



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2019 – 05:25 PM EDT

PDB ID : 4Z3S  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with antibiotic A201A, mRNA and three tRNAs in the A, P and E sites at 2.65Å resolution  
Authors : Polikanov, Y.S.; Starosta, A.L.; Juetten, M.F.; Altman, R.B.; Terry, D.S.; Lu, W.; Burnett, B.J.; Dinos, G.; Reynolds, K.; Blanchard, S.C.; Steitz, T.A.; Wilson, D.N.  
Deposited on : 2015-03-31  
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

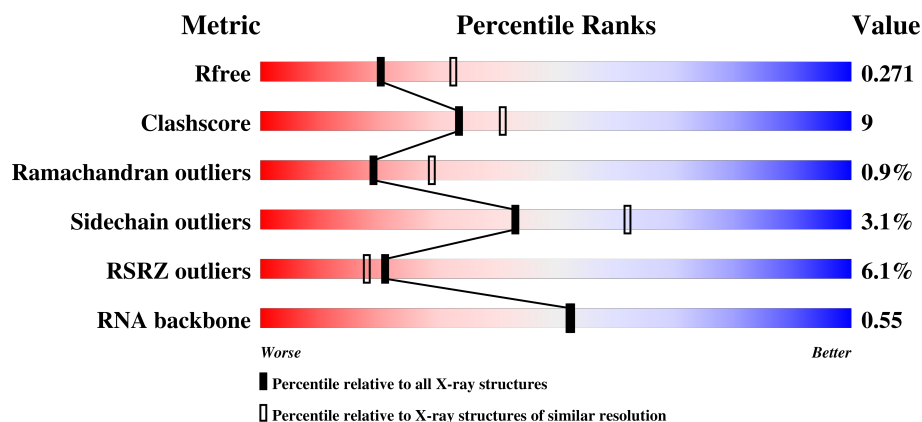
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	111664	1112 (2.68-2.64)
Clashscore	122126	1151 (2.68-2.64)
Ramachandran outliers	120053	1133 (2.68-2.64)
Sidechain outliers	120020	1133 (2.68-2.64)
RSRZ outliers	108989	1098 (2.68-2.64)
RNA backbone	2636	1047 (3.00-2.32)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>2%</div> <div>63%</div> <div>28%</div> <div>7%</div> <div>.</div> </div>
1	2A	2915	<div> <div>2%</div> <div>52%</div> <div>36%</div> <div>8%</div> <div>.</div> <div>.</div> </div>
2	1B	121	<div> <div>76%</div> <div>17%</div> <div>5%</div> <div>.</div> <div>.</div> </div>
2	2B	121	<div> <div>43%</div> <div>42%</div> <div>14%</div> <div>.</div> </div>

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

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

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

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

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Mol	Chain	Length	Quality of chain
53	1v	27	
53	2v	27	
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
54	5MU	2y	54	-	-	-	X
56	MG	1A	3342	-	-	-	X
56	MG	1A	3640	-	-	-	X
56	MG	1P	204	-	-	-	X
56	MG	2A	3163	-	-	-	X
56	MG	2A	3225	-	-	-	X
56	MG	2A	3467	-	-	-	X
56	MG	2A	3470	-	-	-	X
56	MG	2A	3633	-	-	-	X
56	MG	2A	3642	-	-	-	X
56	MG	2Z	8001	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299169 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			

- 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			
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
			1429	916	256	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			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			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			
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			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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	14	Total	C	N	O	P	0	0	0
			281	125	51	91	14			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1588	713	285	515	73	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
54	2w	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	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
			1635	731	295	531	76	2			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1635	731	295	531	76	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	7	Total	Mg	0	0
			7	7		
56	17	1	Total	Mg	0	0
			1	1		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	2	Total	Mg	0	0
			2	2		
56	1N	6	Total	Mg	0	0
			6	6		
56	20	3	Total	Mg	0	0
			3	3		
56	18	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	2	Total 2	Mg 2	0	0
56	13	1	Total 1	Mg 1	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1P	4	Total 4	Mg 4	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2w	3	Total 3	Mg 3	0	0
56	2a	202	Total 202	Mg 202	0	0
56	1E	8	Total 8	Mg 8	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2F	7	Total 7	Mg 7	0	0
56	16	2	Total 2	Mg 2	0	0
56	28	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1W	4	Total 4	Mg 4	0	0
56	1A	929	Total 929	Mg 929	0	0
56	1t	1	Total 1	Mg 1	0	0
56	2p	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	2P	1	Total 1	Mg 1	0	0
56	1X	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	12	2	Total 2	Mg 2	0	0
56	1y	7	Total 7	Mg 7	0	0
56	1S	1	Total 1	Mg 1	0	0
56	25	2	Total 2	Mg 2	0	0
56	2T	1	Total 1	Mg 1	0	0
56	1D	9	Total 9	Mg 9	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	0	0
56	27	1	Total 1	Mg 1	0	0
56	2G	1	Total 1	Mg 1	0	0
56	1I	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	1V	4	Total 4	Mg 4	0	0
56	2X	1	Total 1	Mg 1	0	0
56	1w	5	Total 5	Mg 5	0	0
56	1a	235	Total 235	Mg 235	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	15	5	Total 5	Mg 5	0	0
56	1x	15	Total 15	Mg 15	0	0
56	2j	2	Total 2	Mg 2	0	0
56	1R	2	Total 2	Mg 2	0	0

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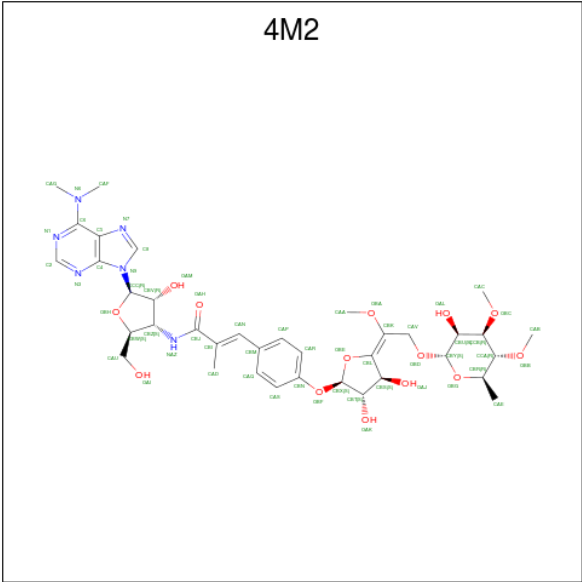
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1s	1	Total 1	Mg 1	0	0
56	1m	1	Total 1	Mg 1	0	0
56	2U	1	Total 1	Mg 1	0	0
56	1G	5	Total 5	Mg 5	0	0
56	2O	2	Total 2	Mg 2	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1d	1	Total 1	Mg 1	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2l	3	Total 3	Mg 3	0	0
56	2g	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2x	3	Total 3	Mg 3	0	0
56	2R	2	Total 2	Mg 2	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	2D	4	Total 4	Mg 4	0	0
56	2q	2	Total 2	Mg 2	0	0
56	1U	4	Total 4	Mg 4	0	0
56	1O	3	Total 3	Mg 3	0	0
56	1r	1	Total 1	Mg 1	0	0
56	19	2	Total 2	Mg 2	0	0
56	1l	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2V	4	Total 4	Mg 4	0	0
56	1F	8	Total 8	Mg 8	0	0
56	10	6	Total 6	Mg 6	0	0
56	1g	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	1Q	5	Total 5	Mg 5	0	0
56	2A	671	Total 671	Mg 671	0	0
56	23	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	1B	25	Total 25	Mg 25	0	0
56	1c	1	Total 1	Mg 1	0	0
56	2v	2	Total 2	Mg 2	0	0

- Molecule 57 is 3'-deoxy-3'-{[(2E)-3-(4-{[(4Z)-6-O-(6-deoxy-3,4-di-O-methyl-alpha-D-manno pyranosyl)-5-O-methyl-alpha-D-threo-hex-4-enofuranosyl]oxy}phenyl)-2-methylprop-2-enoyl]amino}-N,N-dimethyladenosine (three-letter code: 4M2) (formula: C<sub>37</sub>H<sub>50</sub>N<sub>6</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1A	1	Total	C	N	O	0	0
			57	37	6	14		
57	2A	1	Total	C	N	O	0	0
			57	37	6	14		

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1	Total	K	0	0
			1	1		
58	2A	1	Total	K	0	0
			1	1		

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

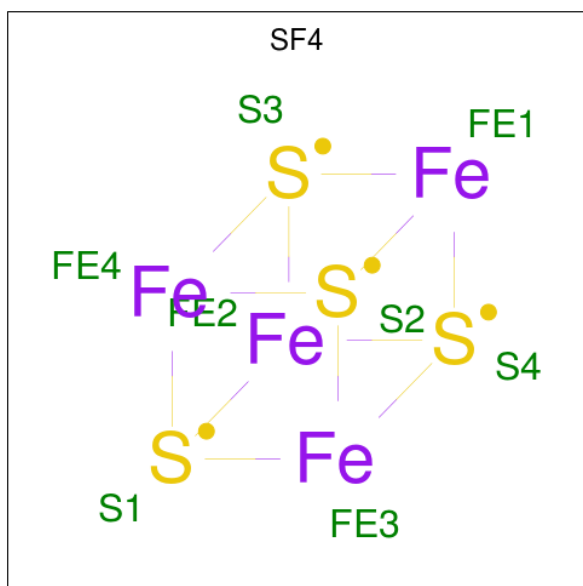
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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		
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:  $\text{Fe}_4\text{S}_4$ ).



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	1741	Total 1741	O 1741	0	0
61	1B	49	Total 49	O 49	0	0
61	1D	21	Total 21	O 21	0	0
61	1E	27	Total 27	O 27	0	0
61	1F	22	Total 22	O 22	0	0
61	1G	3	Total 3	O 3	0	0
61	1I	1	Total 1	O 1	0	0
61	1N	6	Total 6	O 6	0	0
61	1O	4	Total 4	O 4	0	0
61	1P	21	Total 21	O 21	0	0
61	1Q	5	Total 5	O 5	0	0
61	1R	5	Total 5	O 5	0	0
61	1S	6	Total 6	O 6	0	0
61	1T	13	Total 13	O 13	0	0
61	1U	12	Total 12	O 12	0	0
61	1V	10	Total 10	O 10	0	0
61	1W	6	Total 6	O 6	0	0
61	1X	4	Total 4	O 4	0	0
61	1Y	4	Total 4	O 4	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	6	Total 6	O 6	0	0
61	11	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	12	4	Total 4	O 4	0	0
61	13	5	Total 5	O 5	0	0
61	15	1	Total 1	O 1	0	0
61	17	6	Total 6	O 6	0	0
61	18	10	Total 10	O 10	0	0
61	19	2	Total 2	O 2	0	0
61	1a	309	Total 309	O 309	0	0
61	1d	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	3	Total 3	O 3	0	0
61	1m	1	Total 1	O 1	0	0
61	1o	2	Total 2	O 2	0	0
61	1p	2	Total 2	O 2	0	0
61	1q	1	Total 1	O 1	0	0
61	1r	1	Total 1	O 1	0	0
61	1v	6	Total 6	O 6	0	0
61	1w	6	Total 6	O 6	0	0
61	1x	13	Total 13	O 13	0	0
61	1y	5	Total 5	O 5	0	0
61	2A	1031	Total 1031	O 1031	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2B	10	Total 10	O 10	0	0
61	2D	16	Total 16	O 16	0	0
61	2E	10	Total 10	O 10	0	0
61	2F	7	Total 7	O 7	0	0
61	2I	2	Total 2	O 2	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	14	Total 14	O 14	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	3	Total 3	O 3	0	0
61	2U	1	Total 1	O 1	0	0
61	2V	2	Total 2	O 2	0	0
61	2W	1	Total 1	O 1	0	0
61	2X	3	Total 3	O 3	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	6	Total 6	O 6	0	0
61	21	5	Total 5	O 5	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0

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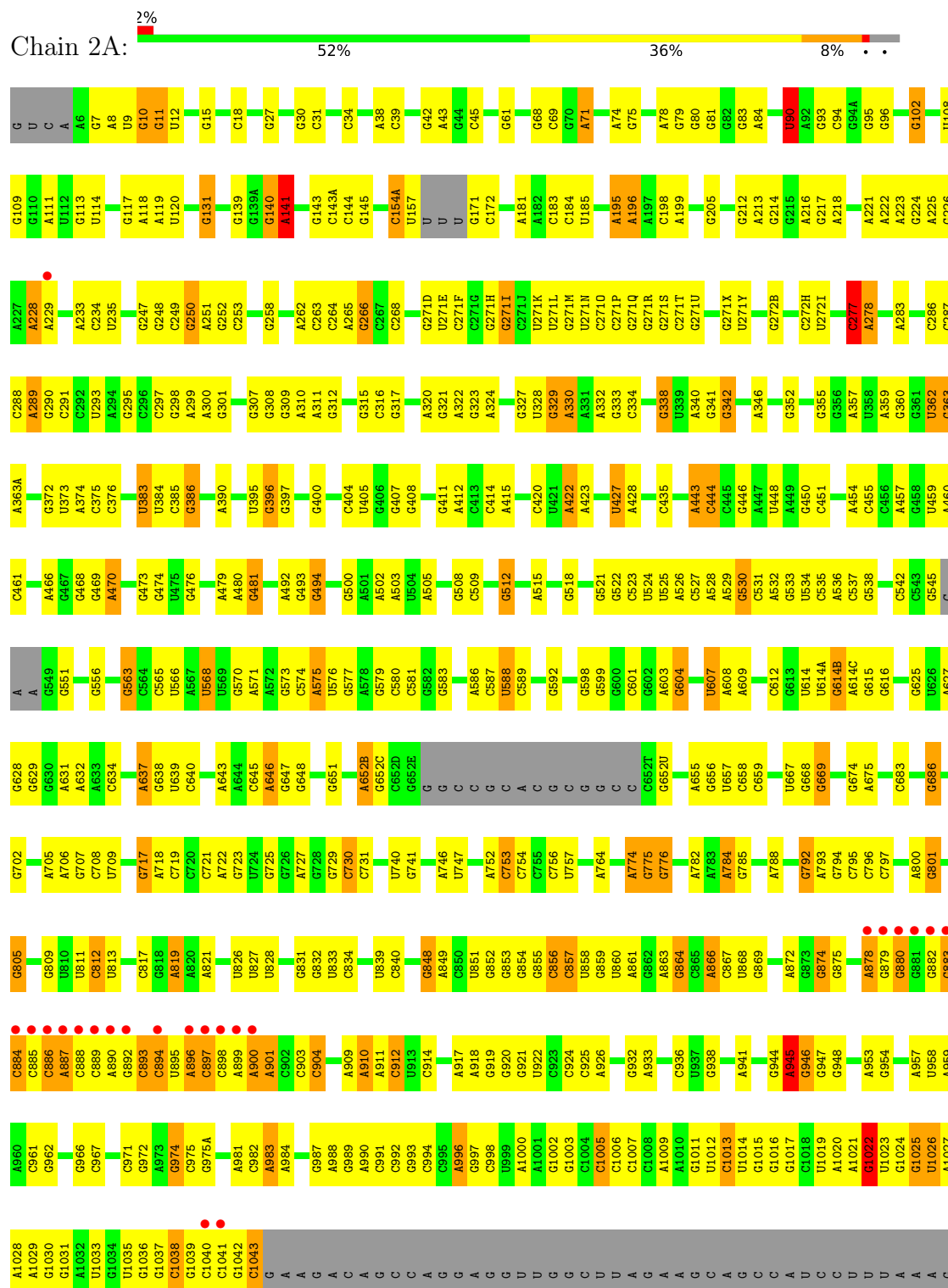
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	25	3	Total 3	O 3	0	0
61	27	3	Total 3	O 3	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
61	2a	203	Total 203	O 203	0	0
61	2d	4	Total 4	O 4	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	3	Total 3	O 3	0	0
61	2o	1	Total 1	O 1	0	0
61	2p	2	Total 2	O 2	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	2	Total 2	O 2	0	0
61	2v	3	Total 3	O 3	0	0
61	2x	6	Total 6	O 6	0	0



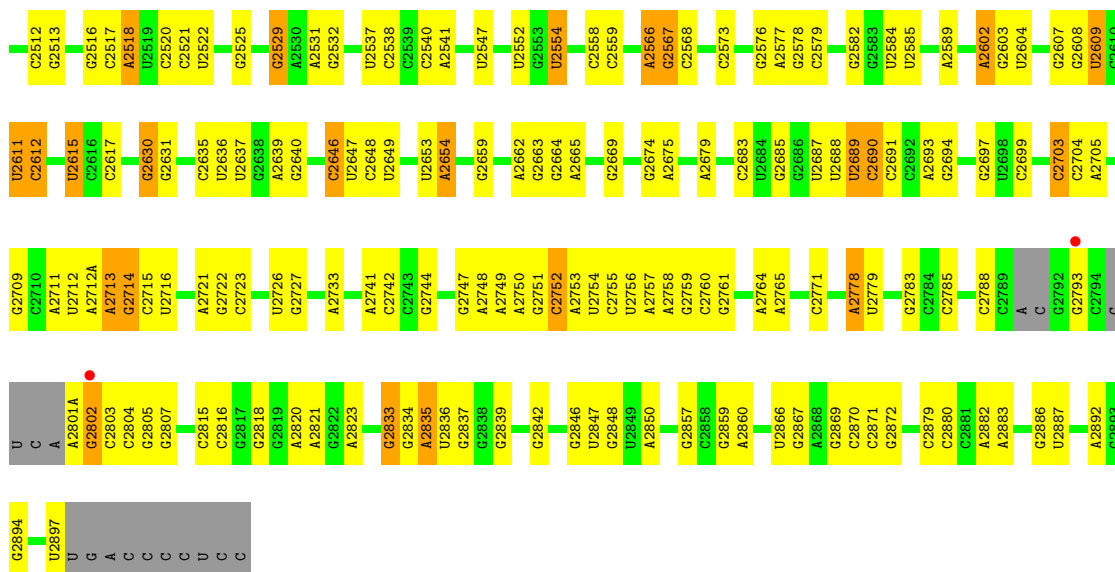
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- Molecule 1: 23S Ribosomal RNA



G2410	A2328	U2244	G2162	G2100	G1997	U1779	A1641	A	G1443	G1256	U1165	A
G2417	G2329	G2251	C2163	G2101	G1998	A1780	G1642	C1536	G1444	A1359	C1166	G
A2418	G2330	G2251	G2164	U2102	C1999	A1781	A1445	G1537	A1445	A1360	G1171	U
U2419	G2331	G2265	G2165	C2103	G2000	C1782	G1647	G1538	G1263	A1262	G	U
G2420	U2332	U2265	U2166	G2104	A2001	A1783	C1648	G1539	A1265	G1264	A	C
A2425	A2333	G2265	U2167	C2105	G2002	A1784	A1652	A1542	G1448	A1365	U	G
G2426	G2334	G2168	G2168	G2106	C2006	A1785	A1652	C1543	A1449	A1366	G	U
G2429	A2335	A2169	A2170	G2110	G1899	A1786	A1653	C1543	A1367	A1267	U	A
A2430	G2337	A2171	A2171	C2111	A1900	A1786	A1654	C1544	A1268	A1267	A	A
U2431	G2340	A2172	A2172	G2112	G1903	C1790	A1665	U1453	G1368	A1269	C1178	U
A2435	U2344	A2173	A2173	G2113	G2012	A1791	A1666	G1455	G1369	C1270	C1179	A
G2436	G2345	C2174	C2174	U2114	A2013	U1794	G1667	C1546	C1370	A1271	C1180	U
U2438	G2347	G2175	G2175	G2115	G1906	C1795	G1667	C1547	G1371	A1272	G	C
A2439	U2348	A2176	A2176	G2116	A1913	U1796	G1674	C1557	U1372	U1273	U	U
G2440	G2349	A2177	A2177	C2117	C1914	U1797	A1558	C1558	G1377	A1278	G1184	C
G2441	G2350	C2178	C2178	U2118	G2018	U1798	U1688	A1566	G1377	A1278	C1185	C
G2445	G2351	U2180	U2180	A2119	A1927	U1799	U1689	A1567	A1468	A1286	C1186	A
G2446	G2352	G2181	G2181	G2120	A1928	C1800	U1690	A1567	A1469	A1287	U1187	C
G2447	G2353	G2182	G2182	G2121	G1929	G1801	U1693	A1568	A1470	A1288	A1189	U
G2448	G2354	C2183	C2183	U2122	U2022	A1802	C1694	G1569	A1471	U1289	G	G
G2449	G2355	G2184	G2184	G2123	A1932	C1804	G1696	U1578	G1482	U1292	U	U
G2450	G2356	G2185	G2185	G2124	A1932	C1804	G1696	U1578	G1482	U1292	C	C
G2451	G2357	G2186	G2186	G2125	G1933	U1805	G1697	A1579	C1386	C1293	G	G
G2452	G2358	G2187	G2187	G2126	A2030	A1698	G1697	A1580	U1394	C1293	A	A
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G2454	G2360	C2189	C2189	G2128	A2033	A1700	G1697	A1581	A1395	A1204	U	U
G2455	G2361	G2190	G2190	G2129	A2034	A1701	G1697	C1582	A1395	U1205	U	U
G2456	G2362	G2191	G2191	U2130	G2035	G1814	G1702	A1583	U1396	A1205	G	G
G2457	G2363	G2192	G2192	G2131	C2036	A1815	G1703	C1403	C1403	A1210	G	G
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G2459	G2365	G2194	G2194	U2133	A2042	G1826	G1704	U1405	U1405	G1218	U	U
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G2463	G2369	U2203	U2203	C2137	C2050	C1830	U1721	C1505	C1505	C1221A	G	G
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G2465	G2371	G2206	G2206	C2140	C2055	C1836	U1739	A1507	A1507	U1313	U	U
G2466	G2372	G2207	G2207	G2141	C2056	C1837	U1740	A1508	A1508	C1314	C	C
G2467	G2373	G2208	G2208	C2142	G2069	A1858	A1741	C1509	C1509	C1315	U	U
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G2469	G2375	G2223	G2223	C2145	G2061	G1860	G1756	A1509B	A1509B	A1317	U	U
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G2471	G2377	G2225	G2225	G2147	C2064	A1848	G1746	G1514	G1514	G1332	U	U
G2472	G2378	G2226	G2226	G2148	C2065	G1857	G1754	G1515	G1515	C1333	U	U
G2473	G2379	G2227	G2227	G2149	C2066	A1857	A1755	G1518	G1518	G1334	U	U
G2474	G2380	G2228	G2228	U2150	G2069	A1858	G1756	U1519	U1519	U1335	U	U
G2475	G2381	G2229	G2229	G2151	G2070	G1860	A1762	G1520	G1520	A1336	U	U
G2476	G2382	U2232	U2232	G2152	A2071	A1876	G1763	G1527	G1527	G1337	U	U
G2477	G2383	U2233	U2233	G2153	A2071	A1877	G1764	G1528	G1528	U1340	U	U
G2478	G2384	G2235	G2235	G2154	G1984	G1878	G1764	A1528A	A1528A	U1341	U	U
G2479	G2385	G2236	G2236	G2155	U2074	G1882	G1772	A1529	A1529	C1345	U	U
G2480	G2386	G2237	G2237	G2156	U2075	G1883	G1773	C1530	C1530	G1248	U	U
G2481	G2387	G2238	G2238	G2157	G2078	G1884	G1774	C1531	C1531	G1250	U	U
G2482	G2388	G2239	G2239	G2158	U2079	A1885	G1775	C1532	C1532	U1382	U	U
G2483	G2389	G2240	G2240	G2159	U1995	A1886	U1776	C1533	C1533	A1353	U	U
G2484	G2390	G2241	G2241	G2160	C1996	C1886	U1778	C1534	C1534	A1254	U	U
G2485	G2391	G2242	G2242	G2161	C1996	C1886	U1778	C1535	C1535	G1355	U	U





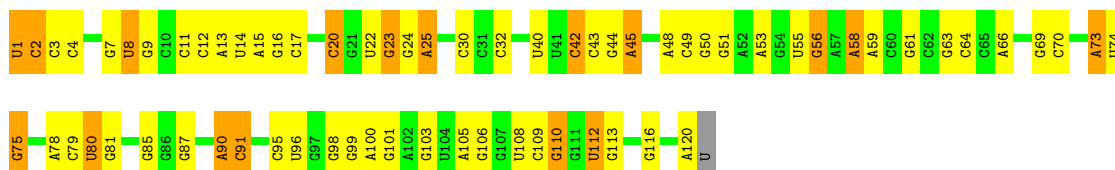
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 76% 17% 5% ..



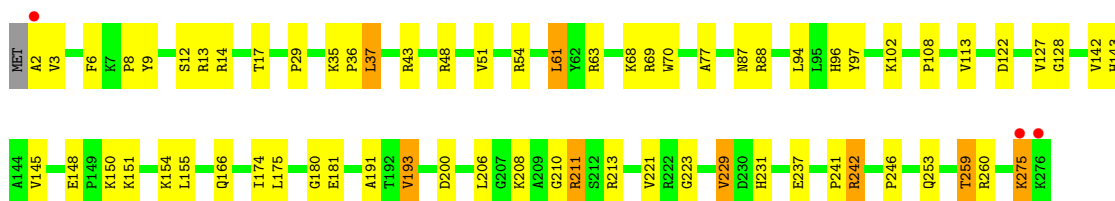
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 43% 42% 14% .



• Molecule 3: 50S ribosomal protein L2

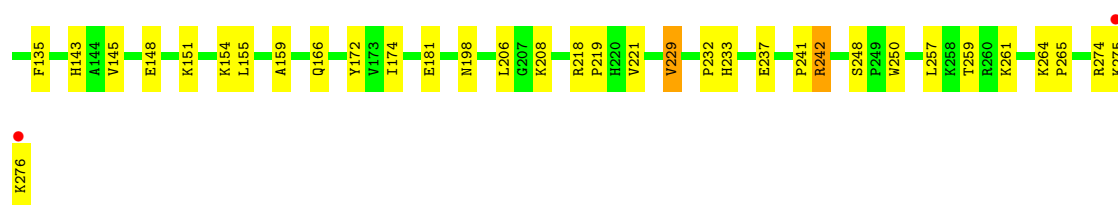
Chain 1D: 75% 21% .



• Molecule 3: 50S ribosomal protein L2

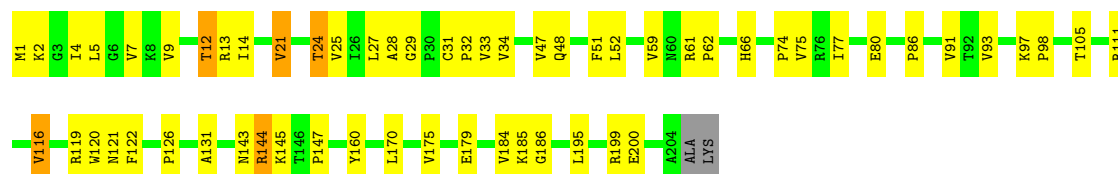
Chain 2D: 75% 23% .





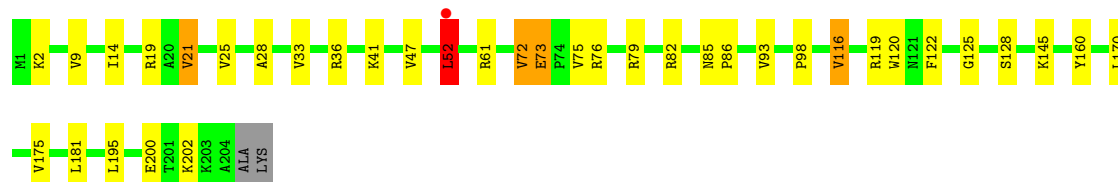
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 70% 26% ..



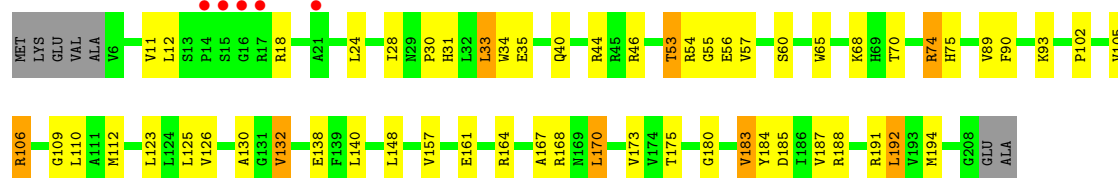
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 81% 16% ..



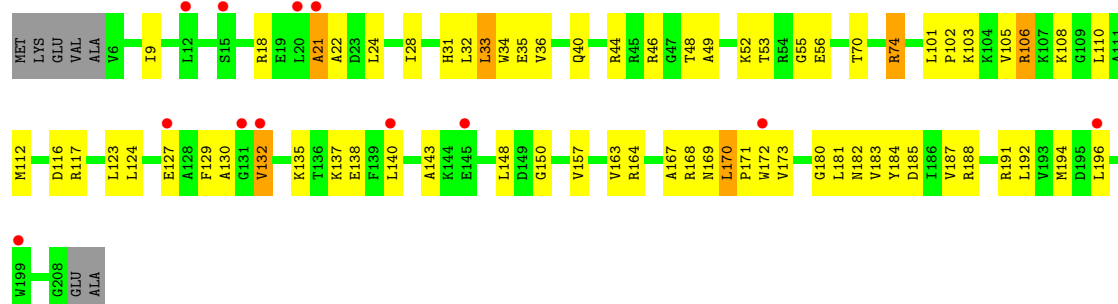
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 2% 69% 24% ..

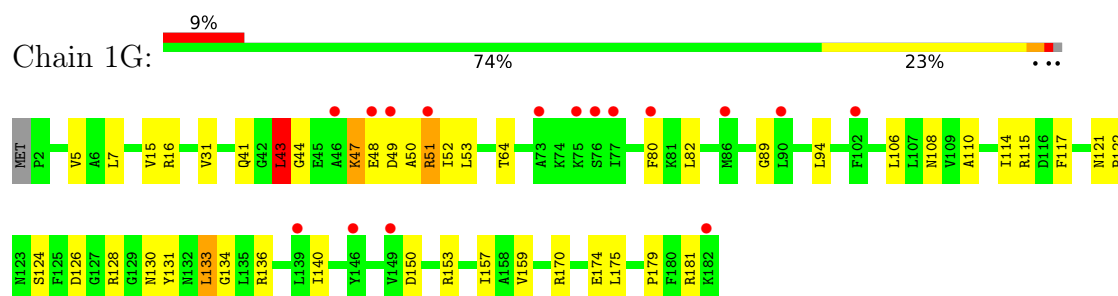


• Molecule 5: 50S ribosomal protein L4

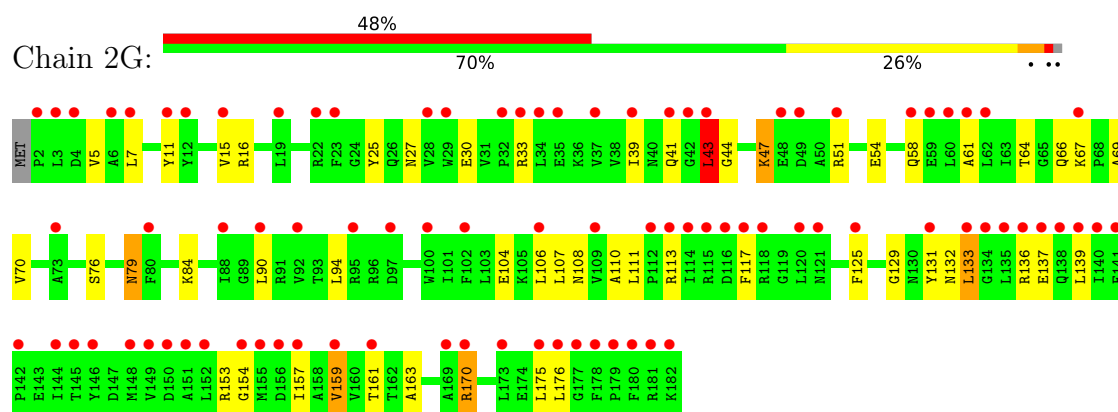
Chain 2F: 6% 64% 30% ..



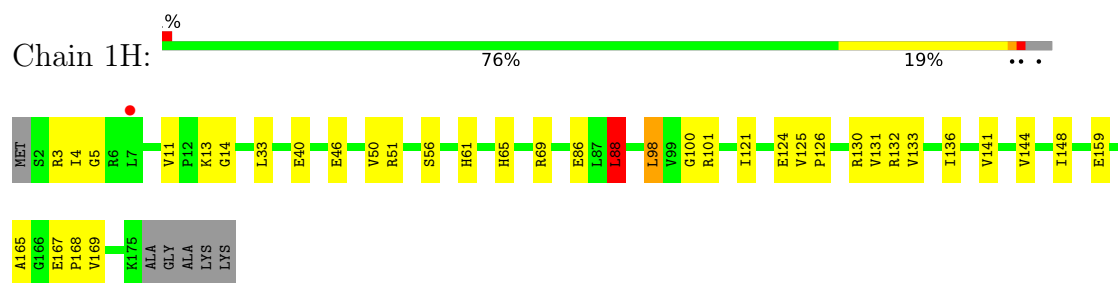
- Molecule 6: 50S ribosomal protein L5



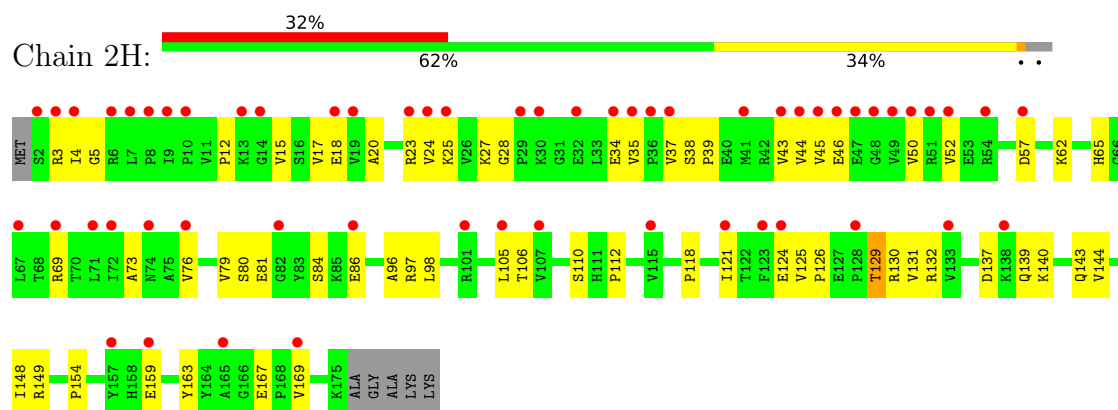
- Molecule 6: 50S ribosomal protein L5



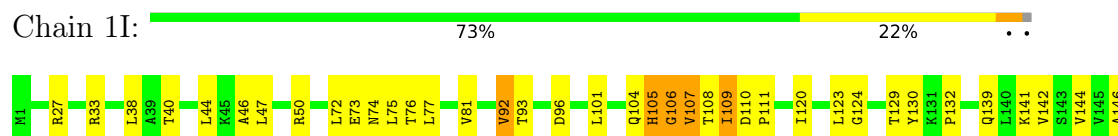
- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6

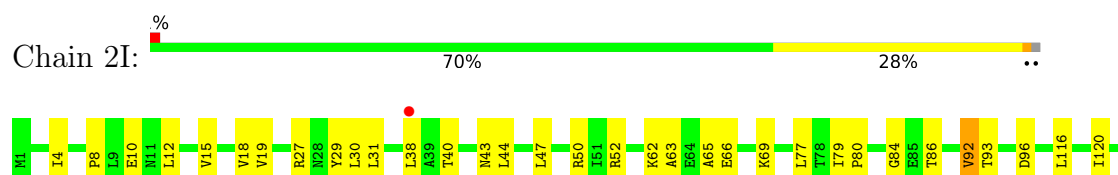


- Molecule 8: 50S ribosomal protein L9



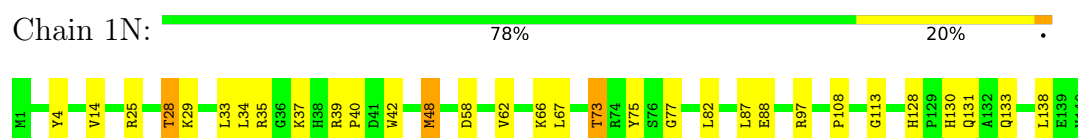
GLN  
GLU

- Molecule 8: 50S ribosomal protein L9

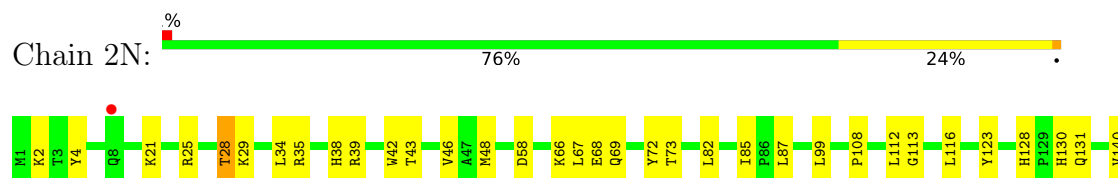


L123  
G124  
Y130  
K131  
P132  
H133  
T138  
Q139  
L140  
K141  
V142  
S143  
V144  
V145  
GLN  
GLU

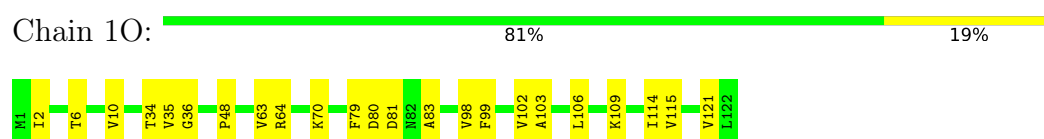
- Molecule 9: 50S ribosomal protein L13



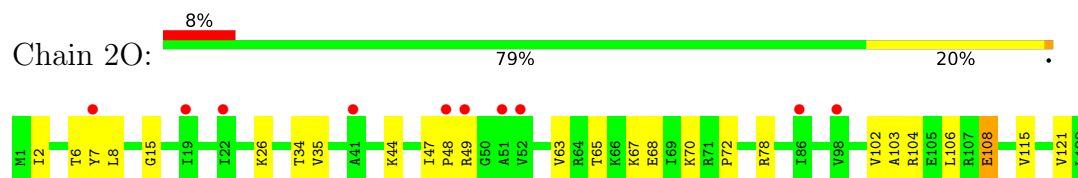
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14

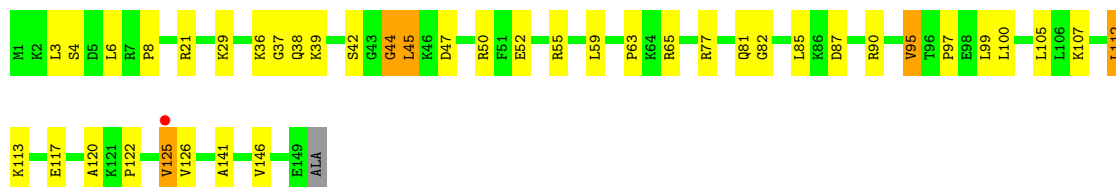
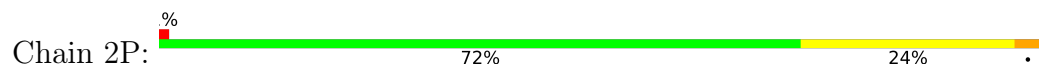


- Molecule 11: 50S ribosomal protein L15

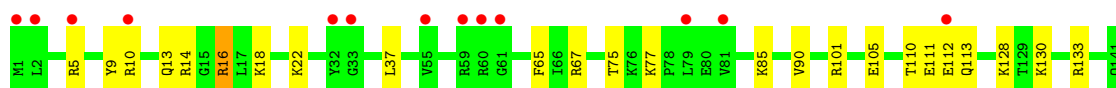
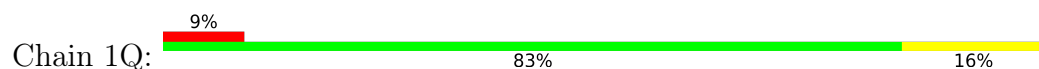




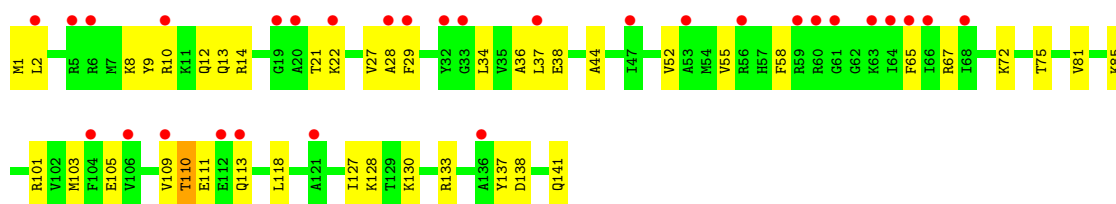
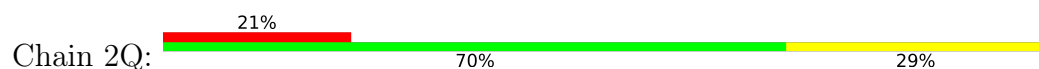
- Molecule 11: 50S ribosomal protein L15



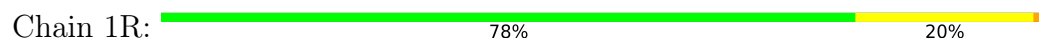
- Molecule 12: 50S ribosomal protein L16



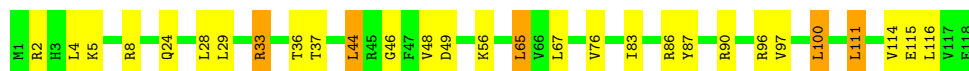
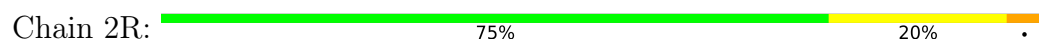
- Molecule 12: 50S ribosomal protein L16




- Molecule 13: 50S ribosomal protein L17

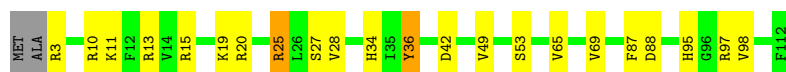


- Molecule 13: 50S ribosomal protein L17




- Molecule 14: 50S ribosomal protein L18

Chain 1S:  79% 18% ..




