



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2018 – 09:10 PM EST

PDB ID : 6CFJ
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with histidyl-CAM and bound to mRNA and A-, P-, and E-site tRNAs at 2.8Å resolution
Authors : Tereshchenkov, A.G.; Dobosz-Bartoszek, M.; Osterman, I.A.; Marks, J.; Sergeeva, V.A.; Kasatsky, P.; Komarova, E.S.; Stavrianidi, A.N.; Rodin, I.A.; Konevega, A.L.; Sergiev, P.V.; Sumbatyan, N.V.; Mankin, A.S.; Bogdanov, A.A.; Polikanov, Y.S.
Deposited on : 2018-02-15
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

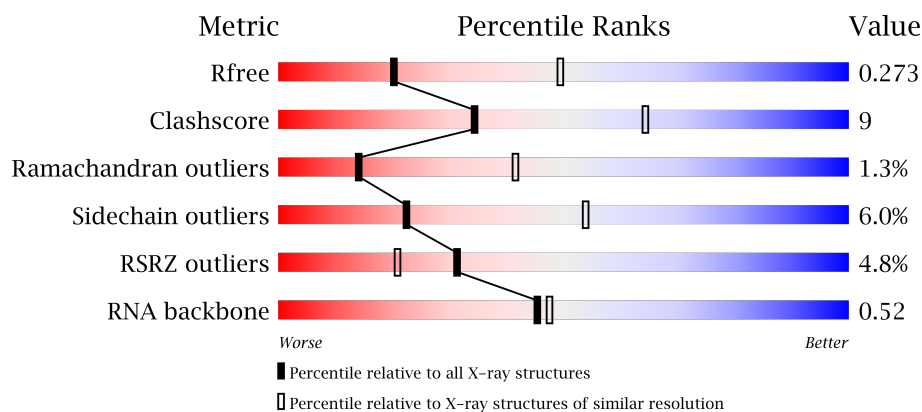
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


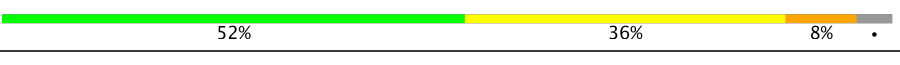


The reported resolution of this entry is 2.80 Å.

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



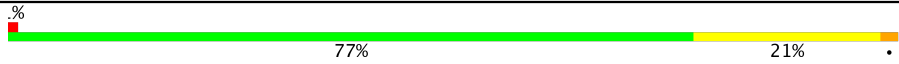


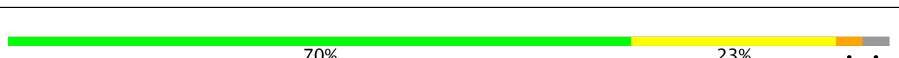
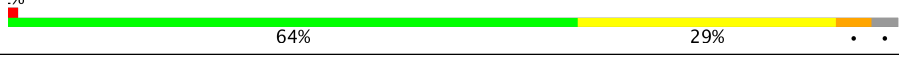

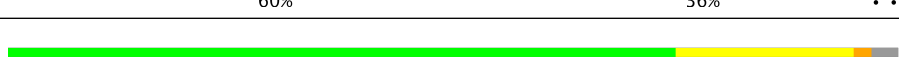


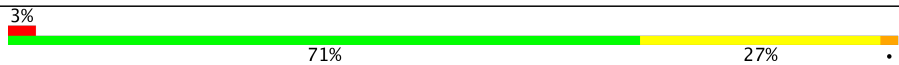
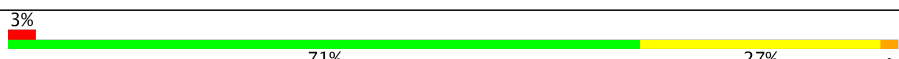



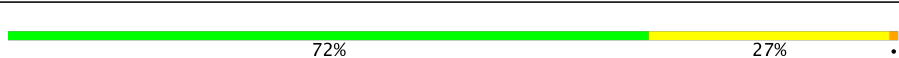

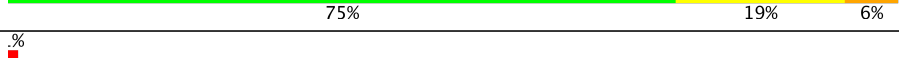






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)
RNA backbone	2435	1007 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	
1	2A	2915	
2	1B	121	
2	2B	121	

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

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

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

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Mol	Chain	Length	Quality of chain
40	2i	128	<div> <div>54%</div> <div>96%</div> <div>..</div> </div>
41	1j	105	<div> <div>25%</div> <div>87%</div> <div>6% 8%</div> </div>
41	2j	105	<div> <div>35%</div> <div>83%</div> <div>9% 9%</div> </div>
42	1k	129	<div> <div>%</div> <div>84%</div> <div>12%</div> </div>
42	2k	129	<div> <div>5%</div> <div>82%</div> <div>6% 12%</div> </div>
43	1l	132	<div> <div></div> <div>84%</div> <div>8% 8%</div> </div>
43	2l	132	<div> <div>6%</div> <div>89%</div> <div>8%</div> </div>
44	1m	126	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
44	2m	126	<div> <div>13%</div> <div>93%</div> <div>..</div> </div>
45	1n	61	<div> <div>16%</div> <div>89%</div> <div>10%</div> </div>
45	2n	61	<div> <div>67%</div> <div>90%</div> <div>8%</div> </div>
46	1o	89	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
46	2o	89	<div> <div>%</div> <div>96%</div> <div>...</div> </div>
47	1p	88	<div> <div>6%</div> <div>89%</div> <div>5% 7%</div> </div>
47	2p	88	<div> <div>%</div> <div>90%</div> <div>7%</div> </div>
48	1q	105	<div> <div>3%</div> <div>90%</div> <div>6%</div> </div>
48	2q	105	<div> <div>19%</div> <div>90%</div> <div>5% 6%</div> </div>
49	1r	88	<div> <div>5%</div> <div>73%</div> <div>5% 23%</div> </div>
49	2r	88	<div> <div>2%</div> <div>75%</div> <div>23%</div> </div>
50	1s	93	<div> <div>%</div> <div>86%</div> <div>11%</div> </div>
50	2s	93	<div> <div>17%</div> <div>84%</div> <div>5% 11%</div> </div>
51	1t	106	<div> <div>13%</div> <div>83%</div> <div>8% 9%</div> </div>
51	2t	106	<div> <div>17%</div> <div>80%</div> <div>10% 9%</div> </div>
52	1u	27	<div> <div>15%</div> <div>81%</div> <div>15%</div> </div>
52	2u	27	<div> <div>44%</div> <div>81%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	101	-	-	-	X
56	MG	15	101	-	-	-	X
56	MG	16	103	-	-	-	X
56	MG	17	103	-	-	-	X
56	MG	18	101	-	-	-	X
56	MG	1A	3030	-	-	-	X
56	MG	1A	3031	-	-	-	X
56	MG	1A	3034	-	-	-	X
56	MG	1A	3037	-	-	-	X
56	MG	1A	3042	-	-	-	X
56	MG	1A	3068	-	-	-	X
56	MG	1A	3087	-	-	-	X
56	MG	1A	3095	-	-	-	X
56	MG	1A	3096	-	-	-	X
56	MG	1A	3102	-	-	-	X
56	MG	1A	3111	-	-	-	X
56	MG	1A	3113	-	-	-	X
56	MG	1A	3140	-	-	-	X
56	MG	1A	3141	-	-	-	X
56	MG	1A	3148	-	-	-	X
56	MG	1A	3154	-	-	-	X
56	MG	1A	3160	-	-	-	X
56	MG	1A	3171	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3173	-	-	-	X
56	MG	1A	3174	-	-	-	X
56	MG	1A	3175	-	-	-	X
56	MG	1A	3178	-	-	-	X
56	MG	1A	3179	-	-	-	X
56	MG	1A	3186	-	-	-	X
56	MG	1A	3199	-	-	-	X
56	MG	1A	3214	-	-	-	X
56	MG	1A	3217	-	-	-	X
56	MG	1A	3221	-	-	-	X
56	MG	1A	3222	-	-	-	X
56	MG	1A	3224	-	-	-	X
56	MG	1A	3252	-	-	-	X
56	MG	1A	3253	-	-	-	X
56	MG	1A	3269	-	-	-	X
56	MG	1A	3302	-	-	-	X
56	MG	1A	3304	-	-	-	X
56	MG	1A	3328	-	-	-	X
56	MG	1A	3337	-	-	-	X
56	MG	1A	3362	-	-	-	X
56	MG	1A	3375	-	-	-	X
56	MG	1A	3377	-	-	-	X
56	MG	1A	3393	-	-	-	X
56	MG	1A	3412	-	-	-	X
56	MG	1A	3422	-	-	-	X
56	MG	1A	3427	-	-	-	X
56	MG	1A	3430	-	-	-	X
56	MG	1A	3451	-	-	-	X
56	MG	1A	3454	-	-	-	X
56	MG	1A	3455	-	-	-	X
56	MG	1A	3456	-	-	-	X
56	MG	1A	3480	-	-	-	X
56	MG	1A	3483	-	-	-	X
56	MG	1A	3485	-	-	-	X
56	MG	1A	3492	-	-	-	X
56	MG	1A	3505	-	-	-	X
56	MG	1A	3526	-	-	-	X
56	MG	1A	3550	-	-	-	X
56	MG	1A	3560	-	-	-	X
56	MG	1A	3567	-	-	-	X
56	MG	1A	3625	-	-	-	X
56	MG	1A	3680	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3685	-	-	-	X
56	MG	1A	3689	-	-	-	X
56	MG	1A	3696	-	-	-	X
56	MG	1A	3704	-	-	-	X
56	MG	1A	3736	-	-	-	X
56	MG	1A	3739	-	-	-	X
56	MG	1A	3749	-	-	-	X
56	MG	1A	3751	-	-	-	X
56	MG	1A	3753	-	-	-	X
56	MG	1A	3756	-	-	-	X
56	MG	1A	3757	-	-	-	X
56	MG	1A	3772	-	-	-	X
56	MG	1A	3783	-	-	-	X
56	MG	1A	3799	-	-	-	X
56	MG	1A	3887	-	-	-	X
56	MG	1A	3932	-	-	-	X
56	MG	1A	3960	-	-	-	X
56	MG	1A	3994	-	-	-	X
56	MG	1A	4008	-	-	-	X
56	MG	1A	4014	-	-	-	X
56	MG	1A	4020	-	-	-	X
56	MG	1A	4023	-	-	-	X
56	MG	1A	4024	-	-	-	X
56	MG	1A	4026	-	-	-	X
56	MG	1A	4031	-	-	-	X
56	MG	1A	4032	-	-	-	X
56	MG	1A	4034	-	-	-	X
56	MG	1A	4036	-	-	-	X
56	MG	1A	4038	-	-	-	X
56	MG	1A	4039	-	-	-	X
56	MG	1A	4040	-	-	-	X
56	MG	1A	4041	-	-	-	X
56	MG	1A	4045	-	-	-	X
56	MG	1A	4046	-	-	-	X
56	MG	1A	4047	-	-	-	X
56	MG	1A	4049	-	-	-	X
56	MG	1A	4050	-	-	-	X
56	MG	1A	4055	-	-	-	X
56	MG	1A	4060	-	-	-	X
56	MG	1A	4061	-	-	-	X
56	MG	1A	4063	-	-	-	X
56	MG	1B	207	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1D	304	-	-	-	X
56	MG	1D	308	-	-	-	X
56	MG	1D	312	-	-	-	X
56	MG	1D	314	-	-	-	X
56	MG	1E	302	-	-	-	X
56	MG	1E	311	-	-	-	X
56	MG	1F	301	-	-	-	X
56	MG	1F	302	-	-	-	X
56	MG	1F	304	-	-	-	X
56	MG	1F	305	-	-	-	X
56	MG	1F	309	-	-	-	X
56	MG	1N	201	-	-	-	X
56	MG	1N	204	-	-	-	X
56	MG	1N	205	-	-	-	X
56	MG	1P	201	-	-	-	X
56	MG	1Q	201	-	-	-	X
56	MG	1R	203	-	-	-	X
56	MG	1R	204	-	-	-	X
56	MG	1Y	503	-	-	-	X
56	MG	1a	3014	-	-	-	X
56	MG	1a	3015	-	-	-	X
56	MG	1a	3038	-	-	-	X
56	MG	1a	3042	-	-	-	X
56	MG	1a	3108	-	-	-	X
56	MG	1a	3214	-	-	-	X
56	MG	1e	201	-	-	-	X
56	MG	1x	102	-	-	-	X
56	MG	25	502	-	-	-	X
56	MG	2A	3024	-	-	-	X
56	MG	2A	3054	-	-	-	X
56	MG	2A	3066	-	-	-	X
56	MG	2A	3072	-	-	-	X
56	MG	2A	3091	-	-	-	X
56	MG	2A	3109	-	-	-	X
56	MG	2A	3125	-	-	-	X
56	MG	2A	3127	-	-	-	X
56	MG	2A	3138	-	-	-	X
56	MG	2A	3180	-	-	-	X
56	MG	2A	3247	-	-	-	X
56	MG	2A	3267	-	-	-	X
56	MG	2A	3271	-	-	-	X
56	MG	2A	3299	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3317	-	-	-	X
56	MG	2A	3323	-	-	-	X
56	MG	2A	3325	-	-	-	X
56	MG	2A	3329	-	-	-	X
56	MG	2A	3343	-	-	-	X
56	MG	2A	3382	-	-	-	X
56	MG	2A	3395	-	-	-	X
56	MG	2A	3398	-	-	-	X
56	MG	2A	3447	-	-	-	X
56	MG	2A	3458	-	-	-	X
56	MG	2A	3464	-	-	-	X
56	MG	2A	3472	-	-	-	X
56	MG	2A	3478	-	-	-	X
56	MG	2A	3495	-	-	-	X
56	MG	2A	3552	-	-	-	X
56	MG	2A	3570	-	-	-	X
56	MG	2A	3583	-	-	-	X
56	MG	2A	3624	-	-	-	X
56	MG	2A	3654	-	-	-	X
56	MG	2A	3661	-	-	-	X
56	MG	2A	3662	-	-	-	X
56	MG	2A	3697	-	-	-	X
56	MG	2A	3732	-	-	-	X
56	MG	2A	3742	-	-	-	X
56	MG	2A	3749	-	-	-	X
56	MG	2A	3755	-	-	-	X
56	MG	2B	3008	-	-	-	X
56	MG	2D	303	-	-	-	X
56	MG	2D	306	-	-	-	X
56	MG	2D	307	-	-	-	X
56	MG	2F	303	-	-	-	X
56	MG	2U	202	-	-	-	X
56	MG	2U	203	-	-	-	X
56	MG	2U	204	-	-	-	X
56	MG	2a	1627	-	-	-	X
56	MG	2a	1655	-	-	-	X
56	MG	2a	1676	-	-	-	X
56	MG	2a	1693	-	-	-	X
56	MG	2a	1694	-	-	-	X
56	MG	2a	1714	-	-	-	X
56	MG	2a	1761	-	-	-	X
56	MG	2a	1822	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	EZG	1A	4030	-	-	-	X
58	EZG	2A	3746	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299109 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1273	G	UNK	conflict	GB 37223181
2A	1227	G	UNK	conflict	GB 37223181

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			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
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
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
49	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1x	8	4SU	G	conflict	GB 205271127
2x	8	4SU	G	conflict	GB 205271127

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	10	Total	Mg	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	17	5	Total 5	Mg 5	0	0
56	2d	2	Total 2	Mg 2	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1N	5	Total 5	Mg 5	0	0
56	20	3	Total 3	Mg 3	0	0
56	18	3	Total 3	Mg 3	0	0
56	2W	3	Total 3	Mg 3	0	0
56	1Y	2	Total 2	Mg 2	0	0
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1P	3	Total 3	Mg 3	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2l	4	Total 4	Mg 4	0	0
56	1q	1	Total 1	Mg 1	0	0
56	2a	233	Total 233	Mg 233	0	0
56	1E	13	Total 13	Mg 13	0	0
56	1b	2	Total 2	Mg 2	0	0
56	25	3	Total 3	Mg 3	0	0
56	2F	4	Total 4	Mg 4	0	0
56	16	3	Total 3	Mg 3	0	0
56	28	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2e	1	Total Mg 1 1	0	0
56	1W	5	Total Mg 5 5	0	0
56	1A	1063	Total Mg 1063 1063	0	0
56	1t	1	Total Mg 1 1	0	0
56	1n	2	Total Mg 2 2	0	0
56	2P	1	Total Mg 1 1	0	0
56	1X	6	Total Mg 6 6	0	0
56	12	2	Total Mg 2 2	0	0
56	1y	4	Total Mg 4 4	0	0
56	1S	3	Total Mg 3 3	0	0
56	1p	1	Total Mg 1 1	0	0
56	2T	3	Total Mg 3 3	0	0
56	1D	14	Total Mg 14 14	0	0
56	23	1	Total Mg 1 1	0	0
56	1e	1	Total Mg 1 1	0	0
56	2G	1	Total Mg 1 1	0	0
56	1I	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	1V	3	Total Mg 3 3	0	0
56	2X	2	Total Mg 2 2	0	0
56	1w	11	Total Mg 11 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1a	215	Total 215	Mg 215	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	15	6	Total 6	Mg 6	0	0
56	1x	15	Total 15	Mg 15	0	0
56	2j	2	Total 2	Mg 2	0	0
56	1R	5	Total 5	Mg 5	0	0
56	1s	1	Total 1	Mg 1	0	0
56	1m	1	Total 1	Mg 1	0	0
56	2U	6	Total 6	Mg 6	0	0
56	1G	5	Total 5	Mg 5	0	0
56	2O	2	Total 2	Mg 2	0	0
56	11	5	Total 5	Mg 5	0	0
56	2r	2	Total 2	Mg 2	0	0
56	21	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2w	9	Total 9	Mg 9	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2x	5	Total 5	Mg 5	0	0
56	2R	4	Total 4	Mg 4	0	0
56	1Z	4	Total 4	Mg 4	0	0
56	2D	7	Total 7	Mg 7	0	0

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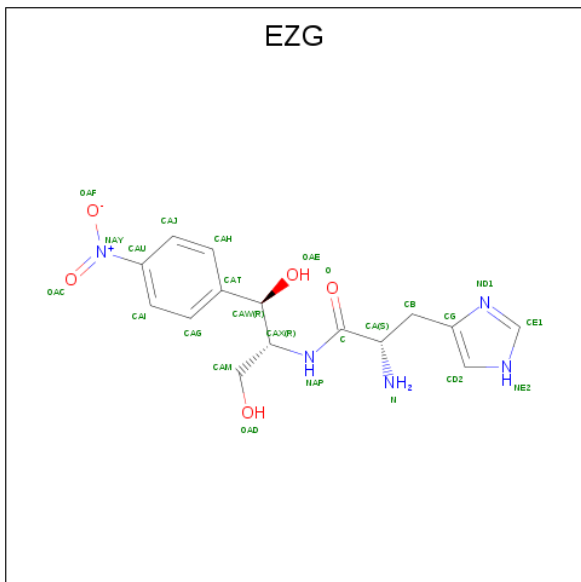
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2q	4	Total Mg 4 4	0	0
56	1U	6	Total Mg 6 6	0	0
56	1O	7	Total Mg 7 7	0	0
56	1r	1	Total Mg 1 1	0	0
56	19	1	Total Mg 1 1	0	0
56	1l	3	Total Mg 3 3	0	0
56	2V	2	Total Mg 2 2	0	0
56	1F	9	Total Mg 9 9	0	0
56	10	5	Total Mg 5 5	0	0
56	2t	1	Total Mg 1 1	0	0
56	1Q	5	Total Mg 5 5	0	0
56	2A	754	Total Mg 754 754	0	0
56	2Z	1	Total Mg 1 1	0	0
56	1B	38	Total Mg 38 38	0	0
56	2y	7	Total Mg 7 7	0	0
56	27	2	Total Mg 2 2	0	0
56	2v	5	Total Mg 5 5	0	0

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 58 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-L-histidinamide (three-letter code: EZG) (formula: C₁₅H₁₉N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1A	1	Total	C	N	O	0	0
			25	15	5	5		
58	2A	1	Total	C	N	O	0	0
			25	15	5	5		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

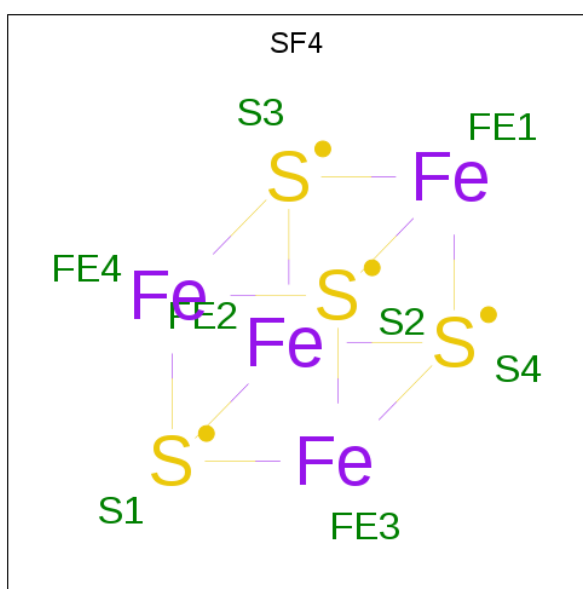
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	24	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1433	Total	O	0	0
			1433	1433		
61	1B	65	Total	O	0	0
			65	65		
61	1D	24	Total	O	0	0
			24	24		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1E	30	Total 30	O 30	0	0
61	1F	10	Total 10	O 10	0	0
61	1G	8	Total 8	O 8	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	2	Total 2	O 2	0	0
61	1N	6	Total 6	O 6	0	0
61	1O	8	Total 8	O 8	0	0
61	1P	18	Total 18	O 18	0	0
61	1Q	12	Total 12	O 12	0	0
61	1R	12	Total 12	O 12	0	0
61	1S	4	Total 4	O 4	0	0
61	1T	7	Total 7	O 7	0	0
61	1U	9	Total 9	O 9	0	0
61	1V	8	Total 8	O 8	0	0
61	1W	8	Total 8	O 8	0	0
61	1X	8	Total 8	O 8	0	0
61	1Y	2	Total 2	O 2	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	10	Total 10	O 10	0	0
61	11	7	Total 7	O 7	0	0
61	12	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	4	Total 4	O 4	0	0
61	15	5	Total 5	O 5	0	0
61	16	2	Total 2	O 2	0	0
61	17	9	Total 9	O 9	0	0
61	18	7	Total 7	O 7	0	0
61	1a	315	Total 315	O 315	0	0
61	1b	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1g	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	6	Total 6	O 6	0	0
61	1m	1	Total 1	O 1	0	0
61	1n	1	Total 1	O 1	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	6	Total 6	O 6	0	0
61	1w	20	Total 20	O 20	0	0
61	1x	14	Total 14	O 14	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	885	Total 885	O 885	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2B	26	Total 26	O 26	0	0
61	2D	18	Total 18	O 18	0	0
61	2E	14	Total 14	O 14	0	0
61	2F	18	Total 18	O 18	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	1	Total 1	O 1	0	0
61	2P	12	Total 12	O 12	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	3	Total 3	O 3	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	1	Total 1	O 1	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	4	Total 4	O 4	0	0
61	21	8	Total 8	O 8	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0
61	25	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	26	1	Total 1	O 1	0	0
61	27	4	Total 4	O 4	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
61	2a	258	Total 258	O 258	0	0
61	2c	1	Total 1	O 1	0	0
61	2d	3	Total 3	O 3	0	0
61	2e	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	6	Total 6	O 6	0	0
61	2o	1	Total 1	O 1	0	0
61	2p	2	Total 2	O 2	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	5	Total 5	O 5	0	0
61	2u	1	Total 1	O 1	0	0
61	2v	2	Total 2	O 2	0	0
61	2w	2	Total 2	O 2	0	0
61	2x	6	Total 6	O 6	0	0

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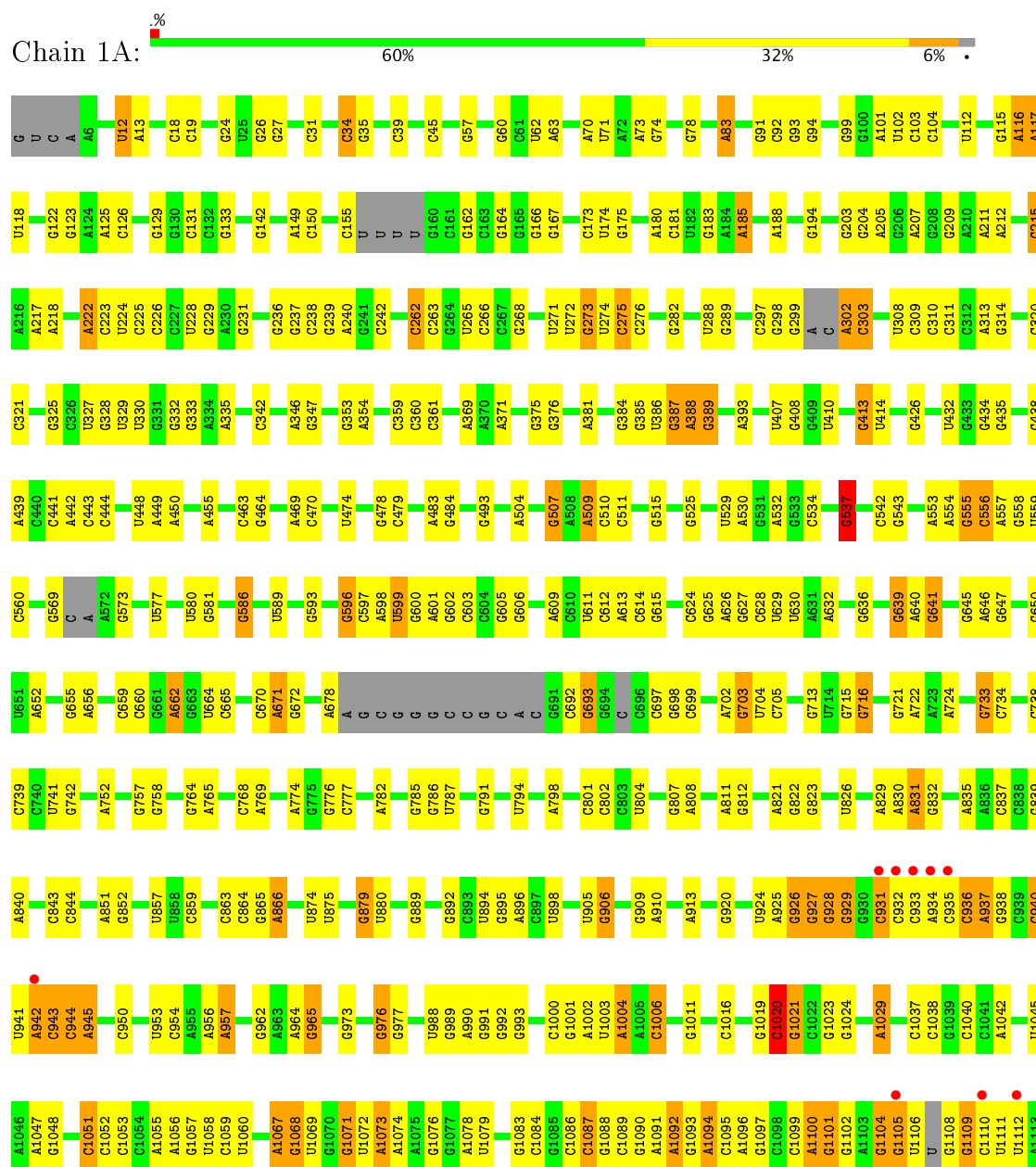
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2y	18	Total	O	0	0
			18	18		

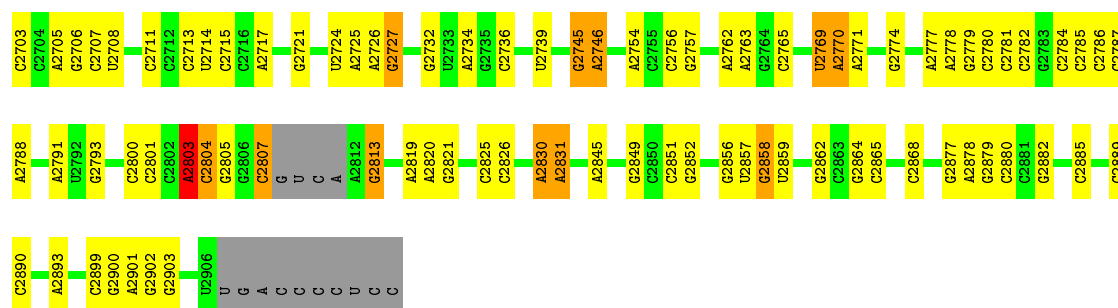
3 Residue-property plots

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

• Molecule 1: 23S Ribosomal RNA

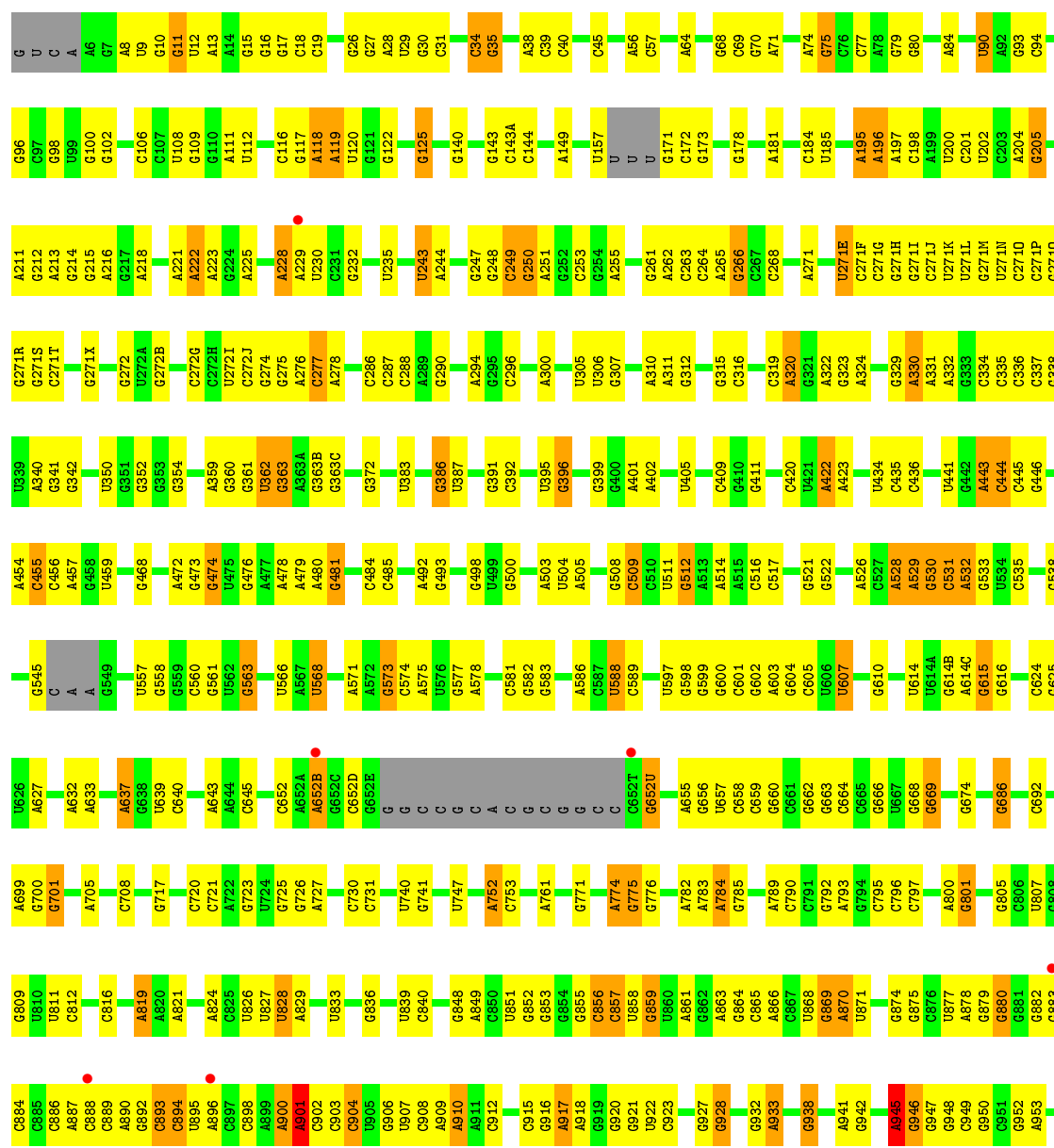


G2579	G2483	C2367	G2109	C2001	G1859	G1760	G1640	C1547	G1426	G1305	G1184	G1114
G2584	G2484	G2370	G2116	G2006	A1860	G1761	C1653	G1552	A1430	G1310	C1185	A1115
C2585	G2182	G2371	G2117	G2006	G1871	G1761	A1653	A1552	A1431	A1311	U1186	A1116
G2586	G2183	G2372	G2118	G2013	G1871	G1766	A1654	A1553	G1432	G1312	U1187	G1117
G2587	G2184	G2373	G2119	G2014	A1878	A1767	A1655	A1554	C1433	U1313	A1188	C1118
G2588	G2185	G2374	G2120	G2015	A1879	A1770	A1656	A1555	G1434	A1314	A1189	C1119
A2589	G2186	G2375	G2121	U2015	A1879	A1770	A1657	A1556	G1435	G1317	G1197	G1120
C2590	G2187	G2376	G2122	G2019	G1892	A1770	A1658	U1560	U1436	G1318	C1198	C1121
G2591	G2188	G2377	G2123	G2020	G1892	G1776	A1660	C1561	A1441	A1319	C1199	C1122
A2592	G2189	G2378	G2124	G2021	G1896	G1776	A1661	C1562	A1442	A1320	G1200	A1123
G2593	G2190	G2379	G2125	G2022	G1899	G1787	G1668	G1567	U1442	A1321	C1125	C1125
C2594	G2191	G2380	G2126	G2023	A1899	G1787	G1669	U1568	C1445	G1206	U1127	U1127
G2595	G2192	G2381	G2127	G2024	C1904	A1793	G1674	U1569	G1446	G1331	U1211	U1211
G2596	G2193	G2382	G2128	G2025	G1905	G1794	G1675	G1570	U1451	G1332	U1212	A1132
G2597	G2194	G2383	G2129	G2026	G1905	G1795	G1680	G1571	U1452	G1333	U1213	A1133
G2598	G2195	G2384	G2130	G2027	G1911	G1800	G1681	G1572	C1453	G1334	A1134	A1134
G2599	G2196	G2385	G2131	G2028	G1915	A1804	G1682	A1574	G1462	U1338	G1135	G1135
G2600	G2197	G2386	G2132	G2029	G1921	A1804	G1683	A1575	C1463	G1339	G1216	G1216
G2601	G2198	G2387	G2133	G2030	G1921	A1804	G1684	A1576	U1340	G1341	G1217	U1136
G2602	G2199	G2388	G2134	G2031	G1922	G1807	G1685	C1577	U1466	G1342	G1218	G1218
G2603	G2200	G2389	G2135	G2032	G1928	U1810	G1686	C1578	G1467	C1343	A1219	C1138
G2604	G2201	G2390	G2136	G2033	G1935	A1811	G1687	C1579	G1468	G1221	U1221	U1139
G2605	G2202	G2391	G2137	G2034	A1935	A1811	G1688	G	U1346	A1222	A1222	U1140
G2606	G2203	G2392	G2138	G2035	A1936	A1811	G1689	U	A1473	C1223	C1223	A1141
G2607	G2204	G2393	G2139	G2036	C1936	A1811	G1690	C	A1474	C1224	U1143	U1143
G2608	G2205	G2394	G2140	G2037	G1941	A1817	G1691	G1584	G1475	G1349	U1228	C1146
G2609	G2206	G2395	G2141	G2038	C1942	A1817	G1692	G1585	U1484	G1355	U1147	U1147
G2610	G2207	G2396	G2142	G2039	G1949	A1820	G1693	G1586	A1485	G1356	U1148	C1148
G2611	G2208	G2397	G2143	G2040	A1950	A1821	G1700	C1593	A1486	U1357	U1232	C1149
G2612	G2209	G2398	G2144	G2041	G1951	A1822	A1701	C1594	A1487	U1358	U1233	A1149
G2613	G2210	G2399	G2145	G2042	G1952	A1823	G1702	A1601	A1488	U1359	A1234	U1151
G2614	G2211	G2400	G2146	G2043	G1953	U1825	G1703	G1602	G1495	U1375	G1245	U1152
G2615	G2212	G2401	G2147	G2044	U1956	U1826	G1704	G1603	G1496	C1379	C1246	G1153
G2616	G2213	G2402	G2148	G2045	C1956	U1827	G1705	A1605	G1497	U1387	U1255	U1154
G2617	G2214	G2403	G2149	G2046	A1959	U1828	A1711	G1606	U1501	U1388	U1256	C1155
G2618	G2215	G2404	G2150	G2047	A1960	U1829	G1714	U1502	G1502	G1389	U1257	A1157
G2619	G2216	G2405	G2151	G2048	A1961	U1830	G1715	G1513	G1513	G1390	C1263	G1158
G2620	G2217	G2406	G2152	G2049	U1973	U1831	G1716	C1514	G1514	U1391	U1159	U1159
G2621	G2218	G2407	G2153	G2050	A1974	U1832	G1717	U1515	U1392	G1273	G1160	G1160
G2622	G2219	G2408	G2154	G2051	A1975	U1833	G1718	A1616	A1399	G1274	G1161	G1161
G2623	G2220	G2409	G2155	G2052	G1976	U1834	G1719	A1617	A1400	G1275	G1162	G1162
G2624	G2221	G2410	G2156	G2053	U1977	U1835	G1720	A1618	G1401	U1285	C1163	C1163
G2625	G2222	G2411	G2157	G2054	U1978	U1836	G1721	G1529	G1402	U1286	C1164	C1164
G2626	G2223	G2412	G2158	G2055	U1979	U1837	G1722	G1530	A1403	U1287	G1165	G1165
G2627	G2224	G2413	G2159	G2056	U1980	U1838	G1723	U1535	A1404	A1288	G1166	G1166
G2628	G2225	G2414	G2160	G2057	A1981	U1839	G1724	U1536	A1405	U1289	G1167	G1167
G2629	G2226	G2415	G2161	G2058	A1982	U1840	G1725	A1537	A1406	G1291	A1175	A1175
G2630	G2227	G2416	G2162	G2059	A1983	U1841	G1726	A1538	A1407	U1292	U1176	U1176
G2631	G2228	G2417	G2163	G2060	A1984	U1842	G1727	A1539	A1408	U1293	C1180	C1180
G2632	G2229	G2418	G2164	G2061	A1985	U1843	G1728	A1540	A1409	U1294	G1181	G1181
G2633	G2230	G2419	G2165	G2062	A1986	U1844	G1729	A1541	A1410	U1295	G1182	G1182
G2634	G2231	G2420	G2166	G2063	A1987	U1845	G1730	A1542	A1411	U1296	G1302	G1302
G2635	G2232	G2421	G2167	G2064	A1988	U1846	G1731	A1543	A1412	U1297	U1297	U1297
G2636	G2233	G2422	G2168	G2065	A1989	U1847	G1732	A1544	A1413	U1298	U1298	U1298
G2637	G2234	G2423	G2169	G2066	A1990	U1848	G1733	A1545	A1414	U1299	U1299	U1299
G2638	G2235	G2424	G2170	G2067	A1991	U1849	G1734	A1546	A1415	U1300	U1300	U1300
G2639	G2236	G2425	G2171	G2068	A1992	U1850	G1735	A1547	A1416	U1301	U1301	U1301
G2640	G2237	G2426	G2172	G2069	A1993	U1851	G1736	A1548	A1417	U1302	U1302	U1302
G2641	G2238	G2427	G2173	G2070	A1994	U1852	G1737	A1549	A1418	U1303	U1303	U1303
G2642	G2239	G2428	G2174	G2071	A1995	U1853	G1738	A1550	A1419	U1304	U1304	U1304
G2643	G2240	G2429	G2175	G2072	A1996	U1854	G1739	A1551	A1420	U1305	U1305	U1305
G2644	G2241	G2430	G2176	G2073	A1997	U1855	G1740	A1552	A1421	U1306	U1306	U1306
G2645	G2242	G2431	G2177	G2074	A1998	U1856	G1741	A1553	A1422	U1307	U1307	U1307
G2646	G2243	G2432	G2178	G2075	A1999	U1857	G1742	A1554	A1423	U1308	U1308	U1308
G2647	G2244	G2433	G2179	G2076	A2000	U1858	G1743	A1555	A1424	U1309	U1309	U1309
G2648	G2245	G2434	G2180	G2077	A2001	U1859	G1744	A1556	A1425	U1310	U1310	U1310
G2649	G2246	G2435	G2181	G2078	A2002	U1860	G1745	A1557	A1426	U1311	U1311	U1311
G2650	G2247	G2436	G2182	G2079	A2003	U1861	G1746	A1558	A1427	U1312	U1312	U1312
G2651	G2248	G2437	G2183	G2080	A2004	U1862	G1747	A1559	A1428	U1313	U1313	U1313
G2652	G2249	G2438	G2184	G2081	A2005	U1863	G1748	A1560	A1429	U1314	U1314	U1314
G2653	G2250	G2439	G2185	G2082	A2006	U1864	G1749	A1561	A1430	U1315	U1315	U1315
G2654	G2251	G2440	G2186	G2083	A2007	U1865	G1750	A1562	A1431	U1316	U1316	U1316
G2655	G2252	G2441	G2187	G2084	A2008	U1866	G1751	A1563	A1432	U1317	U1317	U1317
G2656	G2253	G2442	G2188	G2085	A2009	U1867	G1752	A1564	A1433	U1318	U1318	U1318
G2657	G2254	G2443	G2189	G2086	A2010	U1868	G1753	A1565	A1434	U1319	U1319	U1319
G2658	G2255	G2444	G2190	G2087	A2011	U1869	G1754	A1566	A1435	U1320	U1320	U1320
G2659	G2256	G2445	G2191	G2088	A2012	U1870	G1755	A1567	A1436	U1321	U1321	U1321
G2660	G2257	G2446	G2192	G2089	A2013	U1871	G1756	A1568	A1437	U1322	U1322	U1322
G2661	G2258	G2447	G2193	G2090	A2014	U1872	G1757	A1569	A1438	U1323	U1323	U1323
G2662	G2259	G2448	G2194	G2091	A2015	U1873	G1758	A1570	A1439	U1324	U1324	U1324
G2663	G2260	G2449	G2195	G2092	A2016	U1874	G1759	A1571	A1440	U1325	U1325	U1325
G2664	G2261	G2450	G2196	G2093	A2017	U1875	G1760	A1572	A1441	U1326	U1326	U1326
G2665	G2262	G2451	G2197	G2094	A2018	U1876	G1761	A1573	A1442	U1327	U1327	U1327
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G2667	G2264	G2453	G2199	G2096	A2020	U1878	G1763	A1575	A1444	U1329	U1329	U1329
G2668	G2265	G2454	G2200	G2097	A2021	U1879	G1764	A1576	A1445	U1330	U1330	U1330
G2669	G2266	G2455	G2201	G2098	A2022	U1880	G1765	A1577	A1446	U1331	U1331	U1331
G2670	G2267	G2456	G2202	G2099	A2023	U1881	G1766	A1578	A1447	U1332	U1332	U1332
G2671	G2268	G2457	G2203	G2100	A2024	U1882	G1767	A1579	A1448	U1333	U1333	U1333
G2672	G2269	G2458	G2204	G2101	A2025	U1883	G1768	A1580	A1449	U1334	U1334	U1334
G2673	G2270	G2459	G2205	G2102	A2026	U1884	G1769	A1581	A1450	U1335	U1335	U1335
G2674	G2271	G2460	G2206	G2103	A2027	U1885	G1770	A1582	A1451	U1336	U1336	U1336
G2675	G2272	G2461	G2207	G2104	A2028	U1886	G1771	A1583	A1452	U1337	U1337	U1337
G2676	G2273	G2462	G2208	G2105	A2029	U1887	G1772	A1584	A1453	U1338	U1338	U1338
G2677	G2274	G2463	G2209	G2106	A2030	U1888	G1773	A1585	A1454	U1339	U1339	U1339
G2678	G2275	G2464	G2210	G2107	A2031	U1889	G1774	A1586	A1455	U1340	U1340	U1340
G2679	G2276	G2465	G2211	G2108	A2032	U1890	G1775	A1587	A1456	U1341	U1341	U1341
G2680	G2277	G2466	G2212	G2109	A2033	U1891	G1776	A1588	A1457	U1342	U1342	U1342
G2681	G2278	G2467	G2213	G2110	A2034	U1892	G1777	A1589	A1458	U1343	U1343	U1343
G26												

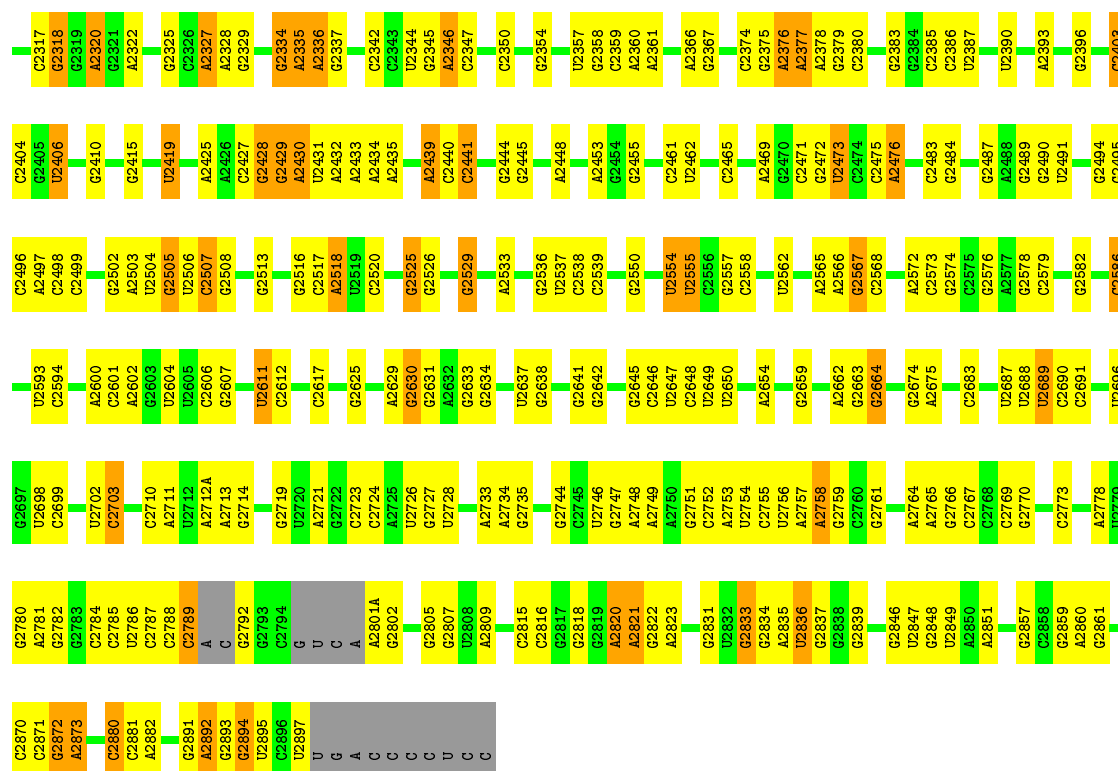


• Molecule 1: 23S Ribosomal RNA

Chain 2A: 52% 36% 8%

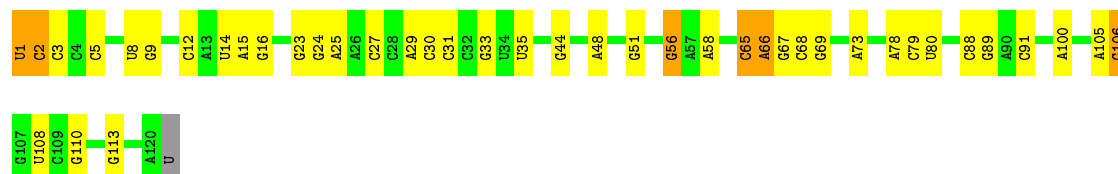


G2206	A1966	C1830	A1722	C1617	C1530	G1442	G1347	A1247	G1169	C1038	G956
G2207	C1967	G1831	U1739	G1622	C1531	G1445	U1352	G1248	G1170	G1039	A957
A2208	C2140	G1835	G1740	G1627	C1532	A1448	A1353	G1249	G1171	C1040	U988
U2218	A1970	G1836	G1746	G1627	C1533	A1449	A1354	G1250	G	C1041	A959
G2224	A1971	C1836	G1751	G1628	U	G1450	A1359	G1251	U	C1042	A960
A2225	G1973	G1838	G1751	U1629	C1536	G1450A	A1360	G1252	A	G1043	G961
C2226	G1973	G1839	G1751	U1629	G1537	C1451	A1367	G1253	G	G	G962
A2227	C1983	G1839	G1754	C1636	G1538	C1451	A1367	A1254	C	A	
	U2074	A1847	G1754	A1637	G1539	G1455	G1363	G1255	A	A	G966
G2230	U1991	A1848	G1755	C1637	G1542	G1455	G1364	G1256	G	A	
U2233	G1992	A1848	G1756	C1638	C1543	A1460	A1365	G1260	G	A	G974
G2234	U1993	G1857	G1757	U1639	C1543	G1461	A1366	G1261	U	C	C975
	C1996	G1866	A1759	C1640	C1546	C1462	A1367	A1262	G	A	A980
G2238	C1997	A1876	A1762	G1647	C1547	C1462	C1370	G1263	G	C	
G2239	G1998	G1877	G1763	C1648	C1548	C1467	G1371	G1264	U	A	A983
	A2001	G1878	G1764	G1651	C1557	C1468	U1372	A1265	G	A	G986
U2243	G2002	C1879	G1769	G1652	A1558	G1469	A1379	G1266	U	A	G987
	G2010	C1882	A1773	A1654	A1559	G1470	G1380	U1267	G	A	
U2249	U2099	A1889	A1773	C1658	A1566	G1475	A1384	A1268	U	G	A990
G2250	G2100	A1890	A1780	C1663	A1567	C1476	G1385	G1270	U	G	G991
G2251	G2101	A1890	A1780	G1663	G1568	A1477	C1386	G1271	U	U	G992
G2252	G2102	A1890	A1780	C1663	A1569	G1478	C1386	A1272	G	U	G993
G2253	C2103	G1899	A1783	C1663	A1569	G1478	C1386	U1273	G	G	G994
	G2104	A1900	A1784	A1664	A1572	U1481	U1394	A1274	C	C	G995
G2262	C2105	A1901	A1784	A1664	A1572	G1482	U1405	A1284	U	U	A996
	G2106	A1901	A1786	A1669	U1578	G1482	U1405	G1285	U	U	U999
A2268	G2107	G1906	A1786	A1669	A1579	A1486	U1405	G1286	U	A	A1000
A2269	C2108	G1906	A1786	A1669	A1579	A1486	U1406	A1287	G	A	A1001
G2270	U2022	G1906	A1786	A1669	A1579	A1486	U1406	A1287	G	A	G1002
G2271	G2023	A1912	A1791	G1675	A1580	G1487	G1410	U1292	C	A	G1003
	G2024	A1913	A1791	G1675	A1581	G1487	G1410	C1293	U	G	
A2274	G2025	C1914	U1794	U1680	C1582	U1489	G1412	G1298	U	C	C1007
C2275	C2026	A1915	C1795	U1680	C1583	U1490	A1412	G1299	U	C	
G2276	C2026	A1916	U1796	G1681	C1584	U1490	G1413	G1299	U	C	
	A2031	A1916	C1797	G1681	C1584	U1490	G1413	G1299	U	C	
G2277	G2032	C1920	U1798	G1682	A1586	A1493	G1416	G1298	G	G	A1010
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G2279	U2034	G1921	G1799	C1684	C1588	A1495	G1417	U1300	C	C	U1012
	G2035	A1916	C1800	C1684	C1589	A1496	G1418	A1301	U	A	C1013
C2283	G2036	A1916	C1801	U1689	U1590	U1497	A1419	A1302	U	U	G1016
	G2037	A1916	A1802	A1690	G1593	A1507	U1420	G1303	C	C	G1017
A2287	G2038	G1930	G1804	U1692	C1594	A1508	G1421	G1309	U	U	C1018
U2291	C2039	A1936	U1805	U1693	G1595	C1509	G1422	G1310	U	U	U1019
C2292	U2041	A1937	C1806	U1693	C1596	A1509A	G1424	G1311	U	U	A1020
	G2042	A1938	C1806	U1693	C1596	A1509B	G1425	U1312	A	A	A1021
U2296	C2043	U1939	G1811	G1695	C1599	G1510	G1426	G1313	U	A	G1022
C2297	C2044	U1939	G1812	G1697	C1599	G1511	A1427	G1314	A	A	U1023
A2298			G1813	A1698	A1603	C1511	G1428	C1315	G	G	G1024
G2299			G1814	G1699	A1603	G1517	G1429	G1325	A	A	G1025
G2300	A2051	C1947	A1815	G1699	C1607	U1523	C1430	G1325	G	G	U1026
	G2052	A1961	G1816	A1700	A1608	U1523	U1431	A1237	U	U	A1027
A2305	G2053	U1955	G1817	G1702	A1609	G1524	A1434	G1238	U	U	G1028
C2306	G2055	C1968	U1818	G1703	A1610	G1525	G1435	U1240	C	C	A1029
G2307	G2056	C1968	U1818	G1703	A1610	G1526	G1435	A1241	G	G	G1030
G2308			G1824	C1711	G1613	G1527	G1436	A1242	U	U	G1031
A2309	A2059	U1963	A1825	C1712	A1614	A1528	C1437	G1243	A	A	U1032
G2310	G2060	G1964	G1826	G1721	A1615	A1528A	G1441	G1244	A	A	U1033
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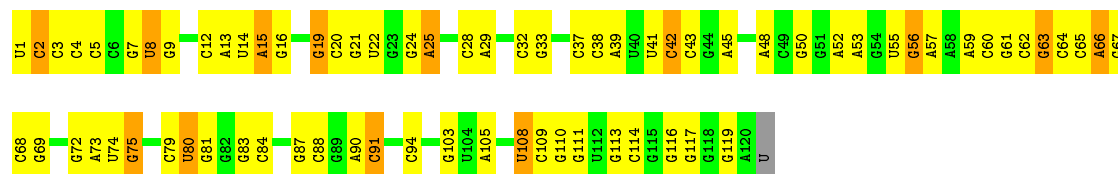
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 64% 30% 5% •



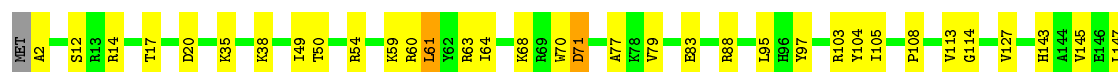
• Molecule 2: 5S Ribosomal RNA

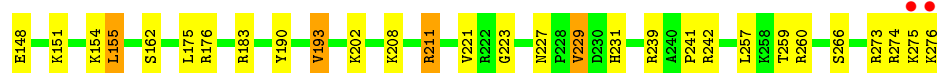
Chain 2B: 39% 50% 11% •



• Molecule 3: 50S ribosomal protein L2

Chain 1D: 77% 21% •





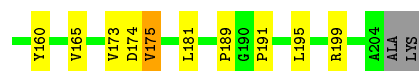
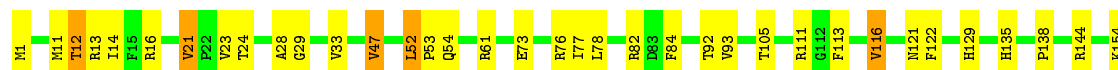
• Molecule 3: 50S ribosomal protein L2

Chain 2D: 78% 20%



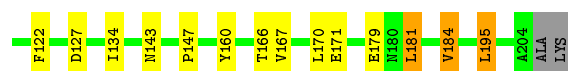
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 77% 19%



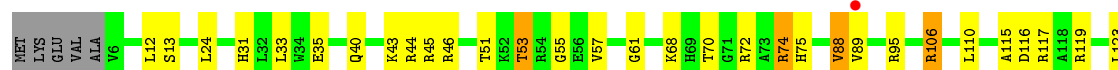
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 74% 19% 5%



• Molecule 5: 50S ribosomal protein L4

Chain 1F: 70% 23%



• Molecule 5: 50S ribosomal protein L4

Chain 2F: 64% 29%





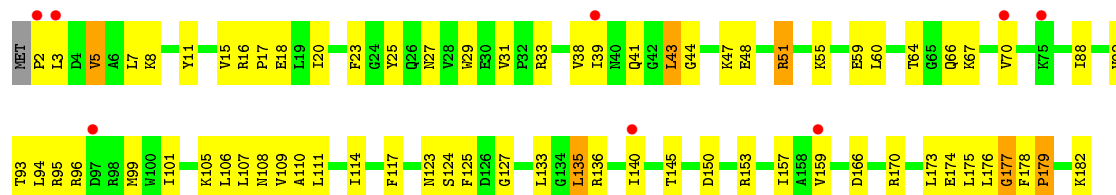
- Molecule 6: 50S ribosomal protein L5

Chain 1G: 73% 24% ..



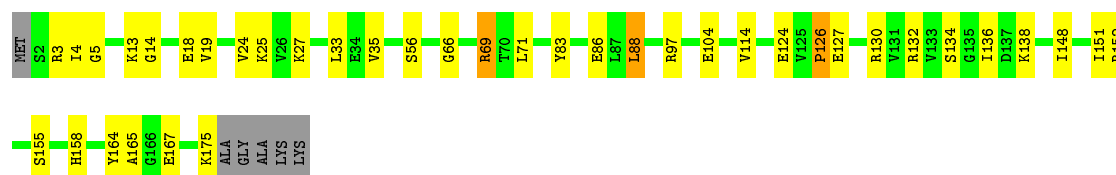
- Molecule 6: 50S ribosomal protein L5

Chain 2G: 4% 60% 36% ..



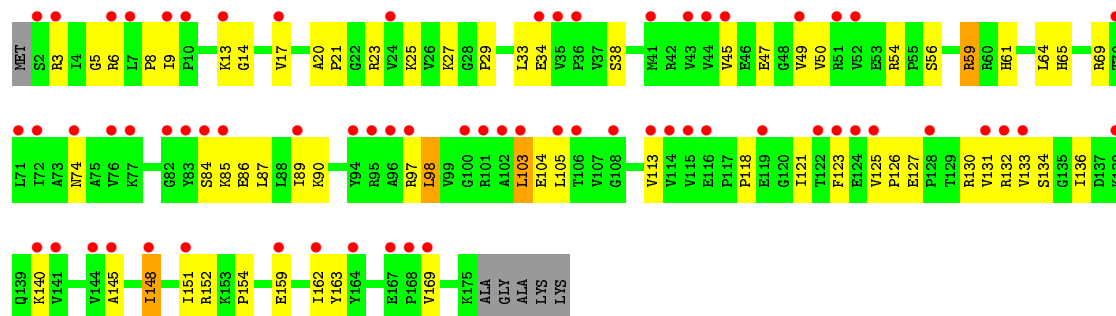
- Molecule 7: 50S ribosomal protein L6

Chain 1H: 75% 20% ..



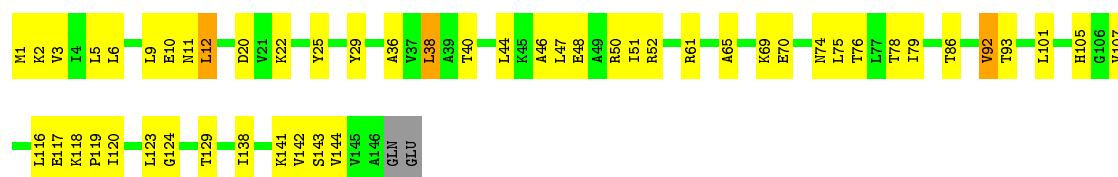
- Molecule 7: 50S ribosomal protein L6

Chain 2H: 37% 62% 33% ..

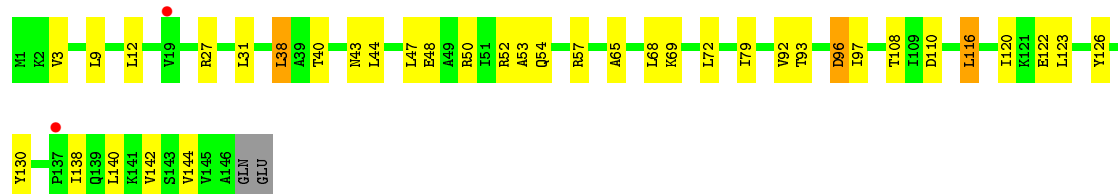
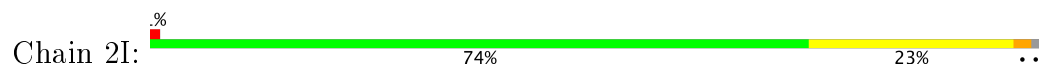


- Molecule 8: 50S ribosomal protein L9

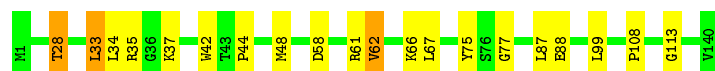
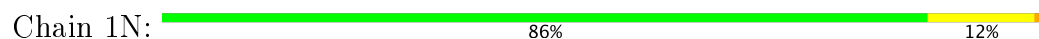
Chain 1I: 64% 32% ..



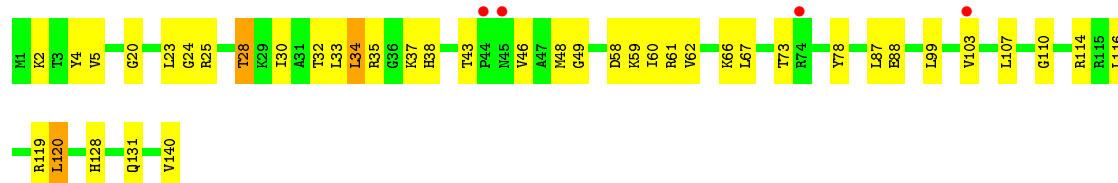
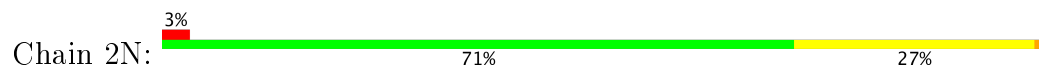
• Molecule 8: 50S ribosomal protein L9



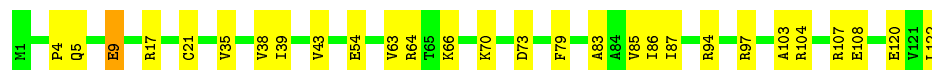
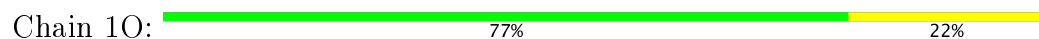
• Molecule 9: 50S ribosomal protein L13



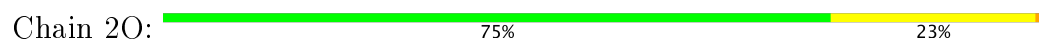
• Molecule 9: 50S ribosomal protein L13



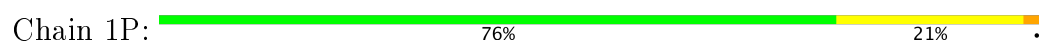
• Molecule 10: 50S ribosomal protein L14

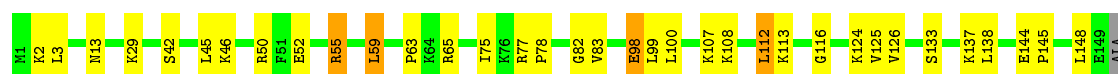


• Molecule 10: 50S ribosomal protein L14

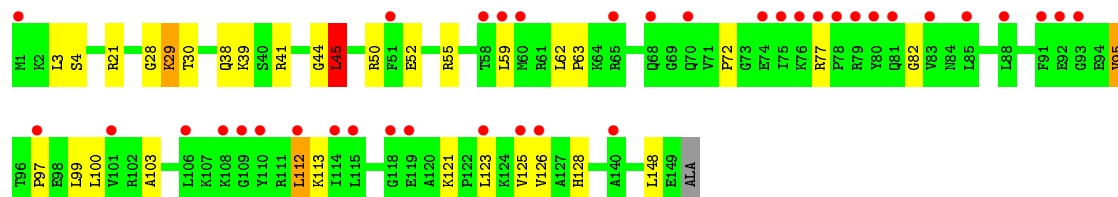
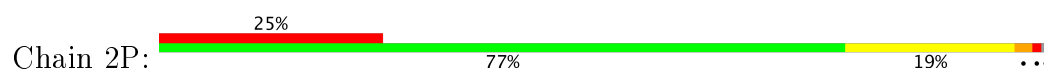


• Molecule 11: 50S ribosomal protein L15

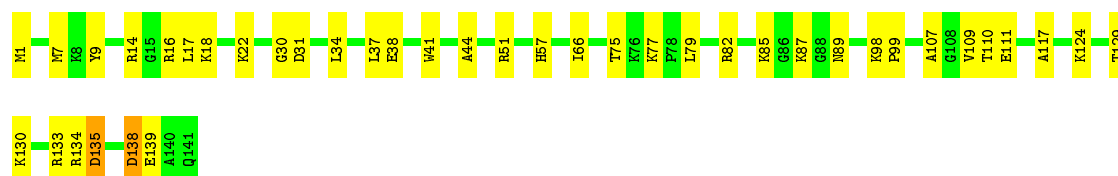




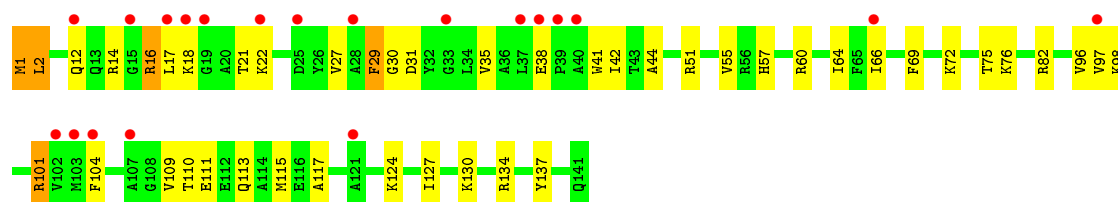
• Molecule 11: 50S ribosomal protein L15



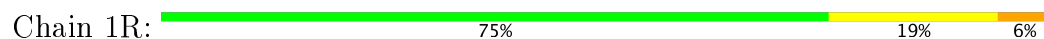
• Molecule 12: 50S ribosomal protein L16



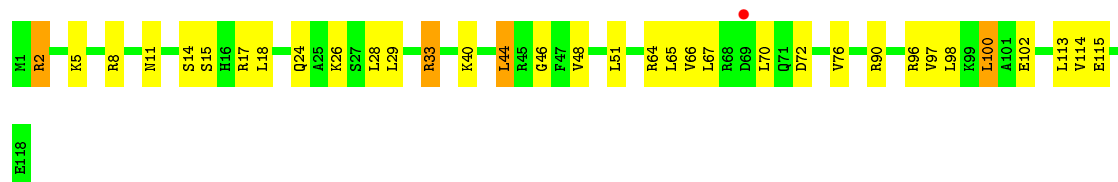
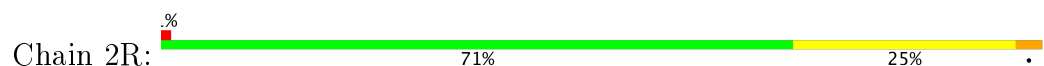
• Molecule 12: 50S ribosomal protein L16



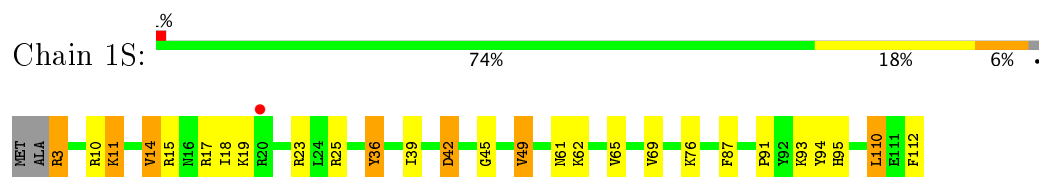
• Molecule 13: 50S ribosomal protein L17



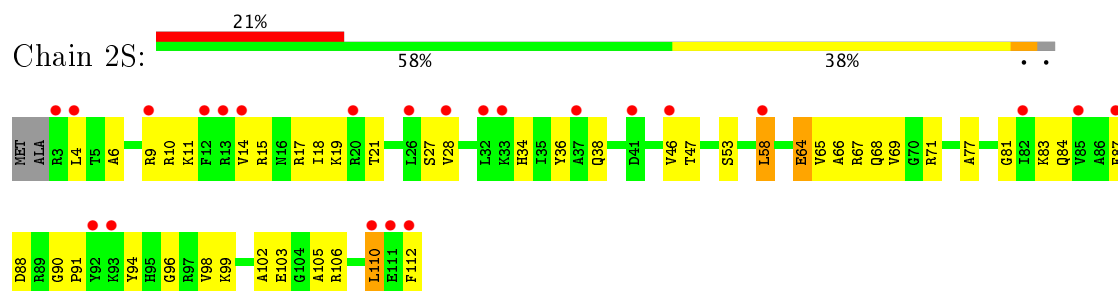
• Molecule 13: 50S ribosomal protein L17



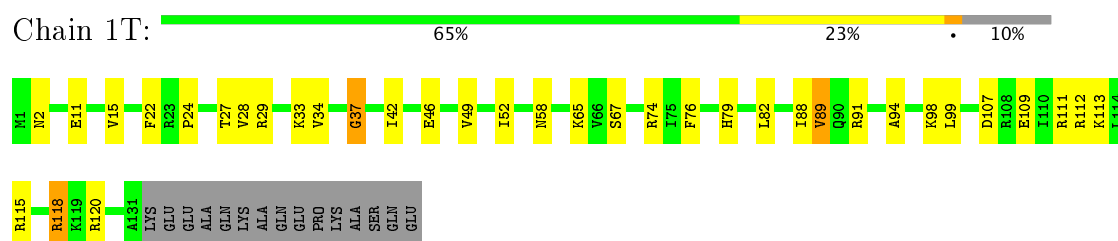
- Molecule 14: 50S ribosomal protein L18



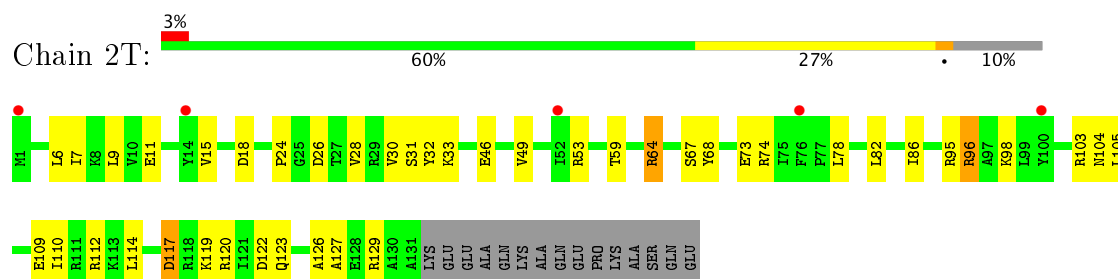
- Molecule 14: 50S ribosomal protein L18



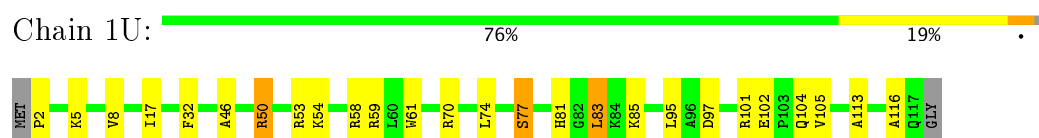
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



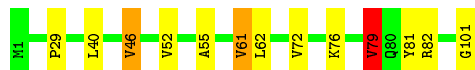
- Molecule 16: 50S ribosomal protein L20





- Molecule 17: 50S ribosomal protein L21

Chain 1V: 87% 10% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V: 82% 13% 5%



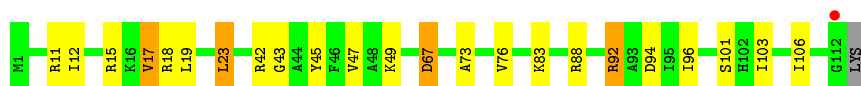
- Molecule 18: 50S ribosomal protein L22

Chain 1W: 83% 16% ..



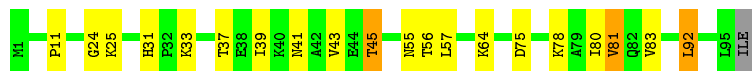
- Molecule 18: 50S ribosomal protein L22

Chain 2W: 79% 17% ..



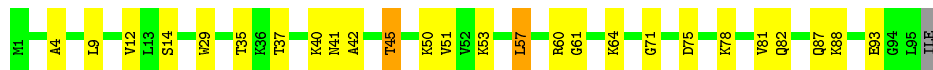
- Molecule 19: 50S ribosomal protein L23

Chain 1X: 78% 18% ..



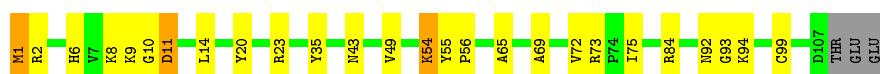
- Molecule 19: 50S ribosomal protein L23

Chain 2X: 72% 25% ..

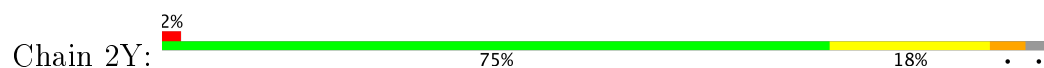


- Molecule 20: 50S ribosomal protein L24

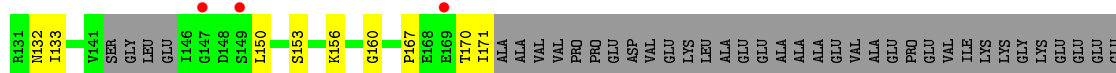
Chain 1Y: 74% 21% ..



