2.3
34	2d	110	PHE	2.3
52	2v	603	GLU	2.3
9	1O	103	ALA	2.3
1	1A	652(S)	C	2.3
1	1A	1675	C	2.3
32	2b	108	ILE	2.3
53	2w	129	ILE	2.3
27	26	39	TYR	2.3
33	2c	165	THR	2.3
41	2k	25	TYR	2.3
1	1A	2793	G	2.2
37	2g	4	ARG	2.2
4	1E	11	MET	2.2
4	1E	118	LYS	2.2
4	1E	156	MET	2.2
10	2P	69	GLY	2.2
39	1i	6	GLY	2.2
9	1O	11	ALA	2.2
35	1e	76	ILE	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	1D	168	ARG	2.2
44	2n	37	PHE	2.2
44	2n	46	GLU	2.2
53	2w	158	GLU	2.2
32	2b	232	PRO	2.2
52	2v	629	GLY	2.2
11	2Q	132	VAL	2.2
27	16	2	ALA	2.2
33	2c	61	ALA	2.2
45	2o	38	ARG	2.2
31	1a	954	G	2.2
34	2d	98	GLU	2.2
53	2w	2	THR	2.2
3	1D	231	HIS	2.2
35	1e	70	PRO	2.2
44	2n	49	HIS	2.2
22	2l	5	CYS	2.2
41	1k	95	ILE	2.2
41	2k	73	MET	2.2
47	2q	56	VAL	2.2
52	2v	659	LEU	2.2
9	1O	23	ARG	2.2
9	2O	49	ARG	2.2
31	1a	1531	A	2.2
52	2v	572	TYR	2.2
47	2q	69	LYS	2.2
1	1A	2511	U	2.2
41	2k	88	GLY	2.2
44	2n	13	THR	2.2
53	1w	154	THR	2.2
25	24	22	ILE	2.2
4	1E	120	TRP	2.2
14	1T	41	ARG	2.2
1	1A	2505	G	2.2
1	2A	1989	G	2.2
31	2a	1475	G	2.2
31	2a	1516	G	2.2
47	2q	67	LYS	2.2
32	1b	72	GLY	2.2
1	2A	2169	A	2.2
6	2G	97	ASP	2.2
31	1a	983	A	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	2j	94	VAL	2.2
50	1t	71	THR	2.2
1	2A	387	U	2.2
9	1O	108	GLU	2.2
52	2v	400	GLU	2.2
52	1v	475	ASN	2.2
33	1c	118	GLN	2.2
52	1v	543	GLN	2.2
52	2v	549	ALA	2.2
52	2v	565	VAL	2.2
33	2c	10	PHE	2.2
44	2n	15	LYS	2.2
54	2y	10	G	2.2
16	2V	94	LEU	2.2
24	23	47	VAL	2.2
31	1a	814	A	2.2
31	1a	697	U	2.2
38	1h	111	ILE	2.2
14	2T	22	PHE	2.2
31	1a	1226	C	2.2
33	2c	123	GLN	2.2
39	2i	82	ALA	2.2
4	2E	128	SER	2.2
33	2c	51	GLY	2.2
9	2O	94	ARG	2.2
41	2k	100	ALA	2.2
52	1v	525	PHE	2.2
31	2a	1497	G	2.2
3	2D	169	GLU	2.2
3	2D	194	GLY	2.2
14	2T	36	GLU	2.2
35	2e	82	VAL	2.2
44	2n	56	VAL	2.2
52	2v	433	GLU	2.2
52	2v	450	ILE	2.2
41	1k	69	ALA	2.2
41	1k	75	TYR	2.2
3	2D	206	LEU	2.2
10	2P	57	THR	2.2
43	2m	97	PRO	2.2
14	1T	48	ILE	2.2
32	2b	115	LEU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	2c	6	HIS	2.2
46	1p	34	GLU	2.2
49	2s	77	THR	2.2
33	2c	59	ARG	2.2
31	1a	1368	G	2.2
31	2a	782	A	2.2
31	2a	1342	C	2.2
41	2k	111	ASP	2.2
42	2l	55	VAL	2.2
47	2q	53	LEU	2.2
48	1r	31	LEU	2.2
55	1z	18	C	2.2
52	2v	86	GLY	2.2
1	2A	2099	U	2.2
8	1N	140	VAL	2.2
33	2c	18	TRP	2.2
43	1m	15	VAL	2.2
52	2v	389	LEU	2.2
54	2y	50	U	2.2
6	1G	144	ILE	2.2
14	2T	65	LYS	2.2
19	2Y	46	LYS	2.2
31	1a	1513	A	2.2
40	2j	48	THR	2.2
41	1k	45	GLY	2.2
52	1v	-34	ARG	2.2
52	2v	508	GLY	2.2
41	1k	64	ALA	2.2
41	2k	65	ALA	2.2
42	1l	22	SER	2.2
31	2a	1214	C	2.2
3	2D	261	LYS	2.2
4	1E	152	LYS	2.2
9	2O	98	VAL	2.2
9	2O	106	LEU	2.2
37	2g	13	GLN	2.2
41	1k	109	VAL	2.2
48	2r	26	LEU	2.2
52	1v	608	VAL	2.2
24	13	2	PRO	2.2
32	1b	202	PRO	2.2
8	2N	127	ASP	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	1O	56	ASP	2.2
9	1O	65	THR	2.2
47	2q	97	SER	2.2
9	1O	32	TYR	2.2
52	1v	538	TYR	2.2
33	1c	206	GLU	2.2
35	1e	80	ILE	2.2
39	2i	6	GLY	2.2
28	27	1	MET	2.2
31	1a	998	G	2.2
31	2a	812	C	2.2
54	2y	13	C	2.2
9	1O	97	ARG	2.2
29	18	26	LYS	2.2
37	1g	95	ARG	2.2
42	2l	39	VAL	2.2
9	1O	27	GLY	2.1
1	1A	752	A	2.1
7	2H	57	ASP	2.1
14	2T	74	ARG	2.1
27	26	14	THR	2.1
33	2c	4	LYS	2.1
34	1d	112	VAL	2.1
38	2h	73	ASP	2.1
48	2r	21	LYS	2.1
53	2w	144	ALA	2.1
9	2O	121	VAL	2.1
11	2Q	76	LYS	2.1
14	1T	100	TYR	2.1
26	15	58	LEU	2.1
33	2c	111	LEU	2.1
38	1h	112	LEU	2.1
53	1w	156	ARG	2.1
10	2P	42	SER	2.1
33	1c	18	TRP	2.1
39	1i	74	ILE	2.1
43	2m	78	ILE	2.1
50	2t	55	ILE	2.1
52	1v	529	ILE	2.1
19	2Y	58	GLY	2.1
1	1A	1669	A	2.1
20	2Z	59	LEU	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	11	25	LYS	2.1
22	21	4	VAL	2.1
42	1l	47	LYS	2.1
1	2A	201	C	2.1
7	2H	72	ILE	2.1
31	2a	248	C	2.1
1	2A	958	U	2.1
1	2A	2167	U	2.1
4	2E	130	GLY	2.1
11	2Q	138	ASP	2.1
31	2a	926	G	2.1
48	2r	62	GLU	2.1
54	1x	29	G	2.1
3	2D	245	PRO	2.1
4	1E	114	ALA	2.1
4	1E	104	VAL	2.1
37	2g	44	TYR	2.1
39	2i	79	LEU	2.1
52	1v	-48	VAL	2.1
44	2n	61	TRP	2.1
5	2F	81	PRO	2.1
35	1e	119	LEU	2.1
52	2v	550	MET	2.1
19	2Y	40	GLU	2.1
4	1E	127	ASP	2.1
35	2e	16	THR	2.1
20	2Z	39	VAL	2.1
46	2p	18	ARG	2.1
1	1A	1938	A	2.1
1	2A	204	A	2.1
4	1E	160	TYR	2.1
52	2v	255	ILE	2.1
35	2e	47	LYS	2.1
52	1v	-45	LYS	2.1
52	1v	494	GLU	2.1
5	1F	74	ARG	2.1
14	1T	103	ARG	2.1
28	17	47	ARG	2.1
31	2a	1049	U	2.1
34	1d	66	ARG	2.1
54	1x	60	U	2.1
50	2t	12	ALA	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
29	28	33	ASN	2.1
52	1v	582	PHE	2.1
7	2H	167	GLU	2.1
37	2g	55	GLY	2.1
5	2F	167	ALA	2.1
7	2H	171	LEU	2.1
35	1e	48	ALA	2.1
39	1i	119	ALA	2.1
5	2F	83	PHE	2.1
31	1a	1341	U	2.1
41	1k	27	ASN	2.1
1	1A	886	C	2.1
44	1n	15	LYS	2.1
3	2D	235	GLY	2.1
16	2V	42	GLY	2.1
3	1D	37	LEU	2.1
11	2Q	37	LEU	2.1
14	1T	114	LEU	2.1
40	2j	70	ARG	2.1
1	2A	381	G	2.1
1	2A	2396	G	2.1
8	1N	109	LYS	2.1
9	1O	37	ASP	2.1
11	2Q	129	THR	2.1
31	1a	953	G	2.1
35	2e	13	ILE	2.1
40	2j	89	ASP	2.1
42	2l	45	PRO	2.1
31	2a	1044	A	2.1
33	1c	16	ARG	2.1
34	1d	183	GLY	2.1
44	1n	20	ALA	2.1
9	1O	7	TYR	2.1
31	1a	1051	C	2.1
33	2c	14	ILE	2.1
40	1j	91	PRO	2.1
4	1E	196	VAL	2.1
18	1X	92	LEU	2.1
34	1d	148	VAL	2.1
39	1i	106	ALA	2.1
52	1v	427	ALA	2.1
31	1a	1034	G	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	2Z	121	HIS	2.1
31	1a	1358	U	2.1
4	1E	146	THR	2.1
9	2O	23	ARG	2.1
10	2P	94	GLU	2.1
34	1d	168	ARG	2.1
53	2w	148	HIS	2.1
44	2n	14	PRO	2.1
9	2O	13	ASN	2.1
52	2v	527	ASN	2.1
10	2P	110	TYR	2.1
26	15	8	LYS	2.1
22	11	19	GLN	2.1
7	2H	133	VAL	2.1
14	1T	40	THR	2.1
22	21	29	GLY	2.1
33	2c	46	GLU	2.1
35	1e	22	GLY	2.1
37	1g	59	LEU	2.1
39	1i	100	GLY	2.1
42	1l	29	GLY	2.1
1	2A	1918	A	2.1
1	2A	2120	G	2.1
4	1E	192	ASN	2.1
33	1c	72	LYS	2.1
53	1w	42	LYS	2.1
9	2O	7	TYR	2.1
1	2A	253	C	2.1
1	2A	2177	C	2.1
8	2N	11	PRO	2.1
9	2O	4	PRO	2.1
14	1T	82	LEU	2.1
29	28	54	GLU	2.1
8	2N	1	MET	2.1
10	1P	29	LYS	2.1
21	20	15	ASP	2.1
37	2g	60	LYS	2.1
52	2v	546	ILE	2.1
52	1v	-56	ASN	2.1
52	2v	666	ARG	2.1
1	2A	2189	U	2.1
21	20	38	VAL	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	1D	237	GLU	2.1
7	2H	62	LYS	2.0
9	1O	66	LYS	2.0
11	2Q	15	GLY	2.1
16	2V	35	LEU	2.1
34	2d	101	LEU	2.1
34	2d	135	LEU	2.1
54	1x	12	U	2.1
52	1v	90	PHE	2.1
20	2Z	170	THR	2.0
31	1a	1047	G	2.0
52	1v	490	PRO	2.0
37	2g	125	MET	2.0
53	1w	55	ILE	2.0
54	1y	5	G	2.0
41	1k	54	ARG	2.0
31	1a	1501	C	2.0
31	1a	1514	C	2.0
32	1b	93	VAL	2.0
9	1O	79	PHE	2.0
9	1O	113	LYS	2.0
9	2O	55	GLY	2.0
22	11	84	GLY	2.0
52	2v	545	GLY	2.0
4	1E	126	PRO	2.0
9	1O	60	ALA	2.0
9	1O	93	PRO	2.0
17	1W	89	ALA	2.0
39	2i	61	ALA	2.0
47	2q	30	PRO	2.0
9	1O	12	ASP	2.0
34	2d	27	TYR	2.0
38	2h	93	VAL	2.0
10	1P	44	GLY	2.0
15	2U	89	GLU	2.0
34	1d	200	GLU	2.0
1	1A	2049	G	2.0
31	1a	1206	G	2.0
31	2a	80	G	2.0
31	2a	1031	G	2.0
1	1A	2129	C	2.0
3	1D	239	ARG	2.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
53	2w	150	SER	2.0
1	2A	1923	U	2.0
9	1O	80	ASP	2.0
20	2Z	36	LYS	2.0
32	2b	220	ASP	2.0
40	2j	58	ASP	2.0
45	2o	47	LYS	2.0
40	2j	98	ILE	2.0
41	1k	77	MET	2.0
49	2s	78	ARG	2.0
53	2w	64	ARG	2.0
49	1s	58	VAL	2.0
54	1x	14	A	2.0
10	1P	51	PHE	2.0
6	2G	177	GLY	2.0
1	2A	385	C	2.0
1	2A	1904	G	2.0
1	2A	2165	G	2.0
3	2D	247	ALA	2.0
31	2a	1045	C	2.0
31	2a	1526	G	2.0
39	2i	87	GLN	2.0
20	2Z	53	ILE	2.0
34	2d	5	ILE	2.0
42	1l	30	ALA	2.0
4	1E	203	LYS	2.0
1	1A	676	A	2.0
9	2O	103	ALA	2.0
20	2Z	124	ILE	2.0
31	1a	959	A	2.0
40	2j	60	ARG	2.0
52	1v	473	ASP	2.0
5	2F	156	LEU	2.0
32	2b	139	LYS	2.0
41	1k	122	LYS	2.0
1	1A	745	G	2.0
1	1A	2146	C	2.0
20	1Z	10	ARG	2.0
21	20	44	ARG	2.0
21	20	74	ARG	2.0
31	1a	973	G	2.0
31	2a	1491	G	2.0

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Mol	Chain	Res	Type	RSRZ
33	1c	30	ARG	2.0
48	2r	55	ARG	2.0
54	1x	18	G	2.0
3	1D	3	VAL	2.0
3	2D	53	PHE	2.0
33	1c	111	LEU	2.0
49	2s	66	MET	2.0
47	2q	70	ARG	2.0
52	1v	552	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	PSU	2x	55	20/21	0.34	1.03	240,240,240,240	0
54	PSU	2y	32	20/21	0.50	0.37	220,220,220,220	0
54	7MG	1x	46	24/25	0.52	0.32	203,203,203,203	0
54	PSU	2y	55	20/21	0.52	0.47	279,279,279,279	0
54	5MU	2x	54	21/22	0.54	0.72	237,237,237,237	0
54	4SU	2x	8	20/21	0.61	1.10	239,239,239,239	0
54	5MU	2y	54	21/22	0.62	0.74	276,276,276,276	0
54	7MG	2y	46	24/25	0.65	0.39	261,261,261,261	0
54	7MG	2x	46	24/25	0.66	1.03	241,241,241,241	0
54	4SU	1x	8	20/21	0.66	0.35	199,199,199,199	0
54	PSU	1y	32	20/21	0.66	0.43	188,188,188,188	0
54	PSU	1x	55	20/21	0.68	0.32	194,194,194,194	0
54	5MU	1y	54	21/22	0.69	0.17	236,236,236,236	0
54	MIA	2y	37	22/30	0.69	0.39	208,208,208,208	0
1	PSU	2A	1911	20/21	0.73	0.25	158,158,158,158	0
54	PSU	1y	55	20/21	0.73	0.14	240,240,240,240	0
54	4SU	2y	8	20/21	0.74	0.32	259,259,259,259	0
54	PSU	2x	32	20/21	0.75	0.66	214,214,214,214	0
31	5MC	2a	967	21/22	0.76	0.15	216,216,216,216	0
54	MIA	2x	37	22/30	0.78	0.72	192,192,192,192	0
54	MIA	1y	37	22/30	0.79	0.32	175,175,175,175	0
54	PSU	2y	39	20/21	0.79	0.67	212,212,212,212	0
54	5MU	1x	54	21/22	0.80	0.32	193,193,193,193	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PSU	1A	1911	20/21	0.80	0.29	130,130,130,130	0
54	MIA	1x	37	22/30	0.81	0.50	163,163,163,163	0
54	PSU	1x	32	20/21	0.81	0.65	184,184,184,184	0
54	PSU	2x	39	20/21	0.82	0.99	204,204,204,204	0
54	7MG	1y	46	24/25	0.82	0.33	222,222,222,222	0
54	4SU	1y	8	20/21	0.82	0.34	217,217,217,217	0
31	2MG	1a	1207	24/25	0.83	0.31	209,209,209,209	0
54	PSU	1x	39	20/21	0.83	0.39	173,173,173,173	0
31	5MC	2a	1404	21/22	0.84	0.35	156,156,156,156	0
1	5MU	2A	1915	21/22	0.84	0.36	169,169,169,169	0
1	PSU	2A	1917	20/21	0.84	0.30	164,164,164,164	0
31	4OC	2a	1402	22/23	0.84	0.28	165,165,165,165	0
31	PSU	1a	516	20/21	0.85	0.15	144,144,144,144	0
31	5MC	1a	967	21/22	0.85	0.41	188,188,188,188	0
31	5MC	2a	1407	21/22	0.85	0.41	157,157,157,157	0
31	MA6	2a	1518	24/25	0.86	0.48	149,149,149,149	0
31	2MG	2a	1207	24/25	0.86	0.23	232,232,232,232	0
31	5MC	1a	1407	21/22	0.87	0.24	129,129,129,129	0
1	PSU	1A	1917	20/21	0.87	0.15	138,138,138,138	0
31	M2G	1a	966	25/26	0.88	0.37	184,184,184,184	0
31	UR3	2a	1498	21/22	0.89	0.34	158,158,158,158	0
31	PSU	2a	516	20/21	0.89	0.14	166,166,166,166	0
31	MA6	2a	1519	24/25	0.89	0.54	148,148,148,148	0
31	7MG	2a	527	24/25	0.90	0.18	155,155,155,155	0
31	5MC	2a	1400	21/22	0.90	0.44	182,182,182,182	0
1	OMC	2A	1920	21/22	0.90	0.32	153,153,153,153	0
42	0TD	2l	92	10/11	0.90	0.66	155,155,155,155	0
42	0TD	1l	92	10/11	0.90	0.36	132,132,132,132	0
31	7MG	1a	527	24/25	0.90	0.21	133,133,133,133	0
31	M2G	2a	966	25/26	0.91	0.19	211,211,211,211	0
1	PSU	1A	2605	20/21	0.91	0.33	69,69,69,69	0
1	5MU	1A	1915	21/22	0.91	0.17	142,142,142,142	0
54	PSU	1y	39	20/21	0.91	0.34	177,177,177,177	0
31	5MC	1a	1404	21/22	0.91	0.27	126,126,126,126	0
1	2MA	1A	2503	23/24	0.91	0.39	58,58,58,58	0
1	PSU	2A	2605	20/21	0.92	0.26	95,95,95,95	0
1	2MU	2A	2552	21/23	0.92	0.25	105,105,105,105	0
1	OMG	2A	2251	24/25	0.92	0.18	106,106,106,106	0
1	5MU	1A	1939	21/22	0.93	0.24	74,74,74,74	0
1	5MC	2A	1962	21/22	0.93	0.15	112,112,112,112	0
1	OMC	1A	1920	21/22	0.93	0.27	126,126,126,126	0
31	4OC	1a	1402	22/23	0.93	0.22	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MU	2A	1939	21/22	0.94	0.23	101,101,101,101	0
31	UR3	1a	1498	21/22	0.94	0.25	133,133,133,133	0
1	5MC	1A	1962	21/22	0.94	0.21	81,81,81,81	0
1	2MU	1A	2552	21/23	0.95	0.28	71,71,71,71	0
1	OMG	1A	2251	24/25	0.95	0.25	62,62,62,62	0
31	5MC	1a	1400	21/22	0.95	0.25	153,153,153,153	0
1	2MA	2A	2503	23/24	0.95	0.22	95,95,95,95	0
31	MA6	1a	1518	24/25	0.95	0.28	123,123,123,123	0
31	MA6	1a	1519	24/25	0.96	0.27	122,122,122,122	0
1	5MC	1A	1942	21/22	0.96	0.24	81,81,81,81	0
1	5MC	2A	1942	21/22	0.96	0.17	112,112,112,112	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3246	1/1	-0.24	0.56	153,153,153,153	0
56	MG	2g	202	1/1	-0.23	0.63	185,185,185,185	0
56	MG	2a	1801	1/1	-0.17	0.39	215,215,215,215	0
56	MG	2a	1763	1/1	-0.14	0.14	240,240,240,240	0
56	MG	2a	1766	1/1	-0.13	0.46	261,261,261,261	0
56	MG	2a	1767	1/1	-0.10	0.38	276,276,276,276	0
56	MG	2a	1765	1/1	-0.08	0.28	250,250,250,250	0
56	MG	1a	1854	1/1	-0.07	0.67	229,229,229,229	0
56	MG	2A	3252	1/1	-0.07	0.40	127,127,127,127	0
56	MG	2a	1684	1/1	-0.04	0.77	161,161,161,161	0
56	MG	2x	108	1/1	-0.02	0.66	245,245,245,245	0
56	MG	2m	202	1/1	-0.01	0.66	230,230,230,230	0
56	MG	2A	3122	1/1	0.01	1.52	117,117,117,117	0
56	MG	2x	105	1/1	0.03	2.65	237,237,237,237	0
56	MG	2a	1828	1/1	0.06	0.71	163,163,163,163	0
56	MG	1a	1730	1/1	0.09	0.52	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2a	1785	1/1	0.15	1.07	228,228,228,228	0
56	MG	1a	1670	1/1	0.16	0.41	137,137,137,137	0
56	MG	2A	3184	1/1	0.16	0.70	135,135,135,135	0
56	MG	2Q	202	1/1	0.17	0.41	132,132,132,132	0
56	MG	2r	301	1/1	0.19	0.52	139,139,139,139	0
56	MG	2a	1602	1/1	0.19	0.41	151,151,151,151	0
56	MG	2p	102	1/1	0.19	0.70	148,148,148,148	0
56	MG	2a	1714	1/1	0.20	0.67	143,143,143,143	0
56	MG	1a	1823	1/1	0.20	0.26	211,211,211,211	0
56	MG	2y	106	1/1	0.20	0.70	263,263,263,263	0
56	MG	2A	3245	1/1	0.21	0.64	111,111,111,111	0
56	MG	2i	202	1/1	0.21	0.20	255,255,255,255	0
56	MG	2A	3681	1/1	0.22	0.42	119,119,119,119	0
56	MG	2g	203	1/1	0.22	0.25	214,214,214,214	0
56	MG	2A	3517	1/1	0.22	0.42	132,132,132,132	0
56	MG	2g	201	1/1	0.23	0.23	229,229,229,229	0
56	MG	2a	1761	1/1	0.26	0.31	210,210,210,210	0
56	MG	2A	3552	1/1	0.26	0.51	105,105,105,105	0
56	MG	1a	1637	1/1	0.27	0.23	119,119,119,119	0
56	MG	2a	1706	1/1	0.28	0.48	150,150,150,150	0
56	MG	2A	3830	1/1	0.28	0.73	125,125,125,125	0
56	MG	2a	1664	1/1	0.28	0.48	150,150,150,150	0
56	MG	1a	1899	1/1	0.28	0.26	149,149,149,149	0
56	MG	2a	1659	1/1	0.29	0.33	117,117,117,117	0
56	MG	1b	305	1/1	0.29	0.60	166,166,166,166	0
56	MG	2a	1674	1/1	0.29	0.88	127,127,127,127	0
56	MG	2A	3597	1/1	0.30	0.18	120,120,120,120	0
56	MG	2a	1887	1/1	0.30	0.66	134,134,134,134	0
56	MG	1a	1782	1/1	0.30	0.36	127,127,127,127	0
56	MG	1a	1685	1/1	0.31	0.54	173,173,173,173	0
56	MG	2a	1800	1/1	0.31	0.18	220,220,220,220	0
56	MG	1A	4503	1/1	0.31	0.56	102,102,102,102	0
56	MG	1a	1803	1/1	0.32	0.74	125,125,125,125	0
56	MG	2a	1760	1/1	0.33	0.21	220,220,220,220	0
56	MG	2l	204	1/1	0.34	0.50	136,136,136,136	0
56	MG	2l	206	1/1	0.34	0.53	145,145,145,145	0
56	MG	2A	3629	1/1	0.34	0.61	114,114,114,114	0
56	MG	1a	1768	1/1	0.34	0.51	122,122,122,122	0
56	MG	2a	1661	1/1	0.35	0.33	145,145,145,145	0
56	MG	2a	1677	1/1	0.35	0.26	166,166,166,166	0
56	MG	2B	208	1/1	0.36	0.93	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1899	1/1	0.36	0.59	125,125,125,125	0
56	MG	2a	1669	1/1	0.37	0.70	140,140,140,140	0
56	MG	2A	3071	1/1	0.37	0.68	129,129,129,129	0
56	MG	2Q	206	1/1	0.37	0.45	118,118,118,118	0
56	MG	2A	3692	1/1	0.38	0.41	133,133,133,133	0
56	MG	1s	103	1/1	0.39	0.23	203,203,203,203	0
56	MG	2A	3390	1/1	0.40	0.21	116,116,116,116	0
56	MG	2Z	401	1/1	0.40	0.44	142,142,142,142	0
56	MG	2A	3387	1/1	0.41	0.33	123,123,123,123	0
56	MG	2A	3574	1/1	0.41	0.56	253,253,253,253	0
56	MG	2A	3795	1/1	0.41	0.38	109,109,109,109	0
56	MG	1a	1681	1/1	0.41	0.30	158,158,158,158	0
56	MG	1x	301	1/1	0.41	0.22	193,193,193,193	0
56	MG	2A	3639	1/1	0.41	0.44	118,118,118,118	0
56	MG	2T	302	1/1	0.42	0.33	124,124,124,124	0
56	MG	2a	1844	1/1	0.42	0.29	238,238,238,238	0
56	MG	1q	201	1/1	0.42	0.83	115,115,115,115	0
56	MG	2A	3083	1/1	0.42	1.40	115,115,115,115	0
56	MG	2A	3022	1/1	0.43	0.41	126,126,126,126	0
56	MG	2a	1776	1/1	0.43	0.48	197,197,197,197	0
56	MG	1a	1669	1/1	0.43	0.46	124,124,124,124	0
56	MG	2a	1709	1/1	0.44	0.59	156,156,156,156	0
56	MG	1A	4516	1/1	0.44	0.87	118,118,118,118	0
56	MG	2A	3680	1/1	0.44	0.24	114,114,114,114	0
56	MG	1a	1671	1/1	0.44	0.22	139,139,139,139	0
56	MG	1a	1776	1/1	0.44	0.52	122,122,122,122	0
56	MG	2a	1686	1/1	0.44	0.32	150,150,150,150	0
56	MG	1a	1777	1/1	0.44	0.49	128,128,128,128	0
56	MG	1a	1725	1/1	0.45	0.33	117,117,117,117	0
56	MG	1a	1843	1/1	0.45	0.48	281,281,281,281	0
56	MG	2B	217	1/1	0.45	0.34	177,177,177,177	0
56	MG	1a	1908	1/1	0.45	0.84	131,131,131,131	0
56	MG	2m	203	1/1	0.45	0.10	238,238,238,238	0
56	MG	2A	3536	1/1	0.46	0.78	123,123,123,123	0
56	MG	2A	3097	1/1	0.46	0.53	99,99,99,99	0
56	MG	2A	3248	1/1	0.46	0.51	123,123,123,123	0
56	MG	2a	1607	1/1	0.46	0.60	142,142,142,142	0
56	MG	2B	227	1/1	0.46	0.39	132,132,132,132	0
56	MG	1a	1910	1/1	0.46	0.50	127,127,127,127	0
56	MG	2A	3531	1/1	0.46	0.28	138,138,138,138	0
56	MG	1A	4307	1/1	0.47	0.52	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	23	103	1/1	0.47	0.41	112,112,112,112	0
56	MG	2e	202	1/1	0.47	0.21	153,153,153,153	0
56	MG	2A	3538	1/1	0.47	0.21	134,134,134,134	0
56	MG	2A	3631	1/1	0.47	0.37	113,113,113,113	0
56	MG	2s	102	1/1	0.47	0.42	247,247,247,247	0
56	MG	2u	103	1/1	0.47	0.20	238,238,238,238	0
56	MG	2a	1654	1/1	0.47	0.35	132,132,132,132	0
56	MG	1A	4518	1/1	0.47	0.91	122,122,122,122	0
56	MG	1A	4052	1/1	0.47	0.59	92,92,92,92	0
56	MG	1n	102	1/1	0.48	0.32	210,210,210,210	0
56	MG	2A	3087	1/1	0.48	0.37	121,121,121,121	0
56	MG	1A	4054	1/1	0.48	0.81	95,95,95,95	0
56	MG	2A	3770	1/1	0.48	0.76	87,87,87,87	0
56	MG	2B	224	1/1	0.48	0.20	128,128,128,128	0
56	MG	2a	1716	1/1	0.48	0.95	135,135,135,135	0
56	MG	1n	101	1/1	0.49	0.20	207,207,207,207	0
56	MG	1a	1906	1/1	0.49	0.44	121,121,121,121	0
56	MG	2a	1668	1/1	0.49	1.01	151,151,151,151	0
56	MG	2A	3116	1/1	0.49	1.38	127,127,127,127	0
56	MG	1A	4060	1/1	0.49	0.56	72,72,72,72	0
56	MG	2A	3385	1/1	0.49	0.36	120,120,120,120	0
56	MG	2y	101	1/1	0.49	0.52	154,154,154,154	0
56	MG	1g	302	1/1	0.49	0.33	194,194,194,194	0
56	MG	2F	303	1/1	0.50	0.57	126,126,126,126	0
56	MG	1a	1900	1/1	0.50	0.30	134,134,134,134	0
56	MG	2A	3016	1/1	0.50	0.95	118,118,118,118	0
56	MG	2A	3556	1/1	0.50	0.59	96,96,96,96	0
56	MG	2u	101	1/1	0.50	0.69	221,221,221,221	0
56	MG	2y	109	1/1	0.50	0.27	247,247,247,247	0
56	MG	2B	232	1/1	0.51	0.52	144,144,144,144	0
56	MG	1A	4889	1/1	0.51	0.51	61,61,61,61	0
56	MG	2a	1786	1/1	0.52	0.53	234,234,234,234	0
56	MG	2a	1909	1/1	0.52	0.22	225,225,225,225	0
56	MG	2A	3282	1/1	0.52	0.37	107,107,107,107	0
56	MG	1B	223	1/1	0.52	0.57	97,97,97,97	0
56	MG	2a	1627	1/1	0.52	0.51	153,153,153,153	0
56	MG	1A	4790	1/1	0.52	0.48	99,99,99,99	0
56	MG	1A	4891	1/1	0.52	0.34	109,109,109,109	0
56	MG	2A	3421	1/1	0.53	0.26	146,146,146,146	0
56	MG	2A	3562	1/1	0.53	0.40	90,90,90,90	0