- Molecule 14: 50S ribosomal protein L18

Chain 2S:  82% 15% ..



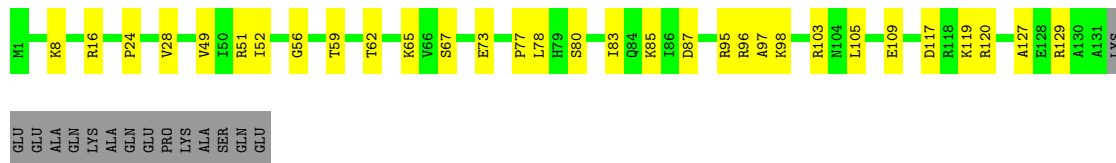
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  74% 16% 10%




- Molecule 15: 50S ribosomal protein L19

Chain 2T:  68% 21% 10%




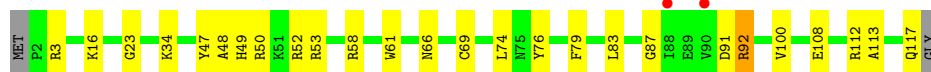
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  82% 16% .




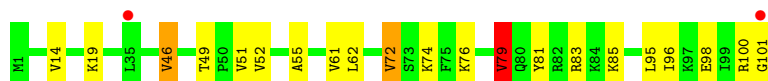
- Molecule 16: 50S ribosomal protein L20

Chain 2U:  76% 21% ..

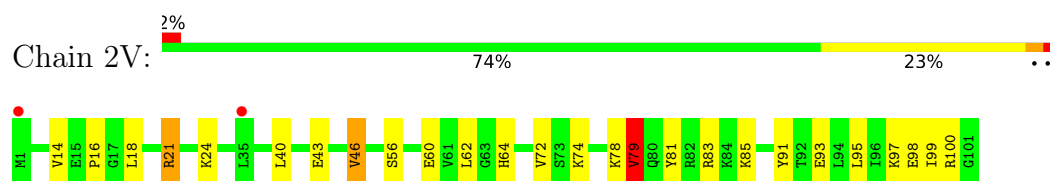


- Molecule 17: 50S ribosomal protein L21

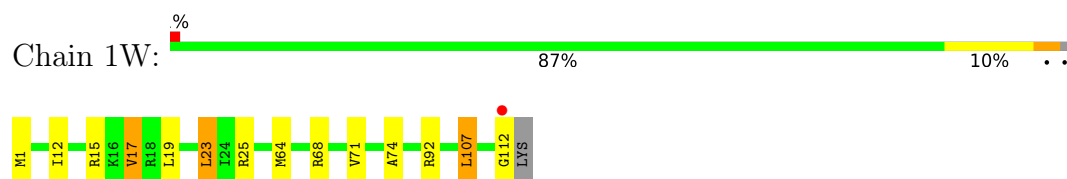
Chain 1V:  79% 18% ..



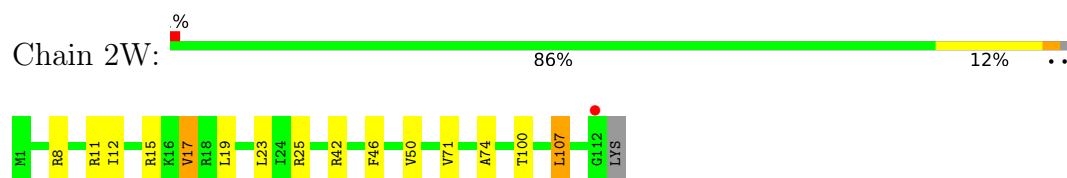
- Molecule 17: 50S ribosomal protein L21



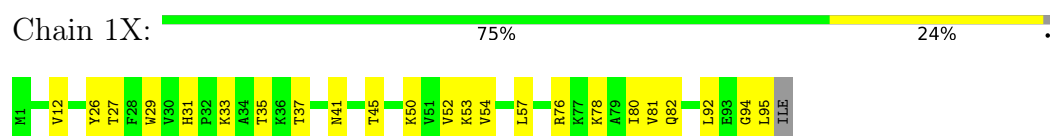
- Molecule 18: 50S ribosomal protein L22



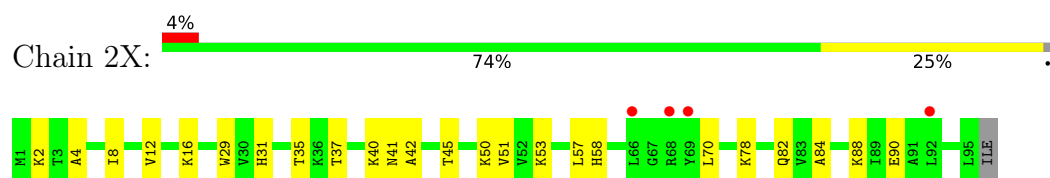
- Molecule 18: 50S ribosomal protein L22



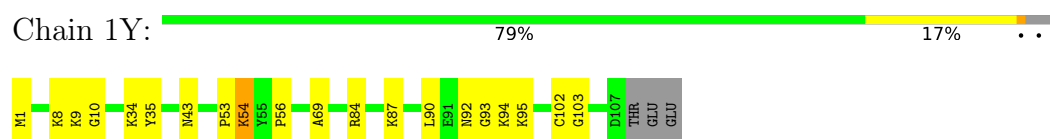
- Molecule 19: 50S ribosomal protein L23



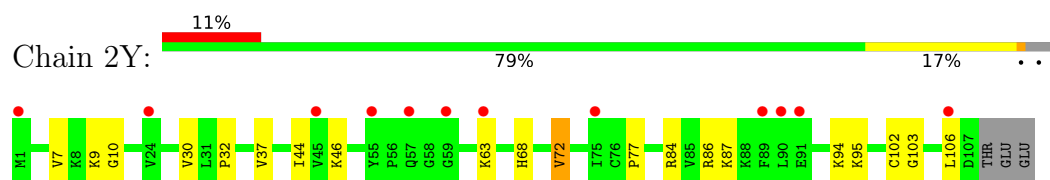
- Molecule 19: 50S ribosomal protein L23



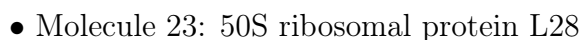
- Molecule 20: 50S ribosomal protein L24



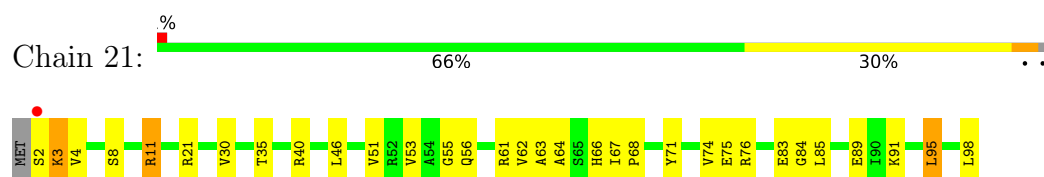
- Molecule 20: 50S ribosomal protein L24



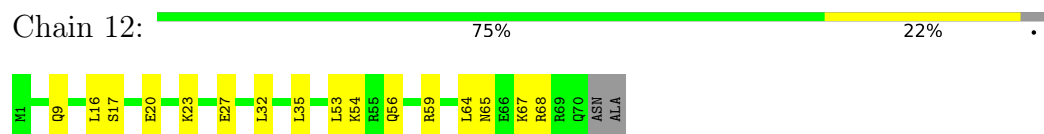
- Molecule 21: 50S ribosomal protein L25



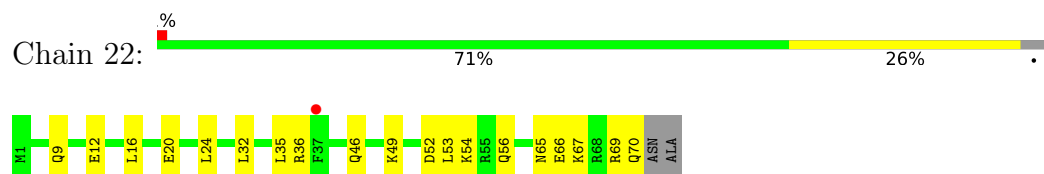




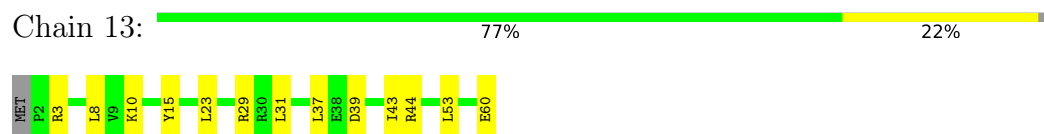
- Molecule 24: 50S ribosomal protein L29



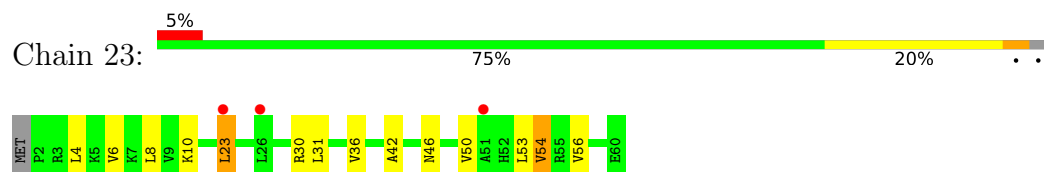
- Molecule 24: 50S ribosomal protein L29



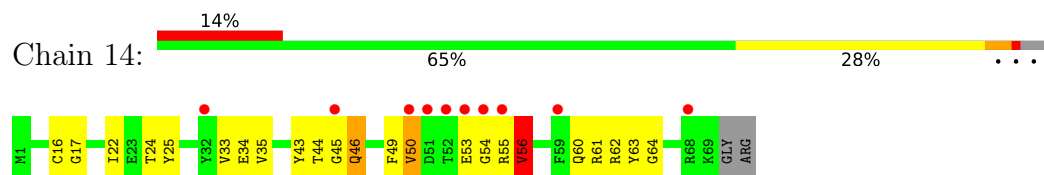
- Molecule 25: 50S ribosomal protein L30



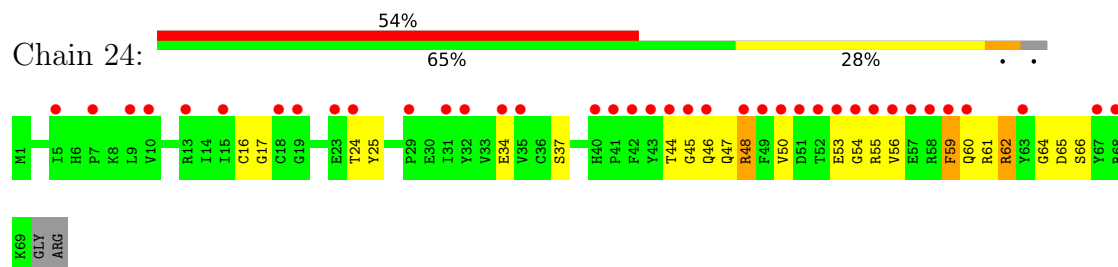
- Molecule 25: 50S ribosomal protein L30



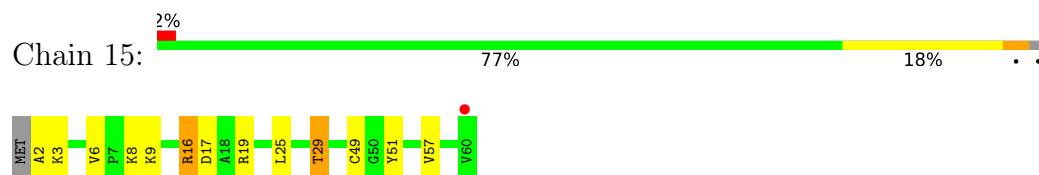
- Molecule 26: 50S ribosomal protein L31



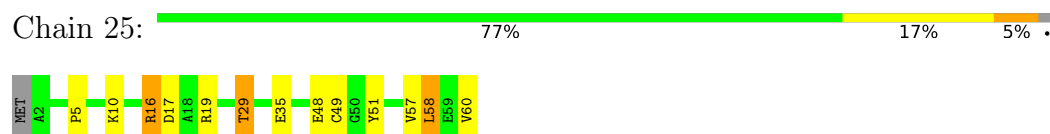
- Molecule 26: 50S ribosomal protein L31



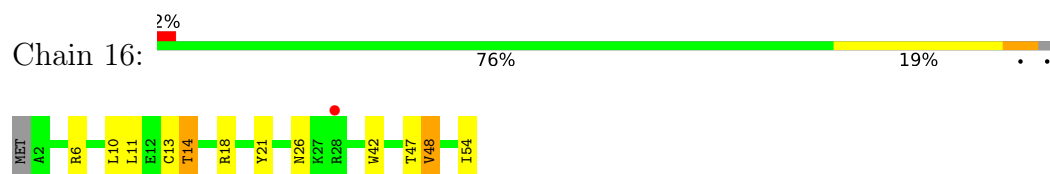
- Molecule 27: 50S ribosomal protein L32



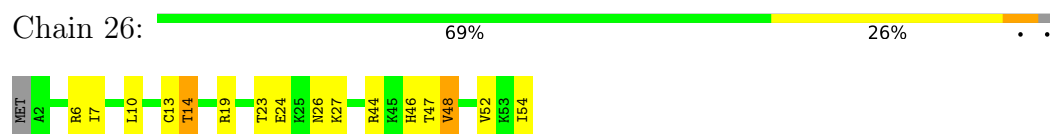
- Molecule 27: 50S ribosomal protein L32



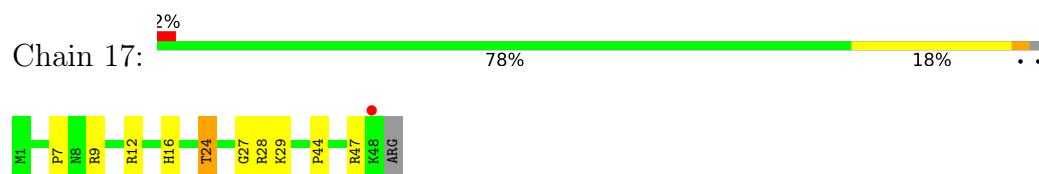
- Molecule 28: 50S ribosomal protein L33



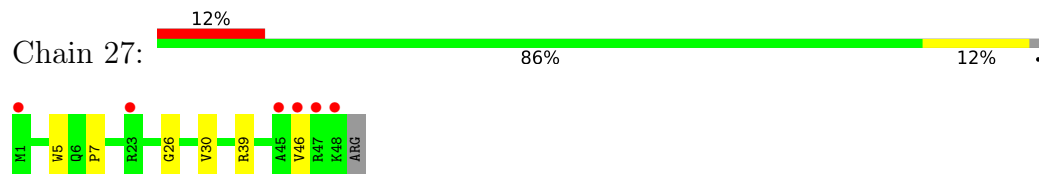
- Molecule 28: 50S ribosomal protein L33



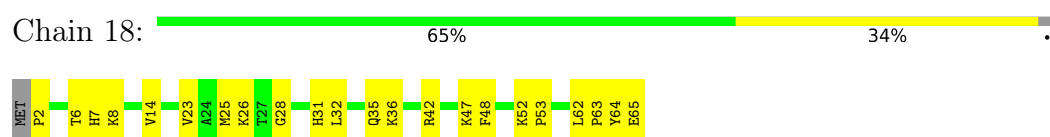
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34

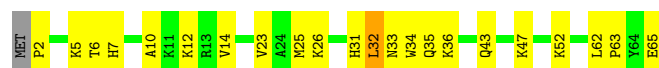


- Molecule 30: 50S ribosomal protein L35



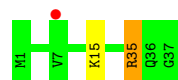
- Molecule 30: 50S ribosomal protein L35

Chain 28:  65% 32% ..



- Molecule 31: 50S ribosomal protein L36

Chain 19:  3% 95% ..




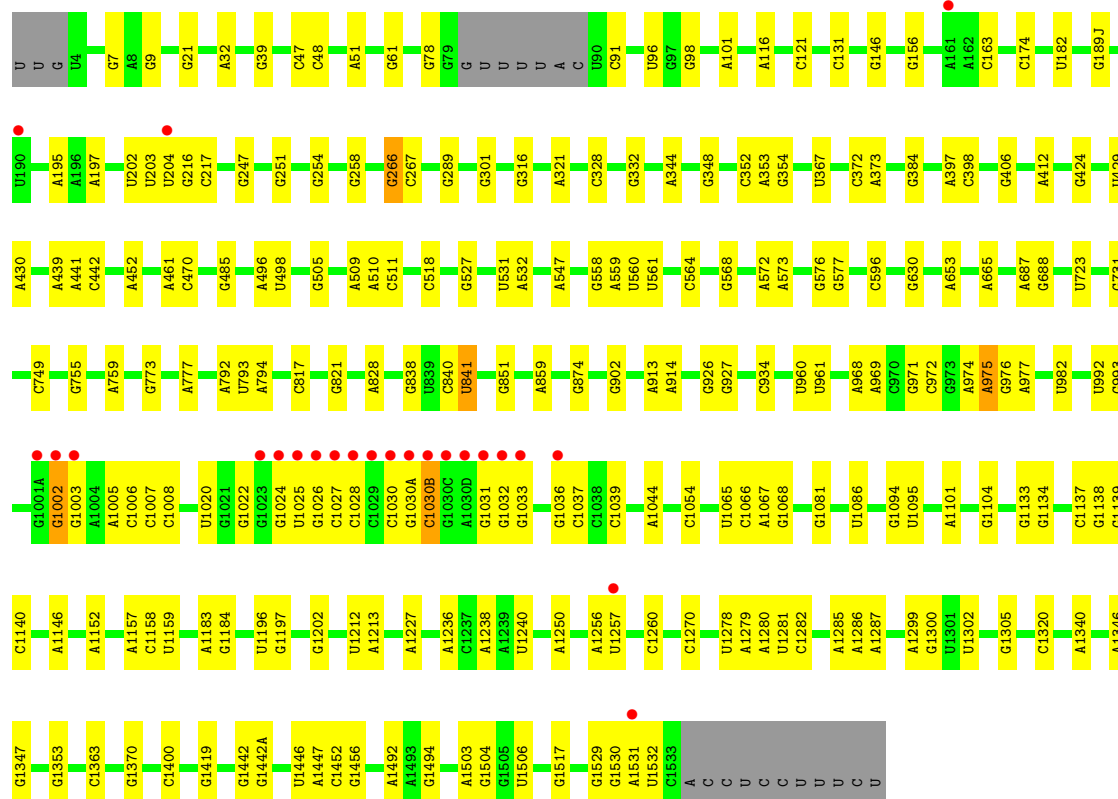
- Molecule 31: 50S ribosomal protein L36

Chain 29:  8% 65% 35%




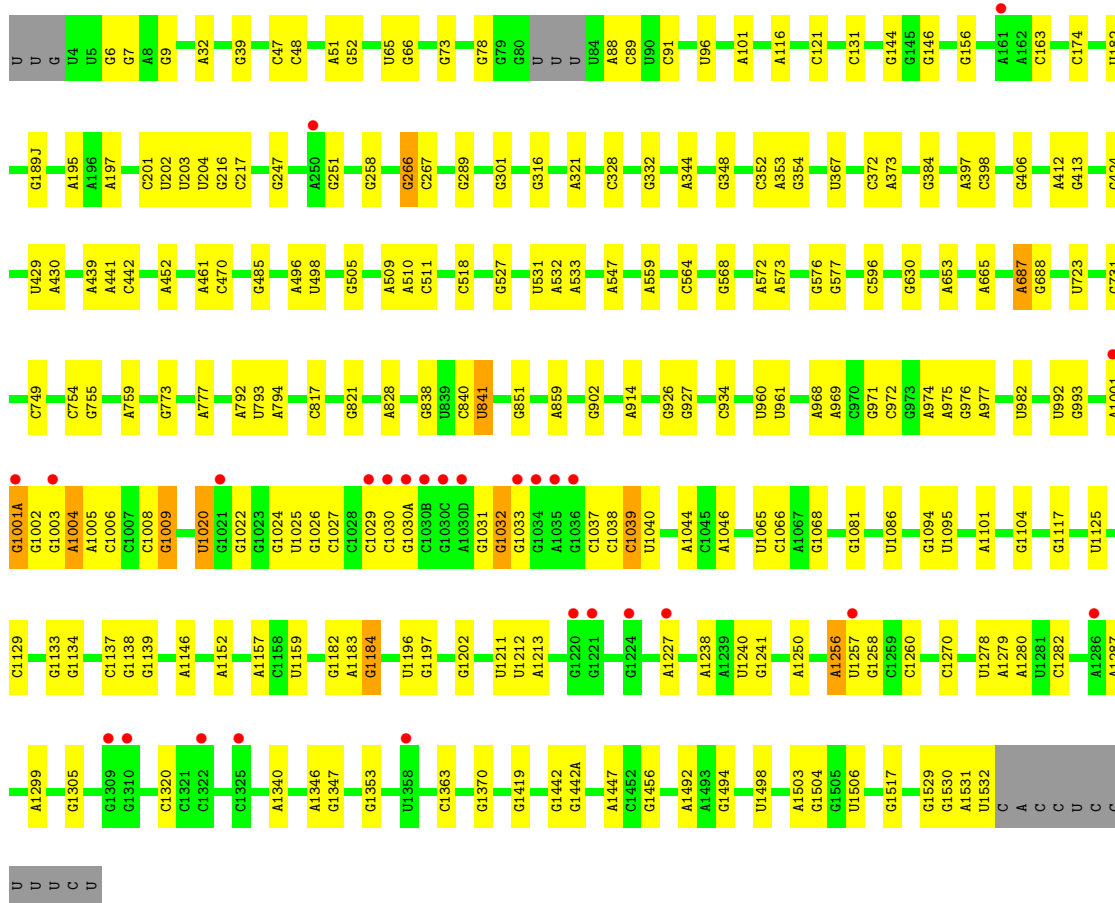
- Molecule 32: 16S Ribosomal RNA

Chain 1a:  2% 84% 15% .



- Molecule 32: 16S Ribosomal RNA

Chain 2a:  2% 84% 14% ..



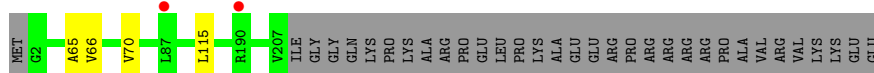
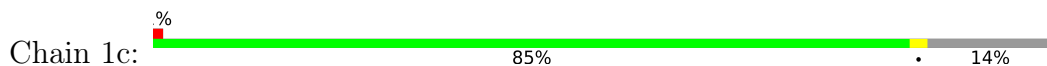
- Molecule 33: 30S ribosomal protein S2



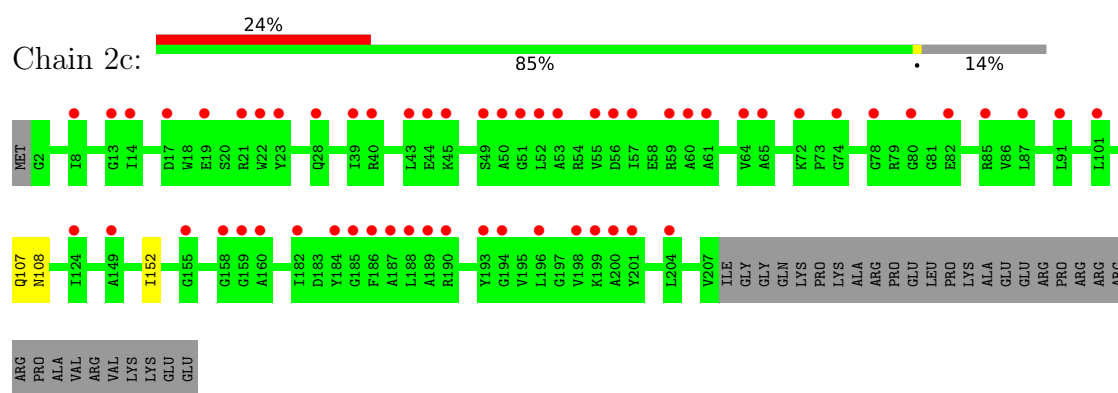
- Molecule 33: 30S ribosomal protein S2



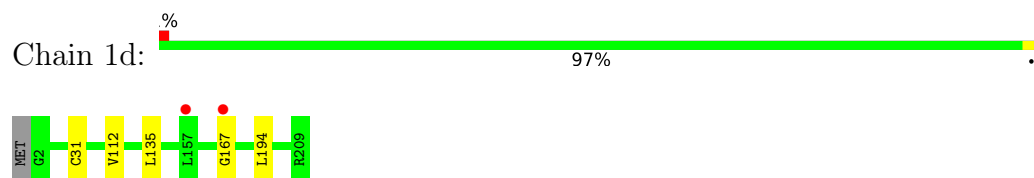
- Molecule 34: 30S ribosomal protein S3



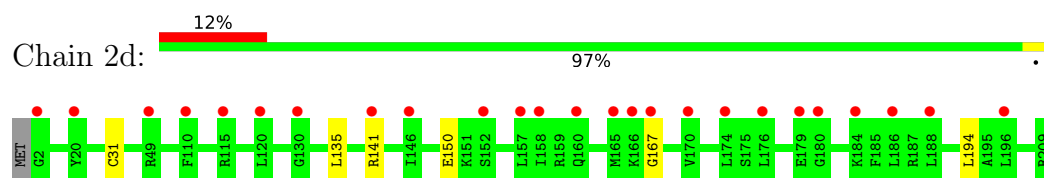
- Molecule 34: 30S ribosomal protein S3



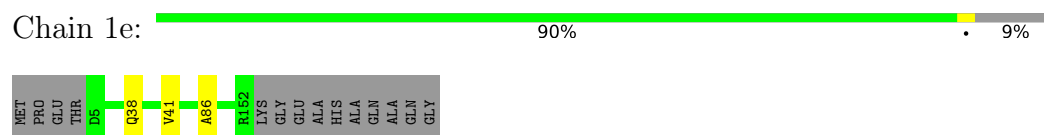
- Molecule 35: 30S ribosomal protein S4



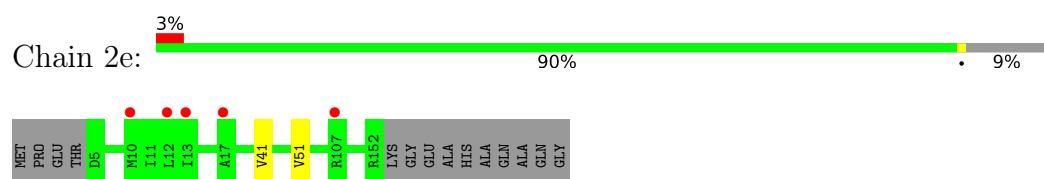
- Molecule 35: 30S ribosomal protein S4



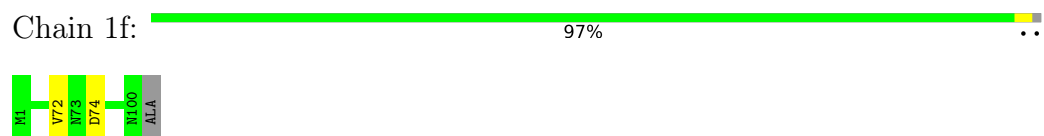
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6

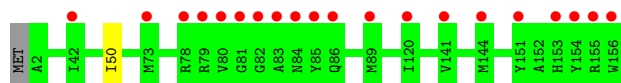


- Molecule 37: 30S ribosomal protein S6

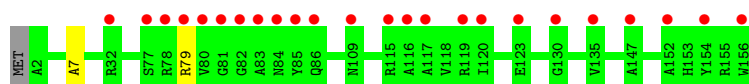




- Molecule 38: 30S ribosomal protein S7



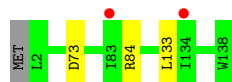
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8



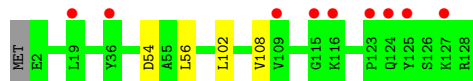
- Molecule 39: 30S ribosomal protein S8



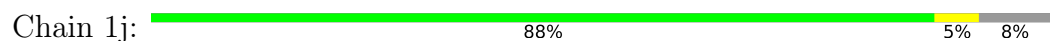
- Molecule 40: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S9

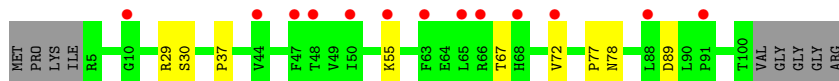
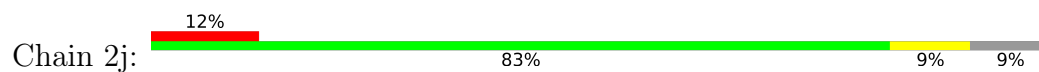


- Molecule 41: 30S ribosomal protein S10

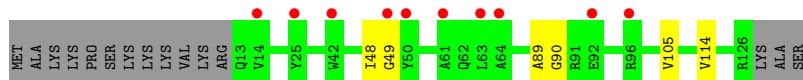
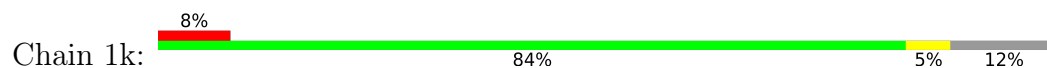




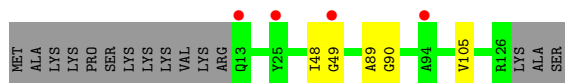
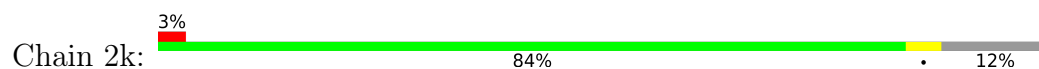
- Molecule 41: 30S ribosomal protein S10



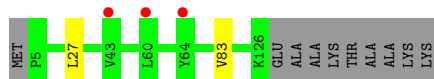
- Molecule 42: 30S ribosomal protein S11



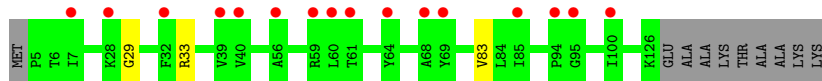
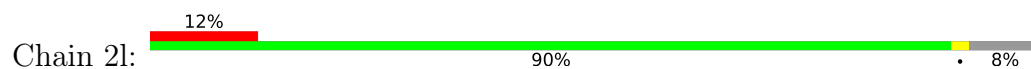
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12

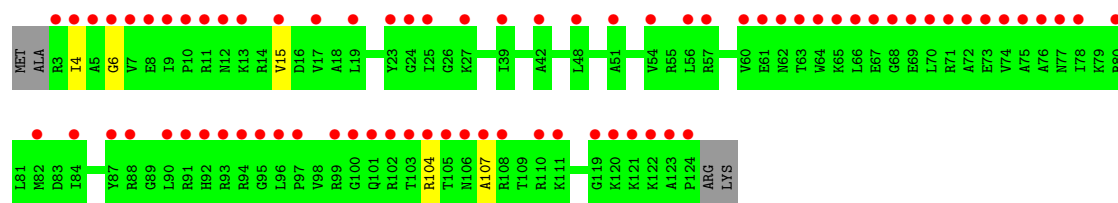


- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13

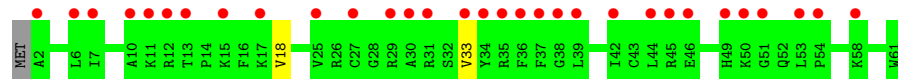




- Molecule 45: 30S ribosomal protein S14 type Z



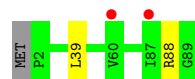
- Molecule 45: 30S ribosomal protein S14 type Z



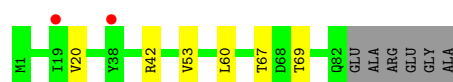
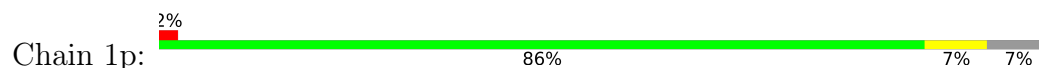
- Molecule 46: 30S ribosomal protein S15



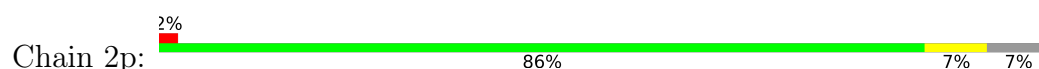
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

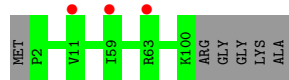


- Molecule 47: 30S ribosomal protein S16

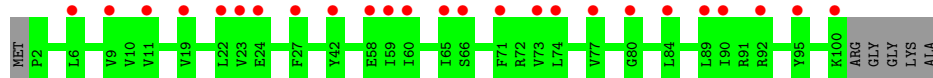




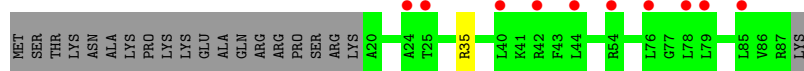
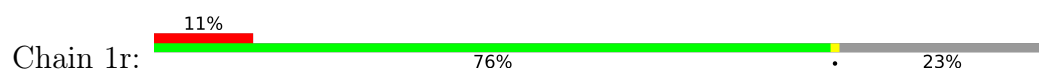
- Molecule 48: 30S ribosomal protein S17



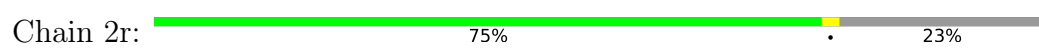
- Molecule 48: 30S ribosomal protein S17



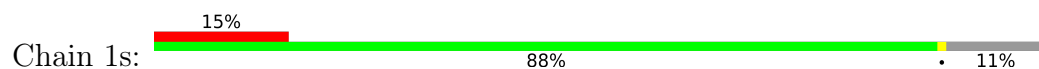
- Molecule 49: 30S ribosomal protein S18



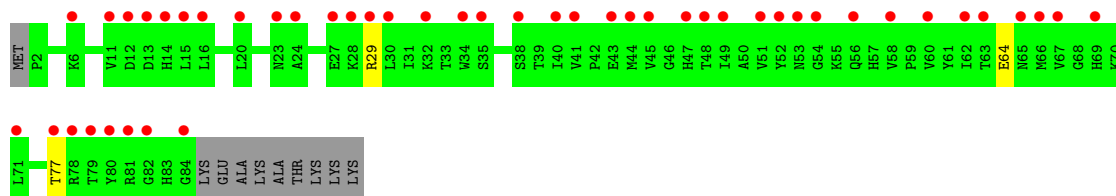
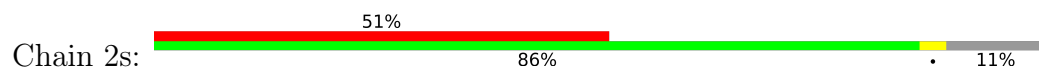
- Molecule 49: 30S ribosomal protein S18



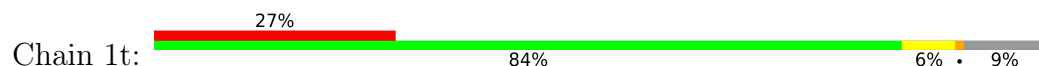
- Molecule 50: 30S ribosomal protein S19



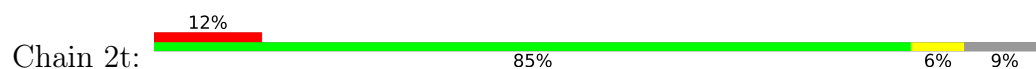
- Molecule 50: 30S ribosomal protein S19



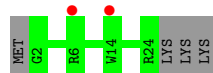
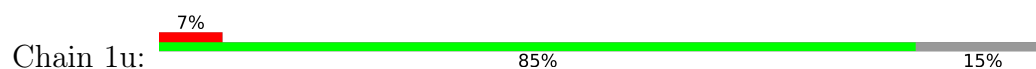
- Molecule 51: 30S ribosomal protein S20



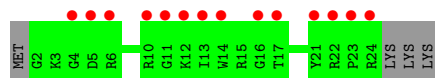
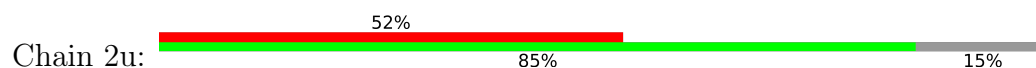
- Molecule 51: 30S ribosomal protein S20



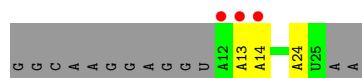
- Molecule 52: 30S ribosomal protein Thx



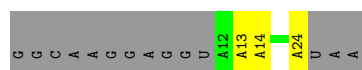
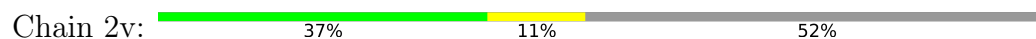
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