- Molecule 20: 50S ribosomal protein L24

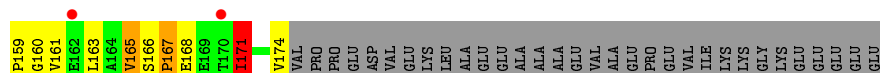
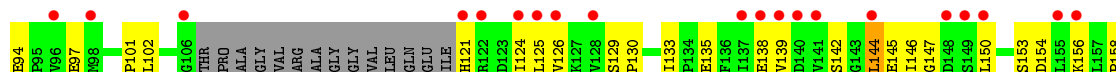


- Molecule 21: 50S ribosomal protein L25

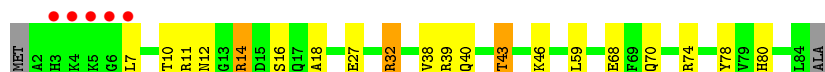
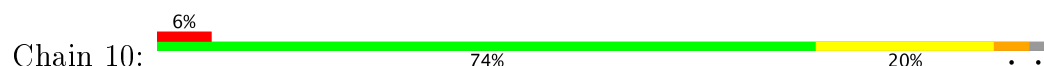


GLU

- Molecule 21: 50S ribosomal protein L25



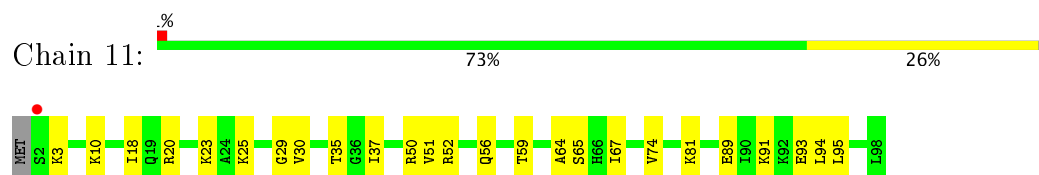
- Molecule 22: 50S ribosomal protein L27



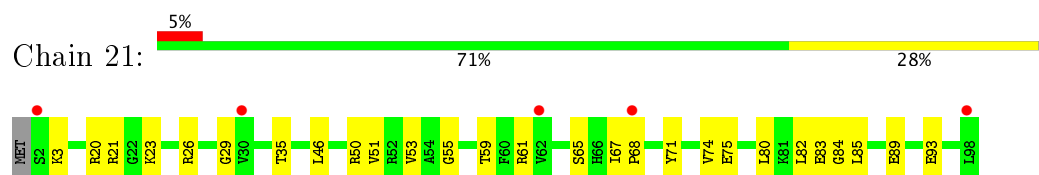
- Molecule 22: 50S ribosomal protein L27



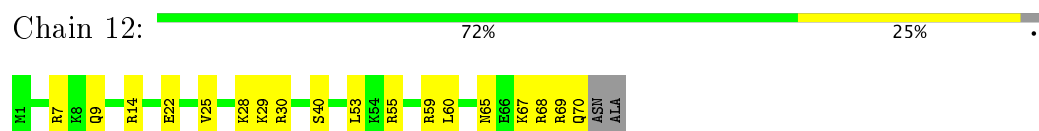
- Molecule 23: 50S ribosomal protein L28



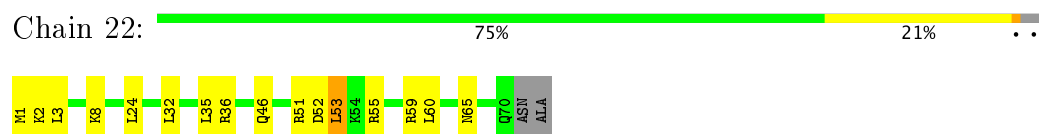
- Molecule 23: 50S ribosomal protein L28



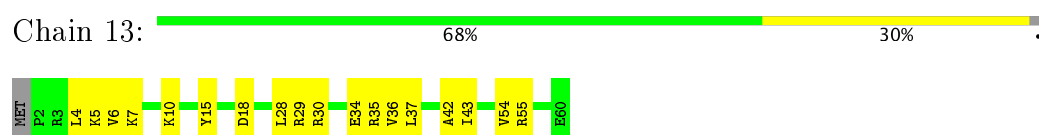
- Molecule 24: 50S ribosomal protein L29



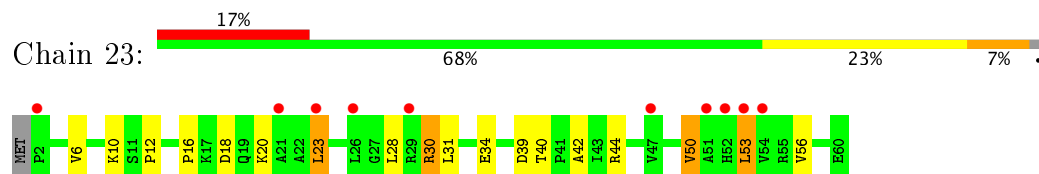
- Molecule 24: 50S ribosomal protein L29



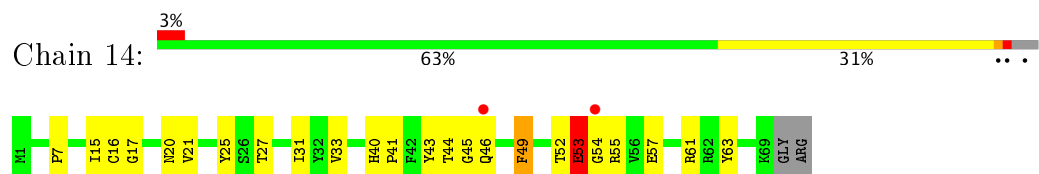
- Molecule 25: 50S ribosomal protein L30



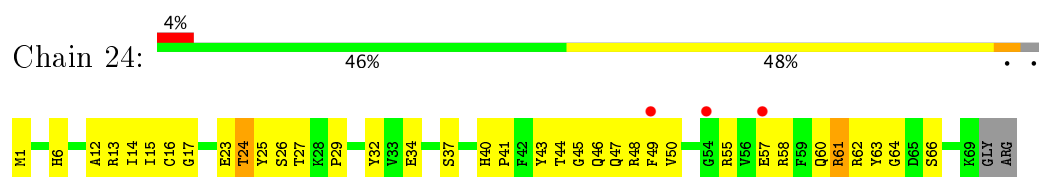
- Molecule 25: 50S ribosomal protein L30



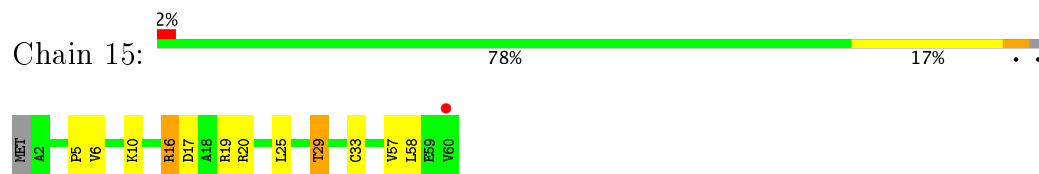
- Molecule 26: 50S ribosomal protein L31



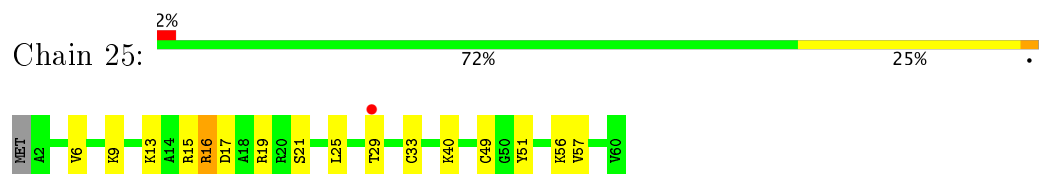
- Molecule 26: 50S ribosomal protein L31



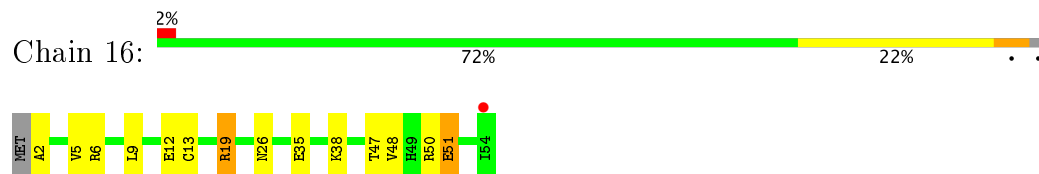
- Molecule 27: 50S ribosomal protein L32



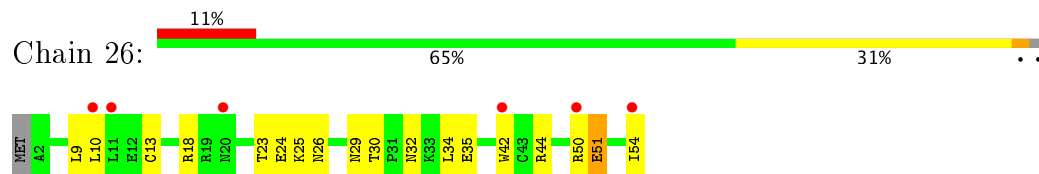
- Molecule 27: 50S ribosomal protein L32



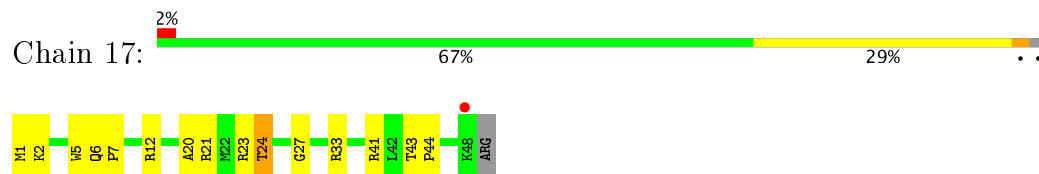
- Molecule 28: 50S ribosomal protein L33



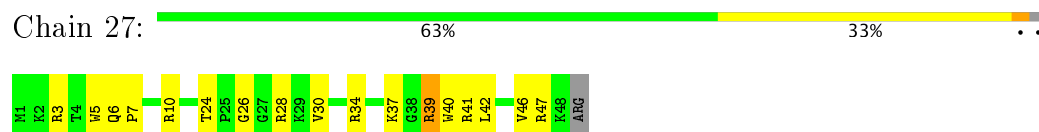
- Molecule 28: 50S ribosomal protein L33



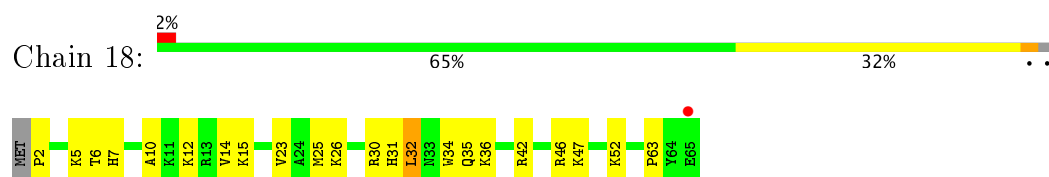
- Molecule 29: 50S ribosomal protein L34



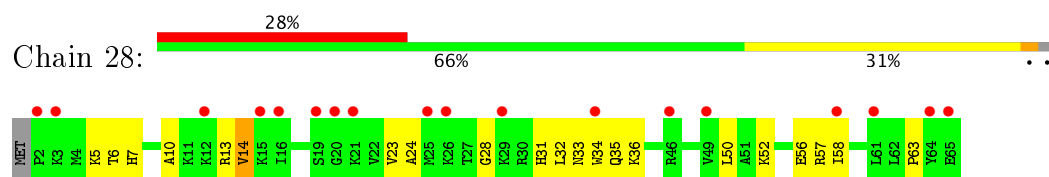
- Molecule 29: 50S ribosomal protein L34



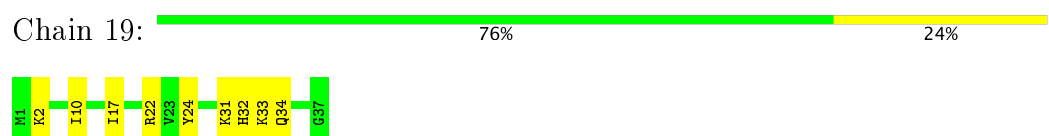
- Molecule 30: 50S ribosomal protein L35



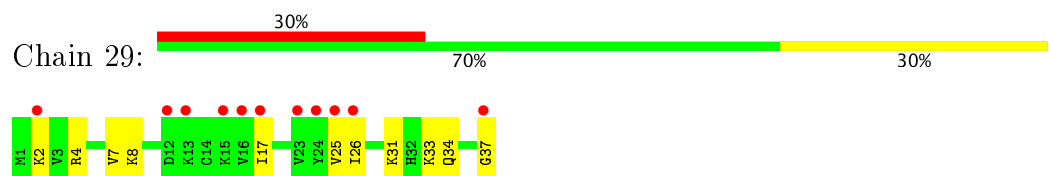
- Molecule 30: 50S ribosomal protein L35



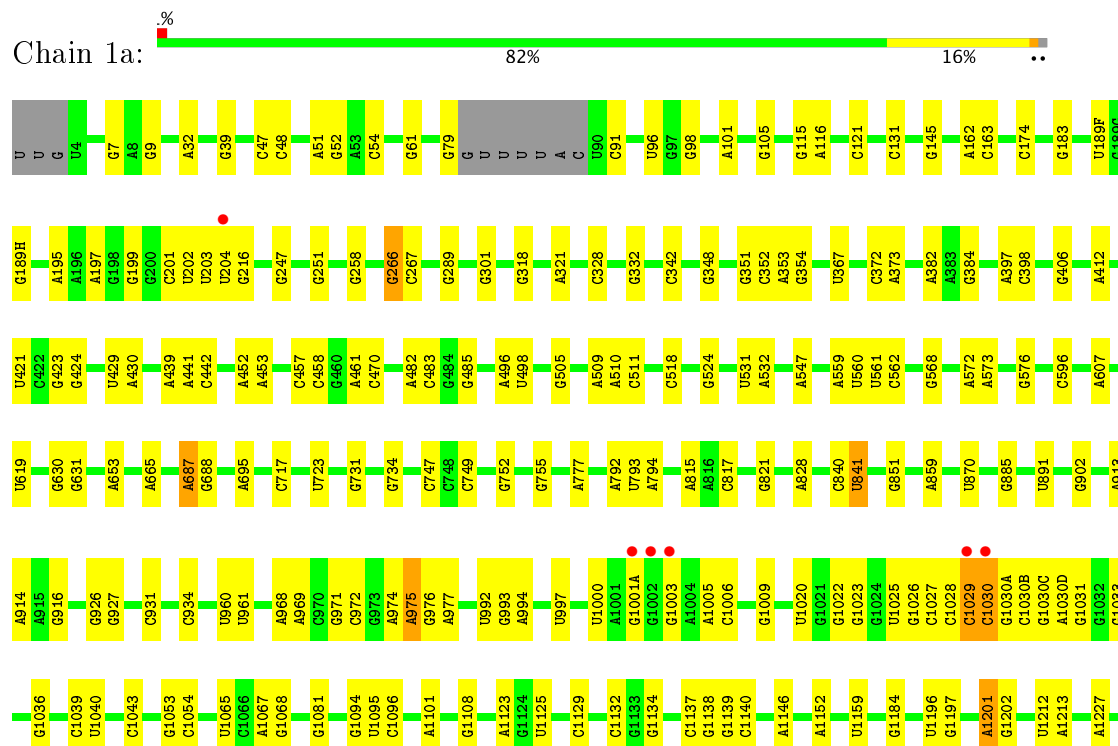
- Molecule 31: 50S ribosomal protein L36

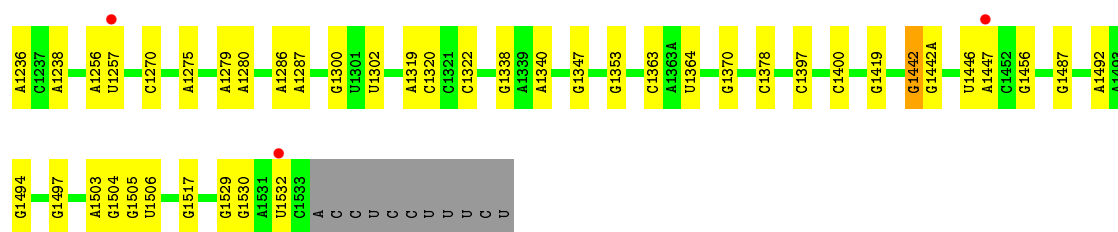


- Molecule 31: 50S ribosomal protein L36

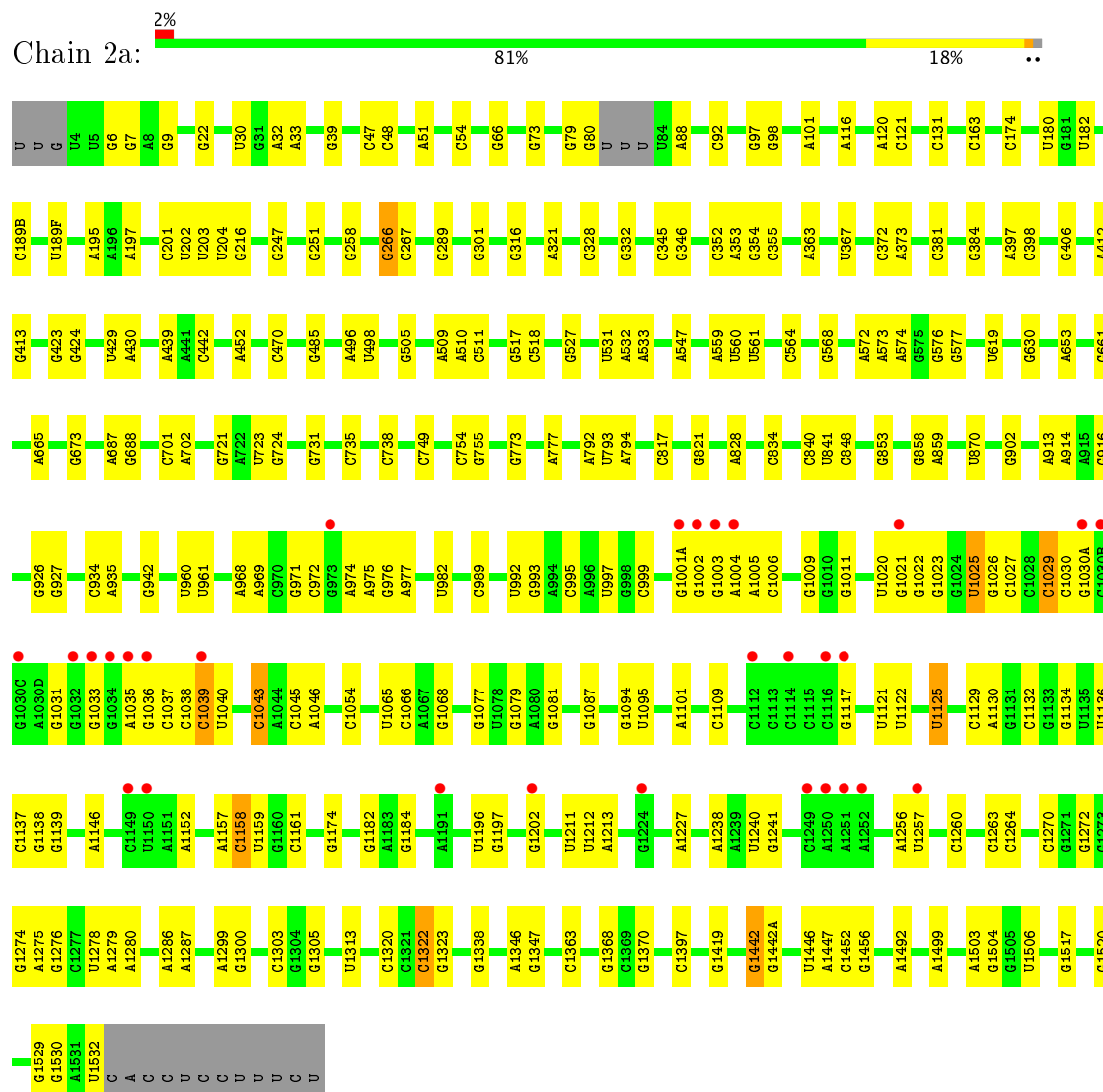


- Molecule 32: 16S Ribosomal RNA

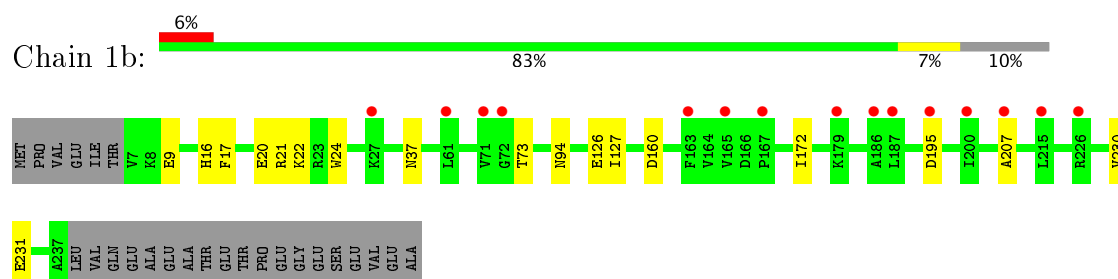




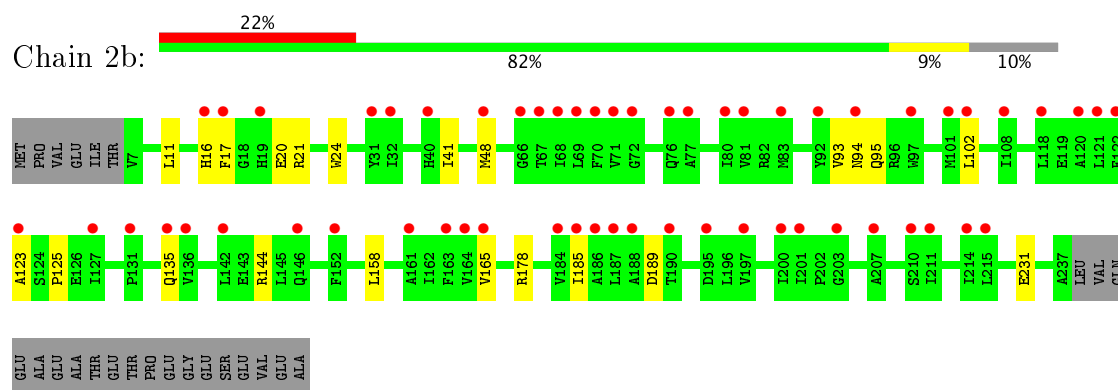
• Molecule 32: 16S Ribosomal RNA



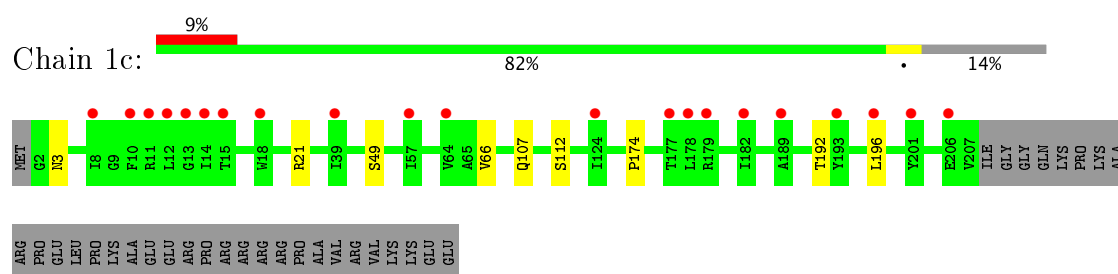
• Molecule 33: 30S ribosomal protein S2



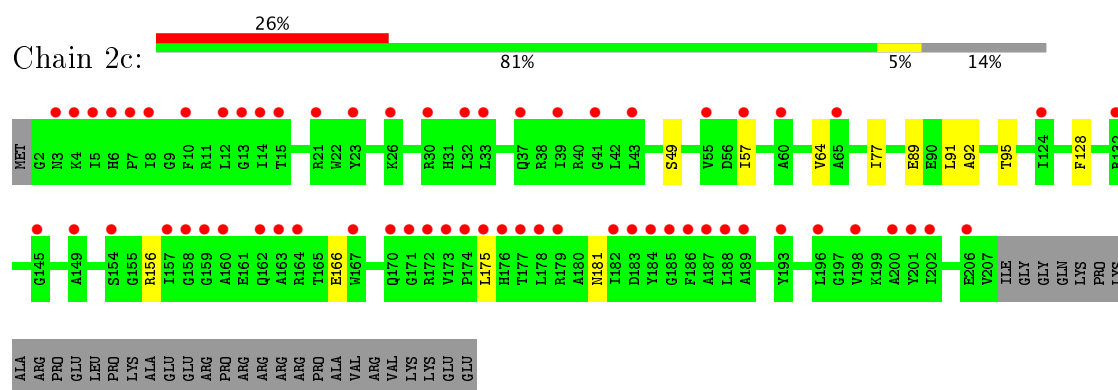
- Molecule 33: 30S ribosomal protein S2



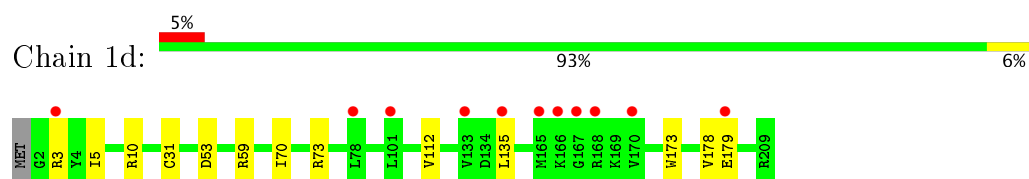
- Molecule 34: 30S ribosomal protein S3



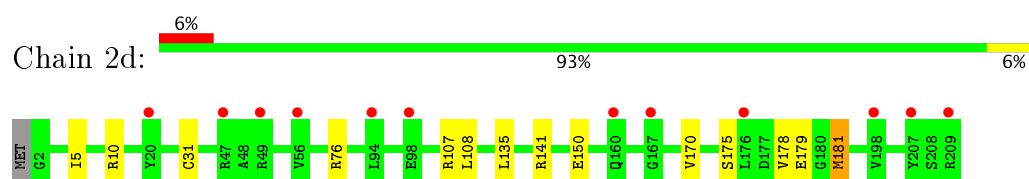
- Molecule 34: 30S ribosomal protein S3



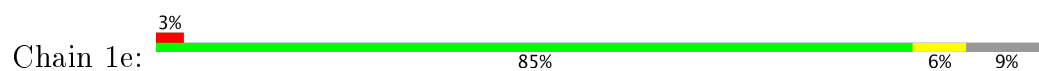
- Molecule 35: 30S ribosomal protein S4



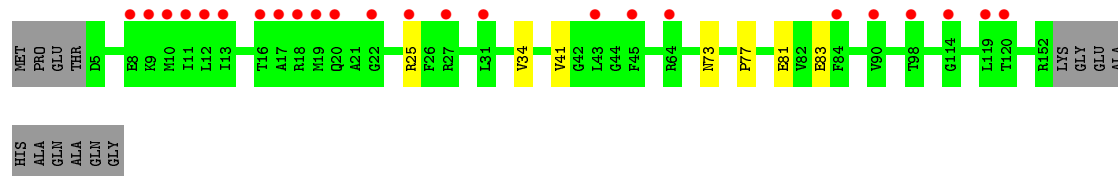
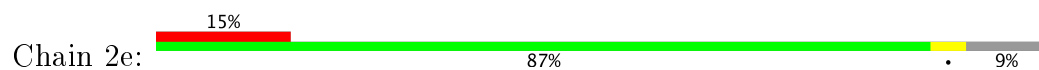
- Molecule 35: 30S ribosomal protein S4



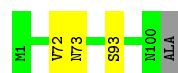
- Molecule 36: 30S ribosomal protein S5



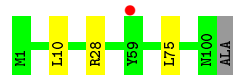
- Molecule 36: 30S ribosomal protein S5



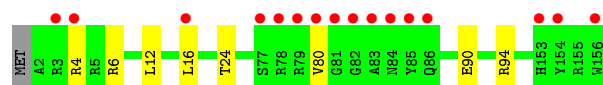
- Molecule 37: 30S ribosomal protein S6



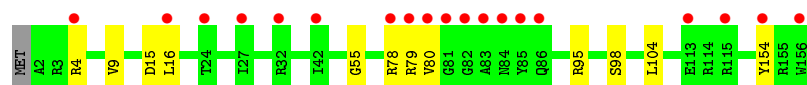
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

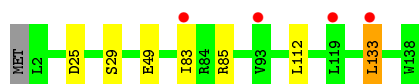


- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

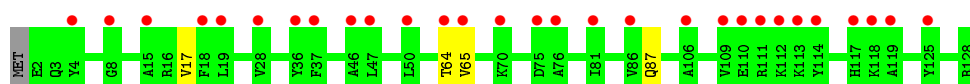




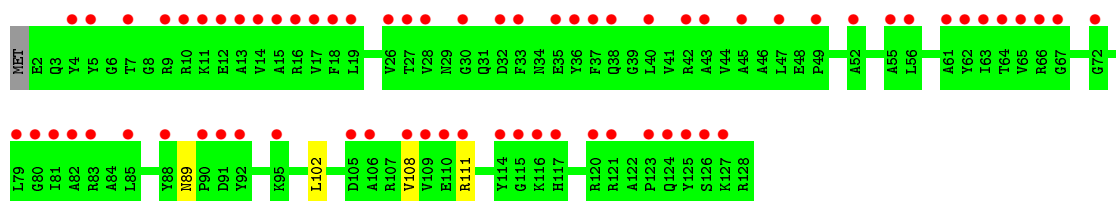
- Molecule 39: 30S ribosomal protein S8



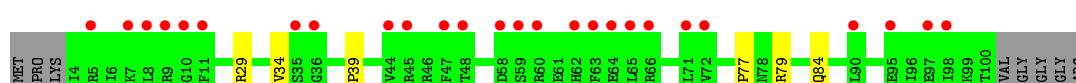
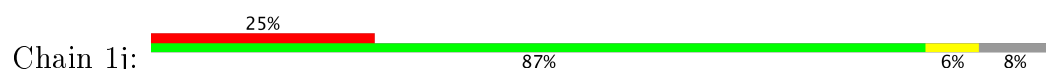
- Molecule 40: 30S ribosomal protein S9



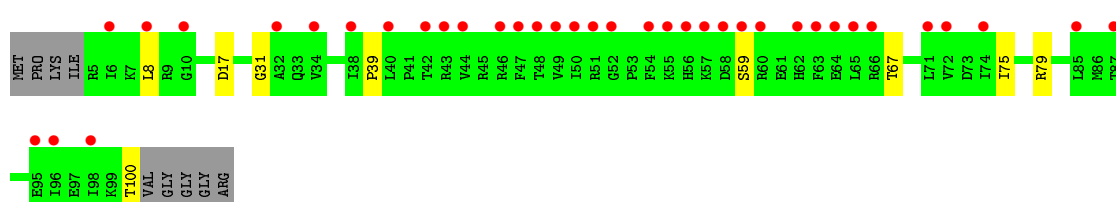
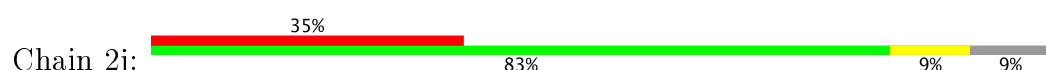
- Molecule 40: 30S ribosomal protein S9



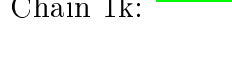
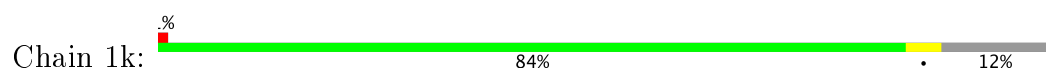
- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10

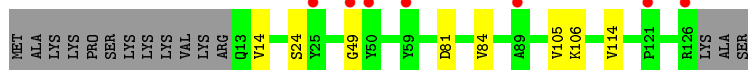
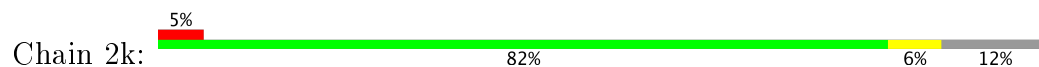


- Molecule 42: 30S ribosomal protein S11

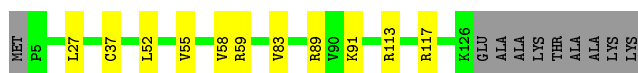
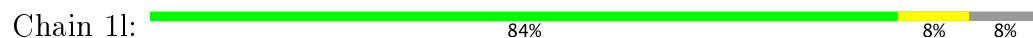




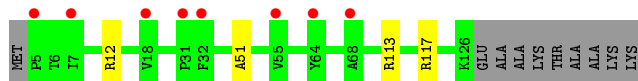
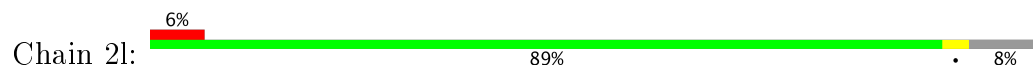
- Molecule 42: 30S ribosomal protein S11



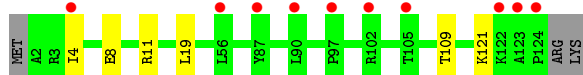
- Molecule 43: 30S ribosomal protein S12



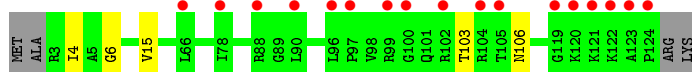
- Molecule 43: 30S ribosomal protein S12



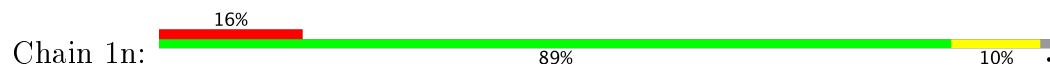
- Molecule 44: 30S ribosomal protein S13



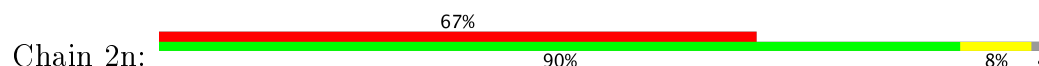
- Molecule 44: 30S ribosomal protein S13

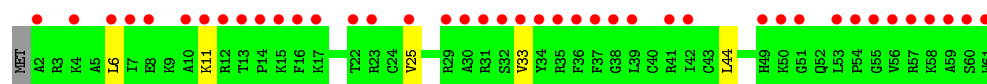


- Molecule 45: 30S ribosomal protein S14 type Z

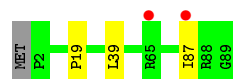


- Molecule 45: 30S ribosomal protein S14 type Z





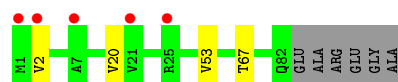
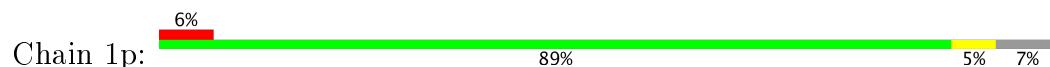
- Molecule 46: 30S ribosomal protein S15



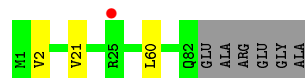
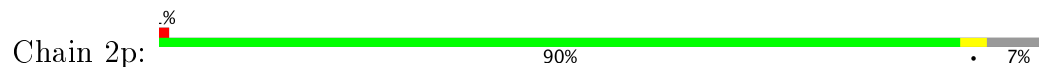
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



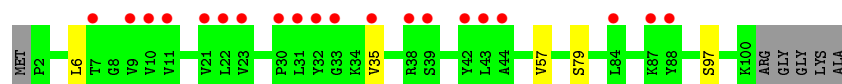
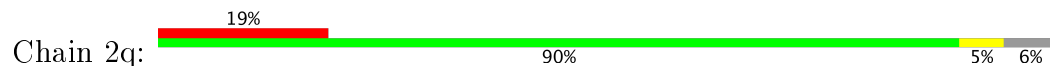
- Molecule 47: 30S ribosomal protein S16



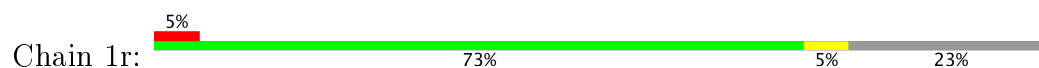
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

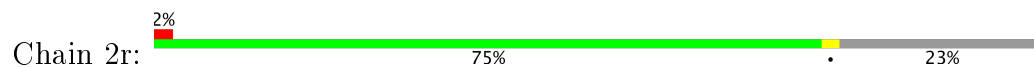


- Molecule 49: 30S ribosomal protein S18

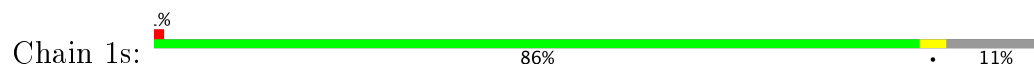




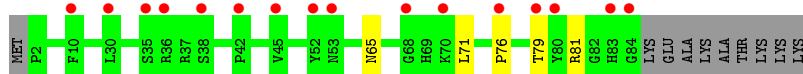
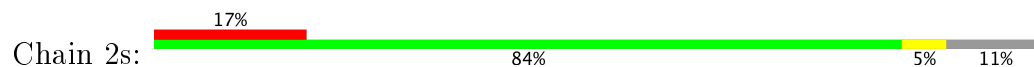
- Molecule 49: 30S ribosomal protein S18



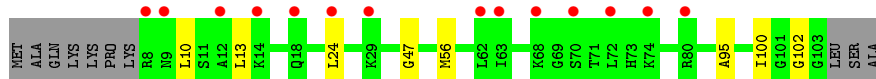
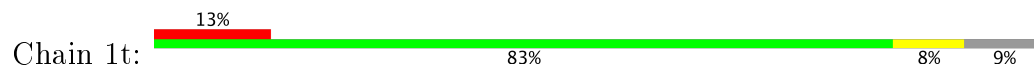
- Molecule 50: 30S ribosomal protein S19



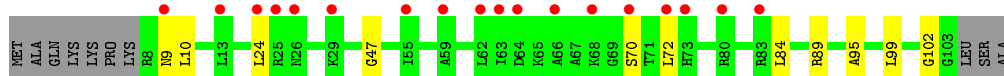
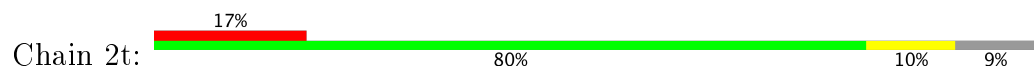
- Molecule 50: 30S ribosomal protein S19



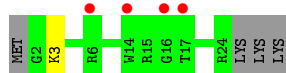
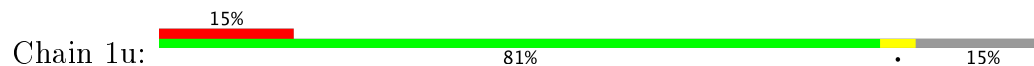
- Molecule 51: 30S ribosomal protein S20



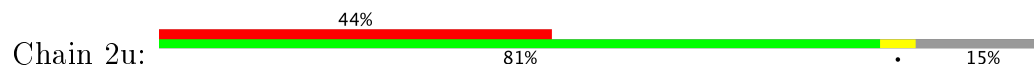
- Molecule 51: 30S ribosomal protein S20

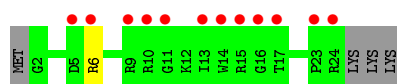


- Molecule 52: 30S ribosomal protein Thx

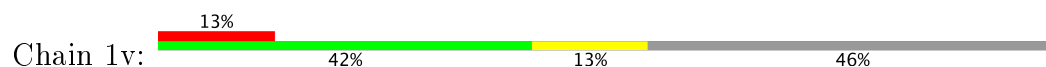


- Molecule 52: 30S ribosomal protein Thx





- Molecule 53: mRNA



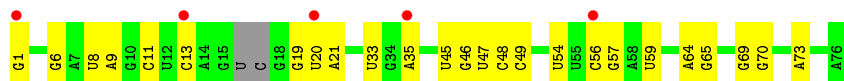
- Molecule 53: mRNA



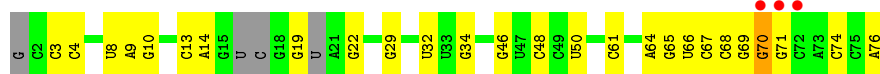
- Molecule 54: A-site and E-site tRNAs



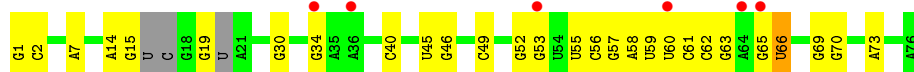
- Molecule 54: A-site and E-site tRNAs



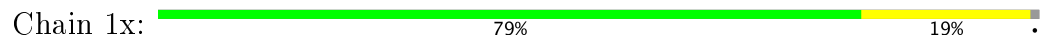
- Molecule 54: A-site and E-site tRNAs



- Molecule 54: A-site and E-site tRNAs

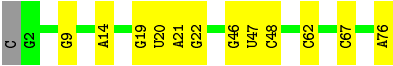
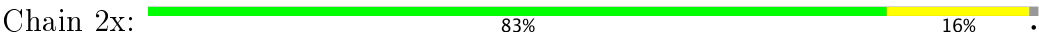


- Molecule 55: P-site tRNA





● Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.78Å 449.83Å 622.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.54 – 2.80 181.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (152.54-2.80) 94.0 (181.84-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.214 , 0.269 0.221 , 0.273	Depositor DCC
R_{free} test set	67418 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299109	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.50	0/69009	0.96	49/107712 (0.0%)
1	2A	0.39	0/67293	0.89	43/105034 (0.0%)
2	1B	0.45	1/2882 (0.0%)	0.88	0/4494
2	2B	0.40	1/2879 (0.0%)	0.92	2/4487 (0.0%)
3	1D	0.35	0/2186	0.55	0/2944
3	2D	0.34	0/2186	0.55	0/2944
4	1E	0.35	0/1592	0.56	0/2149
4	2E	0.30	0/1592	0.51	0/2149
5	1F	0.33	0/1619	0.53	0/2193
5	2F	0.31	0/1615	0.50	0/2188
6	1G	0.30	0/1448	0.49	0/1957
6	2G	0.29	0/1453	0.48	1/1963 (0.1%)
7	1H	0.33	0/1356	0.51	0/1834
7	2H	0.31	0/1356	0.49	1/1834 (0.1%)
8	1I	0.29	0/1112	0.48	0/1514
8	2I	0.28	0/1079	0.47	0/1475
9	1N	0.34	0/1144	0.50	0/1543
9	2N	0.28	0/1144	0.47	0/1543
10	1O	0.36	0/943	0.55	0/1269
10	2O	0.31	0/943	0.52	0/1269
11	1P	0.35	0/1152	0.55	0/1533
11	2P	0.31	0/1152	0.53	0/1533
12	1Q	0.33	0/1143	0.51	0/1527
12	2Q	0.29	0/1143	0.49	0/1527
13	1R	0.32	0/982	0.53	0/1312
13	2R	0.28	0/982	0.49	0/1312
14	1S	0.31	0/883	0.52	0/1176
14	2S	0.29	0/880	0.49	0/1172
15	1T	0.32	0/1105	0.51	0/1477
15	2T	0.28	0/1097	0.47	0/1468
16	1U	0.36	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.43	0/1301
17	1V	0.34	0/782	0.56	0/1049
17	2V	0.29	0/782	0.53	0/1049
18	1W	0.34	0/897	0.54	0/1205
18	2W	0.30	0/897	0.51	0/1205
19	1X	0.35	0/764	0.56	0/1025
19	2X	0.30	0/764	0.54	1/1025 (0.1%)
20	1Y	0.34	0/819	0.54	0/1095
20	2Y	0.32	0/819	0.51	0/1095
21	1Z	0.32	0/1267	0.52	0/1717
21	2Z	0.30	0/1299	0.51	0/1763
22	10	0.35	0/662	0.55	0/881
22	20	0.32	0/662	0.49	0/881
23	11	0.34	0/762	0.52	0/1014
23	21	0.31	0/762	0.54	0/1014
24	12	0.33	0/590	0.46	0/781
24	22	0.27	0/590	0.43	0/781
25	13	0.33	0/474	0.50	0/635
25	23	0.28	0/469	0.46	0/630
26	14	0.35	0/565	0.59	0/761
26	24	0.30	0/545	0.50	0/737
27	15	0.36	0/469	0.54	0/635
27	25	0.32	0/469	0.50	0/635
28	16	0.35	0/460	0.53	0/613
28	26	0.31	0/456	0.51	0/608
29	17	0.34	0/426	0.55	0/561
29	27	0.32	0/426	0.54	0/561
30	18	0.34	0/525	0.56	0/691
30	28	0.31	0/525	0.49	0/691
31	19	0.34	0/310	0.53	0/407
31	29	0.30	0/310	0.51	0/407
32	1a	0.36	0/35795	0.88	25/55864 (0.0%)
32	2a	0.36	2/35886 (0.0%)	0.90	38/56005 (0.1%)
33	1b	0.29	0/1881	0.47	0/2542
33	2b	0.30	0/1860	0.50	0/2518
34	1c	0.29	0/1572	0.47	0/2126
34	2c	0.29	0/1566	0.47	0/2119
35	1d	0.29	0/1685	0.46	0/2262
35	2d	0.29	0/1704	0.47	0/2284
36	1e	0.30	0/1145	0.49	0/1543
36	2e	0.29	0/1149	0.52	0/1548
37	1f	0.29	0/823	0.48	0/1115
37	2f	0.30	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.30	0/1250	0.46	0/1679
38	2g	0.28	0/1254	0.43	0/1683
39	1h	0.29	0/1108	0.47	0/1494
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.29	0/1002	0.47	0/1346
40	2i	0.29	0/997	0.49	0/1343
41	1j	0.27	0/722	0.47	0/982
41	2j	0.29	0/727	0.50	0/988
42	1k	0.27	0/844	0.47	0/1145
42	2k	0.27	0/848	0.47	0/1149
43	1l	0.31	0/937	0.52	0/1260
43	2l	0.30	0/937	0.55	0/1260
44	1m	0.28	0/969	0.46	0/1302
44	2m	0.28	0/961	0.49	0/1291
45	1n	0.31	0/501	0.47	0/664
45	2n	0.33	0/501	0.50	0/664
46	1o	0.27	0/739	0.42	0/985
46	2o	0.28	0/739	0.46	0/985
47	1p	0.28	0/697	0.50	0/939
47	2p	0.27	0/693	0.47	0/935
48	1q	0.28	0/836	0.48	0/1117
48	2q	0.29	0/836	0.47	0/1117
49	1r	0.30	0/560	0.46	0/746
49	2r	0.28	0/560	0.46	0/746
50	1s	0.29	0/667	0.52	0/900
50	2s	0.30	0/661	0.56	0/893
51	1t	0.28	0/730	0.48	0/965
51	2t	0.27	0/729	0.42	0/965
52	1u	0.28	0/203	0.50	0/266
52	2u	0.30	0/203	0.50	0/266
53	1v	0.38	0/310	0.88	0/480
53	2v	0.49	0/310	0.94	0/480
54	1w	0.51	1/1606 (0.1%)	1.05	5/2497 (0.2%)
54	1y	0.53	1/1606 (0.1%)	1.14	7/2497 (0.3%)
54	2w	0.47	0/1556	1.17	4/2418 (0.2%)
54	2y	0.54	1/1583 (0.1%)	1.09	2/2459 (0.1%)
55	1x	0.48	0/1725	1.09	12/2689 (0.4%)
55	2x	0.45	0/1725	1.09	10/2689 (0.4%)
All	All	0.40	7/316686 (0.0%)	0.83	200/474113 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	1	G	OP3-P	-10.33	1.48	1.61
54	1y	1	G	OP3-P	-10.31	1.48	1.61
54	2y	1	G	OP3-P	-10.09	1.49	1.61
2	1B	1	U	OP3-P	-10.05	1.49	1.61
2	2B	1	U	OP3-P	-10.04	1.49	1.61
32	2a	1272	G	C6-N1	-8.32	1.33	1.39
32	2a	1272	G	N1-C2	-7.58	1.31	1.37