56	MG	1a	1706	1/1	0.53	0.65	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3579	1/1	0.53	0.68	115,115,115,115	0
56	MG	2A	3590	1/1	0.53	0.29	171,171,171,171	0
56	MG	1a	1634	1/1	0.53	0.60	117,117,117,117	0
56	MG	2a	1794	1/1	0.54	0.67	168,168,168,168	0
56	MG	1A	4809	1/1	0.54	0.99	58,58,58,58	0
56	MG	1A	4282	1/1	0.54	0.51	69,69,69,69	0
56	MG	2a	1826	1/1	0.54	0.52	162,162,162,162	0
56	MG	2A	3817	1/1	0.54	0.21	139,139,139,139	0
56	MG	1A	4756	1/1	0.54	0.75	106,106,106,106	0
56	MG	2A	3833	1/1	0.54	0.22	111,111,111,111	0
56	MG	2m	201	1/1	0.54	0.89	166,166,166,166	0
56	MG	1A	5014	1/1	0.54	0.42	71,71,71,71	0
56	MG	1A	4048	1/1	0.54	0.66	103,103,103,103	0
56	MG	2i	204	1/1	0.55	0.48	241,241,241,241	0
56	MG	1a	1682	1/1	0.55	0.62	197,197,197,197	0
56	MG	2a	1735	1/1	0.55	0.43	132,132,132,132	0
56	MG	1a	1895	1/1	0.55	0.38	121,121,121,121	0
56	MG	2a	1789	1/1	0.55	0.35	233,233,233,233	0
56	MG	2B	201	1/1	0.55	0.37	115,115,115,115	0
56	MG	2h	202	1/1	0.55	0.11	180,180,180,180	0
56	MG	2a	1768	1/1	0.55	0.43	260,260,260,260	0
56	MG	1A	4259	1/1	0.56	0.46	61,61,61,61	0
56	MG	2A	3206	1/1	0.56	0.48	120,120,120,120	0
56	MG	1A	4452	1/1	0.56	0.29	64,64,64,64	0
56	MG	2a	1636	1/1	0.56	0.38	150,150,150,150	0
56	MG	2x	103	1/1	0.56	0.57	192,192,192,192	0
56	MG	23	102	1/1	0.57	0.34	124,124,124,124	0
56	MG	2A	3502	1/1	0.57	0.46	104,104,104,104	0
56	MG	2O	301	1/1	0.57	0.15	136,136,136,136	0
56	MG	1A	4038	1/1	0.57	0.58	81,81,81,81	0
56	MG	2o	301	1/1	0.57	0.67	118,118,118,118	0
56	MG	2A	3832	1/1	0.57	0.27	121,121,121,121	0
56	MG	2A	3284	1/1	0.57	0.43	97,97,97,97	0
56	MG	2A	3137	1/1	0.57	0.42	134,134,134,134	0
56	MG	1a	1709	1/1	0.58	0.32	107,107,107,107	0
56	MG	2A	3403	1/1	0.58	0.61	219,219,219,219	0
56	MG	1a	1780	1/1	0.58	0.83	124,124,124,124	0
56	MG	1a	1731	1/1	0.58	0.26	136,136,136,136	0
56	MG	2g	206	1/1	0.58	0.53	216,216,216,216	0
56	MG	2A	3329	1/1	0.59	0.51	87,87,87,87	0
56	MG	2a	1885	1/1	0.59	0.32	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4519	1/1	0.59	0.66	94,94,94,94	0
56	MG	1a	1792	1/1	0.59	0.62	105,105,105,105	0
56	MG	1b	301	1/1	0.59	0.18	165,165,165,165	0
56	MG	2A	3762	1/1	0.59	0.23	124,124,124,124	0
56	MG	2a	1617	1/1	0.60	0.44	127,127,127,127	0
56	MG	2a	1624	1/1	0.60	0.38	137,137,137,137	0
56	MG	1A	4301	1/1	0.60	0.81	102,102,102,102	0
56	MG	1A	4323	1/1	0.60	0.76	85,85,85,85	0
56	MG	2a	1722	1/1	0.60	0.81	141,141,141,141	0
56	MG	2A	3257	1/1	0.60	0.48	87,87,87,87	0
56	MG	2a	1737	1/1	0.60	0.29	132,132,132,132	0
56	MG	2a	1753	1/1	0.60	0.46	138,138,138,138	0
56	MG	2a	1758	1/1	0.60	0.54	205,205,205,205	0
56	MG	2A	3030	1/1	0.60	0.96	97,97,97,97	0
56	MG	2a	1893	1/1	0.60	0.82	123,123,123,123	0
56	MG	1A	4723	1/1	0.60	0.37	77,77,77,77	0
56	MG	2B	205	1/1	0.60	0.35	119,119,119,119	0
56	MG	2v	703	1/1	0.60	0.25	154,154,154,154	0
56	MG	2A	3761	1/1	0.60	0.37	126,126,126,126	0
56	MG	2B	216	1/1	0.60	0.44	174,174,174,174	0
56	MG	1s	102	1/1	0.60	0.07	229,229,229,229	0
56	MG	28	101	1/1	0.60	1.11	109,109,109,109	0
56	MG	1a	1835	1/1	0.60	0.07	221,221,221,221	0
56	MG	1A	4343	1/1	0.60	0.29	71,71,71,71	0
56	MG	2A	3350	1/1	0.61	0.45	104,104,104,104	0
56	MG	2A	3402	1/1	0.61	0.44	112,112,112,112	0
56	MG	2a	1756	1/1	0.61	0.35	205,205,205,205	0
56	MG	2a	1868	1/1	0.61	0.35	144,144,144,144	0
56	MG	2A	3735	1/1	0.61	0.52	101,101,101,101	0
56	MG	1a	1653	1/1	0.61	0.34	119,119,119,119	0
56	MG	1m	201	1/1	0.61	0.63	216,216,216,216	0
56	MG	2x	106	1/1	0.62	0.26	211,211,211,211	0
56	MG	1a	1615	1/1	0.62	0.61	92,92,92,92	0
56	MG	2a	1913	1/1	0.62	0.24	246,246,246,246	0
56	MG	2B	230	1/1	0.62	0.59	151,151,151,151	0
56	MG	1a	1913	1/1	0.62	0.40	97,97,97,97	0
56	MG	2v	701	1/1	0.63	0.45	171,171,171,171	0
56	MG	2a	1666	1/1	0.63	0.43	133,133,133,133	0
56	MG	2A	3193	1/1	0.63	0.59	107,107,107,107	0
56	MG	28	104	1/1	0.63	0.17	110,110,110,110	0
56	MG	2F	302	1/1	0.63	0.33	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2a	1780	1/1	0.63	0.46	211,211,211,211	0
56	MG	1a	1875	1/1	0.63	0.63	118,118,118,118	0
56	MG	2A	3020	1/1	0.63	0.68	103,103,103,103	0
56	MG	1o	101	1/1	0.63	0.38	113,113,113,113	0
56	MG	2A	3546	1/1	0.64	0.40	97,97,97,97	0
56	MG	2a	1734	1/1	0.64	0.29	127,127,127,127	0
56	MG	2A	3208	1/1	0.64	0.25	118,118,118,118	0
56	MG	2A	3763	1/1	0.64	0.36	133,133,133,133	0
56	MG	1A	4550	1/1	0.64	0.62	89,89,89,89	0
56	MG	2l	202	1/1	0.64	0.27	150,150,150,150	0
56	MG	2a	1754	1/1	0.64	0.56	148,148,148,148	0
56	MG	2A	3529	1/1	0.64	0.47	118,118,118,118	0
56	MG	2A	3566	1/1	0.64	0.36	114,114,114,114	0
56	MG	1A	4138	1/1	0.64	0.36	72,72,72,72	0
56	MG	2A	3689	1/1	0.64	0.27	161,161,161,161	0
56	MG	2A	3112	1/1	0.64	0.97	136,136,136,136	0
56	MG	2A	3440	1/1	0.64	0.61	99,99,99,99	0
56	MG	2A	3383	1/1	0.65	0.40	100,100,100,100	0
56	MG	2A	3583	1/1	0.65	1.00	122,122,122,122	0
56	MG	2A	3831	1/1	0.65	0.35	128,128,128,128	0
56	MG	2A	3423	1/1	0.65	0.16	130,130,130,130	0
56	MG	2A	3724	1/1	0.65	0.43	91,91,91,91	0
56	MG	2a	1771	1/1	0.65	0.25	178,178,178,178	0
56	MG	2a	1773	1/1	0.65	0.32	228,228,228,228	0
56	MG	1a	1649	1/1	0.65	0.74	105,105,105,105	0
56	MG	2A	3802	1/1	0.65	0.36	108,108,108,108	0
56	MG	1a	1684	1/1	0.66	0.91	202,202,202,202	0
56	MG	2A	3612	1/1	0.66	0.43	136,136,136,136	0
56	MG	2a	1710	1/1	0.66	1.10	131,131,131,131	0
56	MG	2a	1711	1/1	0.66	0.37	149,149,149,149	0
56	MG	1A	4291	1/1	0.66	0.59	71,71,71,71	0
56	MG	2A	3094	1/1	0.66	0.55	113,113,113,113	0
56	MG	1D	308	1/1	0.66	0.72	77,77,77,77	0
56	MG	1A	4662	1/1	0.66	0.61	87,87,87,87	0
56	MG	2x	104	1/1	0.66	0.41	219,219,219,219	0
56	MG	1A	4678	1/1	0.66	0.52	86,86,86,86	0
56	MG	2A	3577	1/1	0.66	0.40	143,143,143,143	0
56	MG	2A	3027	1/1	0.66	1.06	123,123,123,123	0
56	MG	1A	4806	1/1	0.66	0.31	73,73,73,73	0
56	MG	1B	205	1/1	0.66	0.41	87,87,87,87	0
56	MG	2A	3758	1/1	0.66	0.09	211,211,211,211	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3076	1/1	0.67	0.93	113,113,113,113	0
56	MG	2A	3461	1/1	0.67	0.41	111,111,111,111	0
56	MG	1u	101	1/1	0.67	0.29	211,211,211,211	0
56	MG	1a	1765	1/1	0.67	0.72	125,125,125,125	0
56	MG	2a	1732	1/1	0.67	0.43	110,110,110,110	0
56	MG	2a	1634	1/1	0.67	0.44	120,120,120,120	0
56	MG	2A	3351	1/1	0.67	0.49	146,146,146,146	0
56	MG	1a	1845	1/1	0.67	0.46	234,234,234,234	0
56	MG	2E	302	1/1	0.67	0.28	96,96,96,96	0
56	MG	1A	4699	1/1	0.67	0.48	75,75,75,75	0
56	MG	2A	3614	1/1	0.67	0.40	102,102,102,102	0
56	MG	2A	3615	1/1	0.67	0.60	138,138,138,138	0
56	MG	2A	3808	1/1	0.67	0.55	173,173,173,173	0
56	MG	2A	3537	1/1	0.67	0.17	73,73,73,73	0
56	MG	1A	4027	1/1	0.67	0.68	62,62,62,62	0
56	MG	1a	1810	1/1	0.67	0.98	100,100,100,100	0
56	MG	2A	3645	1/1	0.67	0.30	116,116,116,116	0
56	MG	2c	301	1/1	0.67	0.17	225,225,225,225	0
56	MG	1A	4861	1/1	0.67	0.63	85,85,85,85	0
56	MG	2a	1697	1/1	0.67	0.24	136,136,136,136	0
56	MG	2A	3136	1/1	0.67	0.50	110,110,110,110	0
56	MG	2A	3263	1/1	0.67	0.67	89,89,89,89	0
56	MG	2g	204	1/1	0.67	0.28	216,216,216,216	0
56	MG	1A	5035	1/1	0.67	0.57	68,68,68,68	0
56	MG	2y	108	1/1	0.67	0.33	245,245,245,245	0
56	MG	2h	201	1/1	0.67	0.14	179,179,179,179	0
56	MG	1a	1807	1/1	0.68	0.36	100,100,100,100	0
56	MG	2a	1921	1/1	0.68	0.50	152,152,152,152	0
56	MG	1A	4970	1/1	0.68	0.35	89,89,89,89	0
56	MG	2A	3205	1/1	0.68	0.26	122,122,122,122	0
56	MG	2A	3828	1/1	0.68	0.44	126,126,126,126	0
56	MG	2a	1798	1/1	0.68	0.35	239,239,239,239	0
56	MG	1D	306	1/1	0.68	1.01	69,69,69,69	0
56	MG	1A	4973	1/1	0.68	0.49	80,80,80,80	0
56	MG	2a	1805	1/1	0.68	0.89	114,114,114,114	0
56	MG	1A	4535	1/1	0.68	0.49	77,77,77,77	0
56	MG	1A	4288	1/1	0.68	0.71	74,74,74,74	0
56	MG	1A	5055	1/1	0.68	0.26	133,133,133,133	0
56	MG	1a	1863	1/1	0.68	0.66	215,215,215,215	0
56	MG	1a	1794	1/1	0.68	0.93	84,84,84,84	0
56	MG	2A	3407	1/1	0.68	0.18	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2y	103	1/1	0.68	0.59	223,223,223,223	0
56	MG	1A	4691	1/1	0.68	0.33	81,81,81,81	0
56	MG	2B	221	1/1	0.68	0.55	122,122,122,122	0
56	MG	1a	1805	1/1	0.68	1.08	140,140,140,140	0
56	MG	2a	1625	1/1	0.69	0.52	148,148,148,148	0
56	MG	1a	1738	1/1	0.69	0.41	148,148,148,148	0
56	MG	1a	1739	1/1	0.69	0.25	144,144,144,144	0
56	MG	2a	1812	1/1	0.69	0.30	126,126,126,126	0
56	MG	1A	4859	1/1	0.69	0.29	72,72,72,72	0
56	MG	2A	3449	1/1	0.69	0.61	84,84,84,84	0
56	MG	1a	1656	1/1	0.69	0.33	102,102,102,102	0
56	MG	2A	3464	1/1	0.69	1.00	129,129,129,129	0
56	MG	1a	1704	1/1	0.69	0.55	125,125,125,125	0
56	MG	1a	1831	1/1	0.69	0.40	152,152,152,152	0
56	MG	2P	203	1/1	0.69	0.67	113,113,113,113	0
56	MG	1A	4600	1/1	0.69	0.58	78,78,78,78	0
56	MG	1B	206	1/1	0.69	0.21	71,71,71,71	0
56	MG	2A	3388	1/1	0.69	0.31	117,117,117,117	0
56	MG	2A	3389	1/1	0.69	0.71	117,117,117,117	0
56	MG	2A	3643	1/1	0.69	0.36	131,131,131,131	0
56	MG	1A	4747	1/1	0.69	0.80	84,84,84,84	0
56	MG	2A	3395	1/1	0.69	0.30	128,128,128,128	0
56	MG	2A	3397	1/1	0.69	0.48	189,189,189,189	0
56	MG	2A	3555	1/1	0.69	0.77	107,107,107,107	0
56	MG	1a	1645	1/1	0.69	0.26	127,127,127,127	0
56	MG	1d	301	1/1	0.69	0.77	128,128,128,128	0
56	MG	2a	1622	1/1	0.69	0.50	156,156,156,156	0
56	MG	2a	1718	1/1	0.69	0.65	136,136,136,136	0
56	MG	1A	4633	1/1	0.69	0.43	71,71,71,71	0
56	MG	1a	1909	1/1	0.70	0.57	136,136,136,136	0
56	MG	2A	3476	1/1	0.70	0.47	116,116,116,116	0
56	MG	2A	3798	1/1	0.70	0.50	98,98,98,98	0
56	MG	1y	105	1/1	0.70	0.29	180,180,180,180	0
56	MG	2A	3199	1/1	0.70	0.29	111,111,111,111	0
56	MG	2A	3398	1/1	0.70	0.40	155,155,155,155	0
56	MG	2A	3091	1/1	0.70	0.68	112,112,112,112	0
56	MG	1O	204	1/1	0.70	2.09	87,87,87,87	0
56	MG	2A	3717	1/1	0.70	0.29	108,108,108,108	0
56	MG	1A	4285	1/1	0.70	0.51	62,62,62,62	0
56	MG	2a	1910	1/1	0.70	0.19	240,240,240,240	0
56	MG	1a	1915	1/1	0.70	0.19	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4303	1/1	0.70	0.28	87,87,87,87	0
56	MG	1A	4706	1/1	0.70	0.44	68,68,68,68	0
56	MG	1a	1786	1/1	0.70	0.37	119,119,119,119	0
56	MG	1A	4714	1/1	0.70	0.61	99,99,99,99	0
56	MG	2A	3647	1/1	0.71	0.86	108,108,108,108	0
56	MG	2A	3675	1/1	0.71	0.57	123,123,123,123	0
56	MG	2A	3826	1/1	0.71	0.57	114,114,114,114	0
56	MG	1a	1884	1/1	0.71	0.39	122,122,122,122	0
56	MG	1a	1814	1/1	0.71	0.27	158,158,158,158	0
56	MG	12	101	1/1	0.71	0.50	84,84,84,84	0
56	MG	1a	1611	1/1	0.71	0.34	99,99,99,99	0
56	MG	2A	3412	1/1	0.71	0.27	105,105,105,105	0
56	MG	2A	3591	1/1	0.71	0.52	191,191,191,191	0
56	MG	1A	4639	1/1	0.71	0.45	71,71,71,71	0
56	MG	1a	1629	1/1	0.71	0.81	101,101,101,101	0
56	MG	2a	1673	1/1	0.71	0.88	167,167,167,167	0
56	MG	2g	205	1/1	0.71	0.22	211,211,211,211	0
56	MG	1a	1844	1/1	0.71	0.37	270,270,270,270	0
56	MG	2a	1676	1/1	0.71	0.45	163,163,163,163	0
56	MG	2A	3548	1/1	0.71	0.25	104,104,104,104	0
56	MG	1A	4888	1/1	0.71	0.43	69,69,69,69	0
56	MG	1A	4935	1/1	0.71	0.35	67,67,67,67	0
56	MG	1a	1672	1/1	0.71	0.28	99,99,99,99	0
56	MG	1A	5033	1/1	0.71	0.80	68,68,68,68	0
56	MG	2A	3477	1/1	0.71	0.49	126,126,126,126	0
56	MG	1a	1763	1/1	0.72	0.58	109,109,109,109	0
56	MG	20	101	1/1	0.72	0.39	128,128,128,128	0
56	MG	2A	3151	1/1	0.72	0.54	97,97,97,97	0
56	MG	2A	3155	1/1	0.72	0.50	100,100,100,100	0
56	MG	2A	3337	1/1	0.72	0.49	91,91,91,91	0
56	MG	2A	3173	1/1	0.72	0.38	87,87,87,87	0
56	MG	2A	3472	1/1	0.72	0.51	99,99,99,99	0
56	MG	19	101	1/1	0.72	0.28	71,71,71,71	0
56	MG	2a	1609	1/1	0.72	0.93	138,138,138,138	0
56	MG	2x	102	1/1	0.72	1.07	107,107,107,107	0
56	MG	1a	1860	1/1	0.72	0.11	214,214,214,214	0
56	MG	2A	3811	1/1	0.72	0.32	115,115,115,115	0
56	MG	2A	3613	1/1	0.72	0.24	122,122,122,122	0
56	MG	1A	4604	1/1	0.72	0.28	67,67,67,67	0
56	MG	2A	3719	1/1	0.72	0.47	134,134,134,134	0
56	MG	1a	1707	1/1	0.72	0.20	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3272	1/1	0.72	0.54	81,81,81,81	0
56	MG	2A	3752	1/1	0.72	0.39	117,117,117,117	0
56	MG	2A	3754	1/1	0.72	0.16	121,121,121,121	0
56	MG	2A	3572	1/1	0.72	0.53	182,182,182,182	0
56	MG	2a	1639	1/1	0.73	0.28	141,141,141,141	0
56	MG	2a	1648	1/1	0.73	0.74	124,124,124,124	0
56	MG	1A	4178	1/1	0.73	0.21	60,60,60,60	0
56	MG	2a	1657	1/1	0.73	0.32	138,138,138,138	0
56	MG	2A	3111	1/1	0.73	0.72	137,137,137,137	0
56	MG	2A	3486	1/1	0.73	0.44	141,141,141,141	0
56	MG	2A	3611	1/1	0.73	0.29	141,141,141,141	0
56	MG	1a	1859	1/1	0.73	0.27	207,207,207,207	0
56	MG	2A	3509	1/1	0.73	0.33	93,93,93,93	0
56	MG	2A	3025	1/1	0.73	1.33	118,118,118,118	0
56	MG	1A	4354	1/1	0.73	0.45	62,62,62,62	0
56	MG	2A	3624	1/1	0.73	0.64	156,156,156,156	0
56	MG	1A	4012	1/1	0.73	0.81	71,71,71,71	0
56	MG	2A	3066	1/1	0.73	0.32	125,125,125,125	0
56	MG	2Z	404	1/1	0.73	0.26	132,132,132,132	0
56	MG	1A	4521	1/1	0.73	0.57	79,79,79,79	0
56	MG	2A	3073	1/1	0.73	0.27	127,127,127,127	0
56	MG	2a	1703	1/1	0.73	0.34	157,157,157,157	0
56	MG	2A	3160	1/1	0.73	1.40	103,103,103,103	0
56	MG	1A	5053	1/1	0.73	0.25	275,275,275,275	0
56	MG	2A	3327	1/1	0.73	0.77	91,91,91,91	0
56	MG	13	301	1/1	0.73	0.45	65,65,65,65	0
56	MG	2a	1606	1/1	0.73	0.72	137,137,137,137	0
56	MG	2A	3333	1/1	0.73	0.26	98,98,98,98	0
56	MG	2a	1845	1/1	0.73	0.20	229,229,229,229	0
56	MG	2a	1608	1/1	0.73	0.81	135,135,135,135	0
56	MG	2a	1873	1/1	0.73	0.18	157,157,157,157	0
56	MG	2A	3428	1/1	0.73	0.18	166,166,166,166	0
56	MG	2A	3191	1/1	0.73	0.47	92,92,92,92	0
56	MG	1A	4927	1/1	0.73	0.49	87,87,87,87	0
56	MG	2A	3451	1/1	0.73	0.43	99,99,99,99	0
56	MG	1A	4330	1/1	0.73	0.31	77,77,77,77	0
56	MG	2a	1748	1/1	0.73	0.64	114,114,114,114	0
56	MG	2A	3372	1/1	0.73	0.25	107,107,107,107	0
56	MG	1A	4549	1/1	0.73	0.62	125,125,125,125	0
56	MG	2A	3753	1/1	0.73	0.35	97,97,97,97	0
56	MG	1A	4742	1/1	0.74	0.38	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2a	1623	1/1	0.74	0.22	182,182,182,182	0
56	MG	2A	3521	1/1	0.74	0.71	105,105,105,105	0
56	MG	2a	1713	1/1	0.74	0.92	143,143,143,143	0
56	MG	1A	4304	1/1	0.74	0.63	81,81,81,81	0
56	MG	1a	1864	1/1	0.74	0.39	211,211,211,211	0
56	MG	2a	1804	1/1	0.74	0.37	107,107,107,107	0
56	MG	2A	3617	1/1	0.74	0.38	102,102,102,102	0
56	MG	2A	3283	1/1	0.74	0.44	108,108,108,108	0
56	MG	1A	5012	1/1	0.74	0.34	115,115,115,115	0
56	MG	1A	4197	1/1	0.74	0.52	94,94,94,94	0
56	MG	1a	1834	1/1	0.74	0.29	210,210,210,210	0
56	MG	1A	4788	1/1	0.74	0.76	107,107,107,107	0
56	MG	2a	1658	1/1	0.74	0.35	122,122,122,122	0
56	MG	2r	302	1/1	0.74	0.25	149,149,149,149	0
56	MG	1A	4715	1/1	0.74	0.27	90,90,90,90	0
56	MG	2A	3431	1/1	0.74	0.82	93,93,93,93	0
56	MG	2A	3346	1/1	0.74	0.36	102,102,102,102	0
56	MG	2A	3077	1/1	0.74	0.70	108,108,108,108	0
56	MG	1A	4677	1/1	0.74	0.78	102,102,102,102	0
56	MG	2w	202	1/1	0.74	0.46	88,88,88,88	0
56	MG	1a	1687	1/1	0.74	0.36	118,118,118,118	0
56	MG	2a	1671	1/1	0.74	0.41	173,173,173,173	0
56	MG	1a	1853	1/1	0.74	0.20	225,225,225,225	0
56	MG	1A	4733	1/1	0.74	0.15	82,82,82,82	0
56	MG	1a	1856	1/1	0.74	0.69	227,227,227,227	0
56	MG	1y	106	1/1	0.74	0.27	173,173,173,173	0
56	MG	1a	1857	1/1	0.74	0.20	211,211,211,211	0
56	MG	2A	3018	1/1	0.74	0.42	124,124,124,124	0
56	MG	2A	3508	1/1	0.74	0.28	97,97,97,97	0
56	MG	2a	1610	1/1	0.74	0.38	141,141,141,141	0
56	MG	1A	4960	1/1	0.74	0.46	91,91,91,91	0
56	MG	2A	3789	1/1	0.75	0.61	97,97,97,97	0
56	MG	2A	3028	1/1	0.75	0.82	133,133,133,133	0
56	MG	2h	203	1/1	0.75	1.01	144,144,144,144	0
56	MG	1a	1912	1/1	0.75	1.11	131,131,131,131	0
56	MG	1A	4948	1/1	0.75	0.70	62,62,62,62	0
56	MG	2A	3408	1/1	0.75	0.26	129,129,129,129	0
56	MG	2A	3582	1/1	0.75	0.71	106,106,106,106	0
56	MG	1A	4768	1/1	0.75	0.31	65,65,65,65	0
56	MG	1A	4538	1/1	0.75	0.84	83,83,83,83	0
56	MG	1a	1796	1/1	0.75	0.36	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2Z	403	1/1	0.75	0.90	130,130,130,130	0
56	MG	2A	3706	1/1	0.75	0.33	94,94,94,94	0
56	MG	2A	3593	1/1	0.75	0.12	129,129,129,129	0
56	MG	23	101	1/1	0.75	0.72	104,104,104,104	0
56	MG	1a	1688	1/1	0.75	0.67	131,131,131,131	0
56	MG	1A	4202	1/1	0.75	0.61	95,95,95,95	0
56	MG	1A	4182	1/1	0.75	0.30	58,58,58,58	0
56	MG	2A	3176	1/1	0.75	0.99	114,114,114,114	0
56	MG	1A	4900	1/1	0.75	0.33	81,81,81,81	0
56	MG	2B	215	1/1	0.75	0.25	164,164,164,164	0
56	MG	1A	4134	1/1	0.75	0.71	72,72,72,72	0
56	MG	1A	4762	1/1	0.75	0.49	71,71,71,71	0
56	MG	2A	3470	1/1	0.75	0.61	104,104,104,104	0
56	MG	2d	301	1/1	0.75	0.51	147,147,147,147	0
56	MG	2A	3299	1/1	0.75	0.56	91,91,91,91	0
56	MG	2f	302	1/1	0.75	0.26	143,143,143,143	0
56	MG	2a	1688	1/1	0.75	0.48	153,153,153,153	0
56	MG	2A	3307	1/1	0.75	1.09	92,92,92,92	0
56	MG	2a	1618	1/1	0.75	0.31	145,145,145,145	0
56	MG	2a	1620	1/1	0.75	0.52	151,151,151,151	0
56	MG	10	101	1/1	0.75	0.43	64,64,64,64	0
56	MG	2A	3783	1/1	0.75	0.79	139,139,139,139	0
56	MG	2z	103	1/1	0.75	1.01	179,179,179,179	0
56	MG	1Z	305	1/1	0.76	0.35	72,72,72,72	0
56	MG	1a	1742	1/1	0.76	0.54	106,106,106,106	0
56	MG	2a	1791	1/1	0.76	0.50	239,239,239,239	0
56	MG	2a	1792	1/1	0.76	0.08	250,250,250,250	0
56	MG	1a	1751	1/1	0.76	0.28	131,131,131,131	0
56	MG	1a	1837	1/1	0.76	0.28	226,226,226,226	0
56	MG	1a	1752	1/1	0.76	0.44	128,128,128,128	0
56	MG	1A	4884	1/1	0.76	0.42	84,84,84,84	0
56	MG	2a	1628	1/1	0.76	0.41	161,161,161,161	0
56	MG	1A	4764	1/1	0.76	0.52	64,64,64,64	0
56	MG	1A	4767	1/1	0.76	0.32	80,80,80,80	0
56	MG	1A	4428	1/1	0.76	1.28	59,59,59,59	0
56	MG	1A	4780	1/1	0.76	0.14	76,76,76,76	0
56	MG	1A	4546	1/1	0.76	0.57	104,104,104,104	0
56	MG	1A	4006	1/1	0.76	0.37	59,59,59,59	0
56	MG	2a	1854	1/1	0.76	0.13	286,286,286,286	0
56	MG	2A	3539	1/1	0.76	0.17	125,125,125,125	0
56	MG	1A	4746	1/1	0.76	0.29	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2a	1881	1/1	0.76	0.40	171,171,171,171	0
56	MG	1B	212	1/1	0.76	0.62	87,87,87,87	0
56	MG	1a	1642	1/1	0.76	0.64	112,112,112,112	0
56	MG	1A	4609	1/1	0.76	0.39	70,70,70,70	0
56	MG	1a	1708	1/1	0.76	0.13	108,108,108,108	0
56	MG	2A	3319	1/1	0.76	0.64	87,87,87,87	0
56	MG	1A	4966	1/1	0.76	0.48	83,83,83,83	0
56	MG	1a	1898	1/1	0.76	1.10	108,108,108,108	0
56	MG	2a	1918	1/1	0.76	0.58	138,138,138,138	0
56	MG	1A	4622	1/1	0.76	0.38	115,115,115,115	0
56	MG	1A	4721	1/1	0.76	0.27	82,82,82,82	0
56	MG	1a	1901	1/1	0.76	0.22	113,113,113,113	0
56	MG	2e	201	1/1	0.76	0.52	122,122,122,122	0
56	MG	1a	1659	1/1	0.76	0.24	118,118,118,118	0
56	MG	1a	1820	1/1	0.76	0.32	205,205,205,205	0
56	MG	2A	3738	1/1	0.76	0.29	96,96,96,96	0
56	MG	2B	218	1/1	0.76	0.44	171,171,171,171	0
56	MG	1P	202	1/1	0.76	0.70	60,60,60,60	0