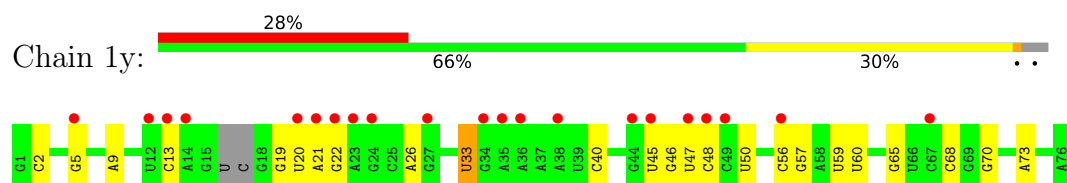
- Molecule 53: mRNA



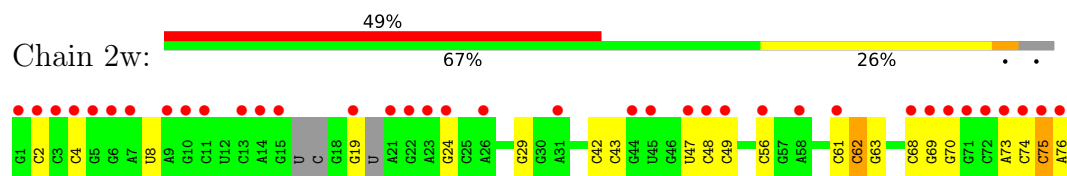
- Molecule 54: A/E-site tRNAs



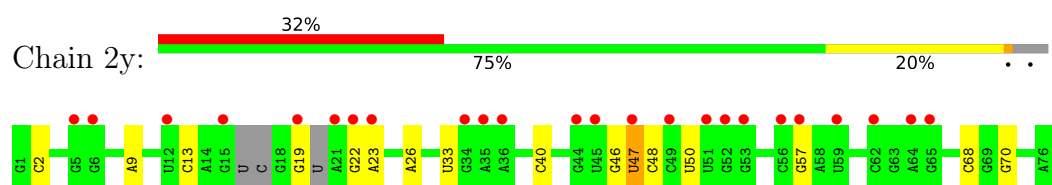
- Molecule 54: A/E-site tRNAs



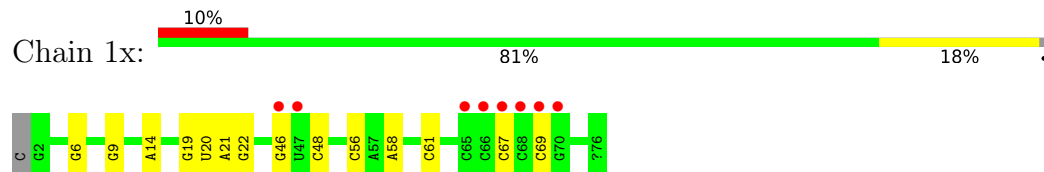
- Molecule 54: A/E-site tRNAs



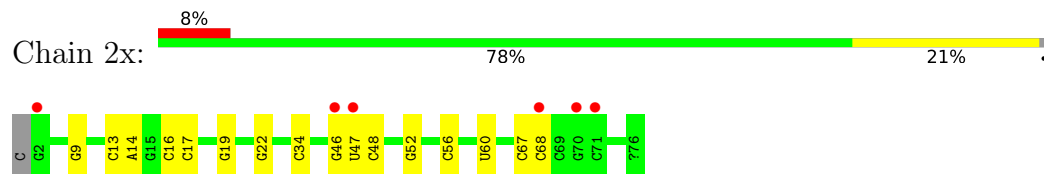
- Molecule 54: A/E-site tRNAs



- 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, $\alpha$ , $\beta$ , $\gamma$	208.89Å 446.22Å 619.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	362.07 – 2.65 362.07 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.5 (362.07-2.65) 98.5 (362.07-2.65)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.226 , 0.271 0.225 , 0.271	Depositor DCC
$R_{free}$ test set	81734 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	299169	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 4M2, 4SU, OMG, 2MU, MIA, MG, SF4, 0TD, ZN, M3O, 2MA, 2MG, 5MC, UR3, MA6, 4OC, M2G, 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	0.94	62/107712 (0.1%)
1	2A	0.42	0/67293	0.92	53/105034 (0.1%)
2	1B	0.43	1/2882 (0.0%)	0.82	0/4494
2	2B	0.48	1/2879 (0.0%)	0.92	1/4487 (0.0%)
3	1D	0.37	0/2186	0.58	0/2944
3	2D	0.34	0/2186	0.56	0/2944
4	1E	0.36	0/1592	0.55	0/2149
4	2E	0.32	0/1592	0.57	1/2149 (0.0%)
5	1F	0.35	0/1619	0.54	0/2193
5	2F	0.32	0/1615	0.55	0/2188
6	1G	0.30	0/1454	0.52	0/1964
6	2G	0.30	0/1453	0.53	0/1963
7	1H	0.31	0/1356	0.52	1/1834 (0.1%)
7	2H	0.28	0/1356	0.52	0/1834
8	1I	0.28	0/1112	0.53	0/1514
8	2I	0.26	0/1079	0.52	0/1475
9	1N	0.34	0/1144	0.52	0/1543
9	2N	0.31	0/1144	0.51	0/1543
10	1O	0.37	0/943	0.53	0/1269
10	2O	0.32	0/943	0.50	0/1269
11	1P	0.36	0/1152	0.59	0/1533
11	2P	0.31	0/1152	0.63	1/1533 (0.1%)
12	1Q	0.36	0/1143	0.53	0/1527
12	2Q	0.33	0/1143	0.54	0/1527
13	1R	0.35	0/982	0.54	0/1312
13	2R	0.31	0/982	0.52	0/1312
14	1S	0.32	0/883	0.54	0/1176
14	2S	0.31	0/880	0.56	0/1172
15	1T	0.32	0/1105	0.51	0/1477
15	2T	0.31	0/1097	0.53	0/1468
16	1U	0.41	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.34	0/977	0.53	0/1301
17	1V	0.38	0/782	0.53	0/1049
17	2V	0.34	0/782	0.53	0/1049
18	1W	0.35	0/897	0.55	0/1205
18	2W	0.33	0/897	0.53	0/1205
19	1X	0.39	0/764	0.59	0/1025
19	2X	0.31	0/764	0.53	0/1025
20	1Y	0.33	0/819	0.56	0/1095
20	2Y	0.31	0/819	0.57	0/1095
21	1Z	0.30	0/1267	0.52	0/1717
21	2Z	0.31	0/1299	0.54	0/1763
22	10	0.37	0/662	0.61	0/881
22	20	0.29	0/662	0.47	0/881
23	11	0.34	0/762	0.49	0/1014
23	21	0.31	0/762	0.51	0/1014
24	12	0.32	0/590	0.50	0/781
24	22	0.30	0/590	0.47	0/781
25	13	0.34	0/474	0.56	0/635
25	23	0.29	0/469	0.52	0/630
26	14	0.33	0/565	0.65	0/761
26	24	0.33	0/545	0.66	0/737
27	15	0.35	0/469	0.59	0/635
27	25	0.32	0/469	0.55	1/635 (0.2%)
28	16	0.35	0/460	0.50	0/613
28	26	0.29	0/456	0.46	0/608
29	17	0.35	0/426	0.58	0/561
29	27	0.36	0/426	0.54	0/561
30	18	0.33	0/525	0.54	0/691
30	28	0.32	0/525	0.51	0/691
31	19	0.38	0/310	0.51	0/407
31	29	0.32	0/310	0.51	0/407
32	1a	0.37	0/35795	0.86	21/55864 (0.0%)
32	2a	0.37	0/35886	0.89	26/56005 (0.0%)
33	1b	0.29	0/1881	0.54	0/2542
33	2b	0.31	0/1860	0.59	0/2518
34	1c	0.27	0/1572	0.47	0/2126
34	2c	0.31	0/1566	0.52	0/2119
35	1d	0.29	0/1685	0.52	0/2262
35	2d	0.30	0/1704	0.51	0/2284
36	1e	0.29	0/1145	0.50	0/1543
36	2e	0.29	0/1149	0.55	0/1548
37	1f	0.29	0/823	0.50	0/1115
37	2f	0.30	0/829	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.28	0/1250	0.48	0/1679
38	2g	0.28	0/1254	0.51	0/1683
39	1h	0.29	0/1108	0.51	0/1494
39	2h	0.27	0/1108	0.53	0/1494
40	1i	0.29	0/1002	0.55	1/1346 (0.1%)
40	2i	0.29	0/997	0.52	0/1343
41	1j	0.27	0/722	0.55	0/982
41	2j	0.30	0/727	0.54	0/988
42	1k	0.27	0/844	0.49	0/1145
42	2k	0.29	0/848	0.50	0/1149
43	1l	0.31	0/937	0.51	0/1260
43	2l	0.29	0/937	0.54	1/1260 (0.1%)
44	1m	0.28	0/969	0.58	0/1302
44	2m	0.29	0/961	0.57	0/1291
45	1n	0.29	0/501	0.50	0/664
45	2n	0.28	0/501	0.52	0/664
46	1o	0.28	0/739	0.49	0/985
46	2o	0.28	0/739	0.48	0/985
47	1p	0.28	0/697	0.54	0/939
47	2p	0.28	0/693	0.53	0/935
48	1q	0.28	0/836	0.50	0/1117
48	2q	0.29	0/836	0.51	0/1117
49	1r	0.29	0/560	0.49	0/746
49	2r	0.27	0/560	0.48	0/746
50	1s	0.27	0/667	0.53	0/900
50	2s	0.33	0/661	0.61	0/893
51	1t	0.27	0/730	0.51	0/965
51	2t	0.28	0/729	0.51	0/965
52	1u	0.27	0/203	0.58	0/266
52	2u	0.29	0/203	0.49	0/266
53	1v	0.34	0/314	0.80	0/487
53	2v	0.38	0/310	0.85	0/480
54	1w	0.42	0/1602	1.08	3/2493 (0.1%)
54	1y	0.43	0/1602	1.11	4/2493 (0.2%)
54	2w	0.43	0/1579	1.02	3/2455 (0.1%)
54	2y	0.45	0/1579	1.05	2/2455 (0.1%)
55	1x	0.52	1/1700 (0.1%)	1.15	18/2650 (0.7%)
55	2x	0.45	0/1700	1.13	8/2650 (0.3%)
All	All	0.40	3/316657 (0.0%)	0.84	207/474074 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
38	2g	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1B	1	U	OP3-P	-10.26	1.48	1.61
2	2B	1	U	OP3-P	-10.14	1.49	1.61
55	1x	22	G	N7-C5	5.84	1.42	1.39

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	46	G	C6-N1-C2	-10.46	118.82	125.10
32	2a	1004	A	O4'-C1'-N9	9.58	115.87	108.20
1	1A	512	G	O4'-C1'-N9	9.34	115.67	108.20
32	1a	254	G	O5'-P-OP1	-9.15	97.46	105.70
1	1A	2682	U	O5'-P-OP2	-8.65	97.92	105.70
32	2a	1020	U	N1-C2-O2	8.48	128.74	122.80
55	1x	22	G	C5-N7-C8	-8.45	100.08	104.30
55	2x	14	A	C4-C5-C6	8.25	121.12	117.00
55	2x	46	G	C6-N1-C2	-8.17	120.20	125.10
55	1x	14	A	C4-C5-C6	8.13	121.07	117.00
1	1A	2167	U	C2-N1-C1'	8.02	127.33	117.70
1	1A	975	C	N1-C2-O2	-7.97	114.12	118.90
1	2A	2149	G	N3-C4-N9	7.82	130.69	126.00
32	1a	1002	G	N3-C4-N9	7.72	130.63	126.00
1	1A	2554	U	O5'-P-OP1	-7.65	98.82	105.70
55	1x	22	G	C4-C5-C6	-7.64	114.21	118.80
32	2a	1001(A)	G	N3-C4-N9	7.63	130.58	126.00
55	1x	14	A	C5-N7-C8	7.60	107.70	103.90
1	1A	1075	C	N1-C2-O2	7.60	123.46	118.90
1	2A	2152	G	C5-C6-O6	-7.58	124.05	128.60
1	1A	1026	U	O5'-P-OP1	-7.53	98.92	105.70
1	1A	2167	U	N3-C2-O2	-7.44	116.99	122.20
32	1a	1002	G	C4-N9-C1'	7.37	136.07	126.50
1	1A	527	C	N1-C2-O2	-7.35	114.49	118.90
1	1A	1086	A	N1-C6-N6	-7.31	114.21	118.60
1	1A	2061	G	O5'-P-OP2	-7.31	99.12	105.70
1	1A	2167	U	N1-C2-O2	7.24	127.86	122.80
55	1x	22	G	N1-C6-O6	-7.20	115.58	119.90
2	2B	80	U	O4'-C1'-N1	7.19	113.95	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1002	G	C8-N9-C1'	-7.17	117.69	127.00
1	1A	588	U	O5'-P-OP2	-7.16	99.25	105.70
1	1A	12	U	C2-N1-C1'	7.04	126.15	117.70
1	2A	2140	C	N1-C2-O2	7.02	123.11	118.90
1	1A	1075	C	C2-N3-C4	6.96	123.38	119.90
55	1x	46	G	C5-C6-N1	6.93	114.97	111.50
1	1A	2028	U	N3-C4-O4	-6.92	114.56	119.40
1	2A	2473	U	C2-N1-C1'	6.90	125.98	117.70
1	1A	1639	U	O5'-P-OP2	-6.86	99.53	105.70
1	2A	1698	A	O4'-C1'-N9	6.80	113.64	108.20
1	1A	801	G	O5'-P-OP2	-6.80	99.58	105.70
1	2A	2140	C	C2-N1-C1'	6.79	126.27	118.80
55	2x	22	G	N1-C6-O6	-6.72	115.87	119.90
1	2A	2139	C	C2-N1-C1'	6.69	126.16	118.80
55	2x	14	A	C5-N7-C8	6.68	107.24	103.90
54	1y	33	U	C2-N1-C1'	6.59	125.61	117.70
1	2A	2152	G	N1-C6-O6	6.59	123.85	119.90
1	2A	2143	C	C2-N3-C4	6.56	123.18	119.90
1	1A	1992	G	P-O3'-C3'	6.52	127.52	119.70
55	1x	22	G	N3-C4-N9	-6.51	122.10	126.00
32	2a	1001(A)	G	C8-N9-C1'	-6.50	118.54	127.00
1	1A	226	G	O4'-C1'-N9	6.45	113.36	108.20
1	2A	2136	C	N1-C2-O2	6.43	122.76	118.90
32	2a	1001(A)	G	C4-N9-C1'	6.42	134.85	126.50
54	1y	33	U	N1-C2-O2	6.40	127.28	122.80
55	1x	14	A	C5-C6-N1	-6.40	114.50	117.70
55	2x	22	G	C5-N7-C8	-6.38	101.11	104.30
1	1A	975	C	O5'-P-OP1	-6.36	99.97	105.70
1	2A	1266	G	C8-N9-C4	6.34	108.94	106.40
1	2A	2149	G	C8-N9-C1'	-6.31	118.80	127.00
1	1A	624	C	O5'-P-OP1	-6.27	100.06	105.70
1	1A	1614	A	O5'-P-OP1	-6.25	100.08	105.70
1	2A	2473	U	N3-C2-O2	-6.22	117.85	122.20
1	1A	1176	G	OP1-P-O3'	6.20	118.83	105.20
32	2a	1039	C	C5-C4-N4	-6.19	115.86	120.20
1	2A	2149	G	C4-N9-C1'	6.16	134.50	126.50
32	2a	841	U	C5-C6-N1	6.14	125.77	122.70
32	1a	560	U	C2-N1-C1'	6.11	125.03	117.70
1	1A	1352	U	O5'-P-OP1	-6.08	100.23	105.70
32	2a	1184	G	N3-C4-N9	6.03	129.62	126.00
1	2A	1313	U	C2-N1-C1'	6.03	124.93	117.70
1	1A	1653	G	P-O3'-C3'	6.02	126.92	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	754	C	C2-N1-C1'	6.01	125.41	118.80
55	1x	22	G	N7-C8-N9	5.96	116.08	113.10
1	1A	2130	U	C5-C6-N1	5.96	125.68	122.70
1	1A	383	U	O4'-C1'-N1	5.95	112.96	108.20
40	1i	50	LEU	CA-CB-CG	5.94	128.96	115.30
1	1A	2848	G	O4'-C1'-N9	5.93	112.94	108.20
32	2a	1029	C	N1-C2-O2	5.93	122.46	118.90
54	2y	23	A	N1-C6-N6	5.91	122.15	118.60
1	1A	2629	A	P-O3'-C3'	5.88	126.75	119.70
1	1A	975	C	C2-N1-C1'	-5.87	112.34	118.80
32	2a	754	C	N1-C2-O2	5.84	122.41	118.90
55	2x	17	C	C2-N1-C1'	5.84	125.23	118.80
1	1A	748	G	C4-N9-C1'	-5.84	118.91	126.50
1	2A	568	U	C5-C4-O4	-5.84	122.40	125.90
1	2A	1204	A	O4'-C1'-N9	5.83	112.87	108.20
1	2A	1300	U	P-O3'-C3'	5.83	126.70	119.70
32	2a	1001(A)	G	N9-C4-C5	-5.83	103.07	105.40
54	1w	1	G	N3-C4-N9	5.82	129.49	126.00
32	1a	1036	G	C4-N9-C1'	5.81	134.06	126.50
1	1A	12	U	N1-C2-O2	5.81	126.87	122.80
32	1a	1007	C	C2-N3-C4	5.78	122.79	119.90
55	2x	22	G	C4-C5-C6	-5.78	115.33	118.80
1	2A	2139	C	N1-C2-O2	5.78	122.36	118.90
32	1a	975	A	O4'-C1'-N9	-5.77	103.58	108.20
1	2A	1992	G	P-O3'-C3'	5.77	126.62	119.70
32	1a	1054	C	C2-N1-C1'	5.75	125.13	118.80
1	2A	1142(A)	A	C2-N3-C4	-5.74	107.73	110.60
55	1x	22	G	C8-N9-C1'	5.73	134.44	127.00
54	1y	56	C	N1-C2-O2	5.71	122.33	118.90
54	2y	47	U	C2-N1-C1'	5.71	124.56	117.70
1	2A	801	G	O5'-P-OP2	-5.71	100.56	105.70
32	1a	841	U	C5-C6-N1	5.70	125.55	122.70
1	2A	2149	G	N9-C4-C5	-5.67	103.13	105.40
1	1A	2501	C	C2-N1-C1'	-5.67	112.56	118.80
1	1A	2006	C	O5'-P-OP1	-5.63	100.63	105.70
32	2a	1020	U	N3-C2-O2	-5.62	118.27	122.20
32	2a	65	U	P-O3'-C3'	5.61	126.44	119.70
32	1a	1002	G	N3-C4-C5	-5.61	125.79	128.60
1	1A	1100	C	C2-N1-C1'	5.59	124.95	118.80
55	1x	14	A	C8-N9-C1'	-5.59	117.64	127.70
1	2A	2689	U	P-O3'-C3'	5.58	126.40	119.70
32	2a	1020	U	C2-N1-C1'	5.58	124.39	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	277	C	N1-C2-O2	5.56	122.24	118.90
1	2A	141	A	N7-C8-N9	5.55	116.58	113.80
32	1a	266	G	P-O3'-C3'	5.55	126.36	119.70
1	1A	570	G	C5-C6-O6	-5.54	125.28	128.60
1	2A	2139	C	C6-N1-C1'	-5.54	114.16	120.80
1	2A	2143	C	N1-C2-O2	5.54	122.22	118.90
1	1A	847	U	C2-N1-C1'	5.53	124.34	117.70
1	1A	1647	G	O4'-C1'-N9	-5.53	103.78	108.20
1	1A	2689	U	N3-C2-O2	-5.51	118.34	122.20
1	1A	372	G	O4'-C1'-N9	5.51	112.60	108.20
1	1A	2790	A	C2-N3-C4	5.50	113.35	110.60
43	2l	29	GLY	N-CA-C	-5.50	99.34	113.10
1	1A	12	U	N3-C2-O2	-5.50	118.35	122.20
1	2A	1639	U	O5'-P-OP2	-5.49	100.76	105.70
1	1A	2455	G	N3-C2-N2	5.45	123.72	119.90
1	1A	2019	A	P-O3'-C3'	5.45	126.24	119.70
32	1a	913	A	P-O3'-C3'	5.45	126.24	119.70
1	1A	1272	A	O5'-P-OP2	-5.44	100.80	105.70
55	1x	22	G	C5-C6-N1	5.43	114.21	111.50
32	2a	1256	A	O4'-C1'-N9	-5.43	103.86	108.20
54	1y	33	U	N3-C2-O2	-5.42	118.41	122.20
1	2A	2155	G	N3-C4-N9	5.42	129.25	126.00
32	1a	558	G	O5'-P-OP1	-5.42	100.83	105.70
55	1x	14	A	C4-N9-C1'	5.41	136.03	126.30
1	2A	1530	C	P-O3'-C3'	5.41	126.19	119.70
32	2a	1032	G	C6-N1-C2	5.39	128.34	125.10
11	2P	44	GLY	C-N-CA	5.39	135.17	121.70
1	1A	2593	U	N3-C4-O4	-5.38	115.64	119.40
32	2a	1032	G	C5-C6-O6	5.38	131.82	128.60
1	1A	1313	U	N3-C2-O2	-5.37	118.44	122.20
1	2A	575	A	O5'-P-OP1	-5.35	100.89	105.70
1	2A	2142	C	N1-C2-O2	5.35	122.11	118.90
55	1x	22	G	C6-C5-N7	5.35	133.61	130.40
32	1a	1030(B)	C	O4'-C1'-N1	5.31	112.45	108.20
1	1A	975	C	C6-N1-C1'	5.31	127.17	120.80
1	2A	228	A	P-O3'-C3'	5.28	126.04	119.70
32	2a	1001	A	N1-C6-N6	-5.28	115.43	118.60
32	2a	1001(A)	G	C6-C5-N7	-5.28	127.23	130.40
1	2A	1698	A	C4-N9-C1'	5.27	135.79	126.30
1	1A	2060	A	C8-N9-C4	5.27	107.91	105.80
32	1a	1030(B)	C	C6-N1-C2	-5.27	118.19	120.30
32	1a	1067	A	P-O3'-C3'	5.26	126.02	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2E	72	VAL	C-N-CA	5.25	134.84	121.70
1	1A	1992	G	O4'-C1'-N9	-5.24	104.01	108.20
32	1a	1285	A	P-O3'-C3'	5.22	125.97	119.70
1	1A	1313	U	C2-N1-C1'	5.22	123.96	117.70
1	2A	2149	G	C6-C5-N7	-5.21	127.27	130.40
7	1H	88	LEU	CA-CB-CG	5.21	127.28	115.30
1	2A	2321	G	C4-N9-C1'	5.21	133.27	126.50
27	25	58	LEU	CA-CB-CG	5.21	127.28	115.30
1	2A	1698	A	C6-C5-N7	-5.21	128.66	132.30
1	2A	383	U	O4'-C1'-N1	5.20	112.36	108.20
32	2a	1040	U	C5-C4-O4	5.19	129.01	125.90
32	1a	21	G	O5'-P-OP1	-5.18	101.04	105.70
1	2A	2148	G	C5-C6-O6	5.18	131.71	128.60
1	2A	945	A	C2-N3-C4	-5.18	108.01	110.60
32	2a	266	G	P-O3'-C3'	5.18	125.92	119.70
1	2A	2140	C	C6-N1-C1'	-5.17	114.59	120.80
54	1w	10	G	N3-C2-N2	-5.17	116.28	119.90
55	1x	46	G	N1-C2-N3	5.17	127.00	123.90
1	2A	2218	U	N1-C2-O2	5.17	126.42	122.80
55	1x	46	G	C5-C6-O6	-5.16	125.50	128.60
1	1A	1075	C	C5-C6-N1	5.16	123.58	121.00
1	1A	2319	G	O4'-C1'-N9	5.14	112.31	108.20
32	2a	1001(A)	G	C4-C5-N7	5.14	112.86	110.80
1	1A	2371	G	C5-C6-N1	5.13	114.07	111.50
1	1A	944	G	N3-C4-N9	5.13	129.08	126.00
1	2A	1558	A	C2-N3-C4	-5.13	108.04	110.60
54	2w	62	C	C5-C6-N1	5.12	123.56	121.00
1	1A	2391	G	O4'-C1'-N9	5.12	112.29	108.20
1	1A	2689	U	P-O3'-C3'	5.12	125.84	119.70
1	2A	2473	U	N1-C2-O2	5.12	126.38	122.80
1	1A	1993	U	O5'-P-OP1	-5.11	101.10	105.70
1	2A	2167	U	N1-C2-O2	5.10	126.37	122.80
1	1A	1177	A	O5'-P-OP1	-5.10	101.11	105.70
55	1x	46	G	N9-C4-C5	5.09	107.44	105.40
32	2a	1039	C	N3-C4-N4	5.08	121.56	118.00
32	2a	1009	G	C6-N1-C2	-5.06	122.06	125.10
32	2a	687	A	P-O3'-C3'	5.05	125.77	119.70
54	2w	75	C	P-O3'-C3'	5.05	125.76	119.70
1	2A	2689	U	N3-C2-O2	-5.04	118.67	122.20
32	1a	1036	G	C8-N9-C1'	-5.04	120.45	127.00
1	2A	1022	G	O4'-C1'-N9	5.03	112.22	108.20
1	2A	512	G	O4'-C1'-N9	5.03	112.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2149	G	N3-C2-N2	5.03	123.42	119.90
32	1a	1158	C	C2-N1-C1'	5.03	124.33	118.80
1	2A	2140	C	N3-C2-O2	-5.02	118.39	121.90
1	2A	2406	U	O4'-C1'-N1	-5.02	104.19	108.20
1	1A	36	G	O5'-P-OP2	-5.01	101.19	105.70
1	1A	788	A	C8-N9-C4	5.01	107.80	105.80
54	1w	72	C	C2-N1-C1'	5.01	124.31	118.80
54	2w	63	G	C5-C6-O6	5.01	131.60	128.60
55	2x	17	C	C6-N1-C2	-5.00	118.30	120.30
1	2A	90	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	2g	79	ARG	Peptide