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-O6	19.26	140.16	128.60
32	2a	1263	C	N1-C2-O2	17.07	129.14	118.90
32	2a	1272	G	N1-C2-N2	-15.02	102.68	116.20
32	2a	1272	G	N3-C2-N2	14.88	130.32	119.90
32	2a	1272	G	N1-C6-O6	-12.36	112.48	119.90
32	2a	1263	C	C2-N3-C4	12.03	125.92	119.90
32	2a	1263	C	N3-C2-O2	-10.82	114.32	121.90
1	2A	2136	C	N1-C2-O2	10.74	125.34	118.90
1	1A	1121	C	N1-C2-O2	10.30	125.08	118.90
32	1a	1025	U	N1-C2-O2	10.04	129.83	122.80
55	1x	46	G	C6-N1-C2	-9.76	119.25	125.10
55	2x	46	G	C6-N1-C2	-9.39	119.46	125.10
1	1A	1109	G	C5-C6-O6	9.36	134.22	128.60
2	2B	80	U	O4'-C1'-N1	9.05	115.44	108.20
32	2a	1263	C	C5-C4-N4	8.83	126.38	120.20
32	2a	1039	C	N1-C2-O2	8.79	124.18	118.90
1	1A	1121	C	C2-N3-C4	8.59	124.19	119.90
1	1A	537	G	O4'-C1'-N9	8.48	114.99	108.20
54	1y	64	A	N1-C6-N6	-8.42	113.55	118.60
1	2A	2136	C	N3-C2-O2	-8.36	116.05	121.90
32	2a	1272	G	C5-C6-N1	-8.29	107.35	111.50
1	2A	2473	U	C2-N1-C1'	8.26	127.61	117.70
32	2a	1272	G	C6-N1-C2	8.08	129.95	125.10
55	2x	14	A	C4-C5-C6	8.08	121.04	117.00
54	1y	33	U	C2-N1-C1'	7.97	127.26	117.70
54	1w	47	U	C2-N1-C1'	7.93	127.22	117.70
1	2A	2149	G	N3-C4-N9	7.93	130.76	126.00
1	1A	1045	U	O5'-P-OP2	-7.86	98.63	105.70
54	1y	64	A	C5-C6-N6	7.76	129.91	123.70
32	2a	1263	C	C6-N1-C2	-7.74	117.20	120.30
32	2a	1025	U	N1-C2-O2	7.71	128.19	122.80
32	2a	79	G	C5-C6-O6	7.69	133.21	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C2-N3-C4	-7.57	108.11	111.90
1	1A	12	U	C2-N1-C1'	7.47	126.66	117.70
55	2x	22	G	C5-N7-C8	-7.39	100.60	104.30
1	1A	1686	U	O5'-P-OP2	-7.38	99.06	105.70
32	1a	1030(B)	C	C2-N1-C1'	7.32	126.85	118.80
1	1A	2158	C	C2-N1-C1'	7.23	126.75	118.80
32	2a	1263	C	C5-C6-N1	7.23	124.61	121.00
32	1a	1025	U	N3-C2-O2	-7.21	117.15	122.20
55	2x	14	A	C5-N7-C8	7.20	107.50	103.90
55	1x	14	A	C4-C5-C6	7.03	120.51	117.00
54	1y	56	C	N1-C2-O2	7.01	123.11	118.90
32	1a	1030	C	N1-C2-O2	6.95	123.07	118.90
55	1x	22	G	N1-C6-O6	-6.93	115.74	119.90
32	2a	1272	G	C4-N9-C1'	6.89	135.46	126.50
32	1a	1025	U	C2-N1-C1'	6.83	125.90	117.70
55	1x	46	G	C5-C6-N1	6.79	114.90	111.50
1	1A	1109	G	C6-N1-C2	6.78	129.17	125.10
32	2a	1001(A)	G	N3-C2-N2	6.76	124.63	119.90
1	1A	2177	G	C5-C6-O6	-6.74	124.56	128.60
32	1a	1036	G	N3-C2-N2	-6.68	115.22	119.90
1	2A	801	G	O5'-P-OP2	-6.65	99.72	105.70
32	2a	1263	C	N3-C4-N4	-6.62	113.36	118.00
1	2A	1313	U	C2-N1-C1'	6.60	125.62	117.70
32	2a	1029	C	N1-C2-O2	6.57	122.84	118.90
32	1a	1027	C	N3-C4-C5	-6.53	119.29	121.90
55	2x	14	A	C5-C6-N1	-6.52	114.44	117.70
1	1A	2189	U	C2-N1-C1'	6.51	125.51	117.70
55	1x	14	A	C5-C6-N1	-6.49	114.45	117.70
1	2A	2142	C	C2-N1-C1'	6.43	125.88	118.80
55	2x	22	G	C4-C5-C6	-6.39	114.97	118.80
32	2a	754	C	C2-N1-C1'	6.37	125.81	118.80
55	1x	22	G	C5-N7-C8	-6.35	101.12	104.30
1	2A	504	U	C2-N1-C1'	6.35	125.32	117.70
1	1A	1121	C	C5-C4-N4	6.34	124.64	120.20
1	2A	2149	G	N9-C4-C5	-6.34	102.86	105.40
1	1A	2252	C	N1-C2-O2	6.32	122.69	118.90
55	2x	46	G	C5-C6-N1	6.30	114.65	111.50
1	1A	2177	G	N1-C6-O6	6.29	123.67	119.90
1	2A	1698	A	O4'-C1'-N9	6.26	113.21	108.20
1	1A	1359	U	C2-N1-C1'	6.25	125.20	117.70
55	1x	14	A	C5-N7-C8	6.21	107.01	103.90
32	2a	754	C	N1-C2-O2	6.21	122.63	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1109	G	N3-C2-N2	6.21	124.25	119.90
32	1a	1030(B)	C	N1-C2-O2	6.19	122.61	118.90
1	1A	2014	G	P-O3'-C3'	6.18	127.11	119.70
32	1a	1030	C	C2-N3-C4	6.14	122.97	119.90
1	1A	2158	C	N1-C2-O2	6.13	122.58	118.90
32	2a	1272	G	C8-N9-C1'	-6.13	119.03	127.00
55	1x	22	G	C4-C5-C6	-6.11	115.14	118.80
1	1A	894	U	C2-N1-C1'	6.09	125.00	117.70
1	2A	1614	A	O5'-P-OP1	-6.06	100.24	105.70
32	1a	1030(B)	C	C6-N1-C2	-6.05	117.88	120.30
32	2a	1025	U	N3-C2-O2	-6.03	117.98	122.20
54	1y	33	U	N1-C2-O2	6.03	127.02	122.80
1	1A	1121	C	N3-C2-O2	-6.02	117.68	121.90
1	1A	2858	G	O4'-C1'-N9	6.00	113.00	108.20
1	1A	599	U	O5'-P-OP1	-5.98	100.32	105.70
1	2A	2149	G	C8-N9-C1'	-5.93	119.29	127.00
1	2A	90	U	C2-N1-C1'	5.85	124.72	117.70
32	2a	1001(A)	G	N9-C4-C5	-5.82	103.07	105.40
1	1A	1321	A	N1-C6-N6	5.82	122.09	118.60
32	1a	1029	C	C2-N3-C4	5.82	122.81	119.90
1	1A	2189	U	N1-C2-O2	5.80	126.86	122.80
1	2A	2473	U	N1-C2-O2	5.80	126.86	122.80
1	1A	2158	C	C6-N1-C1'	-5.79	113.85	120.80
32	2a	1043	C	N1-C2-O2	5.79	122.38	118.90
1	2A	2149	G	C4-N9-C1'	5.79	134.03	126.50
32	2a	1039	C	C2-N3-C4	5.78	122.79	119.90
55	1x	22	G	C5-C6-N1	5.77	114.38	111.50
1	1A	1295	U	O5'-P-OP1	-5.76	100.51	105.70
1	1A	1219	A	OP1-P-O3'	5.76	117.88	105.20
32	1a	841	U	C5-C6-N1	5.75	125.57	122.70
1	1A	215	G	O4'-C1'-N9	5.74	112.79	108.20
55	2x	22	G	N3-C4-N9	-5.72	122.56	126.00
32	2a	1001(A)	G	N3-C4-N9	5.72	129.43	126.00
54	2w	67	C	C5-C4-N4	5.70	124.19	120.20
1	2A	614	U	N3-C2-O2	-5.70	118.21	122.20
2	2B	1	U	C2-N1-C1'	5.70	124.54	117.70
1	1A	2001	C	C6-N1-C2	-5.69	118.02	120.30
1	1A	892	G	O4'-C1'-N9	5.68	112.75	108.20
1	2A	2149	G	C6-C5-N7	-5.68	126.99	130.40
1	1A	1311	A	O5'-P-OP2	-5.67	100.60	105.70
32	1a	266	G	P-O3'-C3'	5.65	126.48	119.70
1	1A	1109	G	N1-C6-O6	-5.64	116.51	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1786	A	O4'-C1'-N9	5.64	112.72	108.20
32	2a	1030	C	N1-C2-O2	5.64	122.28	118.90
32	1a	1025	U	C6-N1-C1'	-5.63	113.32	121.20
55	2x	22	G	N3-C4-C5	5.59	131.40	128.60
32	1a	1067	A	P-O3'-C3'	5.58	126.40	119.70
54	2w	70	G	N3-C2-N2	-5.56	116.01	119.90
32	2a	266	G	N3-C4-C5	-5.55	125.83	128.60
54	1y	33	U	C6-N1-C1'	-5.54	113.44	121.20
1	2A	2136	C	C2-N1-C1'	5.52	124.87	118.80
1	2A	2473	U	C6-N1-C1'	-5.52	113.48	121.20
1	1A	2189	U	N3-C2-O2	-5.51	118.34	122.20
1	1A	1388	A	O5'-P-OP2	-5.51	100.74	105.70
55	1x	14	A	C4-N9-C1'	5.46	136.13	126.30
1	1A	840	A	O5'-P-OP2	-5.45	100.79	105.70
55	1x	14	A	C8-N9-C1'	-5.43	117.92	127.70
1	1A	1302	G	N9-C4-C5	-5.43	103.23	105.40
32	2a	1158	C	C2-N1-C1'	5.42	124.77	118.80
7	2H	98	LEU	CA-CB-CG	5.41	127.74	115.30
1	2A	928	G	C6-C5-N7	-5.41	127.16	130.40
1	1A	410	U	C2-N1-C1'	-5.40	111.22	117.70
1	2A	945	A	N1-C6-N6	5.40	121.84	118.60
54	1w	47	U	C5-C6-N1	5.39	125.40	122.70
1	1A	12	U	C5-C6-N1	5.39	125.39	122.70
54	1w	47	U	C6-N1-C1'	-5.38	113.66	121.20
1	2A	228	A	P-O3'-C3'	5.38	126.15	119.70
54	1w	3	C	C2-N1-C1'	5.37	124.71	118.80
1	2A	2142	C	N1-C2-O2	5.37	122.12	118.90
1	2A	2096	U	N1-C2-O2	5.37	126.56	122.80
54	1y	33	U	C5-C6-N1	5.37	125.38	122.70
1	2A	1992	G	P-O3'-C3'	5.36	126.13	119.70
55	2x	22	G	C8-N9-C1'	5.35	133.96	127.00
1	1A	1302	G	C8-N9-C1'	-5.34	120.05	127.00
6	2G	177	GLY	C-N-CA	-5.34	108.34	121.70
1	2A	383	U	O4'-C1'-N1	5.33	112.47	108.20
32	1a	687	A	P-O3'-C3'	5.32	126.09	119.70
1	2A	2335	A	O4'-C1'-N9	5.32	112.45	108.20
1	2A	928	G	N1-C6-O6	5.29	123.07	119.90
32	1a	975	A	O4'-C1'-N9	-5.29	103.97	108.20
1	2A	2149	G	C4-C5-N7	5.28	112.91	110.80
1	2A	2155	G	N9-C4-C5	-5.28	103.29	105.40
32	1a	115	G	P-O3'-C3'	5.27	126.03	119.70
1	2A	2163	C	C6-N1-C2	-5.27	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	7	A	C6-N1-C2	-5.26	115.44	118.60
32	1a	1065	U	P-O3'-C3'	5.26	126.01	119.70
1	2A	2174	C	N1-C2-O2	5.26	122.06	118.90
54	2y	66	U	C5-C4-O4	-5.26	122.74	125.90
1	2A	2848	G	O4'-C1'-N9	5.26	112.41	108.20
1	1A	1807	G	O5'-P-OP2	-5.24	100.98	105.70
32	1a	1030(B)	C	N3-C2-O2	-5.24	118.24	121.90
1	2A	1698	A	C6-C5-N7	-5.23	128.64	132.30
32	1a	1201	A	P-O3'-C3'	5.23	125.98	119.70
32	2a	266	G	P-O3'-C3'	5.23	125.97	119.70
1	1A	2803	A	C2-N3-C4	5.23	113.21	110.60
1	2A	2473	U	N3-C2-O2	-5.23	118.54	122.20
32	2a	1132	C	C2-N1-C1'	5.21	124.53	118.80
1	1A	2485	U	N3-C2-O2	-5.20	118.56	122.20
1	2A	986	C	C6-N1-C2	-5.19	118.22	120.30
32	1a	1036	G	C6-N1-C2	-5.18	121.99	125.10
1	1A	507	G	O4'-C1'-N9	5.18	112.34	108.20
1	2A	528	A	P-O3'-C3'	5.17	125.91	119.70
1	2A	901	A	N7-C8-N9	5.17	116.39	113.80
32	1a	1442	G	N3-C4-C5	-5.17	126.02	128.60
1	1A	1132	A	N1-C6-N6	-5.16	115.50	118.60
32	2a	1272	G	N1-C2-N3	5.16	127.00	123.90
32	1a	1027	C	C6-N1-C1'	5.14	126.97	120.80
54	2w	70	G	N9-C4-C5	5.13	107.45	105.40
1	2A	195	A	P-O3'-C3'	5.12	125.84	119.70
54	2w	10	G	C4-N9-C1'	5.11	133.15	126.50
1	1A	1359	U	N3-C2-O2	-5.11	118.63	122.20
1	1A	12	U	C6-N1-C1'	-5.09	114.07	121.20
1	2A	512	G	O4'-C1'-N9	5.09	112.27	108.20
1	1A	1700	G	C8-N9-C4	-5.09	104.36	106.40
32	2a	1125	U	C2-N1-C1'	5.08	123.80	117.70
54	1w	47	U	N1-C2-O2	5.07	126.35	122.80
32	2a	913	A	P-O3'-C3'	5.07	125.79	119.70
32	2a	1322	C	N1-C2-O2	-5.07	115.86	118.90
55	1x	46	G	N9-C4-C5	5.07	107.43	105.40
19	2X	57	LEU	CA-CB-CG	5.06	126.94	115.30
1	1A	1020	C	N1-C2-O2	-5.05	115.87	118.90
1	2A	2318	G	N3-C4-C5	-5.05	126.08	128.60
1	2A	504	U	N1-C2-O2	5.04	126.33	122.80
1	1A	2561	G	N1-C6-O6	5.03	122.92	119.90
32	2a	1442	G	P-O3'-C3'	5.02	125.72	119.70
32	1a	913	A	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31192	701	0
1	2A	60322	0	30423	818	0
2	1B	2577	0	1305	26	0
2	2B	2575	0	1303	44	0
3	1D	2136	0	2218	48	0
3	2D	2136	0	2218	50	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	39	0
5	1F	1584	0	1625	37	0
5	2F	1580	0	1619	45	0
6	1G	1423	0	1436	29	0
6	2G	1428	0	1438	45	0
7	1H	1330	0	1407	24	0
7	2H	1330	0	1407	44	0
8	1I	1097	0	1140	32	0
8	2I	1064	0	1082	22	0
9	1N	1117	0	1184	14	0
9	2N	1117	0	1184	23	0
10	1O	933	0	996	20	0
10	2O	933	0	996	23	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	37	0
12	1Q	1122	0	1179	27	0
12	2Q	1122	0	1179	32	0
13	1R	968	0	1033	20	0
13	2R	968	0	1033	22	0
14	1S	873	0	927	23	0
14	2S	870	0	923	37	0
15	1T	1091	0	1151	22	0
15	2T	1083	0	1136	27	0
16	1U	959	0	1019	18	0
16	2U	959	0	1019	26	0
17	1V	771	0	830	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	2V	771	0	830	10	0
18	1W	886	0	940	15	0
18	2W	886	0	940	14	0
19	1X	750	0	814	15	0
19	2X	750	0	814	18	0
20	1Y	806	0	881	15	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	16	0
21	2Z	1271	0	1273	39	0
22	10	653	0	674	19	0
22	20	653	0	674	19	0
23	11	755	0	826	15	0
23	21	755	0	826	23	0
24	12	588	0	643	9	0
24	22	588	0	643	13	0
25	13	469	0	518	13	0
25	23	464	0	514	12	0
26	14	552	0	533	13	0
26	24	532	0	503	23	0
27	15	455	0	465	9	0
27	25	455	0	465	14	0
28	16	453	0	473	9	0
28	26	449	0	469	9	0
29	17	418	0	467	9	0
29	27	418	0	467	18	0
30	18	517	0	582	18	0
30	28	517	0	582	19	0
31	19	307	0	335	7	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16339	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1184	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	277	0	140	0	0
53	2v	277	0	140	0	0
54	1w	1592	0	819	0	0
54	1y	1585	0	804	0	0
54	2w	1544	0	788	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	827	0	0
55	2x	1625	0	828	0	0
56	10	5	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	2	0	0	0	0
56	15	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	16	3	0	0	0	0
56	17	5	0	0	0	0
56	18	3	0	0	0	0
56	19	1	0	0	0	0
56	1A	1063	0	0	0	0
56	1B	38	0	0	0	0
56	1D	14	0	0	0	0
56	1E	13	0	0	0	0
56	1F	9	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	5	0	0	0	0
56	1O	7	0	0	0	0
56	1P	3	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	5	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	6	0	0	0	0
56	1V	3	0	0	0	0
56	1W	5	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	2	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	215	0	0	0	0
56	1b	2	0	0	0	0
56	1e	1	0	0	0	0
56	1f	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1p	1	0	0	0	0
56	1q	1	0	0	0	0
56	1r	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	11	0	0	0	0
56	1x	15	0	0	0	0
56	1y	4	0	0	0	0
56	20	3	0	0	0	0
56	21	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	23	1	0	0	0	0
56	25	3	0	0	0	0
56	27	2	0	0	0	0
56	28	2	0	0	0	0
56	2A	754	0	0	0	0
56	2B	21	0	0	0	0
56	2D	7	0	0	0	0
56	2E	10	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	4	0	0	0	0
56	2T	3	0	0	0	0
56	2U	6	0	0	0	0
56	2V	2	0	0	0	0
56	2W	3	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	233	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	4	0	0	0	0
56	2q	4	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	5	0	0	0	0
56	2w	9	0	0	0	0
56	2x	5	0	0	0	0
56	2y	7	0	0	0	0
57	1A	2	0	0	0	0
57	2A	2	0	0	0	0
58	1A	25	0	0	2	0
58	2A	25	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	10	0	0	0	0
61	11	7	0	0	0	0
61	12	2	0	0	0	0
61	13	4	0	0	0	0
61	15	5	0	0	1	0
61	16	2	0	0	0	0
61	17	9	0	0	1	0
61	18	7	0	0	1	0
61	1A	1433	0	0	74	0
61	1B	65	0	0	2	0
61	1D	24	0	0	0	0
61	1E	30	0	0	4	0
61	1F	10	0	0	4	0
61	1G	8	0	0	2	0
61	1H	1	0	0	0	0
61	1I	2	0	0	0	0
61	1N	6	0	0	1	0
61	1O	8	0	0	0	0
61	1P	18	0	0	1	0
61	1Q	12	0	0	0	0
61	1R	12	0	0	0	0
61	1S	4	0	0	0	0
61	1T	7	0	0	0	0
61	1U	9	0	0	0	0
61	1V	8	0	0	0	0
61	1W	8	0	0	0	0
61	1X	8	0	0	1	0
61	1Y	2	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	315	0	0	0	0
61	1b	1	0	0	0	0
61	1e	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	1f	1	0	0	0	0
6l	1g	1	0	0	0	0
6l	1j	1	0	0	0	0
6l	1l	6	0	0	0	0
6l	1m	1	0	0	0	0
6l	1n	1	0	0	0	0
6l	1q	3	0	0	0	0
6l	1u	1	0	0	0	0
6l	1v	6	0	0	0	0
6l	1w	20	0	0	0	0
6l	1x	14	0	0	0	0
6l	1y	2	0	0	0	0
6l	20	4	0	0	0	0
6l	21	8	0	0	0	0
6l	22	1	0	0	0	0
6l	23	1	0	0	0	0
6l	25	4	0	0	0	0
6l	26	1	0	0	0	0
6l	27	4	0	0	0	0
6l	28	4	0	0	0	0
6l	29	1	0	0	0	0
6l	2A	885	0	0	53	0
6l	2B	26	0	0	0	0
6l	2D	18	0	0	4	0
6l	2E	14	0	0	2	0
6l	2F	18	0	0	0	0
6l	2I	4	0	0	0	0
6l	2N	1	0	0	0	0
6l	2P	12	0	0	1	0
6l	2Q	2	0	0	0	0
6l	2R	2	0	0	0	0
6l	2T	6	0	0	0	0
6l	2U	3	0	0	0	0
6l	2V	1	0	0	0	0
6l	2W	3	0	0	0	0
6l	2X	1	0	0	0	0
6l	2Y	1	0	0	1	0
6l	2Z	2	0	0	0	0
6l	2a	258	0	0	0	0
6l	2c	1	0	0	0	0
6l	2d	3	0	0	0	0
6l	2e	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	4	0	0	0	0
61	2l	6	0	0	0	0
61	2o	1	0	0	0	0
61	2p	2	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	5	0	0	0	0
61	2u	1	0	0	0	0
61	2v	2	0	0	0	0
61	2w	2	0	0	0	0
61	2x	6	0	0	0	0
61	2y	18	0	0	0	0
All	All	299109	0	196685	2479	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2479) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2158:C:N4	1:1A:2177:G:H1	1.36	1.21
1:2A:2136:C:N4	1:2A:2155:G:H1	1.46	1.12
1:2A:2129:C:N4	1:2A:2159:G:H1	1.49	1.10
1:1A:1128:U:H3	1:1A:1132:A:N6	1.48	1.09
1:1A:2149:G:H1	1:1A:2183:C:N4	1.54	1.05
1:2A:2138:C:N4	1:2A:2153:G:H1	1.56	1.03
1:2A:1002:G:H1	1:2A:1038:C:N4	42.97	1.02
1:2A:2129:C:H42	1:2A:2159:G:H1	1.04	0.97
1:1A:1128:U:O4	1:1A:1132:A:N1	1.99	0.95
1:2A:2114:A:N6	1:2A:2119:A:N7	2.15	0.95
1:1A:1100:A:N6	1:1A:1151:U:H3	1.65	0.94
1:2A:1002:G:H1	1:2A:1038:C:H42	43.27	0.94
1:2A:2129:C:N3	1:2A:2159:G:N2	2.17	0.92
11:2P:39:LYS:HB2	11:2P:45:LEU:HG	1.50	0.90
1:1A:1100:A:H61	1:1A:1151:U:H3	1.16	0.89
1:1A:2158:C:N3	1:1A:2177:G:N2	2.20	0.89
1:1A:2149:G:H1	1:1A:2183:C:H42	0.88	0.88
1:2A:2143:C:H42	1:2A:2148:G:H1	1.20	0.87
1:2A:2807:G:N1	1:2A:2893:G:O6	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1004:A:N6	1:1A:1037:C:N3	55.45	0.86
1:2A:2136:C:N4	1:2A:2155:G:N1	2.23	0.86
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.09	0.85
1:2A:2138:C:H42	1:2A:2153:G:H1	0.86	0.85
1:1A:1111:U:O2	1:1A:1119:A:N6	2.08	0.85
29:17:24:THR:HG22	29:17:27:GLY:H	1.39	0.85
1:2A:2108:C:H42	1:2A:2181:G:H1	1.19	0.85
1:2A:1422:G:H5"	10:2O:48:PRO:HB3	99.35	0.85
1:1A:656:A:OP1	11:1P:65:ARG:NH1	2.09	0.85
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.58	0.84
20:1Y:92:ASN:HB3	20:1Y:94:LYS:H	1.42	0.84
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.42	0.84
1:2A:2308:G:O6	1:2A:2311:A:N6	2.12	0.83
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.12	0.83
1:2A:2136:C:N3	1:2A:2155:G:N2	2.26	0.83
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.60	0.82
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.14	0.82
1:1A:1118:C:O2	1:1A:1138:C:N4	2.12	0.82
1:1A:1140:U:H1'	1:1A:1143:U:H5	1.44	0.82
1:1A:1117:G:O6	1:1A:1146:C:N4	2.13	0.82
25:13:6:VAL:HG13	25:13:54:VAL:HG11	1.60	0.82
1:1A:2121:U:H3	1:1A:2212:G:H1	1.28	0.82
1:1A:2149:G:N2	1:1A:2183:C:N3	2.27	0.82
1:1A:1104:G:H1	1:1A:1126:C:N4	1.77	0.81
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.63	0.80
1:2A:2136:C:H42	1:2A:2155:G:H1	1.26	0.80
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.63	0.80
1:1A:1001:G:O6	61:1A:4119:HOH:O	1.99	0.80
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.62	0.80
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.14	0.80
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.63	0.79
1:2A:821:A:N1	61:2A:3845:HOH:O	2.15	0.79
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.15	0.79
1:1A:2695:C:O2	10:1O:70:LYS:NZ	2.12	0.79
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.62	0.79
1:1A:641:G:OP1	5:1F:40:GLN:NE2	2.16	0.79
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.63	0.79
1:2A:975:C:OP1	61:2A:3830:HOH:O	2.00	0.78
1:1A:2387:G:N7	61:1A:4143:HOH:O	2.16	0.78
1:2A:2345:G:H4'	1:2A:2346:A:H5"	1.64	0.78
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.13	0.78
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.67	0.77
1:2A:2287:A:H62	1:2A:2344:U:H3	1.32	0.77
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.55	0.77
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.67	0.77
1:2A:1204:A:H2	1:2A:1241:A:H62	1.30	0.77
2:2B:20:C:N4	2:2B:63:G:O6	2.16	0.77
1:1A:1110:C:N3	1:1A:1120:G:O6	2.18	0.77
1:2A:529:A:N6	1:2A:2041:U:O2	2.18	0.77
3:2D:228:PRO:O	61:2D:401:HOH:O	2.01	0.76
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.65	0.76
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.18	0.76
1:2A:1171:G:H1	1:2A:1178:C:H42	1.31	0.76
1:1A:641:G:OP2	5:1F:43:LYS:NZ	2.19	0.76
1:1A:973:G:N7	61:1A:4152:HOH:O	2.18	0.76
1:1A:2162:C:N3	1:1A:2173:G:O6	2.17	0.76
1:1A:1056:A:OP2	61:1A:4120:HOH:O	2.02	0.76
1:1A:2562:G:OP1	61:1A:4122:HOH:O	2.04	0.76
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.19	0.76
6:2G:44:GLY:HA2	6:2G:88:ILE:HB	1.68	0.76
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	1.68	0.75
1:1A:479:C:OP1	61:1A:4121:HOH:O	2.03	0.75
12:1Q:75:THR:HG21	12:1Q:87:LYS:HE3	1.69	0.75
1:2A:2127:G:N2	1:2A:2161:C:N3	2.34	0.75
1:1A:359:C:H4'	20:1Y:73:ARG:HD3	1.67	0.75
1:2A:1689:A:H62	1:2A:1698:A:H2	1.34	0.75
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.69	0.75
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.69	0.75
1:2A:1363:C:OP1	23:21:61:ARG:NH1	2.20	0.75
1:2A:1002:G:N2	1:2A:1038:C:N3	42.23	0.75
1:1A:2164:C:N3	1:1A:2171:G:O6	2.19	0.75
2:2B:87:G:N2	2:2B:90:A:OP2	2.19	0.75
1:1A:2143:G:H1	1:1A:2199:C:H42	1.31	0.75
1:2A:2138:C:N3	1:2A:2153:G:N2	2.29	0.75
2:2B:8:U:N3	2:2B:113:G:O6	2.15	0.75
1:1A:325:G:OP2	20:1Y:84:ARG:NH2	2.19	0.74
1:2A:2721:A:OP1	61:2A:3831:HOH:O	2.05	0.74
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.70	0.74
1:2A:1651:G:OP1	13:2R:40:LYS:NZ	2.20	0.74
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.22	0.74
2:2B:4:C:H42	2:2B:117:G:H1	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:54:GLY:N	26:14:55:ARG:HA	2.02	0.74
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.70	0.74
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.53	0.74
1:2A:761:A:N7	61:2A:3866:HOH:O	2.20	0.74
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.20	0.74
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.21	0.74
12:2Q:109:VAL:HG13	12:2Q:113:GLN:HB3	1.70	0.73
1:1A:1057:G:OP1	16:1U:77:SER:OG	2.05	0.73
22:10:11:ARG:O	22:10:14:ARG:NH2	2.22	0.73
1:1A:1896:G:OP1	61:1A:4124:HOH:O	2.07	0.73
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.21	0.73
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.22	0.72
1:1A:2460:A:OP1	61:1A:4101:HOH:O	2.06	0.72
1:2A:962:G:OP1	61:2A:3812:HOH:O	2.06	0.72
18:1W:65:LEU:HD12	18:1W:68:ARG:HE	1.54	0.72
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.21	0.72
1:1A:2604:G:OP1	61:1A:4123:HOH:O	2.06	0.72
1:1A:2804:C:H2'	1:1A:2805:G:H8	1.55	0.72
1:1A:625:G:O2'	1:1A:702:A:N6	2.23	0.72
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.05	0.72
5:1F:72:ARG:O	61:1F:401:HOH:O	2.08	0.72
7:1H:25:LYS:HD3	7:1H:27:LYS:HE3	1.69	0.72
1:1A:183:G:N7	61:1A:4172:HOH:O	2.21	0.72
17:2V:72:VAL:HG13	17:2V:85:LYS:HB2	1.70	0.72
1:2A:2134:A:OP2	1:2A:2157:G:N2	2.22	0.72
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.72	0.72
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.18	0.72
1:1A:928:G:N2	1:1A:943:C:O2	2.23	0.71
4:2E:127:ASP:OD2	61:2E:401:HOH:O	2.07	0.71
1:1A:1829:U:OP2	3:1D:274:ARG:NH2	2.22	0.71
1:1A:931:C:H42	1:1A:938:G:H1	1.39	0.71
1:2A:2129:C:N4	1:2A:2159:G:N1	2.25	0.71
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.25	0.71
22:10:10:THR:HG22	22:10:12:ASN:H	1.54	0.71
1:1A:303:C:H42	1:1A:385:G:H1	1.39	0.71
2:2B:33:G:H5'	6:2G:2:PRO:HD3	1.72	0.71
1:2A:2127:G:N1	1:2A:2161:C:N4	2.38	0.71
4:2E:48:GLN:HE21	4:2E:78:LEU:HG	1.56	0.71
11:1P:42:SER:O	61:1P:301:HOH:O	2.09	0.71
1:2A:2513:G:N2	4:2E:143:ASN:OD1	2.24	0.71
1:2A:1530:C:H42	1:2A:1539:G:H1	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:66:ASN:HD21	16:2U:70:ARG:HH21	1.39	0.71
1:2A:271(H):G:H1	1:2A:271(P):C:H42	1.39	0.71
1:2A:1434:A:H61	1:2A:1558:A:H62	1.39	0.70
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.08	0.70
1:2A:2143:C:N4	1:2A:2148:G:H1	1.88	0.70
1:2A:2108:C:N4	1:2A:2181:G:H1	1.89	0.70
1:1A:1104:G:N2	1:1A:1126:C:N3	2.37	0.70
1:1A:1299:A:N7	61:1A:4140:HOH:O	2.23	0.70
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.73	0.70
1:1A:1275:G:N7	61:1A:4191:HOH:O	2.24	0.70
1:1A:1552:C:H2'	1:1A:1553:A:H8	1.57	0.70
1:1A:556:C:OP2	61:1A:4125:HOH:O	2.08	0.70
1:2A:1971:A:OP1	61:2A:3832:HOH:O	2.09	0.70
1:2A:307:G:N1	1:2A:310:A:OP2	2.25	0.70
1:1A:692:C:H42	1:1A:698:G:H1	1.39	0.70
1:1A:739:C:O2'	3:1D:38:LYS:NZ	2.25	0.70
5:1F:61:GLY:O	61:1F:402:HOH:O	2.09	0.70
1:1A:2331:G:H22	14:1S:3:ARG:HD3	1.57	0.70
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.24	0.70
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.72	0.70
1:2A:2789:C:O2	1:2A:2894:G:N2	2.25	0.69
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.25	0.69
21:2Z:97:GLU:HB3	21:2Z:125:LEU:HD11	1.74	0.69
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.24	0.69
1:2A:2171:A:N3	1:2A:2172:U:N3	2.39	0.69
20:1Y:11:ASP:N	20:1Y:11:ASP:OD1	2.21	0.69
1:2A:2114:A:N6	1:2A:2115:G:H21	1.89	0.69
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.73	0.69
1:1A:2672:A:N7	7:1H:175:LYS:NZ	2.40	0.69
1:2A:993:G:N7	1:2A:1213:A:N6	49.03	0.69
1:2A:2169:A:H2'	1:2A:2170:A:C8	2.27	0.69
1:1A:1219:A:H4'	1:1A:1220:U:OP1	1.92	0.69
1:1A:2164:C:O2	1:1A:2171:G:N1	2.25	0.69
20:1Y:20:TYR:HB3	20:1Y:23:ARG:HG3	1.73	0.69
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.26	0.69
1:1A:1990:G:OP1	61:1A:4126:HOH:O	2.09	0.69
22:20:10:THR:HG22	22:20:12:ASN:H	1.58	0.69
1:2A:2494:G:H2'	1:2A:2495:G:H8	1.57	0.69
1:1A:646:A:OP2	11:1P:108:LYS:NZ	2.26	0.69
1:2A:2518:A:OP2	61:2A:3834:HOH:O	2.10	0.69
1:1A:1069:U:OP2	61:1A:4109:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.25	0.69
7:2H:125:VAL:HG12	7:2H:131:VAL:HG22	1.75	0.69
8:2I:92:VAL:HG22	8:2I:120:ILE:HB	1.74	0.69
1:1A:889:G:N7	61:1A:4195:HOH:O	2.25	0.69
1:2A:1169:G:N2	1:2A:1181:C:O2	2.26	0.69
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.25	0.69
7:2H:86:GLU:OE2	7:2H:130:ARG:NH1	2.25	0.69
1:2A:2010:G:OP1	61:2A:3833:HOH:O	2.10	0.68
8:2I:43:ASN:ND2	23:21:75:GLU:OE2	2.26	0.68
1:1A:1310:G:OP1	27:15:19:ARG:NH2	2.27	0.68
1:1A:1813:C:OP1	61:1A:4128:HOH:O	2.11	0.68
1:2A:775:G:O3'	61:2A:3835:HOH:O	2.10	0.68
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.76	0.68
1:1A:880:U:O2	11:1P:55:ARG:NH2	2.25	0.68
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.12	0.68
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	1.74	0.68
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.76	0.68
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.74	0.68
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.73	0.68
2:2B:22:U:H3	2:2B:61:G:H1	1.40	0.68
1:1A:1108:G:H1	1:1A:1123:A:H61	1.40	0.68
5:1F:13:SER:OG	5:1F:127:GLU:OE1	2.10	0.68
20:1Y:54:LYS:HA	20:1Y:56:PRO:HD3	1.74	0.68
12:1Q:138:ASP:OD1	12:1Q:138:ASP:N	2.24	0.68
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.27	0.68
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.20	0.68
1:2A:659:C:H2'	1:2A:660:G:H8	1.59	0.68
1:1A:2849:G:H5'	13:1R:46:GLY:HA2	1.76	0.67
24:22:1:MET:N	24:22:52:ASP:OD1	2.26	0.67
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.10	0.67
61:1A:4108:HOH:O	4:1E:135:HIS:NE2	2.27	0.67
1:1A:1232:G:O6	61:1A:4127:HOH:O	2.11	0.67
1:1A:988:U:OP2	61:1A:4129:HOH:O	2.12	0.67
6:1G:125:PHE:O	61:1G:3101:HOH:O	2.12	0.67
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.27	0.67
1:1A:1202:A:OP2	61:1A:4130:HOH:O	2.12	0.67
1:2A:2031:A:N3	1:2A:2455:G:O2'	2.28	0.67
1:1A:1128:U:C4	1:1A:1132:A:N1	2.63	0.67
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.77	0.67
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.29	0.67
7:2H:98:LEU:HA	7:2H:103:LEU:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1132:A:O2'	1:1A:1133:G:N7	2.27	0.67
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.27	0.67
1:2A:731:C:OP2	61:2A:3836:HOH:O	2.12	0.67
1:1A:1310:G:N7	61:1A:4206:HOH:O	2.28	0.67
1:1A:927:G:H2'	1:1A:928:G:H8	1.60	0.67
1:2A:1345:C:OP2	61:2A:3837:HOH:O	2.12	0.67
1:1A:1700:G:H3'	13:1R:2:ARG:HD3	1.77	0.67
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.77	0.67
1:1A:2831:A:OP2	61:1A:4117:HOH:O	2.12	0.67
4:2E:11:MET:HG2	4:2E:24:THR:HB	1.77	0.67
1:2A:1422:G:O3'	10:2O:49:ARG:NH1	99.45	0.67
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.26	0.67
1:2A:1022:G:N2	1:2A:1023:U:O4	2.28	0.66
3:2D:152:GLY:O	61:2D:402:HOH:O	2.14	0.66
1:1A:1485:A:OP1	61:1A:4135:HOH:O	2.14	0.66
1:1A:2058:C:OP1	61:1A:4125:HOH:O	2.13	0.66
3:2D:232:PRO:O	61:2D:403:HOH:O	2.14	0.66
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.60	0.66
14:2S:67:ARG:HG2	14:2S:71:ARG:HD2	1.78	0.66
1:1A:1020:C:OP1	61:1A:4134:HOH:O	2.14	0.66
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.78	0.66
1:1A:1139:G:H3'	1:1A:1140:U:H5''	1.78	0.66
1:1A:2239:A:OP2	61:1A:4138:HOH:O	2.14	0.66
1:1A:2641:A:O2'	1:1A:2642:G:OP2	2.13	0.66
1:1A:925:A:N6	1:1A:945:A:O2'	2.26	0.66
2:1B:58:A:OP2	61:1B:301:HOH:O	2.12	0.66
2:2B:41:U:H5	6:2G:70:VAL:H	1.43	0.66
4:1E:122:PHE:O	61:1E:401:HOH:O	2.14	0.65
1:2A:1762:A:N1	61:2A:3903:HOH:O	2.28	0.65
1:1A:1138:C:H2'	1:1A:1139:G:H5'	1.78	0.65
1:1A:992:G:OP2	61:1A:4137:HOH:O	2.14	0.65
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.78	0.65
6:2G:18:GLU:HG2	6:2G:175:LEU:HD21	1.78	0.65
12:2Q:55:VAL:HG12	12:2Q:64:ILE:HD12	1.78	0.65
26:24:16:CYS:SG	26:24:17:GLY:N	2.70	0.65
1:2A:2141:G:O6	1:2A:2150:U:O2	2.13	0.65
14:2S:68:GLN:HA	14:2S:71:ARG:HD3	1.78	0.65
19:2X:61:GLY:N	19:2X:75:ASP:OD1	2.26	0.65
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.30	0.65
1:1A:1355:G:H4'	29:17:7:PRO:HB2	1.79	0.65
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2094:G:O6	61:1A:4131:HOH:O	2.13	0.65
1:2A:1920:4OC:HM22	1:2A:1921:G:H5'	1.79	0.65
1:1A:857:U:OP1	61:1A:4140:HOH:O	2.14	0.65
1:2A:563:G:OP2	61:2A:3842:HOH:O	2.14	0.65
1:2A:789:A:N1	61:2A:3911:HOH:O	2.29	0.65
6:2G:135:LEU:HD21	6:2G:157:ILE:HD12	1.77	0.65
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.79	0.65
1:1A:133:G:N7	61:1A:4216:HOH:O	2.29	0.65
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.78	0.65
22:20:11:ARG:O	22:20:14:ARG:NH2	2.28	0.65
1:2A:1019:U:H2'	1:2A:1020:A:C8	2.32	0.65
1:2A:826:U:H4'	11:2P:55:ARG:HB3	1.79	0.65
1:1A:1285:G:OP1	61:1A:4132:HOH:O	2.13	0.65
1:1A:1684:A:OP1	61:1A:4139:HOH:O	2.14	0.65
1:1A:2717:A:N3	61:1A:4218:HOH:O	2.29	0.65
1:2A:571:A:OP2	61:2A:3838:HOH:O	2.14	0.65
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.78	0.65
1:2A:1119:C:H2'	1:2A:1120:G:C8	3.65	0.64
1:2A:2582:G:OP2	61:2A:3841:HOH:O	2.14	0.64
1:1A:2227:G:H3'	1:1A:2228:G:C8	2.33	0.64
12:2Q:17:LEU:HD21	12:2Q:41:TRP:HE1	1.62	0.64
1:1A:131:C:O2	1:1A:231:G:N2	72.21	0.64
1:1A:2182:G:O6	1:1A:2183:C:N4	2.30	0.64
1:2A:1958:C:OP2	61:2A:3844:HOH:O	2.15	0.64
1:2A:900:A:H2'	1:2A:901:A:H8	1.63	0.64
18:2W:67:ASP:N	18:2W:67:ASP:OD1	2.24	0.64
1:1A:449:A:OP2	61:1A:4133:HOH:O	2.13	0.64
1:1A:83:A:H5''	20:1Y:8:LYS:HG2	1.78	0.64
16:1U:104:GLN:HE21	16:1U:105:VAL:HG23	1.62	0.64
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.79	0.64
18:2W:73:ALA:HB3	18:2W:106:ILE:HD12	1.80	0.64
1:1A:1099:C:H42	1:1A:1152:G:H1	1.45	0.64
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.79	0.64
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.79	0.64
1:1A:2124:U:H3	1:1A:2209:G:H1	1.44	0.64
1:1A:865:G:OP2	61:1A:4127:HOH:O	2.15	0.64
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	1.79	0.64
1:2A:1920:4OC:O5'	1:2A:1920:4OC:H6	1.98	0.64
1:1A:1313:U:OP1	61:1A:4141:HOH:O	2.15	0.64
1:1A:238:C:O2	30:18:12:LYS:NZ	2.20	0.64
2:2B:28:C:N4	2:2B:56:G:O6	2.20	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:51:G:N7	14:1S:62:LYS:NZ	2.41	0.64
20:1Y:43:ASN:HB3	20:1Y:65:ALA:HB3	1.80	0.64
1:2A:2134:A:O2'	1:2A:2159:G:N2	2.30	0.64
1:1A:1104:G:N1	1:1A:1126:C:N4	2.41	0.64
1:2A:1937:A:OP1	61:2A:3846:HOH:O	2.15	0.64
1:2A:784:A:OP1	61:2A:3840:HOH:O	2.14	0.64
1:1A:555:G:N1	1:1A:2045:G:OP1	2.28	0.63
1:2A:907:U:H4'	12:2Q:101:ARG:HH22	1.63	0.63
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.79	0.63
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.81	0.63
21:2Z:52:SER:OG	21:2Z:54:HIS:ND1	2.29	0.63
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.30	0.63
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.31	0.63
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.79	0.63
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.62	0.63
7:2H:20:ALA:HB2	7:2H:25:LYS:HG2	1.80	0.63
15:2T:59:THR:HG23	15:2T:78:LEU:HB3	1.79	0.63
1:1A:1221:G:H1'	1:1A:1222:A:H5'	1.80	0.63
6:1G:170:ARG:NH2	6:1G:182:LYS:O	2.30	0.63
1:1A:1040:C:OP2	16:1U:54:LYS:NZ	2.30	0.63
19:1X:11:PRO:HB3	19:1X:92:LEU:HD11	1.79	0.63
1:2A:2143:C:H2'	1:2A:2144:U:O4'	1.98	0.63
1:2A:586:A:N1	1:2A:809:G:O2'	2.31	0.63
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.34	0.63
1:2A:2121:G:H1	1:2A:2177:C:N4	1.96	0.63
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.31	0.63
4:2E:24:THR:HG23	4:2E:184:VAL:HG13	1.81	0.63
5:1F:75:HIS:ND1	61:1F:404:HOH:O	2.31	0.63
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.64	0.63
1:2A:2781:A:H5''	1:2A:2782:G:H5'	1.81	0.63
1:1A:2013:U:H2'	1:1A:2014:G:H5''	1.80	0.62
26:24:24:THR:OG1	26:24:25:TYR:N	2.32	0.62
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.81	0.62
28:16:13:CYS:SG	28:16:47:THR:HG21	2.38	0.62
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.33	0.62
1:2A:531:C:OP1	1:2A:561:G:N1	2.32	0.62
1:1A:1140:U:H1'	1:1A:1143:U:C5	2.32	0.62
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.33	0.62
1:2A:2431:U:OP1	61:2A:3849:HOH:O	2.16	0.62
6:2G:60:LEU:HD21	6:2G:92:VAL:HG11	1.82	0.62
1:1A:1087:C:H42	1:1A:1160:G:H1	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2227:G:H3'	1:1A:2228:G:H8	1.63	0.62
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.81	0.62
1:2A:852:G:H2'	1:2A:853:G:H8	1.64	0.62
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.32	0.62
1:1A:1827:U:H2'	1:1A:1828:C:C6	2.34	0.62
1:1A:2156:A:OP1	1:1A:2178:G:N2	2.33	0.62
1:1A:976:G:OP2	1:1A:1358:U:O2'	101.79	0.62
11:2P:62:LEU:O	30:28:13:ARG:NH1	2.33	0.62
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.15	0.62
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.00	0.62
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.81	0.62
5:2F:18:ARG:NH2	5:2F:127:GLU:OE2	2.32	0.62
1:1A:92:C:H2'	1:1A:93:G:C8	3.51	0.62
1:1A:2324:U:H5'	6:1G:88:ILE:HD11	1.80	0.62
10:1O:21:CYS:HB2	10:1O:39:ILE:HD12	1.82	0.62
1:2A:2099:U:H3	1:2A:2190:G:H1	1.46	0.62
1:1A:2172:U:N3	1:1A:2173:G:N7	2.47	0.61
1:1A:831:A:O4'	3:1D:227:ASN:ND2	2.33	0.61
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.82	0.61
11:2P:39:LYS:NZ	61:2P:3101:HOH:O	2.25	0.61
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.34	0.61
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.31	0.61
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.36	0.61
1:2A:441:U:O2	5:2F:46:ARG:NH2	2.32	0.61
3:2D:51:VAL:HG11	3:2D:54:ARG:HE	1.63	0.61
1:1A:1831:C:OP2	3:1D:183:ARG:NH2	2.34	0.61
3:2D:20:ASP:N	3:2D:20:ASP:OD1	2.31	0.61
26:14:15:ILE:O	26:14:33:VAL:N	2.34	0.61
5:1F:44:ARG:NH1	61:1F:403:HOH:O	2.23	0.61
1:2A:2471:C:N4	1:2A:2476:A:O2'	2.31	0.61
1:2A:1310:G:H2'	1:2A:1311:G:H8	3.42	0.61
2:2B:21:G:H1	2:2B:62:C:H42	1.48	0.61
7:2H:23:ARG:NH1	7:2H:34:GLU:OE1	2.34	0.61
23:11:59:THR:O	23:11:91:LYS:NZ	2.24	0.61
1:1A:2825:C:H5'	27:15:29:THR:HG21	1.81	0.61
23:21:46:LEU:HD13	23:21:61:ARG:HD3	1.83	0.61
30:28:28:GLY:O	30:28:36:LYS:NZ	2.29	0.61
25:13:10:LYS:NZ	25:13:15:TYR:OH	2.34	0.61
1:1A:2401:G:H5''	1:1A:2402:U:H5'	1.83	0.61
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.13	0.61
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1633:A:H2'	1:1A:1634:C:C6	2.36	0.60
1:1A:2889:C:OP2	61:1A:4144:HOH:O	2.16	0.60
8:1I:69:LYS:HG3	8:1I:138:ILE:HG12	1.81	0.60
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.16	0.60
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.36	0.60
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.24	0.60
1:1A:1405:A:H2	1:1A:1418:U:O4	1.83	0.60
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.83	0.60
1:2A:10:G:H1'	1:2A:2801(A):A:H62	1.66	0.60
1:2A:509:C:OP1	61:2A:3850:HOH:O	2.16	0.60
14:2S:11:LYS:HE3	14:2S:15:ARG:HH12	1.66	0.60
1:1A:2178:G:H2'	1:1A:2179:G:C2	2.36	0.60
1:2A:1309:G:H4'	29:27:7:PRO:HB2	1.82	0.60
6:2G:48:GLU:O	6:2G:51:ARG:NH1	2.34	0.60
1:1A:1109:G:N2	1:1A:1122:C:O2'	2.34	0.60
1:2A:1653:G:O6	13:2R:11:ASN:ND2	2.34	0.60
2:2B:45:A:O4'	6:2G:95:ARG:NH1	2.35	0.60
2:1B:113:G:N2	14:1S:45:GLY:O	2.26	0.60
1:1A:1040:C:OP1	16:1U:53:ARG:NH2	2.34	0.60
1:1A:2163:G:C4	1:1A:2164:C:H1'	2.36	0.60
1:2A:2250:G:C8	1:2A:2496:C:H5''	2.36	0.60
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.34	0.60
1:1A:2801:C:OP1	4:1E:61:ARG:NH2	2.35	0.60
1:1A:639:G:N2	5:1F:44:ARG:O	2.34	0.60
5:2F:20:LEU:HD13	5:2F:125:LEU:HD22	1.83	0.60
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.65	0.60
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.67	0.60
7:2H:121:ILE:HD11	7:2H:140:LYS:HG2	1.83	0.60
1:2A:1423:G:P	10:2O:49:ARG:HH12	97.19	0.60
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.35	0.60
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.36	0.60
1:2A:1286:A:H8	1:2A:1287:A:H4'	8.01	0.60
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.20	0.60
1:2A:2342:C:O2'	1:2A:2374:C:OP1	2.19	0.60
21:2Z:124:ILE:HD13	21:2Z:163:LEU:HD11	1.84	0.60
1:1A:2457:G:OP1	5:1F:74:ARG:NH2	2.35	0.59
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.02	0.59
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.24	0.59
1:2A:816:C:OP2	61:2A:3854:HOH:O	2.17	0.59
7:2H:84:SER:HB3	7:2H:132:ARG:HH11	1.67	0.59
20:2Y:94:LYS:NZ	61:2Y:601:HOH:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1577:C:H42	1:1A:1586:G:H1	1.49	0.59
1:2A:2432:A:OP2	61:2A:3851:HOH:O	2.17	0.59
1:2A:2052:G:H4'	4:2E:143:ASN:O	2.02	0.59
5:2F:145:GLU:OE1	5:2F:145:GLU:N	2.35	0.59
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.67	0.59
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.35	0.59
1:2A:222:A:OP1	61:2A:3848:HOH:O	2.16	0.59
1:2A:900:A:O2'	1:2A:901:A:OP1	2.17	0.59
5:2F:149:ASP:OD1	5:2F:149:ASP:N	2.30	0.59
11:1P:50:ARG:HD3	30:18:7:HIS:HD2	1.64	0.59
1:1A:1714:G:O2'	1:1A:2013:U:O4	2.19	0.59
31:29:17:ILE:HD12	31:29:26:ILE:HD11	1.84	0.59
1:2A:2659:G:N7	61:2A:3917:HOH:O	2.31	0.59
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.83	0.59
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.31	0.59
1:2A:800:A:OP1	1:2A:800:A:H8	1.86	0.59
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.85	0.59
16:2U:50:ARG:HH22	17:2V:72:VAL:HB	1.68	0.59
21:2Z:130:PRO:HA	21:2Z:133:ILE:HG13	1.84	0.59
1:1A:1539:C:N4	1:1A:2227:G:O2'	2.36	0.59
1:1A:2600:G:OP1	61:1A:4146:HOH:O	2.17	0.59
1:2A:2074:U:O4	61:2A:3839:HOH:O	2.14	0.59
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.21	0.59
1:1A:2140:U:H6	1:1A:2170:G:HO2'	1.51	0.59
1:1A:929:G:H1	1:1A:940:C:H42	1.51	0.59
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.33	0.59
1:2A:740:U:OP1	61:2A:3856:HOH:O	2.17	0.59
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	1.84	0.59
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	1.85	0.59
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.83	0.59
1:1A:1288:A:N1	11:1P:2:LYS:NZ	2.51	0.59
1:1A:1997:G:OP2	61:1A:4147:HOH:O	2.17	0.59
7:1H:97:ARG:NH2	7:1H:104:GLU:OE1	2.35	0.59
1:2A:1183:G:H5''	25:23:30:ARG:HH22	1.67	0.59
11:2P:50:ARG:HD3	30:28:7:HIS:HD2	1.68	0.59
1:2A:2690:C:OP2	13:2R:17:ARG:NH2	2.35	0.59
23:11:18:ILE:HG12	23:11:37:ILE:HG12	1.85	0.58
1:1A:1218:G:O2'	1:1A:1219:A:O4'	2.21	0.58
1:1A:2143:G:H1	1:1A:2199:C:N4	2.00	0.58
6:1G:101:ILE:HG22	6:1G:105:LYS:HE2	1.85	0.58
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:5:LEU:HB2	21:2Z:47:VAL:HG21	1.85	0.58
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.36	0.58
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.84	0.58
1:2A:455:C:N4	1:2A:476:G:O6	20.06	0.58
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.85	0.58
1:2A:908:C:OP2	12:2Q:22:LYS:NZ	2.33	0.58
1:1A:532:A:H2	1:1A:1206:G:H21	76.23	0.58
1:1A:556:C:O2	61:1A:4136:HOH:O	2.14	0.58
16:1U:46:ALA:O	16:1U:50:ARG:HG2	2.04	0.58
1:2A:796:C:H2'	1:2A:797:C:C6	2.38	0.58
25:13:7:LYS:HB2	25:13:34:GLU:HG2	1.85	0.58
1:1A:2260:C:OP2	61:1A:4149:HOH:O	2.17	0.58
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.86	0.58
1:2A:1007:C:N3	1:2A:1022:G:O6	16.40	0.58
1:1A:173:C:H2'	1:1A:174:U:C6	2.38	0.58
5:1F:188:ARG:HA	11:1P:3:LEU:HD11	1.85	0.58
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.85	0.58
1:2A:1371:G:N7	61:2A:3931:HOH:O	2.32	0.58
1:2A:662:G:O2'	1:2A:836:G:OP1	26.21	0.58
8:2I:48:GLU:HB3	8:2I:52:ARG:HH12	1.69	0.58
16:2U:28:ARG:NH1	16:2U:38:THR:OG1	2.35	0.58
1:1A:1305:G:N2	1:1A:1331:G:H1'	39.90	0.58
1:1A:2205:C:H2'	1:1A:2206:G:H8	1.67	0.58
1:1A:223:C:H2'	1:1A:224:U:H6	1.68	0.58
14:1S:39:ILE:HB	14:1S:49:VAL:HG13	1.85	0.58
1:2A:878:A:N6	1:2A:900:A:N7	2.51	0.58
1:2A:1468:C:OP1	61:2A:3852:HOH:O	2.17	0.58
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.67	0.58
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.39	0.58
1:2A:290:G:H1	1:2A:350:U:H3	1.52	0.58
1:1A:713:G:N2	30:18:2:PRO:O	2.37	0.58
27:25:33:CYS:HB2	27:25:40:LYS:HD3	1.86	0.58
1:2A:1023:U:OP2	61:2A:3817:HOH:O	2.17	0.58
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.85	0.57
1:1A:1832:G:OP2	3:1D:154:LYS:NZ	2.35	0.57
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.19	0.57
1:2A:223:A:O2'	1:2A:420:C:O2	2.22	0.57
1:2A:922:U:O2'	22:20:29:GLN:NE2	2.36	0.57
9:2N:30:ILE:HG22	9:2N:34:LEU:HD22	1.84	0.57
1:1A:1111:U:H1'	1:1A:1120:G:C2	2.39	0.57
1:1A:1639:G:H2'	1:1A:1640:G:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1532:C:H41	1:2A:1537:G:H1	1.51	0.57
1:2A:1813:G:O6	61:2A:3858:HOH:O	2.17	0.57
8:2I:140:LEU:HD22	8:2I:142:VAL:HG22	1.86	0.57
10:2O:9:GLU:OE2	10:2O:18:LYS:NZ	2.37	0.57
1:2A:1751:C:HO2'	1:2A:2861:G:HO2'	1.50	0.57
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.86	0.57
9:2N:30:ILE:O	9:2N:34:LEU:N	2.32	0.57
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.52	0.57
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.85	0.57
1:1A:1121:C:H2'	1:1A:1122:C:H5'	1.86	0.57
1:1A:223:C:H2'	1:1A:224:U:C6	2.39	0.57
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.04	0.57
9:2N:20:GLY:HA2	9:2N:61:ARG:HG3	1.85	0.57
21:2Z:138:GLU:H	21:2Z:156:LYS:HE2	1.70	0.57
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.87	0.57
24:12:14:ARG:O	24:12:67:LYS:NZ	2.37	0.57
5:1F:51:THR:HB	5:1F:88:VAL:HG11	1.87	0.57
1:2A:2625:G:O6	61:2A:3843:HOH:O	2.15	0.57
6:2G:29:TRP:O	6:2G:33:ARG:NH1	2.36	0.57
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.87	0.57
17:2V:46:VAL:HG23	17:2V:52:VAL:HG11	1.87	0.57
1:1A:166:G:H2'	1:1A:167:G:C8	3.93	0.57
1:2A:1469:A:OP2	61:2A:3855:HOH:O	2.17	0.57
1:2A:1658:C:OP1	61:2A:3859:HOH:O	2.17	0.57
1:2A:2140:C:H1'	1:2A:2152:G:N2	2.19	0.57
1:2A:863:A:H2'	1:2A:864:G:H8	1.69	0.57
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.86	0.57
1:1A:1435:G:H2'	1:1A:1436:U:C6	3.10	0.57
1:1A:742:G:OP1	1:1A:1426:G:O2'	2.18	0.57
1:2A:1237:A:OP1	61:2A:3863:HOH:O	2.18	0.57
1:2A:947:G:OP2	61:2A:3861:HOH:O	2.18	0.57
13:2R:33:ARG:NH1	13:2R:115:GLU:OE1	2.36	0.57
1:1A:1711:A:OP1	61:1A:4106:HOH:O	2.17	0.57
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.40	0.57
2:1B:88:C:H2'	2:1B:89:G:O4'	2.04	0.57
1:2A:2746:U:OP1	7:2H:85:LYS:NZ	2.29	0.57
1:1A:1342:G:OP1	1:1A:2721:G:O2'	2.16	0.57
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.28	0.57
1:2A:1783:A:HO2'	1:2A:2607:G:HO2'	1.52	0.57
58:2A:3746:EZG:ND1	61:2A:3933:HOH:O	2.33	0.57
22:20:63:VAL:HG21	22:20:83:PRO:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE2	1.87	0.56
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.86	0.56
1:2A:2498:C:H3'	61:2A:3829:HOH:O	2.03	0.56
1:2A:516:C:OP1	27:25:13:LYS:NZ	2.34	0.56
4:2E:76:ARG:NH1	61:2E:403:HOH:O	2.38	0.56
8:2I:38:LEU:HB2	8:2I:40:THR:HG23	1.86	0.56
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.87	0.56
1:1A:493:G:OP1	29:17:33:ARG:NH1	2.38	0.56
1:1A:1159:U:H2'	1:1A:1160:G:C8	2.40	0.56
1:1A:2104:A:H5'	61:1A:4178:HOH:O	2.05	0.56
1:1A:2157:A:H5'	1:1A:2182:G:H4'	1.87	0.56
1:1A:297:C:H2'	1:1A:298:G:H8	1.71	0.56
22:20:10:THR:HG22	22:20:12:ASN:N	2.20	0.56
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.87	0.56
1:2A:1530:C:N4	1:2A:1539:G:H1	2.03	0.56
2:2B:24:G:N7	2:2B:56:G:H2'	2.20	0.56
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.41	0.56
1:1A:166:G:H2'	1:1A:167:G:H8	3.54	0.56
1:1A:174:U:H2'	1:1A:175:G:H8	1.70	0.56
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.88	0.56
2:2B:72:G:O2'	2:2B:105:A:N6	2.37	0.56
1:1A:1217:G:OP2	1:1A:1219:A:N6	2.38	0.56
1:1A:2507:G:H5''	12:1Q:82:ARG:HG2	1.87	0.56
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.40	0.56
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.40	0.56
1:2A:639:U:H2'	1:2A:640:C:C6	2.40	0.56
1:2A:861:A:N3	2:2B:79:C:O2'	2.38	0.56
1:1A:1151:U:H2'	1:1A:1152:G:H8	1.71	0.56
1:1A:2642:G:H2'	1:1A:2643:G:C8	2.40	0.56
1:1A:532:A:N6	1:1A:1206:G:O2'	79.79	0.56
2:1B:8:U:OP1	14:1S:15:ARG:NH2	2.38	0.56
1:2A:1310:G:H2'	1:2A:1311:G:C8	3.86	0.56
1:2A:27:G:O2'	1:2A:28:A:OP2	2.23	0.56
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.86	0.56
1:1A:1716:A:OP2	61:1A:4122:HOH:O	2.18	0.56
1:1A:692:C:N4	1:1A:698:G:H1	2.04	0.56
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.88	0.56
1:2A:1599:C:OP1	61:2A:3857:HOH:O	2.17	0.56
1:2A:218:A:OP2	61:2A:3862:HOH:O	2.18	0.56
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.38	0.56
6:2G:170:ARG:O	6:2G:174:GLU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2367:C:H1'	22:10:39:ARG:HH21	1.70	0.56
1:2A:2121:G:H1	1:2A:2177:C:H42	1.52	0.56
21:2Z:47:VAL:O	21:2Z:50:GLN:NE2	2.39	0.56
1:1A:2177:G:H3'	1:1A:2178:G:C8	2.41	0.56
1:1A:655:G:OP2	30:18:15:LYS:NZ	2.35	0.56
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.19	0.56
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.41	0.56
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.71	0.56
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.36	0.56
21:2Z:92:SER:O	21:2Z:130:PRO:HG3	2.06	0.56
1:1A:1552:C:H2'	1:1A:1553:A:C8	2.41	0.56
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.41	0.56
1:1A:559:U:H2'	1:1A:560:C:C6	2.41	0.56
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.41	0.56
1:2A:882:G:H2'	1:2A:883:G:H8	1.70	0.56
1:1A:2348:A:H61	22:10:43:THR:CG2	2.19	0.55
5:1F:12:LEU:HB3	5:1F:126:VAL:HG12	1.88	0.55
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.05	0.55
8:1I:79:ILE:HB	8:1I:144:VAL:HG12	1.87	0.55
1:1A:1051:C:O2'	9:1N:28:THR:HG21	2.06	0.55
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.87	0.55
1:2A:108:U:H2'	1:2A:109:G:H8	1.71	0.55
1:2A:1270:C:H2'	1:2A:1271:G:C8	6.68	0.55
1:2A:484:C:H2'	1:2A:485:C:H6	1.71	0.55
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.34	0.55
1:1A:122:G:OP1	1:1A:1422:C:O2'	2.15	0.55
1:1A:2584:A:C8	4:1E:144:ARG:HD3	2.41	0.55
1:2A:265:A:C8	1:2A:266:G:H1'	2.40	0.55
28:16:35:GLU:OE2	28:16:50:ARG:NH1	2.39	0.55
1:1A:2158:C:H42	1:1A:2177:G:H1	0.63	0.55
1:1A:2291:G:O6	22:10:14:ARG:HG3	2.07	0.55
8:1I:47:LEU:HG	8:1I:51:ILE:HD11	1.88	0.55
1:2A:1155:A:H5''	16:2U:55:ARG:NH1	2.21	0.55
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.07	0.55
2:2B:43:C:H5''	26:24:1:MET:HG2	1.87	0.55
2:2B:83:G:H1	2:2B:94:C:H42	1.54	0.55
1:1A:2153:G:N2	1:1A:2180:A:N1	2.55	0.55
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.19	0.55
6:1G:45:GLU:OE2	61:1G:3102:HOH:O	2.17	0.55
8:1I:65:ALA:O	8:1I:69:LYS:N	2.39	0.55
19:1X:56:THR:O	61:1X:201:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.41	0.55
1:2A:1266:G:N2	1:2A:1269:A:N7	9.96	0.55
1:2A:2882:A:H5'	13:2R:96:ARG:HG3	1.87	0.55
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.87	0.55
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.36	0.55
1:2A:602:G:O2'	1:2A:655:A:N6	2.39	0.55
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.89	0.55
1:1A:2101:U:O3'	23:11:35:THR:OG1	2.25	0.55
1:1A:71:U:OP1	61:1A:4148:HOH:O	2.17	0.55
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.87	0.55
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	1.88	0.55
6:1G:145:THR:HG23	6:1G:148:MET:HG2	1.89	0.55
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.88	0.55
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.07	0.55
21:2Z:166:SER:O	21:2Z:168:GLU:N	2.39	0.55
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.89	0.55
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.21	0.55
1:1A:1068:G:OP2	1:1A:1068:G:H8	6.89	0.55
1:1A:1320:A:N3	1:1A:1343:C:H1'	2.22	0.55
1:1A:2442:A:H2'	1:1A:2442:A:N3	2.22	0.55
1:1A:2732:G:OP2	61:1A:4153:HOH:O	2.18	0.55
1:1A:879:G:H5'	11:1P:45:LEU:HD21	1.89	0.55
1:2A:2489:G:N2	1:2A:2491:U:O4	2.32	0.55
1:2A:652(D):C:H42	1:2A:652(U):G:H1	1.54	0.55
1:2A:2393:A:H5''	11:2P:63:PRO:HB3	1.89	0.55
1:1A:1100:A:N6	1:1A:1151:U:N3	2.35	0.55
1:2A:111:A:O2'	24:22:65:ASN:ND2	2.34	0.55
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	1.89	0.55
12:2Q:17:LEU:HD21	12:2Q:41:TRP:NE1	2.21	0.55
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.87	0.55
1:1A:1484:U:O2	1:1A:1602:G:N2	2.41	0.54
5:2F:53:THR:HG22	5:2F:56:GLU:HG3	1.88	0.54
14:2S:58:LEU:HD12	14:2S:65:VAL:HG13	1.89	0.54
22:10:38:VAL:HB	22:10:59:LEU:HB2	1.89	0.54
1:1A:2129:C:H42	1:1A:2204:G:H1	1.54	0.54
6:1G:83:ARG:O	6:1G:86:MET:HG3	2.07	0.54
7:1H:148:ILE:HA	7:1H:151:ILE:HD12	1.89	0.54
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.08	0.54
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.07	0.54
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.43	0.54
1:2A:632:A:H2'	1:2A:633:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:656:G:H2'	1:2A:657:U:O4'	2.06	0.54
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.89	0.54
15:2T:122:ASP:O	15:2T:126:ALA:N	2.36	0.54
1:1A:2545:A:H2'	1:1A:2546:A:O4'	2.06	0.54
1:1A:2713:C:OP1	61:1A:4151:HOH:O	2.18	0.54
1:1A:650:G:O6	11:1P:107:LYS:NZ	2.40	0.54
1:1A:2602:A:O3'	3:1D:239:ARG:NH2	2.40	0.54
1:2A:2089:U:H3	1:2A:2230:G:H1	1.54	0.54
1:2A:740:U:H2'	1:2A:741:G:C8	2.41	0.54
2:2B:14:U:O3'	2:2B:108:U:O2'	2.23	0.54
1:1A:1105:G:H2'	1:1A:1106:U:C5	2.43	0.54
1:1A:1829:U:H5'	3:1D:259:THR:CG2	2.36	0.54
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	1.89	0.54
1:2A:2357:U:OP1	22:20:20:ARG:NE	2.34	0.54
1:2A:2357:U:P	22:20:20:ARG:HE	2.30	0.54
15:2T:24:PRO:HA	15:2T:49:VAL:HG23	1.89	0.54
23:11:89:GLU:O	23:11:93:GLU:HG2	2.07	0.54
1:1A:1115:A:H2'	1:1A:1119:A:N7	2.23	0.54
1:1A:2650:G:P	4:1E:82:ARG:HH12	2.31	0.54
1:2A:1183:G:H5''	25:23:30:ARG:NH2	2.23	0.54
1:2A:2128:C:H2'	1:2A:2129:C:O4'	2.06	0.54
1:2A:863:A:H2'	1:2A:864:G:C8	2.42	0.54
1:1A:1346:U:H4'	1:1A:1347:A:H5''	1.88	0.54
1:1A:1514:C:OP2	1:1A:1593:C:O2'	2.25	0.54
1:1A:1904:C:H2'	1:1A:1905:G:O4'	2.08	0.54
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.41	0.54
29:27:34:ARG:HB2	29:27:42:LEU:HD22	1.89	0.54
1:2A:686:G:H8	29:27:6:GLN:O	1.91	0.54
1:2A:108:U:H2'	1:2A:109:G:C8	2.43	0.54
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.26	0.54
1:2A:922:U:H2'	1:2A:923:C:C6	2.43	0.54
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.90	0.54
1:2A:1187:G:OP2	1:2A:1187:G:H8	1.90	0.54
1:2A:624:C:OP1	61:2A:3860:HOH:O	2.17	0.54
1:1A:798:A:OP1	61:1A:4150:HOH:O	2.18	0.54
19:2X:60:ARG:HH22	29:27:47:ARG:NH1	2.05	0.54
1:1A:2307:C:OP1	14:1S:10:ARG:NH1	2.40	0.54
10:1O:38:VAL:HG13	10:1O:87:ILE:HD11	1.90	0.54
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.40	0.54
7:2H:25:LYS:HB3	7:2H:27:LYS:HZ1	1.72	0.54
28:16:9:LEU:HD13	28:16:51:GLU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1347:A:O2'	1:1A:1348:A:H3'	2.06	0.54
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.08	0.54
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.43	0.54
1:2A:624:C:H2'	1:2A:625:G:H8	2.94	0.54
31:19:2:LYS:HE2	31:19:31:LYS:O	2.07	0.53
1:1A:2130:C:H2'	1:1A:2131:U:H6	1.73	0.53
1:1A:586:G:H22	1:1A:601:A:H2	1.56	0.53
11:1P:124:LYS:HA	11:1P:144:GLU:HB3	1.91	0.53
24:22:24:LEU:HD23	24:22:60:LEU:HD21	1.88	0.53
1:2A:1286:A:C8	1:2A:1287:A:H4'	8.12	0.53
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.08	0.53
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.55	0.53
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.90	0.53
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.24	0.53
1:2A:2786:U:OP1	4:2E:69:LYS:NZ	2.34	0.53
22:10:38:VAL:HG12	22:10:40:GLN:HG2	1.91	0.53
29:17:21:ARG:NH1	61:17:5001:HOH:O	2.31	0.53
1:1A:715:G:H5'	1:1A:716:G:OP2	2.09	0.53
13:1R:59:ASP:N	13:1R:59:ASP:OD1	2.42	0.53
25:23:23:LEU:HD13	25:23:50:VAL:HG11	1.90	0.53
1:2A:2495:G:H5''	12:2Q:82:ARG:HG2	1.90	0.53
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.21	0.53
1:1A:174:U:H2'	1:1A:175:G:C8	2.43	0.53
4:1E:111:ARG:HD2	4:1E:160:TYR:CD2	2.44	0.53
1:1A:346:A:OP1	5:1F:168:ARG:HD2	2.08	0.53
7:1H:86:GLU:HB3	7:1H:165:ALA:HB2	1.89	0.53
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.07	0.53
1:2A:784:A:C5	3:2D:229:VAL:HG11	2.44	0.53
1:1A:768:C:H2'	1:1A:769:A:C8	2.44	0.53
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.89	0.53
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	1.91	0.53
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	1.90	0.53
23:21:83:GLU:N	23:21:83:GLU:OE1	2.41	0.53
1:2A:1441:G:O2'	61:2A:3864:HOH:O	2.18	0.53
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.91	0.53
1:2A:568:U:H5'	1:2A:945:A:N1	2.23	0.53
21:2Z:55:HIS:CE1	21:2Z:135:GLU:HG3	2.44	0.53
1:1A:1825:U:H2'	1:1A:1826:C:C6	2.43	0.53
26:24:46:GLN:NE2	26:24:48:ARG:HD3	2.24	0.53
29:27:34:ARG:HH21	29:27:39:ARG:HG2	1.74	0.53
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.43	0.53
1:2A:2137:C:O2'	1:2A:2138:C:OP2	2.25	0.53
1:2A:266:G:H5''	1:2A:268:C:H41	11.64	0.53
14:2S:11:LYS:HG3	14:2S:91:PRO:HD3	1.90	0.53
1:1A:664:U:H2'	1:1A:665:C:C6	2.44	0.53
8:1I:101:LEU:HG	8:1I:107:VAL:HB	1.88	0.53
26:24:60:GLN:O	26:24:62:ARG:NH1	2.41	0.53
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.44	0.53
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.44	0.53
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.08	0.53
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.35	0.53
1:1A:2586:G:OP1	61:1A:4155:HOH:O	2.19	0.53
3:1D:68:LYS:HD3	3:1D:70:TRP:CH2	2.44	0.53
6:1G:126:ASP:HB3	6:1G:130:ASN:HB2	1.91	0.53
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.90	0.53
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.90	0.53
1:1A:1387:U:O2	19:1X:80:ILE:HD12	2.08	0.53
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.08	0.53
1:2A:2807:G:H22	1:2A:2893:G:H1	1.57	0.53
1:2A:848:G:H2'	1:2A:849:A:C8	2.42	0.53
24:12:28:LYS:HD2	24:12:53:LEU:HD21	1.91	0.53
26:14:53:GLU:HB2	26:14:55:ARG:HA	1.91	0.53
1:1A:2504:U:H2'	1:1A:2505:U:C6	2.44	0.53
4:1E:121:ASN:ND2	61:1E:403:HOH:O	2.34	0.53
6:2G:108:ASN:HA	26:24:37:SER:HB2	1.90	0.53
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.42	0.53
5:2F:133:ASN:N	5:2F:138:GLU:OE1	2.42	0.53
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.90	0.53
1:1A:302:A:O2'	1:1A:303:C:OP1	2.25	0.53
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.43	0.53
1:1A:1123:A:H2'	1:1A:1124:U:H4'	1.90	0.52
1:1A:1291:G:OP1	11:1P:13:ASN:ND2	2.29	0.52
2:1B:65:C:HO2'	2:1B:66:A:P	2.31	0.52
2:1B:79:C:H2'	2:1B:80:U:O4'	2.09	0.52
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.09	0.52
22:20:40:GLN:HE21	22:20:57:PHE:HB3	1.73	0.52
1:2A:261:G:HO2'	1:2A:610:G:HO2'	1.53	0.52
11:2P:38:GLN:HG2	11:2P:45:LEU:H	1.74	0.52
12:2Q:1:MET:HG3	12:2Q:44:ALA:HB1	1.91	0.52
1:1A:1006:C:H42	1:1A:1023:G:H1	21.37	0.52
1:1A:149:A:H2'	1:1A:150:C:C6	2.80	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1825:U:H2'	1:1A:1826:C:H6	1.74	0.52
1:1A:2153:G:H5''	1:1A:2154:U:H3'	1.91	0.52
1:1A:906:G:O2'	1:1A:962:G:O6	2.16	0.52
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.42	0.52
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.44	0.52
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.24	0.52
7:2H:33:LEU:HD11	7:2H:136:ILE:HG22	1.92	0.52
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD21	1.91	0.52
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.10	0.52
1:1A:1814:A:H5'	1:1A:2620:G:H4'	1.91	0.52
5:1F:123:LEU:HD13	5:1F:192:LEU:HB3	1.90	0.52
7:1H:24:VAL:O	7:1H:35:VAL:N	2.39	0.52
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.44	0.52
26:24:61:ARG:NH1	26:24:62:ARG:O	2.43	0.52
1:2A:184:C:H2'	1:2A:185:U:C6	2.45	0.52
1:2A:517:C:OP2	27:25:13:LYS:HE2	2.09	0.52
3:2D:274:ARG:O	3:2D:275:LYS:HD2	2.09	0.52
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.90	0.52
10:2O:53:LYS:N	10:2O:56:ASP:OD2	2.38	0.52
10:2O:88:ASN:ND2	10:2O:92:GLU:OE1	2.40	0.52
16:2U:113:ALA:O	16:2U:117:GLN:HG2	2.08	0.52
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.24	0.52
1:1A:1108:G:H1	1:1A:1123:A:N6	2.07	0.52
1:1A:768:C:H2'	1:1A:769:A:H8	1.75	0.52
2:2B:15:A:H5''	2:2B:16:G:H8	1.73	0.52
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.74	0.52
1:1A:1154:U:H2'	1:1A:1155:C:O4'	2.10	0.52
1:1A:2176:G:C2	1:1A:2177:G:H1'	2.45	0.52
1:1A:957:A:H2'	12:1Q:9:TYR:OH	2.08	0.52
1:2A:1012:U:O2	9:2N:25:ARG:NH1	2.43	0.52
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.09	0.52
1:2A:2116:G:N7	1:2A:2166:G:N2	2.57	0.52
1:2A:2168:G:H8	1:2A:2170:A:N7	2.07	0.52
1:2A:2206:G:H8	1:2A:2207:G:N7	2.08	0.52
11:2P:52:GLU:HG3	30:28:57:ARG:HH22	1.74	0.52
12:2Q:30:GLY:O	12:2Q:134:ARG:NH1	2.43	0.52
1:1A:2152:U:H2'	1:1A:2180:A:N1	2.25	0.52
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.74	0.52
8:1I:70:GLU:O	8:1I:74:ASN:HB2	2.09	0.52
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.90	0.52
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2233:U:H2'	1:2A:2234:G:C8	2.44	0.52
1:2A:315:G:H2'	1:2A:316:C:C6	2.45	0.52
1:2A:668:G:H5'	1:2A:669:G:OP2	2.10	0.52
9:2N:116:LEU:O	9:2N:119:ARG:N	2.39	0.52
24:12:9:GLN:HE21	24:12:60:LEU:HD21	1.74	0.52
1:1A:308:U:H2'	1:1A:309:C:C6	2.45	0.52
1:1A:645:G:N3	1:1A:645:G:H5'	2.25	0.52
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.31	0.52
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.91	0.52
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.45	0.52
1:2A:2155:G:C5	1:2A:2156:G:H1'	2.44	0.52
7:2H:3:ARG:HG2	7:2H:6:ARG:HE	1.75	0.52
26:14:16:CYS:SG	26:14:17:GLY:N	2.82	0.52
1:1A:1223:C:H2'	1:1A:1224:C:H6	1.74	0.52
1:1A:2082:A:OP1	61:1A:4156:HOH:O	2.19	0.52
1:1A:2130:C:H2'	1:1A:2131:U:C6	2.45	0.52
1:1A:407:U:H2'	1:1A:408:G:H8	1.75	0.52
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.90	0.52
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.44	0.52
1:2A:920:G:H2'	1:2A:921:G:H8	1.75	0.52
14:2S:10:ARG:O	14:2S:14:VAL:HG12	2.10	0.52
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.92	0.52
8:1I:10:GLU:O	8:1I:12:LEU:N	2.43	0.52
10:1O:120:GLU:HG2	10:1O:122:LEU:HG	1.92	0.52
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.91	0.52
1:2A:2095:C:H2'	1:2A:2096:U:O4'	2.09	0.52
1:2A:300:A:P	20:2Y:86:ARG:HH21	2.33	0.52
10:2O:7:TYR:CE1	10:2O:20:MET:HB2	2.45	0.52
1:1A:1021:G:O2'	1:1A:1202:A:N1	2.38	0.52
1:1A:606:G:N2	1:1A:632:A:N7	49.61	0.52
9:1N:62:VAL:HG21	9:1N:66:LYS:HB2	1.92	0.52
1:2A:335:C:H4'	20:2Y:73:ARG:HD3	1.92	0.52
1:2A:774:A:N3	1:2A:774:A:H2'	2.25	0.52
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	1.92	0.52
1:1A:1451:U:H2'	1:1A:1452:U:C6	2.46	0.51
1:1A:1735:U:O2	1:1A:1747:A:H5'	2.10	0.51
1:1A:2717:A:O2'	1:1A:2862:G:OP1	2.21	0.51
9:1N:62:VAL:HG23	9:1N:66:LYS:HD2	1.91	0.51
16:2U:110:VAL:HG12	16:2U:114:LYS:HE3	1.92	0.51
1:1A:1338:U:H2'	1:1A:1339:C:C6	2.44	0.51
1:1A:1846:A:OP2	3:1D:54:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:11:MET:HG2	4:1E:24:THR:HB	1.91	0.51
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.92	0.51
1:1A:1233:U:H4'	17:1V:79:VAL:HG22	1.92	0.51
2:2B:19:G:H2'	2:2B:20:C:O4'	2.09	0.51
7:2H:8:PRO:O	7:2H:69:ARG:NH2	2.41	0.51
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.92	0.51
1:1A:1055:A:OP2	61:1A:4120:HOH:O	2.19	0.51
1:1A:2175:G:H2'	1:1A:2176:G:C8	2.45	0.51
1:1A:2376:C:H2'	1:1A:2377:G:O4'	2.11	0.51
1:1A:2564:2MU:O5'	1:1A:2564:2MU:H6	2.10	0.51
4:1E:77:ILE:HG12	4:1E:195:LEU:HD22	1.92	0.51
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.11	0.51
1:2A:2127:G:C2	1:2A:2161:C:N3	2.78	0.51
1:2A:2238:G:N3	1:2A:2238:G:H2'	2.26	0.51
1:2A:271(Q):G:H2'	1:2A:271(R):G:H8	1.76	0.51
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.44	0.51
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.92	0.51
9:2N:99:LEU:O	9:2N:103:VAL:HG23	2.10	0.51
17:2V:50:PRO:HG2	17:2V:51:VAL:HG12	1.92	0.51
1:1A:207:A:C2	1:1A:224:U:H4'	2.45	0.51
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.46	0.51
1:1A:2044:U:O2'	1:1A:2629:C:H5'	2.11	0.51
1:1A:2858:G:H1'	1:1A:2877:G:N2	2.25	0.51
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.93	0.51
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.26	0.51
1:1A:24:G:O2'	18:1W:78:GLU:O	2.25	0.51
21:1Z:53:ILE:HG22	21:1Z:71:VAL:HG12	1.92	0.51
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.44	0.51
1:2A:1882:C:H5''	23:21:26:ARG:HH21	1.76	0.51
1:2A:2134:A:HO2'	1:2A:2159:G:N2	2.08	0.51
1:2A:882:G:N2	1:2A:895:U:O2	2.42	0.51
1:2A:2723:C:OP2	4:2E:109:LYS:NZ	2.44	0.51
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.43	0.51
1:1A:1518:A:OP2	1:1A:1567:G:N1	2.37	0.51
1:1A:1705:C:OP1	4:1E:135:HIS:NE2	2.44	0.51
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.45	0.51
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.25	0.51
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.57	0.51
7:2H:90:LYS:HE2	7:2H:159:GLU:HG2	1.91	0.51
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.92	0.51
20:2Y:9:LYS:NZ	20:2Y:28:LYS:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2162:C:H2'	1:1A:2163:G:C8	2.46	0.51
1:1A:2851:C:H2'	1:1A:2852:G:H8	1.75	0.51
1:2A:1226:A:OP1	17:2V:84:LYS:NZ	2.26	0.51
1:2A:2025:C:H2'	1:2A:2026:C:C6	2.46	0.51
1:2A:27:G:N2	1:2A:512:G:H1'	2.25	0.51
1:2A:305:U:H2'	1:2A:306:U:C6	2.46	0.51
1:2A:605:C:O2	1:2A:657:U:O2'	2.23	0.51
20:2Y:1:MET:HE3	20:2Y:2:ARG:H	1.75	0.51
1:1A:2495:C:N3	12:1Q:124:LYS:NZ	2.58	0.51
1:1A:313:A:H2'	1:1A:314:G:O4'	2.10	0.51
8:1I:25:TYR:O	8:1I:29:TYR:HB3	2.09	0.51
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.29	0.51
28:26:10:LEU:HG	28:26:54:ILE:HG13	1.92	0.51
1:2A:1011:G:H1	1:2A:1018:C:H42	17.56	0.51
1:2A:1261:C:OP2	18:2W:83:LYS:NZ	2.27	0.51
1:2A:2203:U:H4'	3:2D:151:LYS:HG2	1.93	0.51
1:2A:484:C:H2'	1:2A:485:C:C6	2.46	0.51
1:2A:909:A:C6	1:2A:912:C:C2	2.99	0.51
15:2T:28:VAL:HG13	15:2T:86:ILE:HG23	1.92	0.51
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.42	0.51
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.91	0.51
1:1A:1121:C:C2'	1:1A:1122:C:H5'	2.40	0.51
1:1A:2153:G:OP1	1:1A:2154:U:O2'	2.19	0.51
1:1A:721:G:O2'	5:1F:74:ARG:HD3	2.10	0.51
7:2H:89:ILE:HG12	7:2H:162:ILE:HG12	1.92	0.51
8:2I:65:ALA:O	8:2I:69:LYS:N	2.42	0.51
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.44	0.51
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.46	0.51
1:1A:2034:G:OP1	18:1W:11:ARG:NH2	2.44	0.51
1:1A:2762:A:OP1	7:1H:3:ARG:NH1	2.44	0.51
1:1A:388:A:H3'	1:1A:389:G:H8	1.75	0.51
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.44	0.51
13:1R:24:GLN:HE22	13:1R:36:THR:HG21	1.76	0.51
1:2A:1159:U:O2'	1:2A:1160:G:OP2	4.78	0.51
1:2A:1270:C:H2'	1:2A:1271:G:H8	6.03	0.51
1:2A:1653:G:H3'	13:2R:2:ARG:HD3	1.92	0.51
1:2A:2149:G:C2	1:2A:2150:U:H1'	2.46	0.51
1:2A:566:U:OP1	17:2V:80:GLN:NE2	2.40	0.51
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.93	0.51
20:2Y:83:THR:OG1	20:2Y:84:ARG:N	2.44	0.51
1:1A:2205:C:H2'	1:1A:2206:G:C8	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2519:C:H2'	1:1A:2520:G:O4'	2.11	0.51
1:2A:122:G:OP1	1:2A:149:A:O2'	2.22	0.51
1:2A:1301:A:H2	1:2A:1626:G:N3	2.08	0.51
1:2A:1711:C:H2'	1:2A:1712:C:H6	1.76	0.51
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.44	0.51
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HG22	1.93	0.51
1:1A:149:A:H2'	1:1A:150:C:H6	2.26	0.50
1:1A:2285:A:H2'	1:1A:2286:A:C8	2.46	0.50
1:1A:2303:U:H2'	1:1A:2304:C:C6	2.45	0.50
1:1A:553:A:O2'	1:1A:554:A:H5'	2.11	0.50
1:1A:909:G:H2'	1:1A:910:A:O4'	2.11	0.50
12:1Q:31:ASP:HA	12:1Q:134:ARG:NH1	2.25	0.50
1:2A:2379:G:HO2'	14:2S:17:ARG:HH12	1.51	0.50
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.11	0.50
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.93	0.50
1:1A:1388:A:O2'	1:1A:1390:G:OP2	2.21	0.50
1:1A:1740:U:H1'	3:1D:14:ARG:NH2	2.26	0.50
1:1A:936:C:H2'	1:1A:937:A:O4'	4.19	0.50
1:1A:964:A:N3	2:1B:80:U:O2'	2.40	0.50
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.29	0.50
1:2A:1180:C:H2'	1:2A:1181:C:H6	1.76	0.50
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.46	0.50
1:2A:1912:A:OP1	61:2A:3865:HOH:O	2.19	0.50
1:2A:2305:A:H1'	6:2G:136:ARG:HB3	1.93	0.50
21:2Z:6:LYS:HZ3	21:2Z:8:TYR:HE2	1.59	0.50
1:1A:1398:U:OP2	61:1A:4158:HOH:O	2.19	0.50
1:1A:2085:C:OP2	61:1A:4159:HOH:O	2.19	0.50
1:1A:2348:A:H61	22:10:43:THR:HG21	1.76	0.50
1:1A:2800:C:H2'	1:1A:2801:C:H6	1.76	0.50
1:1A:636:G:N2	1:1A:640:A:O2'	2.44	0.50
1:1A:989:G:N7	61:1A:4255:HOH:O	2.34	0.50
4:1E:16:ARG:NH1	4:1E:173:VAL:HG13	2.26	0.50
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	1.92	0.50
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.46	0.50
23:21:51:VAL:HG12	23:21:53:VAL:HG23	1.93	0.50
1:2A:597:U:H2'	1:2A:598:G:C8	2.47	0.50
1:2A:824:A:H1'	1:2A:2358:G:N7	2.27	0.50
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.10	0.50
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.26	0.50
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.45	0.50
1:1A:1060:U:OP2	61:1A:4157:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1111:U:H1'	1:1A:1120:G:N1	2.26	0.50
1:1A:1223:C:H2'	1:1A:1224:C:C6	2.46	0.50
1:1A:265:U:H2'	1:1A:266:C:C6	2.46	0.50
19:1X:24:GLY:O	19:1X:83:VAL:HG22	2.12	0.50
21:1Z:132:ASN:HD21	21:1Z:160:GLY:HA3	1.75	0.50
1:2A:287:C:H2'	1:2A:288:C:C6	2.47	0.50
2:2B:66:A:H61	2:2B:109:C:H5''	1.75	0.50
31:19:32:HIS:O	31:19:34:GLN:HG3	2.11	0.50
1:1A:1086:C:H2'	1:1A:1087:C:O4'	2.10	0.50
1:1A:209:G:O2'	1:1A:222:A:N3	2.35	0.50
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.47	0.50
1:1A:2851:C:H2'	1:1A:2852:G:C8	2.47	0.50
23:21:85:LEU:HD23	23:21:89:GLU:HG2	1.92	0.50
1:2A:1029:A:N1	1:2A:2465:C:O2'	2.37	0.50
1:2A:1268:A:H2'	1:2A:1269:A:C8	3.35	0.50
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.46	0.50
1:2A:2453:A:N7	61:2A:3942:HOH:O	2.34	0.50
4:2E:77:ILE:HD11	4:2E:195:LEU:HD22	1.94	0.50
8:2I:50:ARG:O	8:2I:54:GLN:HB2	2.12	0.50
1:1A:1698:G:O6	61:1A:4145:HOH:O	2.17	0.50
1:1A:2227:G:H8	1:1A:2228:G:N7	2.09	0.50
1:1A:2641:A:HO2'	1:1A:2642:G:P	2.31	0.50
3:1D:77:ALA:HA	3:1D:97:TYR:HA	1.94	0.50
4:1E:14:ILE:HG13	4:1E:21:VAL:HG13	1.94	0.50
25:23:6:VAL:HG22	25:23:56:VAL:HG22	1.92	0.50
26:24:13:ARG:HG2	26:24:23:GLU:HA	1.93	0.50
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.27	0.50
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.45	0.50
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.11	0.50
1:1A:2800:C:H2'	1:1A:2801:C:C6	2.46	0.50
5:1F:152:GLU:OE1	5:1F:191:ARG:HD2	2.12	0.50
14:1S:15:ARG:O	14:1S:19:LYS:HG3	2.12	0.50
1:2A:2151:G:C2	1:2A:2152:G:C8	2.99	0.50
1:2A:1983:C:H4'	1:2A:2606:C:H4'	1.93	0.50
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.28	0.50
3:2D:206:LEU:O	3:2D:211:ARG:HD3	2.11	0.50
4:2E:167:VAL:HG22	4:2E:170:LEU:HD11	1.93	0.50
1:1A:1037:C:H2'	1:1A:1038:C:H6	2.13	0.50
1:1A:2198:A:H2'	1:1A:2199:C:C6	2.46	0.50
1:1A:1615:G:H5'	3:1D:60:ARG:HA	1.94	0.50
11:1P:98:GLU:HG3	11:1P:99:LEU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1139:G:H4'	1:2A:1140:C:H5'	4.64	0.50
1:2A:8:A:H2'	1:2A:9:U:C6	2.47	0.50
1:2A:946:G:H2'	1:2A:947:G:C8	2.47	0.50
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.09	0.50
12:2Q:66:ILE:HG12	12:2Q:104:PHE:HD1	1.77	0.50
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.93	0.50
18:2W:23:LEU:HD11	27:25:25:LEU:HB2	1.92	0.50
1:1A:920:G:H1	1:1A:950:C:H42	1.60	0.50
1:1A:99:G:H21	24:12:7:ARG:HH22	1.59	0.50
29:27:26:GLY:O	29:27:30:VAL:HG23	2.12	0.50
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.12	0.50
1:2A:946:G:H2'	1:2A:947:G:H8	1.77	0.50
5:2F:107:LYS:HG3	5:2F:206:ILE:HA	1.94	0.50
10:2O:88:ASN:HD21	10:2O:92:GLU:HB2	1.76	0.50
1:1A:1037:C:H2'	1:1A:1038:C:C6	2.90	0.49
1:1A:1138:C:C2'	1:1A:1139:G:H5'	2.41	0.49
1:1A:18:C:O2'	1:1A:577:U:OP1	2.30	0.49
1:1A:142:G:H1'	19:1X:37:THR:HG21	1.94	0.49
1:2A:1011:G:H1	1:2A:1018:C:N4	17.78	0.49
1:2A:1341:U:OP2	1:2A:1394:U:O2'	2.26	0.49
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.26	0.49
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.47	0.49
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.47	0.49
1:2A:2557:G:H2'	1:2A:2558:C:H6	1.77	0.49
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.47	0.49
1:2A:30:G:H2'	1:2A:31:C:C6	2.47	0.49
2:2B:24:G:H4'	2:2B:25:A:C8	2.47	0.49
13:2R:26:LYS:HD3	13:2R:70:LEU:O	2.12	0.49
1:1A:1834:A:O2'	3:1D:259:THR:HG21	2.12	0.49
1:1A:2143:G:H2'	1:1A:2144:U:C6	2.47	0.49
1:1A:2346:G:O6	22:10:74:ARG:NH2	2.42	0.49
1:1A:2372:A:H2'	1:1A:2373:A:O4'	2.12	0.49
1:1A:2707:C:H2'	1:1A:2708:U:C6	2.47	0.49
1:1A:602:G:H2'	1:1A:603:C:C6	2.47	0.49
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.11	0.49
10:1O:86:ILE:HG22	10:1O:94:ARG:HD3	1.94	0.49
21:1Z:99:TYR:HB3	21:1Z:123:ASP:OD2	2.12	0.49
1:2A:1543:C:H5''	61:2A:4225:HOH:O	2.11	0.49
1:2A:1837:C:O2'	1:2A:1927:A:N3	2.36	0.49
1:2A:2103:C:H2'	1:2A:2104:G:C8	2.47	0.49
1:2A:2336:A:H61	22:20:43:THR:HG22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:34:C:H2'	1:2A:35:G:H8	4.09	0.49
1:1A:302:A:H2'	1:1A:303:C:C6	2.47	0.49
28:26:35:GLU:HG2	28:26:50:ARG:HD3	1.94	0.49
1:2A:833:U:O2'	30:28:57:ARG:NH1	2.45	0.49
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.48	0.49
1:2A:443:A:C5	5:2F:45:ARG:HD2	2.47	0.49
7:2H:3:ARG:HG2	7:2H:6:ARG:NE	2.27	0.49
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.12	0.49
12:2Q:35:VAL:HG12	12:2Q:130:LYS:O	2.12	0.49
1:1A:1821:C:H2'	1:1A:1822:A:C5	2.48	0.49
1:1A:2247:G:H2'	1:1A:2248:C:C6	2.47	0.49
1:1A:2381:A:H2'	1:1A:2382:G:H8	1.77	0.49
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.47	0.49
1:2A:529:A:H2	61:2A:3888:HOH:O	1.96	0.49
1:2A:588:U:H2'	1:2A:589:C:C6	2.47	0.49
1:2A:858:U:O2	1:2A:2268:A:H2'	2.12	0.49
4:2E:50:GLY:HA2	4:2E:77:ILE:O	2.13	0.49
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.95	0.49
1:1A:463:C:H2'	1:1A:464:G:H8	1.75	0.49
1:1A:1834:A:H4'	3:1D:259:THR:HG23	1.95	0.49
1:2A:2127:G:H1	1:2A:2161:C:N4	2.08	0.49
1:2A:38:A:H2'	1:2A:39:C:C6	2.48	0.49
3:2D:127:VAL:HA	3:2D:193:VAL:HG23	1.95	0.49
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.47	0.49
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.22	0.49
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.47	0.49
1:2A:2127:G:C6	1:2A:2161:C:N4	2.80	0.49
1:2A:435:C:H2'	1:2A:436:C:H6	3.68	0.49
1:2A:819:A:OP2	1:2A:1187:G:N2	2.36	0.49
1:2A:848:G:C2	1:2A:933:A:H1'	2.47	0.49
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.93	0.49
9:2N:24:GLY:O	9:2N:28:THR:OG1	2.29	0.49
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.95	0.49
29:17:20:ALA:HA	29:17:23:ARG:HH21	1.78	0.49
1:1A:1186:U:H4'	1:1A:1188:A:O4'	2.13	0.49
1:2A:1486:A:H2'	1:2A:1487:G:H8	1.76	0.49
1:2A:581:C:H2'	1:2A:582:G:C8	2.47	0.49
2:2B:43:C:O2	6:2G:95:ARG:NE	2.42	0.49
1:1A:1074:A:N6	1:1A:1171:G:H2'	2.27	0.49
1:1A:1318:A:H5''	14:1S:3:ARG:NH1	127.09	0.49
1:1A:1495:G:O2'	1:1A:1575:A:N1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:180:A:N1	61:1A:4262:HOH:O	2.35	0.49
1:1A:2262:G:OP1	12:1Q:85:LYS:NZ	2.30	0.49
1:1A:943:C:N3	1:1A:944:C:N4	2.60	0.49
1:1A:1445:C:OP1	19:1X:25:LYS:NZ	2.45	0.49
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.13	0.49
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.46	0.49
1:1A:2402:U:P	30:18:35:GLN:HE22	2.36	0.49
1:1A:155:C:O2	1:1A:166:G:N2	23.52	0.49
1:1A:2123:G:H1	1:1A:2210:C:H42	1.61	0.49
1:1A:1057:G:OP2	16:1U:70:ARG:NH2	2.46	0.49
1:2A:197:A:O2'	61:2A:3847:HOH:O	2.15	0.49
19:2X:41:ASN:O	19:2X:45:THR:HG23	2.13	0.49
1:1A:1136:U:C2	1:1A:1148:C:H1'	2.47	0.49
1:1A:1431:G:O2'	1:1A:1442:U:O2	2.22	0.49
1:1A:1572:G:C6	1:1A:1573:G:C2	3.01	0.49
1:1A:1717:C:O2	4:1E:129:HIS:NE2	2.44	0.49
1:1A:629:U:H4'	1:1A:705:C:H4'	1.95	0.49
1:1A:2417:G:H5''	11:1P:75:ILE:HG21	1.93	0.49
1:2A:75:G:H4'	24:22:55:ARG:HH11	1.77	0.49
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.48	0.49
9:2N:34:LEU:HD21	9:2N:120:LEU:HB2	1.95	0.49
1:1A:225:C:H2'	1:1A:226:C:C6	2.48	0.48
1:1A:2328:C:H1'	6:1G:128:ARG:HH21	1.77	0.48
7:1H:3:ARG:CZ	7:1H:5:GLY:H	2.26	0.48
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.94	0.48
1:2A:1442:G:N3	1:2A:1442:G:H2'	2.83	0.48
1:2A:994:C:O2'	1:2A:996:A:OP1	2.27	0.48
8:2I:48:GLU:HB3	8:2I:52:ARG:NH1	2.28	0.48
21:2Z:150:LEU:HB2	21:2Z:171:ILE:HD11	1.94	0.48
1:1A:449:A:H2'	1:1A:450:A:C8	2.48	0.48
1:1A:515:G:N7	18:1W:49:LYS:NZ	2.60	0.48
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.47	0.48
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.48	0.48
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.30	0.48
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.95	0.48
1:2A:1568:G:H5''	3:2D:61:LEU:HD13	1.96	0.48
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.28	0.48
25:13:37:LEU:HB3	25:13:43:ILE:HD13	1.96	0.48
1:1A:242:C:OP2	30:18:5:LYS:NZ	2.34	0.48
1:1A:2589:A:OP1	61:1A:4163:HOH:O	2.20	0.48
1:1A:589:U:H5''	11:1P:29:LYS:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:87:TYR:OH	13:1R:117:VAL:O	2.26	0.48
1:2A:2317:C:N4	1:2A:2318:G:O6	2.47	0.48
1:2A:336:C:H2'	1:2A:337:C:C6	2.48	0.48
1:2A:578:A:OP2	61:2A:3868:HOH:O	2.20	0.48
2:2B:91:C:H5'	12:2Q:18:LYS:HA	1.94	0.48
1:2A:908:C:P	12:2Q:22:LYS:HZ2	2.34	0.48
1:1A:2391:G:O2'	14:1S:17:ARG:NH2	2.33	0.48
1:1A:715:G:N7	61:1A:4264:HOH:O	2.35	0.48
8:1I:46:ALA:HB1	8:1I:50:ARG:HH22	1.79	0.48
24:22:32:LEU:HD13	24:22:53:LEU:HB3	1.94	0.48
1:2A:1901:A:OP2	3:2D:255:LYS:NZ	2.31	0.48
1:2A:204:A:O3'	1:2A:205:G:H4'	2.14	0.48
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.48	0.48
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.13	0.48
1:2A:514:A:N3	1:2A:581:C:O2'	2.44	0.48
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.26	0.48
6:1G:101:ILE:HD13	26:14:25:TYR:HB2	1.95	0.48
7:1H:3:ARG:HH22	7:1H:66:GLY:N	2.12	0.48
15:1T:107:ASP:OD2	15:1T:111:ARG:NH1	2.46	0.48
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.49	0.48
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.48	0.48
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.13	0.48
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.14	0.48
20:2Y:31:LEU:HD23	20:2Y:31:LEU:HA	1.70	0.48
21:2Z:31:ARG:HH11	21:2Z:94:GLU:HG2	1.78	0.48
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.48	0.48
1:1A:2504:U:H2'	1:1A:2505:U:H6	1.77	0.48
1:1A:993:G:OP1	61:1A:4162:HOH:O	2.20	0.48
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.47	0.48
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.94	0.48
1:2A:1509(B):A:H2'	1:2A:1510:G:H8	1.78	0.48
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.37	0.48
1:2A:903:C:H2'	1:2A:904:C:C6	2.49	0.48
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.14	0.48
6:2G:109:VAL:HG21	26:24:14:ILE:HD13	1.95	0.48
6:2G:173:LEU:HB3	6:2G:178:PHE:CD2	2.48	0.48
19:2X:88:LYS:HG2	19:2X:93:GLU:HG3	1.96	0.48
1:1A:369:A:N3	1:1A:371:A:N6	2.62	0.48
4:1E:29:GLY:HA3	61:1E:408:HOH:O	2.14	0.48
1:2A:2227:A:OP1	3:2D:263:ARG:HD2	2.13	0.48
1:2A:2430:A:OP2	61:2A:3867:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:880:G:H22	1:2A:898:C:H1'	1.77	0.48
1:2A:893:C:H2'	1:2A:894:C:C5	2.48	0.48
21:2Z:166:SER:C	21:2Z:168:GLU:H	2.16	0.48
1:1A:469:A:H1'	1:1A:1246:C:O4'	2.13	0.48
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.95	0.48
21:1Z:4:ARG:HH21	21:1Z:60:GLU:HG2	1.78	0.48
1:2A:1481:U:H3	1:2A:1510:G:H1	1.61	0.48
1:2A:2144:U:H1'	1:2A:2148:G:N2	2.29	0.48
1:2A:2600:A:H2'	1:2A:2601:C:C6	2.49	0.48
1:2A:666:G:OP2	1:2A:725:G:N2	99.34	0.48
1:2A:801:G:O6	5:2F:53:THR:OG1	2.32	0.48
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.13	0.48
20:2Y:91:GLU:OE1	20:2Y:91:GLU:N	2.45	0.48
28:16:12:GLU:OE1	28:16:19:ARG:NH1	2.47	0.48
1:1A:103:C:H2'	1:1A:104:C:H6	1.79	0.48
1:1A:1473:A:H4'	1:1A:1474:C:O4'	2.13	0.48
1:1A:1674:G:H2'	1:1A:1675:U:C6	2.47	0.48
28:26:25:LYS:NZ	28:26:51:GLU:OE2	2.35	0.48
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.48	0.48
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.49	0.48
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.49	0.48
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.48	0.48
1:1A:1634:C:H2'	1:1A:1635:C:H6	1.79	0.48
1:1A:1827:U:H2'	1:1A:1828:C:H6	1.79	0.48
1:1A:2564:2MU:H2'	1:1A:2566:U:OP2	2.14	0.48
1:1A:2745:G:H3'	1:1A:2746:A:O4'	2.14	0.48
1:1A:2784:C:H2'	1:1A:2785:C:C6	2.49	0.48
5:1F:116:ASP:OD2	5:1F:117:ARG:NH1	2.47	0.48
21:1Z:31:ARG:HD3	21:1Z:94:GLU:OE1	2.14	0.48
29:27:30:VAL:O	29:27:34:ARG:HG2	2.13	0.48
1:2A:1973:G:OP1	61:2A:3869:HOH:O	2.20	0.48
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.12	0.48
1:2A:2441:C:OP2	1:2A:2586:C:O2'	2.31	0.48
2:2B:66:A:N6	2:2B:108:U:H3'	2.29	0.48
3:2D:37:LEU:HD13	3:2D:62:TYR:HB2	1.96	0.48
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.29	0.48
1:2A:957:A:H5'	12:2Q:76:LYS:HG3	1.96	0.48
1:2A:560:C:H4'	16:2U:52:ARG:CZ	2.44	0.48
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.46	0.47
1:1A:116:A:C8	1:1A:117:A:C8	3.02	0.47
1:1A:1232:G:H5''	17:1V:81:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:386:U:O2'	1:1A:387:G:H5''	2.13	0.47
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.43	0.47
22:20:51:VAL:N	22:20:62:LEU:HD12	2.29	0.47
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.28	0.47
1:2A:2127:G:N2	1:2A:2161:C:C2	2.82	0.47
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.14	0.47
14:2S:34:HIS:ND1	14:2S:53:SER:OG	2.46	0.47
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.13	0.47
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.96	0.47
1:1A:1633:A:H2'	1:1A:1634:C:H6	1.77	0.47
1:1A:2122:G:H1	1:1A:2211:U:H3	1.62	0.47
1:2A:266:G:H2'	1:2A:266:G:N3	3.18	0.47
1:2A:918:A:N3	2:2B:80:U:H4'	2.29	0.47
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CD1	2.48	0.47
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.95	0.47
1:1A:1078:A:H2	1:1A:1168:G:H22	1.62	0.47
1:1A:1379:C:OP2	61:1A:4167:HOH:O	2.20	0.47
1:1A:31:C:OP1	61:1A:4161:HOH:O	2.20	0.47
8:1I:38:LEU:HD13	8:1I:40:THR:HG23	1.96	0.47
8:1I:48:GLU:HB3	8:1I:52:ARG:HH22	1.78	0.47
15:1T:15:VAL:HG13	15:1T:79:HIS:CE1	2.49	0.47
27:25:16:ARG:HG3	27:25:17:ASP:N	2.29	0.47
1:2A:1213:A:N3	1:2A:1238:G:O2'	2.43	0.47
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.48	0.47
1:2A:511:U:O4	1:2A:512:G:N1	2.47	0.47
1:2A:928:G:H8	1:2A:928:G:O5'	1.96	0.47
2:2B:42:C:O2'	6:2G:67:LYS:O	2.23	0.47
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.14	0.47
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.14	0.47
14:2S:67:ARG:HH12	14:2S:103:GLU:HB2	1.77	0.47
1:1A:1405:A:H5'	1:1A:1405:A:N3	2.29	0.47
1:1A:2108:U:H2'	1:1A:2109:G:C8	2.50	0.47
1:1A:327:U:H2'	1:1A:328:G:C8	2.50	0.47
8:1I:78:THR:HA	8:1I:143:SER:HG	1.80	0.47
26:24:15:ILE:HB	26:24:32:TYR:HD1	1.79	0.47
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.33	0.47
1:2A:2224:G:H4'	1:2A:2226:C:C2	2.48	0.47
1:2A:68:G:H2'	1:2A:69:C:O4'	2.14	0.47
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.49	0.47
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.96	0.47
14:2S:99:LYS:HE2	14:2S:103:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1110:C:H2'	1:1A:1111:U:O4'	2.14	0.47
1:1A:310:C:H2'	1:1A:311:C:C6	2.49	0.47
1:1A:78:G:O6	1:1A:92:C:N4	28.96	0.47
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.96	0.47
9:1N:62:VAL:CG2	9:1N:66:LYS:HB2	2.44	0.47
12:1Q:16:ARG:O	12:1Q:18:LYS:N	2.48	0.47
25:23:16:PRO:HB2	25:23:18:ASP:OD1	2.14	0.47
26:24:12:ALA:HB3	26:24:26:SER:HB3	1.96	0.47
1:2A:1119:C:H2'	1:2A:1120:G:H8	2.93	0.47
1:2A:1270:C:N4	1:2A:1271:G:O6	13.73	0.47
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	1.96	0.47
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.49	0.47
1:2A:2117:A:O2'	1:2A:2118:U:H5''	2.14	0.47
1:2A:2419:U:H5''	30:28:33:ASN:HB2	1.95	0.47
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.78	0.47
1:2A:446:G:OP1	16:2U:3:ARG:NH1	2.48	0.47
1:2A:526:A:N3	1:2A:2044:C:H1'	2.30	0.47
1:2A:573:G:O2'	1:2A:574:C:H3'	2.13	0.47
1:2A:614(C):A:C4	5:2F:180:GLY:HA3	2.49	0.47
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.49	0.47
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.33	0.47
22:10:46:LYS:HD2	22:10:78:TYR:CZ	2.49	0.47
1:1A:1101:G:H2'	1:1A:1102:G:O4'	2.14	0.47
1:1A:1199:C:H2'	1:1A:1200:G:O4'	2.14	0.47
1:1A:1245:C:H5'	61:1A:4421:HOH:O	2.14	0.47
1:1A:2162:C:O2	1:1A:2173:G:N1	2.25	0.47
1:1A:268:G:H4'	23:11:81:LYS:HG2	1.97	0.47
28:26:34:LEU:HB2	28:26:51:GLU:HB3	1.96	0.47
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.50	0.47
1:2A:1434:A:H61	1:2A:1558:A:N6	2.09	0.47
1:2A:2141:G:C5	1:2A:2151:G:C2	3.03	0.47
1:2A:262:A:H2'	1:2A:263:C:O4'	2.14	0.47
1:2A:286:C:H2'	1:2A:287:C:C6	2.50	0.47
3:2D:3:VAL:HG13	3:2D:17:THR:HB	1.96	0.47
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.28	0.47
7:2H:97:ARG:O	7:2H:104:GLU:N	2.44	0.47
29:17:5:TRP:NE1	29:17:7:PRO:HG3	2.29	0.47
1:1A:2857:U:OP1	15:1T:98:LYS:NZ	2.46	0.47
1:1A:698:G:H2'	1:1A:699:C:C6	2.49	0.47
8:1I:123:LEU:HD12	8:1I:144:VAL:HG23	1.97	0.47
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:615:G:OP2	5:2F:43:LYS:NZ	2.22	0.47
1:2A:708:C:H42	1:2A:723:G:H1	1.63	0.47
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.63	0.47
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.41	0.47
7:2H:87:LEU:O	7:2H:131:VAL:N	2.47	0.47
10:2O:119:PRO:HB2	15:2T:68:TYR:CZ	2.50	0.47
1:1A:1441:A:OP1	61:1A:4166:HOH:O	2.20	0.47
1:1A:1775:C:H5'	1:1A:1776:G:OP2	2.14	0.47
1:1A:2162:C:N3	1:1A:2173:G:C6	2.83	0.47
1:1A:2724:U:OP1	1:1A:2727:G:H4'	2.15	0.47
3:1D:95:LEU:HD11	3:1D:105:ILE:HD13	1.95	0.47
15:1T:118:ARG:HD3	15:1T:118:ARG:HA	1.59	0.47
1:2A:2022:U:OP2	27:25:15:ARG:NH2	2.48	0.47
1:2A:2507:C:H5''	1:2A:2573:C:C4	2.49	0.47
1:2A:2674:G:H2'	1:2A:2675:A:C8	2.50	0.47
1:2A:2689:U:P	1:2A:2719:G:H22	2.38	0.47
1:2A:902:C:H2'	1:2A:903:C:H6	1.80	0.47
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.48	0.47
1:1A:1115:A:H1'	1:1A:1142:A:H4'	1.97	0.47
1:1A:1554:A:O2'	1:1A:1555:C:H5''	2.15	0.47
1:1A:905:U:O2	1:1A:2280:A:H2'	2.15	0.47
1:1A:2856:G:H2'	1:1A:2857:U:O4'	2.15	0.47
1:1A:936:C:OP2	1:1A:936:C:H2'	2.14	0.47
1:1A:273:G:N2	8:1I:50:ARG:HH11	2.12	0.47
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.50	0.47
1:2A:1010:A:N3	1:2A:1153:C:H1'	2.29	0.47
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.49	0.47
1:2A:2638:G:OP1	4:2E:82:ARG:NH2	2.31	0.47
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.48	0.47
1:2A:334:C:OP1	1:2A:336:C:N4	2.48	0.47
1:2A:392:C:H5''	1:2A:409:C:H5''	1.97	0.47
15:2T:26:ASP:O	15:2T:49:VAL:HG22	2.15	0.47
1:1A:1617:A:H2'	1:1A:1618:A:C8	2.50	0.47
1:1A:2205:C:O2'	1:1A:2206:G:OP1	2.30	0.47
1:1A:2365:G:H5''	22:10:32:ARG:NH1	2.30	0.47
1:1A:2658:C:H2'	1:1A:2659:U:O4'	2.15	0.47
1:1A:313:A:N6	1:1A:375:G:O2'	2.48	0.47
23:21:21:ARG:HD3	23:21:35:THR:HG21	1.95	0.47
25:23:18:ASP:OD1	25:23:18:ASP:N	2.48	0.47
1:2A:2815:C:C5'	27:25:29:THR:HG21	2.45	0.47
1:2A:2218:U:N3	23:21:55:GLY:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.13	0.47
1:2A:2638:G:P	4:2E:82:ARG:HH12	2.37	0.47
1:2A:34:C:H2'	1:2A:35:G:C8	4.89	0.47
19:2X:9:LEU:HA	24:22:36:ARG:HH21	1.80	0.47
1:1A:1108:G:N2	1:1A:1134:A:C6	2.83	0.47
1:1A:2732:G:O6	61:1A:4169:HOH:O	2.20	0.47
1:1A:843:C:H2'	1:1A:844:C:C6	2.49	0.47
26:24:64:GLY:C	26:24:66:SER:H	2.18	0.47
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.51	0.47
1:2A:1913:A:H4'	1:2A:1914:C:H5''	1.96	0.47
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.30	0.47
1:2A:557:U:H2'	1:2A:558:G:H8	1.80	0.47
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.48	0.47
1:2A:993:G:H1'	17:2V:89:GLN:OE1	2.15	0.47
2:2B:43:C:O4'	6:2G:66:GLN:NE2	2.47	0.47
18:2W:12:ILE:O	18:2W:101:SER:OG	2.30	0.47
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.35	0.47
1:1A:1109:G:C5	1:1A:1110:C:N4	2.84	0.46
1:1A:1137:G:C6	1:1A:1138:C:C4	3.03	0.46
1:1A:1546:G:H2'	1:1A:1547:C:C6	2.50	0.46
1:1A:1660:A:P	1:1A:1660:A:H8	2.38	0.46
1:1A:2671:G:OP1	7:1H:158:HIS:NE2	2.47	0.46
1:1A:580:U:H2'	1:1A:581:G:O4'	2.79	0.46
17:1V:29:PRO:HA	17:1V:61:VAL:HG22	1.97	0.46
22:20:53:MET:HG3	22:20:59:LEU:HD23	1.97	0.46
1:2A:1161:C:H2'	1:2A:1162:G:H8	1.79	0.46
1:2A:117:G:OP2	1:2A:119:A:O2'	2.29	0.46
1:2A:2114:A:H2'	1:2A:2114:A:N3	2.30	0.46
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.62	0.46
1:1A:1299:A:H2'	1:1A:1299:A:N3	4.79	0.46
1:1A:275:C:H2'	1:1A:276:C:C6	2.50	0.46
1:1A:463:C:H2'	1:1A:464:G:C8	2.50	0.46
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.16	0.46
26:24:40:HIS:CD2	26:24:41:PRO:HD2	2.50	0.46
1:2A:2096:U:H3	1:2A:2193:G:H1	1.63	0.46
23:11:91:LYS:HA	23:11:94:LEU:HD12	1.98	0.46
1:1A:1102:G:H21	1:1A:1149:A:H62	1.64	0.46
5:1F:148:LEU:HD13	5:1F:154:VAL:HG21	1.97	0.46
1:2A:1523:U:H2'	1:2A:1524:G:O4'	2.15	0.46
1:2A:443:A:H5''	1:2A:444:C:OP1	2.15	0.46
1:2A:582:G:H2'	1:2A:583:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1836:U:O2	3:1D:50:THR:HB	2.14	0.46
1:1A:2210:C:H2'	1:1A:2211:U:O4'	2.15	0.46
1:1A:1757:C:O2'	1:1A:2868:C:N3	2.43	0.46
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.45	0.46
12:1Q:34:LEU:HD11	12:1Q:129:THR:HB	1.96	0.46
28:26:23:THR:OG1	28:26:24:GLU:N	2.47	0.46
1:2A:1179:C:H2'	1:2A:1180:C:C6	2.51	0.46
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.50	0.46
1:2A:2065:C:H2'	1:2A:2066:C:H6	1.80	0.46
1:2A:2554:U:H2'	1:2A:2555:U:C6	2.50	0.46
1:2A:320:A:H4'	1:2A:322:A:N7	2.30	0.46
1:2A:1799:G:O3'	3:2D:183:ARG:NH1	2.48	0.46
4:2E:54:GLN:OE1	4:2E:55:ASN:N	2.48	0.46
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	1.97	0.46
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	1.96	0.46
1:1A:1688:A:H2'	1:1A:1689:G:O4'	2.16	0.46
1:1A:831:A:N6	3:1D:229:VAL:HG11	2.31	0.46
7:1H:124:GLU:HG3	7:1H:132:ARG:HB3	1.97	0.46
1:1A:1698:G:OP1	13:1R:40:LYS:NZ	2.49	0.46
1:2A:1913:A:H4'	1:2A:1914:C:C5'	2.46	0.46
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.15	0.46
1:2A:2752:C:H2'	1:2A:2753:A:O4'	2.15	0.46
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.50	0.46
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.16	0.46
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.59	0.46
1:1A:1052:C:C2	1:1A:1183:G:N2	2.84	0.46
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.51	0.46
1:1A:1400:A:H2'	1:1A:1401:G:O4'	2.15	0.46
1:1A:1653:C:N4	1:1A:1668:G:OP2	2.44	0.46
1:2A:1027:A:C6	1:2A:1126:A:C4	3.03	0.46
1:2A:1426:G:O2'	1:2A:1572:A:N6	2.45	0.46
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.51	0.46
1:2A:1533:G:N2	1:2A:1536:C:O2'	2.49	0.46
1:2A:200:U:O2	1:2A:386:G:N2	2.48	0.46
1:2A:538:G:H5'	9:2N:5:VAL:HG11	1.98	0.46
1:1A:231:G:C8	30:18:5:LYS:HG2	2.50	0.46
31:19:17:ILE:HD11	31:19:24:TYR:HB2	1.97	0.46
1:1A:2128:G:H2'	1:1A:2129:C:C6	2.51	0.46
1:1A:2298:A:H4'	1:1A:2299:A:O4'	2.16	0.46
1:1A:2370:G:N1	61:1A:4194:HOH:O	2.24	0.46
1:1A:738:C:H2'	1:1A:739:C:C6	3.00	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:831:A:OP2	61:1A:4165:HOH:O	2.20	0.46
12:1Q:85:LYS:HD2	12:1Q:85:LYS:N	2.31	0.46
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.98	0.46
1:1A:2694:U:O2'	15:1T:58:ASN:ND2	2.49	0.46
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.16	0.46
1:2A:1475:G:C2	1:2A:1517:G:C2	3.04	0.46
1:2A:2119:A:C5	1:2A:2170:A:C6	3.04	0.46
1:2A:276:A:H5''	1:2A:277:C:H5'	1.98	0.46
1:2A:340:A:H2'	1:2A:341:G:O4'	2.16	0.46
5:2F:56:GLU:OE1	5:2F:93:LYS:NZ	2.49	0.46
8:2I:53:ALA:O	8:2I:57:ARG:HG2	2.15	0.46
19:2X:35:THR:HG22	19:2X:37:THR:N	2.31	0.46
30:18:52:LYS:HE2	30:18:52:LYS:HB3	1.71	0.46
1:1A:1108:G:P	1:1A:1116:A:H1'	2.56	0.46
12:1Q:85:LYS:HD3	22:10:7:LEU:HD12	1.97	0.46
1:2A:1297:C:H1'	1:2A:1298:C:H5	5.01	0.46
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.30	0.46
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.51	0.46
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.31	0.46
1:2A:243:U:OP1	30:28:6:THR:OG1	2.29	0.46
1:2A:1637:A:H4'	1:2A:2711:A:O2'	2.16	0.46
1:2A:2815:C:H2'	1:2A:2816:C:C6	2.51	0.46
1:2A:952:G:C6	1:2A:966:G:C6	3.04	0.46
1:1A:329:U:H2'	1:1A:330:U:C6	2.50	0.46
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.33	0.46
1:1A:236:G:H4'	1:1A:413:G:C5	2.50	0.46
1:1A:704:U:H2'	1:1A:705:C:C6	2.51	0.46
9:1N:77:GLY:O	61:1N:301:HOH:O	2.20	0.46
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.51	0.46
10:1O:86:ILE:HG21	10:1O:94:ARG:HH11	1.81	0.46
1:2A:1818:U:OP2	3:2D:157:ARG:HD3	2.15	0.46
1:2A:362:U:O2'	1:2A:363:G:H5''	2.16	0.46
1:2A:990:A:H1'	1:2A:1156:A:N3	2.30	0.46
30:18:42:ARG:NH1	61:18:5001:HOH:O	2.13	0.46
1:1A:1110:C:N3	1:1A:1120:G:C6	2.84	0.46
1:1A:2549:U:H2'	1:1A:2550:C:C6	2.51	0.46
1:1A:310:C:H2'	1:1A:311:C:H6	1.81	0.46
3:1D:275:LYS:HG3	3:1D:276:LYS:HB2	1.98	0.46
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.81	0.46
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.51	0.46
7:2H:59:ARG:HD2	7:2H:59:ARG:HA	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:73:GLU:OE2	15:2T:103:ARG:NE	2.48	0.46
16:2U:16:LYS:HB3	16:2U:16:LYS:HE2	1.73	0.46
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.51	0.45
1:1A:801:C:H2'	1:1A:802:C:H6	1.81	0.45
2:1B:14:U:O3'	2:1B:108:U:O2'	2.34	0.45
13:1R:44:LEU:HA	13:1R:44:LEU:HD23	1.85	0.45
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.97	0.45
15:1T:91:ARG:HH11	15:1T:120:ARG:NH1	2.13	0.45
22:20:32:ARG:H	22:20:35:ASN:ND2	2.13	0.45
1:2A:2126:A:H61	1:2A:2162:G:C2'	2.28	0.45
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.31	0.45
1:2A:855:G:H2'	1:2A:856:C:C6	2.51	0.45
5:2F:120:GLU:HG3	5:2F:122:LYS:CG	2.46	0.45
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	1.97	0.45
25:13:18:ASP:OD1	25:13:18:ASP:N	2.49	0.45
26:14:41:PRO:HG3	26:14:49:PHE:CE1	2.52	0.45
1:1A:1000:C:OP1	12:1Q:87:LYS:NZ	2.32	0.45
1:1A:1221:G:H1'	1:1A:1222:A:C5'	2.46	0.45
1:1A:1343:C:OP2	61:1A:4171:HOH:O	2.21	0.45
1:1A:2120:U:H3	1:1A:2213:G:H1	1.62	0.45
1:1A:662:A:OP1	11:1P:133:SER:OG	2.31	0.45
3:1D:35:LYS:HE2	3:1D:64:ILE:HG12	1.98	0.45
6:1G:15:VAL:HG13	6:1G:175:LEU:HB3	1.98	0.45
22:20:48:GLY:H	22:20:51:VAL:HB	1.81	0.45
1:2A:851:U:O2'	25:23:42:ALA:O	2.30	0.45
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.51	0.45
1:2A:1547:C:H2'	1:2A:1548:C:C6	2.51	0.45
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	1.98	0.45
1:2A:2119:A:N6	1:2A:2171:A:C6	2.84	0.45
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.51	0.45
1:2A:531:C:OP1	1:2A:561:G:N2	2.49	0.45
9:2N:103:VAL:O	9:2N:107:LEU:HG	2.16	0.45
10:2O:73:ASP:OD2	15:2T:32:TYR:OH	2.30	0.45
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.98	0.45
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.99	0.45
4:2E:9:VAL:HG23	15:2T:7:ILE:HD11	1.97	0.45
1:1A:1218:G:N2	1:1A:1222:A:OP2	2.43	0.45
1:1A:1831:C:OP1	3:1D:260:ARG:NH2	2.49	0.45
1:1A:2163:G:C6	1:1A:2164:C:C2	3.04	0.45
1:1A:733:G:N2	1:1A:835:A:H61	2.15	0.45
4:1E:191:PRO:HD2	61:1E:410:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:66:LYS:HA	10:1O:79:PHE:O	2.15	0.45
14:1S:61:ASN:O	14:1S:65:VAL:HG23	2.16	0.45
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.69	0.45
1:2A:532:A:N6	1:2A:1206:G:O2'	62.55	0.45
1:2A:2473:U:H2'	1:2A:2473:U:O2	2.15	0.45
1:2A:26:G:C6	1:2A:27:G:N1	2.84	0.45
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.97	0.45
7:2H:25:LYS:HE3	7:2H:27:LYS:HZ1	1.82	0.45
26:14:20:ASN:OD1	26:14:21:VAL:N	2.50	0.45
1:1A:1047:A:H2'	1:1A:1048:G:O4'	2.17	0.45
1:1A:1405:A:C2	1:1A:1418:U:O4	2.67	0.45
1:1A:2096:U:H2'	1:1A:2097:U:C6	2.52	0.45
1:1A:2786:C:H2'	1:1A:2787:C:H6	1.81	0.45
1:1A:320:C:H2'	1:1A:321:C:H6	1.81	0.45
1:1A:671:A:H2'	1:1A:672:G:O4'	2.16	0.45
14:1S:87:PHE:HB2	14:1S:112:PHE:CE1	2.51	0.45
1:1A:1057:G:P	16:1U:77:SER:HG	2.38	0.45
1:2A:752:A:P	29:27:3:ARG:HH22	2.39	0.45
1:2A:1219:G:N2	1:2A:1221:C:N3	2.64	0.45
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.26	0.45
1:2A:1784:A:H5''	61:2A:3978:HOH:O	2.15	0.45
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.17	0.45
1:2A:2734:A:H2'	1:2A:2735:G:O4'	2.17	0.45
1:2A:795:C:H2'	1:2A:796:C:C6	2.52	0.45
3:2D:222:ARG:NH1	3:2D:224:ALA:HB3	2.31	0.45
10:2O:63:VAL:HG11	10:2O:85:VAL:HG23	1.98	0.45
11:2P:121:LYS:HG2	11:2P:123:LEU:HG	1.99	0.45
13:2R:28:LEU:HD22	13:2R:48:VAL:HG21	1.99	0.45
14:2S:94:TYR:CZ	14:2S:99:LYS:HG3	2.51	0.45
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.16	0.45
25:13:6:VAL:HG12	25:13:28:LEU:HD11	1.99	0.45
1:1A:2143:G:OP2	1:1A:2143:G:H8	1.98	0.45
12:1Q:38:GLU:HA	12:1Q:99:PRO:HG3	1.98	0.45
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.16	0.45
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.99	0.45
26:24:40:HIS:HD1	26:24:43:TYR:HD2	1.64	0.45
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.32	0.45
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.16	0.45
1:2A:2190:G:H2'	1:2A:2191:G:O4'	2.16	0.45
1:2A:500:G:N1	1:2A:503:A:OP2	2.50	0.45
1:2A:848:G:C4	1:2A:933:A:H8	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:868:U:C4	1:2A:869:G:N7	2.84	0.45
2:2B:80:U:H2'	2:2B:81:G:C8	2.51	0.45
6:2G:39:ILE:HG12	6:2G:157:ILE:HG12	1.99	0.45
25:13:6:VAL:HG13	25:13:54:VAL:CG1	2.39	0.45
26:14:63:TYR:CD1	26:14:63:TYR:N	2.84	0.45
30:18:32:LEU:O	30:18:36:LYS:HE3	2.17	0.45
1:1A:1110:C:O2	1:1A:1120:G:N1	2.29	0.45
1:1A:1615:G:H5''	3:1D:61:LEU:HD13	1.98	0.45
1:1A:1704:C:H2'	1:1A:1705:C:C6	2.51	0.45
1:1A:441:C:H2'	1:1A:442:A:C8	2.51	0.45
4:1E:54:GLN:HB2	4:1E:76:ARG:HG2	1.99	0.45
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.17	0.45
1:2A:459:U:H4'	29:27:40:TRP:CZ3	2.52	0.45
1:2A:1183:G:H2'	1:2A:1184:G:H8	1.82	0.45
1:2A:118:A:OP2	1:2A:119:A:H5''	2.17	0.45
1:2A:906:G:O4'	12:2Q:29:PHE:HE2	2.00	0.45
6:2G:123:ASN:O	6:2G:125:PHE:N	2.49	0.45
9:2N:33:LEU:HD12	9:2N:38:HIS:CD2	2.52	0.45
12:2Q:42:ILE:HD13	12:2Q:97:VAL:HB	1.97	0.45
13:2R:98:LEU:HB2	13:2R:113:LEU:HD11	1.99	0.45
21:2Z:159:PRO:HA	21:2Z:160:GLY:HA2	1.54	0.45
21:2Z:23:LYS:HD2	21:2Z:40:ASP:HA	1.99	0.45
1:1A:1099:C:N4	1:1A:1152:G:H1	2.11	0.45
1:1A:2171:G:C6	1:1A:2172:U:C2	3.04	0.45
1:1A:613:A:H2'	1:1A:614:C:O4'	2.16	0.45
3:1D:61:LEU:O	3:1D:63:ARG:NH1	2.50	0.45
11:1P:116:GLY:O	11:1P:137:LYS:NZ	2.37	0.45
14:1S:110:LEU:HA	14:1S:110:LEU:HD12	1.78	0.45
13:2R:33:ARG:NH2	27:25:57:VAL:O	2.49	0.45
28:26:18:ARG:HD2	28:26:42:TRP:CD1	2.51	0.45
1:2A:2186:G:H2'	1:2A:2187:G:H8	1.81	0.45
1:2A:2252:G:H2'	1:2A:2253:G:O4'	2.17	0.45
1:2A:2562:U:H4'	10:2O:25:LEU:HD21	1.98	0.45
1:2A:13:A:N6	1:2A:526:A:OP2	2.45	0.45
2:2B:38:C:O2	2:2B:48:A:H1'	2.17	0.45
7:2H:38:SER:HB2	7:2H:64:LEU:HD22	1.99	0.45
24:12:25:VAL:HG13	24:12:29:LYS:HD2	1.98	0.45
25:13:4:LEU:O	25:13:36:VAL:HA	2.17	0.45
26:14:40:HIS:HB3	26:14:43:TYR:CD2	2.52	0.45
1:1A:1099:C:C2	1:1A:1100:A:H1'	2.52	0.45
1:1A:185:A:N3	1:1A:185:A:H2'	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1921:G:H2'	1:1A:1921:G:N3	2.32	0.45
1:1A:2021:C:H4'	1:1A:2736:C:O2	2.17	0.45
1:1A:2134:G:C2	1:1A:2135:U:H1'	2.51	0.45
1:1A:2164:C:N3	1:1A:2171:G:C6	2.85	0.45
12:1Q:1:MET:HB3	12:1Q:44:ALA:HB1	1.99	0.45
1:2A:2390:U:P	30:28:35:GLN:HE22	2.40	0.45
1:2A:2663:G:H3'	1:2A:2664:G:H8	1.81	0.45
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.17	0.45
1:2A:274:G:H2'	1:2A:275:G:C8	2.52	0.45
1:2A:601:C:O2	1:2A:605:C:H4'	2.17	0.45
4:2E:49:LEU:HD21	4:2E:91:VAL:HG21	1.98	0.45
11:2P:39:LYS:CB	11:2P:45:LEU:HG	2.35	0.45
14:2S:105:ALA:O	14:2S:110:LEU:HB2	2.17	0.45
1:1A:1312:G:O5'	18:1W:15:ARG:NH2	2.50	0.45
1:1A:2754:A:OP1	31:19:22:ARG:NH2	2.32	0.45
2:1B:78:A:C2	2:1B:100:A:C4	3.04	0.45
10:1O:63:VAL:HG23	10:1O:64:ARG:HG2	1.99	0.45
13:1R:54:LEU:HA	13:1R:54:LEU:HD12	1.84	0.45
15:1T:22:PHE:HB3	15:1T:88:ILE:HD11	1.98	0.45
1:2A:2792:G:N3	1:2A:2792:G:H2'	2.31	0.45
6:2G:150:ASP:OD1	6:2G:153:ARG:NH2	2.48	0.45
30:18:26:LYS:HG2	30:18:46:ARG:O	2.16	0.45
1:1A:1273:G:C2	1:1A:1274:G:H1'	3.50	0.45
1:1A:2290:A:OP2	22:10:12:ASN:ND2	2.50	0.45
1:1A:2527:C:O2'	1:1A:2528:G:H5'	2.17	0.45
2:1B:91:C:H5'	12:1Q:18:LYS:HG2	1.99	0.45
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.49	0.45
9:1N:67:LEU:HB3	9:1N:88:GLU:HG3	1.98	0.45
1:2A:1628:G:H2'	1:2A:1629:U:C6	2.52	0.45
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	1.98	0.45
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.51	0.45
16:2U:52:ARG:HG3	16:2U:55:ARG:NH2	2.31	0.45
21:2Z:45:ASP:O	21:2Z:49:ARG:HG2	2.17	0.45
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.14	0.45
31:19:10:ILE:HD11	31:19:34:GLN:HE21	1.82	0.44
1:1A:2659:U:H2'	1:1A:2660:C:C6	2.53	0.44
1:1A:2699:U:H2'	1:1A:2700:U:O4'	2.18	0.44
6:1G:11:TYR:OH	6:1G:32:PRO:O	2.30	0.44
11:1P:77:ARG:HB2	11:1P:78:PRO:HD2	1.98	0.44
1:1A:543:G:H4'	18:1W:18:ARG:NE	2.32	0.44
1:1A:794:U:H4'	18:1W:92:ARG:HH22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:55:ASN:O	19:1X:80:ILE:N	2.42	0.44
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.75	0.44
24:22:35:LEU:HD12	24:22:53:LEU:HD12	1.99	0.44
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.25	0.44
1:2A:2152:G:C2	1:2A:2153:G:H1'	2.52	0.44
1:2A:253:C:OP2	30:28:5:LYS:NZ	2.36	0.44
1:2A:70:G:H5''	1:2A:112:U:O2	2.16	0.44
19:2X:50:LYS:HB3	19:2X:87:GLN:HE22	1.82	0.44
1:1A:2734:A:H8	1:1A:2734:A:O5'	2.00	0.44
1:1A:2830:A:OP2	13:1R:2:ARG:NH2	2.51	0.44
16:1U:102:GLU:HB3	16:1U:104:GLN:NE2	2.32	0.44
19:1X:64:LYS:HD3	19:1X:64:LYS:HA	1.82	0.44
26:24:57:GLU:HA	26:24:58:ARG:HA	1.65	0.44
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.51	0.44
1:2A:1161:C:H2'	1:2A:1162:G:C8	2.51	0.44
1:2A:1489:U:HO2'	1:2A:1490:A:H8	1.62	0.44
1:2A:2444:G:OP2	5:2F:68:LYS:NZ	2.35	0.44
1:2A:479:A:HO2'	1:2A:481:G:H8	1.64	0.44
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.31	0.44
11:2P:97:PRO:HG3	11:2P:112:LEU:HD12	1.99	0.44
21:2Z:163:LEU:HG	21:2Z:165:VAL:HG22	1.99	0.44
1:1A:1859:G:OP2	1:1A:1859:G:H8	2.00	0.44
3:1D:127:VAL:HA	3:1D:193:VAL:HG22	2.00	0.44
6:1G:15:VAL:HG21	6:1G:176:LEU:HD23	1.99	0.44
8:1I:6:LEU:HG	8:1I:36:ALA:HA	1.99	0.44
13:1R:56:LYS:NZ	13:1R:90:ARG:O	2.50	0.44
1:2A:1639:U:C2'	1:2A:1640:C:H5''	2.47	0.44
1:2A:211:A:H2'	1:2A:212:G:O4'	2.17	0.44
1:2A:2149:G:C6	1:2A:2150:U:C2	3.05	0.44
1:2A:2427:C:H5''	1:2A:2428:G:OP1	2.17	0.44
1:2A:455:C:N3	1:2A:472:A:H2'	2.32	0.44
1:2A:652(B):A:N6	1:2A:655:A:H1'	2.32	0.44
2:2B:55:U:H2'	2:2B:56:G:O4'	2.17	0.44
18:2W:45:TYR:CZ	18:2W:49:LYS:HE3	2.53	0.44
61:1A:5058:HOH:O	22:10:14:ARG:HB2	2.17	0.44
1:1A:1222:A:H2'	1:1A:1222:A:N3	2.33	0.44
1:1A:757:G:H2'	1:1A:758:G:C8	2.52	0.44
6:1G:61:ALA:HB1	26:14:7:PRO:HG3	1.99	0.44
15:1T:33:LYS:HA	15:1T:42:ILE:HD13	1.99	0.44
18:1W:6:ILE:HA	18:1W:103:ILE:O	2.18	0.44
1:2A:1020:A:N1	1:2A:1141:U:H1'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2872:G:C2	1:2A:2873:A:N6	2.84	0.44
1:2A:307:G:H21	1:2A:330:A:H62	1.66	0.44
6:2G:5:VAL:HG23	6:2G:8:LYS:HB2	2.00	0.44
1:2A:910:A:H62	12:2Q:12:GLN:HA	1.83	0.44
1:2A:747:U:O2'	18:2W:92:ARG:NH1	2.50	0.44
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HG12	2.00	0.44
1:1A:1653:C:H5''	1:1A:1654:A:H5'	1.98	0.44
1:1A:2346:G:H4'	1:1A:2347:A:OP2	2.17	0.44
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.51	0.44
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.20	0.44
16:1U:17:ILE:HG13	16:1U:32:PHE:HE1	1.81	0.44
1:2A:2754:U:O2'	31:29:17:ILE:HD13	2.17	0.44
1:2A:2403:C:N3	1:2A:2415:G:C2	2.86	0.44
1:2A:2494:G:C4	1:2A:2495:G:C8	3.06	0.44
1:2A:27:G:HO2'	1:2A:28:A:P	2.39	0.44
1:2A:324:A:N6	1:2A:338:G:O2'	2.50	0.44
1:2A:942:G:OP1	11:2P:39:LYS:NZ	2.45	0.44
10:2O:80:ASP:OD2	15:2T:64:ARG:NH2	2.44	0.44
20:2Y:73:ARG:HH21	20:2Y:83:THR:C	2.21	0.44
1:1A:1088:G:H2'	1:1A:1089:C:C6	2.52	0.44
1:1A:180:A:H2'	1:1A:181:C:C6	2.52	0.44
1:1A:1830:G:N2	3:1D:155:LEU:HD12	2.32	0.44
3:1D:223:GLY:HA3	3:1D:231:HIS:CE1	2.52	0.44
8:1I:61:ARG:HA	8:1I:61:ARG:HD3	1.61	0.44
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.17	0.44
1:2A:184:C:H2'	1:2A:185:U:H6	1.83	0.44
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.18	0.44
1:2A:2593:U:H2'	1:2A:2594:C:C6	2.52	0.44
1:2A:492:A:H2'	1:2A:493:G:O4'	2.17	0.44
1:2A:597:U:H2'	1:2A:598:G:H8	1.82	0.44
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.50	0.44
11:2P:44:GLY:HA2	11:2P:45:LEU:HB2	2.00	0.44
12:2Q:2:LEU:HG	12:2Q:69:PHE:CE1	2.52	0.44
12:2Q:51:ARG:O	12:2Q:55:VAL:HG13	2.18	0.44
1:1A:1560:U:H2'	1:1A:1561:C:C6	2.53	0.44
1:1A:308:U:H2'	1:1A:309:C:H6	1.80	0.44
1:1A:510:C:H2'	1:1A:511:C:C6	2.53	0.44
1:1A:605:G:H2'	1:1A:606:G:C8	2.52	0.44
27:25:51:TYR:CE2	27:25:56:LYS:HD3	2.52	0.44
1:2A:1218:C:OP2	16:2U:15:LYS:NZ	2.49	0.44
1:2A:1252:G:N3	16:2U:33:ARG:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2833:G:H4'	1:2A:2834:G:OP2	2.17	0.44
1:2A:323:G:O2'	1:2A:1205:U:N3	2.48	0.44
1:2A:330:A:HO2'	1:2A:331:A:H8	1.66	0.44
1:2A:624:C:H2'	1:2A:625:G:C8	3.66	0.44
1:2A:705:A:C2	1:2A:727:A:H1'	2.52	0.44
3:2D:166:GLN:HB2	3:2D:174:ILE:HG22	1.99	0.44
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.47	0.44
9:2N:34:LEU:O	9:2N:49:GLY:HA3	2.17	0.44
13:2R:44:LEU:HD23	13:2R:44:LEU:HA	1.78	0.44
14:2S:4:LEU:HA	14:2S:4:LEU:HD23	1.84	0.44
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.83	0.44
1:1A:1841:A:H2'	1:1A:1842:G:O4'	2.18	0.44
1:1A:2787:C:H2'	1:1A:2788:A:O4'	2.17	0.44
1:1A:2879:G:H2'	1:1A:2880:C:O4'	2.17	0.44
1:1A:942:A:H4'	1:1A:943:C:OP1	2.18	0.44
2:1B:29:A:H2'	2:1B:30:C:O4'	2.18	0.44
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.53	0.44
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.99	0.44
24:22:8:LYS:HA	24:22:8:LYS:HD2	1.79	0.44
1:2A:1022:G:H1	1:2A:1142(A):A:H2	1.64	0.44
1:2A:1027:A:N6	1:2A:1126:A:C4	2.86	0.44
1:2A:1028:A:H2'	1:2A:1029:A:C8	2.53	0.44
1:2A:1217:C:H2'	1:2A:1218:C:O4'	2.61	0.44
1:2A:1263:U:C4	1:2A:1264:G:C6	3.05	0.44
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.53	0.44
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.18	0.44
1:2A:699:A:H2'	1:2A:700:G:O4'	2.17	0.44
1:2A:816:C:N4	1:2A:1192:G:O6	2.51	0.44
1:2A:900:A:C2'	1:2A:901:A:H8	2.27	0.44
1:2A:2773:C:OP1	4:2E:166:THR:OG1	2.34	0.44
9:2N:62:VAL:HG11	9:2N:66:LYS:HB2	1.99	0.44
19:2X:9:LEU:HB2	19:2X:29:TRP:O	2.18	0.44
1:1A:2148:A:H4'	1:1A:2149:G:OP1	2.18	0.44
1:1A:2236:G:H4'	1:1A:2238:C:C2	2.53	0.44
1:1A:2826:C:O2	1:1A:2893:A:O2'	2.35	0.44
1:1A:807:G:OP1	61:1A:4170:HOH:O	2.21	0.44
3:1D:145:VAL:HB	3:1D:155:LEU:HB2	2.00	0.44
7:1H:104:GLU:HG3	7:1H:114:VAL:HG22	2.00	0.44
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.82	0.44
21:1Z:128:VAL:HG23	21:1Z:160:GLY:O	2.17	0.44
1:2A:1016:G:H2'	1:2A:1017:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1242:A:N1	11:2P:4:SER:OG	2.41	0.44
1:2A:1693:U:O3'	3:2D:14:ARG:NH2	2.51	0.44
1:2A:2335:A:C8	1:2A:2337:G:C5	3.06	0.44
1:2A:249:C:H4'	1:2A:250:G:O5'	2.17	0.44
1:2A:2851:A:O2'	13:2R:64:ARG:NH2	2.48	0.44
12:2Q:17:LEU:HD22	12:2Q:96:VAL:HG13	1.99	0.44
19:2X:60:ARG:NH2	29:27:47:ARG:HH12	2.14	0.44
23:11:10:LYS:NZ	23:11:65:SER:OG	2.44	0.43
1:1A:2137:G:H8	1:1A:2137:G:O5'	2.00	0.43
1:1A:2518:U:N3	58:1A:4030:EZG:CG	2.80	0.43
1:1A:624:C:O2'	1:1A:628:C:H5''	2.18	0.43
1:1A:722:A:C8	1:1A:851:A:C6	3.05	0.43
14:1S:3:ARG:HD3	14:1S:3:ARG:HA	1.88	0.43
21:1Z:132:ASN:ND2	21:1Z:160:GLY:HA3	2.33	0.43
25:23:6:VAL:HG12	25:23:28:LEU:HD11	2.00	0.43
30:28:52:LYS:HG2	30:28:56:GLU:OE2	2.17	0.43
1:2A:2161:C:H3'	1:2A:2162:G:C8	2.53	0.43
1:2A:839:U:H2'	1:2A:840:C:C6	2.53	0.43
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	2.00	0.43
7:2H:148:ILE:HG13	7:2H:148:ILE:H	1.50	0.43
14:2S:64:GLU:CD	14:2S:64:GLU:H	3.53	0.43
16:2U:49:HIS:HA	16:2U:52:ARG:HB3	1.98	0.43
19:2X:57:LEU:HD22	19:2X:78:LYS:HE2	2.00	0.43
21:2Z:144:LEU:HD23	21:2Z:145:GLU:H	1.82	0.43
1:1A:1087:C:N4	1:1A:1160:G:H1	2.15	0.43
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.18	0.43
1:1A:2885:C:O2'	15:1T:2:ASN:OD1	2.36	0.43
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.18	0.43
1:2A:1315:C:H42	1:2A:1337:G:H1	1.66	0.43
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.18	0.43
1:2A:320:A:O2'	1:2A:322:A:OP2	2.36	0.43
1:2A:434:U:H2'	1:2A:435:C:C6	6.51	0.43
1:2A:535:C:O3'	16:2U:53:ARG:NH1	2.50	0.43
1:2A:657:U:H2'	1:2A:658:C:C6	2.53	0.43
1:2A:992:C:OP1	16:2U:47:TYR:OH	2.25	0.43
3:2D:253:GLN:HG3	61:2D:412:HOH:O	2.17	0.43
1:1A:1683:C:H2'	1:1A:1684:A:C8	2.53	0.43
1:1A:1973:U:O2	1:1A:1975:A:H8	2.01	0.43
1:1A:2123:G:H2'	1:1A:2124:U:C6	2.53	0.43
2:1B:5:C:O2'	2:1B:27:C:O2	2.35	0.43
10:1O:70:LYS:HE2	10:1O:70:LYS:HB3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	2.00	0.43
18:1W:18:ARG:HG3	18:1W:76:VAL:HB	1.99	0.43
26:24:15:ILE:HB	26:24:32:TYR:CD1	2.54	0.43
26:24:47:GLN:C	26:24:49:PHE:H	2.21	0.43
1:2A:1155:A:H5''	16:2U:55:ARG:HH11	1.83	0.43
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.19	0.43
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.54	0.43
1:2A:478:A:C6	1:2A:480:A:C6	3.07	0.43
1:1A:414:U:P	23:11:20:ARG:HH12	2.40	0.43
26:14:44:THR:O	26:14:46:GLN:N	2.51	0.43
1:1A:1654:A:H1'	1:1A:1656:A:OP2	2.18	0.43
1:1A:2343:G:O2'	1:1A:2348:A:N1	2.45	0.43
1:1A:426:G:OP2	61:1A:4164:HOH:O	2.20	0.43
1:1A:609:A:H5'	5:1F:89:VAL:HG21	2.00	0.43
2:1B:2:C:H2'	2:1B:3:C:H6	1.82	0.43
5:1F:106:ARG:H	5:1F:106:ARG:HG2	1.50	0.43
1:2A:125:G:C6	29:27:10:ARG:HG3	2.53	0.43
1:2A:1528:A:H2'	1:2A:1528(A):A:C8	2.54	0.43
1:2A:1529:G:O6	1:2A:1530:C:N4	2.51	0.43
1:2A:2274:A:C5	1:2A:2276:G:C8	3.05	0.43
1:2A:93:G:H2'	1:2A:94:C:C6	2.53	0.43
4:2E:101:ARG:NH1	4:2E:171:GLU:HB2	2.34	0.43
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.18	0.43
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.51	0.43
1:1A:1387:U:O4'	19:1X:57:LEU:HD23	2.18	0.43
1:1A:1756:U:H2'	1:1A:1757:C:C6	2.53	0.43
1:1A:1935:A:H4'	1:1A:1936:C:H5''	2.00	0.43
1:1A:2372:A:O5'	1:1A:2372:A:H8	2.02	0.43
1:1A:2819:A:H2'	1:1A:2820:A:C8	2.54	0.43
1:1A:332:G:H2'	1:1A:333:G:H8	2.94	0.43
1:1A:703:G:H2'	1:1A:704:U:O4'	2.18	0.43
1:1A:733:G:H8	29:17:6:GLN:O	2.02	0.43
2:1B:23:G:O6	61:1B:302:HOH:O	2.21	0.43
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.19	0.43
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.29	0.43
1:2A:1422:G:H5''	10:2O:48:PRO:CB	100.11	0.43
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.53	0.43
1:2A:212:G:H2'	1:2A:213:A:O4'	2.19	0.43
1:2A:2133:G:O2'	1:2A:2134:A:OP1	2.30	0.43
1:2A:2366:A:H2'	1:2A:2367:G:O4'	2.18	0.43
1:2A:2429:G:OP2	61:2A:3867:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2637:U:H5''	4:2E:82:ARG:NH1	2.34	0.43
3:2D:242:ARG:HG2	3:2D:246:PRO:HG3	1.99	0.43
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.51	0.43
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.18	0.43
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	2.00	0.43
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.45	0.43
1:1A:1410:G:N7	23:11:3:LYS:HD2	2.33	0.43
30:18:23:VAL:CG1	30:18:47:LYS:HB3	2.49	0.43
1:1A:1004:A:H5'	1:1A:1024:G:O6	28.32	0.43
1:1A:1115:A:H4'	1:1A:1116:A:H8	1.83	0.43
1:1A:2769:U:H1'	1:1A:2770:A:H5''	1.99	0.43
1:1A:659:C:H2'	1:1A:660:C:C6	2.54	0.43
2:1B:24:G:N7	2:1B:56:G:H2'	2.33	0.43
2:1B:65:C:O2'	2:1B:66:A:OP1	2.28	0.43
6:1G:46:ALA:HB1	6:1G:50:ALA:O	2.19	0.43
7:1H:3:ARG:HG3	7:1H:4:ILE:N	2.34	0.43
25:23:6:VAL:O	25:23:34:GLU:HA	2.17	0.43
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.18	0.43
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.48	0.43
1:2A:265:A:H8	1:2A:266:G:H1'	1.81	0.43
1:2A:557:U:H2'	1:2A:558:G:C8	2.54	0.43
1:2A:75:G:H4'	24:22:55:ARG:NH1	2.34	0.43
1:2A:859:G:N2	1:2A:917:A:OP2	2.38	0.43
1:2A:956:G:N2	1:2A:959:A:H3'	2.33	0.43
6:2G:111:LEU:HD23	6:2G:117:PHE:CZ	2.53	0.43
6:2G:127:GLY:H	6:2G:166:ASP:CG	2.21	0.43
1:2A:2642:G:H5''	9:2N:78:TYR:CD1	2.53	0.43
14:2S:105:ALA:HB1	14:2S:110:LEU:HD22	2.01	0.43
28:16:2:ALA:HA	28:16:6:ARG:HB2	2.01	0.43
1:1A:1221:G:H21	1:1A:1222:A:H4'	1.84	0.43
1:1A:1851:U:C2	3:1D:202:LYS:HD3	2.53	0.43
10:1O:9:GLU:O	10:1O:83:ALA:HA	2.18	0.43
1:1A:1001:G:H5''	12:1Q:77:LYS:HD2	2.01	0.43
22:20:14:ARG:H	22:20:14:ARG:HG2	1.66	0.43
1:2A:2025:C:H2'	1:2A:2026:C:H6	1.83	0.43
1:2A:2143:C:N3	1:2A:2148:G:N2	2.55	0.43
1:2A:263:C:H2'	1:2A:264:C:O4'	2.19	0.43
1:2A:359:A:H2'	1:2A:360:G:O4'	2.19	0.43
1:2A:864:G:C6	1:2A:865:C:N4	2.87	0.43
2:2B:7:G:H2'	2:2B:8:U:O4'	2.19	0.43
1:1A:1627:A:H8	1:1A:1627:A:OP2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1766:G:H1'	1:1A:1770:A:H61	1.84	0.43
1:1A:596:G:O2'	1:1A:597:C:H3'	2.19	0.43
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	2.00	0.43
8:1I:124:GLY:H	8:1I:144:VAL:HG23	1.82	0.43
10:1O:107:ARG:HD3	15:1T:37:GLY:H	1.84	0.43
18:1W:68:ARG:HH11	18:1W:111:HIS:HA	1.84	0.43
1:2A:1221(A):C:H42	1:2A:1228:G:H1	1.66	0.43
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.18	0.43
1:2A:1669:A:H5''	1:2A:2550:G:OP1	2.17	0.43
1:2A:473:G:H2'	1:2A:474:G:H8	2.78	0.43
1:2A:918:A:C2	2:2B:80:U:H4'	2.53	0.43
20:2Y:28:LYS:HD2	20:2Y:40:GLU:OE1	2.19	0.43
1:1A:1120:G:N1	1:1A:1121:C:H1'	2.34	0.43
1:1A:1514:C:OP2	1:1A:1594:C:H5	2.02	0.43
1:1A:2389:A:H2'	1:1A:2390:A:C8	2.54	0.43
1:1A:442:A:H2'	1:1A:443:C:C6	2.54	0.43
1:1A:776:G:C6	3:1D:208:LYS:HB2	2.54	0.43
1:1A:863:C:H2'	1:1A:864:C:H6	1.83	0.43
3:1D:79:VAL:O	3:1D:114:GLY:N	2.52	0.43
16:1U:97:ASP:OD1	16:1U:101:ARG:NH1	2.51	0.43
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.34	0.43
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.18	0.43
1:2A:332:A:O2'	1:2A:334:C:OP2	2.28	0.43
1:2A:372:G:H8	23:2I:65:SER:O	2.01	0.43
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.19	0.43
6:2G:16:ARG:HB2	6:2G:17:PRO:HD3	2.00	0.43
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.99	0.43
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	2.00	0.43
14:2S:77:ALA:O	14:2S:81:GLY:N	2.52	0.43
15:2T:119:LYS:HG2	15:2T:123:GLN:HE21	1.84	0.43
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	2.00	0.43
25:13:35:ARG:HE	25:13:37:LEU:HD21	1.84	0.43
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.79	0.43
1:1A:1001:G:H2'	1:1A:1002:A:H2'	2.00	0.43
1:1A:2605:U:H2'	1:1A:2606:C:C6	2.54	0.43
30:28:50:LEU:HA	30:28:50:LEU:HD23	1.77	0.43
1:2A:140:G:N2	1:2A:1596:A:H4'	2.33	0.43
1:2A:2175:C:H2'	1:2A:2176:A:O4'	2.18	0.43
1:2A:2100:G:H1	1:2A:2189:U:H3	1.65	0.43
1:2A:271(H):G:H1	1:2A:271(P):C:N4	2.13	0.43
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:275:LYS:HE3	3:2D:276:LYS:O	2.19	0.43
3:2D:275:LYS:HA	3:2D:276:LYS:C	2.40	0.43
1:2A:674:G:O2'	5:2F:74:ARG:HD3	2.19	0.43
6:2G:170:ARG:NH2	6:2G:182:LYS:O	2.52	0.43
7:2H:127:GLU:OE1	7:2H:130:ARG:NE	2.38	0.43
11:2P:59:LEU:HD11	30:28:10:ALA:CB	2.46	0.43
14:2S:66:ALA:O	14:2S:69:VAL:HG12	2.19	0.43
14:2S:14:VAL:HG11	14:2S:90:GLY:O	2.18	0.43
1:1A:1128:U:N3	1:1A:1132:A:N6	2.30	0.42
1:1A:1139:G:H3'	1:1A:1140:U:C5'	2.47	0.42
1:1A:2296:C:OP2	28:16:6:ARG:HG3	2.19	0.42
1:1A:741:U:OP1	3:1D:59:LYS:NZ	2.50	0.42
16:1U:102:GLU:HB3	16:1U:104:GLN:HE22	1.84	0.42
1:1A:1198:C:H1'	16:1U:77:SER:HB3	2.00	0.42
21:1Z:72:ARG:HD3	21:1Z:72:ARG:HA	1.65	0.42
1:2A:1007:C:O2	1:2A:1022:G:N1	18.25	0.42
1:2A:143(A):C:H2'	1:2A:144:C:H6	1.84	0.42
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.19	0.42
1:2A:1965:C:H3'	1:2A:1966:A:H2'	2.01	0.42
1:2A:2023:G:H5'	1:2A:2617:C:H4'	2.01	0.42
1:2A:244:A:C2	1:2A:255:A:C4	3.07	0.42
1:2A:479:A:H4'	1:2A:480:A:OP1	2.18	0.42
9:2N:62:VAL:CG1	9:2N:66:LYS:HB2	2.49	0.42
1:2A:826:U:C4'	11:2P:55:ARG:HB3	2.45	0.42
20:2Y:43:ASN:O	20:2Y:64:GLU:HA	2.19	0.42
1:1A:1102:G:O6	1:1A:1147:U:H5''	2.19	0.42
1:1A:1341:C:H2'	1:1A:1342:G:H8	1.83	0.42
1:1A:2284:U:H5''	1:1A:2285:A:OP1	2.18	0.42
1:1A:262:C:H42	1:1A:282:G:H1	1.66	0.42
1:1A:27:G:N2	1:1A:537:G:H1'	2.34	0.42
5:1F:183:VAL:O	5:1F:187:VAL:HG23	2.18	0.42
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.51	0.42
10:1O:104:ARG:CZ	15:1T:34:VAL:HG11	2.50	0.42
23:21:80:LEU:HB3	23:21:82:LEU:HD21	2.01	0.42
1:2A:1219:G:H1	1:2A:1230:C:H42	1.66	0.42
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	2.00	0.42
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.84	0.42
1:2A:2611:U:OP2	1:2A:2611:U:H3'	2.20	0.42
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.83	0.42
1:1A:1016:C:O2'	1:1A:1029:A:N3	2.45	0.42
1:1A:1212:C:H2'	1:1A:1213:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:125:A:H5''	1:1A:126:C:C6	2.53	0.42
1:1A:1513:G:H2'	1:1A:1594:C:H41	1.83	0.42
1:1A:2158:C:N4	1:1A:2177:G:N1	2.19	0.42
1:1A:2705:A:H2'	1:1A:2706:G:C8	2.54	0.42
1:1A:360:C:H2'	1:1A:361:C:C6	2.55	0.42
4:1E:165:VAL:O	4:1E:189:PRO:HG2	2.19	0.42
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	2.02	0.42
6:1G:159:VAL:HG21	6:1G:173:LEU:HD21	2.02	0.42
8:1I:38:LEU:H	8:1I:38:LEU:HG	1.62	0.42
28:26:10:LEU:HD12	28:26:54:ILE:HA	2.01	0.42
1:2A:1682:G:H1'	1:2A:1762:A:C6	2.54	0.42
1:2A:2108:C:N3	1:2A:2181:G:N2	2.55	0.42
1:2A:2505:G:H2'	1:2A:2576:G:O6	2.18	0.42
1:2A:2600:A:H2'	1:2A:2601:C:H6	1.84	0.42
1:2A:2747:G:OP1	7:2H:74:ASN:ND2	2.51	0.42
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.54	0.42
1:2A:478:A:N1	1:2A:500:G:H4'	2.34	0.42
1:2A:915:C:H3'	1:2A:916:G:H8	1.83	0.42
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.19	0.42
1:2A:1354:A:O3'	3:2D:38:LYS:HE2	2.20	0.42
7:2H:54:ARG:HB3	7:2H:65:HIS:CD2	2.54	0.42
14:2S:71:ARG:H	14:2S:71:ARG:HG3	1.65	0.42
1:1A:1613:A:OP1	3:1D:211:ARG:NH1	2.50	0.42
1:1A:1474:C:O2'	1:1A:1616:A:OP2	2.27	0.42
1:1A:2182:G:C6	1:1A:2183:C:C4	3.06	0.42
1:1A:2224:C:H2'	1:1A:2225:U:O4'	2.20	0.42
1:1A:2603:C:H2'	1:1A:2604:G:C8	2.54	0.42
1:1A:821:A:H2'	1:1A:821:A:N3	2.34	0.42
4:1E:47:VAL:HG22	4:1E:84:PHE:O	2.19	0.42
11:1P:133:SER:O	11:1P:137:LYS:HB2	2.20	0.42
18:1W:11:ARG:C	18:1W:11:ARG:HH11	2.23	0.42
29:27:34:ARG:NH2	29:27:39:ARG:HG2	2.34	0.42
1:2A:1486:A:H2'	1:2A:1487:G:C8	2.54	0.42
1:2A:1613:G:N1	1:2A:1617:C:O2'	2.46	0.42
3:2D:228:PRO:HD3	3:2D:235:GLY:CA	2.50	0.42
4:2E:170:LEU:HB3	4:2E:184:VAL:HG23	2.02	0.42
11:2P:44:GLY:CA	11:2P:45:LEU:HB2	2.49	0.42
14:2S:87:PHE:HB2	14:2S:112:PHE:CE1	2.55	0.42
1:1A:1121:C:O2	1:1A:1122:C:H2'	2.19	0.42
1:1A:1685:C:O3'	1:1A:2721:G:N2	2.53	0.42
1:1A:2314:G:H2'	1:1A:2315:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2429:C:OP1	11:1P:65:ARG:NH2	2.52	0.42
2:1B:16:G:C6	2:1B:69:G:C2	3.08	0.42
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.20	0.42
21:1Z:130:PRO:HA	21:1Z:133:ILE:HG13	2.01	0.42
29:27:37:LYS:HD3	29:27:39:ARG:HD3	2.01	0.42
1:2A:1532:C:N4	1:2A:1537:G:N1	2.68	0.42
1:2A:18:C:H2'	1:2A:19:C:C6	2.55	0.42
1:2A:2270:G:H2'	1:2A:2271:G:O4'	2.20	0.42
1:2A:2432:A:C6	1:2A:2433:A:C6	3.07	0.42
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.20	0.42
1:2A:473:G:H2'	1:2A:474:G:C8	3.34	0.42
1:2A:98:G:P	24:22:2:LYS:HG2	2.60	0.42
5:2F:184:TYR:HE1	11:2P:3:LEU:HD21	1.84	0.42
6:2G:15:VAL:HA	6:2G:175:LEU:HD23	2.02	0.42
7:2H:145:ALA:HA	7:2H:148:ILE:HD12	2.01	0.42
15:2T:114:LEU:HD23	15:2T:114:LEU:HA	1.87	0.42
28:16:6:ARG:HH11	28:16:26:ASN:HB2	1.85	0.42
1:1A:1660:A:C6	18:1W:87:PRO:HB3	2.54	0.42
1:1A:2128:G:H1	1:1A:2205:C:H42	1.66	0.42
1:1A:2180:A:O2'	1:1A:2181:G:OP2	2.32	0.42
1:1A:2418:U:H2'	1:1A:2418:U:H6	1.60	0.42
1:1A:2807:C:N4	1:1A:2813:G:H22	2.17	0.42
1:1A:2819:A:C6	1:1A:2820:A:C6	3.07	0.42
6:1G:174:GLU:HG3	6:1G:180:PHE:CD2	2.55	0.42
22:20:69:PHE:CE1	22:20:79:VAL:HG22	2.55	0.42
29:27:24:THR:O	29:27:28:ARG:HG3	2.20	0.42
11:2P:59:LEU:HD12	30:28:58:ILE:HG12	2.01	0.42
1:2A:271(S):G:H2'	1:2A:271(T):C:C6	2.55	0.42
1:2A:247:G:H4'	1:2A:386:G:C5	2.55	0.42
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	2.01	0.42
18:1W:19:LEU:HB3	27:15:25:LEU:HD11	2.02	0.42
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.49	0.42
1:1A:1056:A:N3	1:1A:1199:C:H1'	2.35	0.42
1:1A:1993:A:C4	3:1D:241:PRO:HD3	2.55	0.42
1:1A:2188:G:N7	1:1A:2190:G:N2	2.68	0.42
1:1A:2193:A:O2'	1:1A:2194:U:H5''	2.20	0.42
1:1A:320:C:H2'	1:1A:321:C:C6	2.55	0.42
1:1A:863:C:H2'	1:1A:864:C:C6	2.54	0.42
3:1D:183:ARG:NH2	3:1D:266:SER:HB2	2.34	0.42
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.55	0.42
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.18	0.42
1:2A:77:C:OP1	24:22:59:ARG:HD3	2.20	0.42
18:2W:43:GLY:O	18:2W:47:VAL:HG23	2.20	0.42
1:1A:2225:U:O2'	1:1A:2226:C:H5'	2.20	0.42
1:1A:2517:G:O6	1:1A:2588:G:H2'	2.20	0.42
1:1A:2821:G:N2	1:1A:2900:G:H1'	2.34	0.42
1:1A:342:C:N4	1:1A:347:G:O6	5.70	0.42
1:1A:599:U:H2'	1:1A:600:G:C8	2.55	0.42
5:1F:164:ARG:HD2	5:1F:175:THR:HG23	2.01	0.42
6:1G:138:GLN:N	6:1G:138:GLN:OE1	2.39	0.42
7:1H:88:LEU:HD23	7:1H:130:ARG:HG2	2.01	0.42
1:2A:1270:C:H4'	1:2A:1325:G:N7	2.35	0.42
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.44	0.42
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.19	0.42
1:2A:2859:G:H2'	1:2A:2860:A:C8	2.55	0.42
1:2A:272(G):C:H42	1:2A:363(C):G:H1	1.68	0.42
1:2A:530:G:O4'	1:2A:530:G:N3	2.52	0.42
1:2A:531:C:H4'	1:2A:532:A:H5''	2.01	0.42
1:2A:848:G:N9	1:2A:933:A:H8	2.18	0.42
2:2B:55:U:O2'	6:2G:27:ASN:ND2	2.42	0.42
1:2A:1805:U:O2	3:2D:50:THR:HB	2.20	0.42
4:2E:52:LEU:O	4:2E:76:ARG:HG3	2.20	0.42
6:2G:111:LEU:HA	6:2G:114:ILE:HD12	2.01	0.42
10:2O:40:VAL:HG22	10:2O:59:LYS:HG2	2.00	0.42
1:2A:2296:U:OP2	14:2S:6:ALA:HB2	2.20	0.42
1:1A:2490:A:H5'	31:19:31:LYS:HE2	2.01	0.42
1:1A:2227:G:H5''	1:1A:2228:G:C8	2.55	0.42
1:1A:2418:U:H2'	1:1A:2418:U:OP2	2.20	0.42
1:1A:2803:A:H5''	1:1A:2804:C:H5''	2.01	0.42
1:1A:692:C:H2'	1:1A:693:G:O4'	2.19	0.42
1:1A:2523:U:O2'	4:1E:138:PRO:O	2.31	0.42
7:1H:152:ARG:HD3	7:1H:152:ARG:HA	1.84	0.42
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.54	0.42
10:1O:17:ARG:HA	10:1O:17:ARG:HD3	1.90	0.42
16:1U:83:LEU:HD13	16:1U:113:ALA:HB2	2.02	0.42
1:2A:1425:G:C6	1:2A:1426:G:C6	3.07	0.42
1:2A:171:G:H2'	1:2A:172:C:H6	1.85	0.42
1:2A:2182:G:H2'	1:2A:2183:C:C6	2.55	0.42
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.19	0.42
1:2A:300:A:H8	1:2A:300:A:O5'	3.03	0.42
8:2I:93:THR:O	8:2I:97:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:120:GLU:HG2	10:2O:122:LEU:HG	2.01	0.42
15:2T:127:ALA:C	15:2T:129:ARG:H	2.22	0.42
1:1A:2283:G:OP1	22:10:18:ALA:HB1	2.20	0.42
27:15:16:ARG:HD2	27:15:20:ARG:NH1	2.35	0.42
27:15:5:PRO:O	61:15:201:HOH:O	2.22	0.42
1:1A:1106:U:N3	1:1A:1108:G:O2'	2.48	0.42
1:1A:2466:G:H1'	61:1A:4665:HOH:O	2.20	0.42
1:1A:2631:C:O2'	4:1E:154:LYS:HB3	2.20	0.42
1:1A:469:A:C5	5:1F:45:ARG:HD2	2.55	0.42
12:1Q:135:ASP:O	12:1Q:139:GLU:HG3	2.20	0.42
23:21:67:ILE:N	23:21:68:PRO:HD2	2.34	0.42
24:22:51:ARG:HG2	24:22:55:ARG:NH2	2.35	0.42
1:2A:1027:A:N6	1:2A:1126:A:N3	2.68	0.42
1:2A:2123:G:H2'	1:2A:2124:G:C8	2.55	0.42
1:2A:2104:G:C2	1:2A:2186:G:C2	3.08	0.42
1:2A:2207:G:H3'	1:2A:2208:A:H5''	2.02	0.42
1:2A:2689:U:H4'	1:2A:2690:C:H5'	2.02	0.42
1:2A:2809:A:N6	1:2A:2891:G:H2'	2.35	0.42
1:2A:581:C:H2'	1:2A:582:G:H8	1.84	0.42
2:2B:28:C:H2'	2:2B:29:A:O4'	2.20	0.42
2:2B:37:C:N4	2:2B:38:C:N3	2.68	0.42
13:2R:100:LEU:HA	13:2R:100:LEU:HD12	1.82	0.42
1:1A:1222:A:O2'	1:1A:1223:C:O4'	2.27	0.41
1:1A:2142:G:C2'	1:1A:2143:G:H5'	2.50	0.41
1:1A:611:U:H2'	1:1A:612:C:C6	2.55	0.41
12:1Q:79:LEU:HD23	12:1Q:79:LEU:HA	1.88	0.41
14:1S:10:ARG:HG2	14:1S:91:PRO:HA	2.01	0.41
14:1S:93:LYS:HG2	14:1S:95:HIS:HB2	2.02	0.41
1:1A:1245:C:H1'	16:1U:2:PRO:HG3	2.01	0.41
26:24:44:THR:O	26:24:46:GLN:N	2.53	0.41
1:2A:118:A:N3	1:2A:178:G:H1'	2.35	0.41
1:2A:196:A:N3	1:2A:196:A:H2'	2.36	0.41
1:2A:2483:C:H2'	1:2A:2484:G:O4'	2.20	0.41
1:2A:571:A:N6	1:2A:2499:C:O3'	2.53	0.41
5:2F:33:LEU:HA	5:2F:33:LEU:HD12	1.74	0.41
11:2P:28:GLY:O	11:2P:30:THR:N	2.53	0.41
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.35	0.41
21:2Z:54:HIS:CG	21:2Z:101:PRO:HG3	2.55	0.41
1:1A:1095:C:H1'	1:1A:1159:U:O2'	2.19	0.41
1:1A:1198:C:H4'	16:1U:77:SER:HA	2.01	0.41
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:18:C:H2'	1:1A:19:C:C6	2.55	0.41
1:1A:2189:U:H2'	1:1A:2190:G:O4'	2.20	0.41
1:1A:478:G:C2	1:1A:484:G:C5	3.08	0.41
1:1A:831:A:C5	3:1D:229:VAL:HG21	2.56	0.41
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	2.01	0.41
13:1R:28:LEU:HD22	13:1R:44:LEU:HD13	2.02	0.41
16:1U:85:LYS:HE3	16:1U:116:ALA:O	2.19	0.41
20:1Y:1:MET:HB3	20:1Y:2:ARG:H	1.69	0.41
1:2A:1364:G:O5'	23:21:3:LYS:HG3	2.20	0.41
25:23:39:ASP:OD1	25:23:44:ARG:NH1	2.50	0.41
1:2A:2130:U:H4'	1:2A:2133:G:H4'	2.02	0.41
1:2A:720:C:H2'	1:2A:721:C:C6	2.56	0.41
1:2A:875:G:N1	1:2A:903:C:C2	2.88	0.41
2:2B:2:C:H5''	2:2B:3:C:OP2	2.20	0.41
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	2.01	0.41
8:2I:68:LEU:O	8:2I:72:LEU:HG	2.20	0.41
14:2S:10:ARG:HH21	14:2S:91:PRO:HB2	1.85	0.41
1:1A:1053:C:OP1	9:1N:37:LYS:NZ	2.49	0.41
1:1A:1432:C:H2'	1:1A:1433:C:C6	2.55	0.41
1:1A:1760:U:H2'	1:1A:1761:G:H8	1.84	0.41
1:1A:1821:C:H5''	1:1A:1822:A:OP1	2.20	0.41
1:1A:2050:U:H2'	1:1A:2051:G:O4'	2.19	0.41
1:1A:26:G:C6	1:1A:27:G:N1	2.89	0.41
2:1B:2:C:H2'	2:1B:3:C:C6	2.55	0.41
9:1N:33:LEU:HD12	9:1N:33:LEU:HA	1.82	0.41
21:1Z:100:VAL:O	21:1Z:123:ASP:HB2	2.19	0.41
1:2A:1450(A):C:N3	1:2A:1451:C:N4	2.68	0.41
1:2A:16:G:H2'	1:2A:17:G:H8	1.85	0.41
1:2A:2659:G:N2	1:2A:2662:A:OP2	2.52	0.41
1:2A:2891:G:H5''	1:2A:2892:A:OP2	2.20	0.41
1:2A:39:C:H2'	1:2A:40:C:C6	2.55	0.41
1:2A:643:A:C8	28:26:44:ARG:NH1	2.88	0.41
1:2A:857:C:H2'	1:2A:858:U:C6	2.55	0.41
1:2A:892:G:H3'	1:2A:893:C:C5'	2.50	0.41
14:2S:19:LYS:HG2	14:2S:19:LYS:H	1.65	0.41
1:1A:898:U:O2'	25:13:42:ALA:O	2.38	0.41
1:1A:1314:A:C2	1:1A:2035:A:C4	3.08	0.41
1:1A:1942:4OC:O5'	1:1A:1942:4OC:H6	2.20	0.41
1:1A:1973:U:O2'	1:1A:1975:A:N7	2.42	0.41
1:1A:2182:G:C6	1:1A:2183:C:N4	2.88	0.41
1:1A:443:C:H2'	1:1A:444:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.55	0.41
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.59	0.41
7:1H:18:GLU:HG2	7:1H:19:VAL:N	2.35	0.41
25:23:12:PRO:HB2	25:23:20:LYS:HE3	2.03	0.41
30:28:33:ASN:HA	30:28:36:LYS:HD2	2.02	0.41
1:2A:2134:A:P	1:2A:2157:G:H22	2.44	0.41
1:2A:2815:C:H2'	1:2A:2816:C:H6	1.84	0.41
1:2A:387:U:OP2	23:21:20:ARG:NH1	2.41	0.41
6:2G:117:PHE:CZ	6:2G:179:PRO:HG2	2.55	0.41
7:2H:118:PRO:HD2	7:2H:121:ILE:HG21	2.01	0.41
8:2I:79:ILE:HB	8:2I:144:VAL:HG12	2.02	0.41
10:2O:88:ASN:ND2	10:2O:92:GLU:HB2	2.35	0.41
24:12:55:ARG:O	24:12:59:ARG:HG3	2.20	0.41
1:1A:794:U:O2	1:1A:2036:A:H1'	2.21	0.41
1:1A:2163:G:N3	1:1A:2164:C:H1'	2.36	0.41
1:1A:2541:G:H5''	1:1A:2542:A:H5''	2.02	0.41
1:1A:785:G:H3'	1:1A:786:G:C8	2.56	0.41
1:1A:928:G:H3'	1:1A:929:G:C8	2.55	0.41
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.86	0.41
22:20:53:MET:HG3	22:20:59:LEU:CD2	2.51	0.41
30:28:14:VAL:HG22	30:28:24:ALA:HB2	2.02	0.41
1:2A:1359:A:H2	1:2A:1372:U:O4	2.04	0.41
1:2A:2161:C:H3'	1:2A:2162:G:H8	1.85	0.41
1:2A:2336:A:H61	22:20:43:THR:CG2	2.33	0.41
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.52	0.41
1:2A:2533:A:O2'	1:2A:2664:G:H5''	2.19	0.41
1:2A:300:A:N3	1:2A:319:C:H1'	2.36	0.41
4:2E:181:LEU:HA	4:2E:181:LEU:HD12	1.72	0.41
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.36	0.41
7:2H:3:ARG:CZ	7:2H:5:GLY:H	2.34	0.41
12:2Q:31:ASP:HA	12:2Q:134:ARG:NH1	2.34	0.41
15:2T:33:LYS:HB3	15:2T:82:LEU:HD23	2.02	0.41
16:2U:61:TRP:CZ2	16:2U:93:LYS:HG3	2.55	0.41
21:2Z:153:SER:HB3	21:2Z:167:PRO:HA	2.02	0.41
1:1A:1011:G:O4'	1:1A:2279:A:N6	2.53	0.41
1:1A:1108:G:H5''	1:1A:1116:A:O2'	2.21	0.41
1:1A:1452:U:H2'	1:1A:1453:C:C6	2.55	0.41
1:1A:2169:G:H3'	1:1A:2169:G:N3	2.36	0.41
1:1A:895:G:H2'	1:1A:896:A:C8	2.56	0.41
4:1E:21:VAL:O	4:1E:23:VAL:HG13	2.20	0.41
4:1E:52:LEU:HA	4:1E:53:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:57:HIS:CD2	12:1Q:117:ALA:HB2	2.56	0.41
19:1X:25:LYS:HA	19:1X:81:VAL:O	2.21	0.41
1:2A:1364:G:P	23:21:3:LYS:HG3	2.61	0.41
1:2A:1430:C:H2'	1:2A:1431:U:H6	1.86	0.41
1:2A:1434:A:H2'	1:2A:1435:G:O4'	2.44	0.41
1:2A:1937:A:H1'	1:2A:1939:5MU:H73	2.03	0.41
1:2A:197:A:N6	1:2A:2430:A:H2'	2.35	0.41
1:2A:2516:G:C6	1:2A:2517:C:C4	3.09	0.41
1:2A:1998:G:H4'	1:2A:2724:C:O2'	2.19	0.41
1:2A:319:C:O2'	1:2A:320:A:H5'	2.20	0.41
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.20	0.41
4:2E:70:ALA:O	4:2E:72:VAL:N	2.52	0.41
5:2F:24:LEU:HD21	5:2F:114:VAL:HG12	2.01	0.41
1:2A:2565:A:H62	10:2O:28:SER:CB	2.34	0.41
10:2O:98:VAL:HG23	10:2O:118:ALA:HA	2.02	0.41
14:2S:64:GLU:HG3	14:2S:64:GLU:H	1.62	0.41
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.53	0.41
1:1A:1073:A:C2	1:1A:2500:A:H5'	2.56	0.41
1:1A:1115:A:H2	1:1A:1141:A:HO2'	1.65	0.41
1:1A:1501:U:OP1	13:1R:77:ARG:NH1	2.40	0.41
1:1A:1698:G:N2	1:1A:2029:C:C2	2.89	0.41
1:1A:27:G:C2	1:1A:537:G:N3	2.88	0.41
1:1A:2864:G:H2'	1:1A:2865:C:C6	2.56	0.41
1:1A:360:C:H2'	1:1A:361:C:H6	1.86	0.41
1:1A:925:A:H3'	1:1A:926:G:C8	2.55	0.41
1:1A:99:G:H21	24:12:7:ARG:NH2	2.17	0.41
1:1A:2455:C:OP1	5:1F:68:LYS:HD3	2.20	0.41
7:1H:126:PRO:HB2	7:1H:127:GLU:H	1.64	0.41
8:1I:76:THR:HG22	8:1I:141:LYS:HE2	2.02	0.41
11:1P:46:LYS:HB3	11:1P:46:LYS:HE3	1.91	0.41
13:1R:37:THR:OG1	13:1R:39:PRO:HD2	2.21	0.41
14:1S:36:TYR:CD2	14:1S:36:TYR:N	2.87	0.41
19:1X:57:LEU:HD12	19:1X:57:LEU:O	2.21	0.41
28:26:26:ASN:O	28:26:29:ASN:N	2.54	0.41
1:2A:1418:G:H8	1:2A:1418:G:O5'	2.04	0.41
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.55	0.41
1:2A:1830:C:H2'	1:2A:1831:G:C8	2.56	0.41
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.21	0.41
1:2A:2633:G:H2'	1:2A:2634:G:O4'	2.21	0.41
1:2A:927:G:H2'	1:2A:928:G:O4'	2.20	0.41
2:2B:38:C:H2'	2:2B:39:A:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:9:ILE:HB	7:2H:50:VAL:HB	2.03	0.41
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.20	0.41
1:1A:1535:U:HO2'	1:1A:1536:A:H8	1.64	0.41
1:1A:704:U:H2'	1:1A:705:C:H6	1.86	0.41
1:1A:782:A:N7	1:1A:808:A:H2	2.18	0.41
7:1H:4:ILE:O	7:1H:69:ARG:HD2	2.21	0.41
10:1O:63:VAL:HG11	10:1O:85:VAL:HG23	2.02	0.41
10:1O:9:GLU:H	10:1O:9:GLU:HG2	1.60	0.41
4:1E:12:THR:HG21	15:1T:11:GLU:HG2	2.03	0.41
15:1T:27:THR:O	15:1T:89:VAL:HG13	2.21	0.41
1:2A:11:G:O5'	1:2A:11:G:H8	2.04	0.41
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.56	0.41
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.41	0.41
8:2I:27:ARG:HD3	23:21:71:TYR:CE2	2.55	0.41
21:2Z:158:PRO:HA	21:2Z:159:PRO:HD3	1.96	0.41
25:13:5:LYS:HG3	25:13:36:VAL:HG22	2.02	0.41
1:1A:1305:G:H22	1:1A:1331:G:H1'	40.17	0.41
1:1A:2144:U:H2'	1:1A:2145:G:O4'	2.21	0.41
1:1A:2518:U:H3	58:1A:4030:EZG:CG	2.33	0.41
1:1A:646:A:H5'	1:1A:647:G:OP2	2.21	0.41
12:1Q:37:LEU:HD21	12:1Q:130:LYS:CE	2.51	0.41
1:1A:509:A:O2'	20:1Y:49:VAL:O	2.30	0.41
26:24:48:ARG:HA	26:24:48:ARG:HD2	1.81	0.41
1:2A:1002:G:C2	1:2A:1003:G:C8	4.05	0.41
1:2A:80:G:H1	1:2A:106:C:H42	1.67	0.41
1:2A:1683:C:H2'	1:2A:1684:C:C6	2.56	0.41
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.55	0.41
1:2A:2784:C:H2'	1:2A:2785:C:H6	1.85	0.41
1:2A:2787:C:H2'	1:2A:2788:C:C6	2.56	0.41
1:2A:659:C:H2'	1:2A:660:G:C8	2.47	0.41
7:2H:105:LEU:O	7:2H:113:VAL:N	2.44	0.41
1:2A:2847:U:OP2	15:2T:98:LYS:NZ	2.54	0.41
21:2Z:7:ALA:HB3	21:2Z:61:LEU:HD12	2.03	0.41
1:1A:1228:G:O2'	25:13:29:ARG:NH1	2.54	0.41
1:1A:1094:A:N1	1:1A:1158:G:O2'	2.38	0.41
1:1A:1096:A:H2'	1:1A:1097:G:O4'	2.21	0.41
1:1A:1400:A:H4'	3:1D:38:LYS:HZ3	1.86	0.41
1:1A:1468:G:H1'	1:1A:1542:A:N1	2.36	0.41
1:1A:1820:A:H2'	1:1A:1821:C:O4'	2.21	0.41
1:1A:2179:G:H4'	1:1A:2180:A:OP1	2.20	0.41
1:1A:225:C:H2'	1:1A:226:C:H6	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2756:C:OP1	31:19:33:LYS:NZ	2.43	0.41
1:1A:407:U:H2'	1:1A:408:G:C8	2.54	0.41
1:1A:764:G:H2'	1:1A:765:A:O4'	2.21	0.41
1:1A:1849:U:O4	3:1D:154:LYS:HD2	2.20	0.41
8:1I:5:LEU:H	8:1I:5:LEU:HD12	1.86	0.41
8:1I:86:THR:HG22	8:1I:123:LEU:H	1.86	0.41
19:1X:39:ILE:O	19:1X:43:VAL:HG23	2.21	0.41
26:24:26:SER:OG	26:24:27:THR:N	2.54	0.41
1:2A:116:C:H2'	1:2A:117:G:O4'	2.20	0.41
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.56	0.41
1:2A:1260:G:C6	1:2A:1261:C:C4	3.09	0.41
1:2A:1818:U:H2'	3:2D:157:ARG:HD2	2.03	0.41
1:2A:2526:G:O3'	31:29:33:LYS:NZ	2.54	0.41
1:2A:1638:C:H5''	1:2A:2710:C:O2'	2.20	0.41
1:2A:521:G:H2'	1:2A:522:G:H8	1.85	0.41
1:2A:2728:U:O2'	4:2E:22:PRO:HG2	2.21	0.41
17:2V:15:GLU:O	17:2V:18:LEU:HB3	2.21	0.41
25:13:54:VAL:HG12	25:13:55:ARG:N	2.36	0.41
26:14:16:CYS:HA	26:14:33:VAL:O	2.20	0.41
1:1A:101:A:C6	1:1A:102:U:C4	3.09	0.41
1:1A:2297:C:OP2	28:16:6:ARG:HD3	2.21	0.41
1:1A:239:G:C6	1:1A:240:A:C6	3.09	0.41
1:1A:2524:C:H2'	1:1A:2525:G:O4'	2.21	0.41
1:1A:1686:U:H4'	1:1A:2711:C:H4'	2.03	0.41
1:1A:2859:U:H4'	1:1A:2878:A:C2	2.56	0.41
1:1A:34:C:H5''	1:1A:35:G:OP2	2.20	0.41
1:1A:826:U:OP1	3:1D:49:ILE:HG13	2.21	0.41
1:1A:866:A:C4	1:1A:1234:A:C2	3.09	0.41
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	2.02	0.41
3:1D:68:LYS:HB2	3:1D:70:TRP:CE2	2.55	0.41
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	2.02	0.41
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.54	0.41
14:1S:76:LYS:H	14:1S:76:LYS:HG3	1.70	0.41
15:1T:94:ALA:HB1	15:1T:99:LEU:HD21	2.03	0.41
1:2A:98:G:H5''	24:22:3:LEU:HG	2.02	0.41
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.61	0.41
31:29:2:LYS:HD3	31:29:4:ARG:NH2	2.35	0.41
1:2A:2019:A:O3'	16:2U:27:LEU:HD12	2.20	0.41
1:2A:1759:A:H1'	1:2A:2711:A:C2	2.56	0.41
1:2A:2788:C:H5''	4:2E:61:ARG:HH21	1.86	0.41
1:2A:401:A:H2'	1:2A:402:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:56:A:H2'	1:2A:57:C:O4'	2.21	0.41
1:2A:949:C:H2'	1:2A:950:G:C8	2.56	0.41
2:2B:68:C:H2'	2:2B:69:G:H8	1.84	0.41
3:2D:66:ASP:HB2	3:2D:103:ARG:HD3	2.03	0.41
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.51	0.41
21:2Z:28:MET:HA	21:2Z:88:PHE:O	2.22	0.41
1:1A:1118:C:H5''	1:1A:1119:A:OP1	2.21	0.40
1:1A:1068:G:C5	1:1A:1185:C:C4	3.08	0.40
1:1A:1197:G:O3'	16:1U:81:HIS:HB2	2.21	0.40
1:1A:1680:G:C6	1:1A:1682:G:C4	3.09	0.40
1:1A:1810:U:H2'	61:1A:4292:HOH:O	2.20	0.40
1:1A:2039:U:O2	27:15:10:LYS:HB2	2.21	0.40
1:1A:2274:U:H5	22:10:16:SER:HB3	1.86	0.40
1:1A:965:G:N2	1:1A:2281:A:OP2	2.52	0.40
1:1A:2803:A:H5'	1:1A:2902:G:H21	1.86	0.40
1:1A:752:A:C2	1:1A:774:A:H1'	2.56	0.40
1:1A:1660:A:N1	18:1W:87:PRO:HB3	2.36	0.40
23:21:46:LEU:HD23	23:21:46:LEU:HA	1.91	0.40
23:21:89:GLU:O	23:21:93:GLU:HG2	2.21	0.40
1:2A:1007:C:N3	1:2A:1022:G:C6	16.79	0.40
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.21	0.40
1:2A:2516:G:C6	1:2A:2517:C:N4	2.90	0.40
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.56	0.40
1:2A:422:A:H2'	1:2A:423:A:C8	2.56	0.40
1:2A:600:G:N2	1:2A:605:C:O3'	2.54	0.40
7:2H:20:ALA:CB	7:2H:25:LYS:HG2	2.49	0.40
7:2H:17:VAL:O	7:2H:45:VAL:HG11	2.20	0.40
8:2I:9:LEU:HD22	8:2I:12:LEU:HD12	2.03	0.40
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.20	0.40
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.56	0.40
12:2Q:2:LEU:HD12	12:2Q:2:LEU:HA	1.82	0.40
1:1A:2390:A:H4'	14:1S:23:ARG:NH1	2.35	0.40
1:1A:273:G:O2'	1:1A:274:U:H5''	2.21	0.40
1:1A:2780:C:H2'	1:1A:2781:C:H6	1.85	0.40
1:1A:954:C:OP1	12:1Q:22:LYS:HB3	2.21	0.40
2:1B:68:C:H2'	2:1B:69:G:O4'	2.20	0.40
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	2.03	0.40
10:1O:43:VAL:HG12	10:1O:54:GLU:HA	2.03	0.40
14:1S:11:LYS:HE2	14:1S:15:ARG:HH12	1.86	0.40
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	2.03	0.40
1:2A:987:G:O2'	1:2A:1000:A:N3	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1139:G:O3'	9:2N:24:GLY:HA3	2.21	0.40
1:2A:117:G:C6	1:2A:119:A:C6	3.09	0.40
1:2A:1525:G:H2'	1:2A:1526:G:O4'	2.69	0.40
1:2A:1780:A:N6	61:2A:4058:HOH:O	2.54	0.40
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.84	0.40
1:2A:201:C:H2'	1:2A:202:U:H2'	5.71	0.40
1:2A:2019:A:H2	1:2A:2035:G:H22	1.68	0.40
1:2A:2207:G:H2'	1:2A:2208:A:C2	2.57	0.40
1:2A:218:A:C2	1:2A:235:U:H4'	2.56	0.40
1:2A:663:G:C6	1:2A:664:C:C4	3.09	0.40
1:2A:79:G:H2'	1:2A:80:G:C8	2.60	0.40
1:2A:828:U:H2'	1:2A:829:A:C8	2.56	0.40
2:2B:59:A:H2'	2:2B:60:C:O4'	2.22	0.40
6:2G:107:LEU:HD23	6:2G:111:LEU:HD13	2.04	0.40
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.54	0.40
11:2P:128:HIS:CD2	11:2P:148:LEU:HD11	2.56	0.40
15:2T:64:ARG:NH1	15:2T:103:ARG:HG2	2.36	0.40
21:2Z:102:LEU:HD23	21:2Z:139:VAL:HG21	2.03	0.40
27:15:16:ARG:HG2	27:15:16:ARG:HH11	1.85	0.40
1:1A:1067:A:H3'	1:1A:1067:A:N3	2.36	0.40
1:1A:1091:A:OP1	1:1A:1092:A:H3'	2.21	0.40
1:1A:791:G:N2	1:1A:1497:G:O3'	58.34	0.40
1:1A:2116:G:OP1	8:1I:22:LYS:HD2	2.21	0.40
1:1A:2143:G:O6	1:1A:2198:A:N6	2.54	0.40
1:1A:2899:C:H2'	1:1A:2900:G:O4'	2.21	0.40
1:1A:434:G:H2'	1:1A:435:G:H8	1.86	0.40
1:1A:927:G:H2'	1:1A:928:G:C8	2.47	0.40
1:2A:468:G:N7	29:27:39:ARG:NH2	2.69	0.40
1:2A:1404:C:H2'	1:2A:1405:U:H6	1.87	0.40
1:2A:1547:C:H2'	1:2A:1548:C:H6	1.87	0.40
1:2A:2173:A:H5''	1:2A:2174:C:OP2	2.22	0.40
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.56	0.40
1:2A:882:G:H1	1:2A:894:C:H42	1.69	0.40
1:2A:947:G:H2'	1:2A:948:G:C8	2.56	0.40
11:2P:38:GLN:HG2	11:2P:45:LEU:N	2.36	0.40
16:2U:66:ASN:ND2	16:2U:70:ARG:HH21	2.12	0.40
21:2Z:126:VAL:HG13	21:2Z:161:VAL:HG23	2.03	0.40
1:1A:2661:U:H2'	1:1A:2662:U:C6	2.56	0.40
1:1A:504:A:N1	1:1A:525:G:H4'	2.36	0.40
2:1B:44:G:C2	2:1B:48:A:C2	3.09	0.40
22:20:70:GLN:HG2	22:20:72:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2249:U:N3	1:2A:2253:G:OP2	2.48	0.40
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.56	0.40
1:2A:250:G:C6	1:2A:251:A:C6	3.09	0.40
1:2A:2525:G:N2	1:2A:2539:C:C2	2.89	0.40
1:2A:2648:C:H2'	1:2A:2649:U:H6	1.87	0.40
1:2A:271:A:N6	1:2A:271(X):G:H1'	2.36	0.40
1:2A:395:U:O2'	1:2A:396:G:N7	2.43	0.40
1:2A:700:G:H2'	1:2A:701:G:O4'	2.21	0.40
1:2A:870:A:H5'	1:2A:871:U:OP2	2.21	0.40
5:2F:23:ASP:O	5:2F:24:LEU:HD12	2.21	0.40
6:2G:23:PHE:HB2	6:2G:25:TYR:CE2	2.56	0.40
11:2P:100:LEU:HA	11:2P:103:ALA:HB3	2.03	0.40
16:2U:68:ALA:O	16:2U:71:GLN:HB2	2.21	0.40
19:2X:64:LYS:HD3	19:2X:64:LYS:HA	1.80	0.40
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.56	0.40
30:18:23:VAL:HG13	30:18:47:LYS:HB3	2.03	0.40
1:1A:1116:A:N6	1:1A:1142:A:N3	2.70	0.40
1:1A:2230:U:O4'	23:11:52:ARG:NH2	2.43	0.40
1:1A:228:U:H2'	1:1A:229:G:O4'	2.21	0.40
1:1A:2408:G:OP1	23:11:25:LYS:NZ	2.33	0.40
1:1A:593:G:H2'	1:1A:2052:A:C5	2.57	0.40
1:1A:734:C:OP1	29:17:2:LYS:NZ	2.55	0.40
1:1A:757:G:H2'	1:1A:758:G:H8	1.85	0.40
1:1A:830:A:H2'	1:1A:830:A:N3	2.36	0.40
5:1F:53:THR:HG22	5:1F:55:GLY:N	2.34	0.40
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.50	0.40
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.57	0.40
8:1I:47:LEU:O	8:1I:51:ILE:HG13	2.21	0.40
21:1Z:15:PRO:O	21:1Z:19:ARG:HG3	2.21	0.40
1:2A:1878:G:C5	1:2A:1879:C:C4	3.09	0.40
1:2A:2298:A:N6	1:2A:2318:G:C8	2.89	0.40
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.57	0.40
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.86	0.40
1:2A:561:G:HO2'	16:2U:45:TYR:HE1	1.69	0.40
1:2A:637:A:C6	1:2A:652:C:H4'	2.56	0.40
2:2B:33:G:N3	2:2B:50:G:N2	2.70	0.40
3:2D:155:LEU:HA	3:2D:155:LEU:HD23	4.50	0.40
6:2G:55:LYS:O	6:2G:59:GLU:N	2.28	0.40
6:2G:96:ARG:O	6:2G:99:MET:HB3	2.22	0.40
7:2H:123:PHE:CE1	7:2H:133:VAL:HG22	2.57	0.40
10:2O:4:PRO:O	10:2O:5:GLN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	254 (93%)	18 (7%)	1 (0%)	38	72
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	32	67
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	32	67
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	32	67
5	2F	201/210 (96%)	184 (92%)	13 (6%)	4 (2%)	9	28
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	28	62
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	6	19
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	28	62
7	2H	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	11	34
8	1I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	25	59
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	25	59
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	126 (91%)	9 (6%)	3 (2%)	8	26
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	11	34
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	134 (91%)	11 (8%)	2 (1%)	13	39
12	1Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	25	59
12	2Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	25	59
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	11	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	20	52
14	2S	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	9	30
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	22	55
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	22	55
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	18	50
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	18	50
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	18	50
20	2Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	9	30
21	1Z	148/206 (72%)	133 (90%)	14 (10%)	1 (1%)	25	59
21	2Z	156/206 (76%)	132 (85%)	19 (12%)	5 (3%)	5	16
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	15	44
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	63 (93%)	4 (6%)	1 (2%)	12	37
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	10	32
26	14	67/71 (94%)	55 (82%)	8 (12%)	4 (6%)	2	5
26	24	67/71 (94%)	50 (75%)	13 (19%)	4 (6%)	2	5
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	44 (86%)	7 (14%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	27	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	8	26
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
33	1b	229/256 (90%)	192 (84%)	27 (12%)	10 (4%)	3	9
33	2b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	3	12
34	1c	204/239 (85%)	190 (93%)	11 (5%)	3 (2%)	12	37
34	2c	204/239 (85%)	173 (85%)	25 (12%)	6 (3%)	5	18
35	1d	206/209 (99%)	190 (92%)	13 (6%)	3 (2%)	12	37
35	2d	206/209 (99%)	187 (91%)	15 (7%)	4 (2%)	9	30
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	13	39
36	2e	146/162 (90%)	131 (90%)	14 (10%)	1 (1%)	25	59
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	138 (90%)	12 (8%)	3 (2%)	9	28
38	2g	153/156 (98%)	135 (88%)	15 (10%)	3 (2%)	9	28
39	1h	135/138 (98%)	129 (96%)	4 (3%)	2 (2%)	12	37
39	2h	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	12	37
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
40	2i	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	10
41	2j	94/105 (90%)	79 (84%)	11 (12%)	4 (4%)	3	10
42	1k	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	20	52
42	2k	112/129 (87%)	103 (92%)	6 (5%)	3 (3%)	6	20
43	1l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	22	55
43	2l	119/132 (90%)	103 (87%)	15 (13%)	1 (1%)	22	55
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	102 (85%)	15 (12%)	3 (2%)	6	22
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	15	44
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	15	44
47	1p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	14	41
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	18	50
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	15	44
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	6	22
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2	7
51	2t	94/106 (89%)	83 (88%)	5 (5%)	6 (6%)	1	4
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	8
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11370/12128 (94%)	10425 (92%)	802 (7%)	143 (1%)	14	41