56	MG	2A	3107	1/1	0.77	0.45	166,166,166,166	0
56	MG	2a	1675	1/1	0.77	0.32	166,166,166,166	0
56	MG	2D	301	1/1	0.77	0.33	74,74,74,74	0
56	MG	1a	1621	1/1	0.77	0.81	97,97,97,97	0
56	MG	1A	5052	1/1	0.77	0.39	267,267,267,267	0
56	MG	1A	4373	1/1	0.77	0.42	64,64,64,64	0
56	MG	1a	1852	1/1	0.77	0.53	224,224,224,224	0
56	MG	1A	4075	1/1	0.77	0.58	83,83,83,83	0
56	MG	2a	1769	1/1	0.77	0.31	269,269,269,269	0
56	MG	1a	1812	1/1	0.77	0.33	88,88,88,88	0
56	MG	1A	4242	1/1	0.77	0.38	71,71,71,71	0
56	MG	10	104	1/1	0.77	0.42	79,79,79,79	0
56	MG	1A	4895	1/1	0.77	1.00	59,59,59,59	0
56	MG	1A	4329	1/1	0.77	0.31	73,73,73,73	0
56	MG	2B	203	1/1	0.77	0.54	131,131,131,131	0
56	MG	2B	204	1/1	0.77	0.25	130,130,130,130	0
56	MG	2a	1790	1/1	0.77	0.13	249,249,249,249	0
56	MG	20	104	1/1	0.77	0.14	122,122,122,122	0
56	MG	2A	3174	1/1	0.77	0.38	109,109,109,109	0
56	MG	1a	1833	1/1	0.77	0.28	201,201,201,201	0
56	MG	1A	4736	1/1	0.77	0.28	61,61,61,61	0
56	MG	2A	3482	1/1	0.77	0.49	117,117,117,117	0
56	MG	2A	3305	1/1	0.77	0.69	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1a	1867	1/1	0.77	0.11	227,227,227,227	0
56	MG	1A	4647	1/1	0.77	0.34	68,68,68,68	0
56	MG	1A	4361	1/1	0.77	0.25	84,84,84,84	0
56	MG	2A	3204	1/1	0.77	0.55	111,111,111,111	0
56	MG	2A	3801	1/1	0.77	0.13	128,128,128,128	0
56	MG	2a	1757	1/1	0.77	0.28	211,211,211,211	0
56	MG	1A	4689	1/1	0.78	0.26	89,89,89,89	0
56	MG	1A	4297	1/1	0.78	0.39	99,99,99,99	0
56	MG	2a	1912	1/1	0.78	0.42	137,137,137,137	0
56	MG	1a	1911	1/1	0.78	0.78	105,105,105,105	0
56	MG	1a	1705	1/1	0.78	0.36	122,122,122,122	0
56	MG	1A	4068	1/1	0.78	0.73	84,84,84,84	0
56	MG	2A	3695	1/1	0.78	0.62	84,84,84,84	0
56	MG	2A	3131	1/1	0.78	1.02	130,130,130,130	0
56	MG	2A	3416	1/1	0.78	0.37	114,114,114,114	0
56	MG	2A	3021	1/1	0.78	0.96	112,112,112,112	0
56	MG	1A	4500	1/1	0.78	0.39	69,69,69,69	0
56	MG	2A	3146	1/1	0.78	0.61	87,87,87,87	0
56	MG	2A	3302	1/1	0.78	0.53	100,100,100,100	0
56	MG	2a	1651	1/1	0.78	0.14	142,142,142,142	0
56	MG	2A	3739	1/1	0.78	0.69	103,103,103,103	0
56	MG	2A	3747	1/1	0.78	0.25	107,107,107,107	0
56	MG	2A	3576	1/1	0.78	0.38	151,151,151,151	0
56	MG	1a	1606	1/1	0.78	0.15	115,115,115,115	0
56	MG	2A	3442	1/1	0.78	0.38	108,108,108,108	0
56	MG	1B	214	1/1	0.78	0.48	69,69,69,69	0
56	MG	2h	204	1/1	0.78	0.13	164,164,164,164	0
56	MG	1a	1865	1/1	0.78	0.08	224,224,224,224	0
56	MG	2A	3161	1/1	0.78	1.06	100,100,100,100	0
56	MG	1g	301	1/1	0.78	0.21	186,186,186,186	0
56	MG	1A	4985	1/1	0.78	0.99	73,73,73,73	0
56	MG	2T	301	1/1	0.78	0.20	124,124,124,124	0
56	MG	2A	3781	1/1	0.78	0.20	80,80,80,80	0
56	MG	1A	4579	1/1	0.78	0.34	56,56,56,56	0
56	MG	2A	3338	1/1	0.78	0.37	86,86,86,86	0
56	MG	2A	3181	1/1	0.78	0.32	114,114,114,114	0
56	MG	2a	1683	1/1	0.78	0.82	158,158,158,158	0
56	MG	2q	201	1/1	0.78	0.57	124,124,124,124	0
56	MG	1A	4009	1/1	0.78	0.79	79,79,79,79	0
56	MG	2A	3800	1/1	0.78	0.87	151,151,151,151	0
56	MG	1a	1840	1/1	0.78	0.09	237,237,237,237	0
56	MG	2a	1696	1/1	0.78	0.35	161,161,161,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4121	1/1	0.78	0.49	81,81,81,81	0
56	MG	2a	1821	1/1	0.78	0.20	143,143,143,143	0
56	MG	2a	1824	1/1	0.78	0.37	158,158,158,158	0
56	MG	1A	4933	1/1	0.78	0.65	102,102,102,102	0
56	MG	2A	3084	1/1	0.78	0.50	115,115,115,115	0
56	MG	1A	4540	1/1	0.78	0.35	77,77,77,77	0
56	MG	1a	1850	1/1	0.78	0.76	113,113,113,113	0
56	MG	2a	1604	1/1	0.78	0.18	148,148,148,148	0
56	MG	1a	1745	1/1	0.78	0.52	122,122,122,122	0
56	MG	2A	3244	1/1	0.78	0.24	104,104,104,104	0
56	MG	1A	4765	1/1	0.78	0.67	60,60,60,60	0
56	MG	2A	3105	1/1	0.78	0.53	155,155,155,155	0
56	MG	2A	3661	1/1	0.78	0.27	105,105,105,105	0
56	MG	2A	3834	1/1	0.78	0.14	115,115,115,115	0
56	MG	2a	1733	1/1	0.78	0.18	125,125,125,125	0
56	MG	2a	1905	1/1	0.78	0.97	218,218,218,218	0
56	MG	1A	4950	1/1	0.79	0.22	61,61,61,61	0
56	MG	1A	4047	1/1	0.79	0.44	69,69,69,69	0
56	MG	1a	1686	1/1	0.79	0.18	116,116,116,116	0
56	MG	1A	4464	1/1	0.79	0.43	66,66,66,66	0
56	MG	2A	3194	1/1	0.79	0.17	109,109,109,109	0
56	MG	1a	1622	1/1	0.79	0.98	99,99,99,99	0
56	MG	2A	3465	1/1	0.79	0.64	129,129,129,129	0
56	MG	1A	4153	1/1	0.79	0.29	55,55,55,55	0
56	MG	2a	1745	1/1	0.79	0.16	162,162,162,162	0
56	MG	1A	4667	1/1	0.79	0.24	75,75,75,75	0
56	MG	2a	1663	1/1	0.79	0.79	143,143,143,143	0
56	MG	1A	4327	1/1	0.79	0.31	66,66,66,66	0
56	MG	2A	3841	1/1	0.79	0.32	146,146,146,146	0
56	MG	1A	5006	1/1	0.79	0.81	74,74,74,74	0
56	MG	2a	1876	1/1	0.79	0.32	147,147,147,147	0
56	MG	27	101	1/1	0.79	0.63	90,90,90,90	0
56	MG	1y	101	1/1	0.79	0.33	87,87,87,87	0
56	MG	1A	4511	1/1	0.79	0.39	68,68,68,68	0
56	MG	1A	4772	1/1	0.79	0.46	70,70,70,70	0
56	MG	1P	203	1/1	0.79	0.23	68,68,68,68	0
56	MG	2a	1901	1/1	0.79	0.90	171,171,171,171	0
56	MG	1Q	201	1/1	0.79	0.44	70,70,70,70	0
56	MG	2A	3512	1/1	0.79	0.42	94,94,94,94	0
56	MG	2A	3019	1/1	0.79	0.90	112,112,112,112	0
56	MG	1A	4681	1/1	0.79	0.25	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4616	1/1	0.79	0.23	86,86,86,86	0
56	MG	1A	5051	1/1	0.79	0.20	192,192,192,192	0
56	MG	1b	304	1/1	0.79	0.44	173,173,173,173	0
56	MG	1A	4036	1/1	0.79	0.72	76,76,76,76	0
56	MG	2a	1700	1/1	0.79	0.73	140,140,140,140	0
56	MG	2x	107	1/1	0.79	1.42	131,131,131,131	0
56	MG	1A	4042	1/1	0.79	0.29	58,58,58,58	0
56	MG	1d	305	1/1	0.79	0.26	142,142,142,142	0
56	MG	2A	3034	1/1	0.79	0.86	100,100,100,100	0
56	MG	2A	3057	1/1	0.79	0.73	96,96,96,96	0
56	MG	1A	5054	1/1	0.79	0.30	142,142,142,142	0
56	MG	1A	4750	1/1	0.79	0.37	68,68,68,68	0
56	MG	2A	3805	1/1	0.79	0.26	100,100,100,100	0
57	ZN	2Y	203	1/1	0.79	0.08	153,153,153,153	0
56	MG	2a	1682	1/1	0.80	0.66	131,131,131,131	0
56	MG	1A	4822	1/1	0.80	0.61	82,82,82,82	0
56	MG	1R	203	1/1	0.80	0.90	52,52,52,52	0
56	MG	2A	3133	1/1	0.80	1.15	143,143,143,143	0
56	MG	2A	3732	1/1	0.80	0.32	95,95,95,95	0
56	MG	1Z	301	1/1	0.80	0.39	80,80,80,80	0
56	MG	1A	4192	1/1	0.80	0.37	68,68,68,68	0
56	MG	2A	3142	1/1	0.80	1.06	102,102,102,102	0
56	MG	2B	213	1/1	0.80	0.26	151,151,151,151	0
56	MG	2A	3745	1/1	0.80	0.44	112,112,112,112	0
56	MG	2A	3143	1/1	0.80	0.35	89,89,89,89	0
56	MG	1A	4404	1/1	0.80	0.55	70,70,70,70	0
56	MG	2i	203	1/1	0.80	0.12	234,234,234,234	0
56	MG	2A	3608	1/1	0.80	0.21	111,111,111,111	0
56	MG	1A	4962	1/1	0.80	0.53	69,69,69,69	0
56	MG	2a	1808	1/1	0.80	0.56	102,102,102,102	0
56	MG	1a	1666	1/1	0.80	0.32	116,116,116,116	0
56	MG	1A	4275	1/1	0.80	0.33	65,65,65,65	0
56	MG	1A	4514	1/1	0.80	0.46	81,81,81,81	0
56	MG	2a	1719	1/1	0.80	0.13	151,151,151,151	0
56	MG	2A	3168	1/1	0.80	0.61	90,90,90,90	0
56	MG	2A	3768	1/1	0.80	0.30	90,90,90,90	0
56	MG	1A	4621	1/1	0.80	0.55	114,114,114,114	0
56	MG	2F	301	1/1	0.80	0.27	133,133,133,133	0
56	MG	2a	1860	1/1	0.80	0.47	153,153,153,153	0
56	MG	1A	4126	1/1	0.80	0.40	78,78,78,78	0
56	MG	1A	4294	1/1	0.80	0.36	84,84,84,84	0
56	MG	2A	3312	1/1	0.80	0.33	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3632	1/1	0.80	0.77	110,110,110,110	0
56	MG	2A	3637	1/1	0.80	0.45	88,88,88,88	0
56	MG	1A	4696	1/1	0.80	0.26	72,72,72,72	0
56	MG	1D	307	1/1	0.80	0.16	99,99,99,99	0
56	MG	2A	3550	1/1	0.80	0.21	104,104,104,104	0
56	MG	2A	3188	1/1	0.80	0.27	103,103,103,103	0
56	MG	1a	1819	1/1	0.80	0.34	204,204,204,204	0
56	MG	1A	4917	1/1	0.80	1.15	62,62,62,62	0
56	MG	1A	4485	1/1	0.80	0.19	61,61,61,61	0
56	MG	1a	1829	1/1	0.80	0.11	194,194,194,194	0
56	MG	1A	4700	1/1	0.80	0.25	79,79,79,79	0
56	MG	2A	3573	1/1	0.80	0.23	282,282,282,282	0
56	MG	2A	3023	1/1	0.80	0.77	120,120,120,120	0
56	MG	1A	4520	1/1	0.80	0.49	75,75,75,75	0
56	MG	2A	3713	1/1	0.80	0.19	112,112,112,112	0
56	MG	2a	1678	1/1	0.80	0.41	167,167,167,167	0
56	MG	2a	1775	1/1	0.80	0.30	208,208,208,208	0
56	MG	1a	1601	1/1	0.81	0.22	73,73,73,73	0
56	MG	1A	4626	1/1	0.81	0.49	95,95,95,95	0
56	MG	2a	1635	1/1	0.81	0.12	147,147,147,147	0
56	MG	2a	1796	1/1	0.81	0.41	111,111,111,111	0
56	MG	1a	1677	1/1	0.81	0.52	157,157,157,157	0
56	MG	2A	3242	1/1	0.81	0.21	106,106,106,106	0
56	MG	1A	5020	1/1	0.81	0.57	69,69,69,69	0
56	MG	2a	1649	1/1	0.81	0.30	143,143,143,143	0
56	MG	1A	4395	1/1	0.81	0.43	63,63,63,63	0
56	MG	2a	1729	1/1	0.81	0.28	124,124,124,124	0
56	MG	1A	4942	1/1	0.81	0.18	79,79,79,79	0
56	MG	1a	1827	1/1	0.81	0.24	190,190,190,190	0
56	MG	1a	1828	1/1	0.81	0.34	175,175,175,175	0
56	MG	2l	201	1/1	0.81	0.48	132,132,132,132	0
56	MG	2A	3487	1/1	0.81	0.23	145,145,145,145	0
56	MG	2A	3062	1/1	0.81	0.31	85,85,85,85	0
56	MG	1A	4881	1/1	0.81	0.40	82,82,82,82	0
56	MG	2a	1746	1/1	0.81	0.37	120,120,120,120	0
56	MG	1A	4697	1/1	0.81	0.87	68,68,68,68	0
56	MG	1A	4584	1/1	0.81	0.39	105,105,105,105	0
56	MG	1A	4730	1/1	0.81	0.69	71,71,71,71	0
56	MG	2a	1869	1/1	0.81	0.50	151,151,151,151	0
56	MG	2A	3609	1/1	0.81	0.15	132,132,132,132	0
56	MG	1a	1699	1/1	0.81	0.31	118,118,118,118	0
56	MG	2a	1672	1/1	0.81	0.38	181,181,181,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3742	1/1	0.81	0.45	91,91,91,91	0
56	MG	2A	3528	1/1	0.81	0.25	106,106,106,106	0
56	MG	1V	201	1/1	0.81	0.42	74,74,74,74	0
56	MG	2A	3751	1/1	0.81	0.12	101,101,101,101	0
56	MG	1A	4374	1/1	0.81	0.40	94,94,94,94	0
56	MG	2a	1904	1/1	0.81	0.26	245,245,245,245	0
56	MG	1A	5059	1/1	0.81	0.45	86,86,86,86	0
56	MG	2a	1906	1/1	0.81	0.22	240,240,240,240	0
56	MG	1A	4495	1/1	0.81	0.61	78,78,78,78	0
56	MG	1A	4712	1/1	0.81	0.30	76,76,76,76	0
56	MG	1A	4916	1/1	0.81	0.22	73,73,73,73	0
56	MG	2A	3101	1/1	0.81	0.59	133,133,133,133	0
56	MG	1A	4834	1/1	0.81	0.53	72,72,72,72	0
56	MG	17	103	1/1	0.81	0.56	73,73,73,73	0
56	MG	1A	4848	1/1	0.81	0.33	74,74,74,74	0
56	MG	2A	3640	1/1	0.81	0.36	127,127,127,127	0
56	MG	2A	3642	1/1	0.81	0.33	132,132,132,132	0
56	MG	1a	1809	1/1	0.81	0.31	127,127,127,127	0
56	MG	2y	110	1/1	0.81	0.40	248,248,248,248	0
56	MG	2A	3340	1/1	0.81	0.69	75,75,75,75	0
56	MG	2f	304	1/1	0.81	0.77	137,137,137,137	0
56	MG	29	101	1/1	0.82	0.20	130,130,130,130	0
56	MG	2a	1782	1/1	0.82	1.08	205,205,205,205	0
56	MG	2a	1783	1/1	0.82	1.14	174,174,174,174	0
56	MG	1S	202	1/1	0.82	1.27	92,92,92,92	0
56	MG	1A	4524	1/1	0.82	0.35	74,74,74,74	0
56	MG	1A	4862	1/1	0.82	0.65	74,74,74,74	0
56	MG	2a	1695	1/1	0.82	0.77	146,146,146,146	0
56	MG	1a	1735	1/1	0.82	0.57	150,150,150,150	0
56	MG	2A	3347	1/1	0.82	0.28	99,99,99,99	0
56	MG	1A	4453	1/1	0.82	0.21	66,66,66,66	0
56	MG	1A	4163	1/1	0.82	0.19	57,57,57,57	0
56	MG	2A	3358	1/1	0.82	0.16	97,97,97,97	0
56	MG	2a	1799	1/1	0.82	0.26	238,238,238,238	0
56	MG	1B	202	1/1	0.82	0.18	114,114,114,114	0
56	MG	1B	203	1/1	0.82	0.50	95,95,95,95	0
56	MG	1A	4785	1/1	0.82	1.19	70,70,70,70	0
56	MG	2k	201	1/1	0.82	0.21	158,158,158,158	0
56	MG	1a	1674	1/1	0.82	0.19	134,134,134,134	0
56	MG	1A	4402	1/1	0.82	0.15	73,73,73,73	0
56	MG	1A	4710	1/1	0.82	0.34	73,73,73,73	0
56	MG	2B	223	1/1	0.82	0.17	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4802	1/1	0.82	0.40	73,73,73,73	0
56	MG	2A	3393	1/1	0.82	0.29	132,132,132,132	0
56	MG	2a	1723	1/1	0.82	1.05	118,118,118,118	0
56	MG	1a	1771	1/1	0.82	0.35	135,135,135,135	0
56	MG	1A	4997	1/1	0.82	0.15	80,80,80,80	0
56	MG	1A	4087	1/1	0.82	0.32	69,69,69,69	0
56	MG	2q	202	1/1	0.82	0.37	149,149,149,149	0
56	MG	2A	3269	1/1	0.82	0.40	94,94,94,94	0
56	MG	2E	303	1/1	0.82	0.29	81,81,81,81	0
56	MG	2A	3635	1/1	0.82	0.31	103,103,103,103	0
56	MG	2A	3773	1/1	0.82	0.22	115,115,115,115	0
56	MG	1A	4010	1/1	0.82	0.48	73,73,73,73	0
56	MG	1a	1916	1/1	0.82	0.41	146,146,146,146	0
56	MG	2A	3785	1/1	0.82	0.34	119,119,119,119	0
56	MG	1A	4820	1/1	0.82	0.45	72,72,72,72	0
56	MG	1A	4920	1/1	0.82	0.33	61,61,61,61	0
56	MG	2A	3414	1/1	0.82	0.52	117,117,117,117	0
56	MG	1O	205	1/1	0.82	0.34	112,112,112,112	0
56	MG	1A	4040	1/1	0.82	0.16	93,93,93,93	0
56	MG	2A	3654	1/1	0.82	1.27	115,115,115,115	0
56	MG	1A	4562	1/1	0.82	0.40	65,65,65,65	0
56	MG	2A	3673	1/1	0.82	0.80	133,133,133,133	0
56	MG	1a	1798	1/1	0.82	0.45	118,118,118,118	0
56	MG	1a	1802	1/1	0.82	0.58	142,142,142,142	0
56	MG	1A	4631	1/1	0.82	0.39	70,70,70,70	0
56	MG	1R	201	1/1	0.82	0.54	68,68,68,68	0
56	MG	2A	3446	1/1	0.82	0.85	84,84,84,84	0
56	MG	1a	1646	1/1	0.82	0.80	116,116,116,116	0
56	MG	2z	102	1/1	0.82	0.14	175,175,175,175	0
56	MG	2a	1680	1/1	0.82	0.42	162,162,162,162	0
56	MG	1A	4505	1/1	0.82	0.40	92,92,92,92	0
56	MG	1v	701	1/1	0.83	0.74	117,117,117,117	0
56	MG	2a	1647	1/1	0.83	0.37	139,139,139,139	0
56	MG	1A	4763	1/1	0.83	0.26	69,69,69,69	0
56	MG	1A	4165	1/1	0.83	0.40	56,56,56,56	0
56	MG	1A	4858	1/1	0.83	1.08	58,58,58,58	0
56	MG	1a	1734	1/1	0.83	0.74	147,147,147,147	0
56	MG	2A	3015	1/1	0.83	0.69	112,112,112,112	0
56	MG	2A	3106	1/1	0.83	0.40	170,170,170,170	0
56	MG	1a	1801	1/1	0.83	0.35	105,105,105,105	0
56	MG	1T	204	1/1	0.83	0.28	115,115,115,115	0
56	MG	1a	1623	1/1	0.83	0.13	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3214	1/1	0.83	0.35	93,93,93,93	0
56	MG	2A	3497	1/1	0.83	0.59	79,79,79,79	0
56	MG	2A	3767	1/1	0.83	0.64	93,93,93,93	0
56	MG	2A	3367	1/1	0.83	0.34	92,92,92,92	0
56	MG	2A	3217	1/1	0.83	0.30	91,91,91,91	0
56	MG	2Q	201	1/1	0.83	0.26	126,126,126,126	0
56	MG	2A	3221	1/1	0.83	0.20	114,114,114,114	0
56	MG	2A	3224	1/1	0.83	0.22	119,119,119,119	0
56	MG	1A	5024	1/1	0.83	0.27	55,55,55,55	0
56	MG	1A	4703	1/1	0.83	0.55	64,64,64,64	0
56	MG	2V	201	1/1	0.83	0.34	129,129,129,129	0
56	MG	1a	1917	1/1	0.83	0.24	128,128,128,128	0
56	MG	2A	3793	1/1	0.83	0.45	116,116,116,116	0
56	MG	1a	1636	1/1	0.83	0.19	120,120,120,120	0
56	MG	1A	4094	1/1	0.83	0.29	68,68,68,68	0
56	MG	20	103	1/1	0.83	0.48	97,97,97,97	0
56	MG	2A	3532	1/1	0.83	0.24	118,118,118,118	0
56	MG	2A	3533	1/1	0.83	0.41	124,124,124,124	0
56	MG	2A	3249	1/1	0.83	0.32	128,128,128,128	0
56	MG	1A	5036	1/1	0.83	0.20	72,72,72,72	0
56	MG	2A	3649	1/1	0.83	0.57	110,110,110,110	0
56	MG	1A	4130	1/1	0.83	0.49	58,58,58,58	0
56	MG	1A	4219	1/1	0.83	0.44	61,61,61,61	0
56	MG	2A	3823	1/1	0.83	0.41	95,95,95,95	0
56	MG	2A	3664	1/1	0.83	0.31	112,112,112,112	0
56	MG	2A	3672	1/1	0.83	0.11	120,120,120,120	0
56	MG	2A	3264	1/1	0.83	0.59	81,81,81,81	0
56	MG	1a	1767	1/1	0.83	0.29	133,133,133,133	0
56	MG	2a	1838	1/1	0.83	0.06	244,244,244,244	0
56	MG	1a	1822	1/1	0.83	0.11	215,215,215,215	0
56	MG	2A	3152	1/1	0.83	0.25	96,96,96,96	0
56	MG	2a	1849	1/1	0.83	0.13	142,142,142,142	0
56	MG	2a	1853	1/1	0.83	0.41	269,269,269,269	0
56	MG	1A	4812	1/1	0.83	0.30	72,72,72,72	0
56	MG	2a	1857	1/1	0.83	0.19	145,145,145,145	0
56	MG	2a	1612	1/1	0.83	0.32	141,141,141,141	0
56	MG	1A	4987	1/1	0.83	0.42	62,62,62,62	0
56	MG	2A	3842	1/1	0.83	0.25	99,99,99,99	0
56	MG	2A	3292	1/1	0.83	0.75	79,79,79,79	0
56	MG	2A	3298	1/1	0.83	0.58	94,94,94,94	0
56	MG	2A	3424	1/1	0.83	0.35	142,142,142,142	0
56	MG	1a	1775	1/1	0.83	0.32	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2B	207	1/1	0.83	1.03	161,161,161,161	0
56	MG	18	102	1/1	0.83	0.33	66,66,66,66	0
56	MG	2a	1894	1/1	0.83	0.47	151,151,151,151	0
56	MG	1A	4988	1/1	0.83	0.50	79,79,79,79	0
56	MG	1a	1662	1/1	0.83	0.37	123,123,123,123	0
56	MG	1A	4776	1/1	0.83	0.65	96,96,96,96	0
56	MG	2a	1749	1/1	0.83	0.39	115,115,115,115	0
56	MG	1A	4305	1/1	0.83	0.58	82,82,82,82	0
57	ZN	24	102	1/1	0.83	0.08	230,230,230,230	0
56	MG	2A	3222	1/1	0.84	0.54	112,112,112,112	0
56	MG	1A	4265	1/1	0.84	0.37	61,61,61,61	0
56	MG	2A	3381	1/1	0.84	0.23	98,98,98,98	0
56	MG	2N	201	1/1	0.84	0.48	113,113,113,113	0
56	MG	1a	1770	1/1	0.84	0.42	101,101,101,101	0
56	MG	1A	4396	1/1	0.84	0.26	72,72,72,72	0
56	MG	1T	205	1/1	0.84	0.30	109,109,109,109	0
56	MG	2f	301	1/1	0.84	0.70	138,138,138,138	0
56	MG	1A	4610	1/1	0.84	0.19	60,60,60,60	0
56	MG	2A	3516	1/1	0.84	0.67	82,82,82,82	0
56	MG	2a	1779	1/1	0.84	0.53	183,183,183,183	0
56	MG	1a	1626	1/1	0.84	0.68	98,98,98,98	0
56	MG	1A	4013	1/1	0.84	0.36	81,81,81,81	0
56	MG	1A	4403	1/1	0.84	0.36	62,62,62,62	0
56	MG	2Y	201	1/1	0.84	0.75	113,113,113,113	0
56	MG	2A	3255	1/1	0.84	0.21	126,126,126,126	0
56	MG	1a	1784	1/1	0.84	0.67	124,124,124,124	0
56	MG	1a	1869	1/1	0.84	0.09	226,226,226,226	0
56	MG	2A	3399	1/1	0.84	0.43	194,194,194,194	0
56	MG	1a	1678	1/1	0.84	0.21	162,162,162,162	0
56	MG	2i	201	1/1	0.84	0.58	245,245,245,245	0
56	MG	1i	201	1/1	0.84	0.38	212,212,212,212	0
56	MG	2A	3043	1/1	0.84	0.27	113,113,113,113	0
56	MG	1l	301	1/1	0.84	0.63	133,133,133,133	0
56	MG	2a	1691	1/1	0.84	0.55	139,139,139,139	0
56	MG	2A	3825	1/1	0.84	1.48	97,97,97,97	0
56	MG	2A	3058	1/1	0.84	0.24	85,85,85,85	0
56	MG	1a	1832	1/1	0.84	0.18	189,189,189,189	0
56	MG	2a	1699	1/1	0.84	0.41	138,138,138,138	0
56	MG	1A	4334	1/1	0.84	0.28	73,73,73,73	0
56	MG	2A	3418	1/1	0.84	0.48	117,117,117,117	0
56	MG	1A	4175	1/1	0.84	0.27	60,60,60,60	0
56	MG	1O	203	1/1	0.84	0.25	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4435	1/1	0.84	0.20	65,65,65,65	0
56	MG	1s	101	1/1	0.84	1.12	216,216,216,216	0
56	MG	2A	3078	1/1	0.84	0.24	119,119,119,119	0
56	MG	2A	3082	1/1	0.84	0.30	126,126,126,126	0
56	MG	1A	4698	1/1	0.84	0.76	70,70,70,70	0
56	MG	1a	1902	1/1	0.84	0.56	135,135,135,135	0
56	MG	1a	1903	1/1	0.84	0.47	121,121,121,121	0
56	MG	2A	3196	1/1	0.84	0.52	92,92,92,92	0
56	MG	1A	4921	1/1	0.84	0.26	71,71,71,71	0
56	MG	2v	702	1/1	0.84	0.11	183,183,183,183	0
56	MG	2B	209	1/1	0.84	0.45	77,77,77,77	0
56	MG	2A	3462	1/1	0.84	0.76	104,104,104,104	0
56	MG	1A	4191	1/1	0.84	0.17	67,67,67,67	0
56	MG	1a	1754	1/1	0.84	0.29	100,100,100,100	0
56	MG	2A	3466	1/1	0.84	0.80	129,129,129,129	0
56	MG	2A	3099	1/1	0.84	0.14	152,152,152,152	0
56	MG	2B	220	1/1	0.84	0.16	140,140,140,140	0
56	MG	2A	3598	1/1	0.84	0.16	121,121,121,121	0
56	MG	2A	3605	1/1	0.84	0.19	105,105,105,105	0
56	MG	2a	1637	1/1	0.84	0.32	146,146,146,146	0
56	MG	2A	3607	1/1	0.84	0.16	127,127,127,127	0
56	MG	2a	1900	1/1	0.84	0.42	174,174,174,174	0
56	MG	2B	225	1/1	0.84	0.18	132,132,132,132	0
56	MG	1A	4314	1/1	0.84	0.46	107,107,107,107	0
56	MG	2A	3755	1/1	0.84	0.12	130,130,130,130	0
56	MG	2A	3473	1/1	0.84	0.63	131,131,131,131	0
56	MG	1A	4300	1/1	0.84	0.49	90,90,90,90	0
56	MG	2A	3008	1/1	0.84	0.58	94,94,94,94	0
56	MG	1A	4287	1/1	0.84	0.58	50,50,50,50	0
56	MG	2a	1879	1/1	0.85	0.53	150,150,150,150	0
56	MG	2A	3493	1/1	0.85	0.54	134,134,134,134	0
56	MG	2a	1884	1/1	0.85	0.31	168,168,168,168	0
56	MG	2A	3044	1/1	0.85	0.37	107,107,107,107	0