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

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	31193	638	0
1	2A	60322	0	30423	877	0
2	1B	2577	0	1305	19	0
2	2B	2575	0	1303	50	0
3	1D	2136	0	2218	54	0
3	2D	2136	0	2218	54	0
4	1E	1559	0	1618	39	0
4	2E	1559	0	1618	24	0
5	1F	1584	0	1625	39	0
5	2F	1580	0	1619	53	0
6	1G	1429	0	1447	32	0
6	2G	1428	0	1438	43	0
7	1H	1330	0	1407	24	0
7	2H	1330	0	1407	41	0
8	1I	1097	0	1140	26	0
8	2I	1064	0	1082	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	1N	1117	0	1184	23	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	18	0
10	2O	933	0	996	20	0
11	1P	1135	0	1211	27	0
11	2P	1135	0	1212	40	0
12	1Q	1122	0	1179	20	0
12	2Q	1122	0	1179	33	0
13	1R	968	0	1033	17	0
13	2R	968	0	1033	26	0
14	1S	873	0	927	19	0
14	2S	870	0	923	16	0
15	1T	1091	0	1151	13	0
15	2T	1083	0	1136	17	0
16	1U	959	0	1019	13	0
16	2U	959	0	1019	24	0
17	1V	771	0	830	14	0
17	2V	771	0	830	19	0
18	1W	886	0	940	9	0
18	2W	886	0	940	9	0
19	1X	750	0	814	16	0
19	2X	750	0	814	15	0
20	1Y	806	0	881	13	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	23	0
21	2Z	1271	0	1273	45	0
22	10	653	0	674	16	0
22	20	653	0	674	17	0
23	11	755	0	826	13	0
23	21	755	0	826	22	0
24	12	588	0	643	12	0
24	22	588	0	643	16	0
25	13	469	0	518	9	0
25	23	464	0	514	10	0
26	14	552	0	533	17	0
26	24	532	0	503	14	0
27	15	455	0	465	11	0
27	25	455	0	465	11	0
28	16	453	0	473	8	0
28	26	449	0	469	13	0
29	17	418	0	467	7	0
29	27	418	0	467	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	18	517	0	582	16	0
30	28	517	0	582	16	0
31	19	307	0	335	2	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16340	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	1185	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	281	0	139	0	0
53	2v	277	0	140	0	0
54	1w	1588	0	820	0	0
54	1y	1581	0	805	0	0
54	2w	1561	0	796	0	0
54	2y	1561	0	796	0	0
55	1x	1635	0	838	0	0
55	2x	1635	0	837	0	0
56	10	6	0	0	0	0
56	11	2	0	0	0	0
56	12	2	0	0	0	0
56	13	1	0	0	0	0
56	15	5	0	0	0	0
56	16	2	0	0	0	0
56	17	1	0	0	0	0
56	18	1	0	0	0	0
56	19	2	0	0	0	0
56	1A	929	0	0	0	0
56	1B	25	0	0	0	0
56	1D	9	0	0	0	0
56	1E	8	0	0	0	0
56	1F	8	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	3	0	0	0	0
56	1P	4	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	2	0	0	0	0
56	1S	1	0	0	0	0
56	1T	2	0	0	0	0
56	1U	4	0	0	0	0
56	1V	4	0	0	0	0
56	1W	4	0	0	0	0
56	1X	4	0	0	0	0
56	1Y	2	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	235	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1b	2	0	0	0	0
56	1c	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	1	0	0	0	0
56	1f	1	0	0	0	0
56	1g	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	1	0	0	0	0
56	1n	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	5	0	0	0	0
56	1x	15	0	0	0	0
56	1y	7	0	0	0	0
56	20	3	0	0	0	0
56	21	3	0	0	0	0
56	23	1	0	0	0	0
56	25	2	0	0	0	0
56	27	1	0	0	0	0
56	28	2	0	0	0	0
56	2A	671	0	0	0	0
56	2B	21	0	0	0	0
56	2D	4	0	0	0	0
56	2E	7	0	0	0	0
56	2F	7	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	2	0	0	0	0
56	2T	1	0	0	0	0
56	2U	1	0	0	0	0
56	2V	4	0	0	0	0
56	2X	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	202	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	2	0	0	0	0
56	2p	1	0	0	0	0
56	2q	2	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	2	0	0	0	0
56	2w	3	0	0	0	0
56	2x	3	0	0	0	0
57	1A	57	0	50	5	0
57	2A	57	0	50	5	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	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
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	6	0	0	0	0
61	11	3	0	0	0	0
61	12	4	0	0	1	0
61	13	5	0	0	0	0
61	15	1	0	0	0	0
61	17	6	0	0	0	0
61	18	10	0	0	1	0
61	19	2	0	0	0	0
61	1A	1741	0	0	69	0
61	1B	49	0	0	1	0
61	1D	21	0	0	1	0
61	1E	27	0	0	2	0
61	1F	22	0	0	1	0
61	1G	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1I	1	0	0	0	0
61	1N	6	0	0	0	0
61	1O	4	0	0	0	0
61	1P	21	0	0	1	0
61	1Q	5	0	0	0	0
61	1R	5	0	0	0	0
61	1S	6	0	0	0	0
61	1T	13	0	0	0	0
61	1U	12	0	0	0	0
61	1V	10	0	0	0	0
61	1W	6	0	0	1	0
61	1X	4	0	0	1	0
61	1Y	4	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	309	0	0	0	0
61	1d	1	0	0	0	0
61	1g	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	3	0	0	0	0
61	1m	1	0	0	0	0
61	1o	2	0	0	0	0
61	1p	2	0	0	0	0
61	1q	1	0	0	0	0
61	1r	1	0	0	0	0
61	1v	6	0	0	0	0
61	1w	6	0	0	0	0
61	1x	13	0	0	0	0
61	1y	5	0	0	0	0
61	20	6	0	0	0	0
61	21	5	0	0	0	0
61	22	1	0	0	0	0
61	23	1	0	0	0	0
61	25	3	0	0	0	0
61	27	3	0	0	0	0
61	28	4	0	0	0	0
61	29	1	0	0	0	0
61	2A	1031	0	0	89	0
61	2B	10	0	0	1	0
61	2D	16	0	0	4	0
61	2E	10	0	0	1	0
61	2F	7	0	0	0	0
61	2I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2N	1	0	0	0	0
61	2O	1	0	0	0	0
61	2P	14	0	0	2	0
61	2Q	1	0	0	0	0
61	2R	2	0	0	0	0
61	2T	3	0	0	0	0
61	2U	1	0	0	0	0
61	2V	2	0	0	0	0
61	2W	1	0	0	1	0
61	2X	3	0	0	0	0
61	2Y	1	0	0	1	0
61	2Z	2	0	0	0	0
61	2a	203	0	0	0	0
61	2d	4	0	0	0	0
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	4	0	0	0	0
61	2l	3	0	0	0	0
61	2o	1	0	0	0	0
61	2p	2	0	0	0	0
61	2r	1	0	0	0	0
61	2t	2	0	0	0	0
61	2v	3	0	0	0	0
61	2x	6	0	0	0	0
All	All	299169	0	196828	2456	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 (2456) 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:1082:U:H3	1:1A:1086:A:N6	1.56	1.02
1:1A:1082:U:N3	1:1A:1086:A:N6	2.09	1.01
1:1A:1082:U:O4	1:1A:1086:A:N1	1.95	0.99
1:2A:1002:G:H1	1:2A:1038:C:N4	43.03	0.97
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.50	0.94
1:2A:1002:G:H1	1:2A:1038:C:H42	43.41	0.94
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.10	0.92
1:2A:2129:C:H42	1:2A:2159:G:H1	1.01	0.92
1:1A:1359:A:N1	1:1A:1372:U:N3	2.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2099:U:H3	1:1A:2190:G:H1	1.18	0.91
22:20:10:THR:HG22	22:20:12:ASN:H	1.34	0.91
1:1A:2135:A:H61	1:1A:2157:G:H21	1.16	0.90
20:1Y:92:ASN:HB3	20:1Y:94:LYS:H	1.36	0.90
29:17:24:THR:HG22	29:17:27:GLY:H	1.37	0.89
3:2D:242:ARG:HH11	3:2D:242:ARG:HG3	1.33	0.88
1:2A:198:C:OP2	61:2A:9701:HOH:O	1.91	0.88
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	99.40	0.88
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.07	0.88
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.07	0.88
16:2U:76:TYR:OH	16:2U:92:ARG:NH1	2.06	0.87
1:2A:195:A:N7	61:2A:9701:HOH:O	2.08	0.87
1:1A:1670:C:OP1	61:1A:4001:HOH:O	1.94	0.86
1:1A:1082:U:H3	1:1A:1086:A:H61	0.87	0.86
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.07	0.86
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.09	0.85
22:10:10:THR:HG22	22:10:12:ASN:H	1.40	0.85
1:2A:1204:A:H2	1:2A:1241:A:H62	1.21	0.85
1:2A:882:G:N2	1:2A:894:C:N3	2.23	0.85
1:2A:2129:C:N4	1:2A:2159:G:H1	1.72	0.85
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.09	0.84
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.39	0.84
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.59	0.84
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.09	0.84
1:2A:1002:G:N2	1:2A:1038:C:N3	42.62	0.84
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.59	0.84
1:2A:987:G:H1	1:2A:1218:C:H42	46.44	0.83
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.61	0.83
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.12	0.83
1:1A:279:C:H42	1:1A:361:G:H1	1.27	0.82
1:1A:400:G:N7	61:1A:4018:HOH:O	2.11	0.82
1:1A:998:C:OP1	61:1A:4002:HOH:O	1.98	0.82
1:2A:1315:C:OP2	61:2A:9702:HOH:O	1.97	0.82
4:1E:77:ILE:HD13	4:1E:195:LEU:HD11	1.59	0.82
1:1A:958:U:OP2	12:1Q:14:ARG:NH1	2.13	0.82
1:1A:2140:C:H42	1:1A:2151:G:H1	1.27	0.81
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.14	0.81
1:2A:2124:G:H1	1:2A:2174:C:H42	1.27	0.81
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.13	0.81
1:2A:397:G:N7	61:2A:9730:HOH:O	2.13	0.80
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2N:123:TYR:HH	9:2N:130:HIS:HE2	1.18	0.80
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.15	0.80
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.00	0.79
1:2A:2499:C:OP2	61:2A:9704:HOH:O	2.00	0.79
1:1A:847:U:OP2	61:1A:4003:HOH:O	2.00	0.79
1:2A:1648:C:OP1	61:2A:9703:HOH:O	1.99	0.79
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.62	0.79
1:1A:1754:C:OP1	15:1T:96:ARG:NH1	2.16	0.79
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.64	0.79
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.15	0.78
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.14	0.78
1:1A:1422:G:H5''	10:1O:48:PRO:HB3	99.38	0.78
1:2A:2104:G:H1	1:2A:2185:C:H42	1.32	0.78
1:2A:1286:A:H2'	1:2A:1287:A:H4'	6.47	0.78
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.49	0.78
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.17	0.77
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.65	0.77
1:1A:1070:A:N7	1:1A:1096:A:O2'	2.17	0.77
1:1A:266:G:H5''	1:1A:268:C:H41	11.25	0.76
1:2A:1171:G:H1	1:2A:1178:C:H42	1.33	0.76
1:2A:1689:A:H62	1:2A:1698:A:H2	1.34	0.76
1:2A:81:G:N7	61:2A:9748:HOH:O	2.19	0.76
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.68	0.76
1:2A:2042:A:OP1	61:2A:9705:HOH:O	2.02	0.76
1:2A:83:G:H1	1:2A:102:G:HO2'	1.33	0.76
1:2A:1153:C:OP2	61:2A:9707:HOH:O	2.04	0.75
1:1A:1013:C:OP2	61:1A:4004:HOH:O	2.02	0.75
12:1Q:16:ARG:HG2	12:1Q:18:LYS:HG3	1.68	0.75
1:2A:2297:C:O2	1:2A:2321:G:N2	2.18	0.75
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.69	0.75
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.19	0.75
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.16	0.74
1:2A:2268:A:OP1	61:2A:9706:HOH:O	2.03	0.74
1:2A:833:U:O2	11:2P:55:ARG:NH2	2.19	0.74
1:1A:2822:G:N7	61:1A:4046:HOH:O	2.20	0.74
1:2A:1023:U:OP2	61:2A:9708:HOH:O	2.05	0.74
1:2A:740:U:OP2	61:2A:9711:HOH:O	2.06	0.74
1:1A:2448:A:OP1	61:1A:4005:HOH:O	2.05	0.74
1:2A:2139:C:H42	1:2A:2152:G:H1	1.34	0.74
1:2A:2685:G:O6	61:2A:9713:HOH:O	2.06	0.74
7:2H:124:GLU:HB2	7:2H:132:ARG:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.05	0.74
21:1Z:151:HIS:O	21:1Z:153:SER:N	2.20	0.74
1:2A:2615:U:OP1	61:2A:9712:HOH:O	2.06	0.74
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.70	0.73
1:1A:2763:G:OP2	61:1A:4007:HOH:O	2.05	0.73
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.22	0.73
1:2A:990:A:OP2	61:2A:9710:HOH:O	2.05	0.73
1:1A:1602:U:O4	61:1A:4006:HOH:O	2.05	0.73
1:2A:2287:A:H62	1:2A:2344:U:H3	1.35	0.73
1:2A:249:C:O2	30:28:12:LYS:NZ	2.21	0.73
1:2A:921:G:O6	61:2A:9709:HOH:O	2.05	0.73
1:1A:1365:A:O2'	23:11:11:ARG:NH2	2.19	0.73
1:2A:2310:A:N1	6:2G:79:ASN:ND2	2.37	0.73
1:1A:1014:U:OP2	61:1A:4004:HOH:O	2.07	0.72
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.70	0.72
1:2A:1042:G:H1	1:2A:1113:U:H3	1.37	0.72
1:2A:2126:A:N6	1:2A:2163:C:O4'	2.22	0.72
1:1A:2171:A:HO2'	1:1A:2172:U:H6	1.36	0.72
1:2A:1024:G:OP2	61:2A:9708:HOH:O	2.07	0.72
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.70	0.72
1:1A:882:G:H1	1:1A:894:C:H42	1.37	0.72
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.22	0.72
17:2V:72:VAL:HG13	17:2V:85:LYS:HB2	1.70	0.72
25:13:3:ARG:NH1	25:13:60:GLU:OE2	2.21	0.72
1:2A:11:G:N7	61:2A:9768:HOH:O	2.22	0.72
1:1A:2447:G:OP2	61:1A:4010:HOH:O	2.06	0.72
1:1A:1007:C:OP2	61:1A:4011:HOH:O	2.08	0.72
1:1A:2407:G:OP1	61:1A:4009:HOH:O	2.06	0.72
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.23	0.72
1:1A:880:G:N2	1:1A:898:C:N3	2.33	0.71
11:2P:95:VAL:HA	11:2P:99:LEU:HD21	1.71	0.71
1:1A:1986:A:OP1	61:1A:4012:HOH:O	2.08	0.71
1:2A:1890:A:OP2	61:2A:9714:HOH:O	2.08	0.71
1:1A:1754:C:H5	15:1T:96:ARG:HH21	1.39	0.71
1:2A:1309:G:H4'	29:27:7:PRO:HB2	1.72	0.71
1:2A:988:A:N7	61:2A:9770:HOH:O	2.23	0.71
3:2D:237:GLU:OE2	61:2D:401:HOH:O	2.08	0.71
5:2F:18:ARG:NH1	5:2F:127:GLU:OE2	2.23	0.71
1:1A:880:G:H1	1:1A:898:C:H42	1.36	0.71
1:2A:2049:G:N7	61:2A:9773:HOH:O	2.23	0.71
1:2A:271(R):G:OP1	23:21:76:ARG:NH1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1653:G:H3'	13:2R:2:ARG:HD3	1.73	0.71
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.38	0.71
1:2A:323:G:HO2'	1:2A:1205:U:H3	1.35	0.71
1:2A:775:G:O3'	61:2A:9717:HOH:O	2.09	0.71
1:1A:2228:G:O6	61:1A:4008:HOH:O	2.06	0.71
3:2D:232:PRO:O	61:2D:402:HOH:O	2.09	0.71
7:2H:98:LEU:HG	7:2H:125:VAL:HG22	1.71	0.71
1:2A:526:A:OP1	61:2A:9718:HOH:O	2.09	0.71
2:2B:66:A:H61	2:2B:109:C:H5''	1.55	0.71
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.73	0.71
1:1A:1237:A:OP1	61:1A:4013:HOH:O	2.09	0.70
5:2F:132:VAL:HA	5:2F:138:GLU:HB3	1.72	0.70
1:1A:11:G:H2'	1:1A:12:U:H5''	1.73	0.70
13:1R:28:LEU:HD12	13:1R:44:LEU:HD13	1.72	0.70
21:1Z:120:ILE:O	21:1Z:121:HIS:ND1	2.24	0.70
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.74	0.70
7:1H:86:GLU:OE2	7:1H:130:ARG:NH1	2.24	0.70
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.22	0.70
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.25	0.70
1:2A:948:G:OP1	61:2A:9715:HOH:O	2.08	0.70
1:2A:542:C:H42	1:2A:551:G:H1	1.38	0.70
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH12	1.57	0.70
7:2H:18:GLU:HB3	7:2H:25:LYS:HB2	1.72	0.70
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.24	0.70
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.57	0.70
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.24	0.70
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.27	0.70
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.72	0.69
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.24	0.69
1:2A:1783:A:N7	61:2A:9787:HOH:O	2.26	0.69
1:1A:592:G:O6	61:1A:4015:HOH:O	2.10	0.69
3:2D:76:PRO:HB2	3:2D:116:GLN:HE21	1.57	0.69
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.24	0.69
1:2A:962:G:OP1	61:2A:9715:HOH:O	2.08	0.69
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.74	0.69
1:2A:11:G:H2'	1:2A:12:U:H5'	1.74	0.69
1:2A:1973:G:OP1	61:2A:9719:HOH:O	2.09	0.69
6:2G:11:TYR:OH	6:2G:16:ARG:NH1	2.24	0.69
9:2N:68:GLU:HG3	9:2N:69:GLN:HG3	1.73	0.69
13:2R:28:LEU:HD12	13:2R:44:LEU:HD13	1.74	0.69
26:24:53:GLU:HG2	26:24:54:GLY:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2154:G:C2	1:1A:2155:G:H1'	2.28	0.69
1:1A:668:G:N7	61:1A:4065:HOH:O	2.25	0.69
1:1A:927:G:N7	61:1A:4067:HOH:O	2.25	0.69
1:2A:2251:OMG:OP1	61:2A:9723:HOH:O	2.11	0.69
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.28	0.69
1:1A:2250:G:OP1	12:1Q:85:LYS:NZ	2.23	0.69
1:1A:2384:G:OP2	22:10:55:ARG:NH1	2.22	0.69
1:1A:947:G:OP2	61:1A:4020:HOH:O	2.11	0.69
6:1G:50:ALA:O	6:1G:52:ILE:N	2.26	0.69
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	1.75	0.69
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.75	0.69
1:1A:674:G:OP2	61:1A:4019:HOH:O	2.11	0.69
1:2A:1022:G:N2	1:2A:1023:U:O4	2.25	0.69
1:1A:1062:G:H8	1:1A:1070:A:H5''	1.58	0.68
11:1P:42:SER:O	61:1P:301:HOH:O	2.10	0.68
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.26	0.68
1:2A:1186:G:OP2	61:2A:9710:HOH:O	2.10	0.68
1:1A:248:G:OP1	61:1A:4014:HOH:O	2.10	0.68
1:2A:1622:G:OP2	61:2A:9721:HOH:O	2.10	0.68
1:2A:476:G:O6	61:2A:9720:HOH:O	2.10	0.68
1:1A:2350:C:OP2	61:1A:4017:HOH:O	2.11	0.68
20:1Y:54:LYS:HA	20:1Y:56:PRO:HD3	1.76	0.68
1:2A:792:G:O6	61:2A:9716:HOH:O	2.08	0.68
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.26	0.68
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.12	0.68
1:1A:2049:G:N7	61:1A:4072:HOH:O	2.26	0.68
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.76	0.68
1:2A:878:A:N6	1:2A:899:A:O2'	2.27	0.68
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.29	0.68
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.27	0.68
1:2A:1647:G:OP1	61:2A:9703:HOH:O	2.12	0.68
1:2A:2518:A:OP2	61:2A:9722:HOH:O	2.11	0.68
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.76	0.68
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.59	0.68
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.75	0.68
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.76	0.68
1:2A:1314:C:OP1	61:2A:9702:HOH:O	2.10	0.68
1:1A:1653:G:H3'	13:1R:2:ARG:HD3	1.76	0.67
12:2Q:67:ARG:O	12:2Q:101:ARG:NH2	2.27	0.67
1:2A:2141:G:O6	1:2A:2150:U:O2	2.13	0.67
1:1A:1062:G:C8	1:1A:1070:A:H5''	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.30	0.67
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.75	0.67
1:1A:72:U:OP1	61:1A:4016:HOH:O	2.11	0.67
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.60	0.67
1:2A:1418:G:OP2	61:2A:9725:HOH:O	2.12	0.67
1:2A:1840:G:OP2	61:2A:9727:HOH:O	2.13	0.67
1:2A:2121:G:H1	1:2A:2177:C:H42	1.42	0.67
1:2A:2223:G:OP1	3:2D:172:TYR:OH	2.11	0.67
18:1W:68:ARG:HH12	18:1W:112:GLY:H	1.41	0.67
1:2A:1332:G:OP1	61:2A:9702:HOH:O	2.11	0.67
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.30	0.67
1:2A:2721:A:OP1	61:2A:9729:HOH:O	2.13	0.67
1:1A:1124:C:OP1	61:1A:4021:HOH:O	2.13	0.66
1:1A:84:A:H5'	20:1Y:8:LYS:HG2	1.76	0.66
1:2A:1141:U:OP1	9:2N:25:ARG:NH1	2.26	0.66
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.60	0.66
1:1A:1059:G:H1	1:1A:1079:C:H42	1.41	0.66
24:12:16:LEU:HB3	24:12:20:GLU:HG3	1.77	0.66
1:1A:1762:A:N1	61:1A:4078:HOH:O	2.28	0.66
1:2A:1603:A:OP1	61:2A:9724:HOH:O	2.12	0.66
1:2A:563:G:OP2	61:2A:9726:HOH:O	2.12	0.66
1:1A:2136:C:N3	1:1A:2155:G:N2	2.43	0.66
1:2A:1395:A:OP1	61:2A:9724:HOH:O	2.13	0.66
1:1A:2136:C:N4	1:1A:2155:G:N1	2.44	0.66
17:2V:56:SER:H	17:2V:100:ARG:HB2	1.60	0.66
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.28	0.66
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.25	0.66
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.76	0.66
14:2S:14:VAL:O	14:2S:18:ILE:HG12	1.96	0.66
22:10:11:ARG:O	22:10:14:ARG:NH2	2.28	0.66
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.77	0.66
24:12:59:ARG:NH2	61:12:201:HOH:O	2.29	0.66
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.23	0.66
9:1N:73:THR:HG23	9:1N:82:LEU:HD11	1.78	0.66
1:1A:1676:A:N7	61:1A:4083:HOH:O	2.29	0.66
1:2A:1271:G:OP2	61:2A:9703:HOH:O	2.14	0.66
21:2Z:93:ASP:HB3	21:2Z:131:ARG:HH22	1.61	0.66
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.31	0.65
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.15	0.65
1:2A:1300:U:H4'	1:2A:1301:A:H5'	1.76	0.65
3:1D:237:GLU:OE2	61:1D:401:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2228:G:OP1	3:2D:261:LYS:NZ	2.21	0.65
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.78	0.65
5:1F:44:ARG:NH1	61:1F:401:HOH:O	2.21	0.65
1:2A:2060:A:N3	61:2A:9810:HOH:O	2.30	0.65
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.77	0.65
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.29	0.65
1:2A:1434:A:H61	1:2A:1558:A:H62	1.44	0.65
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.14	0.65
6:2G:79:ASN:OD1	6:2G:79:ASN:N	2.27	0.65
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.31	0.65
1:2A:2048:G:OP1	61:2A:9732:HOH:O	2.14	0.65
1:2A:1026:U:OP1	61:2A:9708:HOH:O	2.15	0.65
1:2A:1830:C:OP2	61:2A:9728:HOH:O	2.13	0.65
14:2S:83:LYS:HG2	14:2S:84:GLN:HG3	1.78	0.65
1:1A:1342:A:OP2	61:1A:4006:HOH:O	2.13	0.65
3:1D:180:GLY:HA3	3:1D:275:LYS:HB2	1.79	0.65
4:1E:119:ARG:HG3	4:1E:160:TYR:HB2	1.79	0.65
1:2A:2171:A:H1'	1:2A:2172:U:C6	2.32	0.65
1:2A:223:A:O2'	1:2A:420:C:O2	2.15	0.65
6:2G:131:TYR:HB3	6:2G:159:VAL:HG13	1.78	0.65
1:1A:1094:U:H1'	1:1A:1097:U:H5	1.62	0.64
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.32	0.64
1:1A:123:G:OP2	61:1A:4022:HOH:O	2.15	0.64
11:2P:126:VAL:HG13	11:2P:146:VAL:HB	1.79	0.64
1:2A:1973:G:OP2	61:2A:9734:HOH:O	2.14	0.64
1:2A:568:U:H5'	1:2A:945:A:N1	2.12	0.64
1:1A:1002:G:C5	1:1A:1003:G:H1'	4.28	0.64
1:1A:2127:G:H21	1:1A:2173:A:H1'	1.61	0.64
1:2A:1568:G:N7	61:2A:9808:HOH:O	2.29	0.64
1:2A:1721:G:H8	1:2A:1741:A:H62	1.45	0.64
1:2A:2349:G:OP1	61:2A:9733:HOH:O	2.14	0.64
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.79	0.64
1:1A:1309:G:H4'	29:17:7:PRO:HB2	1.79	0.64
1:2A:574:C:N3	4:2E:145:LYS:NZ	2.44	0.64
1:1A:2748:A:H5'	7:1H:4:ILE:HD12	1.80	0.64
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.80	0.64
1:2A:2102:U:H3	1:2A:2187:G:H1	1.46	0.64
7:2H:3:ARG:NH1	7:2H:5:GLY:H	1.95	0.64
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.79	0.64
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.80	0.64
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:32:LEU:HD12	24:12:53:LEU:HB3	1.79	0.63
1:2A:1379:A:H4'	1:2A:1380:G:OP2	1.98	0.63
26:24:24:THR:OG1	26:24:25:TYR:N	2.31	0.63
1:1A:503:A:O2'	61:1A:4023:HOH:O	2.15	0.63
20:1Y:34:LYS:NZ	61:1Y:601:HOH:O	2.20	0.63
7:2H:80:SER:OG	7:2H:81:GLU:OE1	2.16	0.63
1:1A:882:G:N2	1:1A:894:C:N3	2.39	0.63
6:1G:115:ARG:HB3	6:1G:136:ARG:HH22	1.63	0.63
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.81	0.63
1:2A:2659:G:N2	1:2A:2662:A:OP2	2.32	0.63
4:2E:72:VAL:HG12	4:2E:73:GLU:O	1.98	0.63
1:2A:2124:G:H1	1:2A:2174:C:N4	1.95	0.63
2:2B:8:U:H3	2:2B:113:G:H1	1.47	0.63
7:2H:23:ARG:NH1	7:2H:34:GLU:OE1	2.32	0.63
1:2A:1278:A:OP1	13:2R:36:THR:HG23	1.99	0.63
23:11:3:LYS:HB2	23:11:61:ARG:HH11	1.64	0.63
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.34	0.63
1:1A:1967:C:OP1	61:1A:4024:HOH:O	2.16	0.63
28:26:14:THR:OG1	28:26:48:VAL:O	2.13	0.63
6:2G:41:GLN:NE2	6:2G:153:ARG:O	2.31	0.63
1:1A:453:C:O2	1:1A:457:A:O2'	2.17	0.63
1:2A:607:U:OP1	5:2F:102:PRO:HA	1.99	0.63
1:2A:2135:A:O4'	1:2A:2159:G:O2'	2.17	0.63
1:1A:1002:G:H3'	1:1A:1003:G:O4'	4.15	0.62
1:1A:2336:A:H61	22:10:43:THR:HG22	1.63	0.62
4:1E:119:ARG:HD3	4:1E:120:TRP:NE1	2.14	0.62
26:24:59:PHE:N	26:24:60:GLN:HB2	2.14	0.62
1:2A:2552:2MU:H2'	1:2A:2554:U:OP2	1.99	0.62
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.26	0.62
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.34	0.62
15:2T:73:GLU:OE2	15:2T:103:ARG:NE	2.32	0.62
1:1A:153:C:OP2	23:11:92:LYS:NZ	2.25	0.62
1:2A:1231:G:H2'	1:2A:1232:G:H8	1.65	0.62
1:2A:2167:U:H2'	1:2A:2168:G:H21	1.64	0.62
12:2Q:12:GLN:HE21	12:2Q:72:LYS:HG3	1.63	0.62
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.79	0.62
17:1V:98:GLU:OE2	17:1V:100:ARG:NH1	2.32	0.62
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.32	0.62
23:21:21:ARG:HD3	23:21:35:THR:HG21	1.80	0.62
12:2Q:109:VAL:HG22	12:2Q:113:GLN:HB3	1.81	0.62
5:1F:34:TRP:CZ2	11:1P:8:PRO:HG3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:43:ASN:ND2	23:21:75:GLU:OE2	2.33	0.62
1:2A:1250:G:OP2	11:2P:21:ARG:NH1	2.33	0.62
1:2A:473:G:H2'	1:2A:474:G:H8	2.67	0.62
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.28	0.62
1:1A:2196:C:OP2	61:1A:4027:HOH:O	2.16	0.62
1:2A:848:G:C4	1:2A:933:A:H8	2.17	0.62
13:1R:33:ARG:NH1	13:1R:115:GLU:OE1	2.32	0.62
1:2A:2137:C:H2'	1:2A:2138:C:C6	2.35	0.62
7:2H:106:THR:HG22	7:2H:112:PRO:HB3	1.82	0.62
1:1A:2691:C:OP2	61:1A:4026:HOH:O	2.16	0.62
1:2A:987:G:H1	1:2A:1218:C:N4	46.03	0.62
1:2A:890:A:H2'	1:2A:892:G:H8	1.65	0.62
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.82	0.62
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.33	0.61
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.33	0.61
1:1A:1020:A:N1	1:1A:1141:U:O2'	2.31	0.61
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.36	0.61
1:1A:278:A:H2'	1:1A:279:C:C6	2.34	0.61
1:2A:131:G:OP1	61:2A:9739:HOH:O	2.16	0.61
57:2A:3673:4M2:H35	57:2A:3673:4M2:H31	1.83	0.61
2:2B:80:U:HO2'	2:2B:81:G:H8	1.48	0.61
14:2S:15:ARG:HB3	14:2S:19:LYS:NZ	2.15	0.61
1:1A:2168:G:O6	1:1A:2171:A:H5''	2.01	0.61
1:1A:2127:G:N2	1:1A:2173:A:H1'	2.15	0.61
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.32	0.61
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.35	0.61
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	1.80	0.61
18:1W:12:ILE:HD13	18:1W:17:VAL:HG13	1.82	0.61
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.82	0.61
1:1A:1671:U:OP2	61:1A:4001:HOH:O	2.16	0.61
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.46	0.61
26:14:53:GLU:HG3	26:14:54:GLY:H	1.65	0.61
1:2A:1958:C:OP2	61:2A:9738:HOH:O	2.16	0.61
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.17	0.61
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.81	0.61
15:2T:16:ARG:NH2	15:2T:83:ILE:O	2.33	0.61
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.47	0.61
1:1A:2140:C:N4	1:1A:2151:G:H1	1.97	0.61
14:1S:34:HIS:ND1	14:1S:53:SER:OG	2.32	0.61
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.14	0.61
2:2B:87:G:N2	2:2B:90:A:OP2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.83	0.61
1:1A:1090:U:C2	1:1A:1102:C:H1'	2.36	0.61
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.64	0.61
1:2A:1639:U:OP1	61:2A:9741:HOH:O	2.16	0.61
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.16	0.61
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.65	0.61
26:14:24:THR:OG1	26:14:25:TYR:N	2.34	0.60
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.35	0.60
1:2A:2169:A:H2'	1:2A:2170:A:C8	2.36	0.60
1:2A:2366:A:H2'	1:2A:2367:G:O4'	2.01	0.60
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.81	0.60
13:2R:36:THR:HG22	13:2R:37:THR:H	1.65	0.60
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.17	0.60
7:1H:101:ARG:NH2	7:1H:121:ILE:O	2.33	0.60
26:24:64:GLY:C	26:24:66:SER:H	2.04	0.60
1:2A:1530:C:H42	1:2A:1539:G:H1	1.49	0.60
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.34	0.60
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.36	0.60
1:1A:1652:A:C2'	1:1A:1653:G:H5'	2.31	0.60
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.82	0.60
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.83	0.60
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.02	0.60
7:2H:28:GLY:HA3	7:2H:79:VAL:HB	1.82	0.60
1:1A:1094:U:H1'	1:1A:1097:U:C5	2.36	0.60
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.34	0.60
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.37	0.60
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.37	0.60
1:2A:2532:G:N2	1:2A:2663:G:O2'	2.34	0.60
9:1N:67:LEU:HA	9:1N:87:LEU:HD22	1.84	0.60
1:2A:10:G:O2'	1:2A:2801(A):A:N6	2.34	0.60
5:2F:40:GLN:HE22	5:2F:182:ASN:HB2	1.67	0.60
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.67	0.60
1:1A:1356:G:N7	61:1A:4100:HOH:O	2.32	0.60
13:1R:36:THR:HG22	13:1R:37:THR:H	1.67	0.60
1:1A:143:G:H4'	19:1X:35:THR:HG21	1.83	0.59
1:1A:548:A:H61	17:1V:19:LYS:H	1.50	0.59
1:1A:1823:G:OP1	3:1D:54:ARG:NH1	2.34	0.59
1:2A:2139:C:N4	1:2A:2152:G:H1	1.99	0.59
1:2A:2330:G:H2'	1:2A:2331:G:O4'	2.02	0.59
1:1A:2135:A:H2	1:1A:2155:G:H1	1.50	0.59
1:2A:2104:G:H1	1:2A:2185:C:N4	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.01	0.59
14:1S:15:ARG:O	14:1S:19:LYS:HG2	2.03	0.59
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.02	0.59
1:2A:451:C:H4'	5:2F:52:LYS:HE2	1.83	0.59
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.35	0.59
6:1G:131:TYR:HB3	6:1G:159:VAL:HG22	1.84	0.59
1:2A:2531:A:H61	1:2A:2662:A:H61	1.51	0.59
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.68	0.59
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.20	0.59
1:2A:991:C:OP2	61:2A:9710:HOH:O	2.17	0.59
7:2H:129:THR:O	7:2H:129:THR:OG1	2.21	0.59
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.02	0.59
1:1A:2793:G:N2	1:1A:2804:C:H1'	2.18	0.59
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.03	0.59
6:2G:39:ILE:HG12	6:2G:157:ILE:HG12	1.85	0.59
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.84	0.59
1:2A:2164:C:H3'	1:2A:2165:G:C8	2.38	0.59
1:2A:2365:G:O6	30:28:43:GLN:NE2	2.34	0.59
1:2A:527:C:N4	1:2A:2779:U:OP2	2.34	0.59
2:2B:24:G:H4'	2:2B:25:A:C8	2.37	0.59
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.83	0.59
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.83	0.59
1:2A:400:G:O6	61:2A:9735:HOH:O	2.16	0.59
30:18:28:GLY:O	30:18:36:LYS:NZ	2.31	0.59
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.37	0.59
1:2A:1021:A:H61	1:2A:1142(A):A:H61	1.51	0.59
2:2B:95:C:H2'	2:2B:96:U:C6	2.37	0.59
28:16:11:LEU:HB2	28:16:21:TYR:HB2	1.84	0.59
1:2A:2166:G:O6	1:2A:2171:A:N6	2.36	0.59
1:2A:839:U:H2'	1:2A:840:C:C6	2.38	0.59
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.37	0.58
57:1A:3894:4M2:H35	57:1A:3894:4M2:H31	1.84	0.58
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.67	0.58
1:2A:450:G:OP2	61:2A:9736:HOH:O	2.16	0.58
26:14:61:ARG:HG3	26:14:62:ARG:H	1.68	0.58
6:1G:48:GLU:HA	6:1G:51:ARG:HE	1.68	0.58
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.84	0.58
1:2A:2453:A:N7	61:2A:9826:HOH:O	2.32	0.58
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.84	0.58
2:2B:40:U:H1'	2:2B:45:A:H61	1.68	0.58
1:2A:534:U:O2'	16:2U:49:HIS:ND1	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	1.84	0.58
1:1A:1991:U:H2'	1:1A:1992:G:H5''	1.83	0.58
1:1A:2124:G:H1	1:1A:2174:C:H42	1.52	0.58
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.85	0.58
1:1A:2134:A:OP1	1:1A:2156:G:N2	2.36	0.58
1:1A:2319:G:H22	14:1S:3:ARG:NE	2.00	0.58
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.39	0.58
1:2A:2842:G:O6	61:2A:9731:HOH:O	2.14	0.58
4:2E:119:ARG:HG3	4:2E:160:TYR:HB2	1.85	0.58
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.36	0.58
18:1W:92:ARG:NH1	61:1W:3103:HOH:O	2.36	0.58
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.35	0.58
1:2A:1857:G:O2'	1:2A:1885:A:N6	2.36	0.58
28:16:13:CYS:SG	28:16:47:THR:HG21	2.44	0.58
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.39	0.58
1:1A:2136:C:N4	1:1A:2155:G:C6	2.72	0.58
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.39	0.58
1:1A:413:C:OP2	61:1A:4030:HOH:O	2.17	0.58
1:1A:272:G:O2'	1:1A:421:U:OP2	2.18	0.58
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.37	0.58
21:1Z:148:ASP:OD1	21:1Z:148:ASP:N	2.36	0.58
21:2Z:39:VAL:HG21	21:2Z:44:PHE:HB2	1.85	0.58
24:22:32:LEU:HD12	24:22:53:LEU:HB3	1.85	0.58
1:2A:323:G:C8	5:2F:171:PRO:HG3	2.38	0.58
1:2A:407:G:N1	1:2A:435:C:N3	50.96	0.58
1:1A:1286:A:H2'	1:1A:1287:A:H4'	6.60	0.58
1:1A:1566:A:OP1	3:1D:211:ARG:NH1	2.37	0.58
1:2A:1971:A:OP1	61:2A:9740:HOH:O	2.16	0.58
1:2A:861:A:N3	2:2B:79:C:O2'	2.34	0.58
7:2H:149:ARG:NH1	7:2H:167:GLU:OE1	2.36	0.58
1:2A:1037:G:H1	1:2A:1118:C:H42	1.51	0.58
1:1A:253:C:O2'	61:1A:4025:HOH:O	2.16	0.58
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.37	0.58
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.69	0.58
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.36	0.58
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	1.84	0.58
19:2X:88:LYS:NZ	19:2X:90:GLU:OE1	2.37	0.58
21:2Z:92:SER:O	21:2Z:130:PRO:HG3	2.03	0.58
1:2A:1288:U:O2'	1:2A:1647:G:N2	2.37	0.57
1:2A:918:A:N6	1:2A:919:G:N3	2.52	0.57
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:7:LEU:HD11	6:2G:107:LEU:HD12	1.86	0.57
10:2O:68:GLU:OE1	10:2O:78:ARG:NH1	2.37	0.57
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.86	0.57
1:1A:1632:A:N7	61:1A:4090:HOH:O	2.32	0.57
1:1A:762:U:OP1	61:1A:4031:HOH:O	2.17	0.57
2:1B:11:C:H3'	2:1B:12:C:C6	2.40	0.57
9:1N:35:ARG:HH21	9:1N:42:TRP:HZ2	1.52	0.57
1:2A:1242:A:N1	11:2P:4:SER:OG	2.36	0.57
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.22	0.57
1:1A:817:C:OP1	61:1A:4034:HOH:O	2.18	0.57
2:1B:23:G:O6	61:1B:3101:HOH:O	2.13	0.57
13:1R:38:VAL:HG22	13:1R:112:ALA:HB2	1.85	0.57
1:2A:1942:5MC:HM53	1:2A:1943:U:C2	2.39	0.57
1:2A:2206:G:H5''	1:2A:2207:G:C5	2.39	0.57
1:1A:1065:U:H2'	1:1A:1073:A:H61	1.69	0.57
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.37	0.57
23:11:91:LYS:HG2	23:11:95:LEU:HD22	1.87	0.57
1:2A:1805:U:O2	3:2D:50:THR:HB	2.04	0.57
1:2A:271(H):G:O2'	1:2A:271(I):G:H8	1.87	0.57
1:2A:898:C:N4	1:2A:899:A:N1	2.52	0.57
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.39	0.57
9:2N:29:LYS:HD2	9:2N:140:VAL:HB	1.87	0.57
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.19	0.57
8:1I:72:LEU:C	8:1I:74:ASN:H	2.06	0.57
1:2A:312:G:O6	61:2A:9737:HOH:O	2.16	0.57
1:1A:1176:G:H1'	1:1A:1177:A:H5''	1.87	0.57
1:1A:1652:A:H2'	1:1A:1653:G:H5'	1.87	0.57
1:1A:2018:G:OP1	27:15:9:LYS:NZ	2.37	0.57
1:1A:2398:U:H2'	1:1A:2399:G:C8	2.40	0.57
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.85	0.57
5:1F:34:TRP:CE2	11:1P:8:PRO:HG3	2.40	0.57
1:2A:1009:A:OP2	61:2A:9745:HOH:O	2.18	0.57
1:2A:83:G:O2'	1:2A:102:G:N2	2.36	0.57
1:2A:1423:G:OP1	10:2O:49:ARG:NH2	97.47	0.57
1:2A:218:A:C2	1:2A:235:U:H4'	2.40	0.57
12:2Q:137:TYR:HE2	21:2Z:49:ARG:HD3	1.70	0.57
1:1A:1069:A:H5'	1:1A:1070:A:OP1	2.05	0.57
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.20	0.57
9:1N:128:HIS:O	9:1N:131:GLN:NE2	2.38	0.57
1:2A:1501:C:H2'	1:2A:1502:C:H6	1.70	0.57
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:612:C:O2	1:2A:629:G:N2	49.90	0.57
1:1A:588:U:H2'	1:1A:589:C:C6	2.39	0.57
1:1A:635:C:O2'	1:1A:639:U:OP1	2.15	0.57
15:1T:112:ARG:HG3	15:1T:115:ARG:HH21	1.69	0.57
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.77	0.57
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.05	0.56
1:1A:764:A:H5''	3:1D:210:GLY:HA2	1.87	0.56
23:21:83:GLU:N	23:21:83:GLU:OE1	2.38	0.56
2:2B:20:C:H42	2:2B:63:G:H1	1.51	0.56
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.21	0.56
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.05	0.56
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.71	0.56
1:1A:1141:U:OP1	9:1N:25:ARG:NH1	2.37	0.56
2:2B:14:U:OP2	2:2B:70:C:O2'	2.18	0.56
4:2E:119:ARG:HD2	4:2E:120:TRP:CE2	2.40	0.56
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.86	0.56
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.40	0.56
1:2A:2882:A:H5'	13:2R:96:ARG:HG3	1.87	0.56
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.40	0.56
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.38	0.56
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.54	0.56
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.04	0.56
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.87	0.56
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.40	0.56
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.40	0.56
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.40	0.56
1:2A:2136:C:H1'	1:2A:2137:C:H5'	1.87	0.56
1:2A:992:C:OP1	16:2U:47:TYR:OH	2.19	0.56
4:2E:2:LYS:HG2	4:2E:200:GLU:HB2	1.87	0.56
1:2A:2340:G:H2'	1:2A:2341:G:H8	1.70	0.56
23:21:4:VAL:HG12	23:21:11:ARG:HB3	1.88	0.56
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.70	0.56
26:14:34:GLU:HG3	26:14:35:VAL:HG12	1.88	0.56
1:1A:1059:G:H1	1:1A:1079:C:N4	2.04	0.56
7:1H:46:GLU:OE2	7:1H:51:ARG:NH2	2.32	0.56
1:1A:956:G:H5''	12:1Q:77:LYS:HD2	1.87	0.56
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.87	0.56
1:2A:323:G:O2'	1:2A:1205:U:N3	2.33	0.56
1:2A:395:U:O2'	1:2A:396:G:N7	2.37	0.56
2:2B:101:G:OP2	61:2B:3101:HOH:O	2.18	0.56
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:12:SER:HB3	3:2D:208:LYS:HB3	1.87	0.56
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.87	0.56
12:2Q:29:PHE:HB3	12:2Q:65:PHE:CD2	2.41	0.56
14:2S:15:ARG:HB3	14:2S:19:LYS:HZ2	1.71	0.56
1:1A:228:A:H8	1:1A:229:A:H5'	1.70	0.56
6:1G:43:LEU:HD11	6:1G:153:ARG:HD2	1.87	0.56
8:1I:46:ALA:HB1	8:1I:50:ARG:HH22	1.70	0.56
1:2A:857:C:H4'	22:20:23:VAL:HG21	1.88	0.56
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.20	0.56
1:2A:2576:G:O2'	1:2A:2579:C:OP2	2.16	0.56
1:2A:7:G:H2'	1:2A:8:A:O4'	2.06	0.56
1:2A:852:G:H2'	1:2A:853:G:H8	1.70	0.56
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.87	0.56
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.39	0.56
26:14:63:TYR:N	26:14:64:GLY:HA2	2.21	0.56
1:1A:2639:A:O3'	9:1N:97:ARG:NH2	2.38	0.56
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.22	0.56
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.36	0.56
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.21	0.55
1:1A:671:C:N4	61:1A:4157:HOH:O	2.38	0.55
23:21:85:LEU:HD23	23:21:89:GLU:HB3	1.87	0.55
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.41	0.55
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.06	0.55
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.40	0.55
1:2A:342:G:O6	61:2A:9744:HOH:O	2.18	0.55
15:1T:117:ASP:OD2	15:1T:120:ARG:NE	2.30	0.55
1:2A:1025:G:O2'	61:2A:9708:HOH:O	2.18	0.55
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.88	0.55
12:1Q:67:ARG:O	12:1Q:101:ARG:NH2	2.39	0.55
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.87	0.55
1:2A:1783:A:OP1	61:2A:9711:HOH:O	2.17	0.55
1:1A:2100:G:H1	1:1A:2189:U:H3	1.53	0.55
1:1A:303:U:O4	61:1A:4032:HOH:O	2.17	0.55
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	1.87	0.55
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.89	0.55
1:2A:1721:G:N1	1:2A:1739:U:OP2	2.39	0.55
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.33	0.55
3:2D:9:TYR:CZ	3:2D:13:ARG:HG2	2.41	0.55
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.88	0.55
12:2Q:21:THR:HG21	12:2Q:101:ARG:HD3	1.88	0.55
1:1A:1055:G:C2	1:1A:1056:G:H1'	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:999:U:OP2	61:1A:4035:HOH:O	2.18	0.55
7:1H:159:GLU:HG2	7:1H:169:VAL:HG11	1.88	0.55
10:1O:64:ARG:HD3	10:1O:79:PHE:CD1	2.42	0.55
1:1A:2882:A:H5'	13:1R:96:ARG:HG3	1.87	0.55
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.07	0.55
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.41	0.55
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.39	0.55
7:2H:86:GLU:OE2	7:2H:130:ARG:NE	2.40	0.55
1:2A:2674:G:H5''	10:2O:26:LYS:HE3	1.88	0.55
1:1A:1173:G:O2'	1:1A:1174:A:O5'	2.24	0.55
1:2A:866:A:H2	1:2A:867:C:C4	2.24	0.55
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.89	0.55
1:2A:2295:C:H5	14:2S:13:ARG:HH12	1.55	0.55
1:1A:1762:A:H2'	61:1A:5424:HOH:O	2.06	0.55
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.23	0.55
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.88	0.55
20:2Y:94:LYS:NZ	61:2Y:601:HOH:O	2.38	0.55
1:1A:2815:C:H5'	27:15:29:THR:HG21	1.88	0.55
1:1A:833:U:O2	11:1P:55:ARG:NH2	2.39	0.55
13:1R:96:ARG:NH1	13:1R:115:GLU:OE2	2.40	0.55
24:22:70:GLN:OE1	24:22:70:GLN:N	2.39	0.55
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.07	0.55
1:2A:1442:G:N3	1:2A:1442:G:H2'	3.01	0.55
1:2A:981:A:OP1	61:2A:9747:HOH:O	2.18	0.55
1:1A:1693:U:O2	3:1D:14:ARG:NH1	2.40	0.55
3:1D:127:VAL:HA	3:1D:193:VAL:HG22	1.89	0.55
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.21	0.55
1:2A:2336:A:H61	22:20:43:THR:CG2	2.20	0.55
1:2A:332:A:O2'	1:2A:334:C:OP2	2.23	0.55
21:2Z:6:LYS:HE3	21:2Z:8:TYR:HE2	1.71	0.55
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.42	0.55
1:1A:458:G:O2'	1:1A:469:G:O6	2.19	0.55
1:1A:987:G:H1	1:1A:1218:C:H42	45.96	0.55
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.88	0.55
1:2A:2833:G:H4'	1:2A:2834:G:OP2	2.07	0.55
8:2I:62:LYS:HE2	8:2I:133:HIS:CE1	2.42	0.55
17:2V:60:GLU:HB2	17:2V:97:LYS:HD3	1.88	0.55
1:1A:530:G:H4'	1:1A:531:C:OP1	2.06	0.54
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.73	0.54
1:2A:2120:G:H2'	1:2A:2121:G:H8	1.71	0.54
30:18:26:LYS:HD3	30:18:48:PHE:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.42	0.54
12:1Q:10:ARG:HH12	12:1Q:90:VAL:H	1.55	0.54
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.42	0.54
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.42	0.54
1:2A:2129:C:N3	1:2A:2159:G:N2	2.45	0.54
5:2F:33:LEU:HD13	5:2F:112:MET:HE2	1.90	0.54
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HG22	1.89	0.54
21:2Z:150:LEU:HB2	21:2Z:171:ILE:HD11	1.89	0.54
1:1A:946:G:OP1	61:1A:4038:HOH:O	2.18	0.54
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.89	0.54
1:2A:1300:U:H4'	1:2A:1301:A:C5'	2.37	0.54
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.42	0.54
1:2A:524:U:H2'	1:2A:525:U:C6	2.43	0.54
1:2A:674:G:H2'	1:2A:675:A:H8	4.75	0.54
2:2B:22:U:H2'	2:2B:23:G:C8	2.43	0.54
18:2W:15:ARG:NH1	61:2W:5001:HOH:O	2.40	0.54
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.42	0.54
6:1G:16:ARG:HH21	6:1G:31:VAL:HG11	1.71	0.54
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE2	1.89	0.54
1:2A:1876:A:H2'	1:2A:1877:A:C8	2.42	0.54
1:2A:2760:C:H1'	7:2H:139:GLN:HE22	1.72	0.54
1:2A:878:A:H61	1:2A:899:A:H1'	1.73	0.54
2:2B:105:A:OP1	21:2Z:72:ARG:NH1	2.41	0.54
1:1A:1094:U:N3	1:1A:1097:U:OP2	2.41	0.54
4:1E:179:GLU:HG3	15:1T:9:LEU:HD21	1.90	0.54
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.08	0.54
2:2B:98:G:H3'	2:2B:99:G:H8	1.73	0.54
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.23	0.54
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.54	0.54
1:2A:708:C:H42	1:2A:723:G:H1	1.54	0.54
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.28	0.54
16:2U:92:ARG:HD3	16:2U:92:ARG:N	2.22	0.54
1:1A:2131:G:H5''	1:1A:2132:U:H3'	1.90	0.54
1:1A:286:C:H2'	1:1A:287:C:C6	2.43	0.54
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.89	0.54
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.08	0.54
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.89	0.54
1:1A:111:A:O2'	24:12:65:ASN:ND2	2.41	0.54
1:1A:2171:A:O2'	1:1A:2172:U:H6	1.89	0.54
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.42	0.54
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.40	0.54
1:2A:601:C:H5'	5:2F:108:LYS:HE3	1.89	0.54
1:2A:900:A:O2'	1:2A:901:A:OP1	2.21	0.54
1:2A:975(A):G:H1'	1:2A:990:A:C2	2.43	0.54
9:2N:72:TYR:N	9:2N:85:ILE:O	2.40	0.54
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.41	0.54
20:2Y:87:LYS:HG2	20:2Y:95:LYS:HD2	1.90	0.54
1:1A:2324:C:H5''	1:1A:2325:G:H5'	1.90	0.54
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.42	0.54
6:1G:44:GLY:O	6:1G:47:LYS:HB2	2.08	0.54
1:2A:2136:C:HO2'	1:2A:2137:C:P	2.31	0.54
1:2A:68:G:H2'	1:2A:69:C:O4'	2.08	0.54
12:2Q:21:THR:HG21	12:2Q:101:ARG:HG2	1.89	0.54
1:1A:1038:C:H42	1:1A:1117:G:H1	1.53	0.54
1:2A:851:U:O2'	25:23:42:ALA:O	2.20	0.54
1:2A:1637:A:OP2	61:2A:9749:HOH:O	2.19	0.54
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.27	0.54
1:2A:910:A:N1	1:2A:2277:G:H1'	2.23	0.54
2:2B:3:C:H2'	2:2B:4:C:C6	2.42	0.54
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.06	0.54
26:14:44:THR:O	26:14:46:GLN:N	2.41	0.53
2:1B:13:A:N1	2:1B:69:G:O2'	2.31	0.53
9:1N:67:LEU:HB3	9:1N:88:GLU:HG3	1.90	0.53
1:2A:1043:C:N4	1:2A:1112:G:O6	2.41	0.53
1:2A:93:G:H2'	1:2A:94:C:C6	2.44	0.53
2:1B:84:C:OP1	25:13:15:TYR:OH	2.16	0.53
1:1A:1068:G:OP2	1:1A:1068:G:H8	5.55	0.53
1:1A:1085:A:H2'	1:1A:1086:A:N3	2.23	0.53
1:1A:271(A):A:N7	1:1A:271(W):G:N2	2.55	0.53
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.90	0.53
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.72	0.53
1:2A:648:G:O2'	1:2A:2351:G:OP1	2.19	0.53
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.08	0.53
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.09	0.53
15:2T:77:PRO:HB2	15:2T:80:SER:HB2	1.91	0.53
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.39	0.53
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.54	0.53
1:1A:1406:U:H2'	1:1A:1407:C:H6	1.73	0.53
1:1A:184:C:H2'	1:1A:185:U:C6	2.44	0.53
17:1V:52:VAL:HG23	17:1V:55:ALA:HB3	1.89	0.53
1:2A:2031:A:N3	1:2A:2455:G:O2'	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2320:A:N6	1:2A:2333:A:H2'	2.23	0.53