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
7	1H	126	PRO
26	14	53	GLU
33	1b	22	LYS
34	1c	107	GLN
38	1g	4	ARG
50	1s	81	ARG
3	2D	3	VAL
6	2G	47	LYS
12	2Q	27	VAL
26	24	45	GLY
29	27	46	VAL
33	2b	16	HIS
33	2b	17	PHE
33	2b	21	ARG
33	2b	125	PRO
36	2e	77	PRO

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Mol	Chain	Res	Type
41	2j	79	ARG
8	1I	11	ASN
20	1Y	54	LYS
26	14	45	GLY
33	1b	126	GLU
36	1e	21	ALA
38	1g	6	ARG
41	1j	79	ARG
43	1l	91	LYS
5	2F	130	ALA
7	2H	47	GLU
7	2H	126	PRO
9	2N	48	MET
10	2O	5	GLN
11	2P	29	LYS
13	2R	14	SER
17	2V	79	VAL
21	2Z	171	ILE
33	2b	95	GLN
33	2b	231	GLU
34	2c	91	LEU
34	2c	156	ARG
35	2d	179	GLU
38	2g	4	ARG
41	2j	75	ILE
42	2k	49	GLY
46	2o	88	ARG
51	2t	9	ASN
51	2t	10	LEU
51	2t	47	GLY
15	1T	37	GLY
17	1V	79	VAL
26	14	61	ARG
33	1b	20	GLU
33	1b	231	GLU
35	1d	173	TRP
35	1d	178	VAL
36	1e	86	ALA
41	1j	29	ARG
41	1j	77	PRO
46	1o	19	PRO
51	1t	47	GLY

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Mol	Chain	Res	Type
51	1t	95	ALA
4	2E	52	LEU
5	2F	21	ALA
6	2G	124	SER
7	2H	29	PRO
8	2I	116	LEU
9	2N	2	LYS
14	2S	84	GLN
20	2Y	102	CYS
20	2Y	103	GLY
21	2Z	167	PRO
26	24	61	ARG
33	2b	20	GLU
33	2b	123	ALA
34	2c	181	ASN
35	2d	181	MET
38	2g	55	GLY
51	2t	95	ALA
4	1E	52	LEU
12	1Q	17	LEU
26	14	57	GLU
33	1b	9	GLU
33	1b	17	PHE
33	1b	21	ARG
33	1b	207	ALA
38	1g	80	VAL
51	1t	100	ILE
52	1u	3	LYS
9	2N	59	LYS
11	2P	45	LEU
13	2R	2	ARG
21	2Z	142	SER
24	22	46	GLN
33	2b	158	LEU
34	2c	64	VAL
34	2c	92	ALA
34	2c	95	THR
35	2d	5	ILE
35	2d	10	ARG
38	2g	80	VAL
41	2j	31	GLY
42	2k	106	LYS

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Mol	Chain	Res	Type
44	2m	106	ASN
50	2s	76	PRO
51	2t	102	GLY
14	1S	94	TYR
33	1b	16	HIS
34	1c	66	VAL
35	1d	179	GLU
39	1h	133	LEU
48	1q	33	GLY
51	1t	10	LEU
5	2F	168	ARG
6	2G	51	ARG
6	2G	179	PRO
15	2T	117	ASP
22	20	12	ASN
26	24	29	PRO
26	24	55	ARG
39	2h	3	THR
43	2l	51	ALA
50	2s	81	ARG
51	2t	99	LEU
21	1Z	156	LYS
47	1p	53	VAL
51	1t	102	GLY
5	2F	133	ASN
10	2O	88	ASN
14	2S	96	GLY
39	1h	83	ILE
42	1k	105	VAL
21	2Z	147	GLY
42	2k	105	VAL
44	2m	4	ILE
33	1b	230	VAL
41	1j	39	PRO
6	2G	177	GLY
41	2j	39	PRO
39	2h	73	ASP
44	2m	6	GLY
34	1c	174	PRO
21	2Z	165	VAL
25	23	50	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	200 (93%)	15 (7%)	18	45
3	2D	215/218 (99%)	206 (96%)	9 (4%)	34	68
4	1E	164/166 (99%)	152 (93%)	12 (7%)	16	42
4	2E	164/166 (99%)	148 (90%)	16 (10%)	9	27
5	1F	160/166 (96%)	144 (90%)	16 (10%)	9	26
5	2F	159/166 (96%)	144 (91%)	15 (9%)	10	29
6	1G	143/156 (92%)	133 (93%)	10 (7%)	18	45
6	2G	143/156 (92%)	134 (94%)	9 (6%)	21	51
7	1H	144/148 (97%)	138 (96%)	6 (4%)	34	68
7	2H	144/148 (97%)	138 (96%)	6 (4%)	34	68
8	1I	113/124 (91%)	104 (92%)	9 (8%)	14	38
8	2I	105/124 (85%)	99 (94%)	6 (6%)	24	56
9	1N	118/119 (99%)	110 (93%)	8 (7%)	18	47
9	2N	118/119 (99%)	108 (92%)	10 (8%)	12	35
10	1O	100/100 (100%)	97 (97%)	3 (3%)	46	80
10	2O	100/100 (100%)	100 (100%)	0	100	100
11	1P	115/116 (99%)	109 (95%)	6 (5%)	27	60
11	2P	115/116 (99%)	111 (96%)	4 (4%)	41	75
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	26	58
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	14	37
13	1R	101/101 (100%)	90 (89%)	11 (11%)	7	22
13	2R	101/101 (100%)	92 (91%)	9 (9%)	11	32
14	1S	86/88 (98%)	78 (91%)	8 (9%)	10	30
14	2S	85/88 (97%)	78 (92%)	7 (8%)	13	37
15	1T	115/127 (91%)	112 (97%)	3 (3%)	51	83
15	2T	113/127 (89%)	105 (93%)	8 (7%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	85 (91%)	8 (9%)	12	34
16	2U	93/94 (99%)	91 (98%)	2 (2%)	57	87
17	1V	80/82 (98%)	73 (91%)	7 (9%)	12	33
17	2V	80/82 (98%)	71 (89%)	9 (11%)	7	20
18	1W	90/92 (98%)	87 (97%)	3 (3%)	43	77
18	2W	90/92 (98%)	83 (92%)	7 (8%)	15	39
19	1X	77/78 (99%)	73 (95%)	4 (5%)	27	60
19	2X	77/78 (99%)	74 (96%)	3 (4%)	37	71
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	23	54
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	17	44
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	11	32
21	2Z	137/179 (76%)	128 (93%)	9 (7%)	19	49
22	10	65/67 (97%)	62 (95%)	3 (5%)	31	65
22	20	65/67 (97%)	63 (97%)	2 (3%)	45	79
23	11	80/83 (96%)	77 (96%)	3 (4%)	38	72
23	21	80/83 (96%)	80 (100%)	0	100	100
24	12	65/67 (97%)	62 (95%)	3 (5%)	31	65
24	22	65/67 (97%)	64 (98%)	1 (2%)	70	92
25	13	51/52 (98%)	50 (98%)	1 (2%)	60	88
25	23	50/52 (96%)	45 (90%)	5 (10%)	9	26
26	14	59/63 (94%)	55 (93%)	4 (7%)	18	47
26	24	53/63 (84%)	49 (92%)	4 (8%)	16	41
27	15	50/52 (96%)	44 (88%)	6 (12%)	6	18
27	25	50/52 (96%)	47 (94%)	3 (6%)	22	54
28	16	51/52 (98%)	47 (92%)	4 (8%)	15	39
28	26	50/52 (96%)	45 (90%)	5 (10%)	9	26
29	17	41/42 (98%)	37 (90%)	4 (10%)	9	27
29	27	41/42 (98%)	39 (95%)	2 (5%)	29	62
30	18	54/55 (98%)	49 (91%)	5 (9%)	10	30
30	28	54/55 (98%)	49 (91%)	5 (9%)	10	30
31	19	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	33 (97%)	1 (3%)	48	81
33	1b	192/220 (87%)	184 (96%)	8 (4%)	34	68
33	2b	187/220 (85%)	174 (93%)	13 (7%)	18	45
34	1c	142/188 (76%)	136 (96%)	6 (4%)	34	68
34	2c	140/188 (74%)	133 (95%)	7 (5%)	28	62
35	1d	169/181 (93%)	159 (94%)	10 (6%)	23	54
35	2d	173/181 (96%)	162 (94%)	11 (6%)	20	50
36	1e	113/123 (92%)	105 (93%)	8 (7%)	17	44
36	2e	114/123 (93%)	108 (95%)	6 (5%)	26	59
37	1f	84/90 (93%)	81 (96%)	3 (4%)	40	74
37	2f	85/90 (94%)	82 (96%)	3 (4%)	41	75
38	1g	119/127 (94%)	114 (96%)	5 (4%)	34	68
38	2g	120/127 (94%)	111 (92%)	9 (8%)	16	41
39	1h	114/119 (96%)	108 (95%)	6 (5%)	26	59
39	2h	114/119 (96%)	107 (94%)	7 (6%)	22	53
40	1i	90/99 (91%)	86 (96%)	4 (4%)	33	67
40	2i	89/99 (90%)	85 (96%)	4 (4%)	32	66
41	1j	66/92 (72%)	64 (97%)	2 (3%)	46	80
41	2j	69/92 (75%)	64 (93%)	5 (7%)	17	43
42	1k	82/99 (83%)	78 (95%)	4 (5%)	29	62
42	2k	83/99 (84%)	78 (94%)	5 (6%)	22	54
43	1l	96/108 (89%)	86 (90%)	10 (10%)	8	24
43	2l	96/108 (89%)	93 (97%)	3 (3%)	45	79
44	1m	93/101 (92%)	87 (94%)	6 (6%)	20	49
44	2m	92/101 (91%)	90 (98%)	2 (2%)	57	87
45	1n	49/50 (98%)	43 (88%)	6 (12%)	6	17
45	2n	49/50 (98%)	44 (90%)	5 (10%)	8	25
46	1o	78/80 (98%)	76 (97%)	2 (3%)	51	83
46	2o	78/80 (98%)	75 (96%)	3 (4%)	38	72
47	1p	69/74 (93%)	66 (96%)	3 (4%)	33	67
47	2p	68/74 (92%)	65 (96%)	3 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	91 (97%)	3 (3%)	44	78
48	2q	94/97 (97%)	89 (95%)	5 (5%)	26	59
49	1r	59/77 (77%)	55 (93%)	4 (7%)	18	47
49	2r	59/77 (77%)	57 (97%)	2 (3%)	42	76
50	1s	69/80 (86%)	67 (97%)	2 (3%)	48	81
50	2s	67/80 (84%)	64 (96%)	3 (4%)	32	66
51	1t	70/82 (85%)	67 (96%)	3 (4%)	33	67
51	2t	70/82 (85%)	65 (93%)	5 (7%)	17	44
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	25	57
All	All	9303/10064 (92%)	8749 (94%)	554 (6%)	22	54

All (554) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	61	LEU
3	1D	71	ASP
3	1D	88	ARG
3	1D	113	VAL
3	1D	147	LEU
3	1D	155	LEU
3	1D	162	SER
3	1D	176	ARG
3	1D	193	VAL
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
3	1D	273	ARG
4	1E	1	MET
4	1E	12	THR
4	1E	21	VAL
4	1E	33	VAL
4	1E	47	VAL
4	1E	73	GLU
4	1E	78	LEU
4	1E	92	THR

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Mol	Chain	Res	Type
4	1E	113	PHE
4	1E	116	VAL
4	1E	175	VAL
4	1E	181	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	95	ARG
5	1F	106	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	161	GLU
5	1F	170	LEU
5	1F	175	THR
5	1F	183	VAL
5	1F	189	THR
5	1F	192	LEU
6	1G	3	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	60	LEU
6	1G	109	VAL
6	1G	126	ASP
6	1G	133	LEU
6	1G	145	THR
6	1G	159	VAL
6	1G	175	LEU
7	1H	56	SER
7	1H	69	ARG
7	1H	71	LEU
7	1H	88	LEU
7	1H	134	SER
7	1H	155	SER
8	1I	1	MET
8	1I	2	LYS
8	1I	9	LEU
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU

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Mol	Chain	Res	Type
8	1I	92	VAL
8	1I	129	THR
8	1I	142	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	35	ARG
9	1N	48	MET
9	1N	62	VAL
9	1N	87	LEU
9	1N	99	LEU
10	1O	9	GLU
10	1O	97	ARG
10	1O	108	GLU
11	1P	55	ARG
11	1P	59	LEU
11	1P	83	VAL
11	1P	98	GLU
11	1P	112	LEU
11	1P	125	VAL
12	1Q	7	MET
12	1Q	89	ASN
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	135	ASP
12	1Q	138	ASP
13	1R	6	SER
13	1R	24	GLN
13	1R	29	LEU
13	1R	36	THR
13	1R	37	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	67	LEU
13	1R	79	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	11	LYS
14	1S	14	VAL
14	1S	36	TYR
14	1S	42	ASP

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Mol	Chain	Res	Type
14	1S	49	VAL
14	1S	69	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	89	VAL
15	1T	118	ARG
16	1U	5	LYS
16	1U	8	VAL
16	1U	50	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	83	LEU
16	1U	95	LEU
17	1V	46	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	17	VAL
18	1W	97	LYS
18	1W	107	LEU
19	1X	45	THR
19	1X	75	ASP
19	1X	81	VAL
19	1X	92	LEU
20	1Y	1	MET
20	1Y	11	ASP
20	1Y	55	TYR
20	1Y	72	VAL
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	33	LEU
21	1Z	41	LEU
21	1Z	61	LEU
21	1Z	72	ARG
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	129	SER

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Mol	Chain	Res	Type
21	1Z	150	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	14	ARG
22	10	32	ARG
22	10	43	THR
23	11	30	VAL
23	11	56	GLN
23	11	95	LEU
24	12	30	ARG
24	12	40	SER
24	12	70	GLN
25	13	30	ARG
26	14	27	THR
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	33	CYS
27	15	57	VAL
27	15	58	LEU
28	16	5	VAL
28	16	19	ARG
28	16	48	VAL
28	16	51	GLU
29	17	1	MET
29	17	24	THR
29	17	41	ARG
29	17	43	THR
30	18	14	VAL
30	18	30	ARG
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
33	1b	24	TRP
33	1b	37	ASN
33	1b	73	THR
33	1b	94	ASN
33	1b	127	ILE
33	1b	160	ASP

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Mol	Chain	Res	Type
33	1b	172	ILE
33	1b	195	ASP
34	1c	3	ASN
34	1c	21	ARG
34	1c	49	SER
34	1c	112	SER
34	1c	192	THR
34	1c	196	LEU
35	1d	3	ARG
35	1d	5	ILE
35	1d	10	ARG
35	1d	31	CYS
35	1d	53	ASP
35	1d	59	ARG
35	1d	70	ILE
35	1d	73	ARG
35	1d	112	VAL
35	1d	135	LEU
36	1e	16	THR
36	1e	31	LEU
36	1e	34	VAL
36	1e	41	VAL
36	1e	45	PHE
36	1e	51	VAL
36	1e	56	GLN
36	1e	91	LEU
37	1f	72	VAL
37	1f	73	ASN
37	1f	93	SER
38	1g	12	LEU
38	1g	16	LEU
38	1g	24	THR
38	1g	90	GLU
38	1g	94	ARG
39	1h	25	ASP
39	1h	29	SER
39	1h	49	GLU
39	1h	85	ARG
39	1h	112	LEU
39	1h	133	LEU
40	1i	17	VAL
40	1i	64	THR

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Mol	Chain	Res	Type
40	1i	65	VAL
40	1i	87	GLN
41	1j	34	VAL
41	1j	84	GLN
42	1k	31	THR
42	1k	48	ILE
42	1k	109	VAL
42	1k	114	VAL
43	1l	27	LEU
43	1l	37	CYS
43	1l	52	LEU
43	1l	55	VAL
43	1l	58	VAL
43	1l	59	ARG
43	1l	83	VAL
43	1l	89	ARG
43	1l	113	ARG
43	1l	117	ARG
44	1m	4	ILE
44	1m	8	GLU
44	1m	11	ARG
44	1m	19	LEU
44	1m	109	THR
44	1m	121	LYS
45	1n	6	LEU
45	1n	13	THR
45	1n	18	VAL
45	1n	23	ARG
45	1n	32	SER
45	1n	35	ARG
46	1o	39	LEU
46	1o	87	ILE
47	1p	2	VAL
47	1p	20	VAL
47	1p	67	THR
48	1q	15	MET
48	1q	35	VAL
48	1q	68	ARG
49	1r	26	LEU
49	1r	31	LEU
49	1r	46	GLU
49	1r	47	THR

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Mol	Chain	Res	Type
50	1s	12	ASP
50	1s	28	LYS
51	1t	13	LEU
51	1t	24	LEU
51	1t	56	MET
3	2D	20	ASP
3	2D	94	LEU
3	2D	106	ILE
3	2D	113	VAL
3	2D	116	GLN
3	2D	142	VAL
3	2D	183	ARG
3	2D	204	ILE
3	2D	242	ARG
4	2E	9	VAL
4	2E	21	VAL
4	2E	23	VAL
4	2E	24	THR
4	2E	27	LEU
4	2E	52	LEU
4	2E	75	VAL
4	2E	78	LEU
4	2E	101	ARG
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	134	ILE
4	2E	181	LEU
4	2E	184	VAL
4	2E	195	LEU
5	2F	12	LEU
5	2F	20	LEU
5	2F	33	LEU
5	2F	53	THR
5	2F	57	VAL
5	2F	74	ARG
5	2F	82	ILE
5	2F	88	VAL
5	2F	132	VAL
5	2F	149	ASP
5	2F	168	ARG
5	2F	170	LEU

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Mol	Chain	Res	Type
5	2F	183	VAL
5	2F	192	LEU
5	2F	201	VAL
6	2G	5	VAL
6	2G	7	LEU
6	2G	31	VAL
6	2G	43	LEU
6	2G	133	LEU
6	2G	135	LEU
6	2G	140	ILE
6	2G	145	THR
6	2G	159	VAL
7	2H	49	VAL
7	2H	59	ARG
7	2H	103	LEU
7	2H	134	SER
7	2H	148	ILE
7	2H	152	ARG
8	2I	38	LEU
8	2I	47	LEU
8	2I	96	ASP
8	2I	108	THR
8	2I	116	LEU
8	2I	123	LEU
9	2N	23	LEU
9	2N	28	THR
9	2N	34	LEU
9	2N	43	THR
9	2N	46	VAL
9	2N	60	ILE
9	2N	73	THR
9	2N	87	LEU
9	2N	120	LEU
9	2N	140	VAL
11	2P	45	LEU
11	2P	95	VAL
11	2P	99	LEU
11	2P	112	LEU
12	2Q	1	MET
12	2Q	2	LEU
12	2Q	16	ARG
12	2Q	21	THR