56	MG	2a	1886	1/1	0.85	0.38	147,147,147,147	0
56	MG	2A	3342	1/1	0.85	0.20	86,86,86,86	0
56	MG	2A	3183	1/1	0.85	0.47	124,124,124,124	0
56	MG	1A	4624	1/1	0.85	0.44	118,118,118,118	0
56	MG	2a	1727	1/1	0.85	0.34	124,124,124,124	0
56	MG	1A	4053	1/1	0.85	0.85	112,112,112,112	0
56	MG	1A	4860	1/1	0.85	0.27	59,59,59,59	0
56	MG	1a	1673	1/1	0.85	0.23	117,117,117,117	0
56	MG	1a	1839	1/1	0.85	0.18	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1614	1/1	0.85	0.24	165,165,165,165	0
56	MG	1B	204	1/1	0.85	0.43	93,93,93,93	0
56	MG	2a	1738	1/1	0.85	0.62	138,138,138,138	0
56	MG	1A	4014	1/1	0.85	0.68	87,87,87,87	0
56	MG	2A	3201	1/1	0.85	0.38	115,115,115,115	0
56	MG	2A	3203	1/1	0.85	0.35	124,124,124,124	0
56	MG	1A	4431	1/1	0.85	0.29	72,72,72,72	0
56	MG	1A	4867	1/1	0.85	0.28	58,58,58,58	0
56	MG	1A	4875	1/1	0.85	0.22	71,71,71,71	0
56	MG	1B	220	1/1	0.85	0.27	79,79,79,79	0
56	MG	1a	1781	1/1	0.85	0.67	110,110,110,110	0
56	MG	2a	1632	1/1	0.85	0.17	137,137,137,137	0
56	MG	2A	3086	1/1	0.85	0.32	119,119,119,119	0
56	MG	1A	4532	1/1	0.85	0.27	45,45,45,45	0
56	MG	2B	212	1/1	0.85	0.47	156,156,156,156	0
56	MG	1A	4640	1/1	0.85	0.33	69,69,69,69	0
56	MG	1A	4644	1/1	0.85	0.34	65,65,65,65	0
56	MG	1A	4798	1/1	0.85	0.35	62,62,62,62	0
56	MG	2A	3243	1/1	0.85	0.26	109,109,109,109	0
56	MG	2A	3098	1/1	0.85	0.25	159,159,159,159	0
56	MG	2A	3565	1/1	0.85	0.28	102,102,102,102	0
56	MG	2A	3737	1/1	0.85	0.53	100,100,100,100	0
56	MG	1A	4037	1/1	0.85	0.70	89,89,89,89	0
56	MG	1a	1627	1/1	0.85	0.38	95,95,95,95	0
56	MG	2a	1777	1/1	0.85	0.68	117,117,117,117	0
56	MG	1A	4894	1/1	0.85	0.47	63,63,63,63	0
56	MG	2A	3743	1/1	0.85	0.43	83,83,83,83	0
56	MG	2a	1781	1/1	0.85	0.23	230,230,230,230	0
56	MG	1a	1630	1/1	0.85	0.84	108,108,108,108	0
56	MG	1A	4804	1/1	0.85	1.06	89,89,89,89	0
56	MG	1A	4298	1/1	0.85	0.51	76,76,76,76	0
56	MG	2D	302	1/1	0.85	0.31	80,80,80,80	0
56	MG	1a	1872	1/1	0.85	0.10	195,195,195,195	0
56	MG	2A	3262	1/1	0.85	0.73	73,73,73,73	0
56	MG	2A	3115	1/1	0.85	0.56	135,135,135,135	0
56	MG	2A	3430	1/1	0.85	0.62	73,73,73,73	0
56	MG	1a	1804	1/1	0.85	0.41	130,130,130,130	0
56	MG	2A	3759	1/1	0.85	0.42	232,232,232,232	0
56	MG	2a	1797	1/1	0.85	0.17	238,238,238,238	0
56	MG	1A	4707	1/1	0.85	0.31	73,73,73,73	0
56	MG	1a	1890	1/1	0.85	0.16	218,218,218,218	0
56	MG	1a	1893	1/1	0.85	0.30	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	5027	1/1	0.85	0.75	63,63,63,63	0
56	MG	1a	1644	1/1	0.85	0.71	120,120,120,120	0
56	MG	1A	4184	1/1	0.85	0.45	61,61,61,61	0
56	MG	1A	4818	1/1	0.85	0.32	69,69,69,69	0
56	MG	2A	3777	1/1	0.85	0.45	100,100,100,100	0
56	MG	1A	4711	1/1	0.85	0.27	78,78,78,78	0
56	MG	1a	1737	1/1	0.85	0.59	74,74,74,74	0
56	MG	2a	1693	1/1	0.85	0.28	141,141,141,141	0
56	MG	1A	4461	1/1	0.85	0.26	78,78,78,78	0
56	MG	2A	3154	1/1	0.85	0.93	92,92,92,92	0
56	MG	2A	3791	1/1	0.85	0.36	93,93,93,93	0
56	MG	1a	1654	1/1	0.85	0.52	120,120,120,120	0
56	MG	2a	1847	1/1	0.85	0.26	160,160,160,160	0
56	MG	1A	4932	1/1	0.85	0.30	153,153,153,153	0
56	MG	1A	4832	1/1	0.85	0.68	71,71,71,71	0
56	MG	2a	1705	1/1	0.85	0.38	150,150,150,150	0
56	MG	1a	1747	1/1	0.85	0.34	149,149,149,149	0
56	MG	1A	4274	1/1	0.85	0.68	51,51,51,51	0
56	MG	1A	4356	1/1	0.85	0.33	75,75,75,75	0
56	MG	2A	3633	1/1	0.85	0.28	110,110,110,110	0
56	MG	1A	5058	1/1	0.85	0.49	100,100,100,100	0
56	MG	28	106	1/1	0.85	0.24	79,79,79,79	0
57	ZN	1n	103	1/1	0.85	0.09	212,212,212,212	0
56	MG	2a	1877	1/1	0.85	0.33	151,151,151,151	0
56	MG	2a	1878	1/1	0.85	0.55	115,115,115,115	0
57	ZN	2n	501	1/1	0.85	0.11	239,239,239,239	0
56	MG	2A	3634	1/1	0.86	0.34	104,104,104,104	0
56	MG	2P	201	1/1	0.86	0.37	100,100,100,100	0
56	MG	1A	4444	1/1	0.86	0.27	76,76,76,76	0
56	MG	2A	3519	1/1	0.86	0.20	91,91,91,91	0
56	MG	1Q	202	1/1	0.86	0.11	67,67,67,67	0
56	MG	1A	4908	1/1	0.86	0.23	64,64,64,64	0
56	MG	2A	3113	1/1	0.86	0.69	140,140,140,140	0
56	MG	1A	4915	1/1	0.86	0.28	85,85,85,85	0
56	MG	1A	4226	1/1	0.86	0.40	81,81,81,81	0
56	MG	2A	3646	1/1	0.86	0.51	110,110,110,110	0
56	MG	1A	4316	1/1	0.86	0.63	85,85,85,85	0
56	MG	2A	3017	1/1	0.86	0.29	111,111,111,111	0
56	MG	2A	3251	1/1	0.86	0.18	123,123,123,123	0
56	MG	1A	5044	1/1	0.86	0.83	52,52,52,52	0
56	MG	1a	1824	1/1	0.86	0.30	213,213,213,213	0
56	MG	2A	3541	1/1	0.86	0.64	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1a	1826	1/1	0.86	0.13	196,196,196,196	0
56	MG	1A	4548	1/1	0.86	0.82	131,131,131,131	0
56	MG	1A	4144	1/1	0.86	0.38	65,65,65,65	0
56	MG	1A	4051	1/1	0.86	0.80	100,100,100,100	0
56	MG	2A	3683	1/1	0.86	0.28	102,102,102,102	0
56	MG	1a	1758	1/1	0.86	0.14	111,111,111,111	0
56	MG	2A	3690	1/1	0.86	0.16	159,159,159,159	0
56	MG	2A	3270	1/1	0.86	0.48	98,98,98,98	0
56	MG	29	102	1/1	0.86	0.27	128,128,128,128	0
56	MG	1A	4841	1/1	0.86	0.48	103,103,103,103	0
56	MG	1A	4638	1/1	0.86	0.32	66,66,66,66	0
56	MG	1A	4551	1/1	0.86	0.40	69,69,69,69	0
56	MG	1A	4425	1/1	0.86	0.14	78,78,78,78	0
56	MG	1A	4490	1/1	0.86	0.34	89,89,89,89	0
56	MG	1A	4581	1/1	0.86	0.29	61,61,61,61	0
56	MG	1A	4778	1/1	0.86	0.19	71,71,71,71	0
56	MG	2a	1822	1/1	0.86	0.27	167,167,167,167	0
56	MG	1A	4650	1/1	0.86	0.42	63,63,63,63	0
56	MG	1A	4659	1/1	0.86	0.39	87,87,87,87	0
56	MG	1b	306	1/1	0.86	0.16	186,186,186,186	0
56	MG	1B	211	1/1	0.86	0.64	82,82,82,82	0
56	MG	2a	1839	1/1	0.86	0.08	241,241,241,241	0
56	MG	2B	214	1/1	0.86	0.25	145,145,145,145	0
56	MG	1A	4492	1/1	0.86	0.30	69,69,69,69	0
56	MG	1A	4882	1/1	0.86	0.35	82,82,82,82	0
56	MG	1a	1783	1/1	0.86	0.25	135,135,135,135	0
56	MG	1A	4214	1/1	0.86	0.29	61,61,61,61	0
56	MG	2a	1731	1/1	0.86	0.36	103,103,103,103	0
56	MG	1A	4602	1/1	0.86	0.29	54,54,54,54	0
56	MG	1A	4526	1/1	0.86	0.32	54,54,54,54	0
56	MG	1m	202	1/1	0.86	0.07	211,211,211,211	0
56	MG	1A	4993	1/1	0.86	0.17	85,85,85,85	0
56	MG	1A	4890	1/1	0.86	0.60	114,114,114,114	0
56	MG	1E	303	1/1	0.86	0.61	62,62,62,62	0
56	MG	2a	1741	1/1	0.86	0.60	174,174,174,174	0
56	MG	1F	301	1/1	0.86	0.35	76,76,76,76	0
56	MG	1A	4531	1/1	0.86	0.34	68,68,68,68	0
56	MG	2a	1643	1/1	0.86	0.20	144,144,144,144	0
56	MG	2A	3355	1/1	0.86	0.26	89,89,89,89	0
56	MG	2A	3207	1/1	0.86	0.32	123,123,123,123	0
56	MG	2D	306	1/1	0.86	1.03	101,101,101,101	0
56	MG	1a	1712	1/1	0.86	0.49	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2a	1653	1/1	0.86	0.36	141,141,141,141	0
56	MG	1A	4170	1/1	0.86	0.52	61,61,61,61	0
56	MG	1A	4311	1/1	0.86	0.59	101,101,101,101	0
56	MG	2z	101	1/1	0.86	0.33	177,177,177,177	0
56	MG	2A	3382	1/1	0.86	0.30	101,101,101,101	0
56	MG	2a	1762	1/1	0.86	0.14	235,235,235,235	0
56	MG	1A	5015	1/1	0.86	0.52	89,89,89,89	0
56	MG	2a	1764	1/1	0.86	0.33	270,270,270,270	0
56	MG	1A	4899	1/1	0.86	0.39	68,68,68,68	0
56	MG	2a	1907	1/1	0.86	0.23	256,256,256,256	0
56	MG	1A	4417	1/1	0.87	0.36	52,52,52,52	0
56	MG	1a	1692	1/1	0.87	0.24	129,129,129,129	0
56	MG	2a	1665	1/1	0.87	0.24	139,139,139,139	0
56	MG	1b	307	1/1	0.87	0.06	164,164,164,164	0
56	MG	1O	201	1/1	0.87	0.48	82,82,82,82	0
56	MG	2A	3185	1/1	0.87	0.45	95,95,95,95	0
56	MG	2A	3332	1/1	0.87	0.28	97,97,97,97	0
56	MG	1A	4136	1/1	0.87	0.66	92,92,92,92	0
56	MG	1A	4779	1/1	0.87	0.23	68,68,68,68	0
56	MG	2Q	204	1/1	0.87	0.54	118,118,118,118	0
56	MG	1A	4119	1/1	0.87	0.41	74,74,74,74	0
56	MG	1A	5042	1/1	0.87	0.23	77,77,77,77	0
56	MG	1a	1795	1/1	0.87	0.47	107,107,107,107	0
56	MG	1A	4636	1/1	0.87	0.35	64,64,64,64	0
56	MG	1a	1641	1/1	0.87	0.22	124,124,124,124	0
56	MG	2A	3492	1/1	0.87	0.35	120,120,120,120	0
56	MG	1A	4866	1/1	0.87	0.34	69,69,69,69	0
56	MG	1a	1723	1/1	0.87	0.45	118,118,118,118	0
56	MG	1A	4003	1/1	0.87	0.50	53,53,53,53	0
56	MG	1A	4390	1/1	0.87	0.31	82,82,82,82	0
56	MG	2a	1793	1/1	0.87	0.20	251,251,251,251	0
56	MG	1A	4956	1/1	0.87	0.25	71,71,71,71	0
56	MG	1a	1647	1/1	0.87	0.73	118,118,118,118	0
56	MG	2A	3373	1/1	0.87	0.39	93,93,93,93	0
56	MG	1A	4743	1/1	0.87	0.16	74,74,74,74	0
56	MG	2A	3100	1/1	0.87	0.22	152,152,152,152	0
56	MG	1A	4799	1/1	0.87	0.47	87,87,87,87	0
56	MG	2A	3523	1/1	0.87	0.28	100,100,100,100	0
56	MG	2A	3524	1/1	0.87	0.32	103,103,103,103	0
56	MG	2A	3526	1/1	0.87	0.09	106,106,106,106	0
56	MG	1A	4436	1/1	0.87	0.25	64,64,64,64	0
56	MG	2l	203	1/1	0.87	0.56	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4032	1/1	0.87	0.25	55,55,55,55	0
56	MG	2A	3233	1/1	0.87	0.31	101,101,101,101	0
56	MG	2A	3666	1/1	0.87	0.37	101,101,101,101	0
56	MG	1a	1894	1/1	0.87	0.72	132,132,132,132	0
56	MG	2A	3109	1/1	0.87	0.23	137,137,137,137	0
56	MG	1y	104	1/1	0.87	0.31	99,99,99,99	0
56	MG	1W	201	1/1	0.87	0.30	72,72,72,72	0
56	MG	1A	4155	1/1	0.87	0.37	60,60,60,60	0
56	MG	1A	4024	1/1	0.87	0.46	78,78,78,78	0
56	MG	2A	3010	1/1	0.87	1.10	88,88,88,88	0
56	MG	2A	3545	1/1	0.87	0.23	97,97,97,97	0
56	MG	1A	4986	1/1	0.87	0.77	64,64,64,64	0
56	MG	1A	4759	1/1	0.87	0.38	74,74,74,74	0
56	MG	2A	3549	1/1	0.87	0.50	96,96,96,96	0
56	MG	1A	4655	1/1	0.87	0.54	82,82,82,82	0
56	MG	1a	1757	1/1	0.87	0.61	107,107,107,107	0
56	MG	2a	1866	1/1	0.87	0.26	138,138,138,138	0
56	MG	1a	1905	1/1	0.87	0.75	108,108,108,108	0
56	MG	1A	4656	1/1	0.87	0.42	80,80,80,80	0
56	MG	1A	4455	1/1	0.87	0.27	75,75,75,75	0
56	MG	2A	3417	1/1	0.87	0.22	117,117,117,117	0
56	MG	1B	219	1/1	0.87	0.15	77,77,77,77	0
56	MG	1A	4824	1/1	0.87	0.21	81,81,81,81	0
56	MG	1B	221	1/1	0.87	0.57	98,98,98,98	0
56	MG	1A	4459	1/1	0.87	0.17	72,72,72,72	0
56	MG	2a	1883	1/1	0.87	0.41	131,131,131,131	0
56	MG	2a	1752	1/1	0.87	0.25	134,134,134,134	0
56	MG	1A	4101	1/1	0.87	0.53	45,45,45,45	0
56	MG	1A	4671	1/1	0.87	0.47	65,65,65,65	0
56	MG	2A	3287	1/1	0.87	0.73	104,104,104,104	0
56	MG	2A	3432	1/1	0.87	0.67	93,93,93,93	0
56	MG	1A	4357	1/1	0.87	0.37	78,78,78,78	0
56	MG	2A	3584	1/1	0.87	0.12	114,114,114,114	0
56	MG	1A	4850	1/1	0.87	0.37	76,76,76,76	0
57	ZN	14	501	1/1	0.87	0.07	172,172,172,172	0
56	MG	2A	3169	1/1	0.87	0.65	81,81,81,81	0
56	MG	1a	1842	1/1	0.87	0.11	78,78,78,78	0
56	MG	2E	305	1/1	0.87	0.14	121,121,121,121	0
56	MG	1E	305	1/1	0.87	0.91	69,69,69,69	0
59	GDP	2v	704	28/28	0.87	0.19	186,186,186,186	0
56	MG	2A	3715	1/1	0.88	0.22	109,109,109,109	0
56	MG	1A	4336	1/1	0.88	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4929	1/1	0.88	0.44	201,201,201,201	0
56	MG	1A	4243	1/1	0.88	0.55	65,65,65,65	0
56	MG	1A	4676	1/1	0.88	0.76	101,101,101,101	0
56	MG	2a	1875	1/1	0.88	0.64	154,154,154,154	0
56	MG	1A	4603	1/1	0.88	0.34	67,67,67,67	0
56	MG	1a	1604	1/1	0.88	0.24	98,98,98,98	0
56	MG	1A	4753	1/1	0.88	0.26	62,62,62,62	0
56	MG	1a	1607	1/1	0.88	0.33	86,86,86,86	0
56	MG	1a	1609	1/1	0.88	0.19	88,88,88,88	0
56	MG	2Q	205	1/1	0.88	1.05	129,129,129,129	0
56	MG	2A	3362	1/1	0.88	0.12	99,99,99,99	0
56	MG	2A	3364	1/1	0.88	0.39	84,84,84,84	0
56	MG	1A	4257	1/1	0.88	0.45	64,64,64,64	0
56	MG	2A	3371	1/1	0.88	0.18	113,113,113,113	0
56	MG	2a	1889	1/1	0.88	0.97	127,127,127,127	0
56	MG	2a	1892	1/1	0.88	0.74	142,142,142,142	0
56	MG	2A	3035	1/1	0.88	0.45	116,116,116,116	0
56	MG	1A	4679	1/1	0.88	0.15	80,80,80,80	0
56	MG	2A	3376	1/1	0.88	0.27	99,99,99,99	0
56	MG	1A	4761	1/1	0.88	0.28	74,74,74,74	0
56	MG	2a	1726	1/1	0.88	0.46	108,108,108,108	0
56	MG	2a	1902	1/1	0.88	0.54	248,248,248,248	0
56	MG	2a	1903	1/1	0.88	0.67	246,246,246,246	0
56	MG	2A	3051	1/1	0.88	1.54	104,104,104,104	0
56	MG	1a	1817	1/1	0.88	0.22	148,148,148,148	0
56	MG	1A	4605	1/1	0.88	0.29	64,64,64,64	0
56	MG	2A	3197	1/1	0.88	0.18	93,93,93,93	0
56	MG	1A	4682	1/1	0.88	0.99	116,116,116,116	0
56	MG	2A	3064	1/1	0.88	0.36	75,75,75,75	0
56	MG	1A	4045	1/1	0.88	0.35	68,68,68,68	0
56	MG	2A	3769	1/1	0.88	0.59	90,90,90,90	0
56	MG	1A	4085	1/1	0.88	0.30	67,67,67,67	0
56	MG	1A	4863	1/1	0.88	0.35	62,62,62,62	0
56	MG	2A	3776	1/1	0.88	0.41	97,97,97,97	0
56	MG	1D	302	1/1	0.88	0.34	57,57,57,57	0
56	MG	1a	1631	1/1	0.88	0.35	126,126,126,126	0
56	MG	2a	1603	1/1	0.88	0.22	151,151,151,151	0
56	MG	1a	1919	1/1	0.88	0.52	144,144,144,144	0
56	MG	2A	3401	1/1	0.88	0.12	89,89,89,89	0
56	MG	2f	303	1/1	0.88	0.35	135,135,135,135	0
56	MG	1A	4086	1/1	0.88	0.37	68,68,68,68	0
56	MG	2a	1755	1/1	0.88	0.10	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4371	1/1	0.88	0.29	74,74,74,74	0
56	MG	2A	3220	1/1	0.88	0.27	115,115,115,115	0
56	MG	2A	3794	1/1	0.88	0.25	113,113,113,113	0
56	MG	1A	4874	1/1	0.88	0.67	87,87,87,87	0
56	MG	1A	4199	1/1	0.88	0.22	218,218,218,218	0
56	MG	2a	1615	1/1	0.88	0.30	145,145,145,145	0
56	MG	1A	4200	1/1	0.88	0.23	69,69,69,69	0
56	MG	2A	3232	1/1	0.88	0.36	95,95,95,95	0
56	MG	2A	3090	1/1	0.88	0.20	110,110,110,110	0
56	MG	1A	4375	1/1	0.88	0.31	65,65,65,65	0
56	MG	1A	5004	1/1	0.88	0.37	89,89,89,89	0
56	MG	2A	3096	1/1	0.88	0.36	98,98,98,98	0
56	MG	1A	4386	1/1	0.88	0.15	64,64,64,64	0
56	MG	1A	4887	1/1	0.88	0.31	67,67,67,67	0
56	MG	2A	3247	1/1	0.88	0.44	113,113,113,113	0
56	MG	2a	1630	1/1	0.88	0.66	123,123,123,123	0
56	MG	1A	4034	1/1	0.88	0.63	69,69,69,69	0
56	MG	1A	4783	1/1	0.88	0.47	70,70,70,70	0
56	MG	2l	205	1/1	0.88	0.27	148,148,148,148	0
56	MG	2A	3250	1/1	0.88	0.59	158,158,158,158	0
56	MG	1a	1760	1/1	0.88	0.23	114,114,114,114	0
56	MG	2A	3102	1/1	0.88	0.24	144,144,144,144	0
56	MG	1A	4393	1/1	0.88	0.33	84,84,84,84	0
56	MG	1A	4151	1/1	0.88	0.32	60,60,60,60	0
56	MG	2p	101	1/1	0.88	0.12	154,154,154,154	0
56	MG	1a	1657	1/1	0.88	0.24	106,106,106,106	0
56	MG	1A	4320	1/1	0.88	0.80	91,91,91,91	0
56	MG	1a	1661	1/1	0.88	0.22	117,117,117,117	0
56	MG	1A	4129	1/1	0.88	0.17	58,58,58,58	0
56	MG	1A	4642	1/1	0.88	0.30	67,67,67,67	0
56	MG	2A	3468	1/1	0.88	0.59	85,85,85,85	0
56	MG	1A	4221	1/1	0.88	0.63	71,71,71,71	0
56	MG	1a	1858	1/1	0.88	0.09	210,210,210,210	0
56	MG	2A	3119	1/1	0.88	0.68	113,113,113,113	0
56	MG	2A	3120	1/1	0.88	0.62	120,120,120,120	0
56	MG	2A	3285	1/1	0.88	0.25	101,101,101,101	0
56	MG	1T	201	1/1	0.88	0.34	66,66,66,66	0
56	MG	2A	3658	1/1	0.88	0.66	112,112,112,112	0
56	MG	2A	3289	1/1	0.88	0.25	107,107,107,107	0
56	MG	1A	5041	1/1	0.88	0.26	79,79,79,79	0
56	MG	2A	3132	1/1	0.88	0.28	141,141,141,141	0
56	MG	1A	4905	1/1	0.88	0.26	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4559	1/1	0.88	0.40	60,60,60,60	0
56	MG	1A	5047	1/1	0.88	0.32	89,89,89,89	0
56	MG	1A	4039	1/1	0.88	0.16	79,79,79,79	0
56	MG	2A	3308	1/1	0.88	0.76	100,100,100,100	0
56	MG	1A	4507	1/1	0.88	0.30	106,106,106,106	0
56	MG	2B	228	1/1	0.88	0.17	145,145,145,145	0
56	MG	2a	1837	1/1	0.88	0.10	240,240,240,240	0
56	MG	1a	1791	1/1	0.88	0.25	116,116,116,116	0
56	MG	1A	4228	1/1	0.88	0.52	109,109,109,109	0
56	MG	2a	1840	1/1	0.88	0.09	228,228,228,228	0
56	MG	2a	1681	1/1	0.88	0.36	165,165,165,165	0
56	MG	1A	4190	1/1	0.88	0.29	68,68,68,68	0
56	MG	2A	3693	1/1	0.88	0.46	86,86,86,86	0
56	MG	2A	3153	1/1	0.88	0.69	80,80,80,80	0
56	MG	2A	3699	1/1	0.88	0.43	107,107,107,107	0
56	MG	1A	4587	1/1	0.88	0.33	72,72,72,72	0
56	MG	1a	1891	1/1	0.88	0.21	89,89,89,89	0
56	MG	1a	1871	1/1	0.89	0.10	199,199,199,199	0
56	MG	2A	3339	1/1	0.89	0.55	72,72,72,72	0
56	MG	2A	3697	1/1	0.89	0.70	128,128,128,128	0
56	MG	2a	1862	1/1	0.89	0.77	155,155,155,155	0
56	MG	2A	3698	1/1	0.89	0.34	108,108,108,108	0
56	MG	1E	308	1/1	0.89	0.50	68,68,68,68	0
56	MG	2E	304	1/1	0.89	0.34	71,71,71,71	0
56	MG	2A	3704	1/1	0.89	0.28	95,95,95,95	0
56	MG	1A	4445	1/1	0.89	0.16	73,73,73,73	0
56	MG	1A	4447	1/1	0.89	0.24	65,65,65,65	0
56	MG	1A	4450	1/1	0.89	0.16	75,75,75,75	0
56	MG	1A	4999	1/1	0.89	0.79	62,62,62,62	0
56	MG	2A	3718	1/1	0.89	0.54	129,129,129,129	0
56	MG	2A	3032	1/1	0.89	0.79	108,108,108,108	0
56	MG	2A	3720	1/1	0.89	0.10	122,122,122,122	0
56	MG	1A	5002	1/1	0.89	0.81	61,61,61,61	0
56	MG	1P	201	1/1	0.89	0.46	53,53,53,53	0
56	MG	1A	4383	1/1	0.89	0.26	65,65,65,65	0
56	MG	1A	4186	1/1	0.89	0.47	59,59,59,59	0
56	MG	2a	1888	1/1	0.89	0.32	136,136,136,136	0
56	MG	1a	1788	1/1	0.89	1.09	118,118,118,118	0
56	MG	2A	3369	1/1	0.89	0.14	84,84,84,84	0
56	MG	1A	4132	1/1	0.89	0.56	61,61,61,61	0
56	MG	2A	3198	1/1	0.89	0.53	100,100,100,100	0
56	MG	2a	1897	1/1	0.89	1.12	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4116	1/1	0.89	0.16	65,65,65,65	0
56	MG	2A	3374	1/1	0.89	0.17	102,102,102,102	0
56	MG	2Z	402	1/1	0.89	1.17	120,120,120,120	0
56	MG	1A	4629	1/1	0.89	0.24	71,71,71,71	0
56	MG	1A	4349	1/1	0.89	0.32	54,54,54,54	0
56	MG	2a	1730	1/1	0.89	0.14	127,127,127,127	0
56	MG	1a	1904	1/1	0.89	0.57	83,83,83,83	0
56	MG	1A	5021	1/1	0.89	0.20	81,81,81,81	0
56	MG	2A	3558	1/1	0.89	0.78	93,93,93,93	0
56	MG	1A	4350	1/1	0.89	0.39	68,68,68,68	0
56	MG	1A	5025	1/1	0.89	0.33	75,75,75,75	0
56	MG	2a	1736	1/1	0.89	0.30	137,137,137,137	0
56	MG	1a	1680	1/1	0.89	0.14	155,155,155,155	0
56	MG	26	101	1/1	0.89	0.93	121,121,121,121	0
56	MG	2a	1740	1/1	0.89	0.11	143,143,143,143	0
56	MG	26	103	1/1	0.89	0.57	119,119,119,119	0
56	MG	2a	1744	1/1	0.89	0.64	95,95,95,95	0
56	MG	2d	302	1/1	0.89	0.13	164,164,164,164	0
56	MG	2d	304	1/1	0.89	0.28	161,161,161,161	0
56	MG	1A	4892	1/1	0.89	0.53	72,72,72,72	0
56	MG	2A	3216	1/1	0.89	0.11	100,100,100,100	0
56	MG	1U	201	1/1	0.89	0.24	61,61,61,61	0
56	MG	1A	4545	1/1	0.89	0.23	65,65,65,65	0
56	MG	1A	4481	1/1	0.89	0.53	78,78,78,78	0
56	MG	1A	4398	1/1	0.89	0.23	75,75,75,75	0
56	MG	1A	4240	1/1	0.89	0.24	60,60,60,60	0
56	MG	2A	3229	1/1	0.89	0.58	73,73,73,73	0
56	MG	2A	3230	1/1	0.89	0.23	87,87,87,87	0
56	MG	2A	3780	1/1	0.89	0.30	90,90,90,90	0
56	MG	2A	3088	1/1	0.89	0.21	72,72,72,72	0
56	MG	1A	4491	1/1	0.89	0.40	86,86,86,86	0
56	MG	1a	1918	1/1	0.89	0.52	142,142,142,142	0
56	MG	1a	1691	1/1	0.89	0.47	117,117,117,117	0
56	MG	1A	4318	1/1	0.89	0.59	81,81,81,81	0
56	MG	2A	3599	1/1	0.89	0.26	122,122,122,122	0
56	MG	1a	1694	1/1	0.89	0.43	125,125,125,125	0
56	MG	2A	3606	1/1	0.89	0.23	137,137,137,137	0
56	MG	1A	4645	1/1	0.89	0.31	66,66,66,66	0
56	MG	1A	5050	1/1	0.89	0.24	173,173,173,173	0
56	MG	1A	4279	1/1	0.89	0.31	64,64,64,64	0
56	MG	2a	1770	1/1	0.89	0.41	237,237,237,237	0
56	MG	1A	4406	1/1	0.89	0.48	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4566	1/1	0.89	0.25	58,58,58,58	0
56	MG	2a	1774	1/1	0.89	0.25	220,220,220,220	0
56	MG	1A	4568	1/1	0.89	0.34	56,56,56,56	0
56	MG	2a	1626	1/1	0.89	0.44	157,157,157,157	0
56	MG	1A	4359	1/1	0.89	0.17	71,71,71,71	0
56	MG	1a	1710	1/1	0.89	0.34	115,115,115,115	0
56	MG	1A	4580	1/1	0.89	0.21	64,64,64,64	0