5:2F:137:LYS:HA	5:2F:140:LEU:HB2	1.91	0.53
1:1A:2121:G:H1	1:1A:2177:C:H42	1.54	0.53
1:1A:639:U:H2'	1:1A:640:C:C6	2.44	0.53
2:1B:88:C:H2'	2:1B:89:G:O4'	2.08	0.53
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.91	0.53
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.73	0.53
1:2A:2185:C:H2'	1:2A:2186:G:O4'	2.07	0.53
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.09	0.53
1:2A:821:A:H2'	1:2A:946:G:H5''	1.90	0.53
27:15:16:ARG:HG3	27:15:17:ASP:N	2.22	0.53
1:1A:2130:U:H2'	1:1A:2131:G:N2	2.23	0.53
1:1A:2206:G:H3'	1:1A:2207:G:N7	2.24	0.53
1:1A:84:A:H5''	20:1Y:8:LYS:HE3	1.89	0.53
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.09	0.53
1:2A:2135:A:N1	1:2A:2156:G:O2'	2.37	0.53
1:2A:328:U:H4'	20:2Y:68:HIS:CG	2.43	0.53
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.90	0.53
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.90	0.53
13:2R:24:GLN:HB3	13:2R:44:LEU:HD11	1.90	0.53
1:1A:1442:G:H2'	1:1A:1442:G:N3	2.92	0.53
1:1A:232:G:H1'	1:1A:262:A:N1	15.31	0.53
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.44	0.53
1:2A:111:A:O2'	24:22:65:ASN:ND2	2.40	0.53
1:2A:113:G:H2'	1:2A:114:U:H6	5.23	0.53
1:2A:2340:G:H2'	1:2A:2341:G:C8	2.44	0.53
1:2A:448:U:O4	1:2A:583:G:H1'	2.09	0.53
1:2A:903:C:H2'	1:2A:904:C:C6	2.43	0.53
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.89	0.53
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.41	0.53
1:1A:1508:A:O2'	1:1A:1509:C:OP1	2.24	0.53
1:1A:2408:U:H2'	1:1A:2409:G:C8	2.44	0.53
1:1A:900:A:H2'	1:1A:901:A:O4'	2.08	0.53
4:1E:59:VAL:HG21	4:1E:74:PRO:HB3	1.90	0.53
1:2A:1754:C:H5	15:2T:96:ARG:NH2	2.06	0.53
1:1A:1647:G:OP1	61:1A:4041:HOH:O	2.19	0.53
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.73	0.53
1:1A:2059:A:C8	1:1A:2503:2MA:HM23	2.44	0.53
1:1A:2879:C:OP2	61:1A:4039:HOH:O	2.19	0.53
1:1A:532:A:N6	1:1A:1206:G:O2'	62.02	0.53
1:1A:548:A:N6	17:1V:19:LYS:H	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.09	0.53
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.24	0.53
1:2A:79:G:H1	1:2A:90:U:H3	29.39	0.53
3:2D:242:ARG:NH1	3:2D:242:ARG:HG3	2.12	0.53
7:2H:159:GLU:HG2	7:2H:169:VAL:HG11	1.89	0.53
16:2U:58:ARG:HA	16:2U:61:TRP:CE3	2.44	0.53
1:1A:2384:G:P	22:10:55:ARG:HH12	2.32	0.53
1:1A:764:A:H5''	3:1D:210:GLY:CA	2.39	0.53
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.91	0.53
21:1Z:45:ASP:O	21:1Z:49:ARG:HG2	2.08	0.53
25:23:8:LEU:HG	25:23:31:LEU:HD23	1.90	0.53
9:2N:67:LEU:HA	9:2N:87:LEU:HD22	1.90	0.53
15:2T:127:ALA:C	15:2T:129:ARG:H	2.12	0.53
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.22	0.52
1:1A:1538:G:H2'	1:1A:1539:G:C8	2.44	0.52
1:1A:747:U:O2	1:1A:2014:A:H1'	2.09	0.52
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.24	0.52
1:2A:1783:A:HO2'	1:2A:2607:G:HO2'	1.57	0.52
5:2F:28:ILE:HG23	5:2F:112:MET:HE3	1.91	0.52
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.90	0.52
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	1.91	0.52
1:1A:131:G:OP1	61:1A:4037:HOH:O	2.18	0.52
1:1A:2198:A:O5'	8:1I:33:ARG:NH2	2.42	0.52
25:23:46:ASN:O	25:23:50:VAL:HG22	2.09	0.52
1:2A:1509(B):A:H2'	1:2A:1510:G:H8	1.74	0.52
1:2A:286:C:H42	1:2A:355:G:H1	1.56	0.52
1:2A:588:U:H2'	1:2A:589:C:C6	2.44	0.52
2:2B:42:C:O2'	6:2G:67:LYS:O	2.21	0.52
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.92	0.52
1:1A:1256:G:O6	61:1A:4028:HOH:O	2.16	0.52
1:1A:1531:C:H42	1:1A:1538:G:H1	1.58	0.52
23:21:91:LYS:HG2	23:21:95:LEU:HD22	1.90	0.52
1:2A:307:G:H21	1:2A:330:A:H62	1.57	0.52
4:2E:98:PRO:HD3	4:2E:175:VAL:HG13	1.91	0.52
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.49	0.52
11:2P:42:SER:O	61:2P:301:HOH:O	2.19	0.52
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.43	0.52
15:2T:105:LEU:HD22	15:2T:109:GLU:HB3	1.91	0.52
28:16:6:ARG:HH12	28:16:26:ASN:HB2	1.74	0.52
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.23	0.52
1:1A:686:G:OP2	61:1A:4040:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:883:G:H22	1:1A:892:G:H1	1.58	0.52
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.45	0.52
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.91	0.52
21:2Z:149:SER:OG	21:2Z:150:LEU:N	2.40	0.52
1:2A:2206:G:H3'	1:2A:2207:G:N7	2.24	0.52
1:2A:2298:A:H1'	1:2A:2321:G:H21	1.74	0.52
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.08	0.52
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.24	0.52
1:2A:614(B):G:N2	5:2F:44:ARG:O	2.39	0.52
6:2G:41:GLN:HB3	6:2G:43:LEU:HD13	1.90	0.52
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.42	0.52
1:1A:2574:G:OP1	61:1A:4036:HOH:O	2.18	0.52
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.43	0.52
26:24:59:PHE:HA	26:24:61:ARG:N	2.24	0.52
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.57	0.52
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.45	0.52
1:2A:796:C:H2'	1:2A:797:C:C6	2.44	0.52
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.09	0.52
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.09	0.52
1:1A:272(H):C:N4	1:1A:363(B):G:O6	2.19	0.52
21:1Z:150:LEU:HD21	21:1Z:154:ASP:HB2	1.92	0.52
1:2A:880:G:H22	1:2A:898:C:H1'	1.75	0.52
1:1A:1512:U:H2'	1:1A:1513:C:C6	2.45	0.52
7:1H:4:ILE:O	7:1H:69:ARG:HD2	2.09	0.52
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.44	0.52
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.45	0.52
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.91	0.52
1:1A:1045:A:H5'	1:1A:1046:A:H5''	1.91	0.52
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.09	0.52
1:2A:1042:G:H2'	1:2A:1043:C:O4'	4.49	0.52
1:2A:1226:A:OP1	16:2U:16:LYS:NZ	2.39	0.52
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.10	0.52
1:2A:1837:C:O2'	1:2A:1927:A:N3	2.36	0.52
1:2A:2314:C:H2'	1:2A:2315:G:H8	1.74	0.52
8:2I:8:PRO:HD3	8:2I:15:VAL:HB	1.91	0.52
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.45	0.52
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.83	0.52
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.45	0.52
1:2A:774:A:N3	1:2A:774:A:H2'	2.25	0.52
12:2Q:138:ASP:OD2	21:2Z:81:ARG:NH1	2.34	0.52
1:1A:2271:G:H5''	22:10:20:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:9:GLN:HE22	24:12:56:GLN:HB3	1.74	0.51
18:1W:23:LEU:HD11	27:15:25:LEU:HB2	1.92	0.51
1:1A:2137:C:H2'	1:1A:2138:C:C6	2.45	0.51
22:20:11:ARG:O	22:20:14:ARG:NH2	2.35	0.51
1:2A:890:A:H2'	1:2A:892:G:C8	2.44	0.51
21:2Z:144:LEU:HD22	21:2Z:174:VAL:HB	1.92	0.51
1:1A:1799:G:OP1	3:1D:260:ARG:NH1	2.41	0.51
1:1A:2106:G:H1	1:1A:2183:C:H42	1.56	0.51
1:1A:226:G:H21	1:1A:228:A:H62	1.58	0.51
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.92	0.51
14:1S:34:HIS:O	14:1S:97:ARG:NH2	2.43	0.51
1:2A:2356:C:H4'	22:20:20:ARG:HG3	1.92	0.51
30:28:10:ALA:HB3	30:28:62:LEU:HD21	1.92	0.51
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.37	0.51
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.45	0.51
1:2A:468:G:N7	29:27:39:ARG:NH2	2.56	0.51
7:2H:25:LYS:HE3	7:2H:27:LYS:HZ3	1.75	0.51
25:13:37:LEU:HB3	25:13:43:ILE:HD13	1.92	0.51
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.10	0.51
1:1A:2804:C:H2'	1:1A:2805:G:C8	2.45	0.51
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	1.92	0.51
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.45	0.51
1:2A:614(C):A:C4	5:2F:180:GLY:HA2	2.45	0.51
1:2A:801:G:OP2	5:2F:55:GLY:HA2	2.11	0.51
19:2X:41:ASN:O	19:2X:45:THR:HG23	2.10	0.51
1:1A:1364:G:P	23:11:3:LYS:HG3	2.50	0.51
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.10	0.51
1:1A:1701:A:OP2	61:1A:4042:HOH:O	2.19	0.51
1:1A:2135:A:N6	1:1A:2157:G:H21	1.96	0.51
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.75	0.51
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.46	0.51
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.92	0.51
10:1O:36:GLY:HA3	10:1O:109:LYS:HD2	1.91	0.51
15:1T:127:ALA:C	15:1T:129:ARG:H	2.13	0.51
2:2B:24:G:H4'	2:2B:25:A:H8	1.73	0.51
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	1.93	0.51
26:14:61:ARG:HG3	26:14:62:ARG:N	2.26	0.51
1:1A:1062:G:H1'	1:1A:1088:A:C8	2.45	0.51
1:1A:1359:A:H2	1:1A:1372:U:O4	1.92	0.51
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.10	0.51
1:1A:2155:G:H5'	1:1A:2156:G:OP2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	1.92	0.51
1:2A:320:A:H4'	1:2A:322:A:N7	2.26	0.51
1:2A:324:A:N6	1:2A:338:G:O2'	2.43	0.51
1:2A:479:A:N3	1:2A:481:G:H5''	2.25	0.51
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.91	0.51
1:1A:1056:G:H5''	1:1A:1057:A:O4'	2.10	0.51
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.46	0.51
1:1A:582:G:H2'	1:1A:583:G:C8	2.46	0.51
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.43	0.51
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.40	0.51
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.91	0.51
1:2A:2167:U:O2'	1:2A:2168:G:O4'	2.28	0.51
1:2A:652(B):A:H61	1:2A:655:A:H1'	1.76	0.51
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.45	0.51
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.11	0.51
21:2Z:6:LYS:HE3	21:2Z:8:TYR:CE2	2.45	0.51
24:12:64:LEU:HD21	24:12:68:ARG:HE	1.75	0.51
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.10	0.51
1:1A:1815:A:OP2	3:1D:54:ARG:NH2	2.43	0.51
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.10	0.51
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.45	0.51
8:1I:104:GLN:O	8:1I:106:GLY:N	2.43	0.51
8:2I:92:VAL:HG11	8:2I:144:VAL:HG11	1.93	0.51
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG12	1.92	0.51
1:1A:2336:A:H61	22:10:43:THR:CG2	2.23	0.51
24:12:32:LEU:HD11	24:12:54:LYS:HG3	1.92	0.51
10:1O:80:ASP:OD2	15:1T:64:ARG:NH2	2.44	0.51
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.10	0.51
24:22:66:GLU:HG2	24:22:69:ARG:HH22	1.76	0.51
11:2P:59:LEU:HD21	30:28:10:ALA:HA	1.93	0.51
1:2A:1782:C:H1'	1:2A:2609:U:H5''	1.93	0.51
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.26	0.51
1:2A:253:C:OP2	30:28:5:LYS:NZ	2.37	0.51
1:2A:571:A:O2'	17:2V:78:LYS:HE2	2.11	0.51
1:1A:897:C:N3	1:1A:898:C:N4	2.58	0.51
7:1H:56:SER:HB3	7:1H:61:HIS:ND1	2.25	0.51
24:22:9:GLN:HE22	24:22:56:GLN:HB3	1.74	0.51
1:2A:1779:U:H2'	61:2A:9787:HOH:O	2.11	0.51
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.46	0.51
1:1A:1801:G:OP2	3:1D:154:LYS:NZ	2.43	0.51
1:1A:548:A:O2'	1:1A:549:G:O5'	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.46	0.51
4:1E:34:VAL:CG2	4:1E:48:GLN:HE21	2.24	0.51
4:1E:7:VAL:HG13	4:1E:27:LEU:HB3	1.93	0.51
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.43	0.51
24:22:32:LEU:HD11	24:22:54:LYS:HG3	1.93	0.51
1:2A:1783:A:H5'	1:2A:2608:G:H4'	1.93	0.51
9:2N:43:THR:HB	9:2N:46:VAL:HG22	1.93	0.51
23:11:83:GLU:N	23:11:83:GLU:OE1	2.44	0.50
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.46	0.50
1:1A:1538:G:H2'	1:1A:1539:G:H8	1.76	0.50
5:1F:148:LEU:HD21	5:1F:191:ARG:HH21	1.75	0.50
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.23	0.50
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.09	0.50
1:1A:1047:G:H2'	1:1A:1110:G:H1	1.76	0.50
10:1O:64:ARG:NH2	10:1O:99:PHE:O	2.44	0.50
31:29:22:ARG:HB2	31:29:24:TYR:HE2	1.76	0.50
1:2A:821:A:N1	61:2A:9837:HOH:O	2.34	0.50
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.74	0.50
1:1A:2141:G:C6	1:1A:2151:G:C2	2.99	0.50
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.52	0.50
1:2A:2165:G:H2'	1:2A:2166:G:H4'	1.93	0.50
1:2A:646:A:H2'	1:2A:647:G:O4'	2.12	0.50
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.92	0.50
7:2H:125:VAL:HG12	7:2H:131:VAL:HG22	1.92	0.50
10:2O:102:VAL:HB	10:2O:106:LEU:HD12	1.93	0.50
1:1A:1106:G:H2'	1:1A:1107:G:O4'	2.11	0.50
1:1A:2151:G:N1	1:1A:2152:G:O6	2.45	0.50
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.19	0.50
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.26	0.50
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.76	0.50
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.11	0.50
1:2A:299:A:N1	1:2A:322:A:O2'	2.36	0.50
1:2A:1501:C:O4'	3:2D:100:GLY:HA2	2.12	0.50
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.93	0.50
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.44	0.50
1:1A:1213:A:N3	1:1A:1238:G:O2'	2.34	0.50
1:2A:1116:C:H2'	1:2A:1117:G:H5''	4.59	0.50
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.46	0.50
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.36	0.50
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.47	0.50
1:2A:2099:U:H2'	1:2A:2100:G:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.46	0.50
3:2D:233:HIS:HA	61:2D:408:HOH:O	2.11	0.50
5:2F:34:TRP:CZ2	11:2P:8:PRO:HG3	2.47	0.50
1:1A:1065:U:C2'	1:1A:1073:A:H61	2.25	0.50
1:1A:1063:G:H1	1:1A:1075:C:H42	1.58	0.50
1:1A:2572:A:N7	4:1E:144:ARG:HD2	2.26	0.50
1:1A:90:U:H4'	1:1A:92:A:H5'	1.94	0.50
8:1I:130:TYR:CE2	8:1I:132:PRO:HB3	2.47	0.50
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.46	0.50
1:2A:444:C:H4'	5:2F:49:ALA:HB2	1.93	0.50
1:2A:530:G:O4'	1:2A:530:G:N3	2.45	0.50
1:2A:958:U:O2	2:2B:90:A:H4'	2.11	0.50
1:1A:1188:U:C2'	1:1A:1189:A:H5'	2.41	0.50
1:1A:576:U:H2'	1:1A:577:G:C8	2.47	0.50
18:1W:68:ARG:NH1	18:1W:112:GLY:H	2.09	0.50
26:24:62:ARG:HH11	26:24:62:ARG:H	1.59	0.50
1:2A:2006:C:H6	1:2A:2006:C:O5'	1.95	0.50
1:2A:924:C:H2'	1:2A:925:C:C6	2.47	0.50
17:2V:62:LEU:CD1	17:2V:95:LEU:HB2	2.42	0.50
28:16:10:LEU:HG	28:16:54:ILE:HG13	1.94	0.50
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.47	0.50
4:1E:5:LEU:HD13	4:1E:77:ILE:HD12	1.94	0.50
1:2A:2697:G:OP1	61:2A:9751:HOH:O	2.19	0.50
1:2A:362:U:O2'	1:2A:363:G:H5''	2.11	0.50
1:2A:586:A:N1	1:2A:809:G:O2'	2.36	0.50
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.93	0.49
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.94	0.49
1:1A:1666:G:C2'	1:1A:1667:G:H5'	2.41	0.49
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.12	0.49
10:1O:98:VAL:HG11	10:1O:114:ILE:HG23	1.94	0.49
1:2A:1591:G:H2'	1:2A:1592:C:C6	2.47	0.49
6:2G:70:VAL:HA	6:2G:90:LEU:HD23	1.94	0.49
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.12	0.49
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.27	0.49
1:2A:1341:U:OP2	1:2A:1394:U:O2'	2.21	0.49
1:2A:1494:A:H2'	1:2A:1495:A:C8	2.47	0.49
1:2A:1882:C:H2'	1:2A:1883:G:O4'	2.11	0.49
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.12	0.49
1:2A:321:G:OP2	5:2F:135:LYS:HD3	2.13	0.49
1:1A:1466:G:O2'	1:1A:1546:C:O2'	2.28	0.49
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:879:G:O5'	1:1A:879:G:H8	1.94	0.49
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.45	0.49
1:2A:1530:C:N4	1:2A:1539:G:H1	2.10	0.49
1:2A:2012:G:OP1	18:2W:11:ARG:NH2	2.45	0.49
1:2A:746:A:HO2'	1:2A:2611:U:HO2'	1.60	0.49
1:2A:2674:G:H2'	1:2A:2675:A:C8	2.48	0.49
1:2A:30:G:H2'	1:2A:31:C:C6	2.48	0.49
5:2F:31:HIS:NE2	5:2F:35:GLU:OE2	2.45	0.49
12:2Q:110:THR:HG23	12:2Q:113:GLN:OE1	2.11	0.49
21:2Z:7:ALA:HB2	21:2Z:59:LEU:HD22	1.93	0.49
1:1A:2279:G:O6	22:10:14:ARG:HG3	2.13	0.49
2:1B:24:G:N7	2:1B:56:G:H2'	2.27	0.49
4:1E:1:MET:HE3	4:1E:199:ARG:HD2	1.95	0.49
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	1.93	0.49
1:2A:111:A:O3'	24:22:65:ASN:ND2	2.40	0.49
2:2B:2:C:H2'	2:2B:3:C:H6	1.77	0.49
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.48	0.49
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.29	0.49
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.76	0.49
5:1F:161:GLU:HG2	5:1F:164:ARG:NH2	2.27	0.49
5:1F:33:LEU:HB3	11:1P:6:LEU:HD21	1.95	0.49
26:24:64:GLY:O	26:24:66:SER:N	2.39	0.49
1:2A:2748:A:H2'	1:2A:2749:A:C8	2.47	0.49
1:2A:2006:C:O2'	1:2A:2823:A:N3	2.45	0.49
21:2Z:145:GLU:HB3	21:2Z:148:ASP:HB2	1.94	0.49
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.94	0.49
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.76	0.49
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.24	0.49
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.48	0.49
1:2A:2506:U:H1'	57:2A:3673:4M2:H29	1.92	0.49
1:2A:309:G:N3	1:2A:329:G:O2'	2.43	0.49
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.13	0.49
21:2Z:28:MET:HA	21:2Z:88:PHE:O	2.12	0.49
24:12:17:SER:N	24:12:20:GLU:OE2	2.39	0.49
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.12	0.49
1:1A:674:G:H1'	5:1F:74:ARG:HD2	1.94	0.49
23:21:3:LYS:HB2	23:21:61:ARG:HH11	1.78	0.49
1:2A:1448:G:H5''	1:2A:1542:A:OP1	2.12	0.49
1:2A:1688:U:H1'	1:2A:1701:A:C6	2.48	0.49
1:2A:2112:G:H2'	1:2A:2113:U:O4'	2.13	0.49
1:2A:288:C:H2'	1:2A:289:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:373:U:H2'	1:2A:374:A:C8	2.47	0.49
2:2B:11:C:H3'	2:2B:12:C:H6	1.77	0.49
5:2F:110:LEU:HD21	5:2F:181:LEU:HD23	1.95	0.49
1:1A:1093:G:H3'	1:1A:1094:U:H5''	1.94	0.49
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.78	0.49
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.94	0.49
1:2A:1470:G:H5''	1:2A:1471:A:OP1	2.13	0.49
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.48	0.49
1:2A:2243:U:O4	61:2A:9743:HOH:O	2.18	0.49
1:2A:2320:A:H61	1:2A:2333:A:H2'	1.77	0.49
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.77	0.49
1:2A:373:U:H2'	1:2A:374:A:H8	1.77	0.49
1:2A:863:A:H2'	1:2A:864:G:C8	2.48	0.49
5:2F:187:VAL:HG12	11:2P:3:LEU:HD12	1.95	0.49
1:2A:300:A:P	20:2Y:86:ARG:HH21	2.36	0.49
1:1A:2857:G:N2	1:1A:2860:A:OP2	2.37	0.49
1:1A:918:A:H5''	2:1B:98:G:O2'	2.12	0.49
1:2A:1430:C:H2'	1:2A:1431:U:H6	1.78	0.49
1:2A:1453:U:O2'	1:2A:1455:G:N7	2.39	0.49
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.42	0.49
1:2A:2218:U:N3	23:21:55:GLY:O	2.46	0.49
1:2A:883:G:O2'	1:2A:884:C:OP1	2.30	0.49
11:2P:81:GLN:NE2	11:2P:105:LEU:O	2.46	0.49
20:2Y:37:VAL:HG21	20:2Y:72:VAL:HG21	1.94	0.49
1:1A:1466:G:HO2'	1:1A:1546:C:HO2'	1.55	0.49
1:1A:1590:U:H2'	1:1A:1591:G:C8	2.48	0.49
4:1E:29:GLY:HA3	61:1E:401:HOH:O	2.13	0.49
1:2A:1235:G:C6	1:2A:1236:G:N1	2.80	0.49
1:2A:141:A:H8	1:2A:1408:C:O2'	1.96	0.49
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.13	0.49
1:2A:2149:G:H3'	1:2A:2150:U:O4'	2.13	0.49
1:2A:2771:C:H5''	4:2E:202:LYS:HD3	1.95	0.49
1:2A:848:G:C4	1:2A:933:A:C8	2.99	0.49
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.45	0.49
1:1A:1094:U:H3	1:1A:1096:A:H3'	1.78	0.48
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.13	0.48
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.13	0.48
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.48	0.48
1:1A:910:A:N1	1:1A:2277:G:H1'	2.28	0.48
28:26:19:ARG:NH2	28:26:52:VAL:HG11	2.27	0.48
1:2A:2742:C:OP1	31:29:35:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.48	0.48
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.13	0.48
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.78	0.48
1:2A:2140:C:H2'	1:2A:2141:G:H5'	1.93	0.48
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.12	0.48
1:2A:2584:U:H2'	1:2A:2585:U:C6	2.48	0.48
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	1.95	0.48
3:2D:166:GLN:HB2	3:2D:174:ILE:HG22	1.94	0.48
9:2N:21:LYS:NZ	9:2N:140:VAL:OXT	2.43	0.48
4:1E:24:THR:HG22	4:1E:186:GLY:O	2.12	0.48
5:1F:110:LEU:HA	5:1F:183:VAL:HG12	1.96	0.48
1:2A:1013:C:H2'	1:2A:1014:U:H6	1.78	0.48
1:2A:184:C:H2'	1:2A:185:U:C6	2.48	0.48
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.48	0.48
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.13	0.48
1:2A:2870:C:H5''	13:2R:65:LEU:HD21	1.95	0.48
1:2A:882:G:H1	1:2A:894:C:H42	1.60	0.48
4:2E:19:ARG:NH1	10:2O:72:PRO:HB3	2.28	0.48
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.47	0.48
1:1A:2742:C:OP1	31:19:35:ARG:HD3	2.13	0.48
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.48	0.48
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.49	0.48
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.93	0.48
4:1E:170:LEU:HB3	4:1E:184:VAL:HG22	1.95	0.48
10:1O:64:ARG:HB2	10:1O:79:PHE:CD2	2.48	0.48
17:1V:62:LEU:HD11	17:1V:95:LEU:HB2	1.95	0.48
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.43	0.48
1:2A:266:G:H2'	1:2A:266:G:N3	3.22	0.48
2:2B:1:U:H2'	2:2B:2:C:C6	2.48	0.48
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.25	0.48
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.95	0.48
8:2I:116:LEU:HD11	8:2I:120:ILE:HG13	1.95	0.48
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.44	0.48
18:2W:25:ARG:NH2	18:2W:74:ALA:O	2.41	0.48
1:1A:1065:U:H1'	1:1A:1074:G:N1	2.28	0.48
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.94	0.48
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.14	0.48
1:1A:289:A:H2'	1:1A:290:G:O4'	2.13	0.48
1:1A:796:C:H2'	1:1A:797:C:C6	2.48	0.48
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.13	0.48
1:2A:224:G:H2'	1:2A:225:A:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:832:G:OP1	61:2A:9756:HOH:O	2.20	0.48
2:2B:1:U:O2'	2:2B:2:C:O5'	2.24	0.48
7:2H:98:LEU:HD11	7:2H:124:GLU:HA	1.96	0.48
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.96	0.48
16:2U:50:ARG:HH12	17:2V:72:VAL:HA	1.79	0.48
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.49	0.48
1:1A:331:A:N1	61:1A:4122:HOH:O	2.35	0.48
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.48	0.48
1:1A:954:G:H5''	12:1Q:13:GLN:HB3	1.95	0.48
1:2A:1376:C:OP1	61:2A:9755:HOH:O	2.20	0.48
1:2A:1501:C:H2'	1:2A:1502:C:C6	2.47	0.48
1:2A:2121:G:H1	1:2A:2177:C:N4	2.09	0.48
1:2A:2154:G:H2'	1:2A:2155:G:H5''	1.94	0.48
1:2A:921:G:H4'	1:2A:2269:A:C5	2.48	0.48
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.14	0.48
6:2G:25:TYR:HB3	6:2G:30:GLU:HB2	1.95	0.48
1:1A:1007:C:OP1	9:1N:37:LYS:NZ	2.47	0.48
1:1A:1231:G:H2'	1:1A:1232:G:C8	2.49	0.48
1:1A:1993:U:OP2	61:1A:4045:HOH:O	2.20	0.48
1:1A:579:G:H2'	1:1A:580:C:C6	2.49	0.48
3:1D:9:TYR:CZ	3:1D:13:ARG:HG2	2.48	0.48
8:1I:77:LEU:HD11	8:1I:101:LEU:HB2	1.95	0.48
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.13	0.48
14:2S:15:ARG:O	14:2S:19:LYS:HD2	2.14	0.48
21:2Z:23:LYS:HD3	21:2Z:40:ASP:HA	1.96	0.48
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.49	0.48
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.24	0.48
6:1G:47:LYS:O	6:1G:51:ARG:HG2	2.14	0.48
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.96	0.48
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.13	0.48
1:2A:407:G:H2'	1:2A:408:G:C8	2.49	0.48
1:2A:604:G:O6	1:2A:634:C:N4	21.67	0.48
7:2H:118:PRO:HG2	7:2H:121:ILE:HG13	1.96	0.48
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.47	0.48
1:1A:1359:A:C2	1:1A:1372:U:O4	2.66	0.48
1:1A:2611:U:H6	1:1A:2611:U:H5'	1.78	0.48
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	1.96	0.48
1:1A:2794:C:N4	1:1A:2802:G:H22	2.11	0.48
9:1N:48:MET:HG2	9:1N:48:MET:O	2.14	0.48
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.96	0.48
1:2A:2336:A:H61	22:20:43:THR:HG21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:22:46:GLN:HB3	24:22:49:LYS:HD3	1.96	0.48
25:23:4:LEU:O	25:23:36:VAL:HA	2.14	0.48
1:2A:2144:U:H1'	1:2A:2148:G:H22	1.78	0.48
1:2A:897:C:H3'	1:2A:898:C:C6	2.48	0.48
2:2B:24:G:N7	2:2B:56:G:H2'	2.29	0.48
2:2B:95:C:H2'	2:2B:96:U:H6	1.79	0.48
26:14:53:GLU:HB2	26:14:55:ARG:C	2.34	0.48
7:1H:133:VAL:HG12	7:1H:141:VAL:HG13	1.95	0.48
8:1I:76:THR:HG22	8:1I:141:LYS:HB2	1.95	0.48
1:2A:2835:A:N3	61:2A:9845:HOH:O	2.35	0.48
1:2A:812:C:H2'	1:2A:813:U:H6	1.77	0.48
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.95	0.48
3:2D:69:ARG:NH1	3:2D:105:ILE:HD13	2.29	0.48
21:2Z:50:GLN:OE1	21:2Z:50:GLN:N	2.47	0.48
21:2Z:5:LEU:HD11	21:2Z:44:PHE:HA	1.96	0.48
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.94	0.48
1:1A:2451:A:C6	57:1A:3894:4M2:H30	2.49	0.48
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.49	0.48
1:1A:2732:G:H3'	1:1A:2733:A:O4'	2.14	0.48
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.94	0.48
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.79	0.48
12:1Q:110:THR:HG23	12:1Q:113:GLN:HB2	1.96	0.48
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.29	0.48
1:2A:359:A:H2'	1:2A:360:G:O4'	2.14	0.48
3:2D:71:ASP:CB	3:2D:103:ARG:HH12	2.27	0.48
7:2H:73:ALA:O	7:2H:76:VAL:HG22	2.13	0.48
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.96	0.48
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.49	0.47
1:1A:2182:G:H2'	1:1A:2183:C:C6	2.49	0.47
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.29	0.47
7:1H:125:VAL:HG22	7:1H:131:VAL:HG22	1.95	0.47
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.96	0.47
14:1S:25:ARG:HD3	14:1S:42:ASP:OD2	2.12	0.47
1:2A:1364:G:P	23:21:3:LYS:HG3	2.53	0.47
1:2A:2099:U:H2'	1:2A:2100:G:C8	2.49	0.47
1:2A:2322:A:H2'	1:2A:2323:G:O4'	2.14	0.47
7:2H:149:ARG:NH2	7:2H:167:GLU:OE2	2.47	0.47
7:2H:24:VAL:HG22	7:2H:35:VAL:HB	1.95	0.47
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.78	0.47
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.47	0.47
12:2Q:1:MET:HG3	12:2Q:44:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:16:LEU:O	24:12:67:LYS:NZ	2.48	0.47
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.49	0.47
1:1A:1540:U:H2'	1:1A:1541:G:O4'	2.14	0.47
1:1A:2404:C:O3'	11:1P:77:ARG:NH2	2.47	0.47
1:1A:247:G:H4'	1:1A:386:G:C5	2.49	0.47
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.39	0.47
5:1F:140:LEU:HD11	5:1F:170:LEU:HD11	1.96	0.47
1:2A:1204:A:H2	1:2A:1241:A:N6	2.01	0.47
1:2A:1772:G:OP1	61:2A:9757:HOH:O	2.20	0.47
1:2A:2748:A:H2'	1:2A:2749:A:H8	1.79	0.47
21:2Z:163:LEU:HG	21:2Z:165:VAL:HG22	1.96	0.47
1:1A:1064:C:N3	1:1A:1074:G:O6	2.47	0.47
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.49	0.47
1:1A:2573:C:H3'	61:1A:4036:HOH:O	2.14	0.47
1:1A:303:U:H2'	1:1A:304:G:H8	1.79	0.47
1:1A:721:C:H2'	1:1A:722:A:C8	2.49	0.47
1:2A:1171:G:N2	1:2A:1178:C:N3	2.45	0.47
1:2A:340:A:H2'	1:2A:341:G:O4'	2.14	0.47
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.21	0.47
11:2P:95:VAL:HG13	11:2P:125:VAL:HB	1.97	0.47
1:1A:1039:G:H1	1:1A:1116:C:H42	1.62	0.47
1:1A:949:C:N4	61:1A:4092:HOH:O	2.47	0.47
4:1E:2:LYS:HG2	4:1E:200:GLU:HB2	1.96	0.47
9:1N:62:VAL:CG1	9:1N:66:LYS:HB2	2.45	0.47
19:1X:35:THR:HG22	19:1X:37:THR:H	1.79	0.47
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.14	0.47
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.15	0.47
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.49	0.47
1:2A:2161:C:H2'	1:2A:2162:G:C8	2.50	0.47
1:2A:725:G:O5'	1:2A:725:G:H8	1.97	0.47
3:2D:37:LEU:HD13	3:2D:87:ASN:ND2	2.28	0.47
1:1A:222:A:H5''	1:1A:421:U:OP1	2.14	0.47
13:2R:33:ARG:NH2	27:25:57:VAL:O	2.44	0.47
1:2A:2155:G:H5'	1:2A:2155:G:H8	1.79	0.47
1:2A:2635:C:OP1	4:2E:79:ARG:NH1	2.38	0.47
1:2A:493:G:OP1	61:2A:9754:HOH:O	2.20	0.47
1:2A:521:G:H2'	1:2A:522:G:C8	2.49	0.47
25:13:39:ASP:OD1	25:13:44:ARG:NH1	2.48	0.47
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.95	0.47
1:1A:464:U:H2'	1:1A:465:G:O4'	2.14	0.47
1:1A:744:G:OP1	61:1A:4044:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.12	0.47
16:1U:86:ALA:O	17:1V:49:THR:HG23	2.14	0.47
1:2A:1171:G:H1	1:2A:1178:C:N4	2.05	0.47
1:2A:2722:G:H5'	13:2R:4:LEU:HD12	1.96	0.47
1:2A:2869:G:H2'	1:2A:2870:C:O4'	2.15	0.47
4:2E:52:LEU:O	4:2E:76:ARG:N	2.41	0.47
8:2I:124:GLY:H	8:2I:144:VAL:HG23	1.80	0.47
13:2R:36:THR:HG22	13:2R:37:THR:N	2.28	0.47
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.15	0.47
1:1A:210:C:OP1	29:17:29:LYS:HD2	2.15	0.47
1:1A:2111:C:OP2	1:1A:2145:C:N4	2.44	0.47
2:1B:66:A:H61	2:1B:109:C:H5'	1.79	0.47
1:1A:614(C):A:C4	5:1F:180:GLY:HA2	2.50	0.47
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.95	0.47
1:2A:1184:G:OP1	25:23:30:ARG:NH1	2.48	0.47
1:2A:1762:A:N1	61:2A:9848:HOH:O	2.36	0.47
2:2B:9:G:H1	2:2B:112:U:H3	1.62	0.47
1:2A:1903:G:OP1	3:2D:241:PRO:HB2	2.14	0.47
5:2F:34:TRP:CE2	11:2P:8:PRO:HG3	2.50	0.47
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.28	0.47
1:1A:1889:A:H2'	1:1A:1890:A:C8	2.49	0.47
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.49	0.47
1:1A:2572:A:C8	4:1E:144:ARG:HD2	2.49	0.47
1:2A:1376:C:OP2	61:2A:9758:HOH:O	2.20	0.47
1:2A:1827:C:O2'	1:2A:1970:A:N3	2.40	0.47
1:2A:2117:A:O2'	1:2A:2118:U:H5''	2.14	0.47
1:2A:2142:C:H42	1:2A:2150:U:H3	1.61	0.47
1:2A:2199:A:H3'	1:2A:2200:C:C6	2.50	0.47
1:2A:1493:C:H5	1:2A:2206:G:H2'	1.79	0.47
1:2A:834:C:O2	1:2A:852:G:N2	38.59	0.47
1:2A:856:C:H2'	1:2A:857:C:C6	2.50	0.47
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.14	0.47
6:2G:27:ASN:HB3	6:2G:30:GLU:HG3	1.96	0.47
21:2Z:126:VAL:HG13	21:2Z:161:VAL:HG23	1.95	0.47
1:1A:2207:G:H2'	1:1A:2208:A:C2	2.49	0.47
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.50	0.47
1:1A:2443:C:OP1	5:1F:68:LYS:HD3	2.14	0.47
1:1A:893:C:H2'	1:1A:894:C:C6	2.50	0.47
5:1F:106:ARG:HG2	5:1F:106:ARG:H	1.44	0.47
1:1A:1030:G:OP2	12:1Q:128:LYS:NZ	2.47	0.47
21:1Z:163:LEU:HD23	21:1Z:167:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.50	0.47
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.15	0.47
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.66	0.47
1:2A:800:A:OP1	1:2A:800:A:H8	1.98	0.47
1:2A:839:U:H2'	1:2A:840:C:H6	1.79	0.47
1:2A:998:C:P	16:2U:92:ARG:HH21	2.37	0.47
26:24:44:THR:O	26:24:46:GLN:N	2.48	0.47
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.49	0.47
1:2A:1927:A:C6	1:2A:1928:A:C6	3.02	0.47
1:2A:2141:G:O6	1:2A:2150:U:C2	2.67	0.47
1:2A:2233:U:H2'	1:2A:2234:G:C8	2.50	0.47
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.14	0.47
1:2A:42:G:H2'	1:2A:43:A:O4'	2.15	0.47
1:2A:323:G:H8	5:2F:171:PRO:HG3	1.78	0.47
10:2O:63:VAL:HB	10:2O:102:VAL:HG12	1.97	0.47
14:2S:64:GLU:H	14:2S:64:GLU:CD	3.74	0.47
26:14:16:CYS:HA	26:14:33:VAL:O	2.15	0.47
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.80	0.47
1:1A:1268:A:C2	1:1A:2013:A:C4	3.03	0.47
1:1A:324:A:N6	1:1A:338:G:O2'	2.48	0.47
1:1A:839:U:H2'	1:1A:840:C:C6	2.49	0.47
27:25:16:ARG:HG3	27:25:17:ASP:N	2.29	0.47
31:29:10:ILE:HD12	31:29:32:HIS:HA	1.96	0.47
1:2A:1421:G:C2	1:2A:1422:G:C8	3.03	0.47
1:2A:1530:C:H1'	1:2A:1531:C:OP1	2.15	0.47
1:2A:1639:U:H4'	1:2A:2699:C:H4'	1.96	0.47
1:2A:154(A):C:H42	1:2A:171:G:H1	1.62	0.47
1:2A:2371:G:O2'	28:26:46:HIS:ND1	2.41	0.47
1:2A:83:G:C2	1:2A:102:G:H1'	2.50	0.47
12:2Q:21:THR:HG21	12:2Q:101:ARG:CD	2.45	0.47
1:1A:1071:G:OP1	1:1A:1071:G:H3'	2.15	0.46
1:1A:1779:U:H2'	61:1A:4549:HOH:O	2.14	0.46
1:1A:256:A:N3	61:1A:4124:HOH:O	2.36	0.46
1:1A:385:C:O2	11:1P:71:VAL:HG21	2.15	0.46
2:1B:1:U:H2'	2:1B:2:C:C6	2.50	0.46
2:1B:66:A:H61	2:1B:108:U:H2'	1.80	0.46
1:2A:1384:A:N3	1:2A:1405:U:H1'	2.30	0.46
1:2A:1545:A:H2'	1:2A:1546:C:O4'	2.15	0.46
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.15	0.46
1:2A:247:G:H4'	1:2A:386:G:C5	2.50	0.46
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1637:A:H4'	1:2A:2711:A:O2'	2.14	0.46
1:2A:863:A:H2'	1:2A:864:G:H8	1.80	0.46
1:1A:1271:G:OP2	61:1A:4041:HOH:O	2.20	0.46
1:1A:1512:U:H2'	1:1A:1513:C:H6	1.80	0.46
1:1A:871:U:OP1	12:1Q:5:ARG:HG3	2.14	0.46
1:2A:521:G:H2'	1:2A:522:G:H8	1.79	0.46
2:2B:20:C:N4	2:2B:63:G:H1	2.12	0.46
1:1A:1371:G:H2'	1:1A:1372:U:C5	2.48	0.46
1:1A:1531:C:N4	1:1A:1538:G:H1	2.12	0.46
1:1A:1740:G:H2'	1:1A:1741:A:H8	1.80	0.46
1:1A:910:A:N3	1:1A:2264:C:O2'	2.44	0.46
1:2A:819:A:C4	1:2A:1189:A:C2	3.04	0.46
1:2A:1805:U:H5''	3:2D:250:TRP:CD2	2.50	0.46
1:2A:2335:A:C8	1:2A:2337:G:C5	3.03	0.46
1:2A:2722:G:H2'	1:2A:2723:C:C6	2.50	0.46
11:2P:45:LEU:HA	11:2P:45:LEU:HD12	1.72	0.46
13:2R:33:ARG:HD2	13:2R:115:GLU:OE1	2.15	0.46
14:2S:26:LEU:HB3	14:2S:87:PHE:HA	1.98	0.46
30:18:42:ARG:HD2	61:18:206:HOH:O	2.15	0.46
1:1A:2136:C:N3	1:1A:2155:G:C2	2.83	0.46
1:1A:466:A:N3	1:1A:683:C:H1'	2.30	0.46
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.15	0.46
8:1I:109:ILE:HD13	8:1I:109:ILE:HA	1.71	0.46
1:2A:265:A:H1'	1:2A:266:G:O4'	2.15	0.46
1:2A:383:U:H2'	1:2A:385:C:H5	1.80	0.46
5:2F:53:THR:HG22	5:2F:56:GLU:CD	2.36	0.46
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.14	0.46
1:1A:1432:C:H2'	1:1A:1433:U:O4'	2.16	0.46
1:1A:243:U:OP1	30:18:6:THR:OG1	2.25	0.46
1:1A:2801(A):A:N3	1:1A:2895:U:H1'	2.30	0.46
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.50	0.46
19:1X:94:GLY:HA3	19:1X:95:LEU:HB2	1.97	0.46
1:2A:1186:G:C2	1:2A:1187:G:H1'	2.50	0.46
1:2A:2125:G:H21	1:2A:2173:A:H62	1.62	0.46
1:2A:272(H):C:H2'	1:2A:272(I):U:C6	2.51	0.46
1:2A:568:U:O4	61:2A:9746:HOH:O	2.18	0.46
1:2A:571:A:N6	1:2A:2499:C:O3'	2.48	0.46
1:1A:1047:G:O2'	1:1A:1048:A:H8	1.99	0.46
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.15	0.46
1:1A:2160:G:O6	1:1A:2161:C:N4	2.49	0.46
5:1F:123:LEU:HD13	5:1F:192:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.96	0.46
26:24:16:CYS:SG	26:24:17:GLY:N	2.88	0.46
1:2A:1403:C:OP1	1:2A:1520:G:N2	2.23	0.46
1:2A:2287:A:N6	1:2A:2344:U:H3	2.07	0.46
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.16	0.46
6:2G:125:PHE:CE2	6:2G:170:ARG:HB2	2.50	0.46
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.16	0.46
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.31	0.46
1:1A:1055:G:H3'	1:1A:1056:G:H8	1.81	0.46
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.77	0.46
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.50	0.46
19:1X:94:GLY:CA	19:1X:95:LEU:HB2	2.45	0.46
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.96	0.46
1:2A:1005:C:O2'	9:2N:28:THR:HG21	2.16	0.46
1:2A:1006:C:C2	1:2A:1138:G:N2	2.84	0.46
1:2A:307:G:N1	1:2A:310:A:OP2	2.47	0.46
1:2A:686:G:N2	1:2A:788:A:H61	2.13	0.46
3:2D:8:PRO:HB3	3:2D:14:ARG:HB2	1.97	0.46
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.15	0.46
1:1A:303:U:H2'	1:1A:304:G:C8	2.50	0.46
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.63	0.46
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	1.97	0.46
1:1A:559:G:H22	16:1U:49:HIS:CE1	2.34	0.46
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.76	0.46
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.74	0.46
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.31	0.46
1:2A:390:A:N6	61:2A:9925:HOH:O	2.48	0.46
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.16	0.46
1:2A:895:U:O3'	1:2A:896:A:H3'	2.16	0.46
1:2A:954:G:H5''	12:2Q:13:GLN:HB3	1.97	0.46
2:2B:32:C:C2	2:2B:51:G:C2	3.04	0.46
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	1.97	0.46
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.51	0.46
1:1A:2612:C:OP2	27:15:2:ALA:N	2.49	0.46
29:17:24:THR:O	29:17:28:ARG:HG3	2.15	0.46
1:1A:1419:A:O2'	1:1A:1421:G:N7	2.39	0.46
1:1A:2267:A:H5''	1:1A:2268:A:H5'	1.97	0.46
1:1A:2570:G:H2'	1:1A:2571:C:O4'	2.16	0.46
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.16	0.46
1:1A:1759:A:H1'	1:1A:2711:A:C2	2.50	0.46
1:1A:1252:G:N2	16:1U:37:GLU:OE2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1297:C:H2'	1:2A:1298:C:C6	2.51	0.46
1:2A:2134:A:H3'	1:2A:2135:A:C8	2.50	0.46
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.50	0.46
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.16	0.46
1:2A:407:G:H2'	1:2A:408:G:H8	1.81	0.46
1:2A:705:A:C2	1:2A:727:A:H1'	2.50	0.46
1:2A:925:C:H2'	1:2A:926:A:H8	1.81	0.46
1:2A:974:G:C4	1:2A:989:G:C2	3.04	0.46
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.47	0.46
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.97	0.46
1:1A:2790:A:H2'	1:1A:2790:A:N3	2.29	0.46
1:1A:1710:C:O2'	1:1A:2858:C:N3	2.41	0.46
1:1A:422:A:H2'	1:1A:423:A:C8	2.51	0.46
5:1F:164:ARG:O	5:1F:168:ARG:HB2	2.15	0.46
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.97	0.46
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.56	0.46
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.51	0.46
1:2A:576:U:H2'	1:2A:577:G:C8	2.51	0.46
1:2A:625:G:N7	11:2P:107:LYS:NZ	2.55	0.46
11:2P:21:ARG:HA	11:2P:21:ARG:HD3	1.72	0.46
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.16	0.46
1:1A:1063:G:H1	1:1A:1075:C:N4	2.13	0.45
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.51	0.45
1:1A:2120:G:O2'	1:1A:2121:G:H5'	2.16	0.45
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.16	0.45
1:1A:562:U:C2	1:1A:572:A:C8	3.04	0.45
1:1A:784:A:H5'	1:1A:785:G:OP1	2.16	0.45
1:1A:882:G:H1	1:1A:894:C:N4	2.08	0.45
2:1B:14:U:OP2	2:1B:70:C:O2'	2.27	0.45
3:1D:242:ARG:HG3	3:1D:242:ARG:NH1	2.16	0.45
1:2A:83:G:N2	1:2A:102:G:H1'	2.31	0.45
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.51	0.45
1:2A:171:G:H2'	1:2A:172:C:C6	2.50	0.45
1:2A:1929:G:H4'	1:2A:1930:G:OP1	2.16	0.45
1:2A:718:A:H3'	1:2A:719:C:H6	1.80	0.45
1:2A:886:C:O2	1:2A:890:A:N6	2.49	0.45
1:2A:898:C:H2'	1:2A:899:A:H5'	1.96	0.45
1:2A:921:G:H2'	1:2A:922:U:C6	2.51	0.45
1:2A:1799:G:O2'	3:2D:181:GLU:OE2	2.24	0.45
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.51	0.45
6:2G:176:LEU:HD23	6:2G:176:LEU:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1178:C:O5'	1:1A:1178:C:H6	1.99	0.45
1:1A:1680:U:O2'	1:1A:1763:G:N7	2.41	0.45
1:1A:1985:G:OP2	61:1A:4049:HOH:O	2.21	0.45
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.99	0.45
8:1I:77:LEU:HG	8:1I:101:LEU:HD13	1.98	0.45
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.16	0.45
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.68	0.45
24:22:35:LEU:HD12	24:22:53:LEU:HD12	1.98	0.45
1:2A:139:G:H2'	1:2A:140:G:N7	2.31	0.45
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.51	0.45
1:2A:494:G:OP1	18:2W:8:ARG:NH1	2.44	0.45
1:2A:746:A:H2'	1:2A:2612:C:H5''	1.98	0.45
1:2A:1695:G:N7	3:2D:14:ARG:NH2	2.64	0.45
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.98	0.45
6:2G:54:GLU:O	6:2G:58:GLN:N	2.42	0.45
16:2U:113:ALA:O	16:2U:117:GLN:HG2	2.15	0.45
1:2A:446:G:OP1	16:2U:3:ARG:NH1	2.49	0.45
17:2V:62:LEU:HD22	17:2V:93:GLU:HG2	1.98	0.45
1:1A:2019:A:O4'	16:1U:34:LYS:HE3	2.16	0.45
1:1A:2116:G:H2'	1:1A:2117:A:C5	2.52	0.45
1:1A:624:C:O2'	1:1A:657:U:OP1	2.31	0.45
1:1A:684:G:OP1	29:17:16:HIS:ND1	2.46	0.45
3:1D:142:VAL:CG1	3:1D:191:ALA:HB1	2.46	0.45
4:1E:121:ASN:ND2	61:1E:402:HOH:O	2.38	0.45
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.32	0.45
13:1R:97:VAL:HG22	13:1R:114:VAL:HG22	1.98	0.45
1:2A:113:G:H2'	1:2A:114:U:C6	5.60	0.45
1:2A:117:G:C6	1:2A:119:A:C6	3.05	0.45
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.24	0.45
1:2A:2135:A:C6	1:2A:2136:C:N4	2.84	0.45
1:2A:833:U:H2'	1:2A:834:C:C6	2.79	0.45
1:2A:863:A:P	12:2Q:22:LYS:HG3	2.56	0.45
1:1A:1913:A:H4'	1:1A:1914:C:H5''	1.98	0.45
1:1A:245:G:O6	30:18:8:LYS:NZ	2.39	0.45
7:1H:144:VAL:O	7:1H:148:ILE:HG13	2.17	0.45
12:1Q:112:GLU:HG3	12:1Q:113:GLN:N	2.30	0.45
19:1X:29:TRP:CZ3	19:1X:76:ARG:HD2	2.51	0.45
1:2A:1204:A:N6	1:2A:1240:U:H2'	2.32	0.45
1:2A:570:G:H2'	1:2A:2030:A:C5	2.52	0.45
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.51	0.45
1:2A:536:A:H2'	1:2A:537:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:918:A:N3	2:2B:80:U:H4'	2.32	0.45
6:2G:11:TYR:O	6:2G:16:ARG:HG2	2.16	0.45
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.39	0.45
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.99	0.45
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.14	0.45
26:14:53:GLU:HB2	26:14:56:VAL:N	2.32	0.45
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.51	0.45
1:1A:1188:U:H2'	1:1A:1189:A:H5'	1.99	0.45
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.51	0.45
1:1A:121:G:H4'	1:1A:149:A:H5'	1.99	0.45
1:1A:221:A:N1	1:1A:265:A:O2'	2.49	0.45
1:1A:223:A:O4'	1:1A:422:A:H5'	2.16	0.45
1:1A:434:U:H2'	1:1A:435:C:C6	6.22	0.45
1:1A:300:A:O2'	1:1A:564:C:N3	73.52	0.45
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.51	0.45
5:1F:167:ALA:HB1	5:1F:173:VAL:HG11	1.98	0.45
1:1A:2305:A:H5''	6:1G:134:GLY:HA3	1.98	0.45
24:22:16:LEU:HB3	24:22:20:GLU:HG3	1.98	0.45
28:26:19:ARG:HH21	28:26:52:VAL:HG11	1.82	0.45
28:26:23:THR:OG1	28:26:24:GLU:N	2.49	0.45
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.50	0.45
1:2A:1775:U:OP1	61:2A:9759:HOH:O	2.21	0.45
1:2A:2155:G:H2'	1:2A:2156:G:H5'	1.99	0.45
1:2A:414:C:H2'	1:2A:415:A:C8	2.51	0.45
1:2A:466:A:N3	1:2A:683:C:H1'	2.32	0.45
1:2A:868:U:C4	1:2A:869:G:N7	2.85	0.45
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.17	0.45
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.99	0.45
1:1A:1310:G:OP2	29:17:9:ARG:NE	2.41	0.45
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.16	0.45
1:1A:596:G:H2'	1:1A:597:U:O4'	2.17	0.45
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.17	0.45
5:1F:123:LEU:HD13	5:1F:192:LEU:HB3	1.99	0.45
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.52	0.45
1:2A:858:U:OP1	22:20:44:ARG:NH2	2.48	0.45
1:2A:108:U:H2'	1:2A:109:G:C8	2.52	0.45
1:2A:1632:A:O5'	1:2A:1632:A:H8	2.00	0.45
1:2A:2354:G:H2'	1:2A:2355:C:H6	1.81	0.45
1:2A:628:G:H2'	1:2A:629:G:C8	2.85	0.45
6:2G:129:GLY:HA3	6:2G:163:ALA:O	2.17	0.45
7:2H:17:VAL:O	7:2H:45:VAL:HG11	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1598:C:O3'	19:2X:35:THR:HG23	2.17	0.45
21:2Z:151:HIS:ND1	21:2Z:168:GLU:O	2.50	0.45
1:1A:2390:U:P	30:18:35:GLN:HE22	2.39	0.45
1:1A:127:A:H5''	1:1A:128:C:C6	2.52	0.45
1:1A:2238:G:H2'	1:1A:2238:G:N3	2.32	0.45
1:1A:2352:A:N6	1:1A:2365:G:O2'	2.49	0.45
1:1A:673:C:OP1	5:1F:54:ARG:NH1	2.48	0.45
2:1B:7:G:H5''	2:1B:7:G:H8	1.82	0.45
24:22:16:LEU:O	24:22:67:LYS:NZ	2.49	0.45
1:2A:1114:G:H2'	1:2A:1115:G:H8	1.81	0.45
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.17	0.45
1:2A:2287:A:O2'	1:2A:2288:A:H3'	2.17	0.45
1:2A:817:C:O2'	1:2A:839:U:OP1	2.29	0.45
2:2B:42:C:C4	2:2B:43:C:C4	3.04	0.45
6:2G:136:ARG:HG3	6:2G:137:GLU:HG3	1.99	0.45
11:2P:122:PRO:HB3	11:2P:141:ALA:O	2.16	0.45
13:2R:44:LEU:HD23	13:2R:44:LEU:HA	1.76	0.45
27:15:49:CYS:SG	27:15:51:TYR:HB2	2.57	0.45
1:1A:1286:A:C8	1:1A:1287:A:H4'	8.20	0.45
1:1A:381:G:O6	61:1A:4047:HOH:O	2.21	0.45
1:1A:515:A:H1'	1:1A:581:C:H1'	1.98	0.45
1:1A:957:A:N1	1:1A:2458:G:H4'	2.32	0.45
6:1G:16:ARG:HH21	6:1G:31:VAL:CG1	2.29	0.45
6:1G:170:ARG:HE	6:1G:174:GLU:CD	2.20	0.45
1:2A:2264:C:N4	22:20:15:ASP:OD2	2.49	0.45
1:2A:1011:G:H1	1:2A:1150:C:H42	1.65	0.45
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.27	0.45
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.50	0.45
1:2A:1468:C:H2'	1:2A:1469:A:C8	2.52	0.45
1:2A:290:G:H2'	1:2A:291:C:C6	2.52	0.45
1:2A:639:U:H2'	1:2A:640:C:C6	2.51	0.45
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	1.99	0.45
1:1A:1903:G:OP1	3:1D:241:PRO:HB2	2.17	0.45
1:1A:2117:A:O2'	1:1A:2118:U:H5''	2.17	0.45
1:1A:34:C:H5''	1:1A:35:G:OP2	2.17	0.45
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	1.98	0.45
1:2A:2400:G:H2'	1:2A:2401:U:H6	1.81	0.45
1:2A:756:C:H2'	1:2A:757:U:O4'	2.52	0.45
1:2A:983:A:C6	1:2A:984:A:N1	2.85	0.45
3:2D:96:HIS:CD2	3:2D:102:LYS:HG2	2.52	0.45
3:2D:76:PRO:CB	3:2D:116:GLN:HE21	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:41:GLN:HG2	6:2G:154:GLY:O	2.17	0.45
8:2I:31:LEU:HD21	8:2I:38:LEU:HD11	1.99	0.45
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.77	0.45
1:1A:647:G:O5'	1:1A:647:G:H8	2.00	0.45
1:1A:800:A:H8	1:1A:800:A:OP1	2.00	0.45