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Mol	Chain	Res	Type
12	2Q	29	PHE
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	101	ARG
12	2Q	110	THR
13	2R	15	SER
13	2R	18	LEU
13	2R	24	GLN
13	2R	29	LEU
13	2R	33	ARG
13	2R	44	LEU
13	2R	65	LEU
13	2R	100	LEU
13	2R	102	GLU
14	2S	21	THR
14	2S	36	TYR
14	2S	46	VAL
14	2S	58	LEU
14	2S	64	GLU
14	2S	83	LYS
14	2S	110	LEU
15	2T	6	LEU
15	2T	31	SER
15	2T	46	GLU
15	2T	64	ARG
15	2T	67	SER
15	2T	74	ARG
15	2T	96	ARG
15	2T	104	ASN
16	2U	74	LEU
16	2U	95	LEU
17	2V	14	VAL
17	2V	18	LEU
17	2V	38	LEU
17	2V	51	VAL
17	2V	52	VAL
17	2V	61	VAL
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
18	2W	11	ARG
18	2W	17	VAL

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Mol	Chain	Res	Type
18	2W	19	LEU
18	2W	23	LEU
18	2W	67	ASP
18	2W	92	ARG
18	2W	96	ILE
19	2X	14	SER
19	2X	45	THR
19	2X	81	VAL
20	2Y	14	LEU
20	2Y	38	ILE
20	2Y	72	VAL
20	2Y	83	THR
20	2Y	84	ARG
20	2Y	99	CYS
21	2Z	27	VAL
21	2Z	33	LEU
21	2Z	38	TYR
21	2Z	40	ASP
21	2Z	86	VAL
21	2Z	129	SER
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	171	ILE
22	20	14	ARG
22	20	27	GLU
24	22	53	LEU
25	23	23	LEU
25	23	30	ARG
25	23	31	LEU
25	23	40	THR
25	23	53	LEU
26	24	24	THR
26	24	34	GLU
26	24	50	VAL
26	24	63	TYR
27	25	6	VAL
27	25	16	ARG
27	25	21	SER
28	26	9	LEU
28	26	13	CYS
28	26	30	THR
28	26	32	ASN

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Mol	Chain	Res	Type
28	26	51	GLU
29	27	39	ARG
29	27	41	ARG
30	28	14	VAL
30	28	23	VAL
30	28	31	HIS
30	28	32	LEU
30	28	34	TRP
31	29	7	VAL
33	2b	11	LEU
33	2b	24	TRP
33	2b	41	ILE
33	2b	48	MET
33	2b	93	VAL
33	2b	94	ASN
33	2b	102	LEU
33	2b	135	GLN
33	2b	144	ARG
33	2b	165	VAL
33	2b	178	ARG
33	2b	185	ILE
33	2b	189	ASP
34	2c	49	SER
34	2c	57	ILE
34	2c	77	ILE
34	2c	89	GLU
34	2c	128	PHE
34	2c	166	GLU
34	2c	175	LEU
35	2d	31	CYS
35	2d	76	ARG
35	2d	107	ARG
35	2d	108	LEU
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	170	VAL
35	2d	175	SER
35	2d	178	VAL
35	2d	181	MET
36	2e	25	ARG
36	2e	34	VAL

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Mol	Chain	Res	Type
36	2e	41	VAL
36	2e	73	ASN
36	2e	81	GLU
36	2e	83	GLU
37	2f	10	LEU
37	2f	28	ARG
37	2f	75	LEU
38	2g	9	VAL
38	2g	15	ASP
38	2g	16	LEU
38	2g	78	ARG
38	2g	79	ARG
38	2g	95	ARG
38	2g	98	SER
38	2g	104	LEU
38	2g	154	TYR
39	2h	2	LEU
39	2h	3	THR
39	2h	12	ARG
39	2h	25	ASP
39	2h	68	ARG
39	2h	87	SER
39	2h	112	LEU
40	2i	89	ASN
40	2i	102	LEU
40	2i	108	VAL
40	2i	111	ARG
41	2j	8	LEU
41	2j	17	ASP
41	2j	59	SER
41	2j	67	THR
41	2j	100	THR
42	2k	14	VAL
42	2k	24	SER
42	2k	81	ASP
42	2k	84	VAL
42	2k	114	VAL
43	2l	12	ARG
43	2l	113	ARG
43	2l	117	ARG
44	2m	15	VAL
44	2m	103	THR

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Mol	Chain	Res	Type
45	2n	6	LEU
45	2n	11	LYS
45	2n	25	VAL
45	2n	33	VAL
45	2n	44	LEU
46	2o	37	ASN
46	2o	51	HIS
46	2o	88	ARG
47	2p	2	VAL
47	2p	21	VAL
47	2p	60	LEU
48	2q	6	LEU
48	2q	35	VAL
48	2q	57	VAL
48	2q	79	SER
48	2q	97	SER
49	2r	37	VAL
49	2r	59	SER
50	2s	65	ASN
50	2s	71	LEU
50	2s	79	THR
51	2t	24	LEU
51	2t	70	SER
51	2t	72	LEU
51	2t	84	LEU
51	2t	89	ARG
52	2u	6	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	79	ASN
8	1I	105	HIS
12	1Q	57	HIS
13	1R	24	GLN
13	1R	71	GLN
14	1S	68	GLN
15	1T	58	ASN

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Mol	Chain	Res	Type
16	1U	104	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	54	HIS
23	11	56	GLN
30	18	35	GLN
33	1b	37	ASN
33	1b	40	HIS
34	1c	6	HIS
34	1c	104	GLN
34	1c	162	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	161	ASN
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
40	1i	3	GLN
40	1i	23	ASN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
44	1m	62	ASN
45	1n	49	HIS
47	1p	13	HIS
50	1s	83	HIS
3	2D	87	ASN
3	2D	112	GLN
3	2D	220	HIS
4	2E	48	GLN
4	2E	66	HIS
5	2F	69	HIS
5	2F	203	GLN
6	2G	66	GLN
7	2H	158	HIS

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Mol	Chain	Res	Type
9	2N	38	HIS
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	57	HIS
12	2Q	123	HIS
14	2S	38	GLN
15	2T	104	ASN
15	2T	123	GLN
19	2X	31	HIS
21	2Z	55	HIS
21	2Z	73	GLN
24	22	65	ASN
26	24	46	GLN
28	26	32	ASN
31	29	20	HIS
33	2b	94	ASN
33	2b	95	GLN
34	2c	6	HIS
34	2c	162	GLN
35	2d	42	GLN
35	2d	116	GLN
35	2d	125	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	68	ASN
38	2g	86	GLN
38	2g	97	GLN
39	2h	82	HIS
40	2i	3	GLN
40	2i	31	GLN
40	2i	58	HIS
46	2o	28	GLN
47	2p	16	HIS
49	2r	63	GLN
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2860/2915 (98%)	472 (16%)	28 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2788/2915 (95%)	502 (18%)	22 (0%)
2	1B	120/121 (99%)	12 (10%)	2 (1%)
2	2B	118/121 (97%)	32 (27%)	0
32	1a	1494/1521 (98%)	243 (16%)	0
32	2a	1498/1521 (98%)	270 (18%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	71/76 (93%)	22 (30%)	0
54	1y	71/76 (93%)	21 (29%)	0
54	2w	68/76 (89%)	24 (35%)	0
54	2y	69/76 (90%)	26 (37%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	9 (12%)	0
All	All	9331/9620 (96%)	1650 (17%)	52 (0%)

All (1650) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	57	G
1	1A	60	G
1	1A	62	U
1	1A	63	A
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	91	G
1	1A	94	G
1	1A	112	U
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	123	G
1	1A	129	G
1	1A	162	G
1	1A	164	G
1	1A	185	A
1	1A	188	A

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Mol	Chain	Res	Type
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	212	A
1	1A	215	G
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	262	C
1	1A	263	C
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	288	U
1	1A	289	G
1	1A	299	G
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	376	G
1	1A	381	A
1	1A	384	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	393	A
1	1A	413	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	448	U
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	483	A
1	1A	507	G
1	1A	529	U
1	1A	530	A

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Mol	Chain	Res	Type
1	1A	534	C
1	1A	537	G
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	615	G
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	678	A
1	1A	693	G
1	1A	697	C
1	1A	703	G
1	1A	716	G
1	1A	724	A
1	1A	733	G
1	1A	777	C
1	1A	787	U
1	1A	804	U
1	1A	811	A
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	859	C

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Mol	Chain	Res	Type
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	879	G
1	1A	906	G
1	1A	913	A
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	928	G
1	1A	929	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	940	C
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	945	A
1	1A	953	U
1	1A	956	A
1	1A	957	A
1	1A	965	G
1	1A	976	G
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1021	G
1	1A	1029	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U

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Mol	Chain	Res	Type
1	1A	1059	C
1	1A	1068	G
1	1A	1071	G
1	1A	1072	U
1	1A	1073	A
1	1A	1076	G
1	1A	1079	U
1	1A	1083	G
1	1A	1084	C
1	1A	1087	C
1	1A	1090	G
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1105	G
1	1A	1112	U
1	1A	1114	G
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1126	C
1	1A	1133	G
1	1A	1134	A
1	1A	1137	G
1	1A	1138	C
1	1A	1139	G
1	1A	1140	U
1	1A	1142	A
1	1A	1146	C
1	1A	1149	A
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1162	C
1	1A	1164	C

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Mol	Chain	Res	Type
1	1A	1175	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1187	U
1	1A	1216	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1256	U
1	1A	1263	C
1	1A	1287	A
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1335	C
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1375	U
1	1A	1388	A
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1441	A
1	1A	1442	U
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1474	C
1	1A	1475	G
1	1A	1485	A
1	1A	1491	A

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Mol	Chain	Res	Type
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1530	G
1	1A	1536	A
1	1A	1539	C
1	1A	1540	A
1	1A	1545	C
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1569	U
1	1A	1571	G
1	1A	1601	A
1	1A	1605	A
1	1A	1606	G
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1658	C
1	1A	1694	G
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1750	G
1	1A	1767	A
1	1A	1776	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1800	G
1	1A	1804	A

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Mol	Chain	Res	Type
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1843	A
1	1A	1847	G
1	1A	1859	G
1	1A	1860	A
1	1A	1871	G
1	1A	1878	A
1	1A	1879	A
1	1A	1892	G
1	1A	1899	A
1	1A	1911	A
1	1A	1915	C
1	1A	1922	A
1	1A	1928	G
1	1A	1941	A
1	1A	1949	A
1	1A	1951	G
1	1A	1952	G
1	1A	1953	U
1	1A	1956	C
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2006	G
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C

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Mol	Chain	Res	Type
1	1A	2074	G
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2118	U
1	1A	2120	U
1	1A	2124	U
1	1A	2132	G
1	1A	2135	U
1	1A	2136	A
1	1A	2141	A
1	1A	2143	G
1	1A	2144	U
1	1A	2148	A
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2169	G
1	1A	2170	G
1	1A	2172	U
1	1A	2177	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2188	G
1	1A	2189	U
1	1A	2190	G
1	1A	2192	A
1	1A	2194	U
1	1A	2195	A

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Mol	Chain	Res	Type
1	1A	2196	C
1	1A	2200	C
1	1A	2203	G
1	1A	2206	G
1	1A	2207	C
1	1A	2211	U
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2230	U
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2285	A
1	1A	2292	G
1	1A	2295	C
1	1A	2299	A
1	1A	2306	C
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2366	G
1	1A	2373	A
1	1A	2384	G
1	1A	2395	G
1	1A	2397	C
1	1A	2408	G
1	1A	2418	U
1	1A	2422	G
1	1A	2430	A
1	1A	2434	A
1	1A	2437	A
1	1A	2441	G

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Mol	Chain	Res	Type
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2483	C
1	1A	2488	A
1	1A	2489	C
1	1A	2490	A
1	1A	2502	G
1	1A	2506	G
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2532	C
1	1A	2537	G
1	1A	2541	G
1	1A	2561	G
1	1A	2566	U
1	1A	2576	A
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2594	G
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2646	G
1	1A	2666	A
1	1A	2681	G
1	1A	2682	A
1	1A	2701	U
1	1A	2702	C
1	1A	2703	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A

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Mol	Chain	Res	Type
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2745	G
1	1A	2746	A
1	1A	2757	G
1	1A	2763	A
1	1A	2765	C
1	1A	2770	A
1	1A	2771	A
1	1A	2774	G
1	1A	2777	A
1	1A	2778	A
1	1A	2779	G
1	1A	2782	C
1	1A	2791	A
1	1A	2793	G
1	1A	2803	A
1	1A	2804	C
1	1A	2807	C
1	1A	2813	G
1	1A	2830	A
1	1A	2831	A
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	9	G
2	1B	12	C
2	1B	15	A
2	1B	25	A
2	1B	35	U
2	1B	56	G
2	1B	66	A
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G

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Mol	Chain	Res	Type
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	54	C
32	1a	61	G
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	145	G
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	183	G
32	1a	189(F)	U
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	318	G
32	1a	321	A
32	1a	328	C

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Mol	Chain	Res	Type
32	1a	332	G
32	1a	342	C
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	382	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	453	A
32	1a	457	C
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	482	A
32	1a	483	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	531	U

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Mol	Chain	Res	Type
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	596	C
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	717	C
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	747	C
32	1a	749	C
32	1a	752	G
32	1a	755	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	885	G

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Mol	Chain	Res	Type
32	1a	891	U
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	997	U
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1026	G
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1040	U

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Mol	Chain	Res	Type
32	1a	1043	C
32	1a	1053	G
32	1a	1054	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1096	C
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1125	U
32	1a	1129	C
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1270	C
32	1a	1275	A
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1300	G
32	1a	1302	U

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Mol	Chain	Res	Type
32	1a	1319	A
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1378	C
32	1a	1397	C
32	1a	1400	5MC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	14	A
53	1v	24	A
54	1w	2	C
54	1w	3	C
54	1w	4	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	14	A
54	1w	19	G

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Mol	Chain	Res	Type
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	62	C
54	1w	68	C
54	1w	70	G
54	1w	71	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	13	C
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	48	C
55	1x	59	A
55	1x	61	C
55	1x	68	C
55	1x	69	C
55	1x	70	G
55	1x	76	A
54	1y	6	G
54	1y	8	4SU
54	1y	9	A
54	1y	11	C
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	35	A
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	54	5MU
54	1y	57	G

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Mol	Chain	Res	Type
54	1y	59	U
54	1y	65	G
54	1y	69	G
54	1y	70	G
54	1y	73	A
1	2A	11	G
1	2A	12	U
1	2A	15	G
1	2A	29	U
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	96	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	125	G
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	198	C
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	243	U
1	2A	248	G
1	2A	249	C

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Mol	Chain	Res	Type
1	2A	250	G
1	2A	266	G
1	2A	271(E)	U
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272	G
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	311	A
1	2A	312	G
1	2A	320	A
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	354	G
1	2A	361	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	391	G
1	2A	396	G
1	2A	399	G
1	2A	405	U
1	2A	411	G
1	2A	422	A
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	474	G

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Mol	Chain	Res	Type
1	2A	481	G
1	2A	498	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	783	A
1	2A	784	A

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Mol	Chain	Res	Type
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	870	A
1	2A	874	G
1	2A	877	U
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
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G

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Mol	Chain	Res	Type
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1122	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1137	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1143	A
1	2A	1144	G
1	2A	1171	G
1	2A	1188	U
1	2A	1208	C
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1244	G
1	2A	1247	A
1	2A	1248	G
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A

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Mol	Chain	Res	Type
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1345	C
1	2A	1347	G
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1441	G
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A

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Mol	Chain	Res	Type
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1511	C
1	2A	1531	C
1	2A	1533	G
1	2A	1542	A
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1588	C
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1663	C
1	2A	1664	A
1	2A	1674	G
1	2A	1676	A
1	2A	1680	U
1	2A	1691	C
1	2A	1694	C
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G

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Mol	Chain	Res	Type
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1806	C
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1866	C
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C

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Mol	Chain	Res	Type
1	2A	2051	A
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2070	G
1	2A	2093	G
1	2A	2099	U
1	2A	2104	G
1	2A	2105	C
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2153	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A

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Mol	Chain	Res	Type
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2171	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2178	C
1	2A	2182	G
1	2A	2183	C
1	2A	2185	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2243	U
1	2A	2262	U
1	2A	2275	C
1	2A	2278	A
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C

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Mol	Chain	Res	Type
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2377	A
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2419	U
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2440	C
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2469	A
1	2A	2476	A
1	2A	2487	G
1	2A	2490	G
1	2A	2497	A
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2536	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2579	C

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Mol	Chain	Res	Type
1	2A	2586	C
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2641	G
1	2A	2654	A
1	2A	2664	G
1	2A	2689	U
1	2A	2691	C
1	2A	2696	U
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2748	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2780	G
1	2A	2789	C
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2892	A

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Mol	Chain	Res	Type
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	15	A
2	2B	19	G
2	2B	25	A
2	2B	32	C
2	2B	42	C
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	57	A
2	2B	63	G
2	2B	64	C
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	84	C
2	2B	88	C
2	2B	91	C
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	114	C
2	2B	116	G
2	2B	119	G
32	2a	6	G
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	30	U
32	2a	32	A
32	2a	33	A

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Mol	Chain	Res	Type
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	54	C
32	2a	66	G
32	2a	73	G
32	2a	80	G
32	2a	88	A
32	2a	92	C
32	2a	97	G
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	131	C
32	2a	163	C
32	2a	174	C
32	2a	180	U
32	2a	182	U
32	2a	189(B)	C
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	301	G
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C

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Mol	Chain	Res	Type
32	2a	346	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	363	A
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C

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Mol	Chain	Res	Type
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	619	U
32	2a	630	G
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	673	G
32	2a	687	A
32	2a	688	G
32	2a	701	C
32	2a	702	A
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	735	C
32	2a	738	C
32	2a	749	C
32	2a	755	G
32	2a	773	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	853	G
32	2a	858	G
32	2a	859	A
32	2a	870	U
32	2a	902	G
32	2a	914	A

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Mol	Chain	Res	Type
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	999	C
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1035	A

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Mol	Chain	Res	Type
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1045	C
32	2a	1046	A
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1087	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1109	C
32	2a	1117	G
32	2a	1121	U
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1161	C
32	2a	1174	G
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G

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Mol	Chain	Res	Type
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1264	C
32	2a	1270	C
32	2a	1274	G
32	2a	1275	A
32	2a	1276	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1303	C
32	2a	1305	G
32	2a	1313	U
32	2a	1320	C
32	2a	1322	C
32	2a	1323	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C

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Mol	Chain	Res	Type
32	2a	1456	G
32	2a	1492	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1532	U
53	2v	13	A
53	2v	14	A
54	2w	3	C
54	2w	4	C
54	2w	8	4SU
54	2w	9	A
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	29	G
54	2w	32	PSU
54	2w	34	G
54	2w	46	7MG
54	2w	48	C
54	2w	50	U
54	2w	61	C
54	2w	64	A
54	2w	65	G
54	2w	66	U
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	74	C
54	2w	76	A
55	2x	9	G
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	47	U

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Mol	Chain	Res	Type
55	2x	48	C
55	2x	62	C
55	2x	67	C
55	2x	76	A
54	2y	2	C
54	2y	14	A
54	2y	15	G
54	2y	19	G
54	2y	30	G
54	2y	34	G
54	2y	40	C
54	2y	45	U
54	2y	46	7MG
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	60	U
54	2y	61	C
54	2y	62	C
54	2y	63	G
54	2y	65	G
54	2y	66	U
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	185	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	716	G
1	1A	811	A
1	1A	913	A

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Mol	Chain	Res	Type
1	1A	941	U
1	1A	1067	A
1	1A	1093	G
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1286	U
1	1A	1554	A
1	1A	1700	G
1	1A	2014	G
1	1A	2156	A
1	1A	2205	C
1	1A	2418	U
1	1A	2442	A
1	1A	2451	A
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
2	1B	65	C
1	2A	34	C
1	2A	195	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G

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Mol	Chain	Res	Type
1	2A	2126	A
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PSU	1A	1933	1	16,21,22	1.53	3 (18%)	20,30,33	3.54	6 (30%)
1	5MU	1A	1937	1	14,22,23	0.75	0	16,32,35	2.10	2 (12%)
1	PSU	1A	1939	1	16,21,22	1.43	1 (6%)	20,30,33	3.63	7 (35%)
1	4OC	1A	1942	1	15,22,24	0.83	1 (6%)	19,31,35	0.91	1 (5%)
1	5MU	1A	1961	1,56	14,22,23	0.67	0	16,32,35	2.11	3 (18%)
1	5MC	1A	1964	1	15,22,23	1.40	1 (6%)	17,32,35	1.25	2 (11%)
1	5MC	1A	1984	1,56	15,22,23	1.42	1 (6%)	17,32,35	0.99	2 (11%)
1	OMG	1A	2263	1,55,56	18,26,27	1.14	2 (11%)	22,38,41	1.99	6 (27%)
1	2MA	1A	2515	1,56	18,25,26	1.57	4 (22%)	17,37,40	1.69	2 (11%)
1	2MU	1A	2564	1,56	14,22,24	0.95	1 (7%)	18,31,36	2.12	1 (5%)
1	PSU	1A	2617	1,56	16,21,22	1.62	3 (18%)	20,30,33	3.51	7 (35%)
32	2MG	1a	1207	32	19,26,27	1.33	2 (10%)	20,38,41	2.36	7 (35%)
32	5MC	1a	1400	32	15,22,23	1.35	1 (6%)	17,32,35	1.26	2 (11%)
32	4OC	1a	1402	32	16,23,24	0.74	0	19,32,35	1.06	1 (5%)
32	5MC	1a	1404	32	15,22,23	1.45	2 (13%)	17,32,35	1.01	1 (5%)
32	5MC	1a	1407	32	15,22,23	1.35	1 (6%)	17,32,35	1.12	1 (5%)
32	UR3	1a	1498	32	14,22,23	0.86	1 (7%)	16,32,35	0.60	0
32	MA6	1a	1518	32	16,26,27	0.94	1 (6%)	18,38,41	2.45	6 (33%)
32	MA6	1a	1519	32	16,26,27	1.01	1 (6%)	18,38,41	2.21	5 (27%)
32	PSU	1a	516	32,56	16,21,22	1.34	2 (12%)	20,30,33	3.54	6 (30%)
32	7MG	1a	527	32	20,26,27	1.79	2 (10%)	22,39,42	2.70	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	1a	966	32	20,27,28	1.48	3 (15%)	21,40,43	2.42	7 (33%)
32	5MC	1a	967	32	15,22,23	1.33	1 (6%)	17,32,35	1.02	1 (5%)
43	0TD	1l	92	43	5,9,10	3.05	2 (40%)	3,11,13	4.01	2 (66%)
54	PSU	1w	32	54	16,21,22	1.31	1 (6%)	20,30,33	3.54	6 (30%)
54	MIA	1w	37	54	23,31,32	1.72	2 (8%)	25,44,47	1.49	5 (20%)
54	PSU	1w	39	54	16,21,22	1.46	1 (6%)	20,30,33	3.44	6 (30%)
54	7MG	1w	46	54	20,26,27	1.54	2 (10%)	22,39,42	2.94	5 (22%)
54	5MU	1w	54	54	14,22,23	0.75	0	16,32,35	2.18	3 (18%)
54	PSU	1w	55	54	16,21,22	1.22	1 (6%)	20,30,33	3.86	6 (30%)
54	4SU	1w	8	54	14,21,22	1.35	2 (14%)	15,30,33	1.39	2 (13%)
55	5MC	1x	32	55	15,22,23	1.39	1 (6%)	17,32,35	1.27	3 (17%)
55	5MU	1x	54	55,56	14,22,23	0.78	0	16,32,35	2.35	3 (18%)
55	PSU	1x	55	55	16,21,22	1.48	1 (6%)	20,30,33	3.65	6 (30%)
55	4SU	1x	8	55	14,21,22	1.49	2 (14%)	15,30,33	2.53	2 (13%)
54	PSU	1y	32	54	16,21,22	1.29	1 (6%)	20,30,33	3.81	6 (30%)
54	MIA	1y	37	54	18,24,32	1.24	2 (11%)	17,35,47	1.85	2 (11%)
54	PSU	1y	39	54	16,21,22	1.30	1 (6%)	20,30,33	3.66	5 (25%)
54	7MG	1y	46	54	20,26,27	1.79	3 (15%)	22,39,42	3.17	7 (31%)
54	5MU	1y	54	54	14,22,23	0.75	1 (7%)	16,32,35	2.33	3 (18%)
54	PSU	1y	55	54	16,21,22	1.47	1 (6%)	20,30,33	3.61	7 (35%)
54	4SU	1y	8	54	14,21,22	1.19	1 (7%)	15,30,33	1.62	2 (13%)
1	PSU	2A	1911	1	16,21,22	1.32	1 (6%)	20,30,33	3.60	7 (35%)
1	5MU	2A	1915	1	14,22,23	0.71	0	16,32,35	2.18	3 (18%)
1	PSU	2A	1917	1	16,21,22	1.44	1 (6%)	20,30,33	3.57	7 (35%)
1	4OC	2A	1920	1	15,22,24	0.75	0	19,31,35	0.94	1 (5%)
1	5MU	2A	1939	1,56	14,22,23	0.73	0	16,32,35	2.17	3 (18%)
1	5MC	2A	1942	1	15,22,23	1.39	1 (6%)	17,32,35	1.05	1 (5%)
1	5MC	2A	1962	1,56	15,22,23	1.37	1 (6%)	17,32,35	1.09	2 (11%)
1	OMG	2A	2251	1,55,56	18,26,27	1.36	2 (11%)	22,38,41	2.02	6 (27%)
1	2MA	2A	2503	1,56	18,25,26	1.50	3 (16%)	17,37,40	1.61	2 (11%)
1	2MU	2A	2552	1,56	14,22,24	1.02	1 (7%)	18,31,36	1.98	1 (5%)
1	PSU	2A	2605	1	16,21,22	1.58	1 (6%)	20,30,33	3.28	6 (30%)
32	2MG	2a	1207	32	19,26,27	1.31	2 (10%)	20,38,41	2.54	9 (45%)
32	5MC	2a	1400	32	15,22,23	1.54	1 (6%)	17,32,35	1.03	1 (5%)
32	4OC	2a	1402	32,56	16,23,24	0.70	0	19,32,35	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1404	32	15,22,23	1.41	1 (6%)	17,32,35	1.18	2 (11%)
32	5MC	2a	1407	32	15,22,23	1.37	1 (6%)	17,32,35	1.21	1 (5%)
32	UR3	2a	1498	32	14,22,23	0.90	1 (7%)	16,32,35	0.77	1 (6%)
32	MA6	2a	1518	32	16,26,27	1.04	1 (6%)	18,38,41	2.33	4 (22%)
32	MA6	2a	1519	32	16,26,27	1.06	1 (6%)	18,38,41	2.22	5 (27%)
32	PSU	2a	516	32	16,21,22	1.23	1 (6%)	20,30,33	3.49	6 (30%)
32	7MG	2a	527	32,56	20,26,27	1.67	2 (10%)	22,39,42	2.73	6 (27%)
32	M2G	2a	966	32	20,27,28	1.44	3 (15%)	21,40,43	2.26	7 (33%)
32	5MC	2a	967	32	15,22,23	1.49	1 (6%)	17,32,35	0.95	2 (11%)
43	0TD	2l	92	43	5,9,10	3.09	2 (40%)	3,11,13	2.73	2 (66%)
54	PSU	2w	32	54	16,21,22	1.19	1 (6%)	20,30,33	3.59	6 (30%)
54	MIA	2w	37	54	20,27,32	1.78	2 (10%)	21,39,47	1.55	5 (23%)
54	PSU	2w	39	54	16,21,22	1.28	1 (6%)	20,30,33	3.71	7 (35%)
54	7MG	2w	46	54	20,26,27	1.69	2 (10%)	22,39,42	2.66	5 (22%)
54	5MU	2w	54	54	14,22,23	0.76	0	16,32,35	2.39	2 (12%)
54	PSU	2w	55	54	16,21,22	1.25	1 (6%)	20,30,33	3.61	6 (30%)
54	4SU	2w	8	54	14,21,22	1.24	1 (7%)	15,30,33	1.33	2 (13%)
55	5MC	2x	32	55	15,22,23	1.38	1 (6%)	17,32,35	1.22	2 (11%)
55	5MU	2x	54	55	14,22,23	0.75	0	16,32,35	2.10	3 (18%)
55	PSU	2x	55	55	16,21,22	1.33	1 (6%)	20,30,33	3.57	6 (30%)
55	4SU	2x	8	55,56	14,21,22	1.28	2 (14%)	15,30,33	2.39	2 (13%)
54	PSU	2y	32	54	16,21,22	1.27	1 (6%)	20,30,33	3.58	7 (35%)
54	MIA	2y	37	54	18,24,32	1.19	2 (11%)	17,35,47	1.91	2 (11%)
54	PSU	2y	39	54	16,21,22	1.49	1 (6%)	20,30,33	4.24	7 (35%)
54	7MG	2y	46	54	20,26,27	1.71	2 (10%)	22,39,42	2.98	6 (27%)
54	5MU	2y	54	54	14,22,23	0.69	0	16,32,35	2.16	3 (18%)
54	PSU	2y	55	54	16,21,22	1.19	2 (12%)	20,30,33	3.77	7 (35%)
54	4SU	2y	8	54	14,21,22	1.25	1 (7%)	15,30,33	1.30	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1937	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	0/5/27/30	0/2/2/2
1	5MU	1A	1961	1,56	-	0/3/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/3/25/26	0/2/2/2
1	5MC	1A	1984	1,56	-	0/3/25/26	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	1A	2515	1,56	-	0/3/25/26	0/3/3/3
1	2MU	1A	2564	1,56	-	0/5/27/28	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	0/7/37/38	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	1l	92	43	-	0/2/12/14	0/0/0/0
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	0/11/33/34	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	0/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/3/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/3/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/3/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/3/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	0/7/37/38	0/3/3/3
54	5MU	1y	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/3/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	2A	1915	1	-	0/3/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	2A	1939	1,56	-	0/3/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/3/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/3/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	2A	2503	1,56	-	0/3/25/26	0/3/3/3
1	2MU	2A	2552	1,56	-	0/5/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	0/7/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	0/7/37/38	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	2l	92	43	-	0/2/12/14	0/0/0/0
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	0/7/37/38	0/3/3/3
54	5MU	2w	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/3/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/3/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/3/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	0/3/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	0/7/37/38	0/3/3/3
54	5MU	2y	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/3/25/26	0/2/2/2

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C2-S10	-6.52	1.70	1.75
54	2w	37	MIA	C2-S10	-6.20	1.70	1.75
43	1l	92	0TD	CB-SB	-5.86	1.69	1.84
43	2l	92	0TD	CB-SB	-5.79	1.69	1.84
1	2A	2605	PSU	C5-C1'	-5.09	1.47	1.52
1	1A	2617	PSU	C5-C1'	-5.00	1.47	1.52
54	2y	39	PSU	C5-C1'	-4.91	1.48	1.52
54	1y	55	PSU	C5-C1'	-4.81	1.48	1.52
1	1A	1933	PSU	C5-C1'	-4.59	1.48	1.52
55	1x	55	PSU	C5-C1'	-4.55	1.48	1.52
54	1w	39	PSU	C5-C1'	-4.48	1.48	1.52
1	2A	1917	PSU	C5-C1'	-4.35	1.48	1.52
54	1w	8	4SU	C4-S4	-4.16	1.59	1.67
1	1A	1939	PSU	C5-C1'	-4.12	1.48	1.52
55	2x	55	PSU	C5-C1'	-3.96	1.48	1.52
54	2y	8	4SU	C4-S4	-3.82	1.60	1.67
54	2w	8	4SU	C4-S4	-3.81	1.60	1.67
54	1y	32	PSU	C5-C1'	-3.76	1.49	1.52
32	1a	516	PSU	C5-C1'	-3.75	1.49	1.52
54	1w	32	PSU	C5-C1'	-3.74	1.49	1.52
1	2A	1911	PSU	C5-C1'	-3.73	1.49	1.52
55	1x	8	4SU	C2-N3	-3.72	1.30	1.38
54	2y	32	PSU	C5-C1'	-3.71	1.49	1.52
55	1x	8	4SU	C4-S4	-3.67	1.60	1.67
54	2w	39	PSU	C5-C1'	-3.65	1.49	1.52
54	1y	39	PSU	C5-C1'	-3.65	1.49	1.52
55	2x	8	4SU	C4-S4	-3.58	1.60	1.67
54	2w	55	PSU	C5-C1'	-3.57	1.49	1.52
54	1y	8	4SU	C4-S4	-3.56	1.60	1.67
54	1w	55	PSU	C5-C1'	-3.49	1.49	1.52
32	2a	516	PSU	C5-C1'	-3.41	1.49	1.52
54	2y	55	PSU	C5-C1'	-3.06	1.49	1.52
54	2w	32	PSU	C5-C1'	-3.04	1.49	1.52
55	2x	8	4SU	C2-N3	-2.55	1.33	1.38
1	2A	2552	2MU	O5'-C5'	-2.29	1.41	1.44
32	1a	516	PSU	O4'-C1'	-2.25	1.41	1.44
1	1A	1942	4OC	O5'-C5'	-2.22	1.41	1.44
54	2y	55	PSU	C2-N1	-2.16	1.33	1.38
1	1A	2564	2MU	C2-N3	-2.16	1.33	1.38
1	1A	2617	PSU	C2-N3	-2.14	1.33	1.38
1	1A	2515	2MA	O5'-C5'	-2.06	1.41	1.44
54	1y	54	5MU	C2-N3	-2.05	1.34	1.38
1	1A	1933	PSU	O4'-C1'	-2.05	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1933	PSU	C2-N1	-2.04	1.34	1.38
1	1A	2617	PSU	C2-N1	-2.01	1.34	1.38
54	1w	8	4SU	C2-N3	-2.01	1.34	1.38
32	1a	1404	5MC	O5'-C5'	-2.01	1.42	1.44
32	1a	1498	UR3	C4-N3	2.08	1.41	1.38
32	2a	1498	UR3	C4-N3	2.09	1.41	1.38
54	1y	46	7MG	C4-N3	2.10	1.37	1.34
54	2y	37	MIA	C2-N3	2.41	1.36	1.32
54	1y	37	MIA	C2-N3	2.55	1.36	1.32
1	2A	2503	2MA	C5-C4	2.85	1.46	1.40
1	1A	2263	OMG	C5-C4	2.87	1.47	1.40
43	1l	92	0TD	CA-C	2.98	1.54	1.50
1	1A	2515	2MA	C5-C4	3.00	1.47	1.40
32	1a	1518	MA6	C5-C4	3.03	1.47	1.40
32	1a	1207	2MG	C5-C4	3.04	1.47	1.40
32	2a	527	7MG	C5-C4	3.07	1.47	1.39
32	1a	966	M2G	C5-C4	3.08	1.47	1.40
32	2a	1207	2MG	C5-C4	3.09	1.47	1.40
32	2a	966	M2G	C5-C4	3.13	1.47	1.40
32	1a	1519	MA6	C5-C4	3.15	1.47	1.40
32	2a	1519	MA6	C5-C4	3.16	1.47	1.40
1	1A	2263	OMG	C6-C5	3.16	1.47	1.41
54	2w	37	MIA	C5-C4	3.21	1.47	1.40
32	2a	966	M2G	C2-N2	3.21	1.40	1.34
1	2A	2251	OMG	C5-C4	3.21	1.47	1.40
54	2w	46	7MG	C5-C4	3.22	1.47	1.39
54	1w	37	MIA	C5-C4	3.25	1.47	1.40
54	1w	46	7MG	C5-C4	3.27	1.48	1.39
32	2a	1518	MA6	C5-C4	3.31	1.48	1.40
54	1y	37	MIA	C5-C4	3.39	1.48	1.40
54	2y	46	7MG	C5-C4	3.41	1.48	1.39
54	2y	37	MIA	C5-C4	3.42	1.48	1.40
1	2A	2503	2MA	C6-N6	3.42	1.35	1.27
32	1a	527	7MG	C5-C4	3.42	1.48	1.39
43	2l	92	0TD	CA-C	3.43	1.54	1.50
1	1A	2515	2MA	C6-N6	3.51	1.35	1.27
54	1y	46	7MG	C5-C4	3.55	1.48	1.39
32	1a	966	M2G	C2-N2	3.69	1.40	1.34
1	2A	2503	2MA	C6-C5	3.72	1.47	1.41
1	1A	2515	2MA	C6-C5	3.90	1.47	1.41
32	2a	966	M2G	C6-C5	3.99	1.48	1.41
32	1a	966	M2G	C6-C5	3.99	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2251	OMG	C6-C5	4.13	1.49	1.41
32	2a	1207	2MG	C6-C5	4.14	1.49	1.41
32	1a	1207	2MG	C6-C5	4.19	1.49	1.41
32	1a	1407	5MC	C5-C4	4.53	1.48	1.41
32	1a	967	5MC	C5-C4	4.62	1.48	1.41
32	2a	1407	5MC	C5-C4	4.62	1.48	1.41
1	2A	1962	5MC	C5-C4	4.69	1.48	1.41
32	1a	1400	5MC	C5-C4	4.70	1.48	1.41
55	1x	32	5MC	C5-C4	4.73	1.48	1.41
1	1A	1964	5MC	C5-C4	4.82	1.48	1.41
55	2x	32	5MC	C5-C4	4.90	1.48	1.41
32	1a	1404	5MC	C5-C4	4.91	1.48	1.41
1	2A	1942	5MC	C5-C4	4.96	1.48	1.41
1	1A	1984	5MC	C5-C4	4.99	1.48	1.41
32	2a	1404	5MC	C5-C4	5.00	1.48	1.41
54	1w	46	7MG	C6-C5	5.14	1.47	1.41
32	2a	967	5MC	C5-C4	5.23	1.49	1.41
32	2a	1400	5MC	C5-C4	5.46	1.49	1.41
54	2y	46	7MG	C6-C5	5.67	1.48	1.41
54	1y	46	7MG	C6-C5	5.91	1.48	1.41
54	2w	46	7MG	C6-C5	5.92	1.48	1.41
32	2a	527	7MG	C6-C5	6.01	1.48	1.41
32	1a	527	7MG	C6-C5	6.49	1.49	1.41

All (328) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	39	PSU	N1-C2-N3	-10.39	120.93	128.40
54	1y	32	PSU	N1-C2-N3	-10.01	121.20	128.40
54	1y	39	PSU	N1-C2-N3	-9.97	121.22	128.40
54	2y	55	PSU	N1-C2-N3	-9.95	121.24	128.40
32	1a	516	PSU	N1-C2-N3	-9.93	121.26	128.40
1	1A	1939	PSU	N1-C2-N3	-9.91	121.27	128.40
54	2w	32	PSU	N1-C2-N3	-9.79	121.36	128.40
1	1A	2617	PSU	N1-C2-N3	-9.74	121.39	128.40
1	2A	1911	PSU	N1-C2-N3	-9.74	121.40	128.40
54	2y	32	PSU	N1-C2-N3	-9.71	121.42	128.40
54	1w	32	PSU	N1-C2-N3	-9.50	121.57	128.40
32	2a	516	PSU	N1-C2-N3	-9.49	121.57	128.40
54	1w	55	PSU	N1-C2-N3	-9.42	121.62	128.40
54	2w	55	PSU	N1-C2-N3	-9.38	121.65	128.40
54	2y	39	PSU	N1-C2-N3	-9.28	121.72	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	55	PSU	C5-C4-N3	-9.24	117.85	125.43
55	2x	55	PSU	N1-C2-N3	-9.23	121.76	128.40
54	2y	39	PSU	C5-C4-N3	-9.18	117.90	125.43
54	1y	32	PSU	C5-C4-N3	-9.07	117.99	125.43
1	1A	1933	PSU	C5-C4-N3	-9.07	117.99	125.43
55	1x	55	PSU	N1-C2-N3	-9.04	121.90	128.40
54	2y	39	PSU	C5-C1'-C2'	-8.95	100.11	115.55
54	2y	55	PSU	C5-C4-N3	-8.93	118.10	125.43
1	2A	1917	PSU	C5-C4-N3	-8.92	118.11	125.43
54	1y	55	PSU	C5-C4-N3	-8.91	118.12	125.43
1	2A	2605	PSU	N1-C2-N3	-8.82	122.05	128.40
54	1w	39	PSU	N1-C2-N3	-8.81	122.06	128.40
54	1w	55	PSU	C5-C4-N3	-8.79	118.22	125.43
1	2A	1917	PSU	N1-C2-N3	-8.78	122.09	128.40
54	1y	39	PSU	C5-C4-N3	-8.68	118.31	125.43
54	1y	55	PSU	N1-C2-N3	-8.62	122.20	128.40
1	1A	1933	PSU	N1-C2-N3	-8.58	122.23	128.40
54	1w	39	PSU	C5-C4-N3	-8.51	118.45	125.43
54	2w	32	PSU	C5-C4-N3	-8.47	118.48	125.43
55	2x	55	PSU	C5-C4-N3	-8.40	118.54	125.43
54	2y	32	PSU	C5-C4-N3	-8.39	118.55	125.43
54	1w	32	PSU	C5-C4-N3	-8.34	118.58	125.43
1	2A	1911	PSU	C5-C4-N3	-8.28	118.64	125.43
32	2a	516	PSU	C5-C4-N3	-8.24	118.67	125.43
1	1A	1939	PSU	C5-C4-N3	-8.15	118.74	125.43
54	2w	55	PSU	C5-C4-N3	-8.06	118.81	125.43
54	2w	39	PSU	C5-C4-N3	-7.97	118.89	125.43
32	1a	516	PSU	C5-C4-N3	-7.79	119.04	125.43
1	1A	2617	PSU	C5-C4-N3	-7.43	119.33	125.43
1	2A	2605	PSU	C5-C4-N3	-7.31	119.43	125.43
32	1a	1518	MA6	N3-C2-N1	-6.53	123.17	128.86
54	2y	37	MIA	N3-C2-N1	-6.46	123.23	128.86
54	1y	37	MIA	N3-C2-N1	-6.41	123.28	128.86
43	1l	92	0TD	CSB-SB-CB	-6.34	89.78	101.60
32	2a	1518	MA6	N3-C2-N1	-6.17	123.49	128.86
54	1w	55	PSU	C5-C1'-C2'	-6.09	105.05	115.55
32	1a	1519	MA6	N3-C2-N1	-6.09	123.56	128.86
55	1x	54	5MU	C5-C4-N3	-5.76	118.88	125.24
54	1y	54	5MU	C5-C4-N3	-5.66	118.99	125.24
54	2w	54	5MU	C5-C4-N3	-5.51	119.16	125.24
54	2y	54	5MU	C5-C4-N3	-5.50	119.18	125.24
54	2y	46	7MG	C5-C6-N1	-5.47	114.79	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	C5-C4-N3	-5.45	119.22	125.24
54	1w	46	7MG	C5-C6-N1	-5.43	114.85	123.37
54	1w	54	5MU	C5-C4-N3	-5.42	119.26	125.24
54	1y	46	7MG	C5-C4-N3	-5.39	117.48	126.47
1	2A	1939	5MU	C5-C4-N3	-5.36	119.33	125.24
32	2a	1519	MA6	N3-C2-N1	-5.35	124.19	128.86
54	1y	46	7MG	C5-C6-N1	-5.25	115.14	123.37
32	1a	527	7MG	C5-C4-N3	-5.18	117.82	126.47
1	2A	1915	5MU	C5-C4-N3	-5.16	119.55	125.24
32	1a	527	7MG	C5-C6-N1	-5.16	115.27	123.37
1	1A	1937	5MU	C5-C4-N3	-5.13	119.58	125.24
54	2y	46	7MG	C5-C4-N3	-5.07	118.00	126.47
1	1A	1961	5MU	C5-C4-N3	-5.04	119.69	125.24
32	2a	527	7MG	C5-C4-N3	-5.02	118.09	126.47
54	2w	46	7MG	C5-C6-N1	-4.91	115.67	123.37
54	1w	46	7MG	C5-C4-N3	-4.77	118.50	126.47
54	1y	55	PSU	C5-C1'-C2'	-4.76	107.33	115.55
54	2w	55	PSU	C5-C1'-C2'	-4.70	107.44	115.55
54	2w	46	7MG	C5-C4-N3	-4.69	118.64	126.47
32	2a	527	7MG	C5-C6-N1	-4.62	116.12	123.37
1	2A	2605	PSU	C5-C6-N1	-4.46	118.61	124.39
55	2x	8	4SU	C5-C4-N3	-4.43	118.14	123.73
1	1A	2617	PSU	C5-C6-N1	-4.36	118.73	124.39
54	1y	55	PSU	C5-C6-N1	-4.35	118.75	124.39
55	1x	8	4SU	C5-C4-N3	-4.32	118.28	123.73
32	1a	1207	2MG	C5-C6-N1	-4.27	117.40	123.48
54	1w	39	PSU	C5-C6-N1	-4.25	118.88	124.39
54	2y	39	PSU	C5-C6-N1	-4.21	118.93	124.39
55	2x	55	PSU	C5-C6-N1	-4.17	118.98	124.39
32	2a	1207	2MG	C6-C5-C4	-4.14	116.72	120.84
32	2a	966	M2G	C5-C6-N1	-4.14	117.59	123.48
32	2a	1207	2MG	C5-C6-N1	-4.14	117.59	123.48
32	2a	1518	MA6	C4-C5-N7	-4.01	105.53	109.41
43	2l	92	0TD	CSB-SB-CB	-4.01	94.12	101.60
32	1a	516	PSU	C5-C6-N1	-3.96	119.25	124.39
32	2a	1402	4OC	CM4-N4-C4	-3.96	119.53	122.94
54	2w	55	PSU	C5-C6-N1	-3.94	119.28	124.39
54	2w	39	PSU	C5-C6-N1	-3.94	119.28	124.39
32	2a	1207	2MG	C4-C5-N7	-3.93	105.61	109.41
54	2y	32	PSU	C5-C6-N1	-3.93	119.29	124.39
55	1x	55	PSU	C5-C6-N1	-3.92	119.31	124.39
1	1A	2263	OMG	C5-C6-N1	-3.89	117.94	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	C4-C5-N7	-3.88	105.66	109.41
1	2A	1917	PSU	C5-C6-N1	-3.87	119.37	124.39
55	1x	55	PSU	C5-C1'-C2'	-3.85	108.91	115.55
32	2a	1519	MA6	C4-C5-N7	-3.81	105.73	109.41
1	1A	1939	PSU	C5-C6-N1	-3.81	119.45	124.39
1	1A	1933	PSU	C5-C6-N1	-3.77	119.50	124.39
1	2A	1917	PSU	C5-C1'-C2'	-3.76	109.07	115.55
54	1y	32	PSU	C5-C1'-C2'	-3.75	109.08	115.55
32	2a	516	PSU	C5-C6-N1	-3.75	119.53	124.39
32	1a	966	M2G	C5-C6-N1	-3.75	118.15	123.48
32	1a	1518	MA6	C4-C5-N7	-3.71	105.82	109.41
1	2A	2251	OMG	C5-C6-N1	-3.69	118.23	123.48
54	1w	37	MIA	C12-N6-C6	-3.67	118.52	123.26
54	1w	55	PSU	C5-C6-N1	-3.67	119.63	124.39
32	2a	966	M2G	C6-C5-C4	-3.66	117.21	120.84
54	1y	39	PSU	C5-C6-N1	-3.66	119.65	124.39
32	2a	1207	2MG	CM2-N2-C2	-3.60	119.25	123.63
54	1w	32	PSU	C5-C6-N1	-3.58	119.75	124.39
54	1y	8	4SU	C5-C4-N3	-3.57	119.22	123.73
32	1a	1207	2MG	C6-C5-C4	-3.57	117.30	120.84
1	2A	2251	OMG	C6-C5-C4	-3.52	117.34	120.84
32	2a	1518	MA6	C9-N6-C6	-3.49	108.94	119.51
1	2A	2251	OMG	C4-C5-N7	-3.45	106.07	109.41
54	1y	32	PSU	C5-C6-N1	-3.40	119.97	124.39
1	2A	1911	PSU	C5-C6-N1	-3.40	119.98	124.39
32	1a	1402	4OC	CM4-N4-C4	-3.39	120.02	122.94
32	1a	1519	MA6	C4-C5-N7	-3.36	106.16	109.41
1	1A	1933	PSU	C5-C1'-C2'	-3.34	109.78	115.55
1	2A	1939	5MU	C5-C6-N1	-3.33	118.54	122.15
32	1a	966	M2G	C6-C5-C4	-3.29	117.57	120.84
32	1a	1518	MA6	C9-N6-C6	-3.26	109.64	119.51
32	1a	966	M2G	CM2-N2-C2	-3.26	118.24	121.34
1	2A	1911	PSU	C5-C1'-C2'	-3.26	109.93	115.55
1	1A	1939	PSU	C5-C1'-C2'	-3.22	109.99	115.55
1	1A	2263	OMG	C6-C5-C4	-3.22	117.64	120.84
32	1a	1519	MA6	C9-N6-C6	-3.19	109.84	119.51
1	1A	1961	5MU	C5-C6-N1	-3.19	118.70	122.15
32	2a	966	M2G	C4-C5-N7	-3.16	106.36	109.41
54	2y	55	PSU	C5-C1'-C2'	-3.15	110.11	115.55
54	2w	32	PSU	C5-C6-N1	-3.13	120.33	124.39
54	2w	37	MIA	C4-C5-N7	-3.09	106.42	109.41
54	2w	37	MIA	C12-N6-C6	-3.09	120.21	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C5-C6-N1	-3.09	117.55	120.64
54	2y	55	PSU	C5-C6-N1	-3.09	120.38	124.39
32	1a	1207	2MG	CM2-N2-C2	-3.08	119.88	123.63
1	1A	2617	PSU	C5-C1'-C2'	-3.06	110.27	115.55
1	1A	2263	OMG	N3-C2-N1	-3.05	123.00	127.46
54	2y	37	MIA	C4-C5-N7	-3.04	106.47	109.41
54	1y	37	MIA	C4-C5-N7	-2.99	106.52	109.41
32	2a	1519	MA6	C9-N6-C6	-2.95	110.57	119.51
32	2a	1400	5MC	C5-C6-N1	-2.88	119.04	122.15
32	1a	966	M2G	C4-C5-N7	-2.84	106.67	109.41
54	1w	37	MIA	C4-C5-N7	-2.83	106.68	109.41
55	2x	55	PSU	C5-C1'-C2'	-2.76	110.79	115.55
54	2w	8	4SU	C5-C4-N3	-2.76	120.25	123.73
32	1a	1518	MA6	C10-N6-C9	-2.75	107.14	116.03
54	1w	8	4SU	C5-C4-N3	-2.71	120.31	123.73
54	1w	46	7MG	C5-C4-N9	-2.71	102.37	106.31
54	2y	8	4SU	C5-C4-N3	-2.68	120.35	123.73
54	2w	39	PSU	C5-C1'-C2'	-2.68	110.93	115.55
1	2A	2503	2MA	C4-C5-N7	-2.68	106.83	109.41
1	1A	2263	OMG	C4-C5-N7	-2.63	106.87	109.41
1	2A	2251	OMG	N3-C2-N1	-2.63	123.62	127.46
54	2w	37	MIA	C5-C6-N1	-2.60	118.05	120.64
54	2w	37	MIA	N3-C2-N1	-2.57	122.23	126.85
32	2a	1207	2MG	C1'-N9-C4	-2.57	122.19	126.64
1	1A	1964	5MC	C5-C6-N1	-2.56	119.37	122.15
1	2A	1962	5MC	C5-C6-N1	-2.53	119.41	122.15
54	1y	46	7MG	C5-C4-N9	-2.53	102.64	106.31
54	1w	37	MIA	N3-C2-N1	-2.51	122.34	126.85
1	2A	2605	PSU	C5-C1'-C2'	-2.50	111.24	115.55
54	1y	54	5MU	C5-C6-N1	-2.46	119.48	122.15
54	1w	54	5MU	C5-C6-N1	-2.46	119.49	122.15
54	1w	32	PSU	C5-C1'-C2'	-2.43	111.36	115.55
32	2a	1404	5MC	C5-C6-N1	-2.39	119.56	122.15
55	1x	32	5MC	C5-C6-N1	-2.39	119.56	122.15
55	2x	54	5MU	C5-C6-N1	-2.38	119.57	122.15
55	2x	32	5MC	C5-C6-N1	-2.35	119.61	122.15
1	1A	1984	5MC	C5-C6-N1	-2.31	119.65	122.15
54	2y	46	7MG	C5-C4-N9	-2.25	103.03	106.31
32	2a	966	M2G	CM2-N2-C2	-2.24	119.21	121.34
1	2A	1915	5MU	C5-C6-N1	-2.21	119.76	122.15
32	1a	1400	5MC	CM5-C5-C4	-2.20	119.39	121.65
54	2y	54	5MU	C5-C6-N1	-2.19	119.78	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	32	PSU	C5-C1'-C2'	-2.16	111.82	115.55
32	2a	527	7MG	C5-C4-N9	-2.14	103.19	106.31
55	1x	54	5MU	C5-C6-N1	-2.14	119.83	122.15
55	1x	32	5MC	CM5-C5-C4	-2.12	119.47	121.65
1	1A	2515	2MA	C4-C5-N7	-2.08	107.40	109.41
32	1a	1518	MA6	C10-N6-C6	-2.06	113.26	119.51
32	2a	1207	2MG	N3-C2-N1	-2.04	123.15	126.23
1	1A	2617	PSU	O2'-C2'-C1'	-2.03	107.61	112.21
32	2a	967	5MC	C5-C6-N1	-2.01	119.98	122.15
1	1A	1984	5MC	N4-C4-N3	2.02	119.99	117.00
43	2l	92	0TD	C-CA-N	2.04	113.97	109.86
32	1a	527	7MG	C2-N3-C4	2.04	119.68	113.95
54	2w	39	PSU	O4'-C1'-C2'	2.05	107.75	104.45
54	2y	55	PSU	O4'-C1'-C2'	2.06	107.75	104.45
1	2A	1917	PSU	O4'-C1'-C2'	2.06	107.76	104.45
54	2y	46	7MG	C2-N3-C4	2.06	119.75	113.95
54	1w	39	PSU	O4'-C1'-C2'	2.07	107.78	104.45
54	2w	46	7MG	C2-N3-C4	2.09	119.81	113.95
32	2a	527	7MG	C2-N3-C4	2.09	119.82	113.95
1	1A	1939	PSU	O4'-C1'-C2'	2.09	107.81	104.45
54	1y	46	7MG	C4-N9-C1'	2.11	131.67	126.58
1	2A	1911	PSU	O4'-C1'-C2'	2.15	107.91	104.45
1	2A	1920	4OC	N4-C4-N3	2.17	120.29	116.64
54	1y	55	PSU	O4'-C1'-C2'	2.17	107.94	104.45
54	2y	32	PSU	O4'-C1'-C2'	2.17	107.94	104.45
32	2a	967	5MC	N4-C4-N3	2.19	120.23	117.00
32	1a	1519	MA6	N1-C6-N6	2.19	119.32	117.00
32	2a	966	M2G	N1-C2-N2	2.21	119.43	117.16
32	1a	1207	2MG	N2-C2-N1	2.21	119.10	116.95
32	2a	516	PSU	O4'-C1'-C2'	2.21	108.00	104.45
1	1A	1942	4OC	N4-C4-N3	2.21	120.37	116.64
54	2w	32	PSU	C4-C5-C1'	2.26	125.52	121.15
43	1l	92	0TD	C-CA-N	2.28	114.46	109.86
54	1y	46	7MG	C2-N3-C4	2.30	120.42	113.95
32	2a	1498	UR3	C3U-N3-C4	2.31	121.21	118.15
32	1a	1404	5MC	N4-C4-N3	2.36	120.48	117.00
1	2A	1962	5MC	N4-C4-N3	2.45	120.62	117.00
55	1x	32	5MC	N4-C4-N3	2.45	120.62	117.00
32	1a	516	PSU	O4'-C1'-C2'	2.49	108.44	104.45
32	2a	1404	5MC	N4-C4-N3	2.50	120.70	117.00
32	2a	1407	5MC	N4-C4-N3	2.68	120.97	117.00
1	1A	1964	5MC	N4-C4-N3	2.76	121.08	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1942	5MC	N4-C4-N3	2.78	121.11	117.00
32	1a	1407	5MC	N4-C4-N3	2.80	121.14	117.00
55	2x	32	5MC	N4-C4-N3	2.85	121.22	117.00
54	2w	37	MIA	C2-N1-C6	2.91	122.04	113.47
32	1a	1400	5MC	N4-C4-N3	3.08	121.55	117.00
32	1a	967	5MC	N4-C4-N3	3.09	121.57	117.00
32	2a	1519	MA6	N1-C6-N6	3.11	120.30	117.00
54	1w	37	MIA	C2-N1-C6	3.12	122.67	113.47
32	2a	1207	2MG	N2-C2-N1	3.28	120.14	116.95
54	2y	39	PSU	O4'-C1'-C5	3.60	115.50	109.93
54	2y	8	4SU	C2-N3-C4	3.64	120.48	115.11
54	2w	8	4SU	C2-N3-C4	3.75	120.64	115.11
1	2A	2251	OMG	C6-N1-C2	3.90	121.67	116.06
1	1A	1933	PSU	C6-N1-C2	3.91	121.62	115.36
1	2A	1917	PSU	C6-N1-C2	3.92	121.64	115.36
32	2a	1519	MA6	C2-N1-C6	4.02	121.69	111.82
32	2a	1207	2MG	C6-N1-C2	4.04	122.42	115.18
1	2A	1911	PSU	C6-N1-C2	4.06	121.86	115.36
55	1x	55	PSU	C6-N1-C2	4.07	121.87	115.36
32	1a	1207	2MG	C6-N1-C2	4.08	122.48	115.18
54	1y	55	PSU	C6-N1-C2	4.08	121.88	115.36
32	1a	966	M2G	N3-C2-N2	4.08	121.36	117.15
54	1w	8	4SU	C2-N3-C4	4.09	121.14	115.11
54	1y	32	PSU	C6-N1-C2	4.11	121.94	115.36
54	1w	55	PSU	C6-N1-C2	4.15	122.00	115.36
54	1w	39	PSU	C6-N1-C2	4.18	122.05	115.36
54	2y	39	PSU	C6-N1-C2	4.19	122.07	115.36
54	2w	32	PSU	C6-N1-C2	4.20	122.09	115.36
32	1a	1519	MA6	C2-N1-C6	4.23	122.20	111.82
32	2a	516	PSU	C6-N1-C2	4.25	122.16	115.36
1	1A	1939	PSU	C6-N1-C2	4.25	122.17	115.36
54	1w	32	PSU	C6-N1-C2	4.26	122.17	115.36
54	1y	39	PSU	C6-N1-C2	4.26	122.18	115.36
55	2x	55	PSU	C6-N1-C2	4.28	122.21	115.36
54	2y	55	PSU	C6-N1-C2	4.30	122.24	115.36
54	2y	32	PSU	C6-N1-C2	4.30	122.25	115.36
1	1A	2263	OMG	C6-N1-C2	4.36	122.33	116.06
54	2w	55	PSU	C6-N1-C2	4.37	122.36	115.36
32	1a	516	PSU	C6-N1-C2	4.41	122.42	115.36
54	2w	39	PSU	C6-N1-C2	4.42	122.44	115.36
1	2A	2605	PSU	C6-N1-C2	4.44	122.46	115.36
32	2a	1518	MA6	C2-N1-C6	4.45	122.74	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	C6-N1-C2	4.45	122.46	116.06
1	1A	2617	PSU	C6-N1-C2	4.56	122.66	115.36
1	1A	2263	OMG	C2-N3-C4	4.57	120.49	115.16
32	1a	527	7MG	C6-N1-C2	4.58	122.64	116.06
54	1y	8	4SU	C2-N3-C4	4.58	121.87	115.11
32	1a	1518	MA6	C2-N1-C6	4.68	123.30	111.82
32	2a	966	M2G	C2-N3-C4	4.82	120.61	115.11
32	1a	1207	2MG	C2-N3-C4	4.86	120.66	115.11
32	2a	1207	2MG	C2-N3-C4	4.98	120.80	115.11
54	2w	46	7MG	C6-N1-C2	4.99	123.23	116.06
1	2A	2251	OMG	C2-N3-C4	5.00	121.00	115.16
32	1a	966	M2G	C6-N1-C2	5.10	122.25	116.18
32	2a	966	M2G	C6-N1-C2	5.16	122.32	116.18
1	2A	2605	PSU	C4-N3-C2	5.30	119.79	115.16
54	1w	46	7MG	C6-N1-C2	5.37	123.78	116.06
1	1A	1961	5MU	C4-N3-C2	5.39	119.87	115.16
55	2x	54	5MU	C4-N3-C2	5.43	119.91	115.16
32	1a	966	M2G	C2-N3-C4	5.43	121.31	115.11
1	2A	2503	2MA	C2-N3-C4	5.54	120.20	115.41
1	2A	1939	5MU	C4-N3-C2	5.54	120.00	115.16
1	1A	2515	2MA	C2-N3-C4	5.73	120.36	115.41
1	1A	2617	PSU	C4-N3-C2	5.85	120.28	115.16
54	2y	46	7MG	C6-N1-C2	5.86	124.49	116.06
54	2y	54	5MU	C4-N3-C2	5.90	120.32	115.16
1	1A	1937	5MU	C4-N3-C2	5.92	120.34	115.16
54	1y	46	7MG	C6-N1-C2	5.94	124.60	116.06
54	1w	54	5MU	C4-N3-C2	5.97	120.38	115.16
54	1y	55	PSU	C4-N3-C2	6.00	120.41	115.16
54	1w	39	PSU	C4-N3-C2	6.18	120.56	115.16
54	2w	55	PSU	C4-N3-C2	6.30	120.67	115.16
1	2A	1915	5MU	C4-N3-C2	6.33	120.69	115.16
55	2x	55	PSU	C4-N3-C2	6.34	120.71	115.16
55	1x	55	PSU	C4-N3-C2	6.43	120.78	115.16
32	2a	516	PSU	C4-N3-C2	6.47	120.82	115.16
54	1w	32	PSU	C4-N3-C2	6.55	120.88	115.16
32	1a	516	PSU	C4-N3-C2	6.55	120.89	115.16
54	2y	32	PSU	C4-N3-C2	6.55	120.89	115.16
1	2A	1917	PSU	C4-N3-C2	6.61	120.94	115.16
1	1A	1933	PSU	C4-N3-C2	6.62	120.95	115.16
54	1y	54	5MU	C4-N3-C2	6.65	120.97	115.16
54	1w	55	PSU	C4-N3-C2	6.77	121.08	115.16
55	1x	54	5MU	C4-N3-C2	6.78	121.09	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	PSU	C4-N3-C2	6.86	121.16	115.16
54	2y	39	PSU	C4-N3-C2	6.93	121.22	115.16
1	2A	1911	PSU	C4-N3-C2	6.93	121.22	115.16
54	2w	32	PSU	C4-N3-C2	6.95	121.24	115.16
54	2w	39	PSU	C4-N3-C2	6.98	121.27	115.16
54	1y	39	PSU	C4-N3-C2	7.09	121.36	115.16
54	2w	54	5MU	C4-N3-C2	7.19	121.45	115.16
54	2y	55	PSU	C4-N3-C2	7.27	121.52	115.16
54	1y	32	PSU	C4-N3-C2	7.36	121.59	115.16
1	2A	2552	2MU	C4-N3-C2	7.62	120.67	114.13
55	2x	8	4SU	C2-N3-C4	7.77	126.58	115.11
1	1A	2564	2MU	C4-N3-C2	8.12	121.10	114.13
54	2w	46	7MG	N3-C4-N9	8.44	137.77	126.98
55	1x	8	4SU	C2-N3-C4	8.47	127.61	115.11
32	1a	527	7MG	N3-C4-N9	8.73	138.13	126.98
32	2a	527	7MG	N3-C4-N9	9.18	138.71	126.98
54	2y	46	7MG	N3-C4-N9	9.37	138.95	126.98
54	1w	46	7MG	N3-C4-N9	9.51	139.12	126.98
54	1y	46	7MG	N3-C4-N9	10.09	139.87	126.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1942	4OC	1	0
1	1A	2564	2MU	2	0
1	2A	1915	5MU	1	0
1	2A	1920	4OC	2	0
1	2A	1939	5MU	2	0
1	2A	2503	2MA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2625 ligands modelled in this entry, 2621 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	EZG	1A	4030	-	21,26,26	2.86	3 (14%)	24,35,35	1.23	3 (12%)
60	SF4	1d	501	35	0,12,12	0.00	-	0,24,24	0.00	-
58	EZG	2A	3746	-	21,26,26	3.59	3 (14%)	24,35,35	1.08	2 (8%)
60	SF4	2d	501	35	0,12,12	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	EZG	1A	4030	-	-	0/24/26/26	0/2/2/2
60	SF4	1d	501	35	-	0/0/48/48	0/6/5/5
58	EZG	2A	3746	-	-	0/24/26/26	0/2/2/2
60	SF4	2d	501	35	-	0/0/48/48	0/6/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4030	EZG	CAT-CAW	-8.56	1.39	1.51
58	2A	3746	EZG	CAT-CAW	-7.82	1.40	1.51
58	1A	4030	EZG	CAU-NAY	-6.12	1.33	1.45
58	2A	3746	EZG	CAU-NAY	-5.88	1.34	1.45
58	1A	4030	EZG	OAC-NAY	7.24	1.35	1.22
58	2A	3746	EZG	OAC-NAY	13.03	1.46	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	2A	3746	EZG	CAX-NAP-C	-2.98	117.83	123.16
58	1A	4030	EZG	CAI-CAG-CAT	-2.62	118.54	121.20
58	1A	4030	EZG	CAM-CAX-NAP	-2.14	105.64	109.38
58	2A	3746	EZG	CAI-CAU-NAY	2.03	120.95	119.41
58	1A	4030	EZG	CAT-CAW-CAX	2.83	116.89	111.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1A	4030	EZG	2	0
58	2A	3746	EZG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.07	16 (0%) 89 86	13, 30, 88, 101	0
1	2A	2789/2915 (95%)	0.07	13 (0%) 90 88	25, 51, 87, 100	0
2	1B	120/121 (99%)	-0.15	0 100 100	23, 43, 57, 85	0
2	2B	120/121 (99%)	-0.14	0 100 100	53, 71, 80, 89	0
3	1D	275/276 (99%)	0.11	2 (0%) 87 83	16, 31, 46, 75	0
3	2D	275/276 (99%)	0.15	0 100 100	23, 43, 56, 66	0
4	1E	204/206 (99%)	0.02	0 100 100	13, 33, 54, 71	0
4	2E	204/206 (99%)	0.24	2 (0%) 82 77	28, 54, 67, 74	0
5	1F	203/210 (96%)	0.00	1 (0%) 90 88	15, 35, 62, 82	0
5	2F	203/210 (96%)	0.17	3 (1%) 74 67	30, 62, 74, 82	0
6	1G	181/182 (99%)	-0.16	0 100 100	35, 51, 69, 78	0
6	2G	181/182 (99%)	0.38	8 (4%) 35 25	56, 72, 78, 83	0
7	1H	174/180 (96%)	-0.13	0 100 100	34, 46, 59, 66	0
7	2H	174/180 (96%)	1.61	67 (38%) 0 0	61, 75, 81, 86	0
8	1I	146/148 (98%)	-0.06	0 100 100	39, 67, 75, 81	0
8	2I	146/148 (98%)	0.13	2 (1%) 75 69	50, 66, 77, 81	0
9	1N	140/140 (100%)	-0.09	0 100 100	21, 35, 55, 68	0
9	2N	140/140 (100%)	0.55	4 (2%) 52 41	43, 58, 72, 75	0
10	1O	122/122 (100%)	-0.03	0 100 100	22, 35, 50, 56	0
10	2O	122/122 (100%)	0.32	0 100 100	43, 54, 67, 70	0
11	1P	149/150 (99%)	0.02	0 100 100	14, 40, 62, 66	0
11	2P	149/150 (99%)	1.23	37 (24%) 1 0	30, 61, 75, 83	0
12	1Q	141/141 (100%)	0.17	0 100 100	22, 36, 49, 72	0
12	2Q	141/141 (100%)	1.00	20 (14%) 3 2	41, 60, 70, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.19	0 100 100	18, 29, 44, 54	0
13	2R	118/118 (100%)	0.29	1 (0%) 86 81	33, 46, 55, 66	0
14	1S	110/112 (98%)	-0.13	1 (0%) 84 79	32, 44, 55, 60	0
14	2S	110/112 (98%)	1.33	23 (20%) 1 1	58, 67, 76, 79	0
15	1T	131/146 (89%)	-0.04	0 100 100	25, 39, 61, 71	0
15	2T	131/146 (89%)	0.42	5 (3%) 41 30	46, 58, 69, 75	0
16	1U	116/118 (98%)	0.03	0 100 100	14, 25, 42, 56	0
16	2U	116/118 (98%)	0.31	1 (0%) 84 79	35, 55, 67, 73	0
17	1V	101/101 (100%)	-0.17	0 100 100	19, 34, 53, 69	0
17	2V	101/101 (100%)	0.06	0 100 100	36, 63, 74, 78	0
18	1W	112/113 (99%)	-0.01	0 100 100	21, 26, 48, 71	0
18	2W	112/113 (99%)	0.23	1 (0%) 84 79	33, 44, 59, 85	0
19	1X	95/96 (98%)	-0.09	0 100 100	19, 31, 53, 75	0
19	2X	95/96 (98%)	0.00	0 100 100	40, 53, 64, 72	0
20	1Y	107/110 (97%)	-0.18	0 100 100	29, 43, 61, 72	0
20	2Y	107/110 (97%)	0.33	2 (1%) 67 58	54, 65, 74, 78	0
21	1Z	154/206 (74%)	0.06	3 (1%) 67 58	35, 57, 79, 85	0
21	2Z	160/206 (77%)	1.31	39 (24%) 1 1	61, 75, 84, 91	0
22	10	83/85 (97%)	0.26	5 (6%) 23 14	18, 31, 51, 56	0
22	20	83/85 (97%)	0.72	9 (10%) 6 3	36, 58, 69, 74	0
23	11	97/98 (98%)	0.21	1 (1%) 82 77	20, 38, 62, 70	0
23	21	97/98 (98%)	0.42	5 (5%) 28 19	35, 50, 68, 73	0
24	12	70/72 (97%)	-0.08	0 100 100	29, 41, 53, 64	0
24	22	70/72 (97%)	-0.09	0 100 100	47, 62, 70, 73	0
25	13	59/60 (98%)	-0.11	0 100 100	19, 31, 54, 72	0
25	23	59/60 (98%)	1.11	10 (16%) 2 1	48, 58, 70, 76	0
26	14	69/71 (97%)	-0.00	2 (2%) 52 41	43, 65, 83, 84	0
26	24	69/71 (97%)	-0.03	3 (4%) 36 26	67, 77, 86, 87	0
27	15	59/60 (98%)	-0.02	1 (1%) 70 63	14, 28, 41, 50	0
27	25	59/60 (98%)	0.09	1 (1%) 70 63	32, 46, 56, 64	0
28	16	53/54 (98%)	0.16	1 (1%) 67 58	27, 36, 50, 55	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.90	6 (11%) 6 3	42, 54, 67, 68	0
29	17	48/49 (97%)	0.13	1 (2%) 64 54	16, 21, 50, 60	0
29	27	48/49 (97%)	0.16	0 100 100	24, 35, 51, 60	0
30	18	64/65 (98%)	0.21	1 (1%) 72 65	21, 27, 37, 55	0
30	28	64/65 (98%)	1.63	18 (28%) 1 0	40, 49, 58, 68	0
31	19	37/37 (100%)	0.55	0 100 100	22, 33, 50, 55	0
31	29	37/37 (100%)	1.50	11 (29%) 1 0	53, 62, 71, 75	0
32	1a	1488/1521 (97%)	0.03	9 (0%) 89 86	32, 59, 86, 102	0
32	2a	1491/1521 (98%)	0.13	29 (1%) 67 58	43, 69, 89, 101	0
33	1b	231/256 (90%)	0.58	15 (6%) 20 12	59, 73, 82, 85	0
33	2b	231/256 (90%)	1.29	57 (24%) 1 0	64, 79, 85, 90	0
34	1c	206/239 (86%)	0.62	21 (10%) 7 4	51, 66, 74, 80	0
34	2c	206/239 (86%)	1.44	63 (30%) 0 0	66, 78, 82, 85	0
35	1d	208/209 (99%)	0.48	11 (5%) 27 18	50, 64, 76, 83	0
35	2d	208/209 (99%)	0.58	12 (5%) 24 15	53, 62, 72, 81	0
36	1e	148/162 (91%)	0.39	5 (3%) 46 34	48, 60, 70, 78	0
36	2e	148/162 (91%)	0.96	24 (16%) 2 1	58, 71, 79, 86	0
37	1f	100/101 (99%)	0.09	0 100 100	48, 60, 69, 70	0
37	2f	100/101 (99%)	0.07	1 (1%) 82 77	51, 63, 70, 76	0
38	1g	155/156 (99%)	0.43	16 (10%) 7 4	51, 62, 74, 88	0
38	2g	155/156 (99%)	0.79	19 (12%) 5 2	62, 71, 78, 84	0
39	1h	137/138 (99%)	0.30	4 (2%) 52 41	48, 61, 67, 72	0
39	2h	137/138 (99%)	0.67	14 (10%) 7 4	64, 71, 77, 85	0
40	1i	127/128 (99%)	1.24	29 (22%) 1 1	46, 69, 77, 83	0
40	2i	127/128 (99%)	2.35	69 (54%) 0 0	68, 77, 82, 88	0
41	1j	97/105 (92%)	1.18	26 (26%) 1 0	52, 71, 78, 83	0
41	2j	96/105 (91%)	1.81	37 (38%) 0 0	70, 78, 85, 87	0
42	1k	114/129 (88%)	0.26	1 (0%) 84 79	40, 58, 72, 79	0
42	2k	114/129 (88%)	0.43	7 (6%) 22 14	49, 66, 74, 78	0
43	1l	121/132 (91%)	0.01	0 100 100	33, 47, 59, 66	0
43	2l	121/132 (91%)	0.53	8 (6%) 19 11	53, 61, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.36	10 (8%) 13 7	47, 59, 70, 74	0
44	2m	122/126 (96%)	0.60	17 (13%) 3 2	62, 75, 81, 85	0
45	1n	60/61 (98%)	1.05	10 (16%) 2 1	50, 59, 67, 71	0
45	2n	60/61 (98%)	2.94	41 (68%) 0 0	68, 77, 81, 87	0
46	1o	88/89 (98%)	0.12	2 (2%) 61 51	44, 59, 70, 75	0
46	2o	88/89 (98%)	-0.09	1 (1%) 80 74	53, 65, 74, 75	0
47	1p	82/88 (93%)	0.51	5 (6%) 22 14	51, 61, 70, 75	0
47	2p	82/88 (93%)	0.29	1 (1%) 79 72	55, 62, 71, 75	0
48	1q	99/105 (94%)	0.34	3 (3%) 51 39	47, 59, 72, 75	0
48	2q	99/105 (94%)	0.98	20 (20%) 1 1	55, 65, 73, 75	0
49	1r	68/88 (77%)	0.32	4 (5%) 23 15	48, 61, 71, 73	0
49	2r	68/88 (77%)	-0.01	2 (2%) 52 41	57, 63, 73, 77	0
50	1s	83/93 (89%)	0.26	1 (1%) 79 72	49, 64, 73, 77	0
50	2s	83/93 (89%)	0.79	16 (19%) 1 1	71, 78, 84, 87	0
51	1t	96/106 (90%)	0.70	14 (14%) 3 1	50, 64, 73, 78	0
51	2t	96/106 (90%)	1.19	18 (18%) 1 1	52, 63, 76, 79	0
52	1u	23/27 (85%)	1.37	4 (17%) 2 1	52, 59, 63, 70	0
52	2u	23/27 (85%)	2.22	12 (52%) 0 0	67, 73, 80, 80	0
53	1v	13/24 (54%)	1.12	3 (23%) 1 1	42, 56, 81, 90	0
53	2v	13/24 (54%)	1.10	2 (15%) 2 1	59, 74, 91, 97	0
54	1w	67/76 (88%)	0.14	5 (7%) 15 8	32, 82, 93, 96	0
54	1y	67/76 (88%)	0.35	5 (7%) 15 8	28, 88, 96, 100	0
54	2w	65/76 (85%)	0.25	3 (4%) 33 23	54, 87, 95, 99	0
54	2y	66/76 (86%)	0.56	6 (9%) 10 5	49, 90, 94, 97	0
55	1x	72/77 (93%)	-0.07	0 100 100	32, 58, 76, 85	0
55	2x	72/77 (93%)	-0.14	0 100 100	45, 71, 81, 83	0
All	All	20875/21748 (95%)	0.29	1008 (4%) 31 21	13, 57, 83, 102	0

All (1008) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	34	TYR	8.6
44	2m	123	ALA	7.6

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Mol	Chain	Res	Type	RSRZ
40	2i	14	VAL	7.4
44	1m	124	PRO	7.1
38	2g	82	GLY	7.1
45	2n	25	VAL	7.0
40	2i	28	VAL	6.9
45	2n	39	LEU	6.9
38	1g	82	GLY	6.8
41	2j	55	LYS	6.7
45	2n	38	GLY	6.6
31	29	37	GLY	6.6
45	2n	2	ALA	6.5
44	2m	124	PRO	6.2
41	1j	10	GLY	6.1
41	2j	47	PHE	6.1
21	2Z	144	LEU	6.0
21	2Z	170	THR	5.6
40	2i	114	TYR	5.6
33	2b	211	ILE	5.5
41	2j	48	THR	5.4
34	2c	201	TYR	5.4
33	2b	201	ILE	5.4
36	2e	10	MET	5.4
34	2c	188	LEU	5.3
44	1m	123	ALA	5.3
40	2i	36	TYR	5.3
44	2m	102	ARG	5.2
30	28	16	ILE	5.2
11	2P	79	ARG	5.2
21	2Z	121	HIS	5.1
40	2i	9	ARG	5.1
41	2j	63	PHE	5.0
41	2j	50	ILE	5.0
36	2e	31	LEU	5.0
33	2b	165	VAL	5.0
34	2c	171	GLY	4.9
7	2H	45	VAL	4.9
33	2b	210	SER	4.9
40	2i	27	THR	4.9
45	2n	35	ARG	4.8
40	2i	115	GLY	4.8
12	2Q	104	PHE	4.8
40	2i	66	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
7	2H	133	VAL	4.8
38	1g	84	ASN	4.8
40	2i	7	THR	4.8
52	2u	15	ARG	4.8
1	2A	229	A	4.8
45	2n	11	LYS	4.8
32	2a	1034	G	4.8
40	2i	62	TYR	4.7
7	2H	7	LEU	4.7
40	2i	19	LEU	4.7
45	2n	12	ARG	4.7
41	2j	54	PHE	4.6
45	2n	61	TRP	4.6
36	2e	11	ILE	4.6
33	2b	187	LEU	4.6
41	2j	62	HIS	4.6
40	2i	108	VAL	4.5
40	2i	125	TYR	4.5
45	2n	37	PHE	4.5
41	2j	65	LEU	4.5
54	2w	71	G	4.5
40	2i	64	THR	4.5
21	2Z	149	SER	4.4
38	1g	85	TYR	4.4
11	2P	118	GLY	4.4
32	2a	1030(B)	C	4.4
22	10	5	LYS	4.4
34	2c	7	PRO	4.4
7	2H	113	VAL	4.4
51	2t	9	ASN	4.3
40	2i	117	HIS	4.3
48	2q	38	ARG	4.3
33	2b	164	VAL	4.3
54	1w	70	G	4.3
45	2n	13	THR	4.3
33	2b	77	ALA	4.3
34	2c	182	ILE	4.2
22	10	6	GLY	4.2
34	2c	157	ILE	4.2
39	2h	133	LEU	4.2
34	2c	170	GLN	4.2
45	2n	7	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
32	2a	1033	G	4.2
40	2i	15	ALA	4.2
40	2i	110	GLU	4.2
34	2c	6	HIS	4.2
21	2Z	126	VAL	4.1
33	2b	163	PHE	4.1
41	2j	46	ARG	4.1
34	1c	196	LEU	4.1
40	2i	26	VAL	4.1
41	2j	52	GLY	4.1
45	2n	31	ARG	4.1
53	2v	12	A	4.1
40	2i	127	LYS	4.1
30	28	65	GLU	4.1
36	2e	20	GLN	4.0
52	2u	16	GLY	4.0
33	2b	71	VAL	4.0
34	2c	8	ILE	4.0
32	2a	1257	U	4.0
40	1i	106	ALA	4.0
12	2Q	22	LYS	4.0
7	2H	2	SER	4.0
21	2Z	51	ALA	4.0
31	29	17	ILE	4.0
44	2m	90	LEU	4.0
12	2Q	103	MET	4.0
21	1Z	149	SER	4.0
11	2P	78	PRO	3.9
52	2u	6	ARG	3.9
41	2j	56	HIS	3.9
34	2c	23	TYR	3.9
34	2c	167	TRP	3.9
40	2i	13	ALA	3.9
40	2i	65	VAL	3.9
40	1i	65	VAL	3.9
34	2c	198	VAL	3.9
3	1D	276	LYS	3.9
47	1p	1	MET	3.8
30	28	61	LEU	3.8
32	2a	1035	A	3.8
34	2c	124	ILE	3.8
45	2n	22	THR	3.8