56	MG	1A	4322	1/1	0.89	0.54	85,85,85,85	0
56	MG	1A	4135	1/1	0.89	0.21	78,78,78,78	0
56	MG	1A	4673	1/1	0.89	0.53	94,94,94,94	0
56	MG	1a	1613	1/1	0.89	0.19	91,91,91,91	0
56	MG	1A	4940	1/1	0.89	0.29	55,55,55,55	0
56	MG	2A	3460	1/1	0.89	0.86	106,106,106,106	0
56	MG	1A	4854	1/1	0.89	0.27	81,81,81,81	0
56	MG	2s	101	1/1	0.89	0.26	250,250,250,250	0
56	MG	2A	3277	1/1	0.89	0.16	88,88,88,88	0
56	MG	2A	3281	1/1	0.89	0.32	104,104,104,104	0
56	MG	1A	4855	1/1	0.89	0.20	59,59,59,59	0
56	MG	1B	208	1/1	0.89	0.34	94,94,94,94	0
56	MG	2a	1795	1/1	0.89	0.37	111,111,111,111	0
56	MG	1B	209	1/1	0.89	0.51	89,89,89,89	0
56	MG	1A	4857	1/1	0.89	0.68	61,61,61,61	0
56	MG	2a	1656	1/1	0.89	0.09	145,145,145,145	0
56	MG	1A	4954	1/1	0.89	0.26	62,62,62,62	0
56	MG	1A	4509	1/1	0.89	0.24	62,62,62,62	0
56	MG	2A	3648	1/1	0.89	0.42	137,137,137,137	0
56	MG	1A	4217	1/1	0.89	0.26	59,59,59,59	0
56	MG	2A	3650	1/1	0.89	0.20	115,115,115,115	0
56	MG	1A	4432	1/1	0.89	0.20	95,95,95,95	0
56	MG	1A	4244	1/1	0.89	0.40	51,51,51,51	0
56	MG	1A	4968	1/1	0.89	0.69	82,82,82,82	0
56	MG	2A	3147	1/1	0.89	0.43	82,82,82,82	0
56	MG	1a	1640	1/1	0.89	0.39	115,115,115,115	0
56	MG	1A	4080	1/1	0.89	0.36	55,55,55,55	0
56	MG	2A	3310	1/1	0.89	0.57	117,117,117,117	0
56	MG	1D	303	1/1	0.89	0.60	82,82,82,82	0
56	MG	2B	222	1/1	0.89	0.23	133,133,133,133	0
56	MG	2A	3678	1/1	0.89	0.38	100,100,100,100	0
56	MG	1a	1764	1/1	0.89	0.35	121,121,121,121	0
56	MG	1A	4380	1/1	0.89	0.29	56,56,56,56	0
56	MG	1A	4984	1/1	0.89	0.25	87,87,87,87	0
56	MG	1A	4684	1/1	0.89	0.56	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4687	1/1	0.89	0.20	88,88,88,88	0
56	MG	1A	4868	1/1	0.89	0.17	62,62,62,62	0
56	MG	1A	4321	1/1	0.90	0.36	102,102,102,102	0
56	MG	2A	3684	1/1	0.90	0.22	94,94,94,94	0
56	MG	1A	4098	1/1	0.90	0.28	53,53,53,53	0
56	MG	2a	1856	1/1	0.90	0.22	147,147,147,147	0
56	MG	2A	3192	1/1	0.90	0.13	99,99,99,99	0
56	MG	2A	3055	1/1	0.90	0.29	102,102,102,102	0
56	MG	1A	4100	1/1	0.90	0.34	66,66,66,66	0
56	MG	1A	4586	1/1	0.90	0.21	73,73,73,73	0
56	MG	2a	1867	1/1	0.90	0.51	79,79,79,79	0
56	MG	1a	1619	1/1	0.90	0.39	95,95,95,95	0
56	MG	2D	303	1/1	0.90	0.22	109,109,109,109	0
56	MG	2a	1870	1/1	0.90	0.21	108,108,108,108	0
56	MG	2a	1872	1/1	0.90	0.58	120,120,120,120	0
56	MG	2A	3530	1/1	0.90	0.13	133,133,133,133	0
56	MG	1A	4886	1/1	0.90	0.52	67,67,67,67	0
56	MG	1A	4066	1/1	0.90	0.34	98,98,98,98	0
56	MG	2a	1698	1/1	0.90	0.39	118,118,118,118	0
56	MG	2A	3067	1/1	0.90	0.32	123,123,123,123	0
56	MG	1A	4589	1/1	0.90	0.29	79,79,79,79	0
56	MG	1A	4131	1/1	0.90	0.34	56,56,56,56	0
56	MG	2A	3075	1/1	0.90	0.08	142,142,142,142	0
56	MG	1a	1719	1/1	0.90	0.98	102,102,102,102	0
56	MG	2a	1707	1/1	0.90	0.18	85,85,85,85	0
56	MG	2A	3540	1/1	0.90	0.28	148,148,148,148	0
56	MG	1A	4529	1/1	0.90	0.91	68,68,68,68	0
56	MG	1A	4660	1/1	0.90	0.68	84,84,84,84	0
56	MG	2A	3727	1/1	0.90	0.60	90,90,90,90	0
56	MG	2a	1890	1/1	0.90	0.31	125,125,125,125	0
56	MG	2A	3377	1/1	0.90	0.50	116,116,116,116	0
56	MG	1A	4661	1/1	0.90	0.61	80,80,80,80	0
56	MG	1E	302	1/1	0.90	0.19	59,59,59,59	0
56	MG	1A	4154	1/1	0.90	0.17	68,68,68,68	0
56	MG	1b	303	1/1	0.90	0.08	166,166,166,166	0
56	MG	1A	4811	1/1	0.90	0.81	63,63,63,63	0
56	MG	1A	4376	1/1	0.90	0.28	61,61,61,61	0
56	MG	2A	3744	1/1	0.90	0.16	105,105,105,105	0
56	MG	1A	4377	1/1	0.90	0.29	80,80,80,80	0
56	MG	1H	201	1/1	0.90	0.24	69,69,69,69	0
56	MG	1A	5019	1/1	0.90	0.47	75,75,75,75	0
56	MG	1A	4606	1/1	0.90	0.33	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3571	1/1	0.90	0.29	172,172,172,172	0
56	MG	1A	4050	1/1	0.90	0.69	100,100,100,100	0
56	MG	20	102	1/1	0.90	0.46	116,116,116,116	0
56	MG	2a	1911	1/1	0.90	0.10	140,140,140,140	0
56	MG	1A	4224	1/1	0.90	0.37	64,64,64,64	0
56	MG	1A	4748	1/1	0.90	0.36	90,90,90,90	0
56	MG	2I	101	1/1	0.90	0.18	110,110,110,110	0
56	MG	1A	4543	1/1	0.90	0.39	83,83,83,83	0
56	MG	1a	1651	1/1	0.90	0.17	121,121,121,121	0
56	MG	1A	5031	1/1	0.90	0.28	88,88,88,88	0
56	MG	2A	3104	1/1	0.90	0.35	53,53,53,53	0
56	MG	1A	4835	1/1	0.90	0.23	63,63,63,63	0
56	MG	2a	1747	1/1	0.90	0.20	122,122,122,122	0
56	MG	1a	1761	1/1	0.90	0.36	112,112,112,112	0
56	MG	1A	4752	1/1	0.90	0.34	63,63,63,63	0
56	MG	1p	101	1/1	0.90	0.18	143,143,143,143	0
56	MG	1A	4925	1/1	0.90	0.17	72,72,72,72	0
56	MG	2A	3774	1/1	0.90	0.46	116,116,116,116	0
56	MG	2A	3595	1/1	0.90	0.09	147,147,147,147	0
56	MG	1a	1658	1/1	0.90	0.20	114,114,114,114	0
56	MG	1A	4847	1/1	0.90	0.37	72,72,72,72	0
56	MG	2A	3260	1/1	0.90	0.33	78,78,78,78	0
56	MG	1A	4499	1/1	0.90	1.38	59,59,59,59	0
56	MG	2A	3425	1/1	0.90	0.38	102,102,102,102	0
56	MG	1A	4385	1/1	0.90	0.50	55,55,55,55	0
56	MG	1a	1664	1/1	0.90	0.34	115,115,115,115	0
56	MG	1A	4757	1/1	0.90	0.88	119,119,119,119	0
56	MG	2A	3121	1/1	0.90	0.43	125,125,125,125	0
56	MG	1A	4501	1/1	0.90	0.35	71,71,71,71	0
56	MG	2A	3797	1/1	0.90	0.36	97,97,97,97	0
56	MG	1A	4625	1/1	0.90	0.56	118,118,118,118	0
56	MG	1U	203	1/1	0.90	0.27	64,64,64,64	0
56	MG	1a	1866	1/1	0.90	0.20	224,224,224,224	0
56	MG	2k	202	1/1	0.90	0.18	124,124,124,124	0
56	MG	2A	3006	1/1	0.90	0.62	101,101,101,101	0
56	MG	2A	3456	1/1	0.90	0.40	83,83,83,83	0
56	MG	2A	3806	1/1	0.90	0.26	114,114,114,114	0
56	MG	1A	4160	1/1	0.90	0.21	50,50,50,50	0
56	MG	2A	3009	1/1	0.90	0.61	94,94,94,94	0
56	MG	1A	4943	1/1	0.90	0.51	61,61,61,61	0
56	MG	2A	3821	1/1	0.90	0.28	89,89,89,89	0
56	MG	2A	3288	1/1	0.90	0.47	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4947	1/1	0.90	0.25	71,71,71,71	0
56	MG	1A	4628	1/1	0.90	0.26	77,77,77,77	0
56	MG	2A	3297	1/1	0.90	0.80	80,80,80,80	0
56	MG	1A	4949	1/1	0.90	0.29	69,69,69,69	0
56	MG	1a	1880	1/1	0.90	0.15	125,125,125,125	0
56	MG	1a	1882	1/1	0.90	0.29	87,87,87,87	0
56	MG	2A	3474	1/1	0.90	0.62	125,125,125,125	0
56	MG	2a	1645	1/1	0.90	0.15	124,124,124,124	0
56	MG	2A	3644	1/1	0.90	0.16	155,155,155,155	0
56	MG	2A	3835	1/1	0.90	0.31	121,121,121,121	0
56	MG	2A	3836	1/1	0.90	0.30	205,205,205,205	0
56	MG	2u	102	1/1	0.90	0.12	241,241,241,241	0
56	MG	2a	1650	1/1	0.90	0.37	136,136,136,136	0
56	MG	1A	4008	1/1	0.90	0.28	71,71,71,71	0
56	MG	1a	1790	1/1	0.90	0.48	87,87,87,87	0
56	MG	2A	3850	1/1	0.90	0.23	109,109,109,109	0
56	MG	2A	3478	1/1	0.90	0.52	127,127,127,127	0
56	MG	2A	3157	1/1	0.90	0.36	102,102,102,102	0
56	MG	1l	101	1/1	0.90	0.84	87,87,87,87	0
56	MG	1A	5060	1/1	0.90	0.52	64,64,64,64	0
56	MG	1A	4239	1/1	0.90	0.22	56,56,56,56	0
56	MG	2a	1806	1/1	0.90	0.23	116,116,116,116	0
56	MG	2a	1807	1/1	0.90	0.26	122,122,122,122	0
56	MG	1A	4955	1/1	0.90	0.31	72,72,72,72	0
56	MG	1A	4449	1/1	0.90	0.23	79,79,79,79	0
56	MG	2A	3500	1/1	0.90	0.33	93,93,93,93	0
56	MG	1A	4061	1/1	0.90	0.41	71,71,71,71	0
56	MG	2A	3671	1/1	0.90	0.23	85,85,85,85	0
56	MG	2A	3504	1/1	0.90	0.30	134,134,134,134	0
56	MG	1A	4451	1/1	0.90	0.22	70,70,70,70	0
56	MG	1A	4198	1/1	0.90	0.51	98,98,98,98	0
56	MG	2A	3676	1/1	0.90	0.61	125,125,125,125	0
56	MG	2B	219	1/1	0.90	0.51	77,77,77,77	0
56	MG	2A	3677	1/1	0.90	0.73	115,115,115,115	0
56	MG	2a	1841	1/1	0.90	0.36	224,224,224,224	0
56	MG	2a	1843	1/1	0.90	0.37	253,253,253,253	0
56	MG	1A	4702	1/1	0.90	0.97	58,58,58,58	0
56	MG	2A	3038	1/1	0.90	0.67	69,69,69,69	0
56	MG	1A	4123	1/1	0.90	0.40	77,77,77,77	0
56	MG	2A	3236	1/1	0.91	0.48	96,96,96,96	0
56	MG	1A	5062	1/1	0.91	0.57	87,87,87,87	0
56	MG	1B	201	1/1	0.91	1.00	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4957	1/1	0.91	0.33	79,79,79,79	0
56	MG	2A	3708	1/1	0.91	0.32	100,100,100,100	0
56	MG	2A	3712	1/1	0.91	0.49	92,92,92,92	0
56	MG	1A	4011	1/1	0.91	0.36	70,70,70,70	0
56	MG	2a	1690	1/1	0.91	0.40	155,155,155,155	0
56	MG	2A	3394	1/1	0.91	0.07	131,131,131,131	0
56	MG	1a	1683	1/1	0.91	0.39	83,83,83,83	0
56	MG	1a	1873	1/1	0.91	0.08	214,214,214,214	0
56	MG	1A	4230	1/1	0.91	0.17	102,102,102,102	0
56	MG	2A	3551	1/1	0.91	0.22	104,104,104,104	0
56	MG	1A	4120	1/1	0.91	0.56	79,79,79,79	0
56	MG	2A	3400	1/1	0.91	0.39	225,225,225,225	0
56	MG	1A	4879	1/1	0.91	0.28	77,77,77,77	0
56	MG	1A	4585	1/1	0.91	0.30	65,65,65,65	0
56	MG	2A	3736	1/1	0.91	0.60	108,108,108,108	0
56	MG	2A	3560	1/1	0.91	0.31	95,95,95,95	0
56	MG	1A	4784	1/1	0.91	0.31	87,87,87,87	0
56	MG	2A	3564	1/1	0.91	0.15	102,102,102,102	0
56	MG	1a	1690	1/1	0.91	0.14	124,124,124,124	0
56	MG	1A	4708	1/1	0.91	0.34	70,70,70,70	0
56	MG	2a	1712	1/1	0.91	0.67	148,148,148,148	0
56	MG	1A	4460	1/1	0.91	0.13	77,77,77,77	0
56	MG	1B	213	1/1	0.91	0.71	88,88,88,88	0
56	MG	1A	4368	1/1	0.91	0.18	63,63,63,63	0
56	MG	2a	1717	1/1	0.91	0.24	143,143,143,143	0
56	MG	1B	216	1/1	0.91	0.45	69,69,69,69	0
56	MG	2A	3575	1/1	0.91	0.46	70,70,70,70	0
56	MG	1A	4463	1/1	0.91	0.26	62,62,62,62	0
56	MG	2A	3419	1/1	0.91	0.47	135,135,135,135	0
56	MG	2a	1896	1/1	0.91	0.56	98,98,98,98	0
56	MG	2A	3420	1/1	0.91	0.33	121,121,121,121	0
56	MG	2A	3581	1/1	0.91	0.18	116,116,116,116	0
56	MG	1A	4652	1/1	0.91	0.45	84,84,84,84	0
56	MG	1A	4592	1/1	0.91	0.18	90,90,90,90	0
56	MG	1A	4370	1/1	0.91	0.25	61,61,61,61	0
56	MG	2A	3150	1/1	0.91	0.40	105,105,105,105	0
56	MG	2A	3765	1/1	0.91	0.13	120,120,120,120	0
56	MG	1A	4472	1/1	0.91	0.40	54,54,54,54	0
56	MG	1A	4724	1/1	0.91	0.29	80,80,80,80	0
56	MG	1A	5003	1/1	0.91	0.27	65,65,65,65	0
56	MG	1a	1718	1/1	0.91	0.79	107,107,107,107	0
56	MG	24	101	1/1	0.91	0.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3037	1/1	0.91	0.81	104,104,104,104	0
56	MG	2A	3156	1/1	0.91	0.40	100,100,100,100	0
56	MG	1A	4072	1/1	0.91	0.21	63,63,63,63	0
56	MG	2A	3448	1/1	0.91	0.83	78,78,78,78	0
56	MG	2a	1920	1/1	0.91	0.19	222,222,222,222	0
56	MG	2A	3040	1/1	0.91	0.34	116,116,116,116	0
56	MG	28	105	1/1	0.91	0.40	119,119,119,119	0
56	MG	2A	3041	1/1	0.91	0.34	117,117,117,117	0
56	MG	2A	3782	1/1	0.91	0.61	139,139,139,139	0
56	MG	1A	4028	1/1	0.91	0.34	58,58,58,58	0
56	MG	1A	4487	1/1	0.91	0.12	75,75,75,75	0
56	MG	2A	3300	1/1	0.91	0.91	96,96,96,96	0
56	MG	1A	4901	1/1	0.91	0.21	61,61,61,61	0
56	MG	1A	4665	1/1	0.91	0.62	78,78,78,78	0
56	MG	1A	5016	1/1	0.91	0.71	81,81,81,81	0
56	MG	1A	4097	1/1	0.91	0.23	57,57,57,57	0
56	MG	1A	4608	1/1	0.91	0.26	70,70,70,70	0
56	MG	2A	3626	1/1	0.91	0.13	158,158,158,158	0
56	MG	2A	3627	1/1	0.91	0.19	165,165,165,165	0
56	MG	1A	4831	1/1	0.91	0.88	109,109,109,109	0
56	MG	1A	4429	1/1	0.91	0.49	54,54,54,54	0
56	MG	2A	3324	1/1	0.91	0.34	87,87,87,87	0
56	MG	1A	4203	1/1	0.91	0.21	61,61,61,61	0
56	MG	2a	1619	1/1	0.91	0.08	68,68,68,68	0
56	MG	1A	4613	1/1	0.91	0.21	70,70,70,70	0
56	MG	2a	1621	1/1	0.91	0.25	162,162,162,162	0
56	MG	2h	205	1/1	0.91	0.46	152,152,152,152	0
56	MG	2A	3809	1/1	0.91	0.72	86,86,86,86	0
56	MG	1A	4078	1/1	0.91	0.41	66,66,66,66	0
56	MG	2a	1772	1/1	0.91	0.51	70,70,70,70	0
56	MG	1A	4845	1/1	0.91	0.52	68,68,68,68	0
56	MG	2A	3818	1/1	0.91	0.21	136,136,136,136	0
56	MG	2A	3335	1/1	0.91	0.31	97,97,97,97	0
56	MG	2A	3483	1/1	0.91	0.87	106,106,106,106	0
56	MG	2A	3484	1/1	0.91	0.47	119,119,119,119	0
56	MG	2a	1778	1/1	0.91	0.85	162,162,162,162	0
56	MG	1a	1836	1/1	0.91	0.07	225,225,225,225	0
56	MG	1A	4497	1/1	0.91	0.21	69,69,69,69	0
56	MG	2a	1633	1/1	0.91	0.37	125,125,125,125	0
56	MG	2A	3490	1/1	0.91	0.60	76,76,76,76	0
56	MG	2A	3491	1/1	0.91	0.64	133,133,133,133	0
56	MG	2a	1784	1/1	0.91	0.42	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4754	1/1	0.91	0.28	62,62,62,62	0
56	MG	1a	1755	1/1	0.91	0.32	100,100,100,100	0
56	MG	2a	1787	1/1	0.91	0.23	231,231,231,231	0
56	MG	2a	1788	1/1	0.91	0.25	229,229,229,229	0
56	MG	1A	5040	1/1	0.91	0.21	78,78,78,78	0
56	MG	1A	4185	1/1	0.91	0.26	62,62,62,62	0
56	MG	2A	3202	1/1	0.91	0.32	114,114,114,114	0
56	MG	1A	4064	1/1	0.91	0.30	69,69,69,69	0
56	MG	1A	4273	1/1	0.91	0.29	69,69,69,69	0
56	MG	2A	3844	1/1	0.91	0.58	107,107,107,107	0
56	MG	1A	4082	1/1	0.91	0.19	58,58,58,58	0
56	MG	2A	3089	1/1	0.91	0.36	122,122,122,122	0
56	MG	2A	3667	1/1	0.91	0.34	93,93,93,93	0
56	MG	1A	4688	1/1	0.91	0.28	65,65,65,65	0
56	MG	1A	4946	1/1	0.91	0.16	52,52,52,52	0
56	MG	2B	206	1/1	0.91	0.72	103,103,103,103	0
56	MG	1a	1766	1/1	0.91	0.34	129,129,129,129	0
56	MG	2a	1803	1/1	0.91	0.22	127,127,127,127	0
56	MG	2A	3095	1/1	0.91	0.29	106,106,106,106	0
56	MG	2A	3522	1/1	0.91	0.49	98,98,98,98	0
56	MG	2a	1662	1/1	0.91	0.14	150,150,150,150	0
56	MG	1A	4026	1/1	0.91	0.29	69,69,69,69	0
56	MG	1A	4117	1/1	0.91	0.38	73,73,73,73	0
56	MG	1A	4308	1/1	0.91	0.68	98,98,98,98	0
56	MG	1A	4280	1/1	0.91	0.43	55,55,55,55	0
56	MG	2y	105	1/1	0.91	0.07	262,262,262,262	0
56	MG	2a	1667	1/1	0.91	0.21	151,151,151,151	0
56	MG	1A	5056	1/1	0.91	0.11	137,137,137,137	0
56	MG	1A	4635	1/1	0.91	0.40	68,68,68,68	0
56	MG	2a	1827	1/1	0.91	1.19	122,122,122,122	0
56	MG	2a	1670	1/1	0.91	0.14	163,163,163,163	0
56	MG	2A	3685	1/1	0.91	0.22	109,109,109,109	0
56	MG	2A	3686	1/1	0.91	0.23	107,107,107,107	0
56	MG	2A	3379	1/1	0.91	0.13	101,101,101,101	0
56	MG	1A	4576	1/1	0.91	0.48	55,55,55,55	0
56	MG	1A	4312	1/1	0.91	1.07	115,115,115,115	0
56	MG	2A	3534	1/1	0.91	0.18	133,133,133,133	0
56	MG	1v	702	1/1	0.91	0.68	91,91,91,91	0
56	MG	2A	3235	1/1	0.91	0.37	97,97,97,97	0
60	K	2A	3001	1/1	0.91	0.95	108,108,108,108	0
56	MG	1A	4961	1/1	0.92	0.14	100,100,100,100	0
56	MG	2a	1846	1/1	0.92	0.26	225,225,225,225	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1B	207	1/1	0.92	0.61	88,88,88,88	0
56	MG	2A	3130	1/1	0.92	0.86	136,136,136,136	0
56	MG	1A	4235	1/1	0.92	0.29	57,57,57,57	0
56	MG	1A	4488	1/1	0.92	0.48	85,85,85,85	0
56	MG	1t	201	1/1	0.92	0.15	42,42,42,42	0
56	MG	2A	3134	1/1	0.92	0.69	83,83,83,83	0
56	MG	2a	1859	1/1	0.92	0.15	160,160,160,160	0
56	MG	2A	3135	1/1	0.92	0.20	105,105,105,105	0
56	MG	2a	1861	1/1	0.92	0.08	153,153,153,153	0
56	MG	2A	3309	1/1	0.92	0.22	108,108,108,108	0
56	MG	2a	1865	1/1	0.92	0.14	119,119,119,119	0
56	MG	1a	1724	1/1	0.92	0.21	126,126,126,126	0
56	MG	1A	4112	1/1	0.92	0.22	59,59,59,59	0
56	MG	2B	229	1/1	0.92	0.17	150,150,150,150	0
56	MG	1A	4149	1/1	0.92	0.66	59,59,59,59	0
56	MG	2B	231	1/1	0.92	0.24	152,152,152,152	0
56	MG	1A	4972	1/1	0.92	0.19	77,77,77,77	0
56	MG	1a	1732	1/1	0.92	0.59	144,144,144,144	0
56	MG	2a	1874	1/1	0.92	0.51	155,155,155,155	0
56	MG	1A	4328	1/1	0.92	0.42	55,55,55,55	0
56	MG	1a	1624	1/1	0.92	0.19	102,102,102,102	0
56	MG	1A	4981	1/1	0.92	0.20	57,57,57,57	0
56	MG	2a	1704	1/1	0.92	0.20	160,160,160,160	0
56	MG	2A	3003	1/1	0.92	0.38	108,108,108,108	0
56	MG	1A	4035	1/1	0.92	0.46	73,73,73,73	0
56	MG	2a	1882	1/1	0.92	0.11	163,163,163,163	0
56	MG	2A	3007	1/1	0.92	0.74	98,98,98,98	0
56	MG	1A	4693	1/1	0.92	0.29	67,67,67,67	0
56	MG	1a	1740	1/1	0.92	0.20	151,151,151,151	0
56	MG	1A	4695	1/1	0.92	0.25	74,74,74,74	0
56	MG	2A	3343	1/1	0.92	0.38	89,89,89,89	0
56	MG	1A	4774	1/1	0.92	0.32	68,68,68,68	0
56	MG	1A	4063	1/1	0.92	0.31	64,64,64,64	0
56	MG	2A	3164	1/1	0.92	0.42	97,97,97,97	0
56	MG	1A	4777	1/1	0.92	0.23	68,68,68,68	0
56	MG	1A	4333	1/1	0.92	0.09	83,83,83,83	0
56	MG	2A	3725	1/1	0.92	0.41	79,79,79,79	0
56	MG	2a	1721	1/1	0.92	0.39	145,145,145,145	0
56	MG	2Q	203	1/1	0.92	0.61	107,107,107,107	0
56	MG	2A	3726	1/1	0.92	0.20	91,91,91,91	0
56	MG	2a	1724	1/1	0.92	0.51	141,141,141,141	0
56	MG	1a	1639	1/1	0.92	0.31	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3729	1/1	0.92	0.30	83,83,83,83	0
56	MG	1a	1862	1/1	0.92	0.23	215,215,215,215	0
56	MG	2A	3733	1/1	0.92	0.27	77,77,77,77	0
56	MG	1A	4015	1/1	0.92	0.83	63,63,63,63	0
56	MG	2A	3179	1/1	0.92	0.74	139,139,139,139	0
56	MG	2A	3542	1/1	0.92	0.15	110,110,110,110	0
56	MG	1A	4379	1/1	0.92	0.74	95,95,95,95	0
56	MG	1A	4560	1/1	0.92	0.17	59,59,59,59	0
56	MG	1A	4701	1/1	0.92	0.34	68,68,68,68	0
56	MG	1A	4502	1/1	0.92	0.44	70,70,70,70	0
56	MG	1A	4786	1/1	0.92	0.17	63,63,63,63	0
56	MG	2a	1739	1/1	0.92	0.39	151,151,151,151	0
56	MG	1A	4637	1/1	0.92	0.12	68,68,68,68	0
56	MG	1a	1648	1/1	0.92	0.41	135,135,135,135	0
56	MG	2b	303	1/1	0.92	0.95	185,185,185,185	0
56	MG	20	106	1/1	0.92	0.07	128,128,128,128	0
56	MG	2A	3750	1/1	0.92	0.16	104,104,104,104	0
56	MG	2A	3553	1/1	0.92	0.15	106,106,106,106	0
56	MG	1A	4310	1/1	0.92	0.68	73,73,73,73	0
56	MG	1a	1874	1/1	0.92	0.32	196,196,196,196	0
56	MG	1A	4504	1/1	0.92	0.19	92,92,92,92	0
56	MG	1a	1879	1/1	0.92	0.20	97,97,97,97	0
56	MG	1A	4897	1/1	0.92	1.03	66,66,66,66	0
56	MG	1A	4337	1/1	0.92	0.28	59,59,59,59	0
56	MG	2A	3760	1/1	0.92	0.28	133,133,133,133	0
56	MG	1A	4506	1/1	0.92	0.49	96,96,96,96	0
56	MG	1a	1774	1/1	0.92	0.46	139,139,139,139	0
56	MG	2A	3046	1/1	0.92	0.29	91,91,91,91	0
56	MG	2A	3391	1/1	0.92	0.12	122,122,122,122	0
56	MG	1A	4339	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	4340	1/1	0.92	0.20	57,57,57,57	0
56	MG	1A	4341	1/1	0.92	0.21	48,48,48,48	0
56	MG	1a	1779	1/1	0.92	0.58	122,122,122,122	0
56	MG	2A	3061	1/1	0.92	0.84	92,92,92,92	0
56	MG	1A	4911	1/1	0.92	0.24	62,62,62,62	0
56	MG	2A	3063	1/1	0.92	0.19	83,83,83,83	0
56	MG	1A	4247	1/1	0.92	0.31	49,49,49,49	0
56	MG	1A	4719	1/1	0.92	0.12	89,89,89,89	0
56	MG	1R	202	1/1	0.92	0.62	56,56,56,56	0
56	MG	1A	4348	1/1	0.92	0.38	62,62,62,62	0
56	MG	2A	3072	1/1	0.92	0.19	133,133,133,133	0
56	MG	1S	201	1/1	0.92	0.58	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	5037	1/1	0.92	0.11	78,78,78,78	0
56	MG	1A	4290	1/1	0.92	0.58	70,70,70,70	0
56	MG	1A	4821	1/1	0.92	0.21	73,73,73,73	0
56	MG	1A	4313	1/1	0.92	0.44	50,50,50,50	0
56	MG	2A	3080	1/1	0.92	0.05	127,127,127,127	0
56	MG	1A	4657	1/1	0.92	0.26	84,84,84,84	0
56	MG	1A	4193	1/1	0.92	0.15	64,64,64,64	0
56	MG	1A	4594	1/1	0.92	0.31	64,64,64,64	0
56	MG	1a	1797	1/1	0.92	0.33	85,85,85,85	0
56	MG	1A	4833	1/1	0.92	0.64	70,70,70,70	0
56	MG	1W	202	1/1	0.92	0.22	55,55,55,55	0
56	MG	1A	4598	1/1	0.92	0.57	59,59,59,59	0
56	MG	1Z	302	1/1	0.92	0.77	98,98,98,98	0
56	MG	1A	4142	1/1	0.92	0.18	66,66,66,66	0
56	MG	2q	204	1/1	0.92	0.61	141,141,141,141	0
56	MG	2A	3439	1/1	0.92	0.45	56,56,56,56	0
56	MG	2A	3816	1/1	0.92	0.40	121,121,121,121	0
56	MG	1A	4837	1/1	0.92	0.19	57,57,57,57	0
56	MG	2A	3441	1/1	0.92	0.19	109,109,109,109	0
56	MG	2t	201	1/1	0.92	0.31	159,159,159,159	0
56	MG	10	102	1/1	0.92	0.36	69,69,69,69	0
56	MG	2A	3628	1/1	0.92	0.53	119,119,119,119	0
56	MG	2A	3444	1/1	0.92	0.30	99,99,99,99	0
56	MG	2A	3254	1/1	0.92	0.09	122,122,122,122	0
56	MG	2A	3447	1/1	0.92	0.53	87,87,87,87	0