8:1I:75:LEU:HD13	8:1I:105:HIS:CE1	2.52	0.45
8:1I:27:ARG:HD3	23:11:71:TYR:CE2	2.52	0.45
24:22:20:GLU:O	24:22:24:LEU:N	2.47	0.45
1:2A:1029:A:N6	1:2A:1125:G:O2'	2.48	0.45
1:2A:1040:C:H2'	1:2A:1041:C:C6	2.52	0.45
1:2A:2750:A:H1'	1:2A:2752:C:N4	2.32	0.45
1:2A:2803:C:H2'	1:2A:2804:C:C6	2.52	0.45
6:2G:108:ASN:O	26:24:37:SER:N	2.49	0.45
25:13:10:LYS:HB3	25:13:53:LEU:HA	1.99	0.44
26:14:16:CYS:SG	26:14:17:GLY:N	2.90	0.44
26:14:62:ARG:HB2	26:14:63:TYR:CD1	2.52	0.44
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.52	0.44
1:1A:414:C:H2'	1:1A:415:A:C8	2.53	0.44
1:2A:1530:C:HO2'	1:2A:1531:C:P	2.38	0.44
1:2A:2313:C:H2'	1:2A:2314:C:C6	2.52	0.44
1:2A:2663:G:H2'	1:2A:2664:G:O4'	2.17	0.44
1:2A:492:A:H2'	1:2A:493:G:O4'	2.17	0.44
2:2B:80:U:O2'	2:2B:81:G:H8	1.99	0.44
7:2H:43:VAL:HA	7:2H:52:VAL:HG22	1.99	0.44
7:2H:52:VAL:O	7:2H:65:HIS:NE2	2.45	0.44
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.17	0.44
13:2R:100:LEU:HD23	13:2R:111:LEU:HB3	1.99	0.44
21:2Z:93:ASP:CB	21:2Z:131:ARG:HH22	2.28	0.44
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.98	0.44
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.82	0.44
1:1A:30:G:H2'	1:1A:31:C:C6	2.52	0.44
1:1A:887:A:H1'	1:1A:889:C:OP2	2.17	0.44
1:1A:902:C:H2'	1:1A:903:C:C6	2.53	0.44
3:1D:43:ARG:HA	3:1D:48:ARG:O	2.16	0.44
8:1I:110:ASP:HA	8:1I:111:PRO:HD2	1.76	0.44
10:1O:102:VAL:HB	10:1O:106:LEU:HD12	1.98	0.44
1:2A:1538:G:H2'	1:2A:1539:G:H8	1.82	0.44
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.17	0.44
1:2A:384:U:H2'	1:2A:385:C:H6	1.82	0.44
1:2A:971:C:H2'	1:2A:972:G:O4'	2.17	0.44
13:2R:87:TYR:OH	13:2R:116:LEU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1035:U:H2'	1:1A:1036:G:C8	2.52	0.44
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.53	0.44
1:1A:2321:G:H5''	1:1A:2322:A:OP2	2.16	0.44
1:1A:299:A:OP2	61:1A:4051:HOH:O	2.21	0.44
1:1A:411:G:C5	11:1P:72:PRO:HB3	2.53	0.44
1:1A:896:A:H4'	1:1A:897:C:OP1	2.17	0.44
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.32	0.44
3:1D:29:PRO:HB3	3:1D:63:ARG:NE	2.31	0.44
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.52	0.44
9:1N:130:HIS:HB3	9:1N:133:GLN:HG2	1.99	0.44
1:1A:637:A:H8	11:1P:117:GLU:HG3	1.82	0.44
17:1V:46:VAL:HG22	17:1V:52:VAL:HG11	2.00	0.44
1:2A:1144:G:H2'	1:2A:1145:C:H6	1.81	0.44
1:2A:1993:U:H4'	4:2E:128:SER:OG	2.17	0.44
1:2A:2158:A:H4'	1:2A:2159:G:OP1	2.17	0.44
1:2A:686:G:H21	1:2A:788:A:H61	1.64	0.44
3:2D:10:THR:OG1	3:2D:13:ARG:HB2	2.17	0.44
3:2D:145:VAL:HB	3:2D:155:LEU:HB2	1.98	0.44
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.51	0.44
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.98	0.44
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.53	0.44
28:16:14:THR:HB	28:16:48:VAL:O	2.17	0.44
1:1A:1007:C:H5''	9:1N:35:ARG:NH1	2.32	0.44
1:1A:1062:G:H5''	1:1A:1070:A:C4'	2.48	0.44
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.52	0.44
1:1A:1878:G:H2'	1:1A:1879:C:C6	2.53	0.44
1:1A:1899:G:H2'	1:1A:1899:G:N3	2.32	0.44
1:1A:226:G:N2	1:1A:228:A:H62	2.16	0.44
2:1B:11:C:H3'	2:1B:12:C:H6	1.83	0.44
3:1D:61:LEU:O	3:1D:63:ARG:NH1	2.50	0.44
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.50	0.44
1:2A:1899:G:O2'	1:2A:1900:A:OP2	2.22	0.44
1:2A:2335:A:O2'	1:2A:2337:G:N7	2.32	0.44
1:2A:2366:A:H3'	1:2A:2367:G:H8	1.82	0.44
57:2A:3673:4M2:CAD	57:2A:3673:4M2:H31	2.48	0.44
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.18	0.44
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.52	0.44
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.50	0.44
16:2U:83:LEU:O	16:2U:87:GLY:N	2.51	0.44
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.99	0.44
1:1A:1087:G:H2'	1:1A:1089:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1094:U:H2'	1:1A:1095:A:C8	2.53	0.44
1:1A:315:G:H2'	1:1A:316:C:C6	2.53	0.44
1:1A:897:C:C2	1:1A:898:C:C5	3.05	0.44
6:1G:47:LYS:HD2	6:1G:80:PHE:O	2.18	0.44
1:2A:2166:G:H3'	1:2A:2167:U:H5''	2.00	0.44
1:2A:2370:G:C6	1:2A:2371:G:C6	3.06	0.44
1:2A:2400:G:H2'	1:2A:2401:U:C6	2.53	0.44
1:2A:566:U:H5''	11:2P:29:LYS:HE3	2.00	0.44
1:2A:966:G:H2'	1:2A:967:C:H6	1.81	0.44
7:2H:57:ASP:O	7:2H:62:LYS:HD2	2.17	0.44
1:2A:2839:G:O2'	13:2R:49:ASP:OD2	2.27	0.44
1:1A:2119:A:O2'	1:1A:2120:G:H5''	2.18	0.44
1:1A:902:C:H2'	1:1A:903:C:H6	1.82	0.44
1:1A:764:A:O4'	3:1D:213:ARG:HG3	2.17	0.44
11:1P:135:LEU:HA	11:1P:135:LEU:HD23	1.73	0.44
1:2A:262:A:H2'	1:2A:263:C:O4'	2.17	0.44
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.53	0.44
1:2A:2715:C:H2'	1:2A:2716:U:O4'	2.17	0.44
2:2B:2:C:H2'	2:2B:3:C:C6	2.53	0.44
15:2T:56:GLY:O	15:2T:59:THR:HG22	2.16	0.44
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.53	0.44
1:1A:1054:A:C6	1:1A:1055:G:C6	3.06	0.44
1:1A:1082:U:C4	1:1A:1086:A:N1	2.78	0.44
4:1E:51:PHE:HB3	4:1E:77:ILE:HD11	1.99	0.44
7:1H:88:LEU:HD22	7:1H:165:ALA:HA	1.99	0.44
1:2A:1638:C:O3'	1:2A:2709:G:N2	2.51	0.44
1:2A:460:A:H2'	1:2A:461:C:O4'	2.18	0.44
2:2B:11:C:OP2	2:2B:12:C:H5	2.01	0.44
6:2G:43:LEU:HB3	6:2G:44:GLY:H	1.57	0.44
7:2H:149:ARG:NH1	7:2H:163:TYR:HA	2.32	0.44
8:2I:27:ARG:HG3	23:21:71:TYR:CZ	2.52	0.44
12:2Q:137:TYR:CE2	21:2Z:49:ARG:HD3	2.52	0.44
7:1H:98:LEU:HD12	7:1H:125:VAL:HG23	2.00	0.44
1:1A:2640:G:P	9:1N:97:ARG:HH22	2.41	0.44
1:2A:667:U:O2	30:28:2:PRO:HD2	2.18	0.44
1:2A:1118:C:H2'	1:2A:1119:C:C6	3.38	0.44
1:2A:1580:A:OP2	1:2A:1580:A:H8	2.01	0.44
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.32	0.44
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.53	0.44
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.52	0.44
1:2A:656:G:H2'	1:2A:657:U:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:69:ARG:HE	3:2D:130:ALA:HB3	1.82	0.44
12:2Q:58:PHE:CE1	12:2Q:109:VAL:HG21	2.53	0.44
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.53	0.44
1:1A:1495:A:H2'	1:1A:1496:A:C8	2.52	0.44
1:1A:2138:C:C2	1:1A:2154:G:C2	3.06	0.44
14:1S:36:TYR:CD2	14:1S:36:TYR:N	2.86	0.44
1:2A:1468:C:H2'	1:2A:1469:A:H8	1.82	0.44
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.18	0.44
1:2A:183:C:N4	1:2A:213:A:H61	2.16	0.44
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.99	0.44
2:2B:78:A:C2	2:2B:100:A:C4	3.05	0.44
2:2B:13:A:O2'	2:2B:14:U:H3'	2.17	0.44
5:2F:33:LEU:HA	5:2F:33:LEU:HD12	1.84	0.44
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.18	0.44
7:2H:97:ARG:HA	7:2H:125:VAL:HG21	2.00	0.44
1:1A:667:U:O2	30:18:2:PRO:HD2	2.18	0.43
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.53	0.43
1:1A:2660:A:H2'	1:1A:2661:G:O4'	2.17	0.43
1:1A:2793:G:H22	1:1A:2804:C:H1'	1.82	0.43
4:1E:98:PRO:HD3	4:1E:175:VAL:HG13	2.00	0.43
11:1P:90:ARG:NH1	11:1P:105:LEU:HD11	2.33	0.43
21:1Z:28:MET:HE1	21:1Z:59:LEU:HD13	2.00	0.43
26:24:48:ARG:HA	26:24:48:ARG:HD3	1.82	0.43
1:2A:1161:C:H2'	1:2A:1162:G:H8	1.83	0.43
1:2A:2116:G:N7	1:2A:2166:G:N2	2.66	0.43
1:2A:2154:G:C2	1:2A:2155:G:C8	3.06	0.43
1:2A:2498:C:H3'	61:2A:9704:HOH:O	2.17	0.43
1:2A:534:U:H2'	1:2A:535:C:C6	2.53	0.43
7:2H:96:ALA:HB2	7:2H:105:LEU:HD23	2.00	0.43
11:2P:39:LYS:HA	11:2P:44:GLY:HA2	2.00	0.43
12:2Q:137:TYR:O	12:2Q:141:GLN:HG2	2.18	0.43
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	1.99	0.43
21:2Z:70:LEU:O	21:2Z:89:PHE:N	2.42	0.43
25:13:3:ARG:HD3	25:13:60:GLU:CD	2.38	0.43
1:1A:1754:C:H5	15:1T:96:ARG:NH2	2.09	0.43
1:1A:1790:C:H5''	1:1A:1791:A:OP1	2.19	0.43
1:1A:403:U:H4'	1:1A:404:C:H5'	2.00	0.43
1:1A:534:U:H2'	1:1A:535:C:C6	2.54	0.43
3:1D:96:HIS:CD2	3:1D:102:LYS:HG2	2.53	0.43
4:1E:170:LEU:HG	4:1E:185:LYS:O	2.17	0.43
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:39:LYS:HD2	11:1P:45:LEU:HD11	2.00	0.43
12:1Q:85:LYS:HD3	22:10:7:LEU:HD13	2.00	0.43
13:1R:14:SER:OG	13:1R:15:SER:N	2.51	0.43
17:1V:55:ALA:HB2	17:1V:101:GLY:HA2	1.99	0.43
1:2A:1006:C:OP1	61:2A:9761:HOH:O	2.21	0.43
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.53	0.43
1:2A:2323:G:O6	61:2A:9752:HOH:O	2.20	0.43
1:2A:2579:C:OP1	61:2A:9753:HOH:O	2.20	0.43
1:2A:2639:A:C2	1:2A:2778:A:C8	3.07	0.43
1:2A:297:C:H2'	1:2A:298:G:O4'	2.19	0.43
1:2A:721:C:H2'	1:2A:722:A:C8	2.53	0.43
1:2A:729:G:H5'	1:2A:730:C:H5''	2.00	0.43
2:2B:73:A:C4	2:2B:105:A:C2	3.06	0.43
5:2F:123:LEU:HD12	5:2F:124:LEU:H	1.83	0.43
1:2A:831:G:O2'	11:2P:38:GLN:OE1	2.36	0.43
16:2U:74:LEU:HD13	16:2U:79:PHE:HB2	2.00	0.43
1:1A:857:C:H4'	22:10:23:VAL:HG21	2.00	0.43
1:1A:1709:U:H2'	1:1A:1710:C:C6	2.53	0.43
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.53	0.43
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.54	0.43
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.18	0.43
1:1A:652(C):G:N2	1:1A:653:A:H1'	2.34	0.43
5:1F:109:GLY:HA2	5:1F:112:MET:HE2	2.00	0.43
9:1N:28:THR:HG22	9:1N:29:LYS:N	2.33	0.43
1:2A:144:C:C2	1:2A:145:G:C8	3.06	0.43
1:2A:1589:C:H2'	1:2A:1590:U:H6	1.84	0.43
1:2A:1600:C:OP1	19:2X:58:HIS:NE2	2.33	0.43
1:2A:2317:C:C4	1:2A:2318:G:N7	2.85	0.43
1:2A:579:G:H2'	1:2A:580:C:C6	2.54	0.43
1:2A:848:G:C2	1:2A:933:A:H1'	2.53	0.43
2:2B:15:A:O4'	2:2B:110:G:C8	2.71	0.43
6:2G:11:TYR:OH	6:2G:33:ARG:HG2	2.18	0.43
6:2G:11:TYR:OH	6:2G:16:ARG:HD3	2.19	0.43
21:2Z:97:GLU:HA	21:2Z:126:VAL:O	2.18	0.43
24:12:35:LEU:HD12	24:12:53:LEU:HD12	2.00	0.43
6:1G:108:ASN:HB3	26:14:22:ILE:HD13	1.99	0.43
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.53	0.43
1:1A:207:A:H2'	1:1A:208:C:O4'	2.17	0.43
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.53	0.43
1:1A:359:A:H2'	1:1A:360:G:O4'	2.19	0.43
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:6:VAL:HG22	25:23:56:VAL:HG13	2.01	0.43
30:28:33:ASN:HA	30:28:36:LYS:HD2	2.00	0.43
1:2A:1527:G:H5''	1:2A:1528:A:OP1	2.19	0.43
1:2A:1641:A:H2'	1:2A:1642:G:O4'	2.18	0.43
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.18	0.43
11:2P:55:ARG:HA	61:2P:303:HOH:O	2.18	0.43
16:2U:34:LYS:HA	16:2U:34:LYS:HD3	1.72	0.43
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.33	0.43
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.18	0.43
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.18	0.43
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	1.99	0.43
10:1O:64:ARG:HD2	10:1O:81:ASP:OD1	2.17	0.43
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.50	0.43
13:2R:33:ARG:HH22	27:25:58:LEU:HA	1.84	0.43
28:26:13:CYS:SG	28:26:47:THR:HG21	2.58	0.43
1:2A:1378:A:O2'	1:2A:1379:A:H5''	2.18	0.43
1:2A:858:U:O2	1:2A:2268:A:H2'	2.18	0.43
1:2A:2274:A:C5	1:2A:2276:G:C8	3.07	0.43
1:2A:250:G:C6	1:2A:251:A:C6	3.06	0.43
1:2A:79:G:O2'	1:2A:346:A:N3	2.42	0.43
1:2A:658:C:H2'	1:2A:659:C:C6	2.53	0.43
1:2A:706:A:H2'	1:2A:707:G:O4'	2.18	0.43
3:2D:124:PRO:HG2	3:2D:129:ASN:ND2	2.34	0.43
3:2D:264:LYS:HA	3:2D:265:PRO:HD3	1.92	0.43
6:2G:125:PHE:CD1	6:2G:131:TYR:HD1	2.35	0.43
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.83	0.43
1:2A:2744:G:N2	7:2H:143:GLN:OE1	2.49	0.43
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.19	0.43
12:2Q:21:THR:CG2	12:2Q:101:ARG:HG2	2.47	0.43
17:2V:98:GLU:CD	17:2V:100:ARG:HH12	2.19	0.43
1:1A:196:A:N3	1:1A:196:A:H2'	2.32	0.43
1:1A:2295:C:OP1	14:1S:10:ARG:NH1	2.51	0.43
1:1A:1999:C:H5''	1:1A:2723:C:O2'	2.19	0.43
1:1A:44:G:H5''	1:1A:45:C:OP1	2.18	0.43
1:1A:524:U:H2'	1:1A:525:U:C6	2.53	0.43
1:1A:573:G:O2'	1:1A:574:C:H3'	2.19	0.43
1:1A:721:C:H2'	1:1A:722:A:H8	1.83	0.43
12:1Q:16:ARG:HE	12:1Q:18:LYS:HD3	1.83	0.43
24:22:32:LEU:HD23	24:22:36:ARG:HH11	1.84	0.43
1:2A:141:A:C8	1:2A:1408:C:O2'	2.67	0.43
1:2A:522:G:C6	1:2A:523:C:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:855:G:C6	1:2A:856:C:C4	3.06	0.43
3:2D:275:LYS:HA	3:2D:276:LYS:C	2.38	0.43
8:2I:63:ALA:HA	8:2I:66:GLU:HB3	2.00	0.43
11:2P:47:ASP:N	11:2P:47:ASP:OD1	4.19	0.43
17:2V:74:LYS:HB2	17:2V:83:ARG:HB2	2.00	0.43
1:2A:480:A:O2'	20:2Y:46:LYS:O	2.30	0.43
24:12:32:LEU:HD11	24:12:54:LYS:CG	2.48	0.43
1:1A:1048:A:OP2	1:1A:1109:C:N4	2.52	0.43
1:1A:1041:C:H42	1:1A:1114:G:H1	1.66	0.43
57:1A:3894:4M2:H28	57:1A:3894:4M2:H27	1.86	0.43
1:1A:765:G:N1	1:1A:812:C:O2'	83.91	0.43
4:1E:111:ARG:HD2	4:1E:160:TYR:CD2	2.54	0.43
10:1O:34:THR:OG1	10:1O:35:VAL:N	2.51	0.43
16:1U:104:GLN:NE2	16:1U:105:VAL:HG23	2.33	0.43
31:29:2:LYS:NZ	31:29:31:LYS:O	2.37	0.43
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.83	0.43
1:2A:2636:U:H1'	1:2A:2783:G:N2	2.34	0.43
1:2A:740:U:H2'	1:2A:741:G:C8	2.54	0.43
16:2U:69:CYS:HB3	16:2U:74:LEU:HD12	2.00	0.43
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.49	0.43
1:1A:2131:G:N3	1:1A:2131:G:H2'	2.34	0.43
1:1A:657:U:H2'	1:1A:658:C:C6	2.54	0.43
3:1D:242:ARG:HD2	3:1D:246:PRO:HG3	2.00	0.43
3:1D:68:LYS:O	3:1D:69:ARG:HB2	2.18	0.43
5:1F:56:GLU:OE2	5:1F:93:LYS:NZ	2.52	0.43
8:1I:106:GLY:HA2	8:1I:107:VAL:O	2.18	0.43
12:1Q:65:PHE:HB2	12:1Q:105:GLU:HB2	2.00	0.43
14:1S:28:VAL:HG11	14:1S:98:VAL:HG13	1.99	0.43
19:1X:50:LYS:HE2	61:1X:201:HOH:O	2.18	0.43
21:1Z:4:ARG:HH21	21:1Z:60:GLU:HG2	1.84	0.43
31:29:29:ASN:HA	31:29:30:PRO:HD3	1.88	0.43
1:2A:108:U:H2'	1:2A:109:G:H8	1.82	0.43
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.18	0.43
1:2A:264:C:O2'	1:2A:265:A:H2'	2.19	0.43
1:2A:407:G:O6	1:2A:435:C:N4	51.62	0.43
1:2A:794:G:H2'	1:2A:795:C:H6	1.83	0.43
1:2A:993:G:N3	1:2A:993:G:H2'	2.91	0.43
11:2P:6:LEU:HD23	11:2P:6:LEU:HA	1.67	0.43
15:2T:78:LEU:O	15:2T:78:LEU:HD23	2.18	0.43
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.53	0.43
1:1A:455:C:N3	1:1A:473:G:H5'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:479:A:N3	1:1A:481:G:H5''	2.33	0.43
5:1F:89:VAL:HG12	5:1F:90:PHE:CD2	2.54	0.43
6:1G:43:LEU:HD12	6:1G:43:LEU:HA	1.80	0.43
14:1S:20:ARG:HD2	14:1S:20:ARG:HA	1.91	0.43
19:1X:12:VAL:HG21	19:1X:27:THR:HG22	2.01	0.43
12:2Q:81:VAL:HB	22:20:7:LEU:HD22	2.01	0.43
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.07	0.43
1:2A:817:C:N4	1:2A:1529:G:O6	111.10	0.43
1:2A:2203:U:O4'	3:2D:151:LYS:HE2	2.19	0.43
1:2A:2505:G:H4'	57:2A:3673:4M2:H23	2.01	0.43
5:2F:183:VAL:O	5:2F:187:VAL:HG23	2.19	0.43
7:2H:4:ILE:O	7:2H:69:ARG:HD2	2.19	0.43
1:1A:1051:G:H2'	1:1A:1052:C:O4'	2.19	0.43
1:1A:1753:G:N1	1:1A:1756:G:OP2	2.49	0.43
1:1A:217:G:H2'	1:1A:218:A:O4'	2.19	0.43
1:1A:245:G:O5'	11:1P:73:GLY:HA2	2.19	0.43
1:1A:876:C:H2'	1:1A:877:U:O4'	2.19	0.43
4:1E:97:LYS:HE2	4:1E:97:LYS:HB3	1.68	0.43
12:1Q:10:ARG:NH1	12:1Q:90:VAL:H	2.16	0.43
1:2A:154(A):C:N4	1:2A:171:G:H1	2.17	0.43
1:2A:2279:G:OP2	22:20:11:ARG:NH1	2.50	0.43
1:2A:2319:G:N1	14:2S:3:ARG:HA	2.34	0.43
1:2A:598:G:H2'	1:2A:599:G:O4'	2.19	0.43
1:2A:196:A:C4	1:2A:805:G:C6	3.07	0.43
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.19	0.43
5:2F:46:ARG:HB3	5:2F:48:THR:HG23	2.01	0.43
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.19	0.43
14:2S:87:PHE:CZ	14:2S:102:ALA:HB2	2.54	0.43
13:1R:33:ARG:NH2	27:15:57:VAL:O	2.23	0.42
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.34	0.42
1:1A:620:G:H5'	1:1A:620:G:N3	2.34	0.42
3:1D:70:TRP:CE2	3:1D:150:LYS:HD3	2.54	0.42
8:1I:77:LEU:HD23	8:1I:104:GLN:NE2	2.34	0.42
14:1S:11:LYS:HD3	14:1S:15:ARG:NH1	2.34	0.42
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.42	0.42
1:2A:1006:C:H2'	1:2A:1007:C:C6	3.46	0.42
1:2A:1336:A:H2'	1:2A:1337:G:H8	1.83	0.42
1:2A:2867:G:OP2	15:2T:119:LYS:NZ	2.46	0.42
1:2A:500:G:N1	1:2A:503:A:OP2	2.46	0.42
1:2A:448:U:C4	1:2A:583:G:H1'	2.54	0.42
1:2A:900:A:HO2'	1:2A:901:A:P	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:866:A:N6	1:2A:914:C:C4	2.87	0.42
4:2E:119:ARG:HG3	4:2E:160:TYR:CG	2.54	0.42
6:2G:131:TYR:CE2	6:2G:133:LEU:HB3	2.54	0.42
8:2I:79:ILE:HA	8:2I:80:PRO:HD2	1.94	0.42
13:2R:97:VAL:HG22	13:2R:114:VAL:HG22	1.99	0.42
1:2A:2019:A:O4'	16:2U:34:LYS:HE3	2.19	0.42
1:2A:996:A:O3'	16:2U:91:ASP:HB2	2.19	0.42
23:11:93:GLU:O	23:11:97:LEU:HG	2.18	0.42
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.52	0.42
30:18:62:LEU:HB3	30:18:65:GLU:CG	2.49	0.42
1:1A:1859:A:N6	1:1A:1883:G:O2'	2.49	0.42
4:1E:9:VAL:HG13	4:1E:25:VAL:O	2.19	0.42
25:23:23:LEU:HD13	25:23:50:VAL:HG11	2.02	0.42
27:25:48:GLU:O	27:25:60:VAL:HG11	2.20	0.42
1:2A:1003:G:N2	1:2A:1153:C:C2	2.87	0.42
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.54	0.42
1:2A:1000:A:C4	1:2A:1155:A:C6	3.07	0.42
1:2A:1859:A:N6	1:2A:1883:G:O2'	2.52	0.42
1:2A:2850:A:OP2	1:2A:2866:U:H5	2.02	0.42
1:2A:747:U:O2	1:2A:2014:A:H1'	2.18	0.42
2:2B:23:G:C2	2:2B:61:G:C2	3.08	0.42
1:2A:2265:U:H4'	12:2Q:13:GLN:HE22	1.84	0.42
22:10:17:GLN:O	22:10:19:LYS:NZ	2.52	0.42
1:1A:2168:G:C6	1:1A:2171:A:C8	3.07	0.42
1:1A:2235:G:H2'	1:1A:2236:C:C6	2.54	0.42
1:1A:2576:G:H1'	61:1A:4364:HOH:O	2.19	0.42
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.52	0.42
4:1E:48:GLN:NE2	4:1E:66:HIS:NE2	2.67	0.42
11:1P:126:VAL:HG12	11:1P:148:LEU:CD2	2.49	0.42
14:1S:87:PHE:HZ	14:1S:98:VAL:HG12	1.84	0.42
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.54	0.42
1:2A:1999:C:H4'	1:2A:2723:C:O2	2.20	0.42
1:2A:2184:G:O2'	1:2A:2185:C:H5'	2.20	0.42
1:2A:833:U:H2'	1:2A:834:C:H6	2.29	0.42
1:2A:848:G:H2'	1:2A:849:A:C8	2.55	0.42
4:2E:125:GLY:O	61:2E:401:HOH:O	2.21	0.42
8:2I:29:TYR:HD2	8:2I:30:LEU:HD23	1.84	0.42
1:1A:1594:G:H2'	1:1A:1595:G:O4'	2.20	0.42
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.39	0.42
1:1A:1914:C:H2'	1:1A:1915:5MU:O4'	2.19	0.42
1:1A:2123:G:H1	1:1A:2175:C:H42	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2124:G:H1	1:1A:2174:C:N4	2.16	0.42
1:1A:2134:A:H62	1:1A:2157:G:H1'	1.84	0.42
1:1A:286:C:H2'	1:1A:287:C:H6	1.84	0.42
1:1A:27:G:N2	1:1A:512:G:H1'	2.35	0.42
1:1A:729:G:C8	3:1D:208:LYS:HD2	2.54	0.42
1:1A:880:G:H2'	1:1A:881:G:H8	1.84	0.42
4:1E:4:ILE:HD12	4:1E:91:VAL:HG12	2.00	0.42
25:23:31:LEU:HA	25:23:31:LEU:HD23	1.92	0.42
1:2A:1002:G:C4	1:2A:1003:G:H8	3.65	0.42
1:2A:1494:A:H2'	1:2A:1495:A:H8	1.85	0.42
1:2A:271(H):G:O6	1:2A:271(Q):G:C6	2.73	0.42
1:2A:39:C:O2	5:2F:46:ARG:NH2	2.52	0.42
1:2A:427:U:OP1	3:2D:13:ARG:NH1	84.83	0.42
1:2A:27:G:N2	1:2A:512:G:H1'	2.33	0.42
3:2D:121:PRO:HB3	3:2D:135:PHE:CE2	2.55	0.42
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	2.01	0.42
6:2G:111:LEU:HD23	6:2G:117:PHE:CZ	2.54	0.42
12:2Q:52:VAL:HA	12:2Q:55:VAL:HG12	2.02	0.42
1:2A:1188:U:C4'	17:2V:79:VAL:HG22	2.46	0.42
27:15:8:LYS:O	27:15:9:LYS:HD2	2.19	0.42
1:1A:113:G:H2'	1:1A:114:U:C6	5.44	0.42
1:1A:1815:A:OP1	1:1A:1815:A:H8	2.01	0.42
1:1A:674:G:H2'	1:1A:675:A:C8	4.96	0.42
1:1A:910:A:C6	1:1A:911:A:C6	3.07	0.42
6:1G:114:ILE:HB	6:1G:117:PHE:HB2	2.02	0.42
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.54	0.42
1:2A:422:A:H2'	1:2A:423:A:C8	2.55	0.42
1:2A:718:A:H3'	1:2A:719:C:C6	2.55	0.42
1:2A:854:G:H2'	1:2A:855:G:H8	1.84	0.42
2:2B:90:A:N7	2:2B:91:C:H1'	2.34	0.42
1:1A:1401:G:H2'	1:1A:1402:C:O4'	2.20	0.42
1:1A:897:C:H2'	1:1A:898:C:C6	2.54	0.42
1:1A:1791:A:H5'	3:1D:206:LEU:HD12	2.02	0.42
7:1H:98:LEU:HD23	7:1H:100:GLY:O	2.20	0.42
10:1O:63:VAL:HB	10:1O:102:VAL:HG12	2.01	0.42
20:1Y:87:LYS:HG3	20:1Y:95:LYS:HD2	2.01	0.42
23:21:98:LEU:HA	23:21:98:LEU:HD23	1.89	0.42
30:28:34:TRP:CG	30:28:35:GLN:N	2.88	0.42
1:2A:1607:C:H4'	1:2A:1608:A:O5'	2.19	0.42
1:2A:1786:A:C4	1:2A:1938:A:C6	3.08	0.42
1:2A:212:G:H2'	1:2A:213:A:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:271(X):G:C2	1:2A:271(Y):U:O4	2.72	0.42
1:2A:108:U:P	1:2A:293:U:HO2'	2.42	0.42
1:2A:469:G:H2'	1:2A:470:A:H5''	2.01	0.42
1:2A:515:A:H1'	1:2A:581:C:H1'	2.02	0.42
1:2A:638:G:H2'	1:2A:639:U:O4'	2.19	0.42
1:2A:2445:G:P	5:2F:74:ARG:HH22	2.39	0.42
12:2Q:27:VAL:O	12:2Q:29:PHE:N	2.53	0.42
21:2Z:14:LYS:HA	21:2Z:15:PRO:HD3	1.84	0.42
26:14:63:TYR:CD1	26:14:63:TYR:N	2.86	0.42
1:1A:1853:A:H2'	1:1A:1854:A:C8	2.55	0.42
1:1A:2632:A:O2'	1:1A:2811:G:O2'	2.24	0.42
1:1A:625:G:O6	11:1P:107:LYS:NZ	2.48	0.42
1:1A:755:C:H2'	1:1A:756:C:C6	2.55	0.42
3:1D:8:PRO:HB3	3:1D:14:ARG:NE	2.35	0.42
4:1E:47:VAL:O	4:1E:80:GLU:HA	2.20	0.42
8:1I:109:ILE:HG23	8:1I:130:TYR:CZ	2.55	0.42
1:2A:1179:C:H2'	1:2A:1180:C:C6	2.55	0.42
1:2A:2050:C:C4	1:2A:2051:A:C6	3.08	0.42
1:2A:307:G:N7	61:2A:9850:HOH:O	2.36	0.42
1:2A:872:A:C8	1:2A:874:G:C8	8.57	0.42
1:2A:909:A:C6	1:2A:912:C:C2	3.07	0.42
3:2D:274:ARG:N	61:2D:405:HOH:O	2.50	0.42
4:2E:72:VAL:HA	4:2E:73:GLU:CB	2.48	0.42
10:2O:104:ARG:NH1	10:2O:104:ARG:HB2	2.35	0.42
10:2O:35:VAL:HG23	10:2O:65:THR:HG23	2.02	0.42
26:14:49:PHE:HB3	26:14:50:VAL:HG12	2.02	0.42
1:1A:1054:A:N6	1:1A:1055:G:O6	2.53	0.42
1:1A:1786:A:H8	61:1A:4341:HOH:O	2.02	0.42
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.34	0.42
1:1A:228:A:C8	1:1A:229:A:H5'	2.51	0.42
1:1A:236:C:H2'	1:1A:237:C:C6	2.55	0.42
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.20	0.42
15:1T:116:ALA:HB1	15:1T:121:ILE:HD11	2.02	0.42
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.51	0.42
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.55	0.42
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.52	0.42
1:2A:1810:A:O5'	1:2A:1810:A:H8	2.03	0.42
1:2A:1895:C:H2'	1:2A:1896:G:O4'	2.19	0.42
1:2A:196:A:N3	1:2A:196:A:H2'	2.35	0.42
1:2A:1999:C:H2'	1:2A:2000:G:O4'	2.19	0.42
1:2A:221:A:N1	1:2A:265:A:O2'	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2393:A:H2'	1:2A:2394:C:O4'	2.19	0.42
1:2A:2503:2MA:H4'	1:2A:2504:U:OP1	2.20	0.42
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.54	0.42
1:2A:2886:G:H2'	1:2A:2887:U:C6	2.54	0.42
1:2A:291:C:O2	1:2A:309:G:N2	48.34	0.42
57:2A:3673:4M2:H27	57:2A:3673:4M2:H28	1.73	0.42
1:2A:669:G:C2	1:2A:801:G:C6	3.08	0.42
1:2A:848:G:N9	1:2A:933:A:H8	2.17	0.42
1:2A:920:G:H2'	1:2A:921:G:H8	1.85	0.42
1:2A:997:G:OP2	16:2U:58:ARG:NH1	2.51	0.42
3:2D:275:LYS:HA	3:2D:275:LYS:HD2	1.85	0.42
6:2G:76:SER:CB	6:2G:84:LYS:H	2.33	0.42
1:1A:2168:G:C6	1:1A:2171:A:H8	2.38	0.42
1:1A:2319:G:C2	14:1S:3:ARG:HA	2.54	0.42
1:1A:2689:U:H4'	1:1A:2690:C:O5'	2.20	0.42
1:1A:2788:C:P	4:1E:61:ARG:HH21	2.42	0.42
57:1A:3894:4M2:CAD	57:1A:3894:4M2:H31	2.48	0.42
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.27	0.42
6:1G:150:ASP:OD1	6:1G:150:ASP:N	2.53	0.42
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.19	0.42
8:1I:109:ILE:HG23	8:1I:130:TYR:OH	2.20	0.42
9:1N:4:TYR:CE2	16:1U:100:VAL:HG11	2.55	0.42
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	2.02	0.42
1:2A:2232:U:OP2	23:21:40:ARG:NH2	2.52	0.42
30:28:23:VAL:CG1	30:28:47:LYS:HB3	2.50	0.42
1:2A:1406:U:H2'	1:2A:1407:C:H6	1.85	0.42
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	2.01	0.42
1:2A:1951:U:O2'	1:2A:1953:A:N7	2.43	0.42
1:2A:2298:A:H1'	1:2A:2321:G:N2	2.34	0.42
1:2A:2485:G:C2	1:2A:2486:G:C8	3.08	0.42
1:2A:2589:A:OP1	61:2A:9763:HOH:O	2.22	0.42
1:2A:2848:G:H1'	1:2A:2867:G:N2	2.35	0.42
1:2A:890:A:N6	1:2A:893:C:H42	2.18	0.42
2:2B:42:C:C6	6:2G:69:ALA:HB2	2.54	0.42
22:10:18:ALA:HB3	22:10:20:ARG:NH1	2.35	0.42
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.53	0.42
1:1A:2346:A:N1	61:1A:4132:HOH:O	2.37	0.42
1:1A:266:G:H2'	1:1A:266:G:N3	3.19	0.42
1:1A:776:G:H4'	1:1A:777:A:O5'	2.20	0.42
1:1A:90:U:H1'	1:1A:92:A:C8	2.54	0.42
1:1A:2032:G:H1'	4:1E:145:LYS:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	2.01	0.42
6:1G:122:PRO:HD3	6:1G:181:ARG:HG2	2.01	0.42
19:1X:26:TYR:HB3	19:1X:92:LEU:HD22	2.02	0.42
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.38	0.42
23:21:62:VAL:HG22	23:21:63:ALA:O	2.19	0.42
29:27:26:GLY:O	29:27:30:VAL:HG23	2.19	0.42
1:2A:1115:G:C2	1:2A:1116:C:C2	3.07	0.42
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.41	0.42
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.28	0.42
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.55	0.42
1:2A:2111:C:OP2	1:2A:2111:C:H6	2.02	0.42
1:2A:2114:A:N6	1:2A:2119:A:N7	2.67	0.42
1:2A:2125:G:N2	1:2A:2173:A:H62	2.17	0.42
1:2A:234:C:H2'	1:2A:235:U:C6	2.55	0.42
1:2A:2815:C:H2'	1:2A:2816:C:H6	1.84	0.42
2:2B:11:C:H3'	2:2B:12:C:C6	2.55	0.42
7:2H:44:VAL:HG12	7:2H:46:GLU:HG3	2.02	0.42
9:2N:73:THR:OG1	9:2N:82:LEU:HD11	2.20	0.42
15:2T:24:PRO:HD3	15:2T:52:ILE:HD12	2.01	0.42
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	2.01	0.42
1:1A:2398:U:H2'	1:1A:2399:G:H8	1.84	0.41
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.38	0.41
1:1A:775:G:O5'	1:1A:777:A:H1'	2.19	0.41
4:1E:31:CYS:HA	4:1E:32:PRO:HD2	1.94	0.41
9:1N:39:ARG:HA	9:1N:40:PRO:HD3	1.93	0.41
1:1A:908:C:OP1	12:1Q:22:LYS:HB3	2.20	0.41
25:23:50:VAL:O	25:23:54:VAL:HB	2.19	0.41
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.20	0.41
1:2A:1710:C:H5'	1:2A:2859:G:H1'	2.01	0.41
1:2A:2193:G:H2'	1:2A:2194:G:O4'	2.20	0.41
1:2A:2238:G:N3	1:2A:2238:G:H2'	2.35	0.41
1:2A:251:A:C5	1:2A:252:G:H1'	2.55	0.41
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.20	0.41
1:2A:2690:C:N4	1:2A:2713:A:H1'	2.34	0.41
1:2A:565:C:H2'	1:2A:566:U:O4'	2.19	0.41
1:2A:885:C:O2'	1:2A:892:G:O6	2.35	0.41
1:2A:903:C:O2'	1:2A:904:C:H5'	2.19	0.41
5:2F:9:ILE:HD13	5:2F:123:LEU:HD23	2.02	0.41
1:2A:2303:G:O2'	6:2G:132:ASN:HB2	2.19	0.41
6:2G:61:ALA:HA	6:2G:66:GLN:O	2.20	0.41
7:2H:12:PRO:O	7:2H:15:VAL:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:18:C:H4'	16:2U:23:GLY:O	2.20	0.41
22:10:82:ARG:HA	22:10:83:PRO:HD3	1.93	0.41
1:1A:1949:G:C6	1:1A:1950:G:C6	3.09	0.41
1:1A:2332:U:O4	61:1A:4029:HOH:O	2.17	0.41
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.56	0.41
1:1A:631:A:H2'	1:1A:632:A:O4'	2.19	0.41
20:1Y:92:ASN:HB3	20:1Y:94:LYS:N	2.18	0.41
1:2A:1504:C:H2'	1:2A:1505:C:C6	2.55	0.41
1:2A:2296:U:H4'	1:2A:2297:C:OP1	2.20	0.41
1:2A:2504:U:OP2	61:2A:9762:HOH:O	2.22	0.41
1:2A:2602:A:H4'	1:2A:2603:G:C5'	2.50	0.41
1:2A:2654:A:N1	1:2A:2665:A:H5''	2.35	0.41
1:2A:81:G:O2'	1:2A:295:G:O2'	2.23	0.41
1:2A:330:A:H2	1:2A:1210:A:O2'	2.03	0.41
1:2A:357:A:H8	1:2A:357:A:O5'	2.03	0.41
1:2A:717:G:H2'	1:2A:718:A:O4'	2.20	0.41
2:2B:40:U:N3	2:2B:44:G:OP2	2.45	0.41
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.43	0.41
6:2G:44:GLY:O	6:2G:47:LYS:HB2	2.20	0.41
21:2Z:161:VAL:O	21:2Z:161:VAL:HG13	2.20	0.41
1:1A:1038:C:N4	1:1A:1117:G:H1	2.17	0.41
1:1A:1227:G:OP1	16:1U:13:LYS:HG2	2.20	0.41
1:1A:1860:G:H2'	1:1A:1861:G:O4'	2.20	0.41
1:1A:2170:A:O5'	1:1A:2170:A:H8	2.03	0.41
1:1A:890:A:H2'	1:1A:892:G:O4'	2.20	0.41
5:1F:183:VAL:O	5:1F:187:VAL:HG23	2.19	0.41
23:21:67:ILE:N	23:21:68:PRO:HD2	2.36	0.41
28:26:7:ILE:HG21	28:26:27:LYS:HD3	2.03	0.41
1:2A:1334:G:C6	1:2A:1335:U:C4	3.08	0.41
1:2A:1359:A:C2	1:2A:1372:U:O4	2.73	0.41
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.55	0.41
1:2A:1703:G:H2'	1:2A:1704:G:C8	2.55	0.41
1:2A:2033:A:O2'	1:2A:2035:G:OP2	2.26	0.41
1:2A:217:G:H2'	1:2A:218:A:O4'	2.19	0.41
1:2A:2475:C:H42	1:2A:2529:G:H22	1.67	0.41
1:2A:2653:U:HO2'	7:2H:110:SER:CB	2.34	0.41
1:2A:776:G:P	61:2A:9717:HOH:O	2.76	0.41
5:2F:129:PHE:HB3	5:2F:132:VAL:HG11	2.03	0.41
8:2I:44:LEU:HD12	8:2I:44:LEU:HA	1.94	0.41
30:18:52:LYS:N	30:18:53:PRO:HD2	2.36	0.41
1:1A:2124:G:H2'	1:1A:2125:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.56	0.41
1:1A:2259:G:C6	1:1A:2260:C:C4	3.08	0.41
1:1A:784:A:OP1	1:1A:2588:G:H5''	2.21	0.41
6:1G:43:LEU:HB2	6:1G:89:GLY:HA2	2.02	0.41
7:1H:167:GLU:HA	7:1H:168:PRO:HD3	1.86	0.41
19:1X:54:VAL:HG22	19:1X:81:VAL:HG12	2.02	0.41
24:22:12:GLU:O	24:22:16:LEU:HG	2.20	0.41
28:26:10:LEU:HD13	28:26:19:ARG:HD3	2.01	0.41
1:2A:1021:A:C2	1:2A:1023:U:C2	3.08	0.41
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.19	0.41
1:2A:2417:C:C4	1:2A:2418:A:N7	2.88	0.41
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.52	0.41
1:2A:375:C:H2'	1:2A:376:C:C6	2.56	0.41
1:2A:886:C:H2'	1:2A:887:A:H1'	2.02	0.41
1:2A:910:A:C6	1:2A:911:A:C6	3.09	0.41
8:2I:65:ALA:HB1	8:2I:132:PRO:HG2	2.02	0.41
21:2Z:73:GLN:HB3	21:2Z:87:ASP:OD2	2.21	0.41
30:18:23:VAL:CG1	30:18:47:LYS:HD3	2.50	0.41
1:1A:1071:G:O2'	1:1A:1089:G:H2'	2.21	0.41
1:1A:1466:G:H2'	1:1A:1547:C:H41	1.85	0.41
1:1A:2577:A:H5'	27:15:3:LYS:HE3	2.01	0.41
1:1A:2626:C:H2'	1:1A:2627:G:O4'	2.20	0.41
1:1A:27:G:C2	1:1A:512:G:N3	2.88	0.41
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.37	0.41
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	2.02	0.41
13:1R:36:THR:HG22	13:1R:37:THR:N	2.35	0.41
18:1W:1:MET:HG3	18:1W:64:MET:SD	2.61	0.41
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.86	0.41
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.21	0.41
1:2A:1885:A:H2'	1:2A:1886:C:O4'	2.20	0.41
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.56	0.41
1:2A:2352:A:N6	1:2A:2365:G:O2'	2.53	0.41
1:2A:2639:A:H2'	1:2A:2640:G:O4'	2.20	0.41
1:2A:328:U:H4'	20:2Y:68:HIS:CD2	2.56	0.41
1:2A:702:G:C2	1:2A:731:C:C2	3.09	0.41
1:2A:855:G:H2'	1:2A:856:C:C6	2.56	0.41
1:2A:883:G:HO2'	1:2A:884:C:P	2.43	0.41
5:2F:196:LEU:HD23	5:2F:196:LEU:HA	1.92	0.41
6:2G:131:TYR:HE2	6:2G:133:LEU:HB3	1.84	0.41
12:2Q:85:LYS:HD2	12:2Q:85:LYS:N	2.35	0.41
22:10:43:THR:HG23	22:10:43:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:987:G:O2'	1:1A:1000:A:N3	2.47	0.41
1:1A:2705:A:O2'	1:1A:2852:G:OP1	2.32	0.41
1:1A:36:G:N3	1:1A:450:G:O2'	2.48	0.41
3:1D:166:GLN:HB2	3:1D:174:ILE:HG22	2.03	0.41
4:1E:14:ILE:HG13	4:1E:21:VAL:HG13	2.03	0.41
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.55	0.41
1:2A:271(S):G:C6	1:2A:271(T):C:C4	3.08	0.41
3:2D:206:LEU:HA	3:2D:206:LEU:HD23	1.77	0.41
1:2A:1816:G:H8	3:2D:62:TYR:CZ	2.39	0.41
8:2I:77:LEU:HB3	8:2I:142:VAL:HG13	2.02	0.41
10:2O:2:ILE:HG21	10:2O:8:LEU:HD11	2.01	0.41
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.55	0.41
19:2X:35:THR:HG22	19:2X:37:THR:H	1.85	0.41
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.21	0.41
1:1A:1226:A:OP1	16:1U:16:LYS:NZ	2.53	0.41
1:1A:2110:G:OP2	1:1A:2110:G:H2'	2.21	0.41
1:1A:2590:A:H2'	1:1A:2591:C:H6	1.85	0.41
1:1A:1654:A:C1'	1:1A:2823:A:H5'	2.51	0.41
1:1A:361:G:N1	1:1A:362:U:O4	2.53	0.41
2:1B:48:A:H4'	14:1S:95:HIS:CD2	2.53	0.41
2:1B:4:C:H2'	2:1B:5:C:O4'	2.21	0.41
5:1F:102:PRO:HB2	5:1F:105:VAL:HG23	2.01	0.41
6:1G:121:ASN:HA	6:1G:122:PRO:HD3	1.91	0.41
26:24:64:GLY:C	26:24:66:SER:N	2.73	0.41
28:26:10:LEU:HG	28:26:54:ILE:HG13	2.01	0.41
1:2A:2078:C:H2'	1:2A:2079:U:C6	2.55	0.41
1:2A:2159:G:N1	1:2A:2160:G:O6	2.54	0.41
1:2A:2165:G:H2'	1:2A:2166:G:C4'	2.51	0.41
1:2A:2228:G:C5	1:2A:2229:C:C4	3.08	0.41
1:2A:277:C:HO2'	1:2A:278:A:P	2.43	0.41
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.20	0.41
1:2A:459:U:OP2	29:27:39:ARG:NH1	2.54	0.41
1:2A:631:A:H2'	1:2A:632:A:O4'	2.20	0.41
1:2A:947:G:H2'	1:2A:948:G:C8	2.55	0.41
5:2F:116:ASP:OD2	5:2F:117:ARG:NH1	2.53	0.41
11:2P:44:GLY:CA	11:2P:45:LEU:HB2	2.50	0.41
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD23	2.03	0.41
1:1A:1094:U:C4	1:1A:1096:A:H5''	2.56	0.41
1:1A:1590:U:H2'	1:1A:1591:G:H8	1.86	0.41
1:1A:1665:A:H2'	1:1A:1666:G:O4'	2.20	0.41
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1915:5MU:H71	1:1A:1915:5MU:OP2	2.21	0.41
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.55	0.41
1:1A:312:G:H5'	1:1A:331:A:O2'	2.20	0.41
7:1H:124:GLU:HB2	7:1H:132:ARG:HB3	2.01	0.41
12:1Q:85:LYS:N	12:1Q:85:LYS:HD2	2.35	0.41
24:22:53:LEU:HA	24:22:53:LEU:HD23	1.86	0.41
1:2A:1418:G:H8	1:2A:1418:G:O5'	2.04	0.41
1:2A:1422:G:C6	1:2A:1423:G:C5	3.09	0.41
1:2A:1906:G:OP2	1:2A:1929:G:O2'	2.37	0.41
8:2I:66:GLU:OE2	8:2I:69:LYS:HD3	2.20	0.41
30:18:6:THR:HG23	30:18:64:TYR:HD2	1.85	0.41
1:1A:1111:A:N3	1:1A:1112:G:H1'	2.36	0.41
1:1A:1203:G:H5'	11:1P:3:LEU:HD23	2.02	0.41
1:1A:184:C:H2'	1:1A:185:U:H6	1.83	0.41
1:1A:2807:G:C2	1:1A:2808:U:C2	3.08	0.41
1:1A:428:A:H8	1:1A:428:A:OP2	2.04	0.41
5:1F:11:VAL:HB	5:1F:18:ARG:HG3	2.03	0.41
7:1H:88:LEU:HD12	7:1H:130:ARG:HG2	2.02	0.41
11:1P:126:VAL:HG12	11:1P:148:LEU:HD22	2.02	0.41
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	2.02	0.41
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	2.02	0.41
1:2A:1227:G:H2'	1:2A:1228:G:O4'	2.21	0.41
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.55	0.41
1:2A:2189:U:H5'	1:2A:2190:G:OP2	2.21	0.41
1:2A:258:G:H1	1:2A:268:C:H42	33.02	0.41
1:2A:2691:C:O3'	1:2A:2871:C:H4'	2.20	0.41
1:2A:2836:U:C4	1:2A:2883:A:N6	2.88	0.41
1:2A:287:C:H2'	1:2A:288:C:C6	2.56	0.41
1:2A:647:G:H2'	1:2A:648:G:O4'	2.21	0.41
9:2N:112:LEU:O	9:2N:116:LEU:HG	2.21	0.41
10:2O:7:TYR:CZ	10:2O:44:LYS:HG3	2.56	0.41
17:2V:14:VAL:HA	17:2V:18:LEU:HD12	2.03	0.41
20:2Y:30:VAL:O	20:2Y:32:PRO:HD3	2.20	0.41
1:1A:2097:C:H2'	1:1A:2098:U:O4'	2.21	0.41
1:1A:2106:G:H2'	1:1A:2107:C:C6	2.56	0.41
1:1A:324:A:H2'	1:1A:325:G:O4'	2.21	0.41
1:1A:363(C):G:H2'	1:1A:363(D):G:C8	2.55	0.41
1:1A:493:G:H2'	1:1A:494:G:O4'	2.19	0.41
5:1F:34:TRP:HA	11:1P:6:LEU:HD13	2.03	0.41
6:1G:126:ASP:OD2	6:1G:130:ASN:ND2	2.47	0.41
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:48:GLU:O	6:1G:51:ARG:HG3	2.21	0.41
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	2.02	0.41
30:28:32:LEU:HA	30:28:32:LEU:HD12	1.89	0.41
1:2A:1006:C:H5'	9:2N:28:THR:HG23	2.03	0.41
1:2A:1262:A:H2	27:25:10:LYS:HD2	1.86	0.41
1:2A:1301:A:C8	1:2A:1303:G:C8	3.09	0.41
1:2A:2104:G:N2	1:2A:2185:C:N3	2.65	0.41
1:2A:225:A:N6	1:2A:226:G:C2	2.89	0.41
1:2A:2287:A:C4	1:2A:2289:G:C8	3.09	0.41
1:2A:2436:G:C5	1:2A:2437:U:C5	3.09	0.41
1:2A:315:G:H2'	1:2A:316:C:C6	2.56	0.41
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	2.02	0.41
10:2O:108:GLU:H	10:2O:108:GLU:HG2	1.56	0.41
1:2A:826:U:H4'	11:2P:55:ARG:HB3	2.03	0.41
19:2X:50:LYS:HB3	19:2X:84:ALA:HB2	2.02	0.41
21:2Z:121:HIS:HB3	21:2Z:123:ASP:O	2.21	0.41
1:1A:1184:G:H5'	25:13:29:ARG:HH11	1.86	0.41
1:1A:1368:G:C2	1:1A:1369:G:C8	3.09	0.41
1:1A:1470:G:H5''	1:1A:1471:A:OP1	2.21	0.41
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.20	0.41
1:1A:2430:A:H5'	1:1A:2431:U:OP2	2.21	0.41
1:1A:817:C:H4'	1:1A:932:G:C5	2.56	0.41
22:20:39:ARG:HA	22:20:39:ARG:HD3	1.90	0.41
22:20:43:THR:O	22:20:43:THR:HG23	2.21	0.41
1:2A:2119:A:C5	1:2A:2170:A:C6	3.09	0.41
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.20	0.41
1:2A:38:A:H2'	1:2A:39:C:C6	2.56	0.41
1:2A:614:U:H5'	1:2A:614(C):A:N6	2.36	0.41
1:2A:79:G:H2'	1:2A:80:G:C8	2.55	0.41
8:2I:52:ARG:HE	8:2I:52:ARG:HB2	1.67	0.41
8:2I:84:GLY:O	8:2I:86:THR:N	2.51	0.41
13:2R:28:LEU:HD13	13:2R:48:VAL:HG21	2.03	0.41
17:2V:21:ARG:HD3	17:2V:91:TYR:CD1	2.55	0.41
1:1A:1065:U:H1'	1:1A:1074:G:C2	2.55	0.40
1:1A:1274:A:N3	1:1A:1297:C:H1'	2.35	0.40
1:1A:228:A:H2'	1:1A:230:U:O4'	2.20	0.40
1:1A:2422:A:HO2'	1:1A:2424:C:H6	1.64	0.40
1:1A:2529:G:H5''	1:1A:2530:A:H5''	2.02	0.40
1:1A:2851:A:H2'	1:1A:2852:G:O4'	2.21	0.40
1:1A:427:U:OP1	3:1D:13:ARG:NH1	84.65	0.40
3:1D:6:PHE:HB3	3:1D:13:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:73:GLU:HG3	8:1I:139:GLN:HB2	2.03	0.40
13:1R:52:ILE:HD11	13:1R:116:LEU:HD22	2.01	0.40
26:24:59:PHE:CD2	26:24:59:PHE:N	2.89	0.40
1:2A:1449:A:H5'	1:2A:1450:G:OP2	2.21	0.40
1:2A:2547:U:C5	1:2A:2566:A:C5	3.08	0.40
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.86	0.40
1:2A:427:U:O3'	1:2A:428:A:H8	2.03	0.40
1:2A:537:C:H2'	1:2A:538:G:H8	1.86	0.40
1:2A:900:A:H2'	1:2A:901:A:H8	1.86	0.40
1:2A:322:A:H3'	5:2F:169:ASN:OD1	2.21	0.40
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.55	0.40
1:1A:754:C:O2'	1:1A:1272:A:N1	2.50	0.40
1:1A:2141:G:C5	1:1A:2142:C:C2	3.09	0.40
1:1A:2584:U:H4'	57:1A:3894:4M2:H46	2.04	0.40
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.55	0.40
1:1A:588:U:H1'	5:1F:90:PHE:CG	2.56	0.40
26:24:62:ARG:HA	26:24:62:ARG:HD3	1.87	0.40
13:2R:33:ARG:NH1	27:25:57:VAL:O	2.54	0.40
1:2A:643:A:C8	28:26:44:ARG:NH1	2.89	0.40
1:2A:1114:G:H2'	1:2A:1115:G:C8	2.56	0.40
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.57	0.40
1:2A:1937:A:H1'	1:2A:1939:5MU:H73	2.03	0.40
1:2A:2149:G:C6	1:2A:2150:U:C2	3.09	0.40
1:2A:2577:A:H5''	1:2A:2578:G:H5'	2.03	0.40
1:2A:271(U):G:N7	61:2A:9859:HOH:O	2.37	0.40
1:2A:500:G:N2	1:2A:502:A:H3'	2.36	0.40
1:2A:608:A:C6	1:2A:609:A:C6	3.09	0.40
2:2B:49:C:H2'	2:2B:50:G:C8	2.56	0.40
5:2F:170:LEU:HA	5:2F:171:PRO:HD3	1.94	0.40
13:2R:83:ILE:O	13:2R:86:ARG:HG2	2.21	0.40
1:1A:360:G:H2'	1:1A:361:G:O4'	2.21	0.40
1:1A:370:G:H4'	1:1A:371:A:OP2	2.21	0.40
1:1A:764:A:N3	3:1D:213:ARG:NH1	2.67	0.40
1:1A:857:C:N4	1:1A:858:U:O4	2.55	0.40
3:1D:145:VAL:HB	3:1D:155:LEU:HB2	2.03	0.40
3:1D:223:GLY:HA3	3:1D:231:HIS:CE1	2.57	0.40
5:1F:12:LEU:HB3	5:1F:126:VAL:HG12	2.04	0.40
8:1I:124:GLY:H	8:1I:144:VAL:HG23	1.86	0.40
9:1N:14:VAL:HG11	9:1N:138:LEU:HD12	2.03	0.40
19:1X:27:THR:OG1	19:1X:80:ILE:HG12	2.22	0.40
21:1Z:120:ILE:H	21:1Z:171:ILE:C	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:93:ASP:OD1	21:1Z:93:ASP:N	2.54	0.40
28:26:6:ARG:HH12	28:26:26:ASN:HB2	1.85	0.40
30:28:62:LEU:HB3	30:28:65:GLU:CG	2.51	0.40
31:29:27:CYS:SG	31:29:28:GLU:N	2.94	0.40
1:2A:2160:G:H2'	1:2A:2161:C:O4'	2.22	0.40
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.57	0.40
1:2A:2430:A:H5'	1:2A:2431:U:OP2	2.21	0.40
1:2A:2521:C:C4	1:2A:2522:U:C4	3.10	0.40
1:2A:2848:G:C8	15:2T:97:ALA:HB2	2.56	0.40
1:2A:753:C:H2'	1:2A:754:C:H6	1.86	0.40
3:2D:232:PRO:HG2	3:2D:248:SER:O	2.20	0.40
11:2P:36:LYS:HB3	11:2P:37:GLY:H	1.76	0.40
15:2T:51:ARG:HB3	15:2T:62:THR:HB	2.02	0.40
16:2U:48:ALA:O	16:2U:52:ARG:HB2	2.21	0.40
17:2V:24:LYS:HG3	17:2V:64:HIS:HD2	1.86	0.40
1:1A:1231:G:H2'	1:1A:1232:G:H8	1.86	0.40
1:1A:1937:A:H1'	1:1A:1939:5MU:H73	2.03	0.40
1:1A:2030:A:H4'	1:1A:2031:A:C8	2.57	0.40
1:1A:2126:A:H4'	1:1A:2127:G:OP1	2.20	0.40
1:1A:271(E):U:H2'	1:1A:271(F):C:H6	1.86	0.40
1:1A:2740:A:C6	1:1A:2764:A:C8	3.09	0.40
4:1E:126:PRO:HB2	4:1E:131:ALA:HB2	2.03	0.40
4:1E:144:ARG:HB3	4:1E:145:LYS:H	1.53	0.40
6:1G:133:LEU:HG	6:1G:157:ILE:HB	2.03	0.40
6:1G:49:ASP:O	6:1G:51:ARG:N	2.54	0.40
8:1I:129:THR:HG22	8:1I:139:GLN:NE2	2.35	0.40
8:1I:81:VAL:O	8:1I:146:ALA:HA	2.22	0.40
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.57	0.40
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.21	0.40
21:1Z:161:VAL:HG22	21:1Z:162:GLU:H	1.85	0.40
1:1A:904:C:O2'	21:1Z:169:GLU:OE2	2.30	0.40
1:2A:2056:G:N2	27:25:5:PRO:HA	2.37	0.40
1:2A:1354:A:H2'	1:2A:1355:G:O4'	2.21	0.40
1:2A:1508:A:H5'	1:2A:1509(A):A:N7	2.36	0.40
1:2A:1993:U:H2'	1:2A:1994:C:O4'	2.20	0.40
1:2A:2126:A:C2	1:2A:2127:G:H1'	2.57	0.40
1:2A:2336:A:H61	22:20:43:THR:HG22	1.87	0.40
1:2A:2516:G:C6	1:2A:2517:C:C4	3.09	0.40
1:2A:579:G:C8	1:2A:2017:U:C4	3.10	0.40
7:2H:38:SER:HA	7:2H:39:PRO:HD3	1.91	0.40
1:2A:637:A:H8	11:2P:117:GLU:HG3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:7:ALA:O	21:2Z:62:PRO:HD3	2.21	0.40
24:12:23:LYS:O	24:12:27:GLU:HG3	2.22	0.40
1:1A:1062:G:C8	1:1A:1088:A:H2'	2.56	0.40
1:1A:1826:G:H2'	1:1A:1827:C:O4'	2.20	0.40
1:1A:2137:C:H2'	1:1A:2138:C:H6	1.87	0.40
1:1A:2702:U:H4'	1:1A:2703:C:OP1	2.20	0.40
1:1A:2871:C:N3	61:1A:4142:HOH:O	2.37	0.40
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.22	0.40
1:1A:79:G:N2	1:1A:90:U:O2	30.45	0.40
6:1G:140:ILE:HD13	6:1G:140:ILE:HA	1.81	0.40
6:1G:53:LEU:HA	6:1G:53:LEU:HD23	1.84	0.40
10:1O:70:LYS:HE2	10:1O:70:LYS:HB3	1.92	0.40
11:1P:47:ASP:N	11:1P:47:ASP:OD1	4.16	0.40
16:1U:48:ALA:O	16:1U:52:ARG:HB2	2.22	0.40
1:1A:295:G:H4'	20:1Y:1:MET:HE3	2.04	0.40
22:20:10:THR:HG22	22:20:12:ASN:N	2.16	0.40
1:2A:1296:G:OP1	1:2A:2709:G:O2'	2.29	0.40
1:2A:1538:G:H2'	1:2A:1539:G:C8	2.56	0.40
1:2A:372:G:O2'	1:2A:400:G:O6	2.29	0.40
1:2A:614(A):U:H4'	1:2A:614(B):G:H5''	2.03	0.40
1:2A:860:U:H1'	1:2A:2268:A:H5'	2.03	0.40
2:2B:58:A:C5	2:2B:59:A:C8	3.09	0.40
1:2A:2637:U:H5''	4:2E:82:ARG:NH1	2.37	0.40
11:2P:85:LEU:HD13	11:2P:120:ALA:HB2	2.03	0.40
15:2T:8:LYS:HD2	15:2T:8:LYS:HA	1.94	0.40
16:2U:108:GLU:O	16:2U:112:ARG:HG3	2.21	0.40
2:2B:103:G:N2	21:2Z:73:GLN:HE22	2.18	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	36	52
3	2D	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	36	52
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	31	46
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	17	26
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	31	46
5	2F	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	17	26
6	1G	179/182 (98%)	167 (93%)	9 (5%)	3 (2%)	10	14
6	2G	179/182 (98%)	167 (93%)	9 (5%)	3 (2%)	10	14
7	1H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	27	41
7	2H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	27	41
8	1I	144/148 (97%)	130 (90%)	11 (8%)	3 (2%)	8	11
8	2I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	24	36
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	24	36
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	24	36
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	24	36
12	1Q	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
12	2Q	139/141 (99%)	135 (97%)	3 (2%)	1 (1%)	24	36
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	17	26
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	17	26
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	2X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	16	24
20	1Y	105/110 (96%)	100 (95%)	3 (3%)	2 (2%)	9	13
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	1Z	148/206 (72%)	131 (88%)	16 (11%)	1 (1%)	24	36
21	2Z	156/206 (76%)	133 (85%)	23 (15%)	0	100	100
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	16	24
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	16	24
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	54 (81%)	10 (15%)	3 (4%)	3	3
26	24	67/71 (94%)	51 (76%)	10 (15%)	6 (9%)	1	0
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	7	11
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	3	4
33	2b	229/256 (90%)	201 (88%)	20 (9%)	8 (4%)	4	5
34	1c	204/239 (85%)	185 (91%)	17 (8%)	2 (1%)	17	26
34	2c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	17	26
35	1d	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	31	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	31	46
36	1e	146/162 (90%)	134 (92%)	11 (8%)	1 (1%)	24	36
36	2e	146/162 (90%)	136 (93%)	10 (7%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	2g	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	24	36
39	1h	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
39	2h	135/138 (98%)	131 (97%)	3 (2%)	1 (1%)	24	36
40	1i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	21	32
40	2i	125/128 (98%)	108 (86%)	15 (12%)	2 (2%)	11	15
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	3
41	2j	94/105 (90%)	81 (86%)	8 (8%)	5 (5%)	2	2
42	1k	112/129 (87%)	103 (92%)	5 (4%)	4 (4%)	4	4
42	2k	112/129 (87%)	104 (93%)	4 (4%)	4 (4%)	4	4
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	7 (6%)	3 (2%)	6	8
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	14	22
47	1p	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	13	20
47	2p	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	13	20
48	1q	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
48	2q	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	14	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	86 (92%)	3 (3%)	5 (5%)	2	2
51	2t	94/106 (89%)	86 (92%)	3 (3%)	5 (5%)	2	2
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11370/12128 (94%)	10690 (94%)	575 (5%)	105 (1%)	19	29