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Mol	Chain	Res	Type	RSRZ
52	2u	11	GLY	3.8
28	26	54	ILE	3.8
40	2i	72	GLY	3.8
13	2R	69	ASP	3.8
21	2Z	48	PHE	3.8
44	2m	122	LYS	3.7
44	2m	104	ARG	3.7
36	2e	18	ARG	3.7
7	2H	103	LEU	3.7
11	2P	123	LEU	3.7
40	2i	124	GLN	3.7
7	2H	76	VAL	3.7
33	2b	200	ILE	3.7
41	2j	58	ASP	3.7
52	2u	14	TRP	3.7
40	1i	76	ALA	3.7
38	2g	81	GLY	3.7
14	2S	26	LEU	3.7
23	11	2	SER	3.7
7	2H	141	VAL	3.6
45	2n	54	PRO	3.6
45	2n	57	ARG	3.6
41	2j	10	GLY	3.6
25	23	51	ALA	3.6
36	2e	12	LEU	3.6
28	26	11	LEU	3.6
38	1g	80	VAL	3.6
31	29	15	LYS	3.6
11	2P	106	LEU	3.6
40	2i	4	TYR	3.6
34	1c	15	THR	3.6
11	2P	85	LEU	3.6
40	2i	126	SER	3.6
45	2n	58	LYS	3.6
41	1j	98	ILE	3.6
1	1A	931	C	3.6
38	2g	154	TYR	3.6
34	2c	187	ALA	3.6
35	2d	47	ARG	3.6
40	2i	109	VAL	3.5
41	1j	35	SER	3.5
7	2H	115	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
34	2c	184	TYR	3.5
36	2e	8	GLU	3.5
22	20	7	LEU	3.5
45	2n	6	LEU	3.5
54	2w	70	G	3.5
51	1t	29	LYS	3.5
34	2c	12	LEU	3.5
34	1c	179	ARG	3.5
38	1g	79	ARG	3.5
33	2b	120	ALA	3.5
11	2P	75	ILE	3.5
14	2S	32	LEU	3.5
40	2i	5	TYR	3.5
34	2c	189	ALA	3.5
34	2c	202	ILE	3.5
34	2c	179	ARG	3.5
33	2b	152	PHE	3.5
7	2H	70	THR	3.4
22	20	2	ALA	3.4
33	2b	80	ILE	3.4
34	2c	60	ALA	3.4
38	1g	83	ALA	3.4
36	2e	119	LEU	3.4
34	2c	14	ILE	3.4
44	2m	120	LYS	3.4
45	2n	53	LEU	3.4
45	1n	2	ALA	3.4
7	2H	94	TYR	3.4
7	2H	114	VAL	3.4
33	2b	108	ILE	3.4
14	2S	14	VAL	3.4
33	2b	16	HIS	3.4
53	2v	24	A	3.4
21	1Z	169	GLU	3.4
34	2c	163	ALA	3.4
39	2h	83	ILE	3.4
36	2e	16	THR	3.4
7	2H	36	PRO	3.4
43	2l	5	PRO	3.4
11	2P	70	GLN	3.4
21	2Z	125	LEU	3.4
35	1d	167	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
52	2u	17	THR	3.4
38	2g	84	ASN	3.3
45	2n	29	ARG	3.3
34	2c	186	PHE	3.3
45	2n	17	LYS	3.3
35	1d	166	LYS	3.3
40	2i	12	GLU	3.3
41	2j	98	ILE	3.3
40	2i	17	VAL	3.3
51	2t	73	HIS	3.3
7	2H	105	LEU	3.3
22	10	4	LYS	3.3
54	1w	71	G	3.3
21	2Z	1	MET	3.3
33	2b	48	MET	3.3
38	2g	156	TRP	3.3
38	2g	4	ARG	3.3
40	1i	113	LYS	3.3
1	1A	1140	U	3.3
40	2i	121	ARG	3.3
7	2H	96	ALA	3.3
34	2c	154	SER	3.3
38	1g	81	GLY	3.3
33	2b	70	PHE	3.3
7	2H	6	ARG	3.3
40	2i	81	ILE	3.3
48	1q	28	PRO	3.3
41	1j	62	HIS	3.3
41	1j	65	LEU	3.3
33	2b	31	TYR	3.2
11	2P	125	VAL	3.2
28	26	10	LEU	3.2
7	2H	3	ARG	3.2
44	2m	88	ARG	3.2
45	2n	33	VAL	3.2
38	1g	156	TRP	3.2
7	2H	159	GLU	3.2
39	2h	2	LEU	3.2
41	2j	85	LEU	3.2
21	2Z	139	VAL	3.2
43	2l	18	VAL	3.2
45	2n	30	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
45	2n	56	VAL	3.2
45	2n	36	PHE	3.2
52	1u	6	ARG	3.2
34	2c	200	ALA	3.2
45	2n	60	SER	3.2
45	2n	15	LYS	3.2
43	2l	7	ILE	3.2
33	2b	197	VAL	3.2
41	2j	71	LEU	3.2
45	2n	14	PRO	3.2
32	2a	1149	C	3.2
54	1w	3	C	3.2
40	1i	117	HIS	3.2
41	2j	44	VAL	3.2
21	2Z	83	PRO	3.2
34	2c	5	ILE	3.1
45	2n	23	ARG	3.1
33	2b	19	HIS	3.1
33	2b	135	GLN	3.1
30	28	64	TYR	3.1
40	2i	116	LYS	3.1
7	2H	52	VAL	3.1
41	2j	49	VAL	3.1
54	1w	72	C	3.1
34	1c	193	TYR	3.1
38	1g	16	LEU	3.1
36	2e	22	GLY	3.1
48	2q	23	VAL	3.1
33	2b	121	LEU	3.1
40	1i	70	LYS	3.1
21	2Z	141	VAL	3.1
21	2Z	150	LEU	3.1
52	2u	13	ILE	3.1
16	2U	90	VAL	3.1
1	2A	2125	G	3.1
1	2A	2155	G	3.1
35	2d	176	LEU	3.1
51	2t	24	LEU	3.1
34	1c	14	ILE	3.1
36	2e	9	LYS	3.1
40	2i	90	PRO	3.1
44	2m	97	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
21	2Z	47	VAL	3.1
34	2c	37	GLN	3.1
35	1d	168	ARG	3.1
48	2q	22	LEU	3.1
1	1A	1114	G	3.1
44	2m	105	THR	3.1
12	2Q	19	GLY	3.1
34	2c	159	GLY	3.1
36	2e	25	ARG	3.1
40	2i	63	ILE	3.1
7	2H	35	VAL	3.1
33	1b	186	ALA	3.1
36	2e	84	PHE	3.1
11	2P	65	ARG	3.1
21	2Z	140	ASP	3.1
7	2H	162	ILE	3.1
31	29	23	VAL	3.0
50	2s	45	VAL	3.0
40	2i	18	PHE	3.0
51	2t	63	ILE	3.0
32	2a	1001(A)	G	3.0
32	2a	1002	G	3.0
41	1j	97	GLU	3.0
33	2b	66	GLY	3.0
11	2P	83	VAL	3.0
48	2q	30	PRO	3.0
21	2Z	122	ARG	3.0
40	2i	42	ARG	3.0
41	2j	74	ILE	3.0
14	2S	46	VAL	3.0
32	2a	1116	C	3.0
32	1a	1002	G	3.0
11	2P	80	TYR	3.0
40	1i	112	LYS	3.0
1	2A	888	C	3.0
34	2c	33	LEU	3.0
40	1i	47	LEU	3.0
34	1c	13	GLY	3.0
33	2b	146	GLN	3.0
45	1n	57	ARG	3.0
43	2l	64	TYR	3.0
40	2i	37	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
41	1j	71	LEU	3.0
7	2H	131	VAL	3.0
21	2Z	79	ARG	3.0
50	2s	70	LYS	3.0
34	2c	206	GLU	3.0
12	2Q	40	ALA	2.9
40	1i	4	TYR	2.9
41	1j	8	LEU	2.9
14	2S	33	LYS	2.9
22	20	3	HIS	2.9
34	2c	149	ALA	2.9
34	2c	160	ALA	2.9
11	2P	115	LEU	2.9
14	2S	93	LYS	2.9
33	2b	94	ASN	2.9
44	2m	78	ILE	2.9
52	1u	17	THR	2.9
33	2b	136	VAL	2.9
40	2i	16	ARG	2.9
7	2H	168	PRO	2.9
33	1b	187	LEU	2.9
33	2b	102	LEU	2.9
51	2t	72	LEU	2.9
35	2d	198	VAL	2.9
33	2b	186	ALA	2.9
33	2b	92	TYR	2.9
12	2Q	102	VAL	2.9
6	2G	3	LEU	2.9
33	2b	142	LEU	2.9
41	2j	51	ARG	2.9
34	2c	39	ILE	2.9
33	2b	215	LEU	2.9
50	2s	80	TYR	2.9
54	2y	36	A	2.9
40	2i	35	GLU	2.9
48	2q	21	VAL	2.9
7	2H	71	LEU	2.9
34	2c	196	LEU	2.9
22	10	3	HIS	2.9
40	2i	123	PRO	2.9
41	1j	5	ARG	2.9
7	2H	164	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	2A	652(B)	A	2.9
28	26	20	ASN	2.9
51	2t	55	ILE	2.9
54	2y	64	A	2.9
12	2Q	97	VAL	2.9
12	2Q	28	ALA	2.9
36	1e	10	MET	2.9
1	1A	932	C	2.9
21	2Z	137	ILE	2.9
51	2t	29	LYS	2.9
48	2q	33	GLY	2.9
50	2s	79	THR	2.8
43	2l	55	VAL	2.8
41	1j	59	SER	2.8
7	2H	10	PRO	2.8
26	24	49	PHE	2.8
33	2b	122	PHE	2.8
48	2q	9	VAL	2.8
51	2t	64	ASP	2.8
41	2j	57	LYS	2.8
7	2H	102	ALA	2.8
7	2H	145	ALA	2.8
25	23	29	ARG	2.8
32	1a	1257	U	2.8
12	2Q	33	GLY	2.8
32	2a	1003	G	2.8
40	2i	32	ASP	2.8
51	1t	14	LYS	2.8
51	1t	74	LYS	2.8
7	2H	169	VAL	2.8
35	1d	170	VAL	2.8
42	2k	50	TYR	2.8
38	2g	79	ARG	2.8
34	1c	18	TRP	2.8
28	26	50	ARG	2.8
35	2d	160	GLN	2.8
38	2g	115	ARG	2.8
51	2t	80	ARG	2.8
52	2u	9	ARG	2.8
34	2c	4	LYS	2.8
7	2H	89	ILE	2.8
40	1i	8	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
40	2i	67	GLY	2.8
11	2P	51	PHE	2.8
25	23	54	VAL	2.8
21	2Z	80	ARG	2.8
21	2Z	138	GLU	2.8
41	1j	60	ARG	2.8
33	2b	123	ALA	2.8
54	2y	65	G	2.8
33	1b	200	ILE	2.8
34	1c	8	ILE	2.8
34	2c	174	PRO	2.8
11	2P	58	THR	2.8
33	2b	69	LEU	2.8
38	2g	16	LEU	2.8
41	2j	66	ARG	2.8
41	2j	95	GLU	2.8
1	1A	1110	C	2.8
38	2g	86	GLN	2.8
26	14	54	GLY	2.8
44	2m	100	GLY	2.8
41	1j	45	ARG	2.8
7	2H	49	VAL	2.8
21	2Z	91	LEU	2.8
40	2i	79	LEU	2.8
26	14	46	GLN	2.8
40	1i	18	PHE	2.7
44	2m	121	LYS	2.7
51	1t	12	ALA	2.7
1	1A	942	A	2.7
33	1b	226	ARG	2.7
12	2Q	66	ILE	2.7
33	2b	214	ILE	2.7
43	2l	32	PHE	2.7
14	2S	58	LEU	2.7
51	1t	18	GLN	2.7
33	2b	161	ALA	2.7
40	2i	61	ALA	2.7
40	1i	81	ILE	2.7
11	2P	126	VAL	2.7
34	2c	32	LEU	2.7
40	1i	75	ASP	2.7
14	2S	13	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
36	2e	17	ALA	2.7
40	2i	111	ARG	2.7
22	20	52	GLY	2.7
32	1a	1030	C	2.7
7	2H	77	LYS	2.7
21	2Z	128	VAL	2.7
22	10	7	LEU	2.7
42	2k	126	ARG	2.7
40	2i	106	ALA	2.7
51	2t	59	ALA	2.7
11	2P	109	GLY	2.7
18	2W	112	GLY	2.7
40	2i	33	PHE	2.7
6	2G	2	PRO	2.7
33	2b	81	VAL	2.7
33	2b	184	VAL	2.7
38	1g	4	ARG	2.7
40	2i	10	ARG	2.7
51	2t	83	ARG	2.7
34	2c	185	GLY	2.7
20	2Y	5	MET	2.7
21	2Z	57	ILE	2.7
1	2A	2127	G	2.7
11	2P	81	GLN	2.7
21	2Z	106	GLY	2.7
50	2s	83	HIS	2.7
34	1c	10	PHE	2.7
51	2t	26	ASN	2.7
40	2i	56	LEU	2.7
41	2j	40	LEU	2.7
51	2t	66	ALA	2.7
40	1i	114	TYR	2.7
27	25	29	THR	2.7
30	28	49	VAL	2.7
33	1b	165	VAL	2.7
34	1c	178	LEU	2.7
33	1b	163	PHE	2.6
35	2d	49	ARG	2.7
1	2A	2173	A	2.6
6	2G	39	ILE	2.6
36	2e	98	THR	2.6
40	1i	64	THR	2.6

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Mol	Chain	Res	Type	RSRZ
7	2H	128	PRO	2.6
35	2d	167	GLY	2.6
34	2c	172	ARG	2.6
11	2P	68	GLN	2.6
9	2N	45	ASN	2.6
41	2j	72	VAL	2.6
33	2b	203	GLY	2.6
34	1c	177	THR	2.6
51	2t	25	ARG	2.6
40	2i	82	ALA	2.6
38	1g	153	HIS	2.6
28	16	54	ILE	2.6
35	1d	165	MET	2.6
1	1A	1142	A	2.6
34	2c	13	GLY	2.6
40	2i	105	ASP	2.6
40	2i	120	ARG	2.6
45	2n	55	GLY	2.6
46	2o	60	VAL	2.6
50	2s	36	ARG	2.6
30	28	29	LYS	2.6
33	1b	207	ALA	2.6
39	2h	111	ILE	2.6
44	1m	90	LEU	2.6
34	2c	158	GLY	2.6
7	2H	13	LYS	2.6
41	2j	64	GLU	2.6
31	29	26	ILE	2.6
45	2n	42	ILE	2.6
11	2P	59	LEU	2.6
25	23	53	LEU	2.6
40	1i	19	LEU	2.6
8	2I	19	VAL	2.6
34	1c	206	GLU	2.6
40	2i	52	ALA	2.6
41	2j	42	THR	2.6
54	2y	53	G	2.6
40	2i	83	ARG	2.6
4	2E	10	GLY	2.6
22	20	75	LEU	2.6
33	1b	27	LYS	2.6
38	1g	78	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
38	2g	32	ARG	2.6
30	28	15	LYS	2.6
30	28	25	MET	2.6
41	1j	64	GLU	2.6
33	2b	188	ALA	2.6
40	1i	111	ARG	2.6
45	2n	41	ARG	2.6
46	1o	87	ILE	2.6
31	29	16	VAL	2.6
34	2c	21	ARG	2.6
40	1i	36	TYR	2.6
41	2j	43	ARG	2.6
11	2P	91	PHE	2.6
45	1n	58	LYS	2.6
7	2H	100	GLY	2.5
7	2H	144	VAL	2.5
38	2g	85	TYR	2.5
9	2N	44	PRO	2.5
51	2t	62	LEU	2.5
11	2P	76	LYS	2.5
45	2n	4	LYS	2.5
7	2H	17	VAL	2.5
42	2k	25	TYR	2.5
43	2l	68	ALA	2.5
7	2H	116	GLU	2.5
33	2b	83	MET	2.5
33	1b	195	ASP	2.5
7	2H	84	SER	2.5
23	21	2	SER	2.5
32	2a	1250	A	2.5
40	2i	92	TYR	2.5
7	2H	34	GLU	2.5
7	2H	108	GLY	2.5
30	28	20	GLY	2.5
49	2r	85	LEU	2.5
39	2h	9	MET	2.5
41	2j	34	VAL	2.5
38	2g	113	GLU	2.5
41	1j	95	GLU	2.5
11	2P	114	ILE	2.5
15	2T	52	ILE	2.5
25	23	26	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
44	1m	56	LEU	2.5
45	1n	56	VAL	2.5
14	2S	37	ALA	2.5
36	1e	132	ALA	2.5
41	1j	36	GLY	2.5
48	2q	32	TYR	2.5
7	2H	151	ILE	2.5
38	2g	27	ILE	2.5
7	2H	74	ASN	2.5
53	1v	13	A	2.5
33	2b	101	MET	2.5
35	2d	56	VAL	2.5
21	2Z	50	GLN	2.5
30	28	2	PRO	2.5
14	2S	111	GLU	2.5
28	26	42	TRP	2.5
30	28	34	TRP	2.5
38	2g	83	ALA	2.5
41	2j	32	ALA	2.5
12	2Q	37	LEU	2.5
33	2b	127	ILE	2.5
42	2k	59	TYR	2.5
35	2d	94	LEU	2.5
1	1A	934	A	2.5
1	2A	896	A	2.5
53	1v	23	A	2.5
14	2S	82	ILE	2.5
40	1i	50	LEU	2.5
41	2j	8	LEU	2.5
7	2H	95	ARG	2.4
7	2H	97	ARG	2.4
21	2Z	72	ARG	2.4
30	28	46	ARG	2.4
7	2H	123	PHE	2.4
1	1A	1141	A	2.4
33	1b	179	LYS	2.4
39	2h	21	LYS	2.4
34	2c	65	ALA	2.4
7	2H	106	THR	2.4
34	1c	12	LEU	2.4
31	29	25	VAL	2.4
33	2b	195	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
7	2H	167	GLU	2.4
11	2P	88	LEU	2.4
34	2c	177	THR	2.4
39	1h	83	ILE	2.4
44	2m	66	LEU	2.4
48	2q	35	VAL	2.4
32	2a	1030(C)	G	2.4
32	2a	1224	G	2.4
51	1t	9	ASN	2.4
34	2c	41	GLY	2.4
41	1j	9	ARG	2.4
21	2Z	156	LYS	2.4
25	23	23	LEU	2.4
51	2t	13	LEU	2.4
5	2F	183	VAL	2.4
39	1h	93	VAL	2.4
22	20	8	GLY	2.4
26	24	54	GLY	2.4
39	2h	15	ASN	2.4
32	2a	1030(A)	G	2.4
31	29	13	LYS	2.4
51	2t	68	LYS	2.4
50	1s	71	LEU	2.4
38	1g	154	TYR	2.4
22	20	69	PHE	2.4
34	2c	10	PHE	2.4
36	2e	45	PHE	2.4
12	2Q	38	GLU	2.4
40	2i	38	GLN	2.4
40	1i	119	ALA	2.4
36	1e	89	ILE	2.4
44	1m	4	ILE	2.4
48	2q	84	LEU	2.4
3	1D	275	LYS	2.4
32	2a	1202	G	2.4
41	1j	66	ARG	2.4
11	2P	119	GLU	2.4
21	2Z	96	VAL	2.4
33	2b	131	PRO	2.4
47	1p	2	VAL	2.4
32	1a	1447	A	2.4
21	2Z	124	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
23	2l	98	LEU	2.4
33	2b	185	ILE	2.4
36	2e	13	ILE	2.4
36	2e	27	ARG	2.4
34	2c	55	VAL	2.4
48	2q	11	VAL	2.4
52	1u	16	GLY	2.4
50	2s	52	TYR	2.4
1	2A	883	G	2.4
32	2a	973	G	2.4
44	1m	105	THR	2.4
14	2S	20	ARG	2.4
54	1y	56	C	2.4
7	2H	82	GLY	2.3
14	2S	87	PHE	2.3
33	2b	40	HIS	2.3
33	2b	72	GLY	2.3
36	1e	81	GLU	2.3
45	2n	49	HIS	2.3
33	1b	167	PRO	2.3
35	2d	20	TYR	2.3
48	2q	42	TYR	2.3
33	2b	207	ALA	2.3
34	2c	164	ARG	2.3
38	2g	78	ARG	2.3
40	1i	15	ALA	2.3
40	2i	80	GLY	2.3
23	2l	62	VAL	2.3
21	2Z	87	ASP	2.3
29	17	48	LYS	2.3
48	2q	7	THR	2.3
49	1r	76	LEU	2.3
7	2H	124	GLU	2.3
14	2S	12	PHE	2.3
1	1A	933	C	2.3
1	2A	2146	C	2.3
21	2Z	86	VAL	2.3
32	2a	1249	C	2.3
41	1j	72	VAL	2.3
11	2P	110	TYR	2.3
32	1a	204	U	2.3
40	2i	45	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
7	2H	119	GLU	2.3
33	2b	118	LEU	2.3
48	2q	31	LEU	2.3
51	2t	70	SER	2.3
41	1j	7	LYS	2.3
41	1j	11	PHE	2.3
27	15	60	VAL	2.3
45	1n	41	ARG	2.3
54	1y	35	A	2.3
32	2a	1150	U	2.3
14	2S	4	LEU	2.3
21	2Z	59	LEU	2.3
39	2h	17	THR	2.3
21	2Z	88	PHE	2.3
45	2n	51	GLY	2.3
50	2s	35	SER	2.3
50	2s	38	SER	2.3
32	2a	1251	A	2.3
26	24	57	GLU	2.3
7	2H	41	MET	2.3
33	1b	215	LEU	2.3
45	2n	10	ALA	2.3
49	1r	78	LEU	2.3
41	1j	63	PHE	2.3
40	1i	118	LYS	2.3
34	2c	175	LEU	2.3
9	2N	74	ARG	2.3
14	2S	3	ARG	2.3
22	20	76	GLY	2.3
7	2H	43	VAL	2.3
45	2n	8	GLU	2.3
52	1u	14	TRP	2.3
11	2P	97	PRO	2.3
40	2i	49	PRO	2.3
50	2s	42	PRO	2.3
1	1A	935	C	2.3
32	2a	1112	C	2.3
34	2c	178	LEU	2.3
44	2m	99	ARG	2.3
48	2q	88	TYR	2.3
54	2w	72	C	2.3
1	1A	1139	G	2.3

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Mol	Chain	Res	Type	RSRZ
5	2F	131	GLY	2.3
7	2H	138	LYS	2.3
33	2b	76	GLN	2.3
23	2l	30	VAL	2.3
34	2c	3	ASN	2.3
49	2r	46	GLU	2.3
7	2H	132	ARG	2.3
6	2G	140	ILE	2.3
34	1c	201	TYR	2.3
34	2c	145	GLY	2.3
35	1d	101	LEU	2.3
51	1t	24	LEU	2.3
14	2S	112	PHE	2.3
54	1y	1	G	2.3
7	2H	24	VAL	2.2
51	1t	70	SER	2.2
36	2e	64	ARG	2.2
32	1a	1532	U	2.2
12	2Q	17	LEU	2.2
12	2Q	39	PRO	2.2
14	2S	110	LEU	2.2
21	1Z	147	GLY	2.2
34	2c	43	LEU	2.2
45	2n	50	LYS	2.2
44	1m	87	TYR	2.2
11	2P	74	GLU	2.2
32	2a	1117	G	2.2
36	1e	86	ALA	2.2
33	2b	32	ILE	2.2
1	2A	2128	C	2.2
12	2Q	12	GLN	2.2
45	1n	50	LYS	2.2
51	1t	68	LYS	2.2
30	28	19	SER	2.2
45	2n	32	SER	2.2
48	2q	39	SER	2.2
1	1A	1112	U	2.2
52	2u	5	ASP	2.2
35	1d	135	LEU	2.2
36	2e	43	LEU	2.2
54	1y	20	U	2.2
30	18	65	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
33	2b	17	PHE	2.2
34	1c	57	ILE	2.2
34	1c	124	ILE	2.2
44	1m	97	PRO	2.2
4	2E	52	LEU	2.2
33	1b	61	LEU	2.2
50	2s	84	GLY	2.2
38	2g	42	ILE	2.2
48	2q	44	ALA	2.2
52	2u	23	PRO	2.2
34	2c	30	ARG	2.2
51	1t	8	ARG	2.2
9	2N	103	VAL	2.2
36	2e	90	VAL	2.2
40	1i	109	VAL	2.2
48	2q	10	VAL	2.2
21	2Z	148	ASP	2.2
34	2c	183	ASP	2.2
38	1g	77	SER	2.2
41	2j	59	SER	2.2
44	2m	96	LEU	2.2
39	2h	84	ARG	2.2
51	1t	63	ILE	2.2
34	2c	173	VAL	2.2
40	1i	110	GLU	2.2
14	2S	9	ARG	2.2
22	20	5	LYS	2.2
38	1g	3	ARG	2.2
39	2h	91	ARG	2.2
40	2i	85	LEU	2.2
7	2H	148	ILE	2.2
33	2b	67	THR	2.2
34	2c	15	THR	2.2
40	1i	46	ALA	2.2
7	2H	83	TYR	2.2
49	1r	38	GLU	2.2
7	2H	51	ARG	2.2
7	2H	85	LYS	2.2
12	2Q	15	GLY	2.2
30	28	21	LYS	2.2
34	1c	11	ARG	2.2
46	1o	65	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
48	2q	87	LYS	2.2
6	2G	97	ASP	2.2
39	1h	133	LEU	2.2
39	2h	16	ALA	2.2
7	2H	122	THR	2.2
36	2e	19	MET	2.2
45	1n	49	HIS	2.2
5	2F	196	LEU	2.2
11	2P	112	LEU	2.2
14	2S	41	ASP	2.2
45	2n	16	PHE	2.2
21	2Z	98	MET	2.2
30	28	3	LYS	2.2
11	2P	93	GLY	2.1
32	2a	1004	A	2.2
34	2c	193	TYR	2.2
38	2g	80	VAL	2.2
40	1i	125	TYR	2.2
21	2Z	155	LEU	2.1
35	1d	78	LEU	2.1
33	2b	97	TRP	2.1
45	1n	61	TRP	2.1
38	1g	86	GLN	2.1
32	1a	1003	G	2.1
40	2i	11	LYS	2.1
11	2P	92	GLU	2.1
35	1d	179	GLU	2.1
42	2k	121	PRO	2.1
5	1F	89	VAL	2.1
41	1j	90	LEU	2.1
34	2c	132	ARG	2.1
47	1p	25	ARG	2.1
36	2e	114	GLY	2.1
41	2j	87	THR	2.1
15	2T	100	TYR	2.1
20	2Y	67	LEU	2.1
40	2i	47	LEU	2.1
35	1d	3	ARG	2.1
41	2j	60	ARG	2.1
41	2j	96	ILE	2.1
47	1p	7	ALA	2.1
50	2s	53	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
33	1b	71	VAL	2.1
34	2c	176	HIS	2.1
40	1i	86	VAL	2.1
1	1A	1105	G	2.1
30	28	26	LYS	2.1
40	2i	95	LYS	2.1
41	1j	48	THR	2.1
48	1q	7	THR	2.1
7	2H	101	ARG	2.1
12	2Q	25	ASP	2.1
41	1j	58	ASP	2.1
47	2p	25	ARG	2.1
7	2H	9	ILE	2.1
1	2A	652(T)	C	2.1
11	2P	101	VAL	2.1
42	2k	49	GLY	2.1
44	2m	119	GLY	2.1
25	23	52	HIS	2.1
33	2b	190	THR	2.1
41	1j	47	PHE	2.1
31	29	12	ASP	2.1
32	1a	1001(A)	G	2.1
40	2i	91	ASP	2.1
12	2Q	121	ALA	2.1
6	2G	75	LYS	2.1
30	28	12	LYS	2.1
32	2a	1039	C	2.1
34	1c	64	VAL	2.1
14	1S	20	ARG	2.1
39	2h	10	LEU	2.1
48	2q	43	LEU	2.1
51	1t	62	LEU	2.1
34	2c	162	GLN	2.1
40	2i	88	TYR	2.1
11	2P	140	ALA	2.1
25	23	21	ALA	2.1
30	28	58	ILE	2.1
41	2j	38	ILE	2.1
44	1m	122	LYS	2.1
14	2S	28	VAL	2.1
14	2S	85	VAL	2.1
25	23	47	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
43	2l	31	PRO	2.1
53	1v	24	A	2.1
32	2a	1114	C	2.1
39	1h	119	LEU	2.1
51	1t	72	LEU	2.1
14	2S	92	TYR	2.1
21	2Z	9	TYR	2.1
31	29	2	LYS	2.1
8	2I	137	PRO	2.1
11	2P	1	MET	2.1
32	2a	1032	G	2.1
47	1p	21	VAL	2.1
50	2s	76	PRO	2.1
32	2a	1252	A	2.1
31	29	24	TYR	2.1
34	1c	39	ILE	2.1
41	2j	6	ILE	2.1
52	2u	24	ARG	2.1
7	2H	44	VAL	2.1
7	2H	125	VAL	2.1
40	1i	28	VAL	2.1
48	1q	98	LEU	2.0
7	2H	72	ILE	2.0
15	2T	14	TYR	2.0
35	2d	209	ARG	2.0
40	2i	55	ALA	2.0
45	2n	59	ALA	2.0
50	2s	68	GLY	2.0
21	2Z	162	GLU	2.0
45	1n	17	LYS	2.0
40	2i	40	LEU	2.0
50	2s	10	PHE	2.0
32	1a	1029	C	2.0
1	2A	1026	U	2.0
33	1b	72	GLY	2.0
34	1c	189	ALA	2.0
34	2c	57	ILE	2.0
39	2h	80	ILE	2.0
51	1t	80	ARG	2.0
34	2c	26	LYS	2.0
37	2f	59	TYR	2.0
38	2g	24	THR	2.0