56	MG	1A	4664	1/1	0.92	0.18	73,73,73,73	0
56	MG	1A	4180	1/1	0.92	0.38	48,48,48,48	0
56	MG	2A	3258	1/1	0.92	0.45	75,75,75,75	0
56	MG	2A	3259	1/1	0.92	0.50	82,82,82,82	0
56	MG	1A	4525	1/1	0.92	0.70	104,104,104,104	0
56	MG	1A	4749	1/1	0.92	0.31	77,77,77,77	0
56	MG	1A	4156	1/1	0.92	0.30	54,54,54,54	0
56	MG	2A	3839	1/1	0.92	0.20	139,139,139,139	0
56	MG	2A	3463	1/1	0.92	0.60	67,67,67,67	0
56	MG	1b	309	1/1	0.92	0.27	171,171,171,171	0
56	MG	2y	102	1/1	0.92	0.20	73,73,73,73	0
56	MG	1a	1697	1/1	0.92	0.25	142,142,142,142	0
56	MG	1d	303	1/1	0.92	0.49	151,151,151,151	0
56	MG	1A	4527	1/1	0.92	0.43	76,76,76,76	0
56	MG	2y	107	1/1	0.92	0.57	207,207,207,207	0
56	MG	1a	1821	1/1	0.92	0.15	202,202,202,202	0
56	MG	1a	1701	1/1	0.92	0.08	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4412	1/1	0.92	0.32	62,62,62,62	0
56	MG	1A	4530	1/1	0.92	0.32	68,68,68,68	0
56	MG	1A	4484	1/1	0.92	0.34	60,60,60,60	0
56	MG	2a	1834	1/1	0.92	0.13	161,161,161,161	0
56	MG	1a	1605	1/1	0.92	0.24	89,89,89,89	0
56	MG	1A	4157	1/1	0.92	0.40	52,52,52,52	0
56	MG	2A	3481	1/1	0.92	0.43	112,112,112,112	0
56	MG	1A	4486	1/1	0.92	0.32	67,67,67,67	0
57	ZN	26	102	1/1	0.92	0.07	130,130,130,130	0
56	MG	1a	1830	1/1	0.92	0.10	194,194,194,194	0
56	MG	2A	3291	1/1	0.92	0.34	75,75,75,75	0
56	MG	1a	1608	1/1	0.92	0.36	69,69,69,69	0
56	MG	2a	1814	1/1	0.93	0.23	142,142,142,142	0
56	MG	1A	4233	1/1	0.93	0.22	65,65,65,65	0
56	MG	1A	4296	1/1	0.93	0.84	82,82,82,82	0
56	MG	2A	3366	1/1	0.93	0.57	82,82,82,82	0
56	MG	1A	4575	1/1	0.93	0.24	56,56,56,56	0
56	MG	1A	4234	1/1	0.93	0.34	59,59,59,59	0
56	MG	1A	4059	1/1	0.93	0.36	72,72,72,72	0
56	MG	2a	1829	1/1	0.93	0.18	147,147,147,147	0
56	MG	2A	3004	1/1	0.93	0.83	93,93,93,93	0
56	MG	2A	3162	1/1	0.93	0.30	102,102,102,102	0
56	MG	2A	3569	1/1	0.93	0.21	96,96,96,96	0
56	MG	2A	3570	1/1	0.93	0.16	167,167,167,167	0
56	MG	2A	3005	1/1	0.93	0.87	102,102,102,102	0
56	MG	1A	4299	1/1	0.93	0.32	95,95,95,95	0
56	MG	1Y	301	1/1	0.93	0.14	85,85,85,85	0
56	MG	2A	3170	1/1	0.93	0.48	90,90,90,90	0
56	MG	2a	1652	1/1	0.93	0.11	142,142,142,142	0
56	MG	1A	4238	1/1	0.93	0.28	59,59,59,59	0
56	MG	1A	5023	1/1	0.93	0.28	58,58,58,58	0
56	MG	1a	1841	1/1	0.93	0.23	231,231,231,231	0
56	MG	2a	1851	1/1	0.93	0.09	145,145,145,145	0
56	MG	2a	1852	1/1	0.93	0.27	45,45,45,45	0
56	MG	2A	3012	1/1	0.93	0.51	108,108,108,108	0
56	MG	1A	4583	1/1	0.93	0.27	56,56,56,56	0
56	MG	1A	4405	1/1	0.93	0.13	71,71,71,71	0
56	MG	1A	4669	1/1	0.93	0.50	89,89,89,89	0
56	MG	1A	4124	1/1	0.93	0.21	76,76,76,76	0
56	MG	2A	3588	1/1	0.93	0.09	127,127,127,127	0
56	MG	1A	4672	1/1	0.93	0.54	67,67,67,67	0
56	MG	1A	4077	1/1	0.93	0.24	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4065	1/1	0.93	0.81	67,67,67,67	0
56	MG	2A	3594	1/1	0.93	0.12	74,74,74,74	0
56	MG	17	101	1/1	0.93	0.40	58,58,58,58	0
56	MG	1a	1855	1/1	0.93	0.81	230,230,230,230	0
56	MG	1A	4049	1/1	0.93	0.43	97,97,97,97	0
56	MG	1A	4081	1/1	0.93	0.29	57,57,57,57	0
56	MG	2A	3604	1/1	0.93	0.15	110,110,110,110	0
56	MG	1A	4106	1/1	0.93	0.33	50,50,50,50	0
56	MG	1a	1733	1/1	0.93	0.12	149,149,149,149	0
56	MG	1A	4775	1/1	0.93	0.32	78,78,78,78	0
56	MG	1a	1861	1/1	0.93	0.25	216,216,216,216	0
56	MG	1A	4133	1/1	0.93	0.37	58,58,58,58	0
56	MG	1A	4108	1/1	0.93	0.34	52,52,52,52	0
56	MG	2A	3411	1/1	0.93	0.34	100,100,100,100	0
56	MG	1A	4433	1/1	0.93	0.15	79,79,79,79	0
56	MG	2A	3413	1/1	0.93	0.17	126,126,126,126	0
56	MG	2A	3039	1/1	0.93	0.65	80,80,80,80	0
56	MG	2A	3415	1/1	0.93	0.28	124,124,124,124	0
56	MG	1A	4022	1/1	0.93	0.78	111,111,111,111	0
56	MG	2A	3625	1/1	0.93	0.55	146,146,146,146	0
56	MG	1A	4363	1/1	0.93	0.13	72,72,72,72	0
56	MG	2A	3042	1/1	0.93	0.34	112,112,112,112	0
56	MG	2A	3215	1/1	0.93	0.21	100,100,100,100	0
56	MG	1A	4781	1/1	0.93	0.45	81,81,81,81	0
56	MG	1a	1744	1/1	0.93	0.28	132,132,132,132	0
56	MG	2A	3218	1/1	0.93	0.16	103,103,103,103	0
56	MG	1a	1870	1/1	0.93	0.14	220,220,220,220	0
56	MG	2B	211	1/1	0.93	0.56	88,88,88,88	0
56	MG	2A	3048	1/1	0.93	0.20	88,88,88,88	0
56	MG	2a	1702	1/1	0.93	0.41	156,156,156,156	0
56	MG	1A	4912	1/1	0.93	0.41	57,57,57,57	0
56	MG	2A	3636	1/1	0.93	0.21	125,125,125,125	0
56	MG	2A	3052	1/1	0.93	0.15	103,103,103,103	0
56	MG	2A	3226	1/1	0.93	0.19	100,100,100,100	0
56	MG	1A	4367	1/1	0.93	0.33	56,56,56,56	0
56	MG	2A	3056	1/1	0.93	0.74	107,107,107,107	0
56	MG	1A	4690	1/1	0.93	0.15	83,83,83,83	0
56	MG	1A	4267	1/1	0.93	0.38	63,63,63,63	0
56	MG	1a	1753	1/1	0.93	0.21	115,115,115,115	0
56	MG	1a	1878	1/1	0.93	0.16	105,105,105,105	0
56	MG	2A	3239	1/1	0.93	0.26	108,108,108,108	0
56	MG	1A	4083	1/1	0.93	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4694	1/1	0.93	0.36	70,70,70,70	0
56	MG	2a	1914	1/1	0.93	0.12	242,242,242,242	0
56	MG	2a	1915	1/1	0.93	0.09	123,123,123,123	0
56	MG	1A	4923	1/1	0.93	0.22	66,66,66,66	0
56	MG	1a	1883	1/1	0.93	0.30	124,124,124,124	0
56	MG	2A	3655	1/1	0.93	0.55	117,117,117,117	0
56	MG	2b	301	1/1	0.93	0.08	199,199,199,199	0
56	MG	2b	302	1/1	0.93	0.14	196,196,196,196	0
56	MG	1A	4448	1/1	0.93	0.44	78,78,78,78	0
56	MG	2A	3660	1/1	0.93	0.34	147,147,147,147	0
56	MG	2A	3458	1/1	0.93	0.44	90,90,90,90	0
56	MG	1a	1625	1/1	0.93	0.39	80,80,80,80	0
56	MG	1A	4926	1/1	0.93	0.40	76,76,76,76	0
56	MG	1A	4797	1/1	0.93	0.40	78,78,78,78	0
56	MG	1A	4069	1/1	0.93	0.31	72,72,72,72	0
56	MG	2E	301	1/1	0.93	0.19	91,91,91,91	0
56	MG	1A	4372	1/1	0.93	0.30	57,57,57,57	0
56	MG	1a	1896	1/1	0.93	0.19	114,114,114,114	0
56	MG	1A	4071	1/1	0.93	0.19	77,77,77,77	0
56	MG	1A	4619	1/1	0.93	0.25	103,103,103,103	0
56	MG	1A	4143	1/1	0.93	0.20	62,62,62,62	0
56	MG	1A	4941	1/1	0.93	0.20	61,61,61,61	0
56	MG	1A	4222	1/1	0.93	0.28	70,70,70,70	0
56	MG	1A	4623	1/1	0.93	0.30	85,85,85,85	0
56	MG	1A	4223	1/1	0.93	0.13	70,70,70,70	0
56	MG	1A	4457	1/1	0.93	0.18	81,81,81,81	0
56	MG	2a	1742	1/1	0.93	0.59	148,148,148,148	0
56	MG	2P	202	1/1	0.93	0.56	127,127,127,127	0
56	MG	1B	215	1/1	0.93	0.33	65,65,65,65	0
56	MG	2A	3480	1/1	0.93	0.31	132,132,132,132	0
56	MG	1A	4058	1/1	0.93	0.68	67,67,67,67	0
56	MG	2A	3093	1/1	0.93	0.35	96,96,96,96	0
56	MG	1B	218	1/1	0.93	0.41	61,61,61,61	0
56	MG	1A	4324	1/1	0.93	0.80	78,78,78,78	0
56	MG	2A	3279	1/1	0.93	0.58	80,80,80,80	0
56	MG	2S	201	1/1	0.93	0.17	87,87,87,87	0
56	MG	1A	4537	1/1	0.93	0.47	66,66,66,66	0
56	MG	2A	3489	1/1	0.93	0.49	53,53,53,53	0
56	MG	1A	4326	1/1	0.93	0.32	67,67,67,67	0
56	MG	1A	4381	1/1	0.93	0.17	72,72,72,72	0
56	MG	1B	224	1/1	0.93	0.50	83,83,83,83	0
56	MG	1B	226	1/1	0.93	0.31	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1655	1/1	0.93	0.18	120,120,120,120	0
56	MG	1A	4542	1/1	0.93	0.21	56,56,56,56	0
56	MG	1A	4286	1/1	0.93	0.22	71,71,71,71	0
56	MG	2A	3503	1/1	0.93	0.37	103,103,103,103	0
56	MG	1A	4148	1/1	0.93	0.22	64,64,64,64	0
56	MG	2A	3505	1/1	0.93	0.32	129,129,129,129	0
56	MG	1A	4090	1/1	0.93	0.36	55,55,55,55	0
56	MG	2A	3721	1/1	0.93	0.29	118,118,118,118	0
56	MG	1A	4722	1/1	0.93	0.39	75,75,75,75	0
56	MG	1A	4965	1/1	0.93	0.23	66,66,66,66	0
56	MG	1A	4840	1/1	0.93	0.21	71,71,71,71	0
56	MG	1a	1799	1/1	0.93	0.16	113,113,113,113	0
56	MG	25	101	1/1	0.93	0.39	45,45,45,45	0
56	MG	1a	1800	1/1	0.93	0.10	119,119,119,119	0
56	MG	1A	4547	1/1	0.93	0.38	129,129,129,129	0
56	MG	1A	4482	1/1	0.93	0.17	61,61,61,61	0
56	MG	2A	3734	1/1	0.93	0.32	108,108,108,108	0
56	MG	1A	4725	1/1	0.93	0.17	73,73,73,73	0
56	MG	1A	4726	1/1	0.93	0.44	79,79,79,79	0
56	MG	1A	4980	1/1	0.93	1.06	59,59,59,59	0
56	MG	1A	4727	1/1	0.93	0.30	82,82,82,82	0
56	MG	2A	3125	1/1	0.93	0.19	81,81,81,81	0
56	MG	2A	3126	1/1	0.93	0.25	138,138,138,138	0
56	MG	1A	4387	1/1	0.93	0.22	81,81,81,81	0
56	MG	1A	4643	1/1	0.93	0.22	64,64,64,64	0
56	MG	2A	3331	1/1	0.93	0.48	91,91,91,91	0
56	MG	2A	3746	1/1	0.93	0.24	93,93,93,93	0
56	MG	1A	4734	1/1	0.93	0.21	64,64,64,64	0
56	MG	2A	3535	1/1	0.93	0.11	141,141,141,141	0
56	MG	1A	4389	1/1	0.93	0.11	78,78,78,78	0
56	MG	1A	4739	1/1	0.93	0.17	74,74,74,74	0
56	MG	2a	1613	1/1	0.93	0.25	147,147,147,147	0
56	MG	1A	4189	1/1	0.93	0.26	60,60,60,60	0
56	MG	1A	4231	1/1	0.93	0.10	72,72,72,72	0
56	MG	1A	4394	1/1	0.93	0.26	60,60,60,60	0
56	MG	2A	3756	1/1	0.93	0.31	137,137,137,137	0
56	MG	1A	4561	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	4864	1/1	0.93	0.19	75,75,75,75	0
56	MG	2A	3544	1/1	0.93	0.22	108,108,108,108	0
56	MG	2A	3144	1/1	0.93	0.33	65,65,65,65	0
56	MG	2A	3344	1/1	0.93	0.23	91,91,91,91	0
56	MG	1A	4865	1/1	0.93	0.33	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	5005	1/1	0.93	0.25	86,86,86,86	0
56	MG	1a	1689	1/1	0.93	0.13	133,133,133,133	0
56	MG	1A	4489	1/1	0.93	0.11	75,75,75,75	0
56	MG	1T	203	1/1	0.93	0.76	62,62,62,62	0
56	MG	2a	1809	1/1	0.93	0.24	122,122,122,122	0
56	MG	1A	5007	1/1	0.93	0.19	92,92,92,92	0
56	MG	2A	3513	1/1	0.94	0.19	85,85,85,85	0
56	MG	1A	4663	1/1	0.94	0.31	89,89,89,89	0
56	MG	2A	3301	1/1	0.94	0.34	96,96,96,96	0
56	MG	1A	4936	1/1	0.94	0.18	61,61,61,61	0
56	MG	2A	3520	1/1	0.94	0.19	91,91,91,91	0
56	MG	1a	1602	1/1	0.94	0.38	77,77,77,77	0
56	MG	2A	3306	1/1	0.94	0.30	85,85,85,85	0
56	MG	2a	1611	1/1	0.94	0.21	143,143,143,143	0
56	MG	1A	4738	1/1	0.94	0.19	70,70,70,70	0
56	MG	2A	3740	1/1	0.94	0.47	88,88,88,88	0
56	MG	1y	102	1/1	0.94	0.44	123,123,123,123	0
56	MG	1A	4278	1/1	0.94	0.41	65,65,65,65	0
56	MG	2a	1817	1/1	0.94	0.12	133,133,133,133	0
56	MG	1A	4836	1/1	0.94	0.29	58,58,58,58	0
56	MG	1A	4466	1/1	0.94	0.24	56,56,56,56	0
56	MG	2A	3138	1/1	0.94	0.49	118,118,118,118	0
56	MG	2A	3139	1/1	0.94	0.20	102,102,102,102	0
56	MG	2A	3141	1/1	0.94	0.27	96,96,96,96	0
56	MG	2A	3328	1/1	0.94	0.18	91,91,91,91	0
56	MG	1z	101	1/1	0.94	0.19	151,151,151,151	0
56	MG	1A	4467	1/1	0.94	0.42	57,57,57,57	0
56	MG	1A	4528	1/1	0.94	0.34	73,73,73,73	0
56	MG	2A	3145	1/1	0.94	0.68	100,100,100,100	0
56	MG	1A	4844	1/1	0.94	0.35	77,77,77,77	0
56	MG	2A	3336	1/1	0.94	0.44	95,95,95,95	0
56	MG	1A	4409	1/1	0.94	0.21	56,56,56,56	0
56	MG	2a	1842	1/1	0.94	0.16	196,196,196,196	0
56	MG	2A	3148	1/1	0.94	0.74	76,76,76,76	0
56	MG	1A	4473	1/1	0.94	0.40	46,46,46,46	0
56	MG	2A	3543	1/1	0.94	0.16	100,100,100,100	0
56	MG	1a	1617	1/1	0.94	0.41	79,79,79,79	0
56	MG	1A	4477	1/1	0.94	0.30	71,71,71,71	0
56	MG	1A	4849	1/1	0.94	0.14	84,84,84,84	0
56	MG	2a	1850	1/1	0.94	0.16	154,154,154,154	0
56	MG	2A	3547	1/1	0.94	0.25	104,104,104,104	0
56	MG	2a	1640	1/1	0.94	0.36	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4479	1/1	0.94	0.31	71,71,71,71	0
56	MG	1A	4141	1/1	0.94	0.29	63,63,63,63	0
56	MG	1A	4958	1/1	0.94	0.31	95,95,95,95	0
56	MG	2A	3349	1/1	0.94	0.20	104,104,104,104	0
56	MG	2a	1858	1/1	0.94	0.29	149,149,149,149	0
56	MG	2A	3775	1/1	0.94	0.19	114,114,114,114	0
56	MG	1A	4959	1/1	0.94	0.49	102,102,102,102	0
56	MG	1A	4414	1/1	0.94	0.36	66,66,66,66	0
56	MG	2A	3779	1/1	0.94	0.37	98,98,98,98	0
56	MG	1A	4306	1/1	0.94	0.19	97,97,97,97	0
56	MG	1A	4021	1/1	0.94	0.55	76,76,76,76	0
56	MG	2A	3359	1/1	0.94	0.33	84,84,84,84	0
56	MG	2A	3559	1/1	0.94	0.33	91,91,91,91	0
56	MG	2A	3360	1/1	0.94	0.38	78,78,78,78	0
56	MG	2A	3561	1/1	0.94	0.36	88,88,88,88	0
56	MG	2a	1871	1/1	0.94	0.33	134,134,134,134	0
56	MG	2A	3361	1/1	0.94	0.29	94,94,94,94	0
56	MG	1A	4241	1/1	0.94	0.47	66,66,66,66	0
56	MG	2A	3363	1/1	0.94	0.39	85,85,85,85	0
56	MG	2A	3166	1/1	0.94	0.69	85,85,85,85	0
56	MG	2A	3567	1/1	0.94	0.13	104,104,104,104	0
56	MG	2A	3365	1/1	0.94	0.38	90,90,90,90	0
56	MG	1A	4309	1/1	0.94	0.46	79,79,79,79	0
56	MG	1A	4685	1/1	0.94	0.51	70,70,70,70	0
56	MG	2a	1880	1/1	0.94	0.17	158,158,158,158	0
56	MG	2A	3024	1/1	0.94	0.74	123,123,123,123	0
56	MG	2A	3171	1/1	0.94	0.46	88,88,88,88	0
56	MG	1A	4544	1/1	0.94	0.19	77,77,77,77	0
56	MG	1A	4107	1/1	0.94	0.27	52,52,52,52	0
56	MG	1a	1762	1/1	0.94	0.42	103,103,103,103	0
56	MG	2A	3178	1/1	0.94	0.48	116,116,116,116	0
56	MG	2A	3814	1/1	0.94	0.31	128,128,128,128	0
56	MG	2A	3578	1/1	0.94	0.49	135,135,135,135	0
56	MG	2A	3029	1/1	0.94	0.82	105,105,105,105	0
56	MG	1A	4378	1/1	0.94	0.27	83,83,83,83	0
56	MG	2A	3380	1/1	0.94	0.12	93,93,93,93	0
56	MG	1A	4975	1/1	0.94	0.17	76,76,76,76	0
56	MG	1A	4976	1/1	0.94	0.24	77,77,77,77	0
56	MG	1a	1877	1/1	0.94	0.15	106,106,106,106	0
56	MG	2A	3186	1/1	0.94	0.35	105,105,105,105	0
56	MG	2A	3829	1/1	0.94	0.17	113,113,113,113	0
56	MG	2A	3036	1/1	0.94	0.66	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2a	1689	1/1	0.94	0.23	156,156,156,156	0
56	MG	1A	4074	1/1	0.94	0.33	78,78,78,78	0
56	MG	1D	305	1/1	0.94	0.30	81,81,81,81	0
56	MG	1A	4183	1/1	0.94	0.14	63,63,63,63	0
56	MG	1a	1881	1/1	0.94	0.11	151,151,151,151	0
56	MG	1A	4692	1/1	0.94	0.54	61,61,61,61	0
56	MG	1A	4627	1/1	0.94	0.37	80,80,80,80	0
56	MG	2a	1908	1/1	0.94	0.16	230,230,230,230	0
56	MG	2A	3603	1/1	0.94	0.13	103,103,103,103	0
56	MG	1a	1772	1/1	0.94	0.05	136,136,136,136	0
56	MG	1a	1885	1/1	0.94	0.11	128,128,128,128	0
56	MG	2A	3200	1/1	0.94	0.19	109,109,109,109	0
56	MG	2A	3845	1/1	0.94	0.82	85,85,85,85	0
56	MG	1a	1889	1/1	0.94	0.18	153,153,153,153	0
56	MG	1A	4773	1/1	0.94	0.28	68,68,68,68	0
56	MG	1A	4227	1/1	0.94	0.20	86,86,86,86	0
56	MG	1a	1892	1/1	0.94	0.42	117,117,117,117	0
56	MG	1E	304	1/1	0.94	0.20	71,71,71,71	0
56	MG	1a	1652	1/1	0.94	0.25	117,117,117,117	0
56	MG	1A	4439	1/1	0.94	0.24	80,80,80,80	0
56	MG	1A	4441	1/1	0.94	0.44	78,78,78,78	0
56	MG	2A	3212	1/1	0.94	0.11	93,93,93,93	0
56	MG	2A	3622	1/1	0.94	0.45	137,137,137,137	0
56	MG	2a	1715	1/1	0.94	0.36	147,147,147,147	0
56	MG	2A	3213	1/1	0.94	0.35	88,88,88,88	0
56	MG	2A	3060	1/1	0.94	0.52	85,85,85,85	0
56	MG	1a	1897	1/1	0.94	0.90	124,124,124,124	0
56	MG	1A	4632	1/1	0.94	0.67	66,66,66,66	0
56	MG	1A	4883	1/1	0.94	0.22	59,59,59,59	0
56	MG	1H	202	1/1	0.94	0.39	76,76,76,76	0
56	MG	2A	3630	1/1	0.94	0.39	102,102,102,102	0
56	MG	2A	3065	1/1	0.94	0.22	117,117,117,117	0
56	MG	1A	4442	1/1	0.94	0.15	75,75,75,75	0
56	MG	1A	4033	1/1	0.94	0.26	70,70,70,70	0
56	MG	2A	3069	1/1	0.94	0.23	149,149,149,149	0
56	MG	2A	3225	1/1	0.94	0.58	113,113,113,113	0
56	MG	1A	4007	1/1	0.94	0.22	64,64,64,64	0
56	MG	2A	3227	1/1	0.94	0.20	94,94,94,94	0
56	MG	1a	1789	1/1	0.94	0.20	111,111,111,111	0
56	MG	1A	4317	1/1	0.94	0.70	106,106,106,106	0
56	MG	1A	4292	1/1	0.94	0.42	96,96,96,96	0
56	MG	1a	1907	1/1	0.94	0.35	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4263	1/1	0.94	0.56	51,51,51,51	0
56	MG	1A	5011	1/1	0.94	0.32	77,77,77,77	0
56	MG	1A	4264	1/1	0.94	0.39	61,61,61,61	0
56	MG	2A	3443	1/1	0.94	0.18	111,111,111,111	0
56	MG	1A	4057	1/1	0.94	0.75	63,63,63,63	0
56	MG	1Q	203	1/1	0.94	0.41	50,50,50,50	0
56	MG	2a	1743	1/1	0.94	0.70	151,151,151,151	0
56	MG	1A	4360	1/1	0.94	0.12	88,88,88,88	0
56	MG	1a	1914	1/1	0.94	0.19	193,193,193,193	0
56	MG	1A	4166	1/1	0.94	0.40	34,34,34,34	0
56	MG	2A	3450	1/1	0.94	0.60	85,85,85,85	0
56	MG	1A	4896	1/1	0.94	1.29	61,61,61,61	0
56	MG	1A	4454	1/1	0.94	0.27	78,78,78,78	0
56	MG	1A	4646	1/1	0.94	0.28	69,69,69,69	0
56	MG	2A	3459	1/1	0.94	0.47	98,98,98,98	0
56	MG	1A	4582	1/1	0.94	0.18	65,65,65,65	0
56	MG	1A	4648	1/1	0.94	0.29	66,66,66,66	0
56	MG	1A	4902	1/1	0.94	0.62	63,63,63,63	0
56	MG	1A	5026	1/1	0.94	0.29	70,70,70,70	0
56	MG	1A	4649	1/1	0.94	0.21	65,65,65,65	0
56	MG	2a	1759	1/1	0.94	0.15	218,218,218,218	0
56	MG	1A	4805	1/1	0.94	0.83	95,95,95,95	0
56	MG	1A	4909	1/1	0.94	0.20	59,59,59,59	0
56	MG	2A	3467	1/1	0.94	0.37	79,79,79,79	0
56	MG	1A	4720	1/1	0.94	0.25	79,79,79,79	0
56	MG	1A	4807	1/1	0.94	0.32	58,58,58,58	0
56	MG	1A	4512	1/1	0.94	0.28	73,73,73,73	0
56	MG	1A	5038	1/1	0.94	0.44	70,70,70,70	0
56	MG	1A	4651	1/1	0.94	0.43	88,88,88,88	0
56	MG	2A	3266	1/1	0.94	0.46	86,86,86,86	0
56	MG	2A	3687	1/1	0.94	0.28	118,118,118,118	0
56	MG	2A	3267	1/1	0.94	0.28	99,99,99,99	0
56	MG	1Z	303	1/1	0.94	0.29	42,42,42,42	0
56	MG	2A	3479	1/1	0.94	0.30	122,122,122,122	0
56	MG	1Z	304	1/1	0.94	0.56	64,64,64,64	0
56	MG	2A	3271	1/1	0.94	0.24	113,113,113,113	0
56	MG	1A	4268	1/1	0.94	0.41	65,65,65,65	0
56	MG	2A	3273	1/1	0.94	0.33	70,70,70,70	0
56	MG	2A	3108	1/1	0.94	0.08	139,139,139,139	0
56	MG	2A	3701	1/1	0.94	0.25	93,93,93,93	0
56	MG	20	105	1/1	0.94	0.06	126,126,126,126	0
56	MG	1a	1700	1/1	0.94	0.16	161,161,161,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3280	1/1	0.94	0.30	89,89,89,89	0
56	MG	2y	104	1/1	0.94	0.13	248,248,248,248	0
56	MG	1A	4815	1/1	0.94	0.52	77,77,77,77	0
56	MG	1a	1703	1/1	0.94	0.10	149,149,149,149	0
56	MG	1A	4816	1/1	0.94	0.33	75,75,75,75	0
56	MG	10	103	1/1	0.94	0.39	72,72,72,72	0
56	MG	1A	4456	1/1	0.94	0.13	80,80,80,80	0
56	MG	1A	4365	1/1	0.94	0.30	58,58,58,58	0
56	MG	1A	4016	1/1	0.94	0.23	68,68,68,68	0
56	MG	1A	4218	1/1	0.94	0.31	58,58,58,58	0
56	MG	1A	4369	1/1	0.94	0.25	61,61,61,61	0
56	MG	28	102	1/1	0.94	0.78	119,119,119,119	0
56	MG	28	103	1/1	0.94	0.53	115,115,115,115	0
56	MG	2A	3722	1/1	0.94	0.11	128,128,128,128	0
56	MG	2A	3123	1/1	0.94	0.23	133,133,133,133	0
56	MG	2A	3295	1/1	0.94	0.27	97,97,97,97	0
56	MG	1A	4593	1/1	0.94	0.39	65,65,65,65	0
56	MG	1A	4173	1/1	0.94	0.14	57,57,57,57	0
56	MG	2A	3129	1/1	0.94	0.74	101,101,101,101	0
56	MG	2A	3103	1/1	0.95	0.58	79,79,79,79	0
56	MG	1A	4118	1/1	0.95	0.62	82,82,82,82	0
56	MG	1A	4846	1/1	0.95	0.22	74,74,74,74	0
56	MG	2X	201	1/1	0.95	0.23	108,108,108,108	0
56	MG	1b	302	1/1	0.95	0.32	165,165,165,165	0
56	MG	2Y	202	1/1	0.95	0.13	137,137,137,137	0
56	MG	2A	3275	1/1	0.95	0.30	83,83,83,83	0
56	MG	1B	222	1/1	0.95	0.19	91,91,91,91	0
56	MG	2A	3278	1/1	0.95	0.33	86,86,86,86	0
56	MG	1A	4401	1/1	0.95	0.22	78,78,78,78	0
56	MG	2A	3691	1/1	0.95	0.26	165,165,165,165	0
56	MG	1A	4745	1/1	0.95	0.22	81,81,81,81	0
56	MG	1A	4137	1/1	0.95	0.15	102,102,102,102	0
56	MG	1A	4601	1/1	0.95	0.13	102,102,102,102	0
56	MG	1A	4232	1/1	0.95	0.28	64,64,64,64	0
56	MG	1A	4963	1/1	0.95	0.43	78,78,78,78	0
56	MG	1A	4964	1/1	0.95	0.38	67,67,67,67	0
56	MG	2A	3700	1/1	0.95	0.20	113,113,113,113	0
56	MG	2A	3488	1/1	0.95	0.42	115,115,115,115	0
56	MG	1A	4670	1/1	0.95	0.26	71,71,71,71	0
56	MG	1e	301	1/1	0.95	0.50	140,140,140,140	0
56	MG	2A	3707	1/1	0.95	0.25	100,100,100,100	0
56	MG	1a	1660	1/1	0.95	0.30	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3709	1/1	0.95	0.23	93,93,93,93	0
56	MG	1A	4046	1/1	0.95	0.28	68,68,68,68	0