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1D	275	LYS
5	1F	130	ALA
6	1G	47	LYS
6	1G	51	ARG
7	1H	126	PRO
21	1Z	152	ALA
33	1b	17	PHE
33	1b	22	LYS
34	1c	65	ALA
42	1k	89	ALA
47	1p	53	VAL
5	2F	130	ALA
6	2G	47	LYS
6	2G	51	ARG
7	2H	126	PRO
11	2P	45	LEU
23	21	3	LYS
26	24	48	ARG
26	24	55	ARG
26	24	62	ARG
29	27	46	VAL
33	2b	16	HIS
33	2b	123	ALA
34	2c	107	GLN
34	2c	108	ASN
42	2k	89	ALA
42	2k	90	GLY
44	2m	107	ALA
47	2p	53	VAL
51	2t	10	LEU
8	1I	105	HIS
8	1I	106	GLY

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Mol	Chain	Res	Type
23	1l	3	LYS
26	14	45	GLY
41	1j	31	GLY
41	1j	77	PRO
42	1k	49	GLY
51	1t	10	LEU
51	1t	47	GLY
51	1t	96	GLY
51	1t	100	ILE
3	2D	3	VAL
4	2E	52	LEU
12	2Q	28	ALA
17	2V	79	VAL
26	24	45	GLY
33	2b	17	PHE
33	2b	21	ARG
33	2b	128	GLU
41	2j	29	ARG
44	2m	4	ILE
51	2t	47	GLY
6	1G	43	LEU
17	1V	79	VAL
20	1Y	53	PRO
26	14	56	VAL
33	1b	9	GLU
33	1b	20	GLU
33	1b	231	GLU
36	1e	86	ALA
41	1j	29	ARG
41	1j	78	ASN
6	2G	43	LEU
19	2X	2	LYS
26	24	47	GLN
26	24	65	ASP
33	2b	20	GLU
33	2b	231	GLU
38	2g	7	ALA
41	2j	30	SER
41	2j	78	ASN
44	2m	6	GLY
50	2s	29	ARG
51	2t	102	GLY