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Mol	Chain	Res	Type	RSRZ
6	2G	70	VAL	2.0
21	2Z	70	LEU	2.0
45	1n	16	PHE	2.0
52	2u	10	ARG	2.0
33	2b	68	ILE	2.0
1	1A	2196	C	2.0
12	2Q	107	ALA	2.0
40	2i	30	GLY	2.0
42	2k	89	ALA	2.0
54	1w	1	G	2.0
54	1y	13	C	2.0
54	2y	60	U	2.0
32	2a	1191	A	2.0
6	2G	159	VAL	2.0
35	1d	133	VAL	2.0
39	2h	19	VAL	2.0
49	1r	39	VAL	2.0
11	2P	77	ARG	2.0
23	21	68	PRO	2.0
25	23	2	PRO	2.0
40	1i	37	PHE	2.0
42	1k	98	LEU	2.0
50	2s	30	LEU	2.0
11	2P	108	LYS	2.0
34	1c	182	ILE	2.0
35	2d	98	GLU	2.0
40	2i	43	ALA	2.0
35	2d	207	TYR	2.0
1	1A	2134	G	2.0
32	2a	1021	G	2.0
32	2a	1036	G	2.0
36	2e	120	THR	2.0
41	1j	44	VAL	2.0
54	2y	34	G	2.0
7	2H	140	LYS	2.0
11	2P	60	MET	2.0
12	2Q	18	LYS	2.0
15	2T	1	MET	2.0
15	2T	76	PHE	2.0
44	1m	102	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	5MU	2x	54	21/22	0.92	0.16	-	77,81,86,94	0
1	2MU	2A	2552	21/23	0.97	0.18	-	31,41,45,52	0
55	5MC	2x	32	21/22	0.94	0.18	-	65,68,73,74	0
1	2MA	1A	2515	23/24	0.98	0.20	-	11,16,19,22	0
1	5MU	2A	1915	21/22	0.93	0.16	-	59,64,71,73	0
32	5MC	1a	1407	21/22	0.97	0.20	-	28,34,39,40	0
43	0TD	2l	92	10/11	0.91	0.30	-	58,64,65,80	0
32	MA6	1a	1518	24/25	0.98	0.20	-	31,38,40,40	0
55	PSU	2x	55	20/21	0.91	0.13	-	67,78,81,81	0
32	M2G	2a	966	25/26	0.94	0.27	-	60,65,72,79	0
54	5MU	2y	54	21/22	0.82	0.33	-	84,91,97,115	0
54	4SU	2y	8	20/21	0.85	0.14	-	83,95,104,112	0
1	PSU	1A	1933	20/21	0.97	0.19	-	30,37,44,45	0
1	5MC	2A	1942	21/22	0.96	0.17	-	49,56,62,66	0
1	PSU	2A	2605	20/21	0.98	0.17	-	27,31,37,38	0
1	5MU	1A	1937	21/22	0.95	0.17	-	43,49,54,56	0
1	4OC	2A	1920	21/23	0.95	0.18	-	53,58,64,66	0
32	5MC	2a	1400	21/22	0.94	0.23	-	60,67,71,73	0
1	PSU	2A	1917	20/21	0.95	0.14	-	55,60,65,69	0
1	PSU	1A	1939	20/21	0.96	0.16	-	38,46,53,54	0
32	MA6	2a	1519	24/25	0.96	0.21	-	47,56,64,66	0
54	PSU	2y	39	20/21	0.88	0.24	-	77,84,98,102	0
54	5MU	1y	54	21/22	0.78	0.32	-	79,87,99,114	0
55	PSU	1x	55	20/21	0.95	0.13	-	53,58,67,72	0
1	PSU	1A	2617	20/21	0.98	0.18	-	16,20,25,28	0
1	2MA	2A	2503	23/24	0.98	0.21	-	24,33,37,46	0
54	PSU	1w	39	20/21	0.97	0.17	-	44,60,69,70	0
54	7MG	1w	46	24/25	0.82	0.15	-	76,87,106,118	0
1	5MC	1A	1984	21/22	0.98	0.17	-	24,31,36,41	0
55	5MC	1x	32	21/22	0.98	0.20	-	44,50,57,66	0
54	7MG	2w	46	24/25	0.83	0.14	-	78,92,98,107	0
55	5MU	1x	54	21/22	0.96	0.14	-	55,62,70,76	0
54	7MG	2y	46	24/25	0.83	0.23	-	83,92,97,112	0
32	PSU	2a	516	20/21	0.93	0.14	-	50,70,74,75	0
54	PSU	2w	39	20/21	0.93	0.19	-	60,73,79,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	UR3	1a	1498	21/22	0.99	0.20	-	27,39,42,46	0
1	OMG	2A	2251	24/25	0.98	0.20	-	32,37,42,45	0
54	PSU	2w	55	20/21	0.92	0.12	-	75,81,89,94	0
32	5MC	1a	1404	21/22	0.97	0.19	-	31,38,42,44	0
54	4SU	1y	8	20/21	0.80	0.20	-	91,96,103,105	0
32	7MG	1a	527	24/25	0.95	0.18	-	34,42,51,55	0
32	4OC	2a	1402	22/23	0.96	0.16	-	52,58,64,67	0
32	5MC	1a	967	21/22	0.98	0.20	-	45,50,58,64	0
54	MIA	2w	37	25/30	0.95	0.17	-	60,68,74,78	0
32	5MC	2a	1404	21/22	0.95	0.17	-	47,51,56,61	0
32	UR3	2a	1498	21/22	0.97	0.18	-	44,50,54,63	0
32	4OC	1a	1402	22/23	0.98	0.18	-	38,42,47,53	0
54	MIA	1y	37	22/30	0.90	0.17	-	70,78,88,93	0
1	5MC	1A	1964	21/22	0.98	0.18	-	30,39,46,50	0
54	PSU	1w	55	20/21	0.92	0.14	-	61,70,79,80	0
32	5MC	2a	967	21/22	0.93	0.30	-	62,67,71,73	0
32	5MC	1a	1400	21/22	0.97	0.21	-	37,47,50,55	0
1	5MU	1A	1961	21/22	0.98	0.18	-	19,23,26,32	0
32	MA6	1a	1519	24/25	0.97	0.20	-	33,39,43,44	0
32	MA6	2a	1518	24/25	0.96	0.19	-	47,59,63,66	0
54	MIA	2y	37	22/30	0.86	0.21	-	69,81,100,111	0
32	7MG	2a	527	24/25	0.94	0.17	-	46,56,67,71	0
54	PSU	1y	32	20/21	0.88	0.19	-	71,81,88,90	0
54	4SU	2w	8	20/21	0.85	0.15	-	85,89,104,109	0
32	5MC	2a	1407	21/22	0.96	0.19	-	44,48,55,60	0
55	4SU	2x	8	20/21	0.93	0.13	-	69,73,78,81	0
54	5MU	2w	54	21/22	0.92	0.12	-	68,75,81,83	0
1	2MU	1A	2564	21/23	0.98	0.19	-	18,23,28,31	0
54	PSU	2y	32	20/21	0.88	0.17	-	69,84,92,94	0
54	PSU	2w	32	20/21	0.93	0.27	-	67,78,88,89	0
54	PSU	1y	55	20/21	0.76	0.28	-	85,93,105,123	0
32	PSU	1a	516	20/21	0.96	0.15	-	32,49,53,54	0
1	5MU	2A	1939	21/22	0.97	0.17	-	34,38,43,44	0
54	PSU	2y	55	20/21	0.80	0.27	-	85,92,104,109	0
1	5MC	2A	1962	21/22	0.97	0.17	-	32,45,48,61	0
54	4SU	1w	8	20/21	0.91	0.12	-	74,81,92,95	0
54	PSU	1y	39	20/21	0.92	0.17	-	70,77,87,90	0
32	2MG	1a	1207	24/25	0.96	0.17	-	57,62,67,68	0
1	4OC	1A	1942	21/23	0.98	0.17	-	32,39,45,47	0
1	PSU	2A	1911	20/21	0.95	0.15	-	50,60,65,67	0
55	4SU	1x	8	20/21	0.96	0.15	-	50,57,65,67	0
32	2MG	2a	1207	24/25	0.95	0.15	-	74,77,86,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	OMG	1A	2263	24/25	0.99	0.17	-	14,18,24,25	0
54	PSU	1w	32	20/21	0.95	0.19	-	57,62,68,69	0
54	5MU	1w	54	21/22	0.97	0.16	-	44,60,67,72	0
32	M2G	1a	966	25/26	0.97	0.23	-	41,48,56,63	0
54	MIA	1w	37	29/30	0.95	0.24	-	41,51,60,64	0
43	0TD	1l	92	10/11	0.94	0.21	-	43,48,51,69	0
54	7MG	1y	46	24/25	0.84	0.22	-	86,94,99,108	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3054	1/1	0.94	0.41	60.37	53,53,53,53	0
56	MG	1A	3739	1/1	0.92	0.34	47.17	29,29,29,29	0
56	MG	1A	3337	1/1	0.97	0.60	42.71	27,27,27,27	0
56	MG	1F	301	1/1	0.98	0.58	37.73	23,23,23,23	0
56	MG	1A	3140	1/1	0.96	0.54	37.39	23,23,23,23	0
56	MG	1A	4032	1/1	0.96	0.49	32.31	30,30,30,30	0
56	MG	1A	3160	1/1	0.95	0.60	28.94	29,29,29,29	0
56	MG	1A	3095	1/1	0.96	0.43	26.12	28,28,28,28	0
56	MG	1A	3199	1/1	0.93	0.52	25.82	32,32,32,32	0
56	MG	1A	3179	1/1	0.92	0.37	25.77	23,23,23,23	0
56	MG	2F	303	1/1	0.90	0.88	24.26	55,55,55,55	0
56	MG	2A	3755	1/1	0.94	0.81	21.97	48,48,48,48	0
56	MG	1A	3427	1/1	0.89	0.67	21.76	29,29,29,29	0
56	MG	1A	4034	1/1	0.97	0.58	21.64	28,28,28,28	0
56	MG	1A	3174	1/1	0.94	0.39	20.80	32,32,32,32	0
56	MG	1A	4049	1/1	0.94	0.78	20.22	30,30,30,30	0
56	MG	1A	4041	1/1	0.83	0.54	19.48	35,35,35,35	0
56	MG	1A	4036	1/1	0.92	0.56	17.74	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3480	1/1	0.86	0.64	16.52	35,35,35,35	0
56	MG	1A	3377	1/1	0.90	0.45	16.24	40,40,40,40	0
56	MG	1A	3302	1/1	0.92	0.77	15.97	32,32,32,32	0
56	MG	1A	4008	1/1	0.95	0.36	15.52	24,24,24,24	0
56	MG	1A	3422	1/1	0.95	0.49	15.45	43,43,43,43	0
56	MG	1A	3154	1/1	0.98	0.44	15.42	31,31,31,31	0
56	MG	2A	3299	1/1	0.92	0.33	15.25	43,43,43,43	0
56	MG	1N	201	1/1	0.93	0.54	14.17	45,45,45,45	0
56	MG	1A	3704	1/1	0.94	0.25	14.02	28,28,28,28	0
56	MG	1A	3253	1/1	0.96	0.71	13.74	24,24,24,24	0
56	MG	2D	306	1/1	0.92	0.67	13.39	43,43,43,43	0
56	MG	2A	3732	1/1	0.99	0.31	12.99	24,24,24,24	0
56	MG	1a	3015	1/1	0.95	0.31	12.96	48,48,48,48	0
56	MG	1A	4055	1/1	0.95	0.66	12.96	31,31,31,31	0
56	MG	25	502	1/1	0.94	0.59	12.95	47,47,47,47	0
56	MG	2A	3343	1/1	0.98	0.28	12.90	36,36,36,36	0
56	MG	1A	4045	1/1	0.91	0.61	12.89	39,39,39,39	0
56	MG	1A	3037	1/1	0.96	0.26	12.71	22,22,22,22	0
56	MG	1A	4024	1/1	0.98	0.35	12.46	43,43,43,43	0
56	MG	1A	3412	1/1	0.95	0.37	12.04	37,37,37,37	0
56	MG	1P	201	1/1	0.96	0.46	11.87	16,16,16,16	0
56	MG	1A	3252	1/1	0.93	0.29	11.78	32,32,32,32	0
56	MG	1A	3454	1/1	0.97	0.37	11.75	30,30,30,30	0
56	MG	2U	202	1/1	0.90	0.81	11.31	55,55,55,55	0
56	MG	1D	304	1/1	0.97	0.68	11.26	43,43,43,43	0
56	MG	1A	3753	1/1	0.96	0.31	11.21	27,27,27,27	0
56	MG	1A	4023	1/1	0.96	0.56	11.11	21,21,21,21	0
56	MG	1A	4060	1/1	0.90	0.62	10.74	19,19,19,19	0
56	MG	2a	1822	1/1	0.85	0.22	10.31	52,52,52,52	0
56	MG	2A	3495	1/1	0.94	0.28	10.29	60,60,60,60	0
56	MG	13	101	1/1	0.94	0.53	10.21	39,39,39,39	0
56	MG	2A	3125	1/1	0.92	0.33	10.18	32,32,32,32	0
56	MG	1A	3030	1/1	0.92	0.59	10.07	20,20,20,20	0
56	MG	1A	3375	1/1	0.98	0.37	10.05	34,34,34,34	0
56	MG	1A	3783	1/1	0.91	0.27	9.95	31,31,31,31	0
56	MG	1A	3214	1/1	0.99	0.31	9.82	32,32,32,32	0
56	MG	1R	203	1/1	0.97	0.49	9.75	34,34,34,34	0
56	MG	1A	3680	1/1	0.85	0.30	9.59	36,36,36,36	0
56	MG	1A	3696	1/1	0.99	0.22	9.56	46,46,46,46	0
56	MG	2U	204	1/1	0.93	0.83	9.56	60,60,60,60	0
56	MG	1A	3068	1/1	0.97	0.35	9.49	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1B	207	1/1	0.93	0.43	9.34	40,40,40,40	0
56	MG	2A	3072	1/1	0.97	0.30	9.12	32,32,32,32	0
56	MG	1A	3148	1/1	0.90	0.27	9.09	26,26,26,26	0
56	MG	1A	3455	1/1	0.86	0.51	9.06	28,28,28,28	0
56	MG	1a	3014	1/1	0.85	0.39	9.04	55,55,55,55	0
56	MG	1A	3887	1/1	0.91	0.23	8.98	16,16,16,16	0
56	MG	1N	204	1/1	0.84	0.60	8.83	46,46,46,46	0
56	MG	2A	3583	1/1	0.94	0.45	8.78	40,40,40,40	0
56	MG	1F	304	1/1	0.96	0.35	8.78	20,20,20,20	0
56	MG	2A	3382	1/1	0.92	0.24	8.73	46,46,46,46	0
56	MG	2A	3478	1/1	0.92	0.60	8.72	38,38,38,38	0
56	MG	1N	205	1/1	0.97	0.48	8.70	48,48,48,48	0
56	MG	1A	3111	1/1	0.95	0.28	8.69	30,30,30,30	0
56	MG	1A	3689	1/1	0.96	0.39	8.52	20,20,20,20	0
56	MG	1E	302	1/1	0.97	0.37	8.31	16,16,16,16	0
56	MG	1A	3034	1/1	0.97	0.22	8.28	12,12,12,12	0
56	MG	2A	3662	1/1	0.98	0.26	8.25	28,28,28,28	0
56	MG	1A	3560	1/1	0.93	0.23	8.24	26,26,26,26	0
56	MG	1A	3304	1/1	0.92	0.43	8.21	41,41,41,41	0
56	MG	2A	3697	1/1	0.92	0.28	8.20	50,50,50,50	0
56	MG	1A	3175	1/1	0.91	0.44	7.95	21,21,21,21	0
56	MG	1A	3173	1/1	0.97	0.29	7.93	34,34,34,34	0
56	MG	1A	3483	1/1	0.98	0.39	7.85	32,32,32,32	0
56	MG	1F	305	1/1	0.96	0.39	7.58	28,28,28,28	0
56	MG	1A	4040	1/1	0.95	0.47	7.46	34,34,34,34	0
56	MG	2A	3323	1/1	0.97	0.43	7.27	31,31,31,31	0
56	MG	17	103	1/1	0.98	0.47	7.23	33,33,33,33	0
56	MG	2A	3091	1/1	0.97	0.29	7.03	38,38,38,38	0
56	MG	1A	4031	1/1	0.96	0.42	6.98	35,35,35,35	0
56	MG	1A	4039	1/1	0.95	0.45	6.85	33,33,33,33	0
56	MG	1x	102	1/1	0.93	0.26	6.83	49,49,49,49	0
56	MG	2B	3008	1/1	0.85	0.30	6.82	59,59,59,59	0
56	MG	1A	3178	1/1	0.99	0.29	6.82	21,21,21,21	0
56	MG	1A	4063	1/1	0.98	0.39	6.79	31,31,31,31	0
56	MG	1A	4020	1/1	0.97	0.30	6.77	50,50,50,50	0
56	MG	1A	4061	1/1	0.95	0.31	6.49	38,38,38,38	0
56	MG	1A	3430	1/1	0.89	0.66	6.43	40,40,40,40	0
56	MG	1A	4014	1/1	0.93	0.34	6.39	33,33,33,33	0
56	MG	1A	4047	1/1	0.89	0.39	6.20	29,29,29,29	0
56	MG	15	101	1/1	0.94	0.38	6.18	27,27,27,27	0
56	MG	1A	3113	1/1	0.96	0.47	6.09	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3994	1/1	0.98	0.27	6.07	21,21,21,21	0
56	MG	2A	3271	1/1	0.95	0.25	6.02	45,45,45,45	0
56	MG	1A	3756	1/1	0.94	0.65	5.98	27,27,27,27	0
56	MG	2A	3654	1/1	0.94	0.26	5.93	33,33,33,33	0
56	MG	1A	3751	1/1	0.94	0.32	5.77	23,23,23,23	0
56	MG	1E	311	1/1	0.96	0.46	5.68	36,36,36,36	0
56	MG	1A	3526	1/1	0.94	0.22	5.67	42,42,42,42	0
56	MG	1A	3736	1/1	0.96	0.24	5.58	16,16,16,16	0
56	MG	1A	3102	1/1	0.95	0.27	5.53	31,31,31,31	0
56	MG	2A	3066	1/1	0.96	0.58	5.52	40,40,40,40	0
56	MG	1A	4038	1/1	0.98	0.49	5.50	31,31,31,31	0
56	MG	2A	3127	1/1	0.93	0.22	5.50	56,56,56,56	0
56	MG	1A	3960	1/1	0.85	0.23	5.49	51,51,51,51	0
56	MG	1A	3328	1/1	0.98	0.41	5.36	25,25,25,25	0
56	MG	1A	3625	1/1	0.96	0.26	5.23	10,10,10,10	0
56	MG	2A	3749	1/1	0.96	0.36	5.20	34,34,34,34	0
56	MG	1A	3171	1/1	0.90	0.24	5.14	29,29,29,29	0
56	MG	2A	3464	1/1	0.96	0.25	5.02	29,29,29,29	0
56	MG	2A	3398	1/1	0.96	0.23	4.93	26,26,26,26	0
56	MG	2a	1714	1/1	0.79	0.28	4.91	68,68,68,68	0
56	MG	1A	4026	1/1	0.98	0.52	4.88	35,35,35,35	0
56	MG	2A	3661	1/1	0.98	0.26	4.85	36,36,36,36	0
56	MG	1a	3038	1/1	0.87	0.20	4.84	55,55,55,55	0
56	MG	1A	3031	1/1	0.98	0.31	4.79	34,34,34,34	0
56	MG	1D	314	1/1	0.95	0.30	4.74	29,29,29,29	0
56	MG	2A	3472	1/1	0.85	0.23	4.72	42,42,42,42	0
56	MG	1A	3456	1/1	0.89	0.41	4.72	33,33,33,33	0
56	MG	1e	201	1/1	0.80	0.37	4.68	59,59,59,59	0
56	MG	2a	1655	1/1	0.95	0.17	4.65	67,67,67,67	0
56	MG	1A	3222	1/1	0.91	0.23	4.62	51,51,51,51	0
56	MG	2a	1627	1/1	0.96	0.22	4.61	53,53,53,53	0
56	MG	1A	4046	1/1	0.95	0.44	4.58	20,20,20,20	0
56	MG	2A	3325	1/1	0.98	0.51	4.56	63,63,63,63	0
56	MG	1A	3393	1/1	0.99	0.23	4.52	24,24,24,24	0
56	MG	2A	3624	1/1	0.94	0.22	4.51	62,62,62,62	0
56	MG	2A	3180	1/1	0.95	0.24	4.43	33,33,33,33	0
56	MG	1A	3217	1/1	0.92	0.29	4.24	19,19,19,19	0
56	MG	1A	3749	1/1	0.92	0.23	4.17	31,31,31,31	0
56	MG	1R	204	1/1	0.92	0.32	4.15	33,33,33,33	0
56	MG	2A	3395	1/1	0.99	0.21	4.13	33,33,33,33	0
56	MG	1F	309	1/1	0.97	0.33	4.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3109	1/1	0.97	0.24	4.09	39,39,39,39	0
56	MG	1Y	503	1/1	0.97	0.40	4.04	42,42,42,42	0
56	MG	1A	3087	1/1	0.92	0.18	4.03	47,47,47,47	0
56	MG	1A	3492	1/1	0.95	0.25	4.00	35,35,35,35	0
56	MG	2A	3329	1/1	0.84	0.22	3.98	46,46,46,46	0
56	MG	2A	3138	1/1	0.98	0.23	3.98	34,34,34,34	0
56	MG	16	103	1/1	0.82	0.53	3.92	56,56,56,56	0
56	MG	2D	307	1/1	0.88	0.27	3.88	35,35,35,35	0
56	MG	1A	3799	1/1	0.94	0.23	3.87	29,29,29,29	0
56	MG	1A	3362	1/1	0.96	0.25	3.81	33,33,33,33	0
56	MG	1A	3451	1/1	0.96	0.28	3.65	24,24,24,24	0
56	MG	2a	1694	1/1	0.83	0.28	3.61	66,66,66,66	0
56	MG	1A	3505	1/1	0.92	0.22	3.59	31,31,31,31	0
56	MG	1A	3757	1/1	0.97	0.24	3.28	22,22,22,22	0
56	MG	2a	1693	1/1	0.91	0.31	3.26	75,75,75,75	0
56	MG	18	101	1/1	0.96	0.34	3.26	37,37,37,37	0
56	MG	1A	3772	1/1	0.93	0.20	3.26	22,22,22,22	0
56	MG	1A	3141	1/1	0.91	0.21	3.26	38,38,38,38	0
56	MG	2A	3247	1/1	0.73	0.13	3.24	63,63,63,63	0
56	MG	1A	3550	1/1	0.96	0.19	3.22	26,26,26,26	0
58	EZG	2A	3746	25/25	0.91	0.32	3.21	35,43,49,51	0
56	MG	2a	1761	1/1	0.92	0.22	3.21	34,34,34,34	0
56	MG	1a	3214	1/1	0.93	0.40	3.13	58,58,58,58	0
56	MG	2A	3447	1/1	0.82	0.22	3.11	27,27,27,27	0
56	MG	1A	3685	1/1	0.98	0.21	3.09	21,21,21,21	0
56	MG	2U	203	1/1	0.85	0.41	3.09	55,55,55,55	0
56	MG	2A	3458	1/1	0.91	0.22	3.08	40,40,40,40	0
56	MG	2D	303	1/1	0.96	0.34	3.06	41,41,41,41	0
56	MG	1A	3269	1/1	0.94	0.21	3.06	35,35,35,35	0
56	MG	1Q	201	1/1	0.96	0.36	3.03	33,33,33,33	0
56	MG	1F	302	1/1	0.97	0.32	2.94	30,30,30,30	0
56	MG	1D	312	1/1	0.98	0.25	2.87	27,27,27,27	0
56	MG	2A	3317	1/1	0.96	0.25	2.80	36,36,36,36	0
56	MG	2A	3552	1/1	0.91	0.20	2.80	35,35,35,35	0
56	MG	2A	3742	1/1	0.91	0.33	2.78	52,52,52,52	0
56	MG	1A	3221	1/1	0.98	0.28	2.73	21,21,21,21	0
56	MG	1A	3932	1/1	0.98	0.23	2.68	13,13,13,13	0
56	MG	1a	3042	1/1	0.95	0.18	2.54	44,44,44,44	0
56	MG	2a	1676	1/1	0.97	0.19	2.50	48,48,48,48	0
56	MG	2A	3267	1/1	0.85	0.20	2.50	52,52,52,52	0
58	EZG	1A	4030	25/25	0.94	0.27	2.48	19,29,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3186	1/1	0.97	0.20	2.40	27,27,27,27	0
56	MG	2A	3570	1/1	0.73	0.20	2.29	56,56,56,56	0
56	MG	1A	3567	1/1	0.98	0.21	2.24	13,13,13,13	0
56	MG	1A	3042	1/1	0.99	0.21	2.18	19,19,19,19	0
56	MG	1A	4050	1/1	0.98	0.29	2.14	26,26,26,26	0
56	MG	2A	3024	1/1	0.89	0.20	2.14	50,50,50,50	0
56	MG	1A	3096	1/1	0.95	0.25	2.11	26,26,26,26	0
56	MG	1A	3485	1/1	0.98	0.21	2.09	21,21,21,21	0
56	MG	1a	3108	1/1	0.95	0.21	2.08	40,40,40,40	0
56	MG	1D	308	1/1	0.99	0.32	2.03	26,26,26,26	0
56	MG	1A	3224	1/1	0.91	0.16	2.01	42,42,42,42	0
56	MG	1A	3866	1/1	0.96	0.23	1.99	20,20,20,20	0
56	MG	2A	3752	1/1	0.90	0.29	1.94	61,61,61,61	0
56	MG	1A	3515	1/1	0.98	0.21	1.93	11,11,11,11	0
56	MG	1A	4052	1/1	0.94	0.40	1.93	31,31,31,31	0
56	MG	2V	3001	1/1	0.94	0.39	1.90	46,46,46,46	0
56	MG	1T	202	1/1	0.92	0.21	1.89	47,47,47,47	0
56	MG	2A	3014	1/1	0.94	0.21	1.86	54,54,54,54	0
56	MG	2A	3452	1/1	0.97	0.22	1.82	32,32,32,32	0
56	MG	1A	3465	1/1	0.86	0.20	1.81	55,55,55,55	0
56	MG	1a	3053	1/1	0.91	0.17	1.81	56,56,56,56	0
56	MG	1B	217	1/1	0.97	0.17	1.78	44,44,44,44	0
56	MG	2A	3578	1/1	0.94	0.20	1.76	27,27,27,27	0
56	MG	1a	3206	1/1	0.85	0.18	1.73	51,51,51,51	0
56	MG	1A	3484	1/1	0.96	0.24	1.68	22,22,22,22	0
56	MG	1A	3182	1/1	0.93	0.20	1.67	33,33,33,33	0
56	MG	2a	1683	1/1	0.95	0.20	1.66	33,33,33,33	0
56	MG	2A	3750	1/1	0.97	0.28	1.61	40,40,40,40	0
56	MG	2A	3304	1/1	0.94	0.20	1.57	49,49,49,49	0
56	MG	1A	3503	1/1	0.96	0.18	1.54	22,22,22,22	0
56	MG	2A	3289	1/1	0.91	0.21	1.46	53,53,53,53	0
56	MG	1x	106	1/1	0.94	0.15	1.45	66,66,66,66	0
56	MG	1A	3038	1/1	0.97	0.22	1.43	25,25,25,25	0
56	MG	2a	1681	1/1	0.83	0.22	1.43	69,69,69,69	0
56	MG	1A	4044	1/1	0.97	0.27	1.41	29,29,29,29	0
56	MG	2A	3385	1/1	0.95	0.20	1.39	27,27,27,27	0
56	MG	2A	3401	1/1	0.97	0.19	1.35	32,32,32,32	0
56	MG	1A	3572	1/1	0.95	0.20	1.35	12,12,12,12	0
56	MG	1U	203	1/1	0.94	0.23	1.34	23,23,23,23	0
56	MG	1P	202	1/1	0.96	0.27	1.33	23,23,23,23	0
56	MG	1A	4066	1/1	0.98	0.23	1.32	35,35,35,35	0
56	MG	1A	3921	1/1	0.92	0.22	1.32	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3192	1/1	0.91	0.17	1.32	54,54,54,54	0
56	MG	1A	3649	1/1	0.96	0.19	1.30	16,16,16,16	0
56	MG	15	106	1/1	0.93	0.24	1.25	19,19,19,19	0
56	MG	1U	204	1/1	0.99	0.26	1.25	23,23,23,23	0
56	MG	2A	3757	1/1	0.91	0.26	1.23	55,55,55,55	0
59	ZN	25	501	1/1	0.98	0.18	1.20	45,45,45,45	0
56	MG	1A	3058	1/1	0.93	0.19	1.20	33,33,33,33	0
56	MG	1A	3070	1/1	0.96	0.17	1.18	23,23,23,23	0
56	MG	2A	3359	1/1	0.96	0.20	1.18	52,52,52,52	0
56	MG	1A	4059	1/1	0.92	0.26	1.18	22,22,22,22	0
56	MG	1A	4064	1/1	0.97	0.26	1.15	30,30,30,30	0
56	MG	2A	3568	1/1	0.87	0.16	1.13	47,47,47,47	0
56	MG	1a	3141	1/1	0.78	0.17	1.13	64,64,64,64	0
56	MG	2D	301	1/1	0.95	0.24	1.09	54,54,54,54	0
56	MG	1A	4005	1/1	0.98	0.22	1.08	10,10,10,10	0
56	MG	1A	3640	1/1	0.85	0.16	1.08	36,36,36,36	0
56	MG	1E	303	1/1	0.98	0.24	1.07	22,22,22,22	0
56	MG	2A	3659	1/1	0.89	0.18	1.07	41,41,41,41	0
56	MG	1A	3656	1/1	0.97	0.19	1.06	25,25,25,25	0
56	MG	2A	3501	1/1	0.86	0.18	1.04	53,53,53,53	0
56	MG	2A	3657	1/1	0.92	0.20	1.02	41,41,41,41	0
56	MG	1A	3300	1/1	0.95	0.18	1.02	29,29,29,29	0
56	MG	2A	3060	1/1	0.97	0.20	1.02	32,32,32,32	0
56	MG	1D	305	1/1	0.97	0.24	1.00	28,28,28,28	0
56	MG	1E	305	1/1	0.97	0.23	0.92	50,50,50,50	0
56	MG	1A	4025	1/1	0.91	0.22	0.91	24,24,24,24	0
56	MG	1D	309	1/1	0.95	0.23	0.87	28,28,28,28	0
56	MG	2R	3002	1/1	0.93	0.25	0.87	56,56,56,56	0
56	MG	1A	3674	1/1	0.91	0.20	0.87	56,56,56,56	0
56	MG	1W	3004	1/1	0.99	0.20	0.87	21,21,21,21	0
56	MG	1A	3590	1/1	0.86	0.22	0.86	36,36,36,36	0
56	MG	1A	4057	1/1	0.98	0.21	0.75	27,27,27,27	0
56	MG	2a	1770	1/1	0.89	0.17	0.74	59,59,59,59	0
56	MG	1a	3145	1/1	0.96	0.22	0.73	48,48,48,48	0
56	MG	2A	3740	1/1	0.97	0.21	0.72	37,37,37,37	0
56	MG	1A	3428	1/1	0.95	0.21	0.72	26,26,26,26	0
56	MG	1S	3002	1/1	0.93	0.20	0.71	36,36,36,36	0
56	MG	2A	3355	1/1	0.99	0.21	0.67	23,23,23,23	0
59	ZN	15	104	1/1	0.99	0.20	0.64	42,42,42,42	0
56	MG	1X	104	1/1	0.98	0.20	0.62	31,31,31,31	0
56	MG	2A	3110	1/1	0.94	0.18	0.61	37,37,37,37	0
56	MG	1A	3837	1/1	0.92	0.19	0.60	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3099	1/1	0.98	0.24	0.60	23,23,23,23	0
56	MG	1A	3537	1/1	0.91	0.18	0.58	30,30,30,30	0
56	MG	2A	3628	1/1	0.93	0.20	0.58	40,40,40,40	0
56	MG	2A	3467	1/1	0.93	0.22	0.57	28,28,28,28	0
56	MG	1A	3565	1/1	0.90	0.19	0.56	26,26,26,26	0
56	MG	1A	3012	1/1	0.98	0.19	0.55	13,13,13,13	0
56	MG	1Q	203	1/1	0.98	0.22	0.53	28,28,28,28	0
56	MG	2A	3244	1/1	0.79	0.18	0.52	47,47,47,47	0
56	MG	1A	3705	1/1	0.93	0.17	0.50	39,39,39,39	0
56	MG	2A	3737	1/1	0.88	0.26	0.47	42,42,42,42	0
56	MG	1F	303	1/1	0.94	0.19	0.47	35,35,35,35	0
56	MG	1A	3971	1/1	0.71	0.14	0.44	65,65,65,65	0
56	MG	2T	3002	1/1	0.90	0.25	0.44	59,59,59,59	0
56	MG	2A	3739	1/1	0.98	0.23	0.43	29,29,29,29	0
56	MG	1A	3792	1/1	0.87	0.18	0.43	19,19,19,19	0
56	MG	2A	3670	1/1	0.96	0.18	0.40	46,46,46,46	0
56	MG	1O	202	1/1	0.97	0.24	0.36	56,56,56,56	0
56	MG	2A	3003	1/1	0.98	0.19	0.35	49,49,49,49	0
56	MG	2A	3485	1/1	0.94	0.22	0.35	56,56,56,56	0
56	MG	1A	3051	1/1	0.97	0.17	0.34	22,22,22,22	0
56	MG	1A	3268	1/1	0.97	0.16	0.33	31,31,31,31	0
56	MG	2A	3630	1/1	0.71	0.18	0.29	55,55,55,55	0
56	MG	2U	205	1/1	0.96	0.23	0.29	49,49,49,49	0
56	MG	2A	3115	1/1	0.88	0.18	0.27	39,39,39,39	0
56	MG	1a	3102	1/1	0.99	0.16	0.26	39,39,39,39	0
56	MG	1A	3116	1/1	0.98	0.17	0.24	26,26,26,26	0
56	MG	1A	3879	1/1	0.95	0.18	0.18	18,18,18,18	0
56	MG	1A	3776	1/1	0.96	0.20	0.14	25,25,25,25	0
56	MG	1A	3579	1/1	0.96	0.18	0.13	31,31,31,31	0
56	MG	2A	3729	1/1	0.96	0.20	0.12	43,43,43,43	0
56	MG	1l	201	1/1	0.94	0.17	0.08	31,31,31,31	0
56	MG	2q	203	1/1	0.84	0.20	0.07	75,75,75,75	0
56	MG	2a	1609	1/1	0.83	0.12	0.05	57,57,57,57	0
56	MG	1p	101	1/1	0.86	0.24	0.01	55,55,55,55	0
56	MG	1A	3310	1/1	0.98	0.17	-0.02	24,24,24,24	0
56	MG	2A	3377	1/1	0.93	0.20	-0.03	37,37,37,37	0
56	MG	1W	3001	1/1	0.96	0.19	-0.08	34,34,34,34	0
56	MG	1A	3528	1/1	0.95	0.15	-0.08	23,23,23,23	0
56	MG	1A	3794	1/1	0.79	0.18	-0.10	18,18,18,18	0
56	MG	1A	3925	1/1	0.97	0.17	-0.10	12,12,12,12	0
56	MG	2T	3001	1/1	0.84	0.26	-0.10	52,52,52,52	0
56	MG	2A	3444	1/1	0.94	0.20	-0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3394	1/1	0.78	0.20	-0.13	29,29,29,29	0
59	ZN	16	102	1/1	0.99	0.17	-0.15	38,38,38,38	0
56	MG	2A	3320	1/1	0.98	0.20	-0.18	17,17,17,17	0
56	MG	2a	1672	1/1	0.94	0.17	-0.18	50,50,50,50	0
56	MG	2a	1710	1/1	0.91	0.15	-0.19	64,64,64,64	0
56	MG	2a	1726	1/1	0.97	0.13	-0.19	64,64,64,64	0
56	MG	2A	3551	1/1	0.91	0.22	-0.22	48,48,48,48	0
56	MG	1a	3074	1/1	0.95	0.16	-0.23	49,49,49,49	0
56	MG	17	101	1/1	0.94	0.19	-0.24	27,27,27,27	0
56	MG	2A	3417	1/1	0.94	0.18	-0.24	35,35,35,35	0
56	MG	1A	3507	1/1	0.98	0.19	-0.25	24,24,24,24	0
59	ZN	2Y	501	1/1	0.97	0.15	-0.26	79,79,79,79	0
56	MG	1A	3641	1/1	0.92	0.18	-0.26	13,13,13,13	0
56	MG	2B	3006	1/1	0.95	0.17	-0.27	65,65,65,65	0
56	MG	2A	3512	1/1	0.96	0.15	-0.28	55,55,55,55	0
56	MG	2A	3381	1/1	0.89	0.18	-0.31	33,33,33,33	0
56	MG	2A	3669	1/1	0.97	0.20	-0.33	27,27,27,27	0
56	MG	1A	3662	1/1	0.98	0.19	-0.34	32,32,32,32	0
56	MG	2A	3124	1/1	0.95	0.18	-0.38	48,48,48,48	0
56	MG	15	102	1/1	0.97	0.19	-0.38	22,22,22,22	0
56	MG	1A	3123	1/1	0.96	0.16	-0.46	21,21,21,21	0
56	MG	1A	3778	1/1	0.97	0.17	-0.46	13,13,13,13	0
56	MG	1U	206	1/1	0.98	0.21	-0.49	16,16,16,16	0
56	MG	1A	3810	1/1	0.98	0.15	-0.49	40,40,40,40	0
56	MG	1A	3928	1/1	0.94	0.17	-0.51	37,37,37,37	0
56	MG	1A	3229	1/1	0.96	0.15	-0.53	28,28,28,28	0
56	MG	2a	1704	1/1	0.90	0.18	-0.53	52,52,52,52	0
56	MG	1a	3139	1/1	0.93	0.21	-0.53	56,56,56,56	0
56	MG	2a	1747	1/1	0.92	0.12	-0.56	56,56,56,56	0
56	MG	1a	3211	1/1	0.95	0.15	-0.56	35,35,35,35	0
56	MG	1A	3771	1/1	0.96	0.18	-0.57	17,17,17,17	0
59	ZN	1Y	501	1/1	0.99	0.14	-0.57	58,58,58,58	0
56	MG	1A	3423	1/1	0.83	0.17	-0.57	38,38,38,38	0
56	MG	1a	3109	1/1	0.90	0.16	-0.58	30,30,30,30	0
56	MG	2A	3754	1/1	0.98	0.26	-0.59	43,43,43,43	0
56	MG	2R	3004	1/1	0.94	0.19	-0.59	49,49,49,49	0
56	MG	1A	3714	1/1	0.95	0.19	-0.62	26,26,26,26	0
56	MG	2A	3449	1/1	0.92	0.11	-0.64	63,63,63,63	0
56	MG	1A	3474	1/1	0.96	0.17	-0.64	38,38,38,38	0
56	MG	1Q	202	1/1	0.97	0.16	-0.66	28,28,28,28	0
56	MG	16	101	1/1	0.88	0.17	-0.67	35,35,35,35	0
56	MG	1a	3155	1/1	0.94	0.18	-0.68	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	1740	1/1	0.73	0.16	-0.69	60,60,60,60	0
56	MG	2q	204	1/1	0.91	0.16	-0.72	65,65,65,65	0
56	MG	2A	3378	1/1	0.94	0.16	-0.72	25,25,25,25	0
56	MG	1A	3935	1/1	0.83	0.15	-0.73	43,43,43,43	0
56	MG	1B	220	1/1	0.87	0.14	-0.74	57,57,57,57	0
56	MG	1A	3934	1/1	0.94	0.16	-0.74	22,22,22,22	0
56	MG	2a	1715	1/1	0.91	0.15	-0.75	50,50,50,50	0
56	MG	2A	3307	1/1	0.87	0.14	-0.75	35,35,35,35	0
56	MG	2A	3545	1/1	0.89	0.18	-0.76	45,45,45,45	0
56	MG	2A	3483	1/1	0.91	0.15	-0.78	59,59,59,59	0
56	MG	1a	3025	1/1	0.97	0.16	-0.78	24,24,24,24	0
59	ZN	19	501	1/1	0.98	0.17	-0.78	42,42,42,42	0
56	MG	1A	3562	1/1	0.95	0.16	-0.79	18,18,18,18	0
56	MG	1D	310	1/1	0.96	0.19	-0.79	33,33,33,33	0
56	MG	1A	3519	1/1	0.98	0.17	-0.79	21,21,21,21	0
56	MG	1A	3039	1/1	0.94	0.18	-0.81	26,26,26,26	0
56	MG	1a	3098	1/1	0.97	0.16	-0.82	39,39,39,39	0
56	MG	2A	3463	1/1	0.96	0.16	-0.85	27,27,27,27	0
60	SF4	2d	501	8/8	0.98	0.15	-0.86	58,60,69,79	0
56	MG	1A	3110	1/1	0.91	0.17	-0.86	27,27,27,27	0
56	MG	1D	307	1/1	0.87	0.17	-0.87	39,39,39,39	0
56	MG	2A	3712	1/1	0.98	0.15	-0.87	35,35,35,35	0
56	MG	1A	3677	1/1	0.98	0.17	-0.90	18,18,18,18	0
56	MG	1a	3164	1/1	0.92	0.13	-0.91	58,58,58,58	0
56	MG	2A	3086	1/1	0.89	0.14	-0.93	62,62,62,62	0
60	SF4	1d	501	8/8	0.98	0.16	-0.94	52,54,61,66	0
56	MG	1R	201	1/1	0.96	0.16	-0.94	36,36,36,36	0
59	ZN	24	501	1/1	0.64	0.09	-0.95	103,103,103,103	0
56	MG	1E	312	1/1	0.98	0.15	-0.96	44,44,44,44	0
59	ZN	14	501	1/1	0.99	0.13	-0.99	70,70,70,70	0
56	MG	12	3002	1/1	0.97	0.19	-1.00	35,35,35,35	0
56	MG	1A	3661	1/1	0.98	0.17	-1.00	18,18,18,18	0
56	MG	2A	3713	1/1	0.96	0.18	-1.01	26,26,26,26	0
56	MG	1D	302	1/1	0.94	0.19	-1.02	21,21,21,21	0
56	MG	1E	308	1/1	0.87	0.17	-1.02	28,28,28,28	0
56	MG	1G	3001	1/1	0.89	0.14	-1.03	29,29,29,29	0
56	MG	1O	203	1/1	0.98	0.16	-1.04	48,48,48,48	0
56	MG	2A	3046	1/1	0.81	0.15	-1.05	58,58,58,58	0
56	MG	1A	3808	1/1	0.95	0.17	-1.05	34,34,34,34	0
56	MG	1A	3796	1/1	0.89	0.17	-1.06	33,33,33,33	0
56	MG	1a	3210	1/1	0.95	0.14	-1.06	41,41,41,41	0
56	MG	1X	105	1/1	0.96	0.16	-1.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3431	1/1	0.94	0.17	-1.08	24,24,24,24	0
56	MG	1U	205	1/1	0.95	0.20	-1.10	23,23,23,23	0
56	MG	1A	3890	1/1	0.95	0.15	-1.11	36,36,36,36	0
56	MG	2A	3380	1/1	0.95	0.17	-1.16	25,25,25,25	0
56	MG	2a	1807	1/1	0.93	0.11	-1.17	61,61,61,61	0
56	MG	1B	228	1/1	0.93	0.15	-1.19	24,24,24,24	0
56	MG	1a	3105	1/1	0.93	0.11	-1.19	59,59,59,59	0
56	MG	2A	3453	1/1	0.97	0.18	-1.20	34,34,34,34	0
56	MG	1r	3001	1/1	0.75	0.16	-1.20	61,61,61,61	0
56	MG	2A	3734	1/1	0.96	0.16	-1.20	25,25,25,25	0
56	MG	1A	3524	1/1	0.95	0.16	-1.20	20,20,20,20	0
59	ZN	1n	501	1/1	0.97	0.11	-1.21	51,51,51,51	0
56	MG	2A	3733	1/1	0.92	0.17	-1.21	30,30,30,30	0
56	MG	1A	3646	1/1	0.94	0.16	-1.22	19,19,19,19	0
56	MG	1A	3795	1/1	0.82	0.16	-1.23	50,50,50,50	0
56	MG	2A	3576	1/1	0.95	0.10	-1.27	52,52,52,52	0
56	MG	2e	3001	1/1	0.96	0.11	-1.28	60,60,60,60	0
56	MG	2A	3357	1/1	0.94	0.15	-1.29	21,21,21,21	0
56	MG	2a	1725	1/1	0.95	0.14	-1.30	49,49,49,49	0
56	MG	19	502	1/1	0.90	0.16	-1.32	39,39,39,39	0
56	MG	2A	3727	1/1	0.96	0.12	-1.35	49,49,49,49	0
56	MG	1a	3114	1/1	0.97	0.10	-1.35	68,68,68,68	0
56	MG	2a	1830	1/1	0.97	0.16	-1.35	71,71,71,71	0
56	MG	1A	3653	1/1	0.90	0.17	-1.35	20,20,20,20	0
56	MG	2A	3076	1/1	0.86	0.13	-1.38	45,45,45,45	0
56	MG	2A	3308	1/1	0.93	0.15	-1.38	54,54,54,54	0
56	MG	2A	3748	1/1	0.95	0.14	-1.38	27,27,27,27	0
56	MG	2d	502	1/1	0.91	0.12	-1.40	58,58,58,58	0
56	MG	1D	311	1/1	0.92	0.14	-1.40	36,36,36,36	0
56	MG	2A	3015	1/1	0.89	0.15	-1.40	37,37,37,37	0
56	MG	2a	1671	1/1	0.88	0.16	-1.41	58,58,58,58	0
56	MG	1a	3007	1/1	0.95	0.18	-1.44	50,50,50,50	0
56	MG	1a	3181	1/1	0.91	0.14	-1.46	41,41,41,41	0
56	MG	2A	3020	1/1	0.96	0.15	-1.48	29,29,29,29	0
56	MG	2F	302	1/1	0.84	0.13	-1.50	50,50,50,50	0
59	ZN	29	501	1/1	0.97	0.07	-1.52	63,63,63,63	0
59	ZN	26	501	1/1	0.98	0.09	-1.53	59,59,59,59	0
56	MG	2a	1736	1/1	0.84	0.11	-1.53	82,82,82,82	0
56	MG	1a	3028	1/1	0.97	0.14	-1.53	37,37,37,37	0
56	MG	1b	3001	1/1	0.97	0.15	-1.55	69,69,69,69	0
56	MG	1t	3001	1/1	0.88	0.20	-1.57	57,57,57,57	0
56	MG	1A	3534	1/1	0.90	0.13	-1.58	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	1766	1/1	0.98	0.14	-1.58	36,36,36,36	0
59	ZN	2n	501	1/1	0.96	0.05	-1.59	93,93,93,93	0
56	MG	2A	3682	1/1	0.89	0.13	-1.61	61,61,61,61	0
56	MG	2A	3510	1/1	0.96	0.11	-1.62	50,50,50,50	0
56	MG	1A	3676	1/1	0.97	0.17	-1.63	31,31,31,31	0
56	MG	1A	3297	1/1	0.88	0.13	-1.64	35,35,35,35	0
56	MG	1a	3213	1/1	0.99	0.15	-1.65	33,33,33,33	0
56	MG	1a	3013	1/1	0.92	0.15	-1.65	45,45,45,45	0
56	MG	2A	3073	1/1	0.90	0.16	-1.66	38,38,38,38	0
56	MG	1A	3758	1/1	0.93	0.13	-1.66	32,32,32,32	0
56	MG	1a	3120	1/1	0.96	0.08	-1.66	43,43,43,43	0
56	MG	1A	3153	1/1	0.98	0.16	-1.68	29,29,29,29	0
56	MG	2a	1731	1/1	0.98	0.09	-1.68	56,56,56,56	0
56	MG	1B	219	1/1	0.97	0.13	-1.69	27,27,27,27	0
56	MG	2l	203	1/1	0.93	0.17	-1.73	62,62,62,62	0
56	MG	1b	3002	1/1	0.94	0.10	-1.73	53,53,53,53	0
56	MG	1S	3001	1/1	0.86	0.18	-1.75	47,47,47,47	0
56	MG	1A	3627	1/1	0.95	0.13	-1.77	26,26,26,26	0
56	MG	2q	201	1/1	0.98	0.07	-1.78	46,46,46,46	0
56	MG	2A	3392	1/1	0.91	0.13	-1.80	33,33,33,33	0
56	MG	1a	3099	1/1	0.93	0.10	-1.80	72,72,72,72	0
56	MG	1a	3051	1/1	0.94	0.12	-1.81	55,55,55,55	0
56	MG	1w	106	1/1	0.90	0.10	-1.84	70,70,70,70	0
56	MG	1A	3585	1/1	0.99	0.16	-1.86	30,30,30,30	0
56	MG	2A	3646	1/1	0.90	0.13	-1.87	59,59,59,59	0
56	MG	1l	105	1/1	0.96	0.11	-1.89	32,32,32,32	0
56	MG	2A	3407	1/1	0.97	0.15	-1.90	35,35,35,35	0
56	MG	1A	3847	1/1	0.96	0.14	-1.90	18,18,18,18	0
56	MG	1a	3031	1/1	0.97	0.06	-1.91	54,54,54,54	0
56	MG	2A	3406	1/1	0.93	0.13	-1.91	40,40,40,40	0
56	MG	1a	3212	1/1	0.94	0.14	-1.91	41,41,41,41	0
56	MG	2A	3571	1/1	0.85	0.10	-1.92	57,57,57,57	0
56	MG	2A	3292	1/1	0.98	0.16	-1.92	31,31,31,31	0
56	MG	1A	3762	1/1	0.92	0.14	-1.93	12,12,12,12	0
56	MG	1A	4062	1/1	0.94	0.13	-1.96	21,21,21,21	0
56	MG	1a	3040	1/1	0.93	0.12	-1.98	41,41,41,41	0
56	MG	2A	3090	1/1	0.97	0.15	-1.98	32,32,32,32	0
56	MG	2X	3002	1/1	0.96	0.14	-1.99	49,49,49,49	0
56	MG	2a	1796	1/1	0.91	0.15	-2.01	54,54,54,54	0
56	MG	1X	106	1/1	0.97	0.14	-2.01	21,21,21,21	0
56	MG	1a	3170	1/1	0.80	0.09	-2.02	66,66,66,66	0
56	MG	2D	305	1/1	0.95	0.10	-2.02	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3912	1/1	0.95	0.15	-2.03	25,25,25,25	0
56	MG	2A	3719	1/1	0.95	0.14	-2.03	70,70,70,70	0
56	MG	2A	3011	1/1	0.93	0.15	-2.05	54,54,54,54	0
56	MG	2A	3155	1/1	0.92	0.09	-2.06	34,34,34,34	0
56	MG	1W	3005	1/1	0.96	0.14	-2.09	21,21,21,21	0
56	MG	2A	3405	1/1	0.97	0.15	-2.09	35,35,35,35	0
56	MG	2f	3001	1/1	0.95	0.11	-2.10	40,40,40,40	0
56	MG	1A	3812	1/1	0.91	0.16	-2.11	43,43,43,43	0
56	MG	2A	3466	1/1	0.92	0.16	-2.11	41,41,41,41	0
56	MG	2A	3716	1/1	0.95	0.09	-2.12	44,44,44,44	0
56	MG	2A	3650	1/1	0.85	0.09	-2.14	52,52,52,52	0
56	MG	2A	3009	1/1	0.96	0.14	-2.15	29,29,29,29	0
56	MG	2a	1774	1/1	0.96	0.15	-2.15	44,44,44,44	0
56	MG	1a	3115	1/1	0.93	0.13	-2.16	48,48,48,48	0
56	MG	1A	3737	1/1	0.93	0.14	-2.17	29,29,29,29	0
56	MG	2A	3455	1/1	0.97	0.15	-2.17	42,42,42,42	0
56	MG	1A	3476	1/1	0.92	0.13	-2.18	27,27,27,27	0
56	MG	2A	3095	1/1	0.95	0.12	-2.18	52,52,52,52	0
56	MG	2A	3668	1/1	0.98	0.12	-2.19	41,41,41,41	0
56	MG	1a	3113	1/1	0.96	0.14	-2.19	40,40,40,40	0
56	MG	1A	3180	1/1	0.96	0.14	-2.19	42,42,42,42	0
56	MG	2A	3029	1/1	0.97	0.14	-2.21	36,36,36,36	0
56	MG	1A	3652	1/1	0.98	0.15	-2.21	23,23,23,23	0
56	MG	2a	1632	1/1	0.95	0.11	-2.23	67,67,67,67	0
56	MG	1A	3626	1/1	0.94	0.14	-2.23	23,23,23,23	0
56	MG	2Q	3001	1/1	0.95	0.07	-2.23	54,54,54,54	0
56	MG	2G	3001	1/1	0.80	0.10	-2.23	60,60,60,60	0
56	MG	2A	3460	1/1	0.93	0.15	-2.24	39,39,39,39	0
56	MG	2A	3523	1/1	0.93	0.14	-2.25	37,37,37,37	0
56	MG	2a	1832	1/1	0.98	0.13	-2.27	37,37,37,37	0
56	MG	2A	3462	1/1	0.96	0.14	-2.28	54,54,54,54	0
56	MG	1A	3592	1/1	0.86	0.14	-2.32	30,30,30,30	0
56	MG	1A	3032	1/1	0.97	0.14	-2.33	26,26,26,26	0
56	MG	2A	3345	1/1	0.95	0.12	-2.39	63,63,63,63	0
56	MG	2a	1663	1/1	0.84	0.13	-2.40	48,48,48,48	0
56	MG	1a	3122	1/1	0.95	0.11	-2.40	40,40,40,40	0
56	MG	2A	3123	1/1	0.94	0.07	-2.40	58,58,58,58	0
56	MG	2a	1759	1/1	0.91	0.17	-2.42	50,50,50,50	0
56	MG	1A	3764	1/1	0.97	0.15	-2.42	24,24,24,24	0
56	MG	1A	3541	1/1	0.97	0.10	-2.43	35,35,35,35	0
56	MG	1G	3003	1/1	0.95	0.11	-2.44	51,51,51,51	0
56	MG	1A	3075	1/1	0.94	0.13	-2.44	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3569	1/1	0.95	0.14	-2.45	17,17,17,17	0
56	MG	1a	3215	1/1	0.97	0.07	-2.47	39,39,39,39	0
56	MG	2t	3001	1/1	0.81	0.09	-2.47	53,53,53,53	0
56	MG	2A	3651	1/1	0.94	0.13	-2.50	42,42,42,42	0
56	MG	2A	3074	1/1	0.96	0.15	-2.50	32,32,32,32	0
56	MG	1A	3197	1/1	0.89	0.13	-2.51	32,32,32,32	0
56	MG	1A	3663	1/1	0.97	0.13	-2.53	43,43,43,43	0
56	MG	2a	1734	1/1	0.98	0.11	-2.56	48,48,48,48	0
56	MG	1A	3827	1/1	0.94	0.13	-2.59	47,47,47,47	0
56	MG	2a	1777	1/1	0.95	0.10	-2.60	55,55,55,55	0
56	MG	2a	1658	1/1	0.93	0.12	-2.60	59,59,59,59	0
56	MG	2A	3443	1/1	0.84	0.14	-2.60	34,34,34,34	0
56	MG	2A	3027	1/1	0.95	0.14	-2.63	32,32,32,32	0
56	MG	1A	3009	1/1	0.98	0.11	-2.65	24,24,24,24	0
56	MG	1A	3707	1/1	0.90	0.12	-2.66	45,45,45,45	0
56	MG	1E	306	1/1	0.88	0.12	-2.66	38,38,38,38	0
56	MG	2A	3411	1/1	0.97	0.14	-2.69	27,27,27,27	0
56	MG	1A	3266	1/1	0.98	0.14	-2.70	24,24,24,24	0
56	MG	1A	3553	1/1	0.96	0.14	-2.71	10,10,10,10	0
56	MG	20	3003	1/1	0.92	0.11	-2.76	56,56,56,56	0
56	MG	2a	1661	1/1	0.87	0.11	-2.77	63,63,63,63	0
56	MG	1A	3631	1/1	0.93	0.16	-2.82	32,32,32,32	0
56	MG	1A	3020	1/1	0.93	0.14	-2.83	18,18,18,18	0
56	MG	1N	202	1/1	0.89	0.13	-2.83	36,36,36,36	0
56	MG	10	104	1/1	0.90	0.12	-2.84	49,49,49,49	0
56	MG	1a	3110	1/1	0.96	0.13	-2.85	50,50,50,50	0
56	MG	1n	503	1/1	0.93	0.08	-2.91	38,38,38,38	0
56	MG	1A	3819	1/1	0.93	0.11	-2.94	29,29,29,29	0
56	MG	1a	3036	1/1	0.91	0.10	-2.95	49,49,49,49	0
56	MG	2a	1689	1/1	0.97	0.08	-2.95	57,57,57,57	0
56	MG	2A	3677	1/1	0.94	0.15	-2.98	48,48,48,48	0
56	MG	1A	3648	1/1	0.92	0.10	-3.00	20,20,20,20	0
56	MG	2a	1665	1/1	0.98	0.16	-3.01	49,49,49,49	0
56	MG	1A	3637	1/1	0.95	0.13	-3.02	20,20,20,20	0
56	MG	2E	306	1/1	0.90	0.12	-3.03	43,43,43,43	0
56	MG	2A	3704	1/1	0.97	0.14	-3.04	37,37,37,37	0
56	MG	1A	4013	1/1	0.94	0.13	-3.04	21,21,21,21	0
56	MG	1a	3002	1/1	0.97	0.10	-3.09	46,46,46,46	0
56	MG	2A	3520	1/1	0.88	0.10	-3.10	52,52,52,52	0
56	MG	1A	3628	1/1	0.93	0.13	-3.11	16,16,16,16	0
56	MG	2a	1789	1/1	0.95	0.09	-3.20	54,54,54,54	0
56	MG	1A	3444	1/1	0.93	0.14	-3.25	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3686	1/1	0.97	0.16	-3.25	18,18,18,18	0
56	MG	2a	1670	1/1	0.94	0.11	-3.26	55,55,55,55	0
56	MG	2A	3717	1/1	0.97	0.11	-3.28	57,57,57,57	0
56	MG	2a	1673	1/1	0.93	0.10	-3.31	57,57,57,57	0
56	MG	1A	3574	1/1	0.95	0.15	-3.31	16,16,16,16	0
56	MG	1A	3644	1/1	0.85	0.14	-3.33	12,12,12,12	0
56	MG	1x	115	1/1	0.90	0.12	-3.33	50,50,50,50	0
56	MG	1a	3143	1/1	0.90	0.08	-3.35	74,74,74,74	0
56	MG	2a	1833	1/1	0.91	0.06	-3.36	62,62,62,62	0
56	MG	1A	3558	1/1	0.91	0.13	-3.38	16,16,16,16	0
56	MG	2A	3715	1/1	0.87	0.09	-3.38	56,56,56,56	0
56	MG	1A	3043	1/1	0.94	0.15	-3.39	19,19,19,19	0
56	MG	2A	3409	1/1	0.94	0.11	-3.39	54,54,54,54	0
56	MG	1A	3481	1/1	0.98	0.12	-3.43	28,28,28,28	0
56	MG	2A	3448	1/1	0.95	0.14	-3.50	33,33,33,33	0
56	MG	2a	1697	1/1	0.84	0.10	-3.52	64,64,64,64	0
56	MG	1A	3668	1/1	0.97	0.14	-3.53	22,22,22,22	0
56	MG	2A	3565	1/1	0.93	0.12	-3.61	45,45,45,45	0
56	MG	1A	3033	1/1	0.96	0.12	-3.63	21,21,21,21	0
56	MG	2E	301	1/1	0.96	0.14	-3.64	33,33,33,33	0
56	MG	2A	3344	1/1	0.97	0.11	-3.67	24,24,24,24	0
56	MG	2A	3143	1/1	0.96	0.13	-3.67	41,41,41,41	0
56	MG	2A	3030	1/1	0.97	0.08	-3.71	25,25,25,25	0
56	MG	2A	3702	1/1	0.74	0.13	-3.73	59,59,59,59	0
56	MG	1a	3019	1/1	0.95	0.10	-3.74	54,54,54,54	0
56	MG	1A	3021	1/1	0.97	0.13	-3.74	29,29,29,29	0
56	MG	1a	3077	1/1	0.90	0.09	-3.74	42,42,42,42	0
56	MG	1A	3184	1/1	0.97	0.14	-3.75	14,14,14,14	0
56	MG	1A	3599	1/1	0.97	0.11	-3.81	15,15,15,15	0
56	MG	2A	3008	1/1	0.90	0.14	-3.82	34,34,34,34	0
56	MG	2A	3144	1/1	0.97	0.10	-3.82	33,33,33,33	0
56	MG	1a	3012	1/1	0.94	0.10	-3.83	41,41,41,41	0
56	MG	2A	3445	1/1	0.93	0.10	-3.90	47,47,47,47	0
56	MG	2A	3606	1/1	0.88	0.12	-3.93	49,49,49,49	0
56	MG	2A	3057	1/1	0.93	0.13	-3.93	47,47,47,47	0
56	MG	1a	3071	1/1	0.97	0.10	-3.96	43,43,43,43	0
56	MG	2A	3744	1/1	0.88	0.10	-3.97	40,40,40,40	0
56	MG	1A	3552	1/1	0.97	0.14	-3.97	23,23,23,23	0
56	MG	2A	3562	1/1	0.92	0.10	-3.98	40,40,40,40	0
56	MG	1A	3962	1/1	0.97	0.08	-4.00	23,23,23,23	0
56	MG	2a	1653	1/1	0.92	0.07	-4.03	67,67,67,67	0
56	MG	2A	3301	1/1	0.95	0.14	-4.03	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	1754	1/1	0.95	0.09	-4.04	61,61,61,61	0
56	MG	1A	3022	1/1	0.97	0.13	-4.05	22,22,22,22	0
56	MG	1a	3126	1/1	0.94	0.12	-4.06	46,46,46,46	0
56	MG	1x	105	1/1	0.95	0.13	-4.06	59,59,59,59	0
56	MG	2A	3360	1/1	0.88	0.13	-4.07	25,25,25,25	0
56	MG	1A	3011	1/1	0.98	0.09	-4.11	20,20,20,20	0
56	MG	1a	3022	1/1	0.91	0.09	-4.12	48,48,48,48	0
56	MG	1A	4035	1/1	0.95	0.10	-4.14	38,38,38,38	0
56	MG	1a	3041	1/1	0.96	0.05	-4.17	51,51,51,51	0
56	MG	2A	3424	1/1	0.99	0.09	-4.18	24,24,24,24	0
56	MG	1a	3039	1/1	0.95	0.10	-4.22	47,47,47,47	0
56	MG	1A	3520	1/1	0.96	0.11	-4.23	11,11,11,11	0
56	MG	2A	3625	1/1	0.93	0.08	-4.24	52,52,52,52	0
56	MG	1A	3807	1/1	0.97	0.11	-4.28	28,28,28,28	0
56	MG	1A	3554	1/1	0.96	0.13	-4.29	14,14,14,14	0
56	MG	2A	3368	1/1	0.97	0.13	-4.32	36,36,36,36	0
56	MG	1a	3205	1/1	0.85	0.12	-4.35	69,69,69,69	0
56	MG	2A	3037	1/1	0.93	0.11	-4.40	61,61,61,61	0
56	MG	2a	1678	1/1	0.91	0.11	-4.46	65,65,65,65	0
56	MG	2A	3535	1/1	0.93	0.14	-4.47	27,27,27,27	0
56	MG	2A	3692	1/1	0.90	0.07	-4.48	52,52,52,52	0
56	MG	2A	3442	1/1	0.94	0.17	-4.49	23,23,23,23	0
56	MG	1A	3634	1/1	0.97	0.12	-4.52	28,28,28,28	0
56	MG	2A	3272	1/1	0.96	0.09	-4.56	33,33,33,33	0
56	MG	2A	3012	1/1	0.96	0.10	-4.60	44,44,44,44	0
56	MG	1U	201	1/1	0.97	0.10	-4.61	20,20,20,20	0
56	MG	1A	3745	1/1	0.97	0.13	-4.67	33,33,33,33	0
56	MG	1A	3605	1/1	0.98	0.09	-4.68	14,14,14,14	0
56	MG	1A	3848	1/1	0.97	0.10	-4.70	34,34,34,34	0
56	MG	1E	313	1/1	0.90	0.10	-4.73	25,25,25,25	0
56	MG	2A	3709	1/1	0.98	0.14	-4.74	40,40,40,40	0
56	MG	2A	3541	1/1	0.96	0.14	-4.79	32,32,32,32	0
56	MG	1A	3670	1/1	0.90	0.11	-4.80	43,43,43,43	0
56	MG	1A	3615	1/1	0.97	0.11	-4.83	12,12,12,12	0
56	MG	1A	3118	1/1	0.93	0.11	-4.85	29,29,29,29	0
56	MG	2A	3077	1/1	0.97	0.10	-4.85	41,41,41,41	0
56	MG	2a	1788	1/1	0.84	0.12	-4.88	55,55,55,55	0
56	MG	2a	1690	1/1	0.94	0.07	-4.93	57,57,57,57	0
56	MG	2A	3375	1/1	0.89	0.11	-5.02	36,36,36,36	0
56	MG	1B	223	1/1	0.96	0.10	-5.03	51,51,51,51	0
56	MG	1a	3009	1/1	0.96	0.10	-5.04	32,32,32,32	0
56	MG	2A	3063	1/1	0.97	0.14	-5.05	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3525	1/1	0.96	0.12	-5.10	9,9,9,9	0
56	MG	2A	3597	1/1	0.96	0.12	-5.12	34,34,34,34	0
56	MG	2A	3354	1/1	0.90	0.14	-5.16	53,53,53,53	0
56	MG	2A	3356	1/1	0.85	0.08	-5.18	42,42,42,42	0
56	MG	1a	3188	1/1	0.95	0.10	-5.19	47,47,47,47	0
56	MG	2A	3521	1/1	0.96	0.07	-5.21	63,63,63,63	0
56	MG	1a	3010	1/1	0.93	0.09	-5.24	45,45,45,45	0
56	MG	2A	3387	1/1	0.97	0.09	-5.24	50,50,50,50	0
56	MG	1a	3169	1/1	0.95	0.09	-5.27	38,38,38,38	0
56	MG	2w	108	1/1	0.98	0.07	-5.28	68,68,68,68	0
56	MG	1A	3888	1/1	0.96	0.14	-5.32	15,15,15,15	0
56	MG	2A	3493	1/1	0.96	0.09	-5.43	28,28,28,28	0
56	MG	1a	3185	1/1	0.99	0.10	-5.44	26,26,26,26	0
56	MG	1A	3660	1/1	0.99	0.09	-5.48	26,26,26,26	0
56	MG	1A	3593	1/1	0.80	0.12	-5.51	30,30,30,30	0
56	MG	2A	3346	1/1	0.92	0.11	-5.52	48,48,48,48	0
56	MG	1a	3158	1/1	0.95	0.06	-5.67	47,47,47,47	0
56	MG	1A	3257	1/1	0.98	0.09	-5.71	34,34,34,34	0
56	MG	1A	3546	1/1	0.96	0.11	-5.74	14,14,14,14	0
56	MG	1A	3942	1/1	0.94	0.10	-5.80	47,47,47,47	0
56	MG	1A	3949	1/1	0.96	0.11	-5.82	18,18,18,18	0
56	MG	1a	3160	1/1	0.96	0.09	-5.83	52,52,52,52	0
56	MG	1A	3196	1/1	0.96	0.12	-5.87	34,34,34,34	0
56	MG	1A	3549	1/1	0.88	0.11	-5.91	30,30,30,30	0
56	MG	1B	206	1/1	0.97	0.07	-5.93	36,36,36,36	0
56	MG	1A	3642	1/1	0.98	0.09	-6.01	34,34,34,34	0
56	MG	2A	3006	1/1	0.93	0.08	-6.05	44,44,44,44	0
56	MG	1A	3288	1/1	0.90	0.08	-6.06	47,47,47,47	0
56	MG	1A	3049	1/1	0.96	0.10	-6.09	21,21,21,21	0
56	MG	2U	201	1/1	0.94	0.08	-6.10	49,49,49,49	0
56	MG	1A	3508	1/1	0.96	0.10	-6.22	26,26,26,26	0
56	MG	1A	3506	1/1	0.88	0.09	-6.30	24,24,24,24	0
56	MG	1A	3701	1/1	0.97	0.10	-6.33	15,15,15,15	0
56	MG	2A	3080	1/1	0.94	0.11	-6.39	28,28,28,28	0
56	MG	1A	3521	1/1	0.94	0.09	-6.48	50,50,50,50	0
56	MG	2A	3486	1/1	0.93	0.12	-6.48	53,53,53,53	0
56	MG	1A	3535	1/1	0.98	0.09	-6.49	23,23,23,23	0
56	MG	2A	3148	1/1	0.97	0.06	-6.50	34,34,34,34	0
56	MG	1A	3216	1/1	0.96	0.14	-6.52	25,25,25,25	0
56	MG	1A	3671	1/1	0.90	0.09	-6.60	14,14,14,14	0
56	MG	2A	3351	1/1	0.94	0.13	-6.67	43,43,43,43	0
56	MG	1A	3836	1/1	0.92	0.09	-6.72	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3815	1/1	0.90	0.08	-6.78	35,35,35,35	0
56	MG	2A	3706	1/1	0.94	0.14	-6.79	42,42,42,42	0
56	MG	1A	3162	1/1	0.97	0.13	-6.80	24,24,24,24	0
56	MG	1A	3441	1/1	0.93	0.07	-6.81	49,49,49,49	0
56	MG	2A	3099	1/1	0.93	0.10	-6.88	38,38,38,38	0
56	MG	2W	203	1/1	0.92	0.12	-6.91	41,41,41,41	0
56	MG	2A	3648	1/1	0.97	0.07	-6.97	46,46,46,46	0
56	MG	1B	224	1/1	0.94	0.09	-7.02	54,54,54,54	0
56	MG	1A	3891	1/1	0.96	0.10	-7.06	33,33,33,33	0
56	MG	2A	3736	1/1	0.97	0.09	-7.13	37,37,37,37	0
56	MG	1A	3885	1/1	0.94	0.12	-7.20	16,16,16,16	0
56	MG	1D	306	1/1	0.96	0.10	-7.29	17,17,17,17	0
56	MG	2A	3026	1/1	0.98	0.10	-7.46	43,43,43,43	0
56	MG	1A	3007	1/1	0.98	0.10	-7.53	12,12,12,12	0
56	MG	2A	3013	1/1	0.93	0.13	-7.65	27,27,27,27	0
56	MG	1A	3941	1/1	0.91	0.09	-7.78	34,34,34,34	0
56	MG	1A	3495	1/1	0.90	0.10	-7.99	31,31,31,31	0
56	MG	1A	3557	1/1	0.99	0.08	-8.00	25,25,25,25	0
56	MG	1A	3060	1/1	0.93	0.08	-8.10	26,26,26,26	0
56	MG	2A	3120	1/1	0.98	0.13	-8.31	38,38,38,38	0
56	MG	2a	1709	1/1	0.90	0.12	-8.50	49,49,49,49	0
56	MG	1A	3188	1/1	0.91	0.10	-8.51	12,12,12,12	0
56	MG	1A	3163	1/1	0.97	0.08	-8.53	24,24,24,24	0
56	MG	1A	3497	1/1	0.98	0.10	-8.98	23,23,23,23	0
56	MG	2A	3540	1/1	0.97	0.09	-9.03	37,37,37,37	0
56	MG	1A	3544	1/1	0.99	0.09	-9.12	12,12,12,12	0
56	MG	1A	3516	1/1	0.87	0.13	-9.70	30,30,30,30	0
56	MG	2A	3473	1/1	0.98	0.10	-9.85	29,29,29,29	0
56	MG	1A	3702	1/1	0.96	0.07	-10.00	23,23,23,23	0
56	MG	1A	3232	1/1	0.95	0.10	-10.57	17,17,17,17	0
56	MG	1A	3937	1/1	0.90	0.10	-10.81	40,40,40,40	0
56	MG	2a	1675	1/1	0.94	0.07	-11.37	53,53,53,53	0
56	MG	2A	3488	1/1	0.96	0.08	-11.45	53,53,53,53	0
56	MG	2A	3504	1/1	0.99	0.08	-12.23	29,29,29,29	0
56	MG	1A	3267	1/1	0.99	0.12	-12.32	24,24,24,24	0
56	MG	2a	1819	1/1	0.92	0.08	-12.83	52,52,52,52	0
56	MG	1A	3220	1/1	0.97	0.08	-14.13	24,24,24,24	0
56	MG	1A	4000	1/1	0.98	0.07	-	29,29,29,29	0
56	MG	1A	3271	1/1	0.90	0.14	-	53,53,53,53	0
56	MG	1V	202	1/1	0.82	0.42	-	44,44,44,44	0
56	MG	1A	3849	1/1	0.92	0.27	-	35,35,35,35	0
56	MG	1A	3187	1/1	0.95	0.08	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3712	1/1	0.93	0.25	-	34,34,34,34	0
56	MG	2A	3038	1/1	0.97	0.16	-	33,33,33,33	0
56	MG	1A	3989	1/1	0.87	0.10	-	49,49,49,49	0
56	MG	1A	3321	1/1	0.88	0.41	-	45,45,45,45	0
56	MG	2A	3698	1/1	0.92	0.16	-	58,58,58,58	0
56	MG	2A	3212	1/1	0.91	0.12	-	59,59,59,59	0
56	MG	2A	3186	1/1	0.87	0.14	-	51,51,51,51	0
56	MG	2A	3275	1/1	0.97	0.09	-	37,37,37,37	0
56	MG	2a	1802	1/1	0.84	0.23	-	69,69,69,69	0
56	MG	1A	3017	1/1	0.97	0.11	-	19,19,19,19	0
56	MG	15	107	1/1	0.86	0.21	-	45,45,45,45	0
56	MG	1a	3061	1/1	0.85	0.14	-	56,56,56,56	0
56	MG	1a	3004	1/1	0.94	0.14	-	50,50,50,50	0
56	MG	1A	3978	1/1	0.98	0.08	-	33,33,33,33	0
56	MG	1A	3015	1/1	0.97	0.16	-	37,37,37,37	0
56	MG	1A	3233	1/1	0.96	0.44	-	35,35,35,35	0
56	MG	1A	3364	1/1	0.98	0.14	-	23,23,23,23	0
56	MG	2A	3334	1/1	0.93	0.28	-	58,58,58,58	0
56	MG	2B	3017	1/1	0.90	0.20	-	61,61,61,61	0
56	MG	1a	3127	1/1	0.97	0.08	-	48,48,48,48	0
56	MG	1a	3076	1/1	0.90	0.17	-	48,48,48,48	0
56	MG	2A	3468	1/1	0.86	0.11	-	40,40,40,40	0
56	MG	1a	3176	1/1	0.91	0.10	-	59,59,59,59	0
56	MG	1A	3782	1/1	0.95	0.09	-	34,34,34,34	0
56	MG	2A	3548	1/1	0.97	0.13	-	51,51,51,51	0
56	MG	1a	3104	1/1	0.93	0.17	-	45,45,45,45	0
56	MG	1a	3129	1/1	0.69	0.15	-	65,65,65,65	0
56	MG	2A	3579	1/1	0.95	0.09	-	51,51,51,51	0
56	MG	2A	3195	1/1	0.91	0.28	-	50,50,50,50	0
56	MG	1A	3139	1/1	0.96	0.19	-	21,21,21,21	0
56	MG	2A	3213	1/1	0.88	0.11	-	50,50,50,50	0
56	MG	2A	3494	1/1	0.95	0.26	-	49,49,49,49	0
56	MG	1A	3255	1/1	0.97	0.11	-	36,36,36,36	0
56	MG	1A	3296	1/1	0.90	0.12	-	37,37,37,37	0
56	MG	2a	1703	1/1	0.98	0.12	-	41,41,41,41	0
56	MG	1A	3284	1/1	0.92	0.20	-	42,42,42,42	0
56	MG	1V	203	1/1	0.95	0.21	-	63,63,63,63	0
56	MG	2A	3278	1/1	0.94	0.14	-	57,57,57,57	0
56	MG	1A	3985	1/1	0.92	0.17	-	60,60,60,60	0
56	MG	1A	3667	1/1	0.98	0.18	-	31,31,31,31	0
56	MG	2A	3031	1/1	0.74	0.28	-	57,57,57,57	0
56	MG	2A	3166	1/1	0.88	0.13	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2g	8001	1/1	0.86	0.15	-	59,59,59,59	0
56	MG	1B	215	1/1	0.94	0.06	-	34,34,34,34	0
56	MG	2x	101	1/1	0.86	0.12	-	52,52,52,52	0
56	MG	2a	1657	1/1	0.91	0.16	-	36,36,36,36	0
56	MG	1A	3595	1/1	0.91	0.14	-	40,40,40,40	0
56	MG	2A	3527	1/1	0.97	0.18	-	52,52,52,52	0
56	MG	1A	3804	1/1	0.81	0.16	-	45,45,45,45	0
56	MG	1A	3645	1/1	0.98	0.11	-	25,25,25,25	0
56	MG	2A	3313	1/1	0.91	0.19	-	41,41,41,41	0
56	MG	2x	104	1/1	0.84	0.13	-	64,64,64,64	0
56	MG	1A	3596	1/1	0.93	0.19	-	44,44,44,44	0
56	MG	2A	3678	1/1	0.94	0.21	-	71,71,71,71	0
56	MG	1A	3874	1/1	0.96	0.16	-	36,36,36,36	0
56	MG	1A	3133	1/1	0.88	0.22	-	43,43,43,43	0
56	MG	1A	3201	1/1	0.67	0.51	-	42,42,42,42	0
56	MG	2A	3116	1/1	0.92	0.11	-	55,55,55,55	0
56	MG	1A	3490	1/1	0.98	0.15	-	26,26,26,26	0
56	MG	2A	3362	1/1	0.97	0.09	-	58,58,58,58	0
56	MG	2A	3157	1/1	0.94	0.11	-	51,51,51,51	0
56	MG	1B	203	1/1	0.94	0.20	-	39,39,39,39	0
56	MG	1A	3904	1/1	0.83	0.15	-	71,71,71,71	0
56	MG	2A	3358	1/1	0.90	0.14	-	47,47,47,47	0
56	MG	2a	1625	1/1	0.96	0.10	-	67,67,67,67	0
56	MG	2A	3168	1/1	0.93	0.11	-	39,39,39,39	0
56	MG	1A	3318	1/1	0.98	0.20	-	46,46,46,46	0
56	MG	1A	3138	1/1	0.97	0.46	-	30,30,30,30	0
56	MG	1A	3538	1/1	0.97	0.06	-	45,45,45,45	0
56	MG	2v	3002	1/1	0.74	0.54	-	67,67,67,67	0
56	MG	1A	3741	1/1	0.87	0.11	-	40,40,40,40	0
56	MG	1A	3858	1/1	0.97	0.17	-	54,54,54,54	0
56	MG	2a	1795	1/1	0.93	0.37	-	64,64,64,64	0
56	MG	1A	3432	1/1	0.89	0.15	-	31,31,31,31	0
56	MG	1A	3672	1/1	0.84	0.22	-	68,68,68,68	0
56	MG	1A	3570	1/1	0.93	0.19	-	57,57,57,57	0
56	MG	1A	3913	1/1	0.95	0.25	-	39,39,39,39	0
56	MG	1a	3044	1/1	0.89	0.15	-	46,46,46,46	0
56	MG	1A	3665	1/1	0.97	0.13	-	12,12,12,12	0
56	MG	2A	3575	1/1	0.97	0.12	-	46,46,46,46	0
56	MG	1A	3027	1/1	0.90	0.36	-	27,27,27,27	0
56	MG	1B	238	1/1	0.97	0.10	-	23,23,23,23	0
56	MG	2A	3112	1/1	0.94	0.12	-	52,52,52,52	0
56	MG	2A	3649	1/1	0.99	0.13	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3317	1/1	0.89	0.47	-	45,45,45,45	0
56	MG	2A	3340	1/1	0.94	0.19	-	30,30,30,30	0
56	MG	2A	3421	1/1	0.94	0.10	-	39,39,39,39	0
56	MG	1A	3386	1/1	0.93	0.10	-	33,33,33,33	0
56	MG	2a	1825	1/1	0.96	0.17	-	56,56,56,56	0
56	MG	1a	3119	1/1	0.96	0.15	-	52,52,52,52	0
56	MG	1A	3193	1/1	0.95	0.19	-	30,30,30,30	0
56	MG	1A	3700	1/1	0.92	0.09	-	27,27,27,27	0
56	MG	2d	503	1/1	0.94	0.12	-	56,56,56,56	0
56	MG	1A	3244	1/1	0.93	0.24	-	34,34,34,34	0
56	MG	1A	3872	1/1	0.93	0.33	-	27,27,27,27	0
56	MG	1A	3119	1/1	0.96	0.18	-	49,49,49,49	0
56	MG	20	3002	1/1	0.89	0.07	-	52,52,52,52	0
56	MG	1x	101	1/1	0.88	0.19	-	54,54,54,54	0
56	MG	1A	3693	1/1	0.98	0.12	-	40,40,40,40	0
56	MG	2A	3197	1/1	0.94	0.14	-	39,39,39,39	0
56	MG	2A	3096	1/1	0.98	0.09	-	42,42,42,42	0
56	MG	2a	1816	1/1	0.97	0.15	-	48,48,48,48	0
56	MG	2A	3305	1/1	0.93	0.15	-	51,51,51,51	0
56	MG	1a	3130	1/1	0.87	0.14	-	46,46,46,46	0
56	MG	1A	3418	1/1	0.95	0.56	-	30,30,30,30	0
56	MG	2A	3207	1/1	0.89	0.28	-	40,40,40,40	0
56	MG	2A	3316	1/1	0.92	0.15	-	53,53,53,53	0
56	MG	2a	1708	1/1	0.89	0.14	-	61,61,61,61	0
56	MG	1A	3806	1/1	0.96	0.11	-	45,45,45,45	0
56	MG	1A	3166	1/1	0.82	0.37	-	31,31,31,31	0
56	MG	2A	3140	1/1	0.78	0.22	-	60,60,60,60	0
56	MG	1A	3326	1/1	0.94	0.17	-	25,25,25,25	0
56	MG	1A	3939	1/1	0.86	0.15	-	44,44,44,44	0
56	MG	1A	3365	1/1	0.93	0.21	-	39,39,39,39	0
56	MG	2a	1620	1/1	0.87	0.21	-	64,64,64,64	0
56	MG	1A	3743	1/1	0.91	0.20	-	42,42,42,42	0
56	MG	1A	3706	1/1	0.94	0.11	-	27,27,27,27	0
56	MG	2a	1809	1/1	0.95	0.15	-	58,58,58,58	0
56	MG	1a	3154	1/1	0.82	0.10	-	59,59,59,59	0
56	MG	1A	3740	1/1	0.95	0.15	-	46,46,46,46	0
56	MG	2B	3019	1/1	0.85	0.30	-	82,82,82,82	0
56	MG	1A	3278	1/1	0.96	0.18	-	40,40,40,40	0
56	MG	2a	1640	1/1	0.36	0.22	-	62,62,62,62	0
56	MG	1A	3360	1/1	0.96	0.18	-	32,32,32,32	0
56	MG	2A	3538	1/1	0.91	0.28	-	49,49,49,49	0
56	MG	2A	3391	1/1	0.96	0.14	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3582	1/1	0.90	0.14	-	44,44,44,44	0
56	MG	1Q	204	1/1	0.86	0.17	-	41,41,41,41	0
56	MG	2A	3428	1/1	0.97	0.17	-	43,43,43,43	0
56	MG	1A	3832	1/1	0.87	0.13	-	69,69,69,69	0
56	MG	2A	3396	1/1	0.89	0.14	-	29,29,29,29	0
56	MG	1A	3651	1/1	0.98	0.12	-	22,22,22,22	0
56	MG	1A	3770	1/1	0.98	0.16	-	12,12,12,12	0
56	MG	1A	3725	1/1	0.96	0.17	-	30,30,30,30	0
56	MG	1A	3864	1/1	0.98	0.23	-	20,20,20,20	0
56	MG	1A	3429	1/1	0.91	0.38	-	29,29,29,29	0
56	MG	1A	3681	1/1	0.91	0.12	-	23,23,23,23	0
56	MG	1a	3147	1/1	0.94	0.05	-	58,58,58,58	0
56	MG	1a	3085	1/1	0.96	0.21	-	33,33,33,33	0
56	MG	1A	3439	1/1	0.88	0.31	-	37,37,37,37	0
56	MG	2a	1786	1/1	0.91	0.12	-	66,66,66,66	0
56	MG	2a	1634	1/1	0.92	0.11	-	59,59,59,59	0
56	MG	2w	103	1/1	0.96	0.09	-	44,44,44,44	0
56	MG	2A	3022	1/1	0.92	0.18	-	38,38,38,38	0
56	MG	1A	3228	1/1	0.94	0.29	-	40,40,40,40	0
56	MG	1A	3816	1/1	0.96	0.27	-	46,46,46,46	0
56	MG	1A	3239	1/1	0.93	0.28	-	38,38,38,38	0
56	MG	1D	303	1/1	0.91	0.27	-	26,26,26,26	0
56	MG	1A	3620	1/1	0.91	0.11	-	49,49,49,49	0
56	MG	1A	3263	1/1	0.89	0.09	-	48,48,48,48	0
56	MG	2A	3237	1/1	0.95	0.15	-	43,43,43,43	0
56	MG	2r	3002	1/1	0.77	0.14	-	64,64,64,64	0
56	MG	2a	1680	1/1	0.95	0.16	-	45,45,45,45	0
56	MG	2a	1775	1/1	0.92	0.15	-	74,74,74,74	0
56	MG	2E	308	1/1	0.97	0.09	-	49,49,49,49	0
56	MG	2A	3525	1/1	0.96	0.27	-	52,52,52,52	0
56	MG	2y	3003	1/1	0.76	0.13	-	59,59,59,59	0
56	MG	1A	3629	1/1	0.95	0.22	-	60,60,60,60	0
56	MG	2a	1612	1/1	0.86	0.11	-	58,58,58,58	0
56	MG	2A	3584	1/1	0.92	0.32	-	50,50,50,50	0
56	MG	2A	3160	1/1	0.80	0.17	-	47,47,47,47	0
56	MG	1a	3193	1/1	0.92	0.16	-	47,47,47,47	0
56	MG	1A	3103	1/1	0.95	0.25	-	33,33,33,33	0
56	MG	1A	3169	1/1	0.87	0.13	-	53,53,53,53	0
56	MG	2A	3036	1/1	0.91	0.19	-	48,48,48,48	0
56	MG	11	103	1/1	0.95	0.08	-	31,31,31,31	0
56	MG	2a	1798	1/1	0.92	0.14	-	60,60,60,60	0
56	MG	2A	3726	1/1	0.95	0.17	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3636	1/1	0.99	0.16	-	21,21,21,21	0
56	MG	1A	3788	1/1	0.95	0.10	-	25,25,25,25	0
56	MG	2A	3566	1/1	0.95	0.13	-	56,56,56,56	0
56	MG	2a	1735	1/1	0.97	0.18	-	50,50,50,50	0
56	MG	2B	3002	1/1	0.75	0.38	-	62,62,62,62	0
56	MG	2a	1712	1/1	0.96	0.09	-	63,63,63,63	0
56	MG	2A	3623	1/1	0.94	0.27	-	46,46,46,46	0
56	MG	1a	3182	1/1	0.96	0.15	-	45,45,45,45	0
56	MG	2a	1824	1/1	0.89	0.18	-	63,63,63,63	0
56	MG	2A	3249	1/1	0.88	0.14	-	54,54,54,54	0
56	MG	1A	3715	1/1	0.93	0.10	-	23,23,23,23	0
56	MG	2A	3590	1/1	0.92	0.15	-	50,50,50,50	0
56	MG	1A	3742	1/1	0.97	0.14	-	28,28,28,28	0
56	MG	1A	3392	1/1	0.97	0.09	-	38,38,38,38	0
56	MG	1A	4058	1/1	0.95	0.24	-	69,69,69,69	0
56	MG	1x	103	1/1	0.85	0.27	-	54,54,54,54	0
56	MG	2A	3184	1/1	0.93	0.30	-	52,52,52,52	0
56	MG	2A	3025	1/1	0.92	0.26	-	54,54,54,54	0
56	MG	1A	3155	1/1	0.97	0.14	-	29,29,29,29	0
56	MG	1A	3850	1/1	0.97	0.40	-	43,43,43,43	0
56	MG	1A	3859	1/1	0.90	0.12	-	61,61,61,61	0
56	MG	2A	3636	1/1	0.75	0.18	-	55,55,55,55	0
56	MG	1A	3963	1/1	0.96	0.08	-	33,33,33,33	0
56	MG	2A	3427	1/1	0.95	0.08	-	46,46,46,46	0
56	MG	1A	3213	1/1	0.96	0.18	-	36,36,36,36	0
56	MG	1D	313	1/1	0.77	0.21	-	52,52,52,52	0
56	MG	2A	3638	1/1	0.83	0.16	-	66,66,66,66	0
56	MG	1A	3371	1/1	0.91	0.23	-	39,39,39,39	0
56	MG	2A	3664	1/1	0.96	0.21	-	41,41,41,41	0
56	MG	1A	3511	1/1	0.92	0.22	-	20,20,20,20	0
56	MG	1A	3402	1/1	0.96	0.08	-	28,28,28,28	0
56	MG	1A	3247	1/1	0.95	0.23	-	27,27,27,27	0
56	MG	1A	4027	1/1	0.88	0.30	-	61,61,61,61	0
56	MG	1A	3250	1/1	0.98	0.31	-	20,20,20,20	0
56	MG	2B	3020	1/1	0.97	0.14	-	54,54,54,54	0
56	MG	1A	3090	1/1	0.97	0.24	-	18,18,18,18	0
56	MG	1a	3107	1/1	0.97	0.20	-	39,39,39,39	0
56	MG	2a	1831	1/1	0.95	0.09	-	53,53,53,53	0
56	MG	1A	3813	1/1	0.96	0.16	-	29,29,29,29	0
56	MG	2A	3673	1/1	0.97	0.17	-	47,47,47,47	0
56	MG	2A	3021	1/1	0.87	0.32	-	58,58,58,58	0
56	MG	2A	3547	1/1	0.89	0.25	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3339	1/1	0.89	0.26	-	48,48,48,48	0
56	MG	1A	3882	1/1	0.78	0.14	-	62,62,62,62	0
56	MG	2A	3181	1/1	0.94	0.16	-	35,35,35,35	0
56	MG	1a	3088	1/1	0.93	0.06	-	57,57,57,57	0
56	MG	1a	3084	1/1	0.85	0.28	-	54,54,54,54	0
56	MG	2A	3130	1/1	0.94	0.20	-	51,51,51,51	0
56	MG	1A	3873	1/1	0.97	0.17	-	42,42,42,42	0
56	MG	2A	3499	1/1	0.95	0.14	-	41,41,41,41	0
56	MG	1A	3241	1/1	0.91	0.14	-	58,58,58,58	0
56	MG	1A	3078	1/1	0.95	0.39	-	26,26,26,26	0
56	MG	2A	3489	1/1	0.91	0.14	-	48,48,48,48	0
56	MG	2A	3242	1/1	0.94	0.13	-	47,47,47,47	0
56	MG	1O	206	1/1	0.93	0.36	-	60,60,60,60	0
56	MG	2A	3399	1/1	0.96	0.20	-	57,57,57,57	0
56	MG	1A	3920	1/1	0.75	0.21	-	39,39,39,39	0
56	MG	1A	3442	1/1	0.97	0.22	-	36,36,36,36	0
56	MG	2A	3171	1/1	0.99	0.05	-	51,51,51,51	0
56	MG	1A	3024	1/1	0.92	0.12	-	32,32,32,32	0
56	MG	2A	3722	1/1	0.93	0.14	-	47,47,47,47	0
56	MG	25	503	1/1	0.90	0.41	-	40,40,40,40	0
56	MG	2A	3019	1/1	0.99	0.19	-	50,50,50,50	0
56	MG	2A	3231	1/1	0.86	0.31	-	49,49,49,49	0
56	MG	2A	3656	1/1	0.90	0.08	-	68,68,68,68	0
56	MG	2A	3544	1/1	0.86	0.24	-	30,30,30,30	0
56	MG	2A	3537	1/1	0.96	0.15	-	46,46,46,46	0
56	MG	1A	3132	1/1	0.97	0.15	-	37,37,37,37	0
56	MG	1a	3156	1/1	0.91	0.16	-	50,50,50,50	0
56	MG	1A	3943	1/1	0.94	0.16	-	38,38,38,38	0
56	MG	2v	3004	1/1	0.88	0.19	-	73,73,73,73	0
56	MG	1A	3106	1/1	0.87	0.54	-	24,24,24,24	0
56	MG	2A	3261	1/1	0.81	0.20	-	50,50,50,50	0
56	MG	1A	3301	1/1	0.93	0.12	-	39,39,39,39	0
56	MG	1A	3194	1/1	0.92	0.21	-	35,35,35,35	0
56	MG	2a	1739	1/1	0.93	0.14	-	57,57,57,57	0
56	MG	2A	3725	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	1A	3769	1/1	0.92	0.16	-	15,15,15,15	0
56	MG	2A	3217	1/1	0.91	0.28	-	51,51,51,51	0
56	MG	1A	3602	1/1	0.98	0.09	-	48,48,48,48	0
56	MG	1A	3327	1/1	0.95	0.18	-	10,10,10,10	0
56	MG	1a	3148	1/1	0.94	0.09	-	55,55,55,55	0
56	MG	2A	3700	1/1	0.96	0.06	-	61,61,61,61	0
56	MG	2A	3016	1/1	0.97	0.20	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3600	1/1	0.95	0.26	-	50,50,50,50	0
56	MG	2A	3152	1/1	0.94	0.18	-	45,45,45,45	0
56	MG	1A	3004	1/1	0.94	0.16	-	21,21,21,21	0
56	MG	2A	3557	1/1	0.98	0.24	-	27,27,27,27	0
56	MG	2a	1785	1/1	0.94	0.15	-	63,63,63,63	0
56	MG	2A	3532	1/1	0.90	0.18	-	62,62,62,62	0
56	MG	1A	3415	1/1	0.89	0.46	-	38,38,38,38	0
56	MG	1A	3013	1/1	0.98	0.10	-	14,14,14,14	0
56	MG	2A	3205	1/1	0.84	0.15	-	55,55,55,55	0
56	MG	1A	3610	1/1	0.97	0.17	-	45,45,45,45	0
56	MG	1A	3997	1/1	0.89	0.20	-	45,45,45,45	0
56	MG	2A	3413	1/1	0.95	0.16	-	55,55,55,55	0
56	MG	1A	3348	1/1	0.98	0.13	-	44,44,44,44	0
56	MG	1A	3500	1/1	0.91	0.16	-	20,20,20,20	0
56	MG	2A	3695	1/1	0.89	0.25	-	58,58,58,58	0
56	MG	1A	3367	1/1	0.82	0.22	-	46,46,46,46	0
56	MG	2a	1781	1/1	0.96	0.10	-	67,67,67,67	0
56	MG	1A	3467	1/1	0.95	0.27	-	49,49,49,49	0
56	MG	2A	3004	1/1	0.94	0.14	-	37,37,37,37	0
56	MG	1A	3790	1/1	0.94	0.37	-	27,27,27,27	0
56	MG	2a	1648	1/1	0.83	0.23	-	63,63,63,63	0
56	MG	11	101	1/1	0.97	0.12	-	28,28,28,28	0
56	MG	2A	3111	1/1	0.90	0.21	-	36,36,36,36	0
56	MG	2A	3753	1/1	0.89	0.55	-	52,52,52,52	0
56	MG	1A	3066	1/1	0.96	0.06	-	22,22,22,22	0
56	MG	17	102	1/1	0.93	0.30	-	31,31,31,31	0
56	MG	2A	3286	1/1	0.87	0.17	-	46,46,46,46	0
56	MG	1a	3072	1/1	0.93	0.09	-	54,54,54,54	0
56	MG	1A	3834	1/1	0.76	0.16	-	51,51,51,51	0
56	MG	2a	1667	1/1	0.82	0.16	-	61,61,61,61	0
56	MG	1A	3727	1/1	0.98	0.05	-	42,42,42,42	0
56	MG	1A	3185	1/1	0.95	0.15	-	26,26,26,26	0
57	K	2A	3327	1/1	0.97	0.11	-	29,29,29,29	0
56	MG	2A	3274	1/1	0.94	0.29	-	45,45,45,45	0
56	MG	2A	3534	1/1	0.98	0.11	-	53,53,53,53	0
56	MG	1a	3162	1/1	0.81	0.22	-	62,62,62,62	0
56	MG	1B	209	1/1	0.90	0.09	-	53,53,53,53	0
56	MG	1a	3166	1/1	0.93	0.08	-	49,49,49,49	0
56	MG	1A	3494	1/1	0.95	0.11	-	35,35,35,35	0
56	MG	1A	3064	1/1	0.98	0.11	-	12,12,12,12	0
56	MG	2A	3400	1/1	0.90	0.25	-	72,72,72,72	0
56	MG	1A	3044	1/1	0.78	0.16	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3170	1/1	0.90	0.08	-	63,63,63,63	0
56	MG	2a	1821	1/1	0.91	0.18	-	66,66,66,66	0
56	MG	2a	1737	1/1	0.93	0.04	-	57,57,57,57	0
56	MG	1A	3453	1/1	0.90	0.38	-	41,41,41,41	0
56	MG	2A	3154	1/1	0.94	0.32	-	51,51,51,51	0
56	MG	1A	3246	1/1	0.84	0.13	-	37,37,37,37	0
57	K	1A	4028	1/1	0.96	0.10	-	40,40,40,40	0
56	MG	2A	3626	1/1	0.94	0.16	-	46,46,46,46	0
56	MG	1A	3529	1/1	0.98	0.09	-	34,34,34,34	0
56	MG	1A	3445	1/1	0.92	0.10	-	47,47,47,47	0
56	MG	2a	1810	1/1	0.96	0.15	-	81,81,81,81	0
56	MG	1A	3612	1/1	0.99	0.09	-	24,24,24,24	0
56	MG	2A	3708	1/1	0.91	0.17	-	63,63,63,63	0
56	MG	1B	213	1/1	0.80	0.85	-	55,55,55,55	0
56	MG	1A	3688	1/1	0.96	0.20	-	21,21,21,21	0
56	MG	2A	3149	1/1	0.97	0.27	-	57,57,57,57	0
56	MG	1A	3352	1/1	0.94	0.18	-	36,36,36,36	0
56	MG	2A	3422	1/1	0.96	0.19	-	49,49,49,49	0
56	MG	1a	3195	1/1	0.96	0.06	-	45,45,45,45	0
56	MG	1R	205	1/1	0.94	0.10	-	34,34,34,34	0
56	MG	2A	3714	1/1	0.85	0.14	-	50,50,50,50	0
56	MG	1A	3958	1/1	0.91	0.17	-	32,32,32,32	0
56	MG	1A	3149	1/1	0.96	0.60	-	28,28,28,28	0
56	MG	1A	3332	1/1	0.90	0.11	-	34,34,34,34	0
56	MG	1a	3020	1/1	0.88	0.09	-	47,47,47,47	0
56	MG	1A	3713	1/1	0.89	0.11	-	48,48,48,48	0
56	MG	1A	3860	1/1	0.93	0.27	-	54,54,54,54	0
56	MG	1A	3025	1/1	0.92	0.27	-	42,42,42,42	0
56	MG	2A	3747	1/1	0.82	0.17	-	35,35,35,35	0
56	MG	1A	3953	1/1	0.93	0.15	-	40,40,40,40	0
56	MG	1A	3270	1/1	0.97	0.09	-	31,31,31,31	0
56	MG	1A	3584	1/1	0.89	0.14	-	44,44,44,44	0
56	MG	2A	3491	1/1	0.77	0.13	-	75,75,75,75	0
56	MG	2A	3319	1/1	0.95	0.13	-	62,62,62,62	0
56	MG	2A	3266	1/1	0.78	0.11	-	54,54,54,54	0
56	MG	2A	3256	1/1	0.79	0.18	-	46,46,46,46	0
56	MG	1B	233	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	1A	3295	1/1	0.96	0.11	-	38,38,38,38	0
56	MG	2B	3001	1/1	0.89	0.56	-	75,75,75,75	0
56	MG	2A	3505	1/1	0.99	0.08	-	42,42,42,42	0
56	MG	2a	1669	1/1	0.93	0.23	-	56,56,56,56	0
56	MG	1A	3190	1/1	0.92	0.08	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3797	1/1	0.90	0.19	-	33,33,33,33	0
56	MG	2A	3490	1/1	0.92	0.07	-	72,72,72,72	0
56	MG	1a	3173	1/1	0.96	0.18	-	39,39,39,39	0
56	MG	1A	3983	1/1	0.98	0.16	-	32,32,32,32	0
56	MG	18	103	1/1	0.95	0.23	-	41,41,41,41	0
56	MG	1A	3833	1/1	0.95	0.14	-	58,58,58,58	0
56	MG	2A	3679	1/1	0.95	0.15	-	49,49,49,49	0
56	MG	1a	3163	1/1	0.95	0.17	-	47,47,47,47	0
56	MG	1A	3883	1/1	0.78	0.21	-	59,59,59,59	0
56	MG	2A	3117	1/1	0.88	0.21	-	61,61,61,61	0
56	MG	2A	3613	1/1	0.90	0.11	-	61,61,61,61	0
56	MG	2A	3581	1/1	0.91	0.12	-	28,28,28,28	0
56	MG	1a	3159	1/1	0.93	0.14	-	41,41,41,41	0
56	MG	2A	3170	1/1	0.90	0.21	-	44,44,44,44	0
56	MG	1A	3131	1/1	0.98	0.12	-	35,35,35,35	0
56	MG	1A	3292	1/1	0.92	0.17	-	43,43,43,43	0
56	MG	2A	3663	1/1	0.93	0.17	-	47,47,47,47	0
56	MG	1A	3400	1/1	0.96	0.17	-	33,33,33,33	0
56	MG	2A	3263	1/1	0.83	0.19	-	54,54,54,54	0
56	MG	1A	3358	1/1	0.97	0.13	-	44,44,44,44	0
56	MG	2a	1617	1/1	0.80	0.15	-	73,73,73,73	0
56	MG	1A	3290	1/1	0.96	0.10	-	46,46,46,46	0
56	MG	2A	3705	1/1	0.90	0.19	-	64,64,64,64	0
56	MG	1A	3509	1/1	0.97	0.18	-	31,31,31,31	0
56	MG	2A	3531	1/1	0.94	0.11	-	60,60,60,60	0
56	MG	1A	3654	1/1	0.98	0.14	-	37,37,37,37	0
56	MG	1A	3127	1/1	0.90	0.15	-	37,37,37,37	0
56	MG	2A	3310	1/1	0.96	0.11	-	58,58,58,58	0
56	MG	2A	3690	1/1	0.88	0.14	-	58,58,58,58	0
56	MG	1A	3172	1/1	0.93	0.40	-	44,44,44,44	0
56	MG	1A	3003	1/1	0.98	0.20	-	19,19,19,19	0
56	MG	2A	3674	1/1	0.98	0.22	-	23,23,23,23	0
56	MG	1A	3001	1/1	0.98	0.09	-	32,32,32,32	0
56	MG	1a	3149	1/1	0.81	0.55	-	76,76,76,76	0
56	MG	2A	3441	1/1	0.88	0.14	-	62,62,62,62	0
56	MG	2A	3416	1/1	0.93	0.13	-	40,40,40,40	0
56	MG	1B	235	1/1	0.95	0.17	-	55,55,55,55	0
56	MG	2a	1639	1/1	0.88	0.21	-	60,60,60,60	0
56	MG	1A	3722	1/1	0.95	0.14	-	29,29,29,29	0
56	MG	2A	3616	1/1	0.85	0.12	-	51,51,51,51	0
56	MG	2A	3517	1/1	0.93	0.09	-	51,51,51,51	0
56	MG	1a	3087	1/1	0.95	0.18	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	1760	1/1	0.93	0.24	-	60,60,60,60	0
56	MG	1A	3695	1/1	0.94	0.21	-	50,50,50,50	0
56	MG	1A	3306	1/1	0.89	0.15	-	43,43,43,43	0
56	MG	1A	3407	1/1	0.94	0.08	-	45,45,45,45	0
56	MG	1a	3052	1/1	0.93	0.10	-	58,58,58,58	0
56	MG	2A	3741	1/1	0.99	0.11	-	39,39,39,39	0
56	MG	2a	1817	1/1	0.95	0.16	-	51,51,51,51	0
56	MG	2A	3224	1/1	0.93	0.16	-	54,54,54,54	0
56	MG	1A	3684	1/1	0.96	0.12	-	44,44,44,44	0
56	MG	2A	3347	1/1	0.90	0.10	-	53,53,53,53	0
56	MG	1f	3001	1/1	0.97	0.11	-	31,31,31,31	0
56	MG	1A	3731	1/1	0.95	0.22	-	16,16,16,16	0
56	MG	2F	301	1/1	0.92	0.16	-	35,35,35,35	0
56	MG	25	504	1/1	0.89	0.36	-	67,67,67,67	0
56	MG	1A	3235	1/1	0.96	0.14	-	22,22,22,22	0
56	MG	2A	3529	1/1	0.90	0.24	-	59,59,59,59	0
56	MG	1A	4015	1/1	0.89	0.19	-	55,55,55,55	0
56	MG	1A	3970	1/1	0.92	0.05	-	53,53,53,53	0
56	MG	2A	3386	1/1	0.91	0.24	-	43,43,43,43	0
56	MG	2A	3652	1/1	0.92	0.16	-	38,38,38,38	0
56	MG	2A	3450	1/1	0.99	0.14	-	37,37,37,37	0
56	MG	2a	1790	1/1	0.98	0.21	-	50,50,50,50	0
56	MG	1a	3047	1/1	0.90	0.28	-	46,46,46,46	0
56	MG	2a	1641	1/1	0.89	0.13	-	53,53,53,53	0
56	MG	1a	3128	1/1	0.93	0.09	-	50,50,50,50	0
56	MG	2A	3549	1/1	0.95	0.15	-	43,43,43,43	0
56	MG	1A	3789	1/1	0.82	0.21	-	44,44,44,44	0
56	MG	1A	3283	1/1	0.88	0.33	-	28,28,28,28	0
56	MG	1A	3487	1/1	0.94	0.13	-	34,34,34,34	0
56	MG	1A	4021	1/1	0.90	0.14	-	47,47,47,47	0
56	MG	1A	4010	1/1	0.97	0.13	-	23,23,23,23	0
56	MG	2y	3007	1/1	0.88	0.14	-	81,81,81,81	0
56	MG	2A	3601	1/1	0.94	0.09	-	53,53,53,53	0
56	MG	2A	3291	1/1	0.98	0.12	-	55,55,55,55	0
56	MG	17	104	1/1	0.98	0.08	-	27,27,27,27	0
56	MG	1A	3159	1/1	0.94	0.34	-	36,36,36,36	0
56	MG	1a	3117	1/1	0.93	0.09	-	27,27,27,27	0
56	MG	1A	3732	1/1	0.98	0.07	-	45,45,45,45	0
56	MG	1A	3518	1/1	0.97	0.11	-	41,41,41,41	0
56	MG	2A	3480	1/1	0.90	0.21	-	47,47,47,47	0
56	MG	2A	3561	1/1	0.97	0.18	-	56,56,56,56	0
56	MG	1A	3901	1/1	0.95	0.30	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	1815	1/1	0.85	0.16	-	61,61,61,61	0
56	MG	2a	1765	1/1	0.91	0.14	-	64,64,64,64	0
56	MG	15	103	1/1	0.96	0.46	-	25,25,25,25	0
56	MG	2A	3079	1/1	0.93	0.09	-	57,57,57,57	0
56	MG	1A	3587	1/1	0.98	0.10	-	12,12,12,12	0
56	MG	2A	3088	1/1	0.79	0.15	-	40,40,40,40	0
56	MG	2A	3614	1/1	0.93	0.12	-	51,51,51,51	0
56	MG	2a	1753	1/1	0.96	0.15	-	45,45,45,45	0
56	MG	2A	3556	1/1	0.98	0.20	-	46,46,46,46	0
56	MG	2a	1823	1/1	0.95	0.09	-	53,53,53,53	0
56	MG	1w	103	1/1	0.85	0.36	-	68,68,68,68	0
56	MG	1a	3165	1/1	0.87	0.09	-	60,60,60,60	0
56	MG	1A	4048	1/1	0.82	0.64	-	31,31,31,31	0
56	MG	2A	3735	1/1	0.90	0.35	-	45,45,45,45	0
56	MG	2A	3199	1/1	0.93	0.12	-	53,53,53,53	0
56	MG	1l	202	1/1	0.81	0.16	-	85,85,85,85	0
56	MG	1A	3752	1/1	0.96	0.44	-	36,36,36,36	0
56	MG	2A	3675	1/1	0.94	0.09	-	62,62,62,62	0
56	MG	2A	3574	1/1	0.95	0.07	-	46,46,46,46	0
56	MG	1A	3073	1/1	0.94	0.48	-	42,42,42,42	0
56	MG	2r	3001	1/1	0.97	0.15	-	56,56,56,56	0
56	MG	27	101	1/1	0.81	0.34	-	44,44,44,44	0
56	MG	1A	3690	1/1	0.97	0.10	-	42,42,42,42	0
56	MG	1A	3992	1/1	0.94	0.18	-	49,49,49,49	0
56	MG	2A	3671	1/1	0.97	0.18	-	29,29,29,29	0
56	MG	1A	3324	1/1	0.95	0.13	-	33,33,33,33	0
56	MG	1A	3319	1/1	0.76	0.23	-	53,53,53,53	0
56	MG	1A	3896	1/1	0.98	0.20	-	42,42,42,42	0
56	MG	1A	3916	1/1	0.88	0.13	-	54,54,54,54	0
56	MG	1B	230	1/1	0.94	0.31	-	42,42,42,42	0
56	MG	1A	3899	1/1	0.95	0.09	-	35,35,35,35	0
56	MG	2A	3106	1/1	0.93	0.08	-	50,50,50,50	0
56	MG	2A	3257	1/1	0.83	0.18	-	57,57,57,57	0
56	MG	1A	3452	1/1	0.97	0.28	-	30,30,30,30	0
56	MG	1A	3387	1/1	0.93	0.20	-	37,37,37,37	0
56	MG	2A	3696	1/1	0.96	0.09	-	39,39,39,39	0
56	MG	2B	3018	1/1	0.89	0.85	-	80,80,80,80	0
56	MG	1x	114	1/1	0.89	0.14	-	67,67,67,67	0
56	MG	2A	3743	1/1	0.92	0.19	-	51,51,51,51	0
56	MG	1A	3936	1/1	0.96	0.08	-	49,49,49,49	0
56	MG	1A	3275	1/1	0.97	0.14	-	25,25,25,25	0
56	MG	1A	3738	1/1	0.98	0.09	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3415	1/1	0.98	0.18	-	47,47,47,47	0
56	MG	2A	3423	1/1	0.97	0.12	-	22,22,22,22	0
56	MG	1A	3956	1/1	0.95	0.07	-	67,67,67,67	0
56	MG	2A	3370	1/1	1.00	0.17	-	44,44,44,44	0
56	MG	1a	3157	1/1	0.93	0.13	-	58,58,58,58	0
56	MG	2A	3496	1/1	0.96	0.11	-	37,37,37,37	0
56	MG	2A	3192	1/1	0.96	0.29	-	54,54,54,54	0
56	MG	2Z	8001	1/1	0.86	0.25	-	73,73,73,73	0
56	MG	1A	3307	1/1	0.94	0.10	-	49,49,49,49	0
56	MG	10	103	1/1	0.93	0.15	-	54,54,54,54	0
56	MG	2E	307	1/1	0.87	0.20	-	60,60,60,60	0
56	MG	2A	3128	1/1	0.81	0.26	-	35,35,35,35	0
56	MG	2A	3644	1/1	0.92	0.14	-	57,57,57,57	0
56	MG	2a	1729	1/1	0.92	0.10	-	61,61,61,61	0
56	MG	1F	308	1/1	0.90	0.11	-	42,42,42,42	0
56	MG	2x	103	1/1	0.80	0.22	-	63,63,63,63	0
56	MG	1A	3718	1/1	0.86	0.20	-	39,39,39,39	0
56	MG	1a	3065	1/1	0.95	0.15	-	41,41,41,41	0
56	MG	1A	3972	1/1	0.98	0.15	-	49,49,49,49	0
56	MG	28	102	1/1	0.73	0.14	-	64,64,64,64	0
56	MG	2A	3082	1/1	0.87	0.18	-	69,69,69,69	0
56	MG	2A	3403	1/1	0.96	0.26	-	29,29,29,29	0
56	MG	1A	3613	1/1	0.95	0.10	-	30,30,30,30	0
56	MG	1A	3128	1/1	0.97	0.31	-	27,27,27,27	0
56	MG	1a	3197	1/1	0.94	0.10	-	39,39,39,39	0
56	MG	1B	201	1/1	0.95	0.10	-	49,49,49,49	0
56	MG	1A	3227	1/1	0.82	0.13	-	49,49,49,49	0
56	MG	2a	1724	1/1	0.86	0.11	-	73,73,73,73	0
56	MG	2A	3010	1/1	0.95	0.18	-	31,31,31,31	0
56	MG	1A	4012	1/1	0.87	0.27	-	47,47,47,47	0
56	MG	2A	3189	1/1	0.95	0.07	-	38,38,38,38	0
56	MG	1B	221	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	1a	3050	1/1	0.88	0.12	-	50,50,50,50	0
56	MG	1a	3100	1/1	0.91	0.11	-	61,61,61,61	0
56	MG	1A	3840	1/1	0.97	0.17	-	32,32,32,32	0
56	MG	2A	3528	1/1	0.94	0.08	-	58,58,58,58	0
56	MG	2A	3035	1/1	0.90	0.15	-	52,52,52,52	0
56	MG	2A	3065	1/1	0.83	0.16	-	52,52,52,52	0
56	MG	1a	3171	1/1	0.96	0.07	-	55,55,55,55	0
56	MG	2a	1718	1/1	0.95	0.14	-	55,55,55,55	0
56	MG	1A	4053	1/1	0.87	0.45	-	42,42,42,42	0