56	MG	1A	4751	1/1	0.95	0.25	71,71,71,71	0
56	MG	2A	3294	1/1	0.95	0.42	91,91,91,91	0
56	MG	1A	4030	1/1	0.95	0.25	58,58,58,58	0
56	MG	2A	3501	1/1	0.95	0.20	104,104,104,104	0
56	MG	2a	1815	1/1	0.95	0.13	85,85,85,85	0
56	MG	2a	1816	1/1	0.95	0.14	156,156,156,156	0
56	MG	1A	4462	1/1	0.95	0.27	74,74,74,74	0
56	MG	2a	1819	1/1	0.95	0.18	150,150,150,150	0
56	MG	2A	3128	1/1	0.95	0.42	130,130,130,130	0
56	MG	1a	1667	1/1	0.95	0.13	132,132,132,132	0
56	MG	1A	4284	1/1	0.95	0.36	65,65,65,65	0
56	MG	2A	3506	1/1	0.95	0.16	149,149,149,149	0
56	MG	1A	4319	1/1	0.95	0.37	68,68,68,68	0
56	MG	1A	4411	1/1	0.95	0.23	50,50,50,50	0
56	MG	1A	4977	1/1	0.95	0.32	78,78,78,78	0
56	MG	2A	3728	1/1	0.95	0.21	83,83,83,83	0
56	MG	1a	1813	1/1	0.95	0.30	91,91,91,91	0
56	MG	1A	4978	1/1	0.95	0.19	60,60,60,60	0
56	MG	1A	4168	1/1	0.95	0.42	50,50,50,50	0
56	MG	1A	4612	1/1	0.95	0.15	62,62,62,62	0
56	MG	1A	4236	1/1	0.95	0.67	55,55,55,55	0
56	MG	1A	4683	1/1	0.95	0.32	55,55,55,55	0
56	MG	2A	3317	1/1	0.95	0.36	81,81,81,81	0
56	MG	1A	4415	1/1	0.95	0.15	74,74,74,74	0
56	MG	2a	1616	1/1	0.95	0.10	139,139,139,139	0
56	MG	2A	3321	1/1	0.95	0.52	86,86,86,86	0
56	MG	2A	3323	1/1	0.95	0.46	89,89,89,89	0
56	MG	2A	3527	1/1	0.95	0.18	111,111,111,111	0
56	MG	1A	4618	1/1	0.95	0.19	95,95,95,95	0
56	MG	1A	4766	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	4989	1/1	0.95	0.23	73,73,73,73	0
56	MG	1A	4990	1/1	0.95	0.21	64,64,64,64	0
56	MG	2A	3330	1/1	0.95	0.20	97,97,97,97	0
56	MG	2a	1855	1/1	0.95	0.07	88,88,88,88	0
56	MG	1A	4992	1/1	0.95	0.37	70,70,70,70	0
56	MG	1A	4876	1/1	0.95	0.26	80,80,80,80	0
56	MG	1A	4686	1/1	0.95	0.14	93,93,93,93	0
56	MG	1A	4475	1/1	0.95	0.16	58,58,58,58	0
56	MG	2a	1629	1/1	0.95	0.28	187,187,187,187	0
56	MG	2A	3002	1/1	0.95	0.64	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4416	1/1	0.95	0.32	57,57,57,57	0
56	MG	2a	1863	1/1	0.95	0.14	162,162,162,162	0
56	MG	1A	4478	1/1	0.95	0.24	71,71,71,71	0
56	MG	1A	4169	1/1	0.95	0.20	57,57,57,57	0
56	MG	1A	4885	1/1	0.95	0.55	92,92,92,92	0
56	MG	2A	3341	1/1	0.95	0.24	86,86,86,86	0
56	MG	1A	4419	1/1	0.95	0.18	55,55,55,55	0
56	MG	1a	1698	1/1	0.95	0.21	120,120,120,120	0
56	MG	2A	3159	1/1	0.95	0.39	100,100,100,100	0
56	MG	2a	1641	1/1	0.95	0.33	146,146,146,146	0
56	MG	1a	1838	1/1	0.95	0.09	231,231,231,231	0
56	MG	1A	4422	1/1	0.95	0.26	52,52,52,52	0
56	MG	2a	1646	1/1	0.95	0.97	120,120,120,120	0
56	MG	2A	3348	1/1	0.95	0.51	90,90,90,90	0
56	MG	1A	4483	1/1	0.95	0.19	66,66,66,66	0
56	MG	2A	3014	1/1	0.95	0.59	108,108,108,108	0
56	MG	1A	4084	1/1	0.95	0.43	61,61,61,61	0
56	MG	2A	3167	1/1	0.95	0.75	99,99,99,99	0
56	MG	1a	1702	1/1	0.95	0.22	181,181,181,181	0
56	MG	2A	3554	1/1	0.95	0.27	89,89,89,89	0
56	MG	1A	4172	1/1	0.95	0.33	58,58,58,58	0
56	MG	2A	3778	1/1	0.95	0.34	97,97,97,97	0
56	MG	1A	4020	1/1	0.95	0.23	73,73,73,73	0
56	MG	1A	4630	1/1	0.95	0.52	56,56,56,56	0
56	MG	2A	3172	1/1	0.95	0.28	91,91,91,91	0
56	MG	1a	1848	1/1	0.95	0.26	178,178,178,178	0
56	MG	1a	1849	1/1	0.95	0.60	149,149,149,149	0
56	MG	2A	3175	1/1	0.95	0.33	58,58,58,58	0
56	MG	2A	3787	1/1	0.95	0.47	125,125,125,125	0
56	MG	2A	3563	1/1	0.95	0.29	90,90,90,90	0
56	MG	1A	4893	1/1	0.95	0.24	65,65,65,65	0
56	MG	2a	1895	1/1	0.95	0.32	156,156,156,156	0
56	MG	2A	3792	1/1	0.95	0.50	130,130,130,130	0
56	MG	1A	4430	1/1	0.95	0.18	61,61,61,61	0
56	MG	2a	1898	1/1	0.95	0.20	160,160,160,160	0
56	MG	1A	4209	1/1	0.95	0.29	55,55,55,55	0
56	MG	1A	5022	1/1	0.95	0.84	122,122,122,122	0
56	MG	2A	3026	1/1	0.95	0.52	117,117,117,117	0
56	MG	1A	4212	1/1	0.95	0.28	51,51,51,51	0
56	MG	1A	4634	1/1	0.95	0.30	59,59,59,59	0
56	MG	1a	1715	1/1	0.95	0.20	123,123,123,123	0
56	MG	1A	4787	1/1	0.95	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4023	1/1	0.95	0.85	110,110,110,110	0
56	MG	1A	4434	1/1	0.95	0.22	58,58,58,58	0
56	MG	1A	5028	1/1	0.95	0.20	70,70,70,70	0
56	MG	1A	4704	1/1	0.95	0.12	77,77,77,77	0
56	MG	2A	3810	1/1	0.95	0.45	145,145,145,145	0
56	MG	1a	1727	1/1	0.95	0.10	127,127,127,127	0
56	MG	1a	1728	1/1	0.95	0.47	143,143,143,143	0
56	MG	2A	3815	1/1	0.95	0.09	136,136,136,136	0
56	MG	1a	1729	1/1	0.95	0.14	143,143,143,143	0
56	MG	2a	1687	1/1	0.95	0.31	162,162,162,162	0
56	MG	2a	1916	1/1	0.95	0.20	63,63,63,63	0
56	MG	1A	4903	1/1	0.95	0.13	61,61,61,61	0
56	MG	1A	5034	1/1	0.95	1.03	67,67,67,67	0
56	MG	1a	1868	1/1	0.95	0.62	214,214,214,214	0
56	MG	2A	3822	1/1	0.95	0.34	91,91,91,91	0
56	MG	2a	1692	1/1	0.95	0.22	149,149,149,149	0
56	MG	2A	3585	1/1	0.95	0.68	114,114,114,114	0
56	MG	2a	1694	1/1	0.95	0.31	146,146,146,146	0
56	MG	2A	3824	1/1	0.95	0.19	99,99,99,99	0
56	MG	2A	3586	1/1	0.95	0.07	120,120,120,120	0
56	MG	2A	3587	1/1	0.95	0.06	123,123,123,123	0
56	MG	16	101	1/1	0.95	0.09	72,72,72,72	0
56	MG	2A	3392	1/1	0.95	0.22	124,124,124,124	0
56	MG	1A	4705	1/1	0.95	0.34	72,72,72,72	0
56	MG	1A	4146	1/1	0.95	0.25	59,59,59,59	0
56	MG	1A	4331	1/1	0.95	0.15	73,73,73,73	0
56	MG	2A	3050	1/1	0.95	0.13	93,93,93,93	0
56	MG	1A	4910	1/1	0.95	0.20	55,55,55,55	0
56	MG	1A	4437	1/1	0.95	0.24	64,64,64,64	0
56	MG	2A	3211	1/1	0.95	0.29	94,94,94,94	0
56	MG	2A	3837	1/1	0.95	0.15	68,68,68,68	0
56	MG	2A	3838	1/1	0.95	0.14	44,44,44,44	0
56	MG	2A	3601	1/1	0.95	0.24	101,101,101,101	0
56	MG	1A	4563	1/1	0.95	0.38	68,68,68,68	0
56	MG	1A	4565	1/1	0.95	0.15	58,58,58,58	0
56	MG	2A	3843	1/1	0.95	0.37	76,76,76,76	0
56	MG	1A	4250	1/1	0.95	0.14	64,64,64,64	0
56	MG	1A	4253	1/1	0.95	0.64	54,54,54,54	0
56	MG	2A	3847	1/1	0.95	0.24	91,91,91,91	0
56	MG	2A	3849	1/1	0.95	0.20	153,153,153,153	0
56	MG	2A	3059	1/1	0.95	0.10	88,88,88,88	0
56	MG	2A	3853	1/1	0.95	0.69	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3410	1/1	0.95	0.25	108,108,108,108	0
56	MG	1A	5049	1/1	0.95	0.65	72,72,72,72	0
56	MG	1a	1746	1/1	0.95	0.12	154,154,154,154	0
56	MG	1A	4079	1/1	0.95	0.40	58,58,58,58	0
56	MG	1a	1748	1/1	0.95	0.17	145,145,145,145	0
56	MG	2a	1728	1/1	0.95	0.21	79,79,79,79	0
56	MG	1a	1749	1/1	0.95	0.31	134,134,134,134	0
56	MG	2A	3223	1/1	0.95	0.10	118,118,118,118	0
56	MG	1A	4443	1/1	0.95	0.28	75,75,75,75	0
56	MG	2B	210	1/1	0.95	0.42	70,70,70,70	0
56	MG	2A	3618	1/1	0.95	0.12	149,149,149,149	0
56	MG	1A	4578	1/1	0.95	0.19	59,59,59,59	0
56	MG	1a	1612	1/1	0.95	0.25	94,94,94,94	0
56	MG	1A	4924	1/1	0.95	0.13	71,71,71,71	0
56	MG	2p	103	1/1	0.95	0.50	152,152,152,152	0
56	MG	2A	3070	1/1	0.95	0.31	156,156,156,156	0
56	MG	1A	4181	1/1	0.95	0.37	45,45,45,45	0
56	MG	1A	4261	1/1	0.95	0.14	63,63,63,63	0
56	MG	1A	4819	1/1	0.95	0.38	119,119,119,119	0
56	MG	2A	3426	1/1	0.95	0.25	93,93,93,93	0
56	MG	1a	1620	1/1	0.95	0.19	98,98,98,98	0
56	MG	2A	3429	1/1	0.95	0.21	117,117,117,117	0
56	MG	1A	4055	1/1	0.95	0.36	86,86,86,86	0
56	MG	2A	3238	1/1	0.95	0.25	108,108,108,108	0
56	MG	1A	4930	1/1	0.95	0.39	110,110,110,110	0
56	MG	2A	3434	1/1	0.95	0.29	95,95,95,95	0
56	MG	2B	226	1/1	0.95	0.09	132,132,132,132	0
56	MG	2A	3437	1/1	0.95	0.17	97,97,97,97	0
56	MG	2A	3241	1/1	0.95	0.59	124,124,124,124	0
56	MG	1A	4931	1/1	0.95	0.27	125,125,125,125	0
56	MG	1A	4110	1/1	0.95	0.22	54,54,54,54	0
56	MG	1A	4091	1/1	0.95	0.32	58,58,58,58	0
56	MG	1A	4823	1/1	0.95	0.48	74,74,74,74	0
56	MG	1A	4653	1/1	0.95	0.28	88,88,88,88	0
56	MG	2A	3085	1/1	0.95	0.13	118,118,118,118	0
56	MG	1A	4937	1/1	0.95	0.17	58,58,58,58	0
56	MG	1A	4938	1/1	0.95	0.32	69,69,69,69	0
56	MG	1A	4828	1/1	0.95	0.21	80,80,80,80	0
56	MG	1A	4266	1/1	0.95	0.20	58,58,58,58	0
56	MG	2A	3652	1/1	0.95	0.12	124,124,124,124	0
56	MG	1A	4728	1/1	0.95	0.18	76,76,76,76	0
56	MG	2A	3453	1/1	0.95	0.53	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3253	1/1	0.95	0.20	128,128,128,128	0
56	MG	1A	4510	1/1	0.95	0.12	69,69,69,69	0
56	MG	2A	3092	1/1	0.95	0.33	118,118,118,118	0
56	MG	2F	304	1/1	0.95	0.15	135,135,135,135	0
56	MG	1a	1638	1/1	0.95	0.43	117,117,117,117	0
56	MG	1A	4732	1/1	0.95	0.21	56,56,56,56	0
56	MG	1A	4113	1/1	0.95	0.32	55,55,55,55	0
56	MG	2A	3668	1/1	0.95	0.38	91,91,91,91	0
56	MG	1A	4114	1/1	0.95	0.25	56,56,56,56	0
56	MG	1A	4093	1/1	0.95	0.31	62,62,62,62	0
56	MG	1A	4737	1/1	0.95	0.16	76,76,76,76	0
56	MG	1A	4953	1/1	0.95	0.19	60,60,60,60	0
56	MG	1A	4515	1/1	0.95	0.33	70,70,70,70	0
57	ZN	29	103	1/1	0.95	0.05	143,143,143,143	0
56	MG	1A	4018	1/1	0.95	0.47	68,68,68,68	0
59	GDP	1v	704	28/28	0.95	0.18	117,117,117,117	0
56	MG	2A	3469	1/1	0.95	0.28	115,115,115,115	0
56	MG	1a	1787	1/1	0.95	0.39	124,124,124,124	0
56	MG	1A	4315	1/1	0.96	0.43	111,111,111,111	0
56	MG	1b	308	1/1	0.96	0.23	162,162,162,162	0
56	MG	2a	1810	1/1	0.96	0.42	129,129,129,129	0
56	MG	2a	1811	1/1	0.96	0.15	129,129,129,129	0
56	MG	1a	1818	1/1	0.96	0.07	186,186,186,186	0
56	MG	1A	4408	1/1	0.96	0.37	57,57,57,57	0
56	MG	1d	302	1/1	0.96	0.17	149,149,149,149	0
56	MG	1A	4791	1/1	0.96	0.43	73,73,73,73	0
56	MG	1a	1603	1/1	0.96	0.17	98,98,98,98	0
56	MG	2A	3766	1/1	0.96	0.73	66,66,66,66	0
56	MG	1A	4969	1/1	0.96	0.23	63,63,63,63	0
56	MG	1e	302	1/1	0.96	0.16	147,147,147,147	0
56	MG	2A	3231	1/1	0.96	0.23	95,95,95,95	0
56	MG	1A	4795	1/1	0.96	0.17	79,79,79,79	0
56	MG	2A	3771	1/1	0.96	0.22	101,101,101,101	0
56	MG	2A	3772	1/1	0.96	0.10	98,98,98,98	0
56	MG	1A	4019	1/1	0.96	0.49	77,77,77,77	0
56	MG	2a	1832	1/1	0.96	0.10	138,138,138,138	0
56	MG	2A	3234	1/1	0.96	0.20	103,103,103,103	0
56	MG	2a	1835	1/1	0.96	0.27	152,152,152,152	0
56	MG	1a	1825	1/1	0.96	0.26	214,214,214,214	0
56	MG	1A	4364	1/1	0.96	0.40	72,72,72,72	0
56	MG	1A	4095	1/1	0.96	0.32	62,62,62,62	0
56	MG	2A	3404	1/1	0.96	0.18	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3405	1/1	0.96	0.28	130,130,130,130	0
56	MG	1A	4031	1/1	0.96	0.17	56,56,56,56	0
56	MG	2A	3240	1/1	0.96	0.30	120,120,120,120	0
56	MG	1A	4588	1/1	0.96	0.26	79,79,79,79	0
56	MG	1a	1714	1/1	0.96	0.28	118,118,118,118	0
56	MG	2A	3784	1/1	0.96	0.35	110,110,110,110	0
56	MG	1A	4522	1/1	0.96	0.24	76,76,76,76	0
56	MG	2A	3786	1/1	0.96	0.18	123,123,123,123	0
56	MG	1A	4590	1/1	0.96	0.78	71,71,71,71	0
56	MG	2A	3788	1/1	0.96	0.23	124,124,124,124	0
56	MG	1A	4523	1/1	0.96	0.38	68,68,68,68	0
56	MG	1a	1721	1/1	0.96	0.12	134,134,134,134	0
56	MG	1B	217	1/1	0.96	0.23	71,71,71,71	0
56	MG	1a	1618	1/1	0.96	0.31	94,94,94,94	0
56	MG	2A	3110	1/1	0.96	0.19	189,189,189,189	0
56	MG	1A	4982	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	4204	1/1	0.96	0.14	64,64,64,64	0
56	MG	1A	4115	1/1	0.96	0.24	62,62,62,62	0
56	MG	1A	4595	1/1	0.96	0.37	62,62,62,62	0
56	MG	1A	4898	1/1	0.96	0.29	60,60,60,60	0
56	MG	2A	3117	1/1	0.96	0.23	134,134,134,134	0
56	MG	2A	3803	1/1	0.96	0.19	112,112,112,112	0
56	MG	2a	1864	1/1	0.96	0.32	161,161,161,161	0
56	MG	2A	3256	1/1	0.96	0.25	92,92,92,92	0
56	MG	2A	3427	1/1	0.96	0.36	95,95,95,95	0
56	MG	1x	302	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	4596	1/1	0.96	0.10	65,65,65,65	0
56	MG	1A	4211	1/1	0.96	0.36	57,57,57,57	0
56	MG	1B	225	1/1	0.96	0.37	92,92,92,92	0
56	MG	2A	3813	1/1	0.96	0.17	126,126,126,126	0
56	MG	1A	4179	1/1	0.96	0.14	60,60,60,60	0
56	MG	1a	1846	1/1	0.96	0.78	193,193,193,193	0
56	MG	2A	3435	1/1	0.96	0.44	97,97,97,97	0
56	MG	2A	3610	1/1	0.96	0.71	114,114,114,114	0
56	MG	1a	1628	1/1	0.96	0.35	101,101,101,101	0
56	MG	2A	3127	1/1	0.96	0.37	135,135,135,135	0
56	MG	1D	301	1/1	0.96	0.28	65,65,65,65	0
56	MG	2A	3268	1/1	0.96	0.25	94,94,94,94	0
56	MG	1A	4420	1/1	0.96	0.24	50,50,50,50	0
56	MG	1A	4421	1/1	0.96	0.13	58,58,58,58	0
56	MG	1a	1632	1/1	0.96	0.18	118,118,118,118	0
56	MG	2A	3619	1/1	0.96	0.20	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3621	1/1	0.96	0.61	95,95,95,95	0
56	MG	1A	4067	1/1	0.96	0.33	86,86,86,86	0
56	MG	1a	1743	1/1	0.96	0.25	139,139,139,139	0
56	MG	1A	4424	1/1	0.96	0.17	61,61,61,61	0
56	MG	1A	4740	1/1	0.96	0.14	79,79,79,79	0
56	MG	1A	4099	1/1	0.96	0.12	69,69,69,69	0
56	MG	1E	301	1/1	0.96	0.18	57,57,57,57	0
56	MG	1A	4825	1/1	0.96	0.16	92,92,92,92	0
56	MG	2A	3454	1/1	0.96	0.17	90,90,90,90	0
56	MG	1A	4245	1/1	0.96	0.23	52,52,52,52	0
56	MG	2A	3457	1/1	0.96	0.46	93,93,93,93	0
56	MG	2A	3140	1/1	0.96	0.29	101,101,101,101	0
56	MG	1A	4829	1/1	0.96	0.25	74,74,74,74	0
56	MG	1A	4830	1/1	0.96	0.28	76,76,76,76	0
56	MG	1A	5009	1/1	0.96	0.25	72,72,72,72	0
56	MG	1A	4675	1/1	0.96	0.23	104,104,104,104	0
56	MG	1A	4536	1/1	0.96	1.13	115,115,115,115	0
56	MG	1a	1756	1/1	0.96	0.20	109,109,109,109	0
56	MG	2A	3641	1/1	0.96	0.26	127,127,127,127	0
56	MG	1A	5013	1/1	0.96	0.55	38,38,38,38	0
56	MG	2a	1701	1/1	0.96	0.24	146,146,146,146	0
56	MG	1A	4246	1/1	0.96	0.20	51,51,51,51	0
56	MG	2B	202	1/1	0.96	0.19	137,137,137,137	0
56	MG	1a	1650	1/1	0.96	0.23	123,123,123,123	0
56	MG	1A	4922	1/1	0.96	0.18	67,67,67,67	0
56	MG	1A	4005	1/1	0.96	0.21	65,65,65,65	0
56	MG	1A	4249	1/1	0.96	0.18	52,52,52,52	0
56	MG	2a	1708	1/1	0.96	0.24	152,152,152,152	0
56	MG	1A	4541	1/1	0.96	0.32	56,56,56,56	0
56	MG	1A	4062	1/1	0.96	0.41	72,72,72,72	0
56	MG	1A	4838	1/1	0.96	0.38	73,73,73,73	0
56	MG	2A	3651	1/1	0.96	0.14	118,118,118,118	0
56	MG	2a	1917	1/1	0.96	0.14	86,86,86,86	0
56	MG	2A	3475	1/1	0.96	0.60	111,111,111,111	0
56	MG	2a	1919	1/1	0.96	0.12	155,155,155,155	0
56	MG	2A	3031	1/1	0.96	0.53	103,103,103,103	0
56	MG	2A	3158	1/1	0.96	0.40	107,107,107,107	0
56	MG	2A	3657	1/1	0.96	0.12	103,103,103,103	0
56	MG	1A	4105	1/1	0.96	0.37	46,46,46,46	0
56	MG	2A	3033	1/1	0.96	0.75	107,107,107,107	0
56	MG	1A	4158	1/1	0.96	0.35	58,58,58,58	0
56	MG	2A	3663	1/1	0.96	0.19	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1769	1/1	0.96	0.20	131,131,131,131	0
56	MG	2A	3163	1/1	0.96	0.22	103,103,103,103	0
56	MG	1A	4620	1/1	0.96	0.20	107,107,107,107	0
56	MG	2A	3315	1/1	0.96	0.20	90,90,90,90	0
56	MG	2A	3485	1/1	0.96	0.35	60,60,60,60	0
56	MG	2A	3316	1/1	0.96	0.26	85,85,85,85	0
56	MG	1A	4258	1/1	0.96	0.19	68,68,68,68	0
56	MG	2A	3318	1/1	0.96	0.48	83,83,83,83	0
56	MG	1A	4089	1/1	0.96	0.31	67,67,67,67	0
56	MG	2A	3320	1/1	0.96	0.62	88,88,88,88	0
56	MG	1a	1773	1/1	0.96	0.32	143,143,143,143	0
56	MG	1A	4934	1/1	0.96	0.33	77,77,77,77	0
56	MG	1a	1663	1/1	0.96	0.27	115,115,115,115	0
56	MG	2A	3682	1/1	0.96	0.39	123,123,123,123	0
56	MG	2A	3495	1/1	0.96	0.26	106,106,106,106	0
56	MG	1A	5030	1/1	0.96	0.32	72,72,72,72	0
56	MG	2A	3499	1/1	0.96	0.16	100,100,100,100	0
56	MG	1a	1665	1/1	0.96	0.12	132,132,132,132	0
56	MG	1A	4162	1/1	0.96	0.17	56,56,56,56	0
56	MG	2A	3688	1/1	0.96	0.61	143,143,143,143	0
56	MG	1A	4438	1/1	0.96	0.09	65,65,65,65	0
56	MG	2A	3047	1/1	0.96	0.26	99,99,99,99	0
56	MG	1A	4140	1/1	0.96	0.27	70,70,70,70	0
56	MG	1A	4164	1/1	0.96	0.27	58,58,58,58	0
56	MG	2A	3334	1/1	0.96	0.31	105,105,105,105	0
56	MG	2A	3694	1/1	0.96	0.53	61,61,61,61	0
56	MG	1A	4070	1/1	0.96	0.21	67,67,67,67	0
56	MG	1A	4552	1/1	0.96	0.25	71,71,71,71	0
56	MG	2A	3511	1/1	0.96	0.19	89,89,89,89	0
56	MG	2A	3182	1/1	0.96	0.50	105,105,105,105	0
56	MG	2A	3054	1/1	0.96	0.20	100,100,100,100	0
56	MG	2A	3514	1/1	0.96	0.12	114,114,114,114	0
56	MG	2A	3702	1/1	0.96	0.25	92,92,92,92	0
56	MG	2A	3515	1/1	0.96	0.35	115,115,115,115	0
56	MG	1U	202	1/1	0.96	0.21	58,58,58,58	0
56	MG	1A	4554	1/1	0.96	0.25	79,79,79,79	0
56	MG	1A	4229	1/1	0.96	0.32	111,111,111,111	0
56	MG	2A	3187	1/1	0.96	0.18	105,105,105,105	0
56	MG	2A	3710	1/1	0.96	0.22	95,95,95,95	0
56	MG	1A	4945	1/1	0.96	0.13	73,73,73,73	0
56	MG	2A	3189	1/1	0.96	0.27	113,113,113,113	0
56	MG	2A	3714	1/1	0.96	0.25	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3345	1/1	0.96	0.36	83,83,83,83	0
56	MG	2A	3716	1/1	0.96	0.24	116,116,116,116	0
56	MG	2A	3190	1/1	0.96	0.47	98,98,98,98	0
56	MG	2s	103	1/1	0.96	0.10	251,251,251,251	0
56	MG	2A	3525	1/1	0.96	0.18	106,106,106,106	0
56	MG	1a	1679	1/1	0.96	0.16	163,163,163,163	0
56	MG	1A	4391	1/1	0.96	0.23	93,93,93,93	0
56	MG	1A	4344	1/1	0.96	0.13	70,70,70,70	0
56	MG	1A	4446	1/1	0.96	0.37	59,59,59,59	0
56	MG	2A	3195	1/1	0.96	0.49	90,90,90,90	0
56	MG	2A	3354	1/1	0.96	0.34	79,79,79,79	0
56	MG	2w	201	1/1	0.96	0.13	84,84,84,84	0
56	MG	1A	4025	1/1	0.96	0.32	67,67,67,67	0
56	MG	2x	101	1/1	0.96	0.87	62,62,62,62	0
56	MG	2A	3356	1/1	0.96	0.30	80,80,80,80	0
56	MG	1A	4196	1/1	0.96	0.32	73,73,73,73	0
56	MG	1A	4269	1/1	0.96	0.15	69,69,69,69	0
56	MG	2A	3730	1/1	0.96	0.36	99,99,99,99	0
56	MG	1A	4353	1/1	0.96	0.28	59,59,59,59	0
56	MG	1A	4572	1/1	0.96	0.18	83,83,83,83	0
56	MG	1A	4573	1/1	0.96	0.18	70,70,70,70	0
56	MG	1A	4399	1/1	0.96	0.14	77,77,77,77	0
56	MG	1A	4871	1/1	0.96	0.24	55,55,55,55	0
56	MG	1A	4270	1/1	0.96	0.34	68,68,68,68	0
56	MG	1A	4577	1/1	0.96	0.08	58,58,58,58	0
56	MG	2A	3074	1/1	0.96	0.15	138,138,138,138	0
56	MG	1A	4272	1/1	0.96	0.31	68,68,68,68	0
56	MG	2A	3370	1/1	0.96	0.20	99,99,99,99	0
56	MG	1a	1806	1/1	0.96	0.19	135,135,135,135	0
56	MG	2A	3209	1/1	0.96	0.24	93,93,93,93	0
56	MG	1a	1695	1/1	0.96	0.07	159,159,159,159	0
56	MG	1a	1808	1/1	0.96	0.40	122,122,122,122	0
56	MG	2A	3079	1/1	0.96	0.15	125,125,125,125	0
56	MG	2a	1601	1/1	0.96	0.18	122,122,122,122	0
56	MG	2A	3748	1/1	0.96	0.33	104,104,104,104	0
56	MG	2A	3749	1/1	0.96	0.24	93,93,93,93	0
56	MG	1a	1696	1/1	0.96	0.13	159,159,159,159	0
56	MG	1A	4029	1/1	0.96	0.27	51,51,51,51	0
56	MG	2a	1802	1/1	0.96	0.27	166,166,166,166	0
56	MG	1A	5063	1/1	0.96	0.16	58,58,58,58	0
56	MG	1A	4128	1/1	0.96	0.20	60,60,60,60	0
56	MG	1A	4145	1/1	0.96	0.47	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3219	1/1	0.96	0.28	110,110,110,110	0
56	MG	1a	1815	1/1	0.96	0.24	171,171,171,171	0
56	MG	2A	3352	1/1	0.97	0.18	89,89,89,89	0
56	MG	1A	4496	1/1	0.97	0.76	60,60,60,60	0
56	MG	2A	3656	1/1	0.97	0.51	109,109,109,109	0
56	MG	1A	5057	1/1	0.97	0.21	170,170,170,170	0
56	MG	2A	3827	1/1	0.97	0.10	105,105,105,105	0
56	MG	2a	1655	1/1	0.97	0.06	142,142,142,142	0
56	MG	1A	4111	1/1	0.97	0.30	49,49,49,49	0
56	MG	1A	4041	1/1	0.97	0.64	74,74,74,74	0
56	MG	1A	4556	1/1	0.97	0.17	58,58,58,58	0
56	MG	2A	3507	1/1	0.97	0.22	128,128,128,128	0
56	MG	1A	4557	1/1	0.97	0.38	58,58,58,58	0
56	MG	2A	3665	1/1	0.97	0.22	129,129,129,129	0
56	MG	1A	4558	1/1	0.97	0.25	66,66,66,66	0
56	MG	1A	4407	1/1	0.97	0.25	52,52,52,52	0
56	MG	1A	4127	1/1	0.97	0.45	63,63,63,63	0
56	MG	1a	1716	1/1	0.97	0.22	120,120,120,120	0
56	MG	1a	1717	1/1	0.97	0.43	110,110,110,110	0
56	MG	1A	4167	1/1	0.97	0.37	58,58,58,58	0