56	MG	2a	1811	1/1	0.93	0.14	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	1711	1/1	0.91	0.24	-	67,67,67,67	0
56	MG	1a	3060	1/1	0.94	0.07	-	50,50,50,50	0
56	MG	2A	3262	1/1	0.93	0.15	-	44,44,44,44	0
56	MG	2a	1608	1/1	0.94	0.14	-	47,47,47,47	0
56	MG	2A	3147	1/1	0.92	0.28	-	50,50,50,50	0
56	MG	1A	3607	1/1	0.98	0.13	-	19,19,19,19	0
56	MG	2A	3364	1/1	0.97	0.08	-	45,45,45,45	0
56	MG	1A	3594	1/1	0.96	0.32	-	46,46,46,46	0
56	MG	1A	3540	1/1	0.96	0.11	-	46,46,46,46	0
56	MG	2a	1698	1/1	0.98	0.07	-	60,60,60,60	0
56	MG	2a	1666	1/1	0.87	0.10	-	51,51,51,51	0
56	MG	2A	3206	1/1	0.92	0.33	-	42,42,42,42	0
56	MG	1A	3664	1/1	0.95	0.19	-	43,43,43,43	0
56	MG	1A	3536	1/1	0.94	0.08	-	25,25,25,25	0
56	MG	1a	3073	1/1	0.88	0.12	-	59,59,59,59	0
56	MG	1n	502	1/1	0.92	0.13	-	51,51,51,51	0
56	MG	1A	3924	1/1	0.91	0.11	-	34,34,34,34	0
56	MG	1A	3384	1/1	0.94	0.08	-	38,38,38,38	0
56	MG	1A	3855	1/1	0.98	0.04	-	49,49,49,49	0
56	MG	1A	4006	1/1	0.90	0.20	-	41,41,41,41	0
56	MG	1A	3608	1/1	0.91	0.20	-	54,54,54,54	0
56	MG	1A	3176	1/1	0.98	0.44	-	25,25,25,25	0
56	MG	1A	3556	1/1	0.97	0.15	-	20,20,20,20	0
56	MG	2A	3352	1/1	0.96	0.10	-	50,50,50,50	0
56	MG	2a	1756	1/1	0.94	0.13	-	43,43,43,43	0
56	MG	2a	1728	1/1	0.94	0.09	-	46,46,46,46	0
56	MG	1w	111	1/1	0.83	0.13	-	69,69,69,69	0
56	MG	1A	3164	1/1	0.97	0.17	-	12,12,12,12	0
56	MG	1A	3678	1/1	0.97	0.16	-	22,22,22,22	0
56	MG	2A	3350	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	2A	3158	1/1	0.83	0.32	-	49,49,49,49	0
56	MG	1A	3370	1/1	0.91	0.22	-	37,37,37,37	0
56	MG	2A	3287	1/1	0.94	0.25	-	47,47,47,47	0
56	MG	1A	3841	1/1	0.94	0.14	-	33,33,33,33	0
56	MG	1A	3842	1/1	0.97	0.07	-	34,34,34,34	0
56	MG	1A	3589	1/1	0.97	0.12	-	23,23,23,23	0
56	MG	1X	103	1/1	0.94	0.25	-	29,29,29,29	0
56	MG	18	102	1/1	0.94	0.12	-	29,29,29,29	0
56	MG	1A	3987	1/1	0.99	0.23	-	36,36,36,36	0
56	MG	2A	3373	1/1	0.94	0.17	-	25,25,25,25	0
56	MG	1A	3914	1/1	0.82	0.21	-	54,54,54,54	0
56	MG	2A	3723	1/1	0.81	0.31	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3425	1/1	0.88	0.14	-	34,34,34,34	0
56	MG	1A	3219	1/1	0.92	0.29	-	19,19,19,19	0
56	MG	1A	4002	1/1	0.95	0.15	-	32,32,32,32	0
56	MG	2A	3269	1/1	0.92	0.14	-	36,36,36,36	0
56	MG	1A	3274	1/1	0.94	0.22	-	40,40,40,40	0
56	MG	1a	3187	1/1	0.95	0.06	-	43,43,43,43	0
56	MG	1a	3097	1/1	0.95	0.08	-	62,62,62,62	0
56	MG	1A	3933	1/1	0.93	0.14	-	54,54,54,54	0
56	MG	1m	201	1/1	0.94	0.10	-	57,57,57,57	0
56	MG	1A	3754	1/1	0.98	0.22	-	22,22,22,22	0
56	MG	1y	104	1/1	0.95	0.13	-	44,44,44,44	0
56	MG	2A	3572	1/1	0.91	0.22	-	66,66,66,66	0
56	MG	1A	3050	1/1	0.92	0.27	-	45,45,45,45	0
56	MG	1A	3889	1/1	0.92	0.14	-	39,39,39,39	0
56	MG	1A	3504	1/1	0.94	0.08	-	48,48,48,48	0
56	MG	2A	3273	1/1	0.91	0.35	-	57,57,57,57	0
56	MG	1a	3174	1/1	0.91	0.08	-	51,51,51,51	0
56	MG	2A	3279	1/1	0.92	0.10	-	64,64,64,64	0
56	MG	1a	3070	1/1	0.98	0.05	-	30,30,30,30	0
56	MG	2a	1659	1/1	0.97	0.12	-	47,47,47,47	0
56	MG	1A	3475	1/1	0.95	0.27	-	28,28,28,28	0
56	MG	1A	3502	1/1	0.97	0.33	-	20,20,20,20	0
56	MG	2a	1603	1/1	0.81	0.17	-	73,73,73,73	0
56	MG	2A	3433	1/1	0.88	0.19	-	60,60,60,60	0
56	MG	2A	3522	1/1	0.97	0.08	-	49,49,49,49	0
56	MG	2A	3594	1/1	0.98	0.12	-	54,54,54,54	0
56	MG	1A	3514	1/1	0.94	0.17	-	21,21,21,21	0
56	MG	1A	3399	1/1	0.96	0.14	-	42,42,42,42	0
56	MG	2R	3003	1/1	0.96	0.15	-	48,48,48,48	0
56	MG	1A	3829	1/1	0.97	0.17	-	43,43,43,43	0
56	MG	1A	3951	1/1	0.86	0.12	-	62,62,62,62	0
56	MG	1B	236	1/1	0.75	0.30	-	65,65,65,65	0
56	MG	2A	3691	1/1	0.92	0.11	-	68,68,68,68	0
56	MG	1A	4033	1/1	0.96	0.60	-	25,25,25,25	0
56	MG	1A	3391	1/1	0.93	0.16	-	46,46,46,46	0
56	MG	1A	3071	1/1	0.92	0.14	-	31,31,31,31	0
56	MG	2A	3069	1/1	0.95	0.23	-	39,39,39,39	0
56	MG	2A	3414	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	1a	3190	1/1	0.91	0.16	-	51,51,51,51	0
56	MG	1A	3545	1/1	0.95	0.15	-	25,25,25,25	0
56	MG	1A	3691	1/1	0.86	0.30	-	55,55,55,55	0
56	MG	1A	3878	1/1	0.92	0.11	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3982	1/1	0.94	0.23	-	46,46,46,46	0
56	MG	1A	3499	1/1	0.98	0.13	-	23,23,23,23	0
56	MG	2A	3145	1/1	0.93	0.15	-	48,48,48,48	0
56	MG	1a	3168	1/1	0.85	0.15	-	63,63,63,63	0
56	MG	1A	4022	1/1	0.95	0.14	-	46,46,46,46	0
56	MG	2A	3440	1/1	0.98	0.13	-	51,51,51,51	0
56	MG	2a	1660	1/1	0.97	0.13	-	59,59,59,59	0
56	MG	2X	3001	1/1	0.94	0.14	-	46,46,46,46	0
56	MG	2A	3042	1/1	0.91	0.15	-	54,54,54,54	0
56	MG	1A	3548	1/1	0.89	0.14	-	52,52,52,52	0
56	MG	1A	3618	1/1	0.91	0.16	-	55,55,55,55	0
56	MG	2A	3083	1/1	0.86	0.10	-	53,53,53,53	0
56	MG	1a	3046	1/1	0.84	0.09	-	54,54,54,54	0
56	MG	2A	3236	1/1	0.97	0.21	-	49,49,49,49	0
56	MG	1P	203	1/1	0.89	0.42	-	33,33,33,33	0
56	MG	2a	1738	1/1	0.81	0.12	-	71,71,71,71	0
56	MG	2A	3228	1/1	0.89	0.39	-	38,38,38,38	0
56	MG	2O	8001	1/1	0.85	0.20	-	56,56,56,56	0
56	MG	1A	3900	1/1	0.90	0.13	-	44,44,44,44	0
56	MG	1A	3682	1/1	0.95	0.09	-	55,55,55,55	0
56	MG	1A	3200	1/1	0.91	0.15	-	44,44,44,44	0
56	MG	2A	3393	1/1	0.98	0.19	-	44,44,44,44	0
56	MG	1A	3305	1/1	0.75	0.20	-	51,51,51,51	0
56	MG	1A	3931	1/1	0.84	0.22	-	47,47,47,47	0
56	MG	1A	3669	1/1	0.99	0.11	-	35,35,35,35	0
56	MG	1A	3573	1/1	0.98	0.09	-	24,24,24,24	0
56	MG	1w	105	1/1	0.95	0.12	-	64,64,64,64	0
56	MG	1l	104	1/1	0.90	0.10	-	59,59,59,59	0
56	MG	2A	3229	1/1	0.82	0.24	-	34,34,34,34	0
56	MG	2A	3241	1/1	0.88	0.18	-	55,55,55,55	0
56	MG	2y	3004	1/1	0.96	0.17	-	36,36,36,36	0
56	MG	1A	3947	1/1	0.89	0.14	-	49,49,49,49	0
56	MG	1A	3409	1/1	0.91	0.15	-	54,54,54,54	0
56	MG	2A	3208	1/1	0.86	0.23	-	49,49,49,49	0
56	MG	1A	3335	1/1	0.94	0.44	-	33,33,33,33	0
56	MG	1A	3694	1/1	0.95	0.08	-	51,51,51,51	0
56	MG	2A	3034	1/1	0.96	0.16	-	56,56,56,56	0
56	MG	1A	3069	1/1	0.98	0.26	-	27,27,27,27	0
56	MG	1A	3666	1/1	0.92	0.05	-	50,50,50,50	0
56	MG	1A	3838	1/1	0.92	0.11	-	53,53,53,53	0
56	MG	1A	4019	1/1	0.97	0.27	-	26,26,26,26	0
56	MG	2A	3434	1/1	0.90	0.16	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3264	1/1	0.95	0.41	-	47,47,47,47	0
56	MG	1A	3635	1/1	0.99	0.22	-	25,25,25,25	0
56	MG	1A	3563	1/1	0.91	0.08	-	35,35,35,35	0
56	MG	1A	3146	1/1	0.95	0.56	-	23,23,23,23	0
56	MG	1A	3272	1/1	0.94	0.12	-	34,34,34,34	0
56	MG	2w	104	1/1	0.95	0.15	-	83,83,83,83	0
56	MG	1A	3437	1/1	0.96	0.11	-	52,52,52,52	0
56	MG	1A	3436	1/1	0.73	0.16	-	62,62,62,62	0
56	MG	1A	3084	1/1	0.98	0.10	-	35,35,35,35	0
56	MG	2D	302	1/1	0.93	0.16	-	39,39,39,39	0
56	MG	1A	3045	1/1	0.97	0.17	-	13,13,13,13	0
56	MG	2a	1705	1/1	0.80	0.13	-	54,54,54,54	0
56	MG	2A	3608	1/1	0.97	0.13	-	48,48,48,48	0
56	MG	2A	3156	1/1	0.87	0.18	-	42,42,42,42	0
56	MG	1A	3460	1/1	0.92	0.10	-	41,41,41,41	0
56	MG	1a	3208	1/1	0.98	0.11	-	42,42,42,42	0
56	MG	1a	3135	1/1	0.94	0.12	-	52,52,52,52	0
56	MG	1A	3421	1/1	0.95	0.46	-	37,37,37,37	0
56	MG	1A	3372	1/1	0.95	0.13	-	35,35,35,35	0
56	MG	2A	3268	1/1	0.96	0.10	-	47,47,47,47	0
56	MG	2A	3225	1/1	0.83	0.18	-	53,53,53,53	0
56	MG	1A	3165	1/1	0.97	0.07	-	31,31,31,31	0
56	MG	2A	3314	1/1	0.94	0.37	-	40,40,40,40	0
56	MG	1A	4051	1/1	0.96	0.22	-	13,13,13,13	0
56	MG	1A	3906	1/1	0.97	0.17	-	60,60,60,60	0
56	MG	1W	3003	1/1	0.95	0.10	-	33,33,33,33	0
56	MG	1A	3826	1/1	0.94	0.16	-	27,27,27,27	0
56	MG	1A	3406	1/1	0.96	0.28	-	48,48,48,48	0
56	MG	2A	3092	1/1	0.90	0.17	-	38,38,38,38	0
56	MG	1A	3823	1/1	0.89	0.13	-	50,50,50,50	0
56	MG	1A	3434	1/1	0.93	0.17	-	47,47,47,47	0
56	MG	1A	3586	1/1	0.89	0.19	-	17,17,17,17	0
56	MG	2a	1604	1/1	0.84	0.16	-	48,48,48,48	0
56	MG	2a	1769	1/1	0.63	0.13	-	75,75,75,75	0
56	MG	2A	3388	1/1	0.97	0.18	-	25,25,25,25	0
56	MG	1A	3466	1/1	0.93	0.17	-	39,39,39,39	0
56	MG	2A	3309	1/1	0.93	0.15	-	52,52,52,52	0
56	MG	1A	3168	1/1	0.94	0.19	-	43,43,43,43	0
56	MG	2A	3043	1/1	0.98	0.10	-	40,40,40,40	0
56	MG	1A	3251	1/1	0.92	0.42	-	25,25,25,25	0
56	MG	2a	1748	1/1	0.89	0.14	-	60,60,60,60	0
56	MG	2A	3185	1/1	0.85	0.19	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3098	1/1	0.93	0.51	-	36,36,36,36	0
56	MG	1A	3617	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	1A	3080	1/1	0.94	0.24	-	41,41,41,41	0
56	MG	1A	3551	1/1	0.95	0.15	-	17,17,17,17	0
56	MG	2y	3002	1/1	0.98	0.14	-	51,51,51,51	0
56	MG	2a	1674	1/1	0.90	0.20	-	55,55,55,55	0
56	MG	1a	3021	1/1	0.95	0.15	-	40,40,40,40	0
56	MG	1A	3844	1/1	0.81	0.08	-	23,23,23,23	0
56	MG	2a	1784	1/1	0.85	0.11	-	66,66,66,66	0
57	K	1A	3486	1/1	0.98	0.07	-	19,19,19,19	0
56	MG	1a	3017	1/1	0.88	0.20	-	57,57,57,57	0
56	MG	2A	3589	1/1	0.97	0.26	-	45,45,45,45	0
56	MG	2A	3107	1/1	0.95	0.17	-	27,27,27,27	0
56	MG	1A	3828	1/1	0.89	0.19	-	62,62,62,62	0
56	MG	2a	1637	1/1	0.71	0.13	-	52,52,52,52	0
56	MG	1a	3063	1/1	0.92	0.16	-	53,53,53,53	0
56	MG	2A	3153	1/1	0.93	0.16	-	49,49,49,49	0
56	MG	2A	3330	1/1	0.98	0.20	-	42,42,42,42	0
56	MG	2A	3546	1/1	0.87	0.15	-	45,45,45,45	0
56	MG	1A	3242	1/1	0.63	0.26	-	59,59,59,59	0
56	MG	2A	3683	1/1	0.93	0.28	-	42,42,42,42	0
56	MG	2A	3312	1/1	0.84	0.17	-	57,57,57,57	0
56	MG	1A	3405	1/1	0.93	0.60	-	46,46,46,46	0
56	MG	2a	1664	1/1	0.91	0.17	-	56,56,56,56	0
56	MG	1a	3132	1/1	0.95	0.08	-	34,34,34,34	0
56	MG	2A	3190	1/1	0.96	0.13	-	44,44,44,44	0
56	MG	2y	3006	1/1	0.34	0.13	-	88,88,88,88	0
56	MG	1a	3006	1/1	0.82	0.20	-	59,59,59,59	0
56	MG	2A	3078	1/1	0.97	0.10	-	54,54,54,54	0
56	MG	2A	3751	1/1	0.97	0.78	-	44,44,44,44	0
56	MG	1w	102	1/1	0.90	0.10	-	76,76,76,76	0
56	MG	2A	3332	1/1	0.72	0.24	-	56,56,56,56	0
56	MG	1A	3606	1/1	0.94	0.18	-	61,61,61,61	0
56	MG	1A	3851	1/1	0.93	0.18	-	44,44,44,44	0
56	MG	2A	3369	1/1	0.98	0.14	-	53,53,53,53	0
56	MG	2A	3121	1/1	0.94	0.15	-	31,31,31,31	0
56	MG	1A	3262	1/1	0.91	0.11	-	33,33,33,33	0
56	MG	2A	3001	1/1	0.89	0.09	-	44,44,44,44	0
56	MG	1A	3675	1/1	0.96	0.15	-	66,66,66,66	0
56	MG	2a	1679	1/1	0.98	0.15	-	44,44,44,44	0
56	MG	1A	3472	1/1	0.92	0.14	-	41,41,41,41	0
56	MG	2a	1645	1/1	0.87	0.61	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3401	1/1	0.95	0.10	-	38,38,38,38	0
56	MG	2A	3100	1/1	0.95	0.15	-	59,59,59,59	0
56	MG	1B	210	1/1	0.84	0.15	-	50,50,50,50	0
56	MG	1A	3236	1/1	0.97	0.21	-	35,35,35,35	0
56	MG	1A	3730	1/1	0.88	0.35	-	42,42,42,42	0
56	MG	1A	3917	1/1	0.98	0.14	-	31,31,31,31	0
56	MG	1A	3809	1/1	0.98	0.09	-	30,30,30,30	0
56	MG	2a	1646	1/1	0.91	0.13	-	71,71,71,71	0
56	MG	2A	3617	1/1	0.96	0.24	-	43,43,43,43	0
56	MG	2A	3379	1/1	0.98	0.09	-	41,41,41,41	0
56	MG	2a	1742	1/1	0.90	0.08	-	70,70,70,70	0
56	MG	2A	3376	1/1	0.88	0.17	-	45,45,45,45	0
56	MG	1A	3825	1/1	0.92	0.48	-	43,43,43,43	0
56	MG	1A	3424	1/1	0.93	0.56	-	32,32,32,32	0
56	MG	2a	1762	1/1	0.90	0.13	-	52,52,52,52	0
56	MG	1A	3231	1/1	0.92	0.27	-	45,45,45,45	0
56	MG	1A	3839	1/1	0.90	0.14	-	34,34,34,34	0
56	MG	2a	1629	1/1	0.95	0.18	-	73,73,73,73	0
56	MG	1A	3621	1/1	0.86	0.17	-	44,44,44,44	0
56	MG	1A	3314	1/1	0.90	0.34	-	42,42,42,42	0
56	MG	1A	3877	1/1	0.96	0.20	-	28,28,28,28	0
56	MG	1A	3632	1/1	0.98	0.29	-	27,27,27,27	0
56	MG	2A	3064	1/1	0.94	0.45	-	44,44,44,44	0
56	MG	2A	3506	1/1	0.93	0.13	-	48,48,48,48	0
56	MG	2a	1755	1/1	0.86	0.06	-	70,70,70,70	0
56	MG	2A	3119	1/1	0.97	0.12	-	41,41,41,41	0
56	MG	1a	3134	1/1	0.92	0.23	-	47,47,47,47	0
56	MG	1A	3359	1/1	0.96	0.12	-	32,32,32,32	0
56	MG	1A	3144	1/1	0.93	0.13	-	37,37,37,37	0
56	MG	1R	202	1/1	0.96	0.08	-	30,30,30,30	0
56	MG	2a	1610	1/1	0.89	0.81	-	63,63,63,63	0
56	MG	2A	3432	1/1	0.94	0.30	-	56,56,56,56	0
56	MG	1a	3116	1/1	0.93	0.09	-	35,35,35,35	0
56	MG	1a	3090	1/1	0.94	0.07	-	41,41,41,41	0
56	MG	2a	1601	1/1	0.98	0.24	-	46,46,46,46	0
56	MG	1a	3083	1/1	0.85	0.19	-	54,54,54,54	0
56	MG	1A	3530	1/1	0.97	0.22	-	25,25,25,25	0
56	MG	1a	3034	1/1	0.98	0.14	-	44,44,44,44	0
56	MG	1G	3005	1/1	0.92	0.08	-	52,52,52,52	0
56	MG	2a	1727	1/1	0.94	0.12	-	87,87,87,87	0
56	MG	1A	3230	1/1	0.82	0.19	-	44,44,44,44	0
56	MG	1A	3482	1/1	0.92	0.28	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	1813	1/1	0.98	0.06	-	54,54,54,54	0
56	MG	1A	3143	1/1	0.85	0.47	-	37,37,37,37	0
56	MG	1A	3376	1/1	0.92	0.23	-	31,31,31,31	0
56	MG	1A	3991	1/1	0.92	0.14	-	66,66,66,66	0
56	MG	2A	3454	1/1	0.95	0.14	-	52,52,52,52	0
56	MG	2A	3665	1/1	0.94	0.11	-	36,36,36,36	0
56	MG	2A	3055	1/1	0.94	0.16	-	44,44,44,44	0
56	MG	1A	3893	1/1	0.97	0.27	-	27,27,27,27	0
56	MG	1A	3591	1/1	0.96	0.16	-	30,30,30,30	0
56	MG	1A	4003	1/1	0.95	0.10	-	32,32,32,32	0
56	MG	1A	3650	1/1	0.95	0.17	-	34,34,34,34	0
56	MG	1A	3345	1/1	0.91	0.17	-	24,24,24,24	0
56	MG	1w	110	1/1	0.72	0.19	-	75,75,75,75	0
56	MG	1A	3996	1/1	0.97	0.17	-	49,49,49,49	0
56	MG	2a	1791	1/1	0.85	0.12	-	69,69,69,69	0
56	MG	1A	3750	1/1	0.95	0.08	-	31,31,31,31	0
56	MG	2A	3141	1/1	0.95	0.13	-	40,40,40,40	0
56	MG	1A	3473	1/1	0.89	0.18	-	42,42,42,42	0
56	MG	1a	3172	1/1	0.96	0.07	-	46,46,46,46	0
56	MG	2B	3005	1/1	0.96	0.10	-	55,55,55,55	0
56	MG	1A	3780	1/1	0.87	0.23	-	44,44,44,44	0
56	MG	1A	3469	1/1	0.91	0.19	-	43,43,43,43	0
56	MG	1x	107	1/1	0.97	0.20	-	46,46,46,46	0
56	MG	1A	3396	1/1	0.94	0.28	-	44,44,44,44	0
56	MG	2a	1614	1/1	0.92	0.09	-	52,52,52,52	0
56	MG	1A	3303	1/1	0.94	0.16	-	44,44,44,44	0
56	MG	1A	3308	1/1	0.83	0.16	-	49,49,49,49	0
56	MG	2q	202	1/1	0.89	0.24	-	59,59,59,59	0
56	MG	2A	3555	1/1	0.98	0.15	-	38,38,38,38	0
56	MG	2A	3610	1/1	0.95	0.12	-	47,47,47,47	0
56	MG	1A	3902	1/1	0.93	0.10	-	55,55,55,55	0
56	MG	2A	3230	1/1	0.95	0.10	-	41,41,41,41	0
56	MG	2a	1652	1/1	0.94	0.09	-	55,55,55,55	0
56	MG	1A	3835	1/1	0.93	0.17	-	42,42,42,42	0
56	MG	2a	1779	1/1	0.95	0.11	-	60,60,60,60	0
56	MG	1A	3470	1/1	0.98	0.17	-	33,33,33,33	0
56	MG	2A	3085	1/1	0.97	0.18	-	48,48,48,48	0
56	MG	2a	1750	1/1	0.68	0.09	-	60,60,60,60	0
56	MG	1A	3208	1/1	0.94	0.14	-	29,29,29,29	0
56	MG	1A	3115	1/1	0.99	0.20	-	39,39,39,39	0
56	MG	1A	3006	1/1	0.96	0.10	-	33,33,33,33	0
56	MG	10	101	1/1	0.97	0.06	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	3175	1/1	0.81	0.09	-	58,58,58,58	0
56	MG	1A	3225	1/1	0.97	0.12	-	40,40,40,40	0
56	MG	1A	3461	1/1	0.88	0.18	-	55,55,55,55	0
56	MG	2B	3015	1/1	0.95	0.14	-	51,51,51,51	0
56	MG	1A	3531	1/1	0.90	0.13	-	19,19,19,19	0
56	MG	1A	3311	1/1	0.94	0.19	-	37,37,37,37	0
56	MG	20	3001	1/1	0.88	0.15	-	52,52,52,52	0
56	MG	2A	3586	1/1	0.78	0.12	-	44,44,44,44	0
56	MG	1A	4065	1/1	0.88	0.12	-	36,36,36,36	0
56	MG	1A	3748	1/1	0.97	0.10	-	38,38,38,38	0
56	MG	1A	3089	1/1	0.94	0.15	-	21,21,21,21	0
56	MG	1A	3249	1/1	0.91	0.35	-	31,31,31,31	0
56	MG	16	104	1/1	0.96	0.14	-	38,38,38,38	0
56	MG	1a	3203	1/1	0.92	0.20	-	69,69,69,69	0
56	MG	1A	3046	1/1	0.96	0.26	-	50,50,50,50	0
56	MG	2B	3003	1/1	0.85	0.20	-	60,60,60,60	0
56	MG	2A	3513	1/1	0.95	0.11	-	52,52,52,52	0
56	MG	2A	3131	1/1	0.87	0.13	-	40,40,40,40	0
56	MG	2A	3331	1/1	0.93	0.16	-	47,47,47,47	0
56	MG	1E	309	1/1	0.97	0.16	-	15,15,15,15	0
56	MG	2a	1688	1/1	0.93	0.13	-	53,53,53,53	0
56	MG	1A	3368	1/1	0.88	0.39	-	39,39,39,39	0
56	MG	1A	3862	1/1	0.96	0.11	-	52,52,52,52	0
56	MG	2E	303	1/1	0.90	0.18	-	50,50,50,50	0
56	MG	1A	3281	1/1	0.94	0.35	-	29,29,29,29	0
56	MG	2A	3218	1/1	0.90	0.15	-	39,39,39,39	0
56	MG	2A	3543	1/1	0.94	0.13	-	45,45,45,45	0
56	MG	1A	3498	1/1	0.96	0.15	-	39,39,39,39	0
56	MG	2A	3293	1/1	0.85	0.28	-	46,46,46,46	0
56	MG	2A	3609	1/1	0.92	0.22	-	36,36,36,36	0
56	MG	2A	3177	1/1	0.90	0.31	-	36,36,36,36	0
56	MG	1A	3289	1/1	0.98	0.15	-	41,41,41,41	0
56	MG	2A	3559	1/1	0.94	0.16	-	61,61,61,61	0
56	MG	2A	3084	1/1	0.96	0.18	-	29,29,29,29	0
56	MG	2A	3429	1/1	0.90	0.22	-	59,59,59,59	0
56	MG	1A	3773	1/1	0.96	0.10	-	15,15,15,15	0
56	MG	1A	3156	1/1	0.98	0.26	-	27,27,27,27	0
56	MG	1A	3894	1/1	0.99	0.09	-	37,37,37,37	0
56	MG	1I	3001	1/1	0.93	0.31	-	64,64,64,64	0
56	MG	2B	3004	1/1	0.95	0.15	-	60,60,60,60	0
56	MG	1a	3008	1/1	0.94	0.18	-	51,51,51,51	0
56	MG	2A	3033	1/1	0.80	0.18	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3416	1/1	0.86	0.15	-	17,17,17,17	0
56	MG	1G	3002	1/1	0.97	0.15	-	39,39,39,39	0
56	MG	2A	3596	1/1	0.95	0.15	-	32,32,32,32	0
56	MG	1a	3058	1/1	0.97	0.07	-	58,58,58,58	0
56	MG	2A	3627	1/1	0.97	0.14	-	50,50,50,50	0
56	MG	28	101	1/1	0.81	0.20	-	49,49,49,49	0
56	MG	1A	3870	1/1	0.97	0.09	-	55,55,55,55	0
56	MG	2A	3497	1/1	0.85	0.18	-	63,63,63,63	0
56	MG	2A	3618	1/1	0.86	0.18	-	71,71,71,71	0
56	MG	1Z	3004	1/1	0.97	0.14	-	41,41,41,41	0
56	MG	1A	3468	1/1	0.94	0.08	-	37,37,37,37	0
56	MG	2A	3136	1/1	0.90	0.15	-	36,36,36,36	0
56	MG	1A	3980	1/1	0.87	0.21	-	62,62,62,62	0
56	MG	1A	3206	1/1	0.96	0.13	-	30,30,30,30	0
56	MG	1A	3254	1/1	0.99	0.29	-	11,11,11,11	0
56	MG	2A	3580	1/1	0.94	0.15	-	39,39,39,39	0
56	MG	2A	3756	1/1	0.93	0.14	-	33,33,33,33	0
56	MG	1A	3334	1/1	0.98	0.21	-	22,22,22,22	0
56	MG	1B	229	1/1	0.89	0.09	-	57,57,57,57	0
56	MG	2A	3672	1/1	0.84	0.26	-	46,46,46,46	0
56	MG	2A	3430	1/1	0.95	0.11	-	53,53,53,53	0
56	MG	1x	104	1/1	0.95	0.21	-	54,54,54,54	0
56	MG	2A	3248	1/1	0.91	0.18	-	44,44,44,44	0
56	MG	2W	201	1/1	0.94	0.16	-	50,50,50,50	0
56	MG	2A	3339	1/1	0.94	0.10	-	58,58,58,58	0
56	MG	2A	3203	1/1	0.96	0.12	-	53,53,53,53	0
56	MG	1A	3256	1/1	0.94	0.10	-	33,33,33,33	0
56	MG	2A	3162	1/1	0.96	0.08	-	54,54,54,54	0
56	MG	1A	3010	1/1	0.96	0.21	-	33,33,33,33	0
56	MG	1A	3072	1/1	0.92	0.31	-	27,27,27,27	0
56	MG	2A	3477	1/1	0.92	0.13	-	64,64,64,64	0
56	MG	2w	105	1/1	0.88	0.14	-	72,72,72,72	0
56	MG	1A	3316	1/1	0.85	0.42	-	34,34,34,34	0
56	MG	1A	3346	1/1	0.87	0.18	-	43,43,43,43	0
56	MG	2A	3113	1/1	0.94	0.21	-	48,48,48,48	0
56	MG	2A	3641	1/1	0.98	0.14	-	50,50,50,50	0
56	MG	1A	3746	1/1	0.90	0.31	-	49,49,49,49	0
56	MG	1A	3522	1/1	0.99	0.15	-	30,30,30,30	0
56	MG	1a	3111	1/1	0.92	0.17	-	45,45,45,45	0
56	MG	1A	3744	1/1	0.92	0.12	-	41,41,41,41	0
56	MG	1A	3077	1/1	0.97	0.44	-	21,21,21,21	0
56	MG	2A	3374	1/1	0.70	0.15	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1B	226	1/1	0.89	0.14	-	67,67,67,67	0
56	MG	2A	3282	1/1	0.94	0.10	-	51,51,51,51	0
56	MG	2A	3349	1/1	0.87	0.17	-	30,30,30,30	0
56	MG	2a	1643	1/1	0.93	0.21	-	61,61,61,61	0
56	MG	2a	1797	1/1	0.88	0.13	-	70,70,70,70	0
56	MG	1A	3817	1/1	0.93	0.13	-	20,20,20,20	0
56	MG	1A	3655	1/1	0.97	0.14	-	11,11,11,11	0
56	MG	2A	3175	1/1	0.78	0.36	-	43,43,43,43	0
56	MG	1a	3125	1/1	0.96	0.12	-	42,42,42,42	0
56	MG	1A	3183	1/1	0.92	0.09	-	39,39,39,39	0
56	MG	2A	3017	1/1	0.91	0.11	-	59,59,59,59	0
56	MG	1A	3603	1/1	0.93	0.16	-	43,43,43,43	0
56	MG	1A	3643	1/1	0.97	0.40	-	29,29,29,29	0
56	MG	1A	3129	1/1	0.95	0.36	-	27,27,27,27	0
56	MG	1A	3658	1/1	0.90	0.10	-	46,46,46,46	0
56	MG	2A	3328	1/1	0.98	0.23	-	45,45,45,45	0
56	MG	1S	3003	1/1	0.86	0.21	-	61,61,61,61	0
56	MG	2A	3553	1/1	0.96	0.09	-	57,57,57,57	0
56	MG	1a	3003	1/1	0.89	0.20	-	56,56,56,56	0
56	MG	1a	3192	1/1	0.89	0.09	-	62,62,62,62	0
56	MG	2A	3667	1/1	0.94	0.11	-	63,63,63,63	0
56	MG	2U	206	1/1	0.96	0.13	-	42,42,42,42	0
56	MG	2A	3588	1/1	0.92	0.09	-	52,52,52,52	0
56	MG	1a	3138	1/1	0.95	0.16	-	66,66,66,66	0
56	MG	1A	3616	1/1	0.95	0.16	-	58,58,58,58	0
56	MG	1a	3001	1/1	0.91	0.14	-	52,52,52,52	0
56	MG	2a	1826	1/1	0.89	0.12	-	55,55,55,55	0
56	MG	2A	3465	1/1	0.99	0.28	-	42,42,42,42	0
56	MG	1A	3350	1/1	0.84	0.31	-	44,44,44,44	0
56	MG	2A	3068	1/1	0.97	0.04	-	35,35,35,35	0
56	MG	2A	3103	1/1	0.90	0.48	-	46,46,46,46	0
56	MG	1A	3074	1/1	0.98	0.32	-	24,24,24,24	0
56	MG	1A	3433	1/1	0.97	0.08	-	50,50,50,50	0
56	MG	17	105	1/1	0.91	0.15	-	34,34,34,34	0
56	MG	1A	3979	1/1	0.95	0.10	-	56,56,56,56	0
56	MG	2a	1607	1/1	0.81	0.18	-	73,73,73,73	0
56	MG	2A	3684	1/1	0.92	0.08	-	68,68,68,68	0
56	MG	2A	3605	1/1	0.94	0.13	-	42,42,42,42	0
56	MG	1A	3218	1/1	0.92	0.07	-	23,23,23,23	0
56	MG	2A	3550	1/1	0.77	0.15	-	58,58,58,58	0
56	MG	1A	3673	1/1	0.94	0.13	-	54,54,54,54	0
56	MG	2a	1743	1/1	0.92	0.10	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	12	3001	1/1	0.92	0.15	-	44,44,44,44	0
56	MG	2A	3101	1/1	0.94	0.17	-	30,30,30,30	0
56	MG	2A	3602	1/1	0.96	0.19	-	62,62,62,62	0
56	MG	2A	3052	1/1	0.88	0.14	-	36,36,36,36	0
56	MG	1A	3959	1/1	0.79	0.12	-	76,76,76,76	0
56	MG	1A	3105	1/1	0.93	0.24	-	30,30,30,30	0
56	MG	2A	3342	1/1	0.96	0.18	-	49,49,49,49	0
56	MG	1A	3158	1/1	0.94	0.17	-	31,31,31,31	0
56	MG	1A	3820	1/1	0.98	0.12	-	35,35,35,35	0
56	MG	1A	3578	1/1	0.97	0.14	-	23,23,23,23	0
56	MG	2A	3585	1/1	0.95	0.20	-	34,34,34,34	0
56	MG	2A	3365	1/1	0.95	0.11	-	38,38,38,38	0
56	MG	2A	3198	1/1	0.77	0.17	-	43,43,43,43	0
56	MG	1A	3142	1/1	0.98	0.12	-	17,17,17,17	0
56	MG	1A	3016	1/1	0.95	0.20	-	40,40,40,40	0
56	MG	2a	1828	1/1	0.95	0.23	-	64,64,64,64	0
56	MG	2A	3402	1/1	0.92	0.15	-	49,49,49,49	0
56	MG	1A	3619	1/1	0.90	0.16	-	36,36,36,36	0
56	MG	1F	307	1/1	0.90	0.12	-	40,40,40,40	0
56	MG	1A	3344	1/1	0.93	0.36	-	31,31,31,31	0
56	MG	1A	3417	1/1	0.91	0.16	-	42,42,42,42	0
56	MG	2A	3173	1/1	0.95	0.14	-	45,45,45,45	0
56	MG	2w	102	1/1	0.86	0.14	-	78,78,78,78	0
56	MG	1O	205	1/1	0.89	0.37	-	57,57,57,57	0
56	MG	1A	3703	1/1	0.95	0.22	-	24,24,24,24	0
56	MG	1A	3491	1/1	0.91	0.19	-	17,17,17,17	0
56	MG	2A	3045	1/1	0.88	0.14	-	55,55,55,55	0
56	MG	1A	3777	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	2A	3132	1/1	0.95	0.07	-	58,58,58,58	0
56	MG	1A	3035	1/1	0.98	0.20	-	24,24,24,24	0
56	MG	2A	3446	1/1	0.92	0.14	-	32,32,32,32	0
56	MG	1A	3926	1/1	0.95	0.16	-	18,18,18,18	0
56	MG	1A	3404	1/1	0.97	0.26	-	28,28,28,28	0
56	MG	1A	3923	1/1	0.92	0.23	-	39,39,39,39	0
56	MG	2l	204	1/1	0.90	0.12	-	43,43,43,43	0
56	MG	1A	3981	1/1	0.94	0.12	-	30,30,30,30	0
56	MG	2v	3003	1/1	0.79	0.20	-	66,66,66,66	0
56	MG	1A	3083	1/1	0.85	0.26	-	55,55,55,55	0
56	MG	1A	3865	1/1	0.98	0.18	-	18,18,18,18	0
56	MG	1O	207	1/1	0.89	0.10	-	54,54,54,54	0
56	MG	1A	3623	1/1	0.97	0.15	-	41,41,41,41	0
56	MG	2a	1716	1/1	0.94	0.18	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1y	101	1/1	0.96	0.10	-	35,35,35,35	0
56	MG	2a	1717	1/1	0.96	0.08	-	66,66,66,66	0
56	MG	2A	3642	1/1	0.96	0.12	-	43,43,43,43	0
56	MG	1B	202	1/1	0.94	0.24	-	42,42,42,42	0
56	MG	27	102	1/1	0.90	0.17	-	47,47,47,47	0
56	MG	1A	3167	1/1	0.96	0.22	-	47,47,47,47	0
56	MG	1A	3209	1/1	0.52	0.29	-	61,61,61,61	0
56	MG	1A	3929	1/1	0.96	0.33	-	35,35,35,35	0
56	MG	2a	1806	1/1	0.78	0.11	-	76,76,76,76	0
56	MG	1A	3390	1/1	0.98	0.10	-	43,43,43,43	0
56	MG	1B	227	1/1	0.96	0.12	-	36,36,36,36	0
56	MG	2A	3067	1/1	0.89	0.22	-	46,46,46,46	0
56	MG	1A	3854	1/1	0.98	0.12	-	46,46,46,46	0
56	MG	2E	304	1/1	0.97	0.20	-	49,49,49,49	0
56	MG	2A	3600	1/1	0.95	0.11	-	56,56,56,56	0
56	MG	1x	109	1/1	0.85	0.11	-	57,57,57,57	0
56	MG	1a	3209	1/1	0.94	0.20	-	60,60,60,60	0
56	MG	1A	3471	1/1	0.95	0.23	-	45,45,45,45	0
56	MG	1A	3998	1/1	0.90	0.13	-	55,55,55,55	0
56	MG	1A	3945	1/1	0.92	0.34	-	30,30,30,30	0
56	MG	2a	1730	1/1	0.93	0.11	-	65,65,65,65	0
56	MG	2A	3341	1/1	0.96	0.17	-	39,39,39,39	0
56	MG	1A	3210	1/1	0.94	0.42	-	25,25,25,25	0
56	MG	1A	3065	1/1	0.84	0.39	-	62,62,62,62	0
56	MG	2A	3363	1/1	0.98	0.15	-	43,43,43,43	0
56	MG	2A	3621	1/1	0.84	0.09	-	49,49,49,49	0
56	MG	2A	3071	1/1	0.88	0.08	-	60,60,60,60	0
56	MG	1A	3277	1/1	0.88	0.13	-	37,37,37,37	0
56	MG	1A	3907	1/1	0.74	0.21	-	39,39,39,39	0
56	MG	1A	3408	1/1	0.81	0.30	-	40,40,40,40	0
56	MG	1A	3026	1/1	0.94	0.13	-	30,30,30,30	0
56	MG	1B	218	1/1	0.93	0.19	-	40,40,40,40	0
56	MG	1a	3121	1/1	0.97	0.15	-	54,54,54,54	0
56	MG	1A	3449	1/1	0.94	0.19	-	52,52,52,52	0
56	MG	1A	3126	1/1	0.96	0.48	-	21,21,21,21	0
56	MG	2A	3214	1/1	0.95	0.08	-	49,49,49,49	0
56	MG	1A	3093	1/1	0.93	0.09	-	31,31,31,31	0
56	MG	1A	3995	1/1	0.98	0.10	-	32,32,32,32	0
56	MG	1a	3018	1/1	0.83	0.30	-	55,55,55,55	0
56	MG	1A	3886	1/1	0.96	0.10	-	24,24,24,24	0
56	MG	2A	3097	1/1	0.90	0.14	-	42,42,42,42	0
56	MG	1a	3080	1/1	0.96	0.23	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1E	307	1/1	0.93	0.55	-	50,50,50,50	0
56	MG	1A	3611	1/1	0.95	0.19	-	45,45,45,45	0
56	MG	2A	3681	1/1	0.91	0.23	-	49,49,49,49	0
56	MG	2A	3615	1/1	0.69	0.34	-	66,66,66,66	0
56	MG	1A	3952	1/1	0.97	0.14	-	50,50,50,50	0
56	MG	1y	102	1/1	0.90	0.09	-	83,83,83,83	0
56	MG	2A	3211	1/1	0.92	0.12	-	68,68,68,68	0
56	MG	2A	3062	1/1	0.97	0.14	-	47,47,47,47	0
56	MG	2A	3687	1/1	0.82	0.29	-	65,65,65,65	0
56	MG	1A	3223	1/1	0.98	0.20	-	34,34,34,34	0
56	MG	1A	3975	1/1	0.95	0.08	-	51,51,51,51	0
56	MG	2a	1622	1/1	0.94	0.40	-	39,39,39,39	0
56	MG	1A	3954	1/1	0.97	0.15	-	53,53,53,53	0
56	MG	1a	3140	1/1	0.96	0.10	-	38,38,38,38	0
56	MG	1A	3884	1/1	0.98	0.08	-	30,30,30,30	0
56	MG	2A	3634	1/1	0.97	0.21	-	48,48,48,48	0
56	MG	2A	3457	1/1	0.69	0.19	-	58,58,58,58	0
56	MG	2A	3253	1/1	0.93	0.54	-	68,68,68,68	0
56	MG	2A	3371	1/1	0.96	0.19	-	22,22,22,22	0
56	MG	2a	1719	1/1	0.89	0.14	-	55,55,55,55	0
56	MG	1A	3055	1/1	0.91	0.12	-	54,54,54,54	0
56	MG	1A	3575	1/1	0.95	0.12	-	11,11,11,11	0
56	MG	1A	3029	1/1	0.94	0.36	-	17,17,17,17	0
56	MG	1A	3211	1/1	0.98	0.23	-	30,30,30,30	0
56	MG	2A	3509	1/1	0.97	0.20	-	52,52,52,52	0
56	MG	1A	3150	1/1	0.99	0.25	-	27,27,27,27	0
56	MG	1A	3108	1/1	0.90	0.15	-	25,25,25,25	0
56	MG	2V	3002	1/1	0.94	0.13	-	56,56,56,56	0
56	MG	2A	3298	1/1	0.93	0.12	-	50,50,50,50	0
56	MG	1A	3961	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	2A	3569	1/1	0.96	0.03	-	63,63,63,63	0
56	MG	1A	3279	1/1	0.95	0.18	-	41,41,41,41	0
56	MG	2A	3137	1/1	0.96	0.08	-	50,50,50,50	0
56	MG	1A	3299	1/1	0.83	0.35	-	28,28,28,28	0
56	MG	1A	3202	1/1	0.93	0.29	-	27,27,27,27	0
56	MG	2a	1800	1/1	0.89	0.23	-	61,61,61,61	0
56	MG	1A	3639	1/1	0.99	0.09	-	39,39,39,39	0
56	MG	1a	3133	1/1	0.95	0.15	-	47,47,47,47	0
56	MG	1A	3088	1/1	0.98	0.20	-	32,32,32,32	0
56	MG	2a	1628	1/1	0.94	0.30	-	49,49,49,49	0
56	MG	1A	3380	1/1	0.91	0.29	-	33,33,33,33	0
56	MG	1A	3040	1/1	0.97	0.06	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2y	3001	1/1	0.76	0.23	-	64,64,64,64	0
56	MG	1A	3245	1/1	0.96	0.46	-	28,28,28,28	0
56	MG	2A	3235	1/1	0.97	0.18	-	40,40,40,40	0
56	MG	1a	3059	1/1	0.88	0.09	-	61,61,61,61	0
56	MG	2A	3216	1/1	0.93	0.16	-	51,51,51,51	0
56	MG	1A	3601	1/1	0.98	0.08	-	24,24,24,24	0
56	MG	1A	3512	1/1	0.92	0.08	-	40,40,40,40	0
56	MG	2a	1611	1/1	0.92	0.10	-	65,65,65,65	0
56	MG	1A	3161	1/1	0.99	0.24	-	20,20,20,20	0
56	MG	1A	3333	1/1	0.89	0.51	-	43,43,43,43	0
56	MG	2A	3335	1/1	0.98	0.11	-	49,49,49,49	0
56	MG	2A	3607	1/1	0.91	0.13	-	48,48,48,48	0
56	MG	1A	3240	1/1	0.96	0.16	-	38,38,38,38	0
56	MG	2A	3563	1/1	0.94	0.19	-	55,55,55,55	0
56	MG	15	105	1/1	0.97	0.46	-	33,33,33,33	0
56	MG	2A	3366	1/1	0.90	0.14	-	67,67,67,67	0
56	MG	1A	3969	1/1	0.95	0.14	-	41,41,41,41	0
56	MG	2A	3126	1/1	0.93	0.17	-	50,50,50,50	0
56	MG	2A	3438	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	1A	3927	1/1	0.97	0.29	-	37,37,37,37	0
56	MG	2A	3191	1/1	0.91	0.14	-	56,56,56,56	0
56	MG	1A	3699	1/1	0.98	0.08	-	25,25,25,25	0
56	MG	2A	3587	1/1	0.74	0.16	-	55,55,55,55	0
56	MG	1A	3723	1/1	0.97	0.10	-	34,34,34,34	0
56	MG	1l	203	1/1	0.92	0.17	-	50,50,50,50	0
56	MG	1A	3191	1/1	0.96	0.21	-	24,24,24,24	0
56	MG	2a	1827	1/1	0.97	0.19	-	58,58,58,58	0
56	MG	2A	3215	1/1	0.76	0.15	-	58,58,58,58	0
56	MG	1A	3683	1/1	0.95	0.28	-	41,41,41,41	0
56	MG	2l	201	1/1	0.93	0.23	-	51,51,51,51	0
56	MG	2a	1812	1/1	0.98	0.11	-	64,64,64,64	0
56	MG	2a	1691	1/1	0.91	0.36	-	56,56,56,56	0
56	MG	1a	3101	1/1	0.90	0.15	-	42,42,42,42	0
56	MG	2a	1733	1/1	0.96	0.12	-	56,56,56,56	0
56	MG	2R	3001	1/1	0.92	0.50	-	58,58,58,58	0
56	MG	1A	3028	1/1	0.96	0.34	-	20,20,20,20	0
56	MG	1A	3821	1/1	0.97	0.11	-	32,32,32,32	0
56	MG	1A	3766	1/1	0.75	0.23	-	36,36,36,36	0
56	MG	1A	3583	1/1	0.97	0.18	-	22,22,22,22	0
56	MG	2A	3418	1/1	0.96	0.06	-	46,46,46,46	0
56	MG	1A	3067	1/1	0.96	0.08	-	22,22,22,22	0
56	MG	2A	3633	1/1	0.97	0.13	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3032	1/1	0.98	0.12	-	41,41,41,41	0
56	MG	1A	3081	1/1	0.96	0.17	-	24,24,24,24	0
56	MG	2A	3410	1/1	0.92	0.31	-	61,61,61,61	0
56	MG	1A	3974	1/1	0.96	0.11	-	50,50,50,50	0
56	MG	1A	3477	1/1	0.96	0.23	-	32,32,32,32	0
56	MG	2a	1803	1/1	0.95	0.08	-	51,51,51,51	0
56	MG	1A	4007	1/1	0.94	0.66	-	39,39,39,39	0
56	MG	1A	3426	1/1	0.91	0.22	-	44,44,44,44	0
56	MG	1a	3124	1/1	0.94	0.13	-	54,54,54,54	0
56	MG	1A	3761	1/1	0.88	0.14	-	48,48,48,48	0
56	MG	2A	3167	1/1	0.90	0.14	-	42,42,42,42	0
56	MG	1a	3035	1/1	0.97	0.22	-	49,49,49,49	0
56	MG	1A	3198	1/1	0.87	0.12	-	43,43,43,43	0
56	MG	1A	3438	1/1	0.91	0.10	-	29,29,29,29	0
56	MG	2A	3240	1/1	0.95	0.12	-	51,51,51,51	0
56	MG	2A	3133	1/1	0.84	0.27	-	44,44,44,44	0
56	MG	1A	3614	1/1	0.97	0.15	-	15,15,15,15	0
56	MG	1A	3863	1/1	0.97	0.11	-	56,56,56,56	0
56	MG	2a	1799	1/1	0.80	0.12	-	59,59,59,59	0
56	MG	2A	3390	1/1	0.91	0.12	-	58,58,58,58	0
56	MG	2a	1613	1/1	0.83	0.15	-	60,60,60,60	0
56	MG	1A	3993	1/1	0.93	0.30	-	44,44,44,44	0
56	MG	1F	306	1/1	0.89	0.18	-	36,36,36,36	0
56	MG	1A	4011	1/1	0.94	0.21	-	37,37,37,37	0
56	MG	1A	3846	1/1	0.97	0.10	-	48,48,48,48	0
56	MG	2B	3021	1/1	0.97	0.18	-	59,59,59,59	0
56	MG	1A	3559	1/1	0.93	0.20	-	15,15,15,15	0
56	MG	1a	3207	1/1	0.87	0.09	-	41,41,41,41	0
56	MG	1A	3130	1/1	0.97	0.23	-	10,10,10,10	0
56	MG	2a	1649	1/1	0.98	0.22	-	41,41,41,41	0
56	MG	1A	3117	1/1	0.90	0.16	-	48,48,48,48	0
56	MG	1A	3397	1/1	0.91	0.15	-	51,51,51,51	0
56	MG	1A	3464	1/1	0.92	0.17	-	39,39,39,39	0
56	MG	1E	310	1/1	0.77	0.15	-	60,60,60,60	0
56	MG	2a	1630	1/1	0.93	0.23	-	57,57,57,57	0
56	MG	2A	3603	1/1	0.93	0.11	-	37,37,37,37	0
56	MG	1A	3542	1/1	0.95	0.16	-	44,44,44,44	0
56	MG	1A	3547	1/1	0.96	0.13	-	22,22,22,22	0
56	MG	2A	3487	1/1	0.95	0.20	-	62,62,62,62	0
56	MG	1Z	3002	1/1	0.81	0.15	-	46,46,46,46	0
56	MG	2A	3193	1/1	0.88	0.12	-	51,51,51,51	0
56	MG	2a	1801	1/1	0.98	0.09	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3048	1/1	0.89	0.12	-	57,57,57,57	0
56	MG	1B	208	1/1	0.78	0.23	-	59,59,59,59	0
56	MG	1X	102	1/1	0.92	0.21	-	35,35,35,35	0
56	MG	1A	3966	1/1	0.98	0.08	-	41,41,41,41	0
56	MG	1A	3443	1/1	0.94	0.15	-	32,32,32,32	0
56	MG	1A	4056	1/1	0.98	0.32	-	33,33,33,33	0
56	MG	1A	3354	1/1	0.95	0.08	-	39,39,39,39	0
56	MG	2F	304	1/1	0.85	0.10	-	64,64,64,64	0
56	MG	2A	3223	1/1	0.89	0.13	-	45,45,45,45	0
56	MG	1A	3489	1/1	0.96	0.22	-	30,30,30,30	0
56	MG	2a	1780	1/1	0.92	0.07	-	57,57,57,57	0
56	MG	1A	3721	1/1	0.90	0.26	-	53,53,53,53	0
56	MG	2A	3361	1/1	0.93	0.11	-	46,46,46,46	0
56	MG	2a	1702	1/1	0.93	0.14	-	56,56,56,56	0
56	MG	1A	3582	1/1	0.95	0.12	-	26,26,26,26	0
56	MG	2A	3061	1/1	0.94	0.17	-	30,30,30,30	0
56	MG	1A	3315	1/1	0.83	0.25	-	37,37,37,37	0
56	MG	2A	3252	1/1	0.90	0.16	-	38,38,38,38	0
56	MG	2A	3660	1/1	0.99	0.13	-	37,37,37,37	0
56	MG	2a	1602	1/1	0.86	0.21	-	54,54,54,54	0
56	MG	1A	3786	1/1	0.92	0.11	-	34,34,34,34	0
56	MG	2A	3210	1/1	0.92	0.35	-	58,58,58,58	0
56	MG	1A	3177	1/1	0.95	0.09	-	34,34,34,34	0
56	MG	1A	3378	1/1	0.94	0.40	-	27,27,27,27	0
56	MG	1A	3496	1/1	0.97	0.09	-	35,35,35,35	0
56	MG	1A	3331	1/1	0.91	0.21	-	39,39,39,39	0
56	MG	1a	3054	1/1	0.97	0.06	-	46,46,46,46	0
56	MG	1A	3076	1/1	0.94	0.25	-	26,26,26,26	0
56	MG	1A	3964	1/1	0.97	0.27	-	45,45,45,45	0
56	MG	1X	101	1/1	0.76	0.09	-	73,73,73,73	0
56	MG	10	102	1/1	0.95	0.23	-	25,25,25,25	0
56	MG	2A	3456	1/1	0.93	0.17	-	26,26,26,26	0
56	MG	1A	3329	1/1	0.93	0.10	-	41,41,41,41	0
56	MG	2A	3420	1/1	0.71	0.23	-	67,67,67,67	0
56	MG	2a	1644	1/1	0.78	0.20	-	62,62,62,62	0
56	MG	1A	3576	1/1	0.95	0.15	-	15,15,15,15	0
56	MG	2A	3643	1/1	0.95	0.08	-	43,43,43,43	0
56	MG	2A	3302	1/1	0.90	0.24	-	43,43,43,43	0
56	MG	1a	3056	1/1	0.95	0.11	-	50,50,50,50	0
56	MG	2A	3536	1/1	0.81	0.14	-	54,54,54,54	0
56	MG	1x	112	1/1	0.95	0.16	-	45,45,45,45	0
56	MG	2a	1763	1/1	0.96	0.10	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3707	1/1	0.94	0.15	-	47,47,47,47	0
56	MG	1x	111	1/1	0.92	0.15	-	64,64,64,64	0
56	MG	2A	3129	1/1	0.99	0.19	-	54,54,54,54	0
56	MG	1A	3294	1/1	0.88	0.21	-	40,40,40,40	0
56	MG	2A	3041	1/1	0.97	0.12	-	46,46,46,46	0
56	MG	2A	3303	1/1	0.96	0.17	-	35,35,35,35	0
56	MG	2y	3005	1/1	0.79	0.09	-	88,88,88,88	0
56	MG	1A	3410	1/1	0.94	0.12	-	45,45,45,45	0
56	MG	2A	3209	1/1	0.97	0.08	-	35,35,35,35	0
56	MG	1a	3198	1/1	0.96	0.25	-	46,46,46,46	0
56	MG	1a	3178	1/1	0.94	0.06	-	54,54,54,54	0
56	MG	1a	3151	1/1	0.95	0.20	-	62,62,62,62	0
56	MG	1A	3189	1/1	1.00	0.11	-	23,23,23,23	0
56	MG	1A	4042	1/1	0.94	0.13	-	40,40,40,40	0
56	MG	1A	3457	1/1	0.94	0.14	-	32,32,32,32	0
56	MG	2A	3194	1/1	0.89	0.21	-	51,51,51,51	0
56	MG	1A	3720	1/1	0.95	0.14	-	41,41,41,41	0
56	MG	2A	3384	1/1	0.91	0.10	-	27,27,27,27	0
56	MG	1A	3984	1/1	0.85	0.11	-	52,52,52,52	0
56	MG	2A	3542	1/1	0.86	0.13	-	36,36,36,36	0
56	MG	1A	3097	1/1	0.97	0.09	-	24,24,24,24	0
56	MG	1A	3755	1/1	0.97	0.20	-	21,21,21,21	0
56	MG	1A	3687	1/1	0.94	0.11	-	33,33,33,33	0
56	MG	2a	1746	1/1	0.95	0.08	-	67,67,67,67	0
56	MG	1A	3450	1/1	0.91	0.11	-	40,40,40,40	0
56	MG	1a	3033	1/1	0.95	0.07	-	57,57,57,57	0
56	MG	1A	3955	1/1	0.91	0.13	-	32,32,32,32	0
56	MG	1x	108	1/1	0.94	0.13	-	61,61,61,61	0
56	MG	2A	3290	1/1	0.95	0.19	-	39,39,39,39	0
56	MG	1A	3716	1/1	0.97	0.10	-	45,45,45,45	0
56	MG	1A	3112	1/1	0.95	0.16	-	40,40,40,40	0
56	MG	2v	3001	1/1	0.98	0.07	-	49,49,49,49	0
56	MG	1A	3802	1/1	0.74	0.22	-	54,54,54,54	0
56	MG	1A	3147	1/1	0.96	0.07	-	50,50,50,50	0
56	MG	1a	3048	1/1	0.90	0.47	-	43,43,43,43	0
56	MG	2A	3622	1/1	0.96	0.11	-	55,55,55,55	0
56	MG	1A	3533	1/1	0.95	0.10	-	47,47,47,47	0
56	MG	1a	3057	1/1	0.91	0.15	-	43,43,43,43	0
56	MG	1A	3880	1/1	0.98	0.26	-	23,23,23,23	0
56	MG	1A	3510	1/1	0.91	0.18	-	50,50,50,50	0
56	MG	1A	3733	1/1	0.96	0.07	-	55,55,55,55	0
56	MG	1A	3905	1/1	0.95	0.07	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	3106	1/1	0.97	0.13	-	52,52,52,52	0
56	MG	1w	104	1/1	0.96	0.07	-	36,36,36,36	0
56	MG	1A	3895	1/1	0.85	0.15	-	71,71,71,71	0
56	MG	2a	1616	1/1	0.81	0.11	-	67,67,67,67	0
56	MG	1A	3571	1/1	0.94	0.12	-	17,17,17,17	0
56	MG	2A	3134	1/1	0.92	0.08	-	51,51,51,51	0
56	MG	1A	3062	1/1	0.95	0.11	-	12,12,12,12	0
56	MG	1a	3027	1/1	0.89	0.24	-	58,58,58,58	0
56	MG	1A	3852	1/1	0.96	0.14	-	55,55,55,55	0
56	MG	1A	3285	1/1	0.95	0.14	-	34,34,34,34	0
56	MG	1a	3037	1/1	0.95	0.15	-	61,61,61,61	0
56	MG	2A	3028	1/1	0.96	0.17	-	42,42,42,42	0
56	MG	1l	102	1/1	0.88	0.21	-	72,72,72,72	0
56	MG	1a	3030	1/1	0.90	0.17	-	43,43,43,43	0
56	MG	1A	3212	1/1	0.96	0.18	-	50,50,50,50	0
56	MG	1A	3915	1/1	0.98	0.07	-	34,34,34,34	0
56	MG	2A	3142	1/1	0.94	0.13	-	46,46,46,46	0
56	MG	1A	3309	1/1	0.88	0.14	-	32,32,32,32	0
56	MG	1A	3909	1/1	0.91	0.20	-	46,46,46,46	0
56	MG	2A	3089	1/1	0.98	0.16	-	40,40,40,40	0
56	MG	2A	3040	1/1	0.95	0.34	-	39,39,39,39	0
56	MG	1W	3002	1/1	0.99	0.16	-	29,29,29,29	0
56	MG	1A	3726	1/1	0.95	0.06	-	35,35,35,35	0
56	MG	1A	3286	1/1	0.98	0.15	-	34,34,34,34	0
56	MG	1A	3824	1/1	0.97	0.13	-	33,33,33,33	0
56	MG	1a	3150	1/1	0.92	0.11	-	65,65,65,65	0
56	MG	2A	3114	1/1	0.99	0.28	-	29,29,29,29	0
56	MG	1a	3194	1/1	0.91	0.08	-	59,59,59,59	0
56	MG	1A	3843	1/1	0.88	0.10	-	66,66,66,66	0
56	MG	2A	3419	1/1	0.95	0.07	-	55,55,55,55	0
56	MG	2A	3243	1/1	0.98	0.17	-	49,49,49,49	0
56	MG	1a	3177	1/1	0.85	0.16	-	57,57,57,57	0
56	MG	2A	3196	1/1	0.82	0.19	-	53,53,53,53	0
56	MG	2A	3437	1/1	0.98	0.24	-	39,39,39,39	0
56	MG	2A	3701	1/1	0.81	0.11	-	50,50,50,50	0
56	MG	1A	3561	1/1	0.97	0.11	-	17,17,17,17	0
56	MG	1a	3202	1/1	0.97	0.06	-	45,45,45,45	0
56	MG	2A	3300	1/1	0.92	0.20	-	58,58,58,58	0
56	MG	1A	3341	1/1	0.81	0.36	-	38,38,38,38	0
56	MG	1A	3977	1/1	0.72	0.13	-	44,44,44,44	0
56	MG	2E	310	1/1	0.97	0.09	-	50,50,50,50	0
56	MG	2a	1706	1/1	0.98	0.06	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2l	202	1/1	0.88	0.43	-	66,66,66,66	0
56	MG	1A	4043	1/1	0.94	0.45	-	23,23,23,23	0
56	MG	1x	110	1/1	0.90	0.12	-	59,59,59,59	0
56	MG	2Q	3002	1/1	0.92	0.21	-	41,41,41,41	0
56	MG	1A	3918	1/1	0.97	0.11	-	33,33,33,33	0
56	MG	1A	3831	1/1	0.92	0.13	-	68,68,68,68	0
56	MG	1A	3577	1/1	0.98	0.13	-	54,54,54,54	0
56	MG	1A	3647	1/1	0.95	0.16	-	16,16,16,16	0
56	MG	1B	231	1/1	0.90	0.23	-	59,59,59,59	0
56	MG	1A	4037	1/1	0.94	0.55	-	28,28,28,28	0
56	MG	1A	4001	1/1	0.94	0.11	-	45,45,45,45	0
56	MG	2A	3515	1/1	0.88	0.19	-	44,44,44,44	0
56	MG	2A	3265	1/1	0.94	0.17	-	46,46,46,46	0
56	MG	2a	1818	1/1	0.91	0.10	-	48,48,48,48	0
56	MG	1a	3118	1/1	0.95	0.09	-	65,65,65,65	0
56	MG	2x	102	1/1	0.96	0.19	-	57,57,57,57	0
56	MG	2a	1682	1/1	0.93	0.09	-	48,48,48,48	0
56	MG	1A	3798	1/1	0.93	0.26	-	45,45,45,45	0
56	MG	2a	1684	1/1	0.91	0.18	-	49,49,49,49	0
56	MG	2A	3389	1/1	0.81	0.20	-	35,35,35,35	0
56	MG	2B	3009	1/1	0.87	0.14	-	63,63,63,63	0
56	MG	10	105	1/1	0.89	0.10	-	50,50,50,50	0
56	MG	1A	3856	1/1	0.97	0.06	-	62,62,62,62	0
56	MG	1A	3414	1/1	0.66	0.28	-	55,55,55,55	0
56	MG	2A	3204	1/1	0.92	0.15	-	43,43,43,43	0
56	MG	2A	3056	1/1	0.94	0.09	-	52,52,52,52	0
56	MG	1A	3048	1/1	0.93	0.45	-	42,42,42,42	0
56	MG	2A	3285	1/1	0.79	0.13	-	58,58,58,58	0
56	MG	2A	3044	1/1	0.89	0.08	-	61,61,61,61	0
56	MG	2A	3070	1/1	0.94	0.15	-	33,33,33,33	0
56	MG	1A	3711	1/1	0.89	0.15	-	44,44,44,44	0
56	MG	1A	3336	1/1	0.93	0.25	-	35,35,35,35	0
56	MG	2v	3005	1/1	0.98	0.15	-	56,56,56,56	0
56	MG	2T	3003	1/1	0.93	0.11	-	41,41,41,41	0
56	MG	2a	1778	1/1	0.91	0.21	-	68,68,68,68	0
56	MG	1A	3630	1/1	0.96	0.24	-	38,38,38,38	0
56	MG	1A	3101	1/1	0.93	0.44	-	28,28,28,28	0
56	MG	1A	3463	1/1	0.93	0.38	-	38,38,38,38	0
56	MG	1A	3803	1/1	0.90	0.34	-	41,41,41,41	0
56	MG	2A	3507	1/1	0.89	0.10	-	67,67,67,67	0
56	MG	2A	3221	1/1	0.91	0.16	-	54,54,54,54	0
56	MG	1A	3609	1/1	0.89	0.08	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3353	1/1	0.98	0.43	-	35,35,35,35	0
56	MG	2A	3470	1/1	0.94	0.22	-	53,53,53,53	0
56	MG	2A	3703	1/1	0.93	0.14	-	50,50,50,50	0
56	MG	2B	3013	1/1	0.70	0.15	-	74,74,74,74	0
56	MG	2A	3283	1/1	0.92	0.14	-	42,42,42,42	0
56	MG	2a	1758	1/1	0.98	0.07	-	52,52,52,52	0
56	MG	1A	3237	1/1	0.91	0.16	-	49,49,49,49	0
56	MG	1T	201	1/1	0.91	0.18	-	42,42,42,42	0
56	MG	2A	3631	1/1	0.98	0.11	-	53,53,53,53	0
56	MG	2A	3348	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	2A	3337	1/1	0.95	0.27	-	27,27,27,27	0
56	MG	1a	3069	1/1	0.82	0.15	-	59,59,59,59	0
56	MG	2a	1814	1/1	0.98	0.14	-	63,63,63,63	0
56	MG	1A	3298	1/1	0.92	0.16	-	40,40,40,40	0
56	MG	1A	3355	1/1	0.89	0.49	-	30,30,30,30	0
56	MG	1A	3383	1/1	0.93	0.18	-	42,42,42,42	0
56	MG	2A	3277	1/1	0.86	0.37	-	54,54,54,54	0
56	MG	1a	3112	1/1	0.92	0.09	-	48,48,48,48	0
56	MG	2A	3514	1/1	0.86	0.22	-	56,56,56,56	0
56	MG	1A	3381	1/1	0.95	0.08	-	46,46,46,46	0
56	MG	2A	3176	1/1	0.91	0.24	-	41,41,41,41	0
56	MG	2A	3728	1/1	0.91	0.17	-	56,56,56,56	0
56	MG	2A	3508	1/1	0.95	0.18	-	57,57,57,57	0
56	MG	2w	101	1/1	0.90	0.18	-	65,65,65,65	0
56	MG	2A	3592	1/1	0.89	0.12	-	43,43,43,43	0
56	MG	1a	3064	1/1	0.86	0.21	-	54,54,54,54	0
56	MG	1A	3724	1/1	0.95	0.10	-	44,44,44,44	0
56	MG	2a	1749	1/1	0.99	0.05	-	55,55,55,55	0
56	MG	1A	3734	1/1	0.97	0.08	-	42,42,42,42	0
56	MG	2A	3639	1/1	0.90	0.22	-	56,56,56,56	0
56	MG	1A	3014	1/1	0.90	0.32	-	27,27,27,27	0
56	MG	2A	3724	1/1	0.96	0.15	-	66,66,66,66	0
56	MG	2a	1752	1/1	0.86	0.16	-	62,62,62,62	0
56	MG	1a	3183	1/1	0.95	0.10	-	51,51,51,51	0
56	MG	2A	3425	1/1	0.84	0.11	-	59,59,59,59	0
56	MG	1A	3747	1/1	0.94	0.08	-	31,31,31,31	0
56	MG	1A	3708	1/1	0.92	0.10	-	42,42,42,42	0
56	MG	2A	3612	1/1	0.87	0.20	-	65,65,65,65	0
56	MG	2A	3053	1/1	0.87	0.14	-	30,30,30,30	0
56	MG	2A	3530	1/1	0.89	0.16	-	64,64,64,64	0
56	MG	1A	3729	1/1	0.97	0.18	-	49,49,49,49	0
56	MG	1A	3018	1/1	0.89	0.14	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1B	205	1/1	0.99	0.30	-	45,45,45,45	0
56	MG	2a	1744	1/1	0.95	0.11	-	67,67,67,67	0
56	MG	1A	3479	1/1	0.90	0.13	-	30,30,30,30	0
56	MG	1a	3094	1/1	0.96	0.26	-	40,40,40,40	0
56	MG	1A	3435	1/1	0.91	0.13	-	56,56,56,56	0
56	MG	2A	3564	1/1	0.95	0.17	-	42,42,42,42	0
56	MG	1A	3857	1/1	0.94	0.16	-	32,32,32,32	0
56	MG	2A	3297	1/1	0.95	0.24	-	51,51,51,51	0
56	MG	1a	3096	1/1	0.88	0.18	-	47,47,47,47	0
56	MG	1v	3001	1/1	0.83	0.11	-	72,72,72,72	0
56	MG	2A	3482	1/1	0.99	0.17	-	38,38,38,38	0
56	MG	2A	3163	1/1	0.75	0.26	-	44,44,44,44	0
56	MG	1w	107	1/1	0.90	0.30	-	64,64,64,64	0
56	MG	2A	3645	1/1	0.95	0.15	-	33,33,33,33	0
56	MG	1A	3940	1/1	0.94	0.10	-	29,29,29,29	0
56	MG	1A	3775	1/1	0.91	0.13	-	41,41,41,41	0
56	MG	2A	3693	1/1	0.98	0.05	-	68,68,68,68	0
56	MG	1A	3356	1/1	0.89	0.19	-	48,48,48,48	0
56	MG	2A	3135	1/1	0.93	0.26	-	49,49,49,49	0
56	MG	1a	3142	1/1	0.91	0.10	-	64,64,64,64	0
56	MG	2A	3658	1/1	0.91	0.17	-	36,36,36,36	0
56	MG	2a	1700	1/1	0.90	0.29	-	62,62,62,62	0
56	MG	2B	3010	1/1	0.87	0.11	-	64,64,64,64	0
56	MG	1A	3312	1/1	0.94	0.24	-	42,42,42,42	0
56	MG	2A	3516	1/1	0.96	0.13	-	62,62,62,62	0
56	MG	1A	3892	1/1	0.98	0.20	-	33,33,33,33	0
56	MG	1A	3908	1/1	0.97	0.14	-	27,27,27,27	0
56	MG	1A	3763	1/1	0.95	0.14	-	22,22,22,22	0
56	MG	2A	3087	1/1	0.84	0.08	-	59,59,59,59	0
56	MG	1A	3967	1/1	0.88	0.27	-	53,53,53,53	0
56	MG	1x	113	1/1	0.98	0.12	-	58,58,58,58	0
56	MG	2A	3383	1/1	0.68	0.22	-	56,56,56,56	0
56	MG	1A	3361	1/1	0.78	0.37	-	57,57,57,57	0
56	MG	2A	3239	1/1	0.96	0.44	-	64,64,64,64	0
56	MG	1A	3488	1/1	0.94	0.12	-	23,23,23,23	0
56	MG	1A	3830	1/1	0.97	0.26	-	39,39,39,39	0
56	MG	2a	1772	1/1	0.81	0.17	-	54,54,54,54	0
56	MG	2A	3461	1/1	0.94	0.15	-	45,45,45,45	0
56	MG	1A	3986	1/1	0.60	0.24	-	67,67,67,67	0
56	MG	1A	3094	1/1	0.89	0.13	-	56,56,56,56	0
56	MG	2A	3731	1/1	0.89	0.11	-	37,37,37,37	0
56	MG	2A	3686	1/1	0.97	0.15	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1B	204	1/1	0.92	0.12	-	29,29,29,29	0
56	MG	2A	3353	1/1	0.74	0.16	-	35,35,35,35	0
56	MG	2A	3511	1/1	0.97	0.14	-	39,39,39,39	0
56	MG	1A	3382	1/1	0.94	0.12	-	41,41,41,41	0
56	MG	1A	3061	1/1	0.94	0.11	-	39,39,39,39	0
56	MG	1B	214	1/1	0.94	0.11	-	42,42,42,42	0
56	MG	2A	3254	1/1	0.93	0.17	-	34,34,34,34	0
56	MG	2a	1631	1/1	0.86	0.09	-	66,66,66,66	0
56	MG	2w	107	1/1	0.98	0.14	-	55,55,55,55	0
56	MG	1A	3845	1/1	0.94	0.30	-	42,42,42,42	0
56	MG	1A	3710	1/1	0.94	0.20	-	28,28,28,28	0
56	MG	1A	3215	1/1	0.92	0.18	-	54,54,54,54	0
56	MG	1B	222	1/1	0.97	0.22	-	48,48,48,48	0
56	MG	1B	234	1/1	0.98	0.06	-	41,41,41,41	0
56	MG	1A	3157	1/1	0.96	0.08	-	50,50,50,50	0
56	MG	2a	1619	1/1	0.96	0.34	-	53,53,53,53	0
56	MG	2A	3165	1/1	0.96	0.19	-	40,40,40,40	0
56	MG	1A	3728	1/1	0.97	0.12	-	39,39,39,39	0
56	MG	1A	3057	1/1	0.86	0.26	-	45,45,45,45	0
56	MG	1A	3005	1/1	0.94	0.13	-	36,36,36,36	0
56	MG	2a	1732	1/1	0.86	0.11	-	56,56,56,56	0
56	MG	1a	3152	1/1	0.96	0.10	-	60,60,60,60	0
56	MG	2A	3326	1/1	0.94	0.11	-	48,48,48,48	0
56	MG	2A	3710	1/1	0.76	0.07	-	76,76,76,76	0
56	MG	2a	1695	1/1	0.93	0.16	-	56,56,56,56	0
56	MG	1A	3965	1/1	0.87	0.16	-	63,63,63,63	0
56	MG	1A	3181	1/1	0.98	0.08	-	43,43,43,43	0
56	MG	2A	3518	1/1	0.89	0.13	-	45,45,45,45	0
56	MG	1a	3068	1/1	0.91	0.14	-	62,62,62,62	0
56	MG	2A	3296	1/1	0.83	0.40	-	54,54,54,54	0
56	MG	1A	3768	1/1	0.95	0.06	-	33,33,33,33	0
56	MG	2A	3619	1/1	0.91	0.09	-	60,60,60,60	0
56	MG	1a	3011	1/1	0.92	0.14	-	41,41,41,41	0
56	MG	1A	3539	1/1	0.96	0.07	-	20,20,20,20	0
56	MG	1A	3347	1/1	0.93	0.14	-	42,42,42,42	0
56	MG	2A	3245	1/1	0.90	0.11	-	59,59,59,59	0
56	MG	2A	3680	1/1	0.95	0.08	-	62,62,62,62	0
56	MG	1A	3431	1/1	0.90	0.41	-	34,34,34,34	0
56	MG	1A	3413	1/1	0.91	0.28	-	55,55,55,55	0
56	MG	2D	304	1/1	0.85	0.14	-	53,53,53,53	0
56	MG	2A	3573	1/1	0.94	0.30	-	37,37,37,37	0
56	MG	2A	3233	1/1	0.93	0.26	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3385	1/1	0.97	0.30	-	29,29,29,29	0
56	MG	2E	305	1/1	0.81	0.14	-	51,51,51,51	0
56	MG	1A	3002	1/1	0.87	0.18	-	46,46,46,46	0
56	MG	2A	3295	1/1	0.95	0.26	-	43,43,43,43	0
56	MG	1A	3276	1/1	0.94	0.17	-	40,40,40,40	0
56	MG	1N	203	1/1	0.90	0.13	-	51,51,51,51	0
56	MG	1A	3922	1/1	0.92	0.09	-	49,49,49,49	0
56	MG	1A	3054	1/1	0.89	0.12	-	26,26,26,26	0
56	MG	1A	3957	1/1	0.93	0.12	-	55,55,55,55	0
56	MG	1A	3638	1/1	0.94	0.15	-	56,56,56,56	0
56	MG	1A	3555	1/1	0.93	0.09	-	29,29,29,29	0
56	MG	2a	1722	1/1	0.84	0.18	-	79,79,79,79	0
56	MG	1A	3822	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	2B	3016	1/1	0.79	0.10	-	54,54,54,54	0
56	MG	1A	3950	1/1	0.95	0.13	-	54,54,54,54	0
56	MG	2a	1623	1/1	0.94	0.14	-	46,46,46,46	0
56	MG	2A	3172	1/1	0.97	0.32	-	48,48,48,48	0
56	MG	2A	3560	1/1	0.80	0.08	-	50,50,50,50	0
56	MG	1A	3063	1/1	0.96	0.31	-	23,23,23,23	0
56	MG	2W	202	1/1	0.77	0.54	-	46,46,46,46	0
56	MG	1A	3910	1/1	0.96	0.10	-	32,32,32,32	0
56	MG	1A	3930	1/1	0.96	0.23	-	33,33,33,33	0
56	MG	2A	3284	1/1	0.96	0.08	-	37,37,37,37	0
56	MG	1A	3019	1/1	0.93	0.16	-	32,32,32,32	0
56	MG	1A	3869	1/1	0.93	0.19	-	19,19,19,19	0
56	MG	2A	3255	1/1	0.93	0.22	-	54,54,54,54	0
56	MG	1A	3853	1/1	0.96	0.07	-	38,38,38,38	0
56	MG	2a	1751	1/1	0.84	0.12	-	87,87,87,87	0
56	MG	2A	3081	1/1	0.95	0.09	-	53,53,53,53	0
56	MG	2A	3039	1/1	0.96	0.15	-	25,25,25,25	0
56	MG	2a	1820	1/1	0.91	0.21	-	60,60,60,60	0
56	MG	1A	3999	1/1	0.96	0.17	-	25,25,25,25	0
56	MG	2A	3321	1/1	0.88	0.21	-	44,44,44,44	0
56	MG	1A	3990	1/1	0.90	0.08	-	38,38,38,38	0
56	MG	2a	1741	1/1	0.97	0.09	-	57,57,57,57	0
56	MG	1A	3100	1/1	0.91	0.20	-	38,38,38,38	0
56	MG	1A	3588	1/1	0.96	0.16	-	32,32,32,32	0
56	MG	2A	3150	1/1	0.96	0.21	-	49,49,49,49	0
56	MG	1a	3045	1/1	0.98	0.11	-	52,52,52,52	0
56	MG	2A	3720	1/1	0.47	0.17	-	97,97,97,97	0
56	MG	1A	3458	1/1	0.73	0.15	-	68,68,68,68	0
56	MG	1A	3976	1/1	0.95	0.09	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3273	1/1	0.94	0.09	-	38,38,38,38	0
56	MG	2A	3604	1/1	0.86	0.10	-	58,58,58,58	0
56	MG	1A	3134	1/1	0.94	0.46	-	30,30,30,30	0
56	MG	2A	3533	1/1	0.95	0.34	-	52,52,52,52	0
56	MG	2A	3333	1/1	0.95	0.12	-	25,25,25,25	0
56	MG	1A	3374	1/1	0.92	0.41	-	40,40,40,40	0
56	MG	1a	3095	1/1	0.98	0.12	-	55,55,55,55	0
56	MG	23	101	1/1	0.92	0.61	-	54,54,54,54	0
56	MG	2a	1633	1/1	0.89	0.11	-	63,63,63,63	0
56	MG	2a	1647	1/1	0.84	0.13	-	80,80,80,80	0
56	MG	2A	3595	1/1	0.93	0.09	-	59,59,59,59	0
56	MG	1A	3008	1/1	0.96	0.16	-	18,18,18,18	0
56	MG	1a	3131	1/1	0.98	0.10	-	38,38,38,38	0
56	MG	2A	3051	1/1	0.99	0.05	-	46,46,46,46	0
56	MG	2A	3611	1/1	0.97	0.14	-	47,47,47,47	0
56	MG	2a	1656	1/1	0.77	0.14	-	68,68,68,68	0
56	MG	1A	3568	1/1	0.89	0.10	-	30,30,30,30	0
56	MG	2A	3251	1/1	0.93	0.20	-	49,49,49,49	0
56	MG	2A	3102	1/1	0.87	0.38	-	44,44,44,44	0
56	MG	2A	3503	1/1	0.93	0.16	-	54,54,54,54	0
56	MG	1A	3532	1/1	0.95	0.16	-	29,29,29,29	0
56	MG	1a	3082	1/1	0.96	0.48	-	41,41,41,41	0
56	MG	1A	3041	1/1	0.98	0.11	-	32,32,32,32	0
56	MG	2A	3093	1/1	0.80	0.13	-	58,58,58,58	0
56	MG	1A	3243	1/1	0.91	0.29	-	25,25,25,25	0
56	MG	1A	3204	1/1	0.95	0.29	-	39,39,39,39	0
56	MG	2A	3164	1/1	0.97	0.37	-	53,53,53,53	0
56	MG	1A	3760	1/1	0.81	0.13	-	44,44,44,44	0
56	MG	1A	3394	1/1	0.96	0.23	-	37,37,37,37	0
56	MG	1B	232	1/1	0.82	0.14	-	66,66,66,66	0
56	MG	2A	3475	1/1	0.98	0.20	-	37,37,37,37	0
56	MG	2a	1687	1/1	0.98	0.05	-	40,40,40,40	0
56	MG	1A	3203	1/1	0.90	0.16	-	27,27,27,27	0
56	MG	1A	3357	1/1	0.82	0.23	-	43,43,43,43	0
56	MG	2A	3554	1/1	0.93	0.14	-	24,24,24,24	0
56	MG	1A	3791	1/1	0.98	0.34	-	23,23,23,23	0
56	MG	1A	3260	1/1	0.97	0.15	-	18,18,18,18	0
56	MG	2A	3492	1/1	0.88	0.22	-	49,49,49,49	0
56	MG	2A	3459	1/1	0.98	0.08	-	50,50,50,50	0
56	MG	2A	3315	1/1	0.98	0.21	-	42,42,42,42	0
56	MG	2A	3685	1/1	0.92	0.14	-	41,41,41,41	0
56	MG	2A	3412	1/1	0.96	0.14	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	3043	1/1	0.91	0.12	-	50,50,50,50	0
56	MG	1E	304	1/1	0.97	0.33	-	22,22,22,22	0
56	MG	2w	106	1/1	0.73	0.33	-	59,59,59,59	0
56	MG	1A	3349	1/1	0.91	0.13	-	39,39,39,39	0
56	MG	2A	3367	1/1	0.97	0.13	-	28,28,28,28	0
56	MG	1A	3135	1/1	0.88	0.27	-	23,23,23,23	0
56	MG	1A	3369	1/1	0.94	0.11	-	38,38,38,38	0
56	MG	1A	3226	1/1	0.76	0.82	-	49,49,49,49	0
56	MG	2A	3238	1/1	0.91	0.14	-	60,60,60,60	0
56	MG	1A	3800	1/1	0.99	0.20	-	54,54,54,54	0
56	MG	1A	3125	1/1	0.95	0.28	-	19,19,19,19	0
56	MG	2Q	3003	1/1	0.87	0.64	-	52,52,52,52	0
56	MG	1A	3373	1/1	0.88	0.12	-	41,41,41,41	0
56	MG	2A	3023	1/1	0.95	0.12	-	41,41,41,41	0
56	MG	1A	3543	1/1	0.96	0.14	-	20,20,20,20	0
56	MG	2A	3258	1/1	0.64	0.17	-	58,58,58,58	0
56	MG	1a	3144	1/1	0.94	0.19	-	66,66,66,66	0
56	MG	1A	3446	1/1	0.96	0.11	-	43,43,43,43	0
56	MG	1a	3153	1/1	0.96	0.10	-	52,52,52,52	0
56	MG	1a	3123	1/1	0.91	0.13	-	60,60,60,60	0
56	MG	2A	3183	1/1	0.90	0.21	-	38,38,38,38	0
56	MG	1A	3056	1/1	0.95	0.15	-	50,50,50,50	0
56	MG	1A	4016	1/1	0.86	0.11	-	55,55,55,55	0
56	MG	1A	3597	1/1	0.95	0.09	-	50,50,50,50	0
56	MG	1A	3398	1/1	0.88	0.12	-	37,37,37,37	0
56	MG	1A	3759	1/1	0.89	0.13	-	32,32,32,32	0
56	MG	1A	3403	1/1	0.96	0.23	-	33,33,33,33	0
56	MG	1A	3657	1/1	0.97	0.13	-	23,23,23,23	0
56	MG	2a	1605	1/1	0.85	0.13	-	61,61,61,61	0
56	MG	1A	3082	1/1	0.95	0.15	-	40,40,40,40	0
56	MG	1a	3180	1/1	0.87	0.10	-	62,62,62,62	0
56	MG	1A	3234	1/1	0.95	0.11	-	43,43,43,43	0
56	MG	2A	3694	1/1	0.97	0.09	-	54,54,54,54	0
56	MG	2A	3146	1/1	0.94	0.15	-	50,50,50,50	0
56	MG	2A	3059	1/1	0.98	0.16	-	35,35,35,35	0
56	MG	1U	202	1/1	0.96	0.11	-	30,30,30,30	0
56	MG	1A	3085	1/1	0.88	0.14	-	13,13,13,13	0
56	MG	2a	1615	1/1	0.85	0.22	-	54,54,54,54	0
56	MG	1A	3091	1/1	0.98	0.18	-	31,31,31,31	0
56	MG	1A	3137	1/1	0.85	0.42	-	40,40,40,40	0
56	MG	2A	3159	1/1	0.92	0.14	-	50,50,50,50	0
56	MG	1A	3291	1/1	0.91	0.21	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3868	1/1	0.97	0.14	-	24,24,24,24	0
56	MG	1A	3023	1/1	0.97	0.16	-	43,43,43,43	0
56	MG	1A	3527	1/1	0.88	0.24	-	66,66,66,66	0
56	MG	13	102	1/1	0.89	0.13	-	46,46,46,46	0
56	MG	1w	109	1/1	0.99	0.41	-	37,37,37,37	0
56	MG	2A	3637	1/1	0.97	0.10	-	53,53,53,53	0
56	MG	2A	3324	1/1	0.97	0.06	-	40,40,40,40	0
56	MG	2a	1723	1/1	0.91	0.14	-	57,57,57,57	0
56	MG	1a	3189	1/1	0.92	0.12	-	53,53,53,53	0
56	MG	2a	1696	1/1	0.91	0.15	-	48,48,48,48	0
56	MG	2a	1692	1/1	0.95	0.32	-	60,60,60,60	0
56	MG	2A	3122	1/1	0.97	0.15	-	26,26,26,26	0
56	MG	2a	1624	1/1	0.92	0.11	-	78,78,78,78	0
56	MG	1a	3200	1/1	0.95	0.15	-	41,41,41,41	0
56	MG	1A	3513	1/1	0.87	0.16	-	29,29,29,29	0
56	MG	2a	1654	1/1	0.94	0.27	-	58,58,58,58	0
56	MG	2A	3372	1/1	0.95	0.23	-	42,42,42,42	0
56	MG	1a	3029	1/1	0.93	0.10	-	49,49,49,49	0
56	MG	2a	1793	1/1	0.92	0.14	-	53,53,53,53	0
56	MG	1a	3136	1/1	0.97	0.12	-	49,49,49,49	0
56	MG	1A	3287	1/1	0.93	0.13	-	30,30,30,30	0
56	MG	2a	1792	1/1	0.85	0.09	-	61,61,61,61	0
56	MG	1A	3805	1/1	0.94	0.20	-	60,60,60,60	0
56	MG	1A	3079	1/1	0.95	0.16	-	32,32,32,32	0
56	MG	2A	3108	1/1	0.93	0.30	-	49,49,49,49	0
56	MG	1A	3205	1/1	0.94	0.59	-	28,28,28,28	0
56	MG	2A	3226	1/1	0.91	0.32	-	42,42,42,42	0
56	MG	1A	3280	1/1	0.92	0.51	-	26,26,26,26	0
56	MG	21	3001	1/1	0.88	0.54	-	36,36,36,36	0
56	MG	1a	3091	1/1	0.93	0.22	-	46,46,46,46	0
56	MG	2A	3050	1/1	0.93	0.14	-	38,38,38,38	0
56	MG	1V	201	1/1	0.93	0.10	-	40,40,40,40	0
56	MG	1A	3787	1/1	0.94	0.14	-	36,36,36,36	0
56	MG	1a	3032	1/1	0.93	0.19	-	54,54,54,54	0
56	MG	2x	105	1/1	0.98	0.14	-	47,47,47,47	0
56	MG	1A	3059	1/1	0.95	0.20	-	36,36,36,36	0
56	MG	1A	3566	1/1	0.89	0.17	-	62,62,62,62	0
56	MG	1A	3207	1/1	0.85	0.28	-	52,52,52,52	0
56	MG	1a	3199	1/1	0.98	0.19	-	47,47,47,47	0
56	MG	1A	3767	1/1	0.95	0.10	-	41,41,41,41	0
56	MG	1A	3811	1/1	0.93	0.08	-	32,32,32,32	0
56	MG	2a	1764	1/1	0.92	0.17	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3092	1/1	0.94	0.17	-	44,44,44,44	0
56	MG	1A	3765	1/1	0.96	0.20	-	19,19,19,19	0
56	MG	2A	3002	1/1	0.86	0.13	-	61,61,61,61	0
56	MG	2A	3049	1/1	0.89	0.12	-	53,53,53,53	0
56	MG	2B	3007	1/1	0.94	0.10	-	56,56,56,56	0
56	MG	1A	3709	1/1	0.94	0.17	-	30,30,30,30	0
56	MG	1A	3659	1/1	0.95	0.20	-	40,40,40,40	0
56	MG	1A	3104	1/1	0.89	0.22	-	45,45,45,45	0
56	MG	2A	3476	1/1	0.93	0.12	-	44,44,44,44	0
56	MG	1a	3079	1/1	0.97	0.14	-	47,47,47,47	0
56	MG	1A	3320	1/1	0.96	0.07	-	48,48,48,48	0
56	MG	1A	3876	1/1	0.92	0.21	-	34,34,34,34	0
56	MG	1A	3462	1/1	0.94	0.31	-	22,22,22,22	0
56	MG	1a	3081	1/1	0.96	0.09	-	67,67,67,67	0
56	MG	2A	3336	1/1	0.97	0.14	-	58,58,58,58	0
56	MG	1A	3322	1/1	0.95	0.36	-	38,38,38,38	0
56	MG	1A	3120	1/1	0.98	0.33	-	29,29,29,29	0
56	MG	2a	1720	1/1	0.94	0.18	-	66,66,66,66	0
56	MG	2A	3688	1/1	0.90	0.14	-	57,57,57,57	0
56	MG	2A	3599	1/1	0.95	0.09	-	61,61,61,61	0
56	MG	2A	3730	1/1	0.87	0.35	-	32,32,32,32	0
56	MG	1D	301	1/1	0.79	0.28	-	44,44,44,44	0
56	MG	2A	3484	1/1	0.90	0.11	-	70,70,70,70	0
56	MG	2A	3202	1/1	0.88	0.14	-	56,56,56,56	0
56	MG	2A	3526	1/1	0.95	0.11	-	49,49,49,49	0
56	MG	1A	3238	1/1	0.92	0.16	-	33,33,33,33	0
56	MG	2a	1776	1/1	0.98	0.11	-	47,47,47,47	0
56	MG	1A	3580	1/1	0.98	0.07	-	18,18,18,18	0
56	MG	2a	1804	1/1	0.91	0.11	-	48,48,48,48	0
56	MG	1A	4054	1/1	0.94	0.48	-	37,37,37,37	0
56	MG	2A	3524	1/1	0.82	0.12	-	61,61,61,61	0
56	MG	2A	3306	1/1	0.97	0.22	-	47,47,47,47	0
56	MG	2A	3227	1/1	0.96	0.09	-	40,40,40,40	0
56	MG	2A	3105	1/1	0.96	0.22	-	34,34,34,34	0
56	MG	1A	3395	1/1	0.98	0.14	-	33,33,33,33	0
56	MG	1a	3075	1/1	0.96	0.11	-	46,46,46,46	0
56	MG	1A	3903	1/1	0.86	0.12	-	23,23,23,23	0
56	MG	1A	3053	1/1	0.98	0.06	-	43,43,43,43	0
56	MG	1a	3049	1/1	0.81	0.16	-	60,60,60,60	0
56	MG	1q	201	1/1	0.92	0.08	-	50,50,50,50	0
56	MG	2A	3182	1/1	0.94	0.64	-	43,43,43,43	0
56	MG	1A	3692	1/1	0.91	0.12	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3469	1/1	0.98	0.29	-	39,39,39,39	0
56	MG	1A	3136	1/1	0.98	0.08	-	21,21,21,21	0
56	MG	1A	4029	1/1	0.94	0.33	-	36,36,36,36	0
56	MG	2A	3397	1/1	0.98	0.12	-	37,37,37,37	0
56	MG	1A	3719	1/1	0.96	0.08	-	47,47,47,47	0
56	MG	2A	3047	1/1	0.97	0.14	-	60,60,60,60	0
56	MG	1A	3411	1/1	0.90	0.12	-	45,45,45,45	0
56	MG	1w	101	1/1	0.87	0.30	-	74,74,74,74	0
56	MG	2a	1651	1/1	0.82	0.08	-	60,60,60,60	0
56	MG	2A	3655	1/1	0.94	0.15	-	53,53,53,53	0
56	MG	2A	3246	1/1	0.96	0.24	-	48,48,48,48	0
56	MG	2A	3294	1/1	0.94	0.28	-	45,45,45,45	0
56	MG	1A	3919	1/1	0.94	0.15	-	42,42,42,42	0
56	MG	1A	3581	1/1	0.94	0.19	-	19,19,19,19	0
56	MG	1A	3313	1/1	0.87	0.39	-	35,35,35,35	0
56	MG	2a	1787	1/1	0.97	0.06	-	53,53,53,53	0
56	MG	1a	3161	1/1	0.86	0.08	-	53,53,53,53	0
56	MG	1A	3258	1/1	0.99	0.20	-	33,33,33,33	0
56	MG	2a	1773	1/1	0.79	0.20	-	70,70,70,70	0
56	MG	1a	3016	1/1	0.97	0.12	-	38,38,38,38	0
56	MG	2a	1626	1/1	0.89	0.08	-	50,50,50,50	0
56	MG	2A	3718	1/1	0.94	0.10	-	56,56,56,56	0
56	MG	2A	3094	1/1	0.85	0.16	-	47,47,47,47	0
56	MG	1A	3440	1/1	0.96	0.33	-	28,28,28,28	0
56	MG	1a	3062	1/1	0.94	0.08	-	36,36,36,36	0
56	MG	2A	3629	1/1	0.98	0.18	-	62,62,62,62	0
56	MG	2a	1768	1/1	0.96	0.05	-	55,55,55,55	0
56	MG	1Z	3003	1/1	0.73	0.17	-	52,52,52,52	0
56	MG	2A	3187	1/1	0.92	0.26	-	54,54,54,54	0
56	MG	1A	3988	1/1	0.94	0.09	-	34,34,34,34	0
56	MG	1a	3137	1/1	0.96	0.15	-	51,51,51,51	0
56	MG	1A	3881	1/1	0.88	0.11	-	44,44,44,44	0
56	MG	1B	212	1/1	0.81	0.29	-	46,46,46,46	0
56	MG	1A	3124	1/1	0.96	0.07	-	33,33,33,33	0
56	MG	2A	3280	1/1	0.87	0.47	-	50,50,50,50	0
56	MG	1a	3103	1/1	0.93	0.07	-	46,46,46,46	0
56	MG	1A	3340	1/1	0.93	0.13	-	47,47,47,47	0
56	MG	2A	3005	1/1	0.95	0.11	-	42,42,42,42	0
56	MG	2A	3232	1/1	0.91	0.12	-	54,54,54,54	0
56	MG	2A	3666	1/1	0.89	0.14	-	46,46,46,46	0
56	MG	2A	3632	1/1	0.94	0.32	-	62,62,62,62	0
56	MG	2A	3169	1/1	0.96	0.07	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3288	1/1	0.99	0.25	-	30,30,30,30	0
56	MG	2a	1677	1/1	0.94	0.15	-	55,55,55,55	0
56	MG	1A	3898	1/1	0.56	0.15	-	71,71,71,71	0
56	MG	1a	3167	1/1	0.94	0.07	-	42,42,42,42	0
56	MG	2A	3220	1/1	0.86	0.12	-	49,49,49,49	0
56	MG	2a	1757	1/1	0.93	0.12	-	48,48,48,48	0
56	MG	1A	3420	1/1	0.92	0.13	-	49,49,49,49	0
56	MG	1A	3779	1/1	0.88	0.10	-	50,50,50,50	0
56	MG	1A	3086	1/1	0.81	0.15	-	55,55,55,55	0
56	MG	2A	3318	1/1	0.90	0.34	-	42,42,42,42	0
56	MG	1A	3501	1/1	0.96	0.21	-	30,30,30,30	0
56	MG	1A	3785	1/1	0.95	0.20	-	35,35,35,35	0
56	MG	1a	3204	1/1	0.98	0.10	-	44,44,44,44	0
56	MG	1A	3293	1/1	0.78	0.23	-	51,51,51,51	0
56	MG	2a	1699	1/1	0.97	0.05	-	58,58,58,58	0
56	MG	1A	3793	1/1	0.99	0.25	-	26,26,26,26	0
56	MG	1a	3024	1/1	0.80	0.16	-	52,52,52,52	0
56	MG	2B	3012	1/1	0.79	0.16	-	75,75,75,75	0
56	MG	1a	3023	1/1	0.94	0.15	-	44,44,44,44	0
56	MG	2B	3011	1/1	0.95	0.14	-	69,69,69,69	0
56	MG	2A	3338	1/1	0.90	0.26	-	42,42,42,42	0
56	MG	1A	4018	1/1	0.91	0.34	-	24,24,24,24	0
56	MG	1A	3265	1/1	0.92	0.18	-	26,26,26,26	0
56	MG	2a	1771	1/1	0.95	0.11	-	62,62,62,62	0
56	MG	1B	237	1/1	0.95	0.16	-	46,46,46,46	0
56	MG	2A	3311	1/1	0.85	0.23	-	50,50,50,50	0
56	MG	1A	3523	1/1	0.82	0.12	-	46,46,46,46	0
56	MG	2A	3259	1/1	0.75	0.20	-	53,53,53,53	0
56	MG	2a	1686	1/1	0.90	0.23	-	67,67,67,67	0
56	MG	2A	3222	1/1	0.93	0.16	-	44,44,44,44	0
56	MG	2A	3721	1/1	0.98	0.07	-	50,50,50,50	0
56	MG	1A	3047	1/1	0.86	0.14	-	50,50,50,50	0
56	MG	1A	3911	1/1	0.97	0.10	-	29,29,29,29	0
56	MG	2A	3007	1/1	0.94	0.10	-	32,32,32,32	0
56	MG	2a	1685	1/1	0.93	0.10	-	53,53,53,53	0
56	MG	1a	3005	1/1	0.95	0.11	-	41,41,41,41	0
56	MG	2A	3426	1/1	0.87	0.18	-	48,48,48,48	0
56	MG	1A	3679	1/1	0.79	0.23	-	14,14,14,14	0
56	MG	2A	3139	1/1	0.91	0.13	-	41,41,41,41	0
56	MG	2A	3471	1/1	0.93	0.20	-	37,37,37,37	0
56	MG	2A	3276	1/1	0.92	0.21	-	58,58,58,58	0
56	MG	1A	3784	1/1	0.97	0.12	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3781	1/1	0.84	0.19	-	51,51,51,51	0
56	MG	1A	3867	1/1	0.93	0.14	-	19,19,19,19	0
56	MG	1A	3338	1/1	0.99	0.22	-	19,19,19,19	0
56	MG	2P	201	1/1	0.97	0.13	-	54,54,54,54	0
56	MG	2a	1829	1/1	0.82	0.30	-	68,68,68,68	0
56	MG	1A	3697	1/1	0.89	0.20	-	27,27,27,27	0
56	MG	1a	3184	1/1	0.97	0.08	-	49,49,49,49	0
56	MG	2a	1782	1/1	0.95	0.14	-	58,58,58,58	0
56	MG	1A	3633	1/1	0.97	0.10	-	52,52,52,52	0
56	MG	2A	3219	1/1	0.91	0.32	-	54,54,54,54	0
56	MG	2a	1662	1/1	0.81	0.11	-	59,59,59,59	0
56	MG	2A	3558	1/1	0.82	0.28	-	50,50,50,50	0
56	MG	2a	1805	1/1	0.96	0.05	-	53,53,53,53	0
56	MG	2A	3498	1/1	0.95	0.06	-	46,46,46,46	0
56	MG	1a	3093	1/1	0.91	0.16	-	49,49,49,49	0
56	MG	1A	3459	1/1	0.80	0.20	-	53,53,53,53	0
56	MG	2A	3502	1/1	0.92	0.16	-	42,42,42,42	0
56	MG	2w	109	1/1	0.74	0.13	-	63,63,63,63	0
56	MG	2A	3620	1/1	0.92	0.09	-	34,34,34,34	0
57	K	2A	3745	1/1	0.97	0.08	-	53,53,53,53	0
56	MG	1A	3478	1/1	0.94	0.20	-	47,47,47,47	0
56	MG	2A	3179	1/1	0.93	0.17	-	45,45,45,45	0
56	MG	1y	103	1/1	0.84	0.26	-	82,82,82,82	0
56	MG	2A	3098	1/1	0.90	0.35	-	68,68,68,68	0
56	MG	1A	3564	1/1	0.94	0.21	-	36,36,36,36	0
56	MG	2A	3479	1/1	0.95	0.15	-	34,34,34,34	0
56	MG	1A	3107	1/1	0.91	0.26	-	24,24,24,24	0
56	MG	2A	3439	1/1	0.81	0.11	-	49,49,49,49	0
56	MG	2B	3014	1/1	0.83	0.31	-	71,71,71,71	0
56	MG	1A	3151	1/1	0.95	0.21	-	36,36,36,36	0
56	MG	2a	1638	1/1	0.91	0.23	-	49,49,49,49	0
56	MG	2a	1650	1/1	0.89	0.16	-	68,68,68,68	0
56	MG	1A	3517	1/1	0.97	0.15	-	28,28,28,28	0
56	MG	1A	3735	1/1	0.89	0.14	-	22,22,22,22	0
56	MG	2j	8002	1/1	0.94	0.05	-	62,62,62,62	0
56	MG	1A	3282	1/1	0.88	0.21	-	56,56,56,56	0
56	MG	2A	3260	1/1	0.96	0.16	-	48,48,48,48	0
56	MG	2A	3640	1/1	0.92	0.23	-	47,47,47,47	0
56	MG	1O	201	1/1	0.90	0.15	-	45,45,45,45	0
56	MG	1B	216	1/1	0.98	0.16	-	42,42,42,42	0
56	MG	1a	3191	1/1	0.94	0.08	-	53,53,53,53	0
56	MG	2A	3738	1/1	0.86	0.17	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3343	1/1	0.97	0.24	-	30,30,30,30	0
56	MG	1A	3973	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	1A	3325	1/1	0.98	0.13	-	33,33,33,33	0
56	MG	2A	3201	1/1	0.76	0.20	-	55,55,55,55	0
56	MG	2a	1642	1/1	0.89	0.21	-	55,55,55,55	0
56	MG	1A	3801	1/1	0.83	0.25	-	71,71,71,71	0
56	MG	1A	3342	1/1	0.95	0.32	-	21,21,21,21	0
56	MG	1a	3086	1/1	0.97	0.07	-	60,60,60,60	0
56	MG	2A	3322	1/1	0.87	0.36	-	55,55,55,55	0
56	MG	2A	3539	1/1	0.86	0.10	-	59,59,59,59	0
56	MG	1B	211	1/1	0.70	0.75	-	45,45,45,45	0
56	MG	1A	3861	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	2A	3577	1/1	0.95	0.21	-	45,45,45,45	0
56	MG	1A	3493	1/1	0.93	0.32	-	23,23,23,23	0
56	MG	2a	1606	1/1	0.96	0.07	-	43,43,43,43	0
56	MG	1A	3363	1/1	0.82	0.17	-	32,32,32,32	0
56	MG	2a	1621	1/1	0.89	0.55	-	65,65,65,65	0
56	MG	2A	3481	1/1	0.92	0.25	-	58,58,58,58	0
56	MG	2a	1635	1/1	0.95	0.15	-	39,39,39,39	0
56	MG	1A	3261	1/1	0.92	0.10	-	35,35,35,35	0
56	MG	1Z	3001	1/1	0.93	0.26	-	42,42,42,42	0
56	MG	1a	3067	1/1	0.95	0.16	-	46,46,46,46	0
56	MG	1A	3109	1/1	0.93	0.41	-	50,50,50,50	0
56	MG	1A	4009	1/1	0.89	0.22	-	41,41,41,41	0
56	MG	1O	204	1/1	0.97	0.10	-	45,45,45,45	0
56	MG	2a	1794	1/1	0.95	0.15	-	58,58,58,58	0
56	MG	2A	3519	1/1	0.97	0.14	-	35,35,35,35	0
56	MG	2A	3404	1/1	0.98	0.18	-	39,39,39,39	0
56	MG	2A	3281	1/1	0.86	0.09	-	60,60,60,60	0
56	MG	1A	3351	1/1	0.95	0.11	-	34,34,34,34	0
56	MG	2A	3711	1/1	0.96	0.07	-	37,37,37,37	0
56	MG	1a	3092	1/1	0.90	0.11	-	55,55,55,55	0
56	MG	1A	3121	1/1	0.90	0.39	-	33,33,33,33	0
56	MG	2A	3699	1/1	0.95	0.11	-	39,39,39,39	0
56	MG	1a	3078	1/1	0.97	0.11	-	48,48,48,48	0
56	MG	1A	3875	1/1	0.96	0.17	-	43,43,43,43	0
56	MG	2A	3635	1/1	0.91	0.14	-	57,57,57,57	0
56	MG	2a	1636	1/1	0.83	0.09	-	66,66,66,66	0
56	MG	2A	3451	1/1	0.96	0.09	-	44,44,44,44	0
56	MG	1A	3698	1/1	0.92	0.12	-	41,41,41,41	0
56	MG	1A	4004	1/1	0.94	0.27	-	55,55,55,55	0
56	MG	1B	225	1/1	0.94	0.17	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3814	1/1	0.97	0.14	-	8,8,8,8	0
56	MG	1w	108	1/1	0.85	0.16	-	66,66,66,66	0
56	MG	2j	8001	1/1	0.83	0.11	-	66,66,66,66	0
56	MG	1A	3366	1/1	0.69	0.29	-	50,50,50,50	0
56	MG	1A	3330	1/1	0.93	0.17	-	28,28,28,28	0
56	MG	1A	3419	1/1	0.96	0.14	-	42,42,42,42	0
56	MG	1A	3145	1/1	0.92	0.62	-	34,34,34,34	0
56	MG	2a	1707	1/1	0.93	0.22	-	68,68,68,68	0
56	MG	1G	3004	1/1	0.94	0.11	-	38,38,38,38	0
56	MG	1A	3122	1/1	0.96	0.13	-	32,32,32,32	0
56	MG	1A	3897	1/1	0.93	0.14	-	44,44,44,44	0
56	MG	2a	1721	1/1	0.95	0.04	-	73,73,73,73	0
56	MG	1A	4017	1/1	0.97	0.41	-	37,37,37,37	0
56	MG	1s	101	1/1	0.93	0.20	-	62,62,62,62	0
56	MG	2A	3653	1/1	0.83	0.22	-	37,37,37,37	0
56	MG	1A	3388	1/1	0.95	0.18	-	30,30,30,30	0
56	MG	1a	3055	1/1	0.92	0.14	-	49,49,49,49	0
56	MG	1a	3196	1/1	0.94	0.06	-	46,46,46,46	0
56	MG	2A	3118	1/1	0.93	0.19	-	42,42,42,42	0
56	MG	2A	3474	1/1	0.95	0.15	-	35,35,35,35	0
56	MG	1a	3201	1/1	0.98	0.06	-	44,44,44,44	0
56	MG	1Q	205	1/1	0.92	0.11	-	28,28,28,28	0
56	MG	2A	3161	1/1	0.93	0.37	-	46,46,46,46	0
56	MG	2A	3676	1/1	0.86	0.13	-	79,79,79,79	0
56	MG	1A	3259	1/1	0.95	0.16	-	45,45,45,45	0
56	MG	1A	3036	1/1	0.90	0.21	-	26,26,26,26	0
56	MG	1A	3447	1/1	0.92	0.32	-	47,47,47,47	0
56	MG	2a	1713	1/1	0.89	0.13	-	48,48,48,48	0
56	MG	2E	302	1/1	0.97	0.09	-	44,44,44,44	0
56	MG	1A	3598	1/1	0.96	0.34	-	48,48,48,48	0
56	MG	2a	1808	1/1	0.87	0.19	-	58,58,58,58	0
56	MG	1A	3948	1/1	0.98	0.09	-	14,14,14,14	0
56	MG	1A	3264	1/1	0.91	0.09	-	39,39,39,39	0
56	MG	2A	3075	1/1	0.92	0.16	-	51,51,51,51	0
56	MG	2A	3250	1/1	0.92	0.15	-	51,51,51,51	0
56	MG	1A	3379	1/1	0.92	0.39	-	53,53,53,53	0
56	MG	1a	3089	1/1	0.85	0.15	-	40,40,40,40	0
56	MG	1A	3717	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	2A	3151	1/1	0.97	0.09	-	47,47,47,47	0
56	MG	1A	3604	1/1	0.97	0.11	-	28,28,28,28	0
56	MG	1A	3624	1/1	0.94	0.13	-	26,26,26,26	0
56	MG	2A	3598	1/1	0.95	0.14	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3591	1/1	0.92	0.12	-	34,34,34,34	0
56	MG	1A	3152	1/1	0.92	0.17	-	43,43,43,43	0
56	MG	1A	3248	1/1	0.82	0.14	-	49,49,49,49	0
56	MG	2O	8002	1/1	0.94	0.12	-	52,52,52,52	0
56	MG	2A	3178	1/1	0.93	0.17	-	44,44,44,44	0
56	MG	2A	3647	1/1	0.97	0.11	-	51,51,51,51	0
56	MG	2A	3188	1/1	0.87	0.12	-	57,57,57,57	0
56	MG	2A	3234	1/1	0.91	0.34	-	47,47,47,47	0
56	MG	1a	3026	1/1	0.84	0.11	-	72,72,72,72	0
56	MG	2E	309	1/1	0.99	0.06	-	41,41,41,41	0
56	MG	1E	301	1/1	0.90	0.59	-	26,26,26,26	0
56	MG	1A	3968	1/1	0.90	0.20	-	55,55,55,55	0
56	MG	1A	3944	1/1	0.88	0.13	-	39,39,39,39	0
56	MG	2A	3436	1/1	0.83	0.14	-	62,62,62,62	0
56	MG	1a	3186	1/1	0.87	0.19	-	48,48,48,48	0
56	MG	1A	3389	1/1	0.94	0.21	-	34,34,34,34	0
56	MG	2a	1767	1/1	0.91	0.08	-	39,39,39,39	0
56	MG	1A	3114	1/1	0.97	0.32	-	22,22,22,22	0
56	MG	2A	3018	1/1	0.91	0.37	-	51,51,51,51	0
56	MG	2A	3104	1/1	0.94	0.12	-	51,51,51,51	0
56	MG	1a	3146	1/1	0.93	0.16	-	64,64,64,64	0
56	MG	1A	3938	1/1	0.92	0.26	-	40,40,40,40	0
56	MG	1a	3066	1/1	0.95	0.10	-	58,58,58,58	0
56	MG	2a	1618	1/1	0.95	0.42	-	51,51,51,51	0
56	MG	2A	3435	1/1	0.94	0.11	-	47,47,47,47	0
56	MG	2A	3200	1/1	0.95	0.24	-	50,50,50,50	0
56	MG	1Y	502	1/1	0.91	0.10	-	67,67,67,67	0
56	MG	1a	3179	1/1	0.99	0.13	-	39,39,39,39	0
56	MG	1A	3622	1/1	0.90	0.08	-	56,56,56,56	0
56	MG	2a	1668	1/1	0.96	0.17	-	55,55,55,55	0
56	MG	2A	3567	1/1	0.95	0.10	-	44,44,44,44	0
56	MG	2a	1701	1/1	0.89	0.10	-	72,72,72,72	0
56	MG	2a	1745	1/1	0.87	0.13	-	64,64,64,64	0
56	MG	1A	3323	1/1	0.94	0.22	-	19,19,19,19	0
56	MG	1A	3195	1/1	0.92	0.49	-	27,27,27,27	0
56	MG	2A	3689	1/1	0.87	0.13	-	56,56,56,56	0
56	MG	2A	3500	1/1	0.97	0.13	-	49,49,49,49	0
56	MG	2a	1783	1/1	0.92	0.11	-	62,62,62,62	0
56	MG	1A	3774	1/1	0.96	0.11	-	56,56,56,56	0
56	MG	1A	3052	1/1	0.87	0.14	-	31,31,31,31	0
56	MG	1A	3448	1/1	0.97	0.18	-	37,37,37,37	0
56	MG	1A	3946	1/1	0.96	0.11	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3270	1/1	0.96	0.33	-	34,34,34,34	0
56	MG	1A	3818	1/1	0.95	0.05	-	21,21,21,21	0
56	MG	2A	3593	1/1	0.93	0.16	-	47,47,47,47	0
56	MG	2A	3058	1/1	0.81	0.20	-	65,65,65,65	0
56	MG	2A	3408	1/1	0.92	0.10	-	53,53,53,53	0
56	MG	1A	3871	1/1	0.97	0.05	-	59,59,59,59	0
56	MG	2A	3174	1/1	0.88	0.24	-	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.