56	MG	2A	3840	1/1	0.97	0.26	117,117,117,117	0
56	MG	1a	1610	1/1	0.97	0.34	90,90,90,90	0
56	MG	2A	3368	1/1	0.97	0.25	100,100,100,100	0
56	MG	2A	3518	1/1	0.97	0.10	96,96,96,96	0
56	MG	1a	1720	1/1	0.97	0.40	124,124,124,124	0
56	MG	2A	3679	1/1	0.97	0.49	106,106,106,106	0
56	MG	1A	4088	1/1	0.97	0.24	66,66,66,66	0
56	MG	1A	4302	1/1	0.97	0.42	80,80,80,80	0
56	MG	1A	4564	1/1	0.97	0.34	56,56,56,56	0
56	MG	1A	4413	1/1	0.97	0.20	63,63,63,63	0
56	MG	1a	1726	1/1	0.97	0.09	127,127,127,127	0
56	MG	1A	4782	1/1	0.97	0.23	81,81,81,81	0
56	MG	1A	4877	1/1	0.97	0.15	81,81,81,81	0
56	MG	2A	3378	1/1	0.97	0.15	106,106,106,106	0
56	MG	1B	210	1/1	0.97	0.54	89,89,89,89	0
56	MG	1A	4878	1/1	0.97	0.34	77,77,77,77	0
56	MG	1A	4332	1/1	0.97	0.34	75,75,75,75	0
56	MG	1A	4103	1/1	0.97	0.26	50,50,50,50	0
56	MG	1A	4569	1/1	0.97	0.32	60,60,60,60	0
56	MG	1A	4974	1/1	0.97	0.11	74,74,74,74	0
56	MG	2A	3386	1/1	0.97	0.21	125,125,125,125	0
56	MG	1a	1847	1/1	0.97	0.12	184,184,184,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3696	1/1	0.97	0.27	105,105,105,105	0
56	MG	1A	4570	1/1	0.97	0.30	60,60,60,60	0
56	MG	1A	4508	1/1	0.97	0.25	70,70,70,70	0
56	MG	1A	4641	1/1	0.97	0.16	79,79,79,79	0
56	MG	2A	3124	1/1	0.97	0.20	125,125,125,125	0
56	MG	1a	1851	1/1	0.97	0.16	175,175,175,175	0
56	MG	1A	4109	1/1	0.97	0.21	54,54,54,54	0
56	MG	2A	3703	1/1	0.97	0.43	94,94,94,94	0
56	MG	1A	4574	1/1	0.97	0.25	57,57,57,57	0
56	MG	2A	3705	1/1	0.97	0.26	98,98,98,98	0
56	MG	1A	4793	1/1	0.97	0.17	108,108,108,108	0
56	MG	1A	4335	1/1	0.97	0.19	76,76,76,76	0
56	MG	1A	4983	1/1	0.97	0.21	56,56,56,56	0
56	MG	1a	1633	1/1	0.97	0.18	109,109,109,109	0
56	MG	2A	3011	1/1	0.97	0.29	104,104,104,104	0
56	MG	2a	1891	1/1	0.97	0.11	157,157,157,157	0
56	MG	2A	3711	1/1	0.97	0.17	95,95,95,95	0
56	MG	1A	4713	1/1	0.97	0.26	55,55,55,55	0
56	MG	2A	3013	1/1	0.97	0.38	118,118,118,118	0
56	MG	1a	1635	1/1	0.97	0.16	121,121,121,121	0
56	MG	1A	4458	1/1	0.97	0.34	60,60,60,60	0
56	MG	1A	4418	1/1	0.97	0.20	52,52,52,52	0
56	MG	2A	3406	1/1	0.97	0.14	140,140,140,140	0
56	MG	1a	1750	1/1	0.97	0.17	134,134,134,134	0
56	MG	2D	304	1/1	0.97	0.13	107,107,107,107	0
56	MG	2D	305	1/1	0.97	0.12	96,96,96,96	0
56	MG	1A	4717	1/1	0.97	0.64	81,81,81,81	0
56	MG	1A	4513	1/1	0.97	0.28	78,78,78,78	0
56	MG	2a	1720	1/1	0.97	0.10	153,153,153,153	0
56	MG	1A	4159	1/1	0.97	0.18	50,50,50,50	0
56	MG	1A	4205	1/1	0.97	0.20	56,56,56,56	0
56	MG	2A	3723	1/1	0.97	0.20	96,96,96,96	0
56	MG	1A	4206	1/1	0.97	0.36	55,55,55,55	0
56	MG	1A	4808	1/1	0.97	0.23	53,53,53,53	0
56	MG	1A	4517	1/1	0.97	0.78	81,81,81,81	0
56	MG	1A	4810	1/1	0.97	0.12	63,63,63,63	0
56	MG	1a	1759	1/1	0.97	0.19	104,104,104,104	0
56	MG	2A	3274	1/1	0.97	0.21	83,83,83,83	0
56	MG	2N	202	1/1	0.97	0.40	84,84,84,84	0
56	MG	1A	4276	1/1	0.97	0.30	67,67,67,67	0
56	MG	2A	3731	1/1	0.97	0.24	86,86,86,86	0
56	MG	2A	3276	1/1	0.97	0.29	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3568	1/1	0.97	0.22	92,92,92,92	0
56	MG	1A	4423	1/1	0.97	0.21	53,53,53,53	0
56	MG	2A	3422	1/1	0.97	0.10	130,130,130,130	0
56	MG	1A	4813	1/1	0.97	0.14	70,70,70,70	0
56	MG	1A	4814	1/1	0.97	0.69	59,59,59,59	0
56	MG	1A	4907	1/1	0.97	0.20	52,52,52,52	0
56	MG	1A	4465	1/1	0.97	0.19	60,60,60,60	0
56	MG	1A	5008	1/1	0.97	0.21	76,76,76,76	0
56	MG	1A	4277	1/1	0.97	0.58	53,53,53,53	0
56	MG	1A	5010	1/1	0.97	0.28	75,75,75,75	0
56	MG	1A	4342	1/1	0.97	0.17	65,65,65,65	0
56	MG	1A	4658	1/1	0.97	0.33	96,96,96,96	0
56	MG	1A	4468	1/1	0.97	0.21	58,58,58,58	0
56	MG	2A	3433	1/1	0.97	0.48	92,92,92,92	0
56	MG	1A	4914	1/1	0.97	0.18	74,74,74,74	0
56	MG	2a	1750	1/1	0.97	0.91	120,120,120,120	0
56	MG	2a	1751	1/1	0.97	0.26	116,116,116,116	0
56	MG	2A	3290	1/1	0.97	0.30	112,112,112,112	0
56	MG	1a	1886	1/1	0.97	0.22	125,125,125,125	0
56	MG	1a	1887	1/1	0.97	0.17	130,130,130,130	0
56	MG	2A	3293	1/1	0.97	0.52	94,94,94,94	0
56	MG	1a	1888	1/1	0.97	0.16	119,119,119,119	0
56	MG	2A	3165	1/1	0.97	0.21	98,98,98,98	0
56	MG	2A	3296	1/1	0.97	0.37	94,94,94,94	0
56	MG	1A	4469	1/1	0.97	0.19	56,56,56,56	0
56	MG	2A	3445	1/1	0.97	0.47	86,86,86,86	0
56	MG	1A	4470	1/1	0.97	0.18	54,54,54,54	0
56	MG	1P	204	1/1	0.97	0.10	88,88,88,88	0
56	MG	1A	4426	1/1	0.97	0.18	77,77,77,77	0
56	MG	1A	4919	1/1	0.97	0.29	62,62,62,62	0
56	MG	2A	3600	1/1	0.97	0.07	118,118,118,118	0
56	MG	2A	3764	1/1	0.97	0.10	151,151,151,151	0
56	MG	2A	3049	1/1	0.97	0.34	94,94,94,94	0
56	MG	2A	3602	1/1	0.97	0.18	97,97,97,97	0
56	MG	2A	3304	1/1	0.97	0.50	127,127,127,127	0
56	MG	27	102	1/1	0.97	0.56	89,89,89,89	0
56	MG	27	103	1/1	0.97	0.12	97,97,97,97	0
56	MG	1A	4122	1/1	0.97	0.40	66,66,66,66	0
56	MG	1A	4251	1/1	0.97	0.23	60,60,60,60	0
56	MG	1A	4826	1/1	0.97	0.39	91,91,91,91	0
56	MG	1a	1668	1/1	0.97	0.07	139,139,139,139	0
56	MG	1A	4476	1/1	0.97	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3177	1/1	0.97	0.47	113,113,113,113	0
56	MG	1A	4666	1/1	0.97	0.49	78,78,78,78	0
56	MG	2A	3313	1/1	0.97	0.22	95,95,95,95	0
56	MG	1A	4741	1/1	0.97	0.28	75,75,75,75	0
56	MG	1A	4252	1/1	0.97	0.40	54,54,54,54	0
56	MG	1A	4281	1/1	0.97	0.30	70,70,70,70	0
56	MG	1A	4096	1/1	0.97	0.36	55,55,55,55	0
56	MG	2q	203	1/1	0.97	0.28	151,151,151,151	0
56	MG	2a	1605	1/1	0.97	0.27	127,127,127,127	0
56	MG	1A	4534	1/1	0.97	0.20	78,78,78,78	0
56	MG	1A	5032	1/1	0.97	0.20	83,83,83,83	0
56	MG	1A	4351	1/1	0.97	0.09	67,67,67,67	0
56	MG	2A	3620	1/1	0.97	0.43	122,122,122,122	0
56	MG	1A	4254	1/1	0.97	0.30	66,66,66,66	0
56	MG	1A	4255	1/1	0.97	0.29	65,65,65,65	0
56	MG	2A	3623	1/1	0.97	0.31	147,147,147,147	0
56	MG	2A	3326	1/1	0.97	0.40	85,85,85,85	0
56	MG	1A	4256	1/1	0.97	0.34	65,65,65,65	0
56	MG	1A	4539	1/1	0.97	0.19	69,69,69,69	0
56	MG	2A	3790	1/1	0.97	0.33	96,96,96,96	0
56	MG	2A	3068	1/1	0.97	0.23	148,148,148,148	0
56	MG	1A	4176	1/1	0.97	0.22	59,59,59,59	0
56	MG	1A	5039	1/1	0.97	0.11	68,68,68,68	0
56	MG	1A	4213	1/1	0.97	0.40	57,57,57,57	0
56	MG	1A	4177	1/1	0.97	0.20	58,58,58,58	0
56	MG	2A	3796	1/1	0.97	0.18	96,96,96,96	0
56	MG	1A	4440	1/1	0.97	0.22	73,73,73,73	0
56	MG	1A	5043	1/1	0.97	0.62	71,71,71,71	0
56	MG	1A	4400	1/1	0.97	0.17	75,75,75,75	0
56	MG	1A	5046	1/1	0.97	0.10	78,78,78,78	0
56	MG	1A	4260	1/1	0.97	0.37	58,58,58,58	0
56	MG	1A	5048	1/1	0.97	0.09	65,65,65,65	0
56	MG	2A	3804	1/1	0.97	0.29	114,114,114,114	0
56	MG	1A	4760	1/1	0.97	0.25	67,67,67,67	0
56	MG	2a	1631	1/1	0.97	0.09	151,151,151,151	0
56	MG	1A	4152	1/1	0.97	0.31	56,56,56,56	0
56	MG	2A	3081	1/1	0.97	0.18	125,125,125,125	0
56	MG	2a	1813	1/1	0.97	0.10	143,143,143,143	0
56	MG	1A	4852	1/1	0.97	0.44	71,71,71,71	0
56	MG	1a	1811	1/1	0.97	0.17	99,99,99,99	0
56	MG	15	102	1/1	0.97	0.21	60,60,60,60	0
56	MG	2A	3812	1/1	0.97	0.45	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1818	1/1	0.97	0.16	156,156,156,156	0
56	MG	1A	4237	1/1	0.97	0.37	73,73,73,73	0
57	ZN	1Y	302	1/1	0.97	0.12	96,96,96,96	0
56	MG	2a	1820	1/1	0.97	0.22	155,155,155,155	0
57	ZN	15	103	1/1	0.97	0.16	74,74,74,74	0
56	MG	1A	4493	1/1	0.97	0.34	68,68,68,68	0
56	MG	2A	3494	1/1	0.97	0.33	134,134,134,134	0
56	MG	17	102	1/1	0.97	0.80	61,61,61,61	0
57	ZN	25	102	1/1	0.97	0.20	119,119,119,119	0
56	MG	1A	4494	1/1	0.97	0.18	78,78,78,78	0
56	MG	2A	3498	1/1	0.97	0.12	102,102,102,102	0
56	MG	2A	3819	1/1	0.97	0.12	42,42,42,42	0
58	SF4	1d	304	8/8	0.97	0.20	150,150,150,150	0
56	MG	18	101	1/1	0.97	0.30	56,56,56,56	0
56	MG	1A	4194	1/1	0.97	0.22	68,68,68,68	0
56	MG	2a	1833	1/1	0.97	0.26	161,161,161,161	0
56	MG	1A	4271	1/1	0.98	0.58	62,62,62,62	0
56	MG	1A	5045	1/1	0.98	0.61	67,67,67,67	0
56	MG	1A	4225	1/1	0.98	0.25	73,73,73,73	0
56	MG	1a	1741	1/1	0.98	0.08	139,139,139,139	0
56	MG	1T	202	1/1	0.98	0.21	83,83,83,83	0
56	MG	1A	4201	1/1	0.98	0.53	70,70,70,70	0
56	MG	1A	4362	1/1	0.98	0.19	67,67,67,67	0
56	MG	2A	3261	1/1	0.98	0.39	80,80,80,80	0
56	MG	2A	3596	1/1	0.98	0.10	100,100,100,100	0
56	MG	1A	4607	1/1	0.98	0.24	67,67,67,67	0
56	MG	1A	4967	1/1	0.98	0.10	83,83,83,83	0
56	MG	1A	4002	1/1	0.98	0.13	65,65,65,65	0
56	MG	2A	3265	1/1	0.98	0.13	90,90,90,90	0
56	MG	1A	4827	1/1	0.98	0.23	69,69,69,69	0
56	MG	2A	3846	1/1	0.98	0.25	108,108,108,108	0
56	MG	1A	4171	1/1	0.98	0.47	49,49,49,49	0
56	MG	2A	3848	1/1	0.98	0.12	61,61,61,61	0
56	MG	2A	3375	1/1	0.98	0.25	103,103,103,103	0
56	MG	1A	4147	1/1	0.98	0.28	57,57,57,57	0
56	MG	2A	3851	1/1	0.98	0.20	110,110,110,110	0
56	MG	2A	3852	1/1	0.98	0.14	96,96,96,96	0
56	MG	1A	4709	1/1	0.98	0.14	68,68,68,68	0
56	MG	1A	4366	1/1	0.98	0.30	60,60,60,60	0
56	MG	1A	4187	1/1	0.98	0.31	67,67,67,67	0
56	MG	1A	4769	1/1	0.98	0.13	72,72,72,72	0
56	MG	1A	4904	1/1	0.98	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4770	1/1	0.98	0.30	65,65,65,65	0
56	MG	1A	4771	1/1	0.98	0.25	70,70,70,70	0
56	MG	2a	1638	1/1	0.98	0.25	148,148,148,148	0
56	MG	2A	3496	1/1	0.98	0.17	99,99,99,99	0
56	MG	1A	4614	1/1	0.98	0.18	71,71,71,71	0
56	MG	1A	4188	1/1	0.98	0.30	68,68,68,68	0
56	MG	2a	1642	1/1	0.98	0.08	143,143,143,143	0
56	MG	1A	4617	1/1	0.98	0.21	98,98,98,98	0
56	MG	2a	1644	1/1	0.98	0.41	125,125,125,125	0
56	MG	2A	3616	1/1	0.98	0.16	93,93,93,93	0
56	MG	1A	4102	1/1	0.98	0.14	53,53,53,53	0
56	MG	1A	4174	1/1	0.98	0.19	59,59,59,59	0
56	MG	1A	4913	1/1	0.98	0.14	72,72,72,72	0
56	MG	1A	4718	1/1	0.98	0.11	99,99,99,99	0
56	MG	2A	3741	1/1	0.98	0.20	85,85,85,85	0
56	MG	1a	1675	1/1	0.98	0.29	124,124,124,124	0
56	MG	1a	1676	1/1	0.98	0.08	151,151,151,151	0
56	MG	15	101	1/1	0.98	0.23	61,61,61,61	0
56	MG	1A	4161	1/1	0.98	0.21	58,58,58,58	0
56	MG	2A	3396	1/1	0.98	0.16	126,126,126,126	0
56	MG	1A	4668	1/1	0.98	0.28	93,93,93,93	0
56	MG	1A	4044	1/1	0.98	0.15	62,62,62,62	0
56	MG	1A	4991	1/1	0.98	0.15	66,66,66,66	0
56	MG	1A	4338	1/1	0.98	0.14	67,67,67,67	0
56	MG	2a	1660	1/1	0.98	0.44	142,142,142,142	0
56	MG	1A	4283	1/1	0.98	0.35	65,65,65,65	0
56	MG	1A	4995	1/1	0.98	0.18	77,77,77,77	0
56	MG	18	103	1/1	0.98	0.19	75,75,75,75	0
56	MG	1A	4139	1/1	0.98	0.27	68,68,68,68	0
56	MG	1A	4998	1/1	0.98	0.16	80,80,80,80	0
56	MG	1A	4851	1/1	0.98	0.24	72,72,72,72	0
56	MG	1A	4533	1/1	0.98	0.32	68,68,68,68	0
56	MG	1A	4674	1/1	0.98	0.24	91,91,91,91	0
56	MG	2A	3638	1/1	0.98	0.10	114,114,114,114	0
56	MG	2A	3409	1/1	0.98	0.09	116,116,116,116	0
56	MG	1A	4215	1/1	0.98	0.42	54,54,54,54	0
56	MG	1A	4216	1/1	0.98	0.21	62,62,62,62	0
56	MG	1a	1693	1/1	0.98	0.14	136,136,136,136	0
56	MG	2A	3303	1/1	0.98	0.19	113,113,113,113	0
56	MG	1a	1785	1/1	0.98	0.33	136,136,136,136	0
56	MG	1A	4729	1/1	0.98	0.36	64,64,64,64	0
56	MG	1A	4928	1/1	0.98	0.15	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4262	1/1	0.98	0.22	66,66,66,66	0
56	MG	1A	4731	1/1	0.98	0.15	54,54,54,54	0
56	MG	1A	4073	1/1	0.98	0.20	71,71,71,71	0
56	MG	1A	4345	1/1	0.98	0.25	65,65,65,65	0
56	MG	2A	3311	1/1	0.98	0.36	102,102,102,102	0
56	MG	1A	4796	1/1	0.98	0.15	100,100,100,100	0
56	MG	2a	1685	1/1	0.98	0.37	167,167,167,167	0
56	MG	2A	3653	1/1	0.98	0.13	117,117,117,117	0
56	MG	2A	3114	1/1	0.98	0.17	153,153,153,153	0
56	MG	1A	4346	1/1	0.98	0.14	72,72,72,72	0
56	MG	1A	4347	1/1	0.98	0.18	66,66,66,66	0
56	MG	1A	4384	1/1	0.98	0.21	66,66,66,66	0
56	MG	2a	1823	1/1	0.98	0.10	153,153,153,153	0
56	MG	2A	3118	1/1	0.98	0.17	135,135,135,135	0
56	MG	2a	1825	1/1	0.98	0.19	169,169,169,169	0
56	MG	2A	3659	1/1	0.98	0.53	149,149,149,149	0
56	MG	1A	4801	1/1	0.98	0.19	76,76,76,76	0
56	MG	1A	5017	1/1	0.98	0.29	68,68,68,68	0
56	MG	1A	4289	1/1	0.98	0.27	68,68,68,68	0
56	MG	2a	1830	1/1	0.98	0.06	147,147,147,147	0
56	MG	2A	3322	1/1	0.98	0.27	88,88,88,88	0
56	MG	1A	4939	1/1	0.98	0.17	71,71,71,71	0
56	MG	1A	4870	1/1	0.98	0.16	54,54,54,54	0
56	MG	2A	3325	1/1	0.98	0.36	88,88,88,88	0
56	MG	2a	1836	1/1	0.98	0.39	124,124,124,124	0
56	MG	1A	4803	1/1	0.98	0.11	101,101,101,101	0
56	MG	2A	3669	1/1	0.98	0.20	92,92,92,92	0
56	MG	2A	3670	1/1	0.98	0.10	92,92,92,92	0
56	MG	2A	3436	1/1	0.98	0.24	104,104,104,104	0
56	MG	1A	4195	1/1	0.98	0.23	68,68,68,68	0
56	MG	2A	3438	1/1	0.98	0.54	79,79,79,79	0
56	MG	2A	3674	1/1	0.98	0.52	145,145,145,145	0
56	MG	1a	1711	1/1	0.98	0.11	125,125,125,125	0
56	MG	1A	4001	1/1	0.98	0.31	65,65,65,65	0
56	MG	1a	1713	1/1	0.98	0.26	109,109,109,109	0
56	MG	2A	3799	1/1	0.98	0.13	116,116,116,116	0
56	MG	2a	1848	1/1	0.98	0.13	157,157,157,157	0
56	MG	1E	307	1/1	0.98	0.38	62,62,62,62	0
56	MG	1A	4944	1/1	0.98	0.17	88,88,88,88	0
56	MG	2A	3557	1/1	0.98	0.22	90,90,90,90	0
56	MG	2A	3228	1/1	0.98	0.14	98,98,98,98	0
56	MG	1A	4220	1/1	0.98	0.29	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4352	1/1	0.98	0.24	61,61,61,61	0
56	MG	1A	4056	1/1	0.98	0.49	66,66,66,66	0
56	MG	2A	3807	1/1	0.98	0.23	132,132,132,132	0
56	MG	1N	201	1/1	0.98	0.35	72,72,72,72	0
56	MG	1A	4591	1/1	0.98	0.13	85,85,85,85	0
56	MG	1A	4880	1/1	0.98	0.20	83,83,83,83	0
56	MG	1a	1722	1/1	0.98	0.53	113,113,113,113	0
56	MG	2A	3452	1/1	0.98	0.53	90,90,90,90	0
56	MG	1a	1816	1/1	0.98	0.33	183,183,183,183	0
56	MG	2a	1725	1/1	0.98	0.12	142,142,142,142	0
56	MG	2A	3237	1/1	0.98	0.15	112,112,112,112	0
56	MG	1A	4392	1/1	0.98	0.08	103,103,103,103	0
56	MG	1A	4951	1/1	0.98	0.20	68,68,68,68	0
56	MG	1A	4952	1/1	0.98	0.16	65,65,65,65	0
56	MG	1A	4004	1/1	0.98	0.52	45,45,45,45	0
56	MG	1A	4125	1/1	0.98	0.35	79,79,79,79	0
57	ZN	16	102	1/1	0.98	0.16	82,82,82,82	0
56	MG	1A	4471	1/1	0.98	0.38	60,60,60,60	0
56	MG	1P	205	1/1	0.98	0.10	95,95,95,95	0
56	MG	1A	4017	1/1	0.98	0.26	69,69,69,69	0
56	MG	1a	1643	1/1	0.98	0.23	130,130,130,130	0
56	MG	1A	4553	1/1	0.98	0.22	91,91,91,91	0
56	MG	2A	3149	1/1	0.98	0.48	110,110,110,110	0
56	MG	1A	4599	1/1	0.98	0.13	60,60,60,60	0
56	MG	1A	4358	1/1	0.98	0.14	72,72,72,72	0
58	SF4	2d	303	8/8	0.98	0.13	166,166,166,166	0
56	MG	1A	4555	1/1	0.98	0.35	57,57,57,57	0
56	MG	1a	1736	1/1	0.98	0.63	145,145,145,145	0
56	MG	1A	4397	1/1	0.98	0.12	72,72,72,72	0
56	MG	1A	4043	1/1	0.99	0.23	56,56,56,56	0
56	MG	2A	3471	1/1	0.99	0.17	113,113,113,113	0
56	MG	2A	3053	1/1	0.99	0.16	96,96,96,96	0
56	MG	1A	4744	1/1	0.99	0.20	69,69,69,69	0
56	MG	1A	4210	1/1	0.99	0.29	58,58,58,58	0
56	MG	1D	304	1/1	0.99	0.44	75,75,75,75	0
56	MG	1A	4716	1/1	0.99	0.20	72,72,72,72	0
56	MG	1v	703	1/1	0.99	0.18	116,116,116,116	0
56	MG	1A	4611	1/1	0.99	0.16	54,54,54,54	0
56	MG	1A	4853	1/1	0.99	0.18	78,78,78,78	0
56	MG	1A	4104	1/1	0.99	0.18	56,56,56,56	0
56	MG	1A	4567	1/1	0.99	0.24	56,56,56,56	0
56	MG	1y	103	1/1	0.99	0.72	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4856	1/1	0.99	0.14	60,60,60,60	0
56	MG	1A	4817	1/1	0.99	0.17	65,65,65,65	0
56	MG	1A	4092	1/1	0.99	0.11	60,60,60,60	0
56	MG	1A	4994	1/1	0.99	0.16	79,79,79,79	0
56	MG	1E	306	1/1	0.99	0.11	83,83,83,83	0
56	MG	1A	4615	1/1	0.99	0.14	67,67,67,67	0
56	MG	1a	1778	1/1	0.99	0.53	126,126,126,126	0
56	MG	1A	4996	1/1	0.99	0.19	71,71,71,71	0
56	MG	1A	4150	1/1	0.99	0.16	59,59,59,59	0
56	MG	1A	4388	1/1	0.99	0.21	79,79,79,79	0
56	MG	1A	4571	1/1	0.99	0.15	79,79,79,79	0
56	MG	1A	5000	1/1	0.99	0.12	63,63,63,63	0
56	MG	1A	5001	1/1	0.99	0.09	65,65,65,65	0
56	MG	2A	3210	1/1	0.99	0.26	93,93,93,93	0
56	MG	1O	202	1/1	0.99	0.47	82,82,82,82	0
56	MG	1A	4906	1/1	0.99	0.15	57,57,57,57	0
56	MG	1A	4076	1/1	0.99	0.18	77,77,77,77	0
56	MG	1A	4325	1/1	0.99	0.22	63,63,63,63	0
56	MG	2A	3353	1/1	0.99	0.20	83,83,83,83	0
56	MG	1A	4789	1/1	0.99	0.26	96,96,96,96	0
56	MG	1A	4758	1/1	0.99	0.23	75,75,75,75	0
56	MG	2A	3820	1/1	0.99	0.15	106,106,106,106	0
56	MG	2A	3580	1/1	0.99	0.27	118,118,118,118	0
56	MG	1A	4207	1/1	0.99	0.32	52,52,52,52	0
56	MG	2A	3357	1/1	0.99	0.08	87,87,87,87	0
56	MG	2A	3662	1/1	0.99	0.15	96,96,96,96	0
56	MG	2A	3286	1/1	0.99	0.20	101,101,101,101	0
56	MG	1a	1614	1/1	0.99	0.10	93,93,93,93	0
56	MG	1a	1793	1/1	0.99	0.12	128,128,128,128	0
56	MG	1A	5061	1/1	0.99	0.12	91,91,91,91	0
56	MG	2A	3510	1/1	0.99	0.07	94,94,94,94	0
56	MG	1a	1616	1/1	0.99	0.11	99,99,99,99	0
56	MG	2A	3589	1/1	0.99	0.13	127,127,127,127	0
56	MG	1A	4792	1/1	0.99	0.14	66,66,66,66	0
56	MG	1A	4869	1/1	0.99	0.23	54,54,54,54	0
56	MG	2A	3592	1/1	0.99	0.23	129,129,129,129	0
56	MG	1A	4597	1/1	0.99	0.09	65,65,65,65	0
56	MG	1A	4474	1/1	0.99	0.26	56,56,56,56	0
56	MG	1A	4872	1/1	0.99	0.17	54,54,54,54	0
56	MG	1A	4873	1/1	0.99	0.16	55,55,55,55	0
56	MG	2A	3757	1/1	0.99	0.20	127,127,127,127	0
56	MG	1A	4918	1/1	0.99	0.19	61,61,61,61	0

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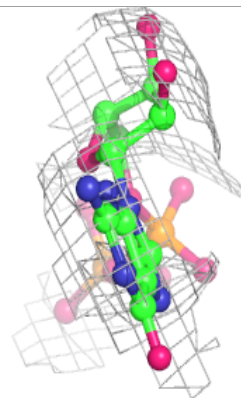
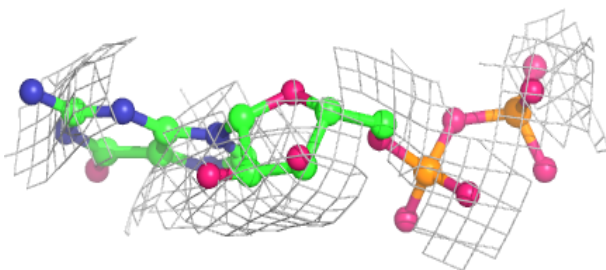
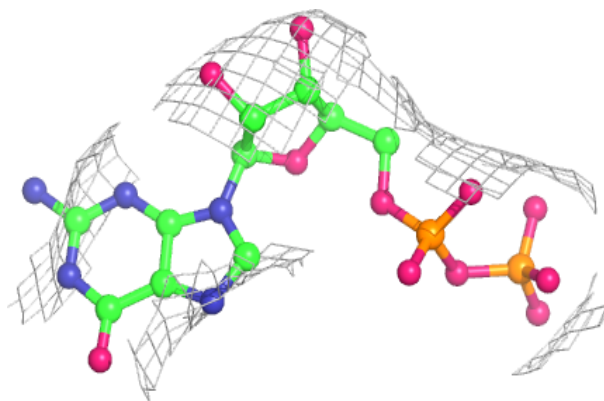
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4293	1/1	0.99	0.25	78,78,78,78	0
56	MG	1A	4248	1/1	0.99	0.20	56,56,56,56	0
56	MG	1A	4295	1/1	0.99	0.34	83,83,83,83	0
56	MG	1A	5018	1/1	0.99	0.21	71,71,71,71	0
56	MG	1A	4410	1/1	0.99	0.43	47,47,47,47	0
56	MG	1A	4800	1/1	0.99	0.22	69,69,69,69	0
56	MG	1A	4498	1/1	0.99	0.30	63,63,63,63	0
56	MG	1A	4735	1/1	0.99	0.13	65,65,65,65	0
56	MG	2a	1831	1/1	0.99	0.06	145,145,145,145	0
56	MG	1A	4971	1/1	0.99	0.14	63,63,63,63	0
56	MG	1A	4680	1/1	0.99	0.15	82,82,82,82	0
56	MG	1A	4839	1/1	0.99	0.19	63,63,63,63	0
56	MG	1A	4654	1/1	0.99	0.10	84,84,84,84	0
56	MG	2A	3455	1/1	0.99	0.15	90,90,90,90	0
56	MG	1a	1876	1/1	0.99	0.08	102,102,102,102	0
56	MG	1A	4427	1/1	0.99	0.25	53,53,53,53	0
56	MG	2A	3384	1/1	0.99	0.34	105,105,105,105	0
57	ZN	19	102	1/1	0.99	0.20	80,80,80,80	0
56	MG	1A	4842	1/1	0.99	0.34	78,78,78,78	0
56	MG	1A	5029	1/1	0.99	0.10	69,69,69,69	0
56	MG	2A	3314	1/1	0.99	0.21	93,93,93,93	0
56	MG	2A	3045	1/1	0.99	0.33	93,93,93,93	0
56	MG	1A	4843	1/1	0.99	0.26	76,76,76,76	0
56	MG	1A	4480	1/1	0.99	0.19	80,80,80,80	0
56	MG	2a	1679	1/1	0.99	0.12	166,166,166,166	0
56	MG	2A	3180	1/1	0.99	0.16	116,116,116,116	0
56	MG	1A	4979	1/1	0.99	0.13	58,58,58,58	0
56	MG	1A	4208	1/1	0.99	0.17	56,56,56,56	0
56	MG	1A	4355	1/1	0.99	0.16	67,67,67,67	0
56	MG	1A	4382	1/1	0.99	0.27	68,68,68,68	0
56	MG	1A	4755	1/1	1.00	0.36	60,60,60,60	0
56	MG	1A	4794	1/1	1.00	0.07	67,67,67,67	0

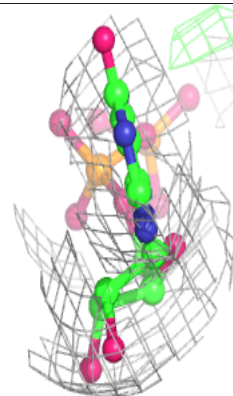
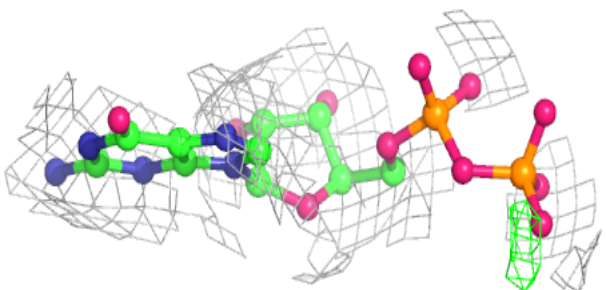
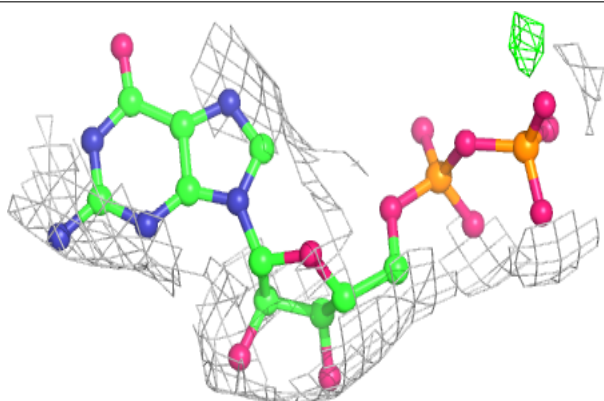
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around GDP 2v 704:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around GDP 1v 704:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.