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Mol	Chain	Res	Type
4	1E	52	LEU
34	1c	66	VAL
40	1i	56	LEU
51	1t	95	ALA
4	2E	73	GLU
5	2F	21	ALA
8	2I	10	GLU
42	2k	49	GLY
46	2o	88	ARG
51	2t	95	ALA
51	2t	100	ILE
20	1Y	54	LYS
33	1b	16	HIS
33	1b	125	PRO
33	1b	126	GLU
35	1d	167	GLY
42	1k	90	GLY
35	2d	167	GLY
40	2i	54	ASP
40	2i	56	LEU
42	2k	105	VAL
8	1I	107	VAL
26	14	46	GLN
33	1b	10	LEU
9	2N	2	LYS
39	2h	73	ASP
41	2j	77	PRO
42	1k	105	VAL
41	2j	37	PRO
11	1P	122	PRO
33	2b	125	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	202 (94%)	13 (6%)	21	33
3	2D	215/218 (99%)	206 (96%)	9 (4%)	32	50
4	1E	164/166 (99%)	157 (96%)	7 (4%)	32	49
4	2E	164/166 (99%)	156 (95%)	8 (5%)	27	42
5	1F	160/166 (96%)	146 (91%)	14 (9%)	11	16
5	2F	159/166 (96%)	150 (94%)	9 (6%)	23	35
6	1G	144/156 (92%)	139 (96%)	5 (4%)	39	57
6	2G	143/156 (92%)	137 (96%)	6 (4%)	32	50
7	1H	144/148 (97%)	142 (99%)	2 (1%)	69	84
7	2H	144/148 (97%)	142 (99%)	2 (1%)	69	84
8	1I	113/124 (91%)	106 (94%)	7 (6%)	20	32
8	2I	105/124 (85%)	100 (95%)	5 (5%)	28	43
9	1N	118/119 (99%)	113 (96%)	5 (4%)	32	50
9	2N	118/119 (99%)	115 (98%)	3 (2%)	50	70
10	1O	100/100 (100%)	99 (99%)	1 (1%)	78	88
10	2O	100/100 (100%)	99 (99%)	1 (1%)	78	88
11	1P	115/116 (99%)	110 (96%)	5 (4%)	32	49
11	2P	115/116 (99%)	112 (97%)	3 (3%)	49	69
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	62	79
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	38	56
13	1R	101/101 (100%)	94 (93%)	7 (7%)	17	27
13	2R	101/101 (100%)	95 (94%)	6 (6%)	21	34
14	1S	86/88 (98%)	82 (95%)	4 (5%)	29	44
14	2S	85/88 (97%)	83 (98%)	2 (2%)	52	71
15	1T	115/127 (91%)	110 (96%)	5 (4%)	32	49
15	2T	113/127 (89%)	110 (97%)	3 (3%)	48	67
16	1U	93/94 (99%)	90 (97%)	3 (3%)	42	60
16	2U	93/94 (99%)	92 (99%)	1 (1%)	76	88
17	1V	80/82 (98%)	75 (94%)	5 (6%)	20	31
17	2V	80/82 (98%)	77 (96%)	3 (4%)	36	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1W	90/92 (98%)	86 (96%)	4 (4%)	31	48
18	2W	90/92 (98%)	85 (94%)	5 (6%)	23	36
19	1X	77/78 (99%)	76 (99%)	1 (1%)	71	85
19	2X	77/78 (99%)	76 (99%)	1 (1%)	71	85
20	1Y	85/91 (93%)	83 (98%)	2 (2%)	52	71
20	2Y	85/91 (93%)	84 (99%)	1 (1%)	74	86
21	1Z	135/179 (75%)	132 (98%)	3 (2%)	55	74
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	55	74
22	10	65/67 (97%)	62 (95%)	3 (5%)	29	45
22	20	65/67 (97%)	63 (97%)	2 (3%)	43	62
23	11	80/83 (96%)	77 (96%)	3 (4%)	36	54
23	21	80/83 (96%)	76 (95%)	4 (5%)	27	41
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	64 (98%)	1 (2%)	67	83
25	13	51/52 (98%)	50 (98%)	1 (2%)	58	77
25	23	50/52 (96%)	48 (96%)	2 (4%)	34	52
26	14	59/63 (94%)	57 (97%)	2 (3%)	40	58
26	24	53/63 (84%)	49 (92%)	4 (8%)	15	24
27	15	50/52 (96%)	47 (94%)	3 (6%)	21	33
27	25	50/52 (96%)	47 (94%)	3 (6%)	21	33
28	16	51/52 (98%)	49 (96%)	2 (4%)	35	53
28	26	50/52 (96%)	48 (96%)	2 (4%)	34	52
29	17	41/42 (98%)	39 (95%)	2 (5%)	27	42
29	27	41/42 (98%)	41 (100%)	0	100	100
30	18	54/55 (98%)	51 (94%)	3 (6%)	23	36
30	28	54/55 (98%)	50 (93%)	4 (7%)	15	24
31	19	34/34 (100%)	33 (97%)	1 (3%)	45	64
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	189 (98%)	3 (2%)	65	81
33	2b	187/220 (85%)	183 (98%)	4 (2%)	56	75
34	1c	142/188 (76%)	140 (99%)	2 (1%)	69	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	2c	140/188 (74%)	139 (99%)	1 (1%)	85	92
35	1d	169/181 (93%)	165 (98%)	4 (2%)	52	71
35	2d	173/181 (96%)	168 (97%)	5 (3%)	45	64
36	1e	113/123 (92%)	111 (98%)	2 (2%)	62	79
36	2e	114/123 (93%)	112 (98%)	2 (2%)	62	79
37	1f	84/90 (93%)	82 (98%)	2 (2%)	52	71
37	2f	85/90 (94%)	83 (98%)	2 (2%)	52	71
38	1g	119/127 (94%)	118 (99%)	1 (1%)	83	92
38	2g	120/127 (94%)	120 (100%)	0	100	100
39	1h	114/119 (96%)	112 (98%)	2 (2%)	62	79
39	2h	114/119 (96%)	112 (98%)	2 (2%)	62	79
40	1i	90/99 (91%)	86 (96%)	4 (4%)	31	48
40	2i	89/99 (90%)	87 (98%)	2 (2%)	55	74
41	1j	66/92 (72%)	65 (98%)	1 (2%)	67	83
41	2j	69/92 (75%)	65 (94%)	4 (6%)	22	34
42	1k	82/99 (83%)	80 (98%)	2 (2%)	52	71
42	2k	83/99 (84%)	82 (99%)	1 (1%)	74	86
43	1l	96/108 (89%)	94 (98%)	2 (2%)	56	75
43	2l	96/108 (89%)	94 (98%)	2 (2%)	56	75
44	1m	93/101 (92%)	91 (98%)	2 (2%)	55	74
44	2m	92/101 (91%)	90 (98%)	2 (2%)	55	74
45	1n	49/50 (98%)	46 (94%)	3 (6%)	20	33
45	2n	49/50 (98%)	47 (96%)	2 (4%)	33	51
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	77 (99%)	1 (1%)	71	85
47	1p	69/74 (93%)	64 (93%)	5 (7%)	16	25
47	2p	68/74 (92%)	63 (93%)	5 (7%)	15	24
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	94 (100%)	0	100	100
49	1r	59/77 (77%)	58 (98%)	1 (2%)	63	80
49	2r	59/77 (77%)	57 (97%)	2 (3%)	40	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	1s	69/80 (86%)	68 (99%)	1 (1%)	69	84
50	2s	67/80 (84%)	65 (97%)	2 (3%)	44	63
51	1t	70/82 (85%)	67 (96%)	3 (4%)	32	49
51	2t	70/82 (85%)	69 (99%)	1 (1%)	69	84
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9304/10064 (92%)	9012 (97%)	292 (3%)	43	62

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	37	LEU
3	1D	61	LEU
3	1D	88	ARG
3	1D	94	LEU
3	1D	113	VAL
3	1D	122	ASP
3	1D	193	VAL
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	33	VAL
4	1E	75	VAL
4	1E	116	VAL
4	1E	144	ARG
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	60	SER
5	1F	70	THR
5	1F	74	ARG
5	1F	106	ARG
5	1F	125	LEU

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Mol	Chain	Res	Type
5	1F	132	VAL
5	1F	170	LEU
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	43	LEU
6	1G	82	LEU
6	1G	133	LEU
7	1H	88	LEU
7	1H	98	LEU
8	1I	38	LEU
8	1I	47	LEU
8	1I	92	VAL
8	1I	108	THR
8	1I	109	ILE
8	1I	123	LEU
8	1I	142	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET
9	1N	73	THR
10	1O	10	VAL
11	1P	59	LEU
11	1P	79	ARG
11	1P	106	LEU
11	1P	112	LEU
11	1P	125	VAL
12	1Q	16	ARG
12	1Q	75	THR
13	1R	29	LEU
13	1R	33	ARG
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	100	LEU
13	1R	111	LEU
14	1S	13	ARG
14	1S	25	ARG
14	1S	36	TYR

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Mol	Chain	Res	Type
14	1S	49	VAL
15	1T	28	VAL
15	1T	34	VAL
15	1T	49	VAL
15	1T	89	VAL
15	1T	128	GLU
16	1U	8	VAL
16	1U	74	LEU
16	1U	108	GLU
17	1V	46	VAL
17	1V	51	VAL
17	1V	61	VAL
17	1V	72	VAL
17	1V	79	VAL
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	107	LEU
19	1X	52	VAL
20	1Y	43	ASN
20	1Y	90	LEU
21	1Z	5	LEU
21	1Z	132	ASN
21	1Z	148	ASP
22	10	14	ARG
22	10	39	ARG
22	10	55	ARG
23	11	11	ARG
23	11	35	THR
23	11	95	LEU
25	13	23	LEU
26	14	50	VAL
26	14	56	VAL
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
28	16	14	THR
28	16	48	VAL
29	17	24	THR
29	17	47	ARG
30	18	14	VAL
30	18	31	HIS

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Mol	Chain	Res	Type
30	18	32	LEU
31	19	35	ARG
33	1b	7	VAL
33	1b	8	LYS
33	1b	158	LEU
34	1c	70	VAL
34	1c	115	LEU
35	1d	31	CYS
35	1d	112	VAL
35	1d	135	LEU
35	1d	194	LEU
36	1e	38	GLN
36	1e	41	VAL
37	1f	72	VAL
37	1f	74	ASP
38	1g	50	ILE
39	1h	112	LEU
39	1h	133	LEU
40	1i	23	ASN
40	1i	42	ARG
40	1i	50	LEU
40	1i	86	VAL
41	1j	5	ARG
42	1k	48	ILE
42	1k	114	VAL
43	1l	27	LEU
43	1l	83	VAL
44	1m	4	ILE
44	1m	32	GLU
45	1n	3	ARG
45	1n	18	VAL
45	1n	33	VAL
47	1p	20	VAL
47	1p	42	ARG
47	1p	60	LEU
47	1p	67	THR
47	1p	69	THR
49	1r	35	ARG
50	1s	4	SER
51	1t	10	LEU
51	1t	15	ARG
51	1t	24	LEU

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Mol	Chain	Res	Type
3	2D	3	VAL
3	2D	37	LEU
3	2D	61	LEU
3	2D	88	ARG
3	2D	94	LEU
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	257	LEU
4	2E	21	VAL
4	2E	33	VAL
4	2E	52	LEU
4	2E	75	VAL
4	2E	116	VAL
4	2E	170	LEU
4	2E	181	LEU
4	2E	195	LEU
5	2F	24	LEU
5	2F	33	LEU
5	2F	70	THR
5	2F	74	ARG
5	2F	106	ARG
5	2F	132	VAL
5	2F	170	LEU
5	2F	191	ARG
5	2F	192	LEU
6	2G	5	VAL
6	2G	43	LEU
6	2G	79	ASN
6	2G	133	LEU
6	2G	159	VAL
6	2G	170	ARG
7	2H	84	SER
7	2H	129	THR
8	2I	47	LEU
8	2I	50	ARG
8	2I	92	VAL
8	2I	123	LEU
8	2I	140	LEU
9	2N	28	THR
9	2N	34	LEU
9	2N	99	LEU

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Mol	Chain	Res	Type
10	2O	108	GLU
11	2P	95	VAL
11	2P	112	LEU
11	2P	125	VAL
12	2Q	2	LEU
12	2Q	10	ARG
12	2Q	75	THR
12	2Q	110	THR
13	2R	29	LEU
13	2R	33	ARG
13	2R	44	LEU
13	2R	65	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	13	ARG
14	2S	110	LEU
15	2T	28	VAL
15	2T	49	VAL
15	2T	95	ARG
16	2U	92	ARG
17	2V	21	ARG
17	2V	46	VAL
17	2V	79	VAL
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	100	THR
18	2W	107	LEU
19	2X	70	LEU
20	2Y	72	VAL
21	2Z	42	VAL
21	2Z	135	GLU
21	2Z	142	SER
22	20	14	ARG
22	20	39	ARG
23	21	11	ARG
23	21	30	VAL
23	21	56	GLN
23	21	95	LEU
24	22	52	ASP
25	23	23	LEU
25	23	54	VAL

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Mol	Chain	Res	Type
26	24	34	GLU
26	24	50	VAL
26	24	56	VAL
26	24	59	PHE
27	25	16	ARG
27	25	29	THR
27	25	35	GLU
28	26	14	THR
28	26	48	VAL
30	28	14	VAL
30	28	26	LYS
30	28	31	HIS
30	28	32	LEU
33	2b	7	VAL
33	2b	94	ASN
33	2b	185	ILE
33	2b	235	SER
34	2c	152	ILE
35	2d	31	CYS
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	194	LEU
36	2e	41	VAL
36	2e	51	VAL
37	2f	21	LEU
37	2f	72	VAL
39	2h	84	ARG
39	2h	133	LEU
40	2i	102	LEU
40	2i	108	VAL
41	2j	55	LYS
41	2j	67	THR
41	2j	72	VAL
41	2j	89	ASP
42	2k	48	ILE
43	2l	33	ARG
43	2l	83	VAL
44	2m	15	VAL
44	2m	104	ARG
45	2n	18	VAL
45	2n	33	VAL

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Mol	Chain	Res	Type
46	2o	39	LEU
47	2p	20	VAL
47	2p	45	THR
47	2p	60	LEU
47	2p	62	VAL
47	2p	69	THR
49	2r	35	ARG
49	2r	37	VAL
50	2s	64	GLU
50	2s	77	THR
51	2t	15	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	69	HIS
6	1G	132	ASN
8	1I	104	GLN
12	1Q	57	HIS
14	1S	95	HIS
16	1U	94	ASN
18	1W	60	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	43	ASN
21	1Z	55	HIS
21	1Z	132	ASN
24	12	9	GLN
24	12	65	ASN
33	1b	40	HIS
34	1c	6	HIS
34	1c	102	ASN
34	1c	176	HIS
35	1d	77	ASN
35	1d	123	HIS
35	1d	161	ASN
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	86	GLN
39	1h	82	HIS

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Mol	Chain	Res	Type
40	1i	23	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
42	1k	99	GLN
43	1l	99	HIS
44	1m	92	HIS
48	1q	26	GLN
50	1s	23	ASN
50	1s	57	HIS
50	1s	69	HIS
50	1s	83	HIS
51	1t	16	HIS
3	2D	116	GLN
5	2F	69	HIS
8	2I	104	GLN
9	2N	38	HIS
9	2N	131	GLN
10	2O	3	GLN
12	2Q	12	GLN
12	2Q	123	HIS
13	2R	91	GLN
14	2S	38	GLN
14	2S	84	GLN
14	2S	95	HIS
16	2U	94	ASN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	55	HIS
21	2Z	73	GLN
24	22	65	ASN
33	2b	40	HIS
33	2b	78	GLN
33	2b	94	ASN
34	2c	6	HIS
34	2c	162	GLN
35	2d	77	ASN
35	2d	123	HIS
35	2d	125	HIS

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Mol	Chain	Res	Type
35	2d	161	ASN
37	2f	13	ASN
37	2f	73	ASN
37	2f	100	ASN
38	2g	64	GLN
38	2g	86	GLN
38	2g	97	GLN
40	2i	58	HIS
40	2i	73	GLN
40	2i	117	HIS
40	2i	124	GLN
42	2k	93	GLN
43	2l	99	HIS
44	2m	77	ASN
46	2o	28	GLN
46	2o	62	GLN
50	2s	65	ASN
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	439 (15%)	28 (0%)
1	2A	2788/2915 (95%)	462 (16%)	26 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1494/1521 (98%)	217 (14%)	0
32	2a	1498/1521 (98%)	225 (15%)	0
53	1v	12/27 (44%)	3 (25%)	0
53	2v	12/27 (44%)	3 (25%)	0
54	1w	71/76 (93%)	27 (38%)	0
54	1y	71/76 (93%)	23 (32%)	0
54	2w	69/76 (90%)	21 (30%)	0
54	2y	69/76 (90%)	15 (21%)	0
55	1x	74/77 (96%)	11 (14%)	0
55	2x	74/77 (96%)	12 (16%)	0
All	All	9331/9626 (96%)	1494 (16%)	55 (0%)

All (1494) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	55	G
1	1A	58	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	93	G
1	1A	94	C
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	198	C
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(C)	C
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	282	A
1	1A	283	A
1	1A	306	U
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G

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Mol	Chain	Res	Type
1	1A	360	G
1	1A	362	U
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	389	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	412	A
1	1A	418	G
1	1A	421	U
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	491	G
1	1A	494	G
1	1A	505	A
1	1A	509	C
1	1A	512	G
1	1A	529	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	534	U
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G

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Mol	Chain	Res	Type
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	740	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	801	G
1	1A	805	G
1	1A	811	U
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	830	G
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	890	A
1	1A	892	G
1	1A	895	U
1	1A	896	A

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Mol	Chain	Res	Type
1	1A	897	C
1	1A	898	C
1	1A	910	A
1	1A	932	G
1	1A	941	A
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	995	C
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1066	U
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1083	U
1	1A	1085	A

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Mol	Chain	Res	Type
1	1A	1088	A
1	1A	1090	U
1	1A	1092	C
1	1A	1094	U
1	1A	1101	U
1	1A	1106	G
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1155	A
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1189	A
1	1A	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1220	A
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1267	U
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1308	A
1	1A	1315	C
1	1A	1320	C
1	1A	1345	C
1	1A	1352	U

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Mol	Chain	Res	Type
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1379	A
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1416	G
1	1A	1417	C
1	1A	1419	A
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1461	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C
1	1A	1496	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1509(B)	A
1	1A	1531	C
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1648	C
1	1A	1653	G

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Mol	Chain	Res	Type
1	1A	1654	A
1	1A	1664	A
1	1A	1667	G
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1748	G
1	1A	1749	A
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A
1	1A	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1929	G
1	1A	1930	G
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1984	G
1	1A	1992	G

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Mol	Chain	Res	Type
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2035	G
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2099	U
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2119	A
1	1A	2121	G
1	1A	2122	U
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2138	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2147	G
1	1A	2148	G
1	1A	2151	G
1	1A	2152	G
1	1A	2155	G

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Mol	Chain	Res	Type
1	1A	2157	G
1	1A	2159	G
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2178	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2269	A
1	1A	2275	C
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2321	G
1	1A	2325	G
1	1A	2334	G
1	1A	2335	A
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G

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Mol	Chain	Res	Type
1	1A	2406	U
1	1A	2410	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2476	A
1	1A	2477	C
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2524	G
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2584	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2761	G
1	1A	2764	A

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Mol	Chain	Res	Type
1	1A	2765	A
1	1A	2778	A
1	1A	2780	G
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	52	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	91	C
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C

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Mol	Chain	Res	Type
32	1a	131	C
32	1a	146	G
32	1a	156	G
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
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	316	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	348	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	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A

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Mol	Chain	Res	Type
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	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	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	564	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	759	A
32	1a	773	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	817	C

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Mol	Chain	Res	Type
32	1a	821	G
32	1a	828	A
32	1a	838	G
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
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	982	U
32	1a	992	U
32	1a	993	G
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1020	U
32	1a	1022	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1031	G

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Mol	Chain	Res	Type
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1039	C
32	1a	1044	A
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1104	G
32	1a	1133	G
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	1157	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
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	1240	U
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1270	C
32	1a	1278	U
32	1a	1279	A

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Mol	Chain	Res	Type
32	1a	1280	A
32	1a	1281	U
32	1a	1282	C
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
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	1452	C
32	1a	1456	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
32	1a	1532	U
53	1v	13	A
53	1v	14	A
53	1v	24	A
54	1w	2	C
54	1w	4	C
54	1w	9	A
54	1w	19	G
54	1w	20	U

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Mol	Chain	Res	Type
54	1w	21	A
54	1w	22	G
54	1w	23	A
54	1w	24	G
54	1w	29	G
54	1w	42	C
54	1w	43	C
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	49	C
54	1w	56	C
54	1w	61	C
54	1w	68	C
54	1w	69	G
54	1w	70	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
54	1w	75	C
54	1w	76	A
55	1x	6	G
55	1x	9	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	48	C
55	1x	56	C
55	1x	58	A
55	1x	61	C
55	1x	67	C
55	1x	69	C
54	1y	2	C
54	1y	5	G
54	1y	9	A
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	22	G
54	1y	26	A

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Mol	Chain	Res	Type
54	1y	33	U
54	1y	40	C
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	50	U
54	1y	57	G
54	1y	59	U
54	1y	60	U
54	1y	65	G
54	1y	68	C
54	1y	70	G
54	1y	73	A
1	2A	9	U
1	2A	10	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	96	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	140	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G

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Mol	Chain	Res	Type
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	271(I)	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	289	A
1	2A	308	G
1	2A	311	A
1	2A	317	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	338	G
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(A)	A
1	2A	386	G
1	2A	396	G
1	2A	404	C
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	427	U
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C

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Mol	Chain	Res	Type
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	494	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	518	G
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	556	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	587	C
1	2A	588	U
1	2A	592	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	646	A
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	709	U
1	2A	717	G
1	2A	730	C
1	2A	752	A

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Mol	Chain	Res	Type
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
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	848	G
1	2A	857	C
1	2A	859	G
1	2A	864	G
1	2A	866	A
1	2A	874	G
1	2A	875	G
1	2A	878	A
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	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	912	C
1	2A	917	A
1	2A	932	G
1	2A	936	C
1	2A	941	A
1	2A	944	G

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Mol	Chain	Res	Type
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	957	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	982	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
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	1043	C
1	2A	1113	U
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1171	G
1	2A	1188	U
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1229	G
1	2A	1248	G
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G

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Mol	Chain	Res	Type
1	2A	1272	A
1	2A	1273	U
1	2A	1289	C
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1320	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1411	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	1436	G
1	2A	1437	C
1	2A	1444	G
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U

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Mol	Chain	Res	Type
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1542	A
1	2A	1543	C
1	2A	1545	A
1	2A	1547	C
1	2A	1548	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1582	C
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1593	G
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1695	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A

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Mol	Chain	Res	Type
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1860	G
1	2A	1876	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
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	1931	U
1	2A	1936	A
1	2A	1938	A
1	2A	1952	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1966	A
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C

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Mol	Chain	Res	Type
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2111	C
1	2A	2116	G
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	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2139	C
1	2A	2140	C
1	2A	2142	C
1	2A	2144	U
1	2A	2146	C
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2160	G
1	2A	2166	G
1	2A	2167	U
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2178	C
1	2A	2185	C
1	2A	2189	U
1	2A	2190	G
1	2A	2198	A

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Mol	Chain	Res	Type
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2235	G
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2313	C
1	2A	2319	G
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2410	G
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2459	A
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A

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Mol	Chain	Res	Type
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G
1	2A	2646	C
1	2A	2654	A
1	2A	2669	G
1	2A	2679	A
1	2A	2689	U
1	2A	2690	C
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	2741	A
1	2A	2751	G
1	2A	2752	C
1	2A	2754	U
1	2A	2757	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A

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Mol	Chain	Res	Type
1	2A	2778	A
1	2A	2793	G
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	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	16	G
2	2B	17	C
2	2B	20	C
2	2B	23	G
2	2B	25	A
2	2B	30	C
2	2B	42	C
2	2B	45	A
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	64	C
2	2B	69	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	90	A
2	2B	91	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	112	U
2	2B	116	G
2	2B	120	A
32	2a	6	G

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Mol	Chain	Res	Type
32	2a	7	G
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	73	G
32	2a	78	G
32	2a	88	A
32	2a	89	C
32	2a	91	C
32	2a	96	U
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	146	G
32	2a	156	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(J)	G
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	217	C
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

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Mol	Chain	Res	Type
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	344	A
32	2a	348	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
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	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	461	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	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	564	C
32	2a	568	G

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Mol	Chain	Res	Type
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	759	A
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	838	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
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

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Mol	Chain	Res	Type
32	2a	977	A
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G
32	2a	1020	U
32	2a	1022	G
32	2a	1024	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1044	A
32	2a	1046	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1104	G
32	2a	1117	G
32	2a	1125	U
32	2a	1129	C
32	2a	1133	G
32	2a	1134	G

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Mol	Chain	Res	Type
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	1159	U
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
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	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1282	C
32	2a	1287	A
32	2a	1299	A
32	2a	1305	G
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1419	G
32	2a	1442	G

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Mol	Chain	Res	Type
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1498	UR3
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	24	A
54	2w	2	C
54	2w	4	C
54	2w	8	4SU
54	2w	19	G
54	2w	24	G
54	2w	29	G
54	2w	42	C
54	2w	43	C
54	2w	47	U
54	2w	48	C
54	2w	49	C
54	2w	56	C
54	2w	61	C
54	2w	62	C
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	73	A
54	2w	74	C
54	2w	75	C
54	2w	76	A
55	2x	9	G
55	2x	13	C
55	2x	16	C
55	2x	19	G

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Mol	Chain	Res	Type
55	2x	34	C
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	56	C
55	2x	60	U
55	2x	67	C
55	2x	68	C
54	2y	2	C
54	2y	9	A
54	2y	13	C
54	2y	19	G
54	2y	22	G
54	2y	26	A
54	2y	33	U
54	2y	40	C
54	2y	46	7MG
54	2y	47	U
54	2y	48	C
54	2y	50	U
54	2y	57	G
54	2y	68	C
54	2y	70	G

All (55) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	800	A
1	1A	827	U
1	1A	1036	G
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G

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Mol	Chain	Res	Type
1	1A	1210	A
1	1A	1442	G
1	1A	1508	A
1	1A	1653	G
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2238	G
1	1A	2406	U
1	1A	2422	A
1	1A	2629	A
1	1A	2689	U
2	1B	1	U
1	2A	195	A
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	587	C
1	2A	752	A
1	2A	774	A
1	2A	856	C
1	2A	883	G
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1300	U
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2126	A
1	2A	2406	U
1	2A	2689	U
1	2A	2756	U



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

86 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	1911	1	16,21,22	1.37	2 (12%)	20,30,33	3.05	5 (25%)
1	5MU	1A	1915	1	13,22,23	0.75	0	14,32,35	1.82	1 (7%)
1	PSU	1A	1917	1	16,21,22	1.30	1 (6%)	20,30,33	3.05	6 (30%)
1	4OC	1A	1920	1	15,22,24	0.79	0	20,31,35	1.45	1 (5%)
1	5MU	1A	1939	1	13,22,23	0.88	1 (7%)	14,32,35	2.05	2 (14%)
1	5MC	1A	1942	1,56	14,22,23	1.49	1 (7%)	17,32,35	1.52	3 (17%)
1	5MC	1A	1962	1,56	14,22,23	1.41	1 (7%)	17,32,35	1.36	2 (11%)
1	OMG	1A	2251	1,55,56	18,26,27	1.35	2 (11%)	22,38,41	2.08	6 (27%)
1	2MA	1A	2503	1,56	16,25,26	1.41	2 (12%)	17,37,40	2.41	3 (17%)
1	2MU	1A	2552	1,56	14,22,24	0.93	0	17,31,36	0.98	2 (11%)
1	PSU	1A	2605	1	16,21,22	1.81	4 (25%)	20,30,33	3.03	6 (30%)
32	2MG	1a	1207	32	18,26,27	1.35	2 (11%)	19,38,41	2.66	8 (42%)
32	5MC	1a	1400	32	14,22,23	1.47	1 (7%)	17,32,35	1.51	2 (11%)
32	4OC	1a	1402	32	16,23,24	0.77	0	20,32,35	0.97	2 (10%)
32	5MC	1a	1404	32	14,22,23	1.42	1 (7%)	17,32,35	1.63	4 (23%)
32	5MC	1a	1407	32	14,22,23	1.52	1 (7%)	17,32,35	1.45	3 (17%)
32	UR3	1a	1498	32	13,22,23	0.78	0	15,32,35	0.65	0
32	MA6	1a	1518	32	16,26,27	1.11	1 (6%)	16,38,41	1.73	5 (31%)
32	MA6	1a	1519	32	16,26,27	1.11	1 (6%)	16,38,41	1.70	4 (25%)
32	PSU	1a	516	32,56	16,21,22	1.50	3 (18%)	20,30,33	2.91	6 (30%)
32	7MG	1a	527	32,56	20,26,27	1.93	4 (20%)	24,39,42	2.69	6 (25%)
32	M2G	1a	966	32	19,27,28	1.42	3 (15%)	20,40,43	2.22	6 (30%)
32	5MC	1a	967	32	14,22,23	1.43	1 (7%)	17,32,35	1.47	3 (17%)
43	0TD	1l	92	43	5,9,10	3.17	2 (40%)	4,11,13	8.18	1 (25%)
54	PSU	1w	32	54,56	16,21,22	1.41	1 (6%)	20,30,33	3.11	6 (30%)
54	MIA	1w	37	54	22,31,32	2.46	3 (13%)	26,44,47	2.56	10 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	PSU	1w	39	54	16,21,22	1.50	1 (6%)	20,30,33	3.02	6 (30%)
54	7MG	1w	46	54	20,26,27	1.95	3 (15%)	24,39,42	2.71	6 (25%)
54	5MU	1w	54	54	13,22,23	0.77	0	14,32,35	2.16	2 (14%)
54	PSU	1w	55	54	16,21,22	1.36	1 (6%)	20,30,33	3.30	6 (30%)
54	4SU	1w	8	54	13,21,22	1.42	2 (15%)	14,30,33	1.49	2 (14%)
55	5MC	1x	32	55	14,22,23	1.51	2 (14%)	17,32,35	1.58	4 (23%)
55	5MU	1x	54	55,56	13,22,23	0.75	0	14,32,35	2.25	1 (7%)
55	PSU	1x	55	55	16,21,22	1.57	1 (6%)	20,30,33	3.12	7 (35%)
55	M3O	1x	76	55,56	27,34,35	1.26	4 (14%)	28,47,50	1.66	4 (14%)
55	4SU	1x	8	55	13,21,22	1.40	2 (15%)	14,30,33	2.89	2 (14%)
54	PSU	1y	32	54	16,21,22	1.35	1 (6%)	20,30,33	3.18	6 (30%)
54	MIA	1y	37	54	17,24,32	1.30	2 (11%)	16,35,47	1.24	2 (12%)
54	PSU	1y	39	54	16,21,22	1.35	2 (12%)	20,30,33	3.13	6 (30%)
54	7MG	1y	46	54	20,26,27	1.99	3 (15%)	24,39,42	2.86	7 (29%)
54	5MU	1y	54	54	13,22,23	0.85	1 (7%)	14,32,35	2.26	2 (14%)
54	PSU	1y	55	54	16,21,22	1.19	1 (6%)	20,30,33	3.04	5 (25%)
54	4SU	1y	8	54	13,21,22	1.37	1 (7%)	14,30,33	1.67	2 (14%)
1	PSU	2A	1911	1	16,21,22	1.36	1 (6%)	20,30,33	3.33	6 (30%)
1	5MU	2A	1915	1	13,22,23	0.74	0	14,32,35	1.89	2 (14%)
1	PSU	2A	1917	1	16,21,22	1.50	1 (6%)	20,30,33	3.22	7 (35%)
1	4OC	2A	1920	1	15,22,24	0.75	0	20,31,35	1.31	1 (5%)
1	5MU	2A	1939	1,56	13,22,23	0.76	0	14,32,35	1.99	2 (14%)
1	5MC	2A	1942	1	14,22,23	1.63	1 (7%)	17,32,35	1.41	2 (11%)
1	5MC	2A	1962	1,56	14,22,23	1.58	1 (7%)	17,32,35	1.43	3 (17%)
1	OMG	2A	2251	1,55,56	18,26,27	1.30	2 (11%)	22,38,41	2.05	6 (27%)
1	2MA	2A	2503	1,56	16,25,26	1.44	3 (18%)	17,37,40	2.11	3 (17%)
1	2MU	2A	2552	1,56	14,22,24	1.11	2 (14%)	17,31,36	0.76	0
1	PSU	2A	2605	1	16,21,22	1.51	1 (6%)	20,30,33	3.09	6 (30%)
32	2MG	2a	1207	32	18,26,27	1.38	2 (11%)	19,38,41	2.65	9 (47%)
32	5MC	2a	1400	32	14,22,23	1.53	1 (7%)	17,32,35	1.43	3 (17%)
32	4OC	2a	1402	32	16,23,24	0.70	0	20,32,35	1.17	1 (5%)
32	5MC	2a	1404	32	14,22,23	1.53	1 (7%)	17,32,35	1.36	3 (17%)
32	5MC	2a	1407	32	14,22,23	1.52	2 (14%)	17,32,35	1.54	2 (11%)
32	UR3	2a	1498	32	13,22,23	0.95	1 (7%)	15,32,35	0.67	0
32	MA6	2a	1518	32	16,26,27	1.11	1 (6%)	16,38,41	1.74	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	MA6	2a	1519	32	16,26,27	1.17	1 (6%)	16,38,41	1.71	4 (25%)
32	PSU	2a	516	32	16,21,22	1.56	2 (12%)	20,30,33	3.11	6 (30%)
32	7MG	2a	527	32,56	20,26,27	1.98	3 (15%)	24,39,42	2.50	6 (25%)
32	M2G	2a	966	32	19,27,28	1.57	3 (15%)	20,40,43	2.21	5 (25%)
32	5MC	2a	967	32	14,22,23	1.57	1 (7%)	17,32,35	1.37	3 (17%)
43	0TD	2l	92	43	5,9,10	3.09	2 (40%)	4,11,13	1.93	1 (25%)
54	PSU	2w	32	54	16,21,22	1.32	1 (6%)	20,30,33	3.15	5 (25%)
54	MIA	2w	37	54	17,24,32	1.30	2 (11%)	16,35,47	1.32	2 (12%)
54	PSU	2w	39	54	16,21,22	1.21	1 (6%)	20,30,33	3.50	6 (30%)
54	7MG	2w	46	54	20,26,27	1.98	3 (15%)	24,39,42	2.47	6 (25%)
54	5MU	2w	54	54	13,22,23	0.75	0	14,32,35	2.33	2 (14%)
54	PSU	2w	55	54	16,21,22	1.28	1 (6%)	20,30,33	3.39	7 (35%)
54	4SU	2w	8	54	13,21,22	1.38	2 (15%)	14,30,33	1.73	2 (14%)
55	5MC	2x	32	55	14,22,23	1.43	1 (7%)	17,32,35	1.49	3 (17%)
55	5MU	2x	54	55	13,22,23	0.77	0	14,32,35	2.10	1 (7%)
55	PSU	2x	55	55	16,21,22	1.33	1 (6%)	20,30,33	3.03	6 (30%)
55	M3O	2x	76	55,56	27,34,35	1.44	4 (14%)	28,47,50	2.04	4 (14%)
55	4SU	2x	8	55	13,21,22	1.41	2 (15%)	14,30,33	2.29	2 (14%)
54	PSU	2y	32	54	16,21,22	1.19	1 (6%)	20,30,33	3.11	6 (30%)
54	MIA	2y	37	54	17,24,32	1.28	2 (11%)	16,35,47	1.34	2 (12%)
54	PSU	2y	39	54	16,21,22	1.28	1 (6%)	20,30,33	3.09	8 (40%)
54	7MG	2y	46	54	20,26,27	1.92	3 (15%)	24,39,42	2.90	7 (29%)
54	5MU	2y	54	54	13,22,23	0.73	0	14,32,35	2.11	1 (7%)
54	PSU	2y	55	54	16,21,22	1.25	1 (6%)	20,30,33	3.11	6 (30%)
54	4SU	2y	8	54	13,21,22	1.37	1 (7%)	14,30,33	1.58	2 (14%)

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	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	1A	1939	1	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1942	1,56	-	0/3/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	0/3/25/26	0/2/2/2
1	OMG	1A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	1A	2503	1,56	-	1/3/25/26	0/3/3/3
1	2MU	1A	2552	1,56	-	0/5/27/28	0/2/2/2
1	PSU	1A	2605	1	-	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	-	2/3/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/7/29/30	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	-	1/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	2/7/37/38	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	1/3/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/2/12/14	-
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	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	M3O	1x	76	55,56	-	9/18/40/41	0/3/3/3
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	-	2/3/25/34	0/3/3/3
54	PSU	1y	39	54	-	1/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
54	5MU	1y	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/3/25/26	0/2/2/2
1	PSU	2A	1911	1	-	1/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/5/27/28	0/3/3/3
1	2MA	2A	2503	1,56	-	1/3/25/26	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	-	2/7/29/30	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	-	2/3/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	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	-	1/2/12/14	-
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/3/25/34	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	3/7/37/38	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	M3O	2x	76	55,56	-	7/18/40/41	0/3/3/3
55	4SU	2x	8	55	-	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	-	2/3/25/34	0/3/3/3
54	PSU	2y	39	54	-	1/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	5/7/37/38	0/3/3/3
54	5MU	2y	54	54	-	2/3/25/26	0/2/2/2
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4SU	2y	8	54	-	0/3/25/26	0/2/2/2

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C2-S10	-7.58	1.69	1.75
54	1w	37	MIA	C13-C14	7.11	1.53	1.32
43	1l	92	0TD	CB-SB	-6.18	1.69	1.84
54	1y	46	7MG	C6-C5	6.06	1.48	1.41
32	2a	527	7MG	C6-C5	6.02	1.48	1.41
54	2w	46	7MG	C6-C5	6.00	1.48	1.41
43	2l	92	0TD	CB-SB	-5.92	1.69	1.84
1	1A	2605	PSU	C5-C1'	-5.79	1.47	1.52
54	2y	46	7MG	C6-C5	5.50	1.47	1.41
54	1w	46	7MG	C6-C5	5.49	1.47	1.41
32	1a	527	7MG	C6-C5	5.49	1.47	1.41
1	2A	1942	5MC	C5-C4	5.44	1.49	1.41
32	2a	967	5MC	C5-C4	5.36	1.49	1.41
1	2A	1962	5MC	C5-C4	5.35	1.49	1.41
32	2a	1404	5MC	C5-C4	5.17	1.48	1.41
32	2a	1400	5MC	C5-C4	5.16	1.48	1.41
54	2y	46	7MG	C5-C4	5.14	1.48	1.38
54	1y	46	7MG	C5-C4	5.11	1.48	1.38
55	1x	55	PSU	C5-C1'	-5.07	1.47	1.52
55	1x	32	5MC	C5-C4	5.03	1.48	1.41
32	1a	1407	5MC	C5-C4	4.98	1.48	1.41
32	2a	516	PSU	C5-C1'	-4.98	1.48	1.52
54	1w	46	7MG	C5-C4	4.96	1.48	1.38
32	2a	1407	5MC	C5-C4	4.95	1.48	1.41
1	1A	1942	5MC	C5-C4	4.93	1.48	1.41
32	1a	1400	5MC	C5-C4	4.88	1.48	1.41
1	1A	1962	5MC	C5-C4	4.85	1.48	1.41
55	2x	32	5MC	C5-C4	4.83	1.48	1.41
32	1a	527	7MG	C5-C4	4.83	1.47	1.38
1	2A	2605	PSU	C5-C1'	-4.81	1.48	1.52
1	2A	1917	PSU	C5-C1'	-4.80	1.48	1.52
32	1a	967	5MC	C5-C4	4.74	1.48	1.41
32	2a	527	7MG	C5-C4	4.70	1.47	1.38
54	1w	39	PSU	C5-C1'	-4.64	1.48	1.52
32	1a	1404	5MC	C5-C4	4.63	1.48	1.41
1	1A	2503	2MA	C6-C5	4.48	1.48	1.41
54	2w	46	7MG	C5-C4	4.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	966	M2G	C6-C5	4.38	1.49	1.41
32	2a	1207	2MG	C6-C5	4.36	1.49	1.41
32	1a	516	PSU	C5-C1'	-4.34	1.48	1.52
55	2x	76	M3O	O3'-C	4.32	1.44	1.34
54	1w	32	PSU	C5-C1'	-4.30	1.48	1.52
32	1a	1207	2MG	C6-C5	4.28	1.48	1.41
1	2A	2503	2MA	C6-C5	4.22	1.47	1.41
55	2x	8	4SU	C4-S4	-4.20	1.59	1.67
1	1A	2251	OMG	C6-C5	4.10	1.48	1.41
54	1w	8	4SU	C4-S4	-4.08	1.60	1.67
54	1y	32	PSU	C5-C1'	-4.03	1.48	1.52
1	2A	2251	OMG	C6-C5	4.03	1.48	1.41
54	2y	8	4SU	C4-S4	-4.00	1.60	1.67
54	1w	55	PSU	C5-C1'	-3.99	1.48	1.52
54	1y	8	4SU	C4-S4	-3.96	1.60	1.67
55	2x	55	PSU	C5-C1'	-3.91	1.48	1.52
1	2A	1911	PSU	C5-C1'	-3.90	1.48	1.52
32	1a	966	M2G	C6-C5	3.90	1.48	1.41
54	2w	32	PSU	C5-C1'	-3.82	1.49	1.52
1	1A	1911	PSU	C5-C1'	-3.82	1.49	1.52
55	1x	76	M3O	O3'-C	3.79	1.43	1.34
54	2w	8	4SU	C4-S4	-3.68	1.60	1.67
54	2w	55	PSU	C5-C1'	-3.66	1.49	1.52
54	2y	55	PSU	C5-C1'	-3.64	1.49	1.52
1	1A	1917	PSU	C5-C1'	-3.51	1.49	1.52
54	2w	46	7MG	C4-N9	-3.50	1.33	1.38
54	1y	39	PSU	C5-C1'	-3.49	1.49	1.52
54	2w	37	MIA	C5-C4	3.42	1.48	1.40
32	2a	527	7MG	C4-N9	-3.38	1.33	1.38
54	2y	37	MIA	C5-C4	3.36	1.48	1.40
54	1w	46	7MG	C4-N9	-3.34	1.33	1.38
32	2a	966	M2G	C5-C4	3.32	1.48	1.40
54	1y	37	MIA	C5-C4	3.31	1.48	1.40
55	2x	76	M3O	C5-C4	-3.28	1.33	1.40
32	2a	966	M2G	C2-N2	3.26	1.40	1.35
55	1x	8	4SU	C2-N3	-3.25	1.31	1.38
55	1x	8	4SU	C4-S4	-3.22	1.61	1.67
54	2y	39	PSU	C5-C1'	-3.22	1.49	1.52
32	2a	1519	MA6	C5-C4	3.21	1.47	1.40
54	1w	37	MIA	C5-C4	3.20	1.47	1.40
32	1a	527	7MG	C4-N9	-3.19	1.34	1.38
1	1A	2251	OMG	C5-C4	3.19	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1518	MA6	C5-C4	3.18	1.47	1.40
54	1y	55	PSU	C5-C1'	-3.16	1.49	1.52
32	1a	1518	MA6	C5-C4	3.14	1.47	1.40
54	2w	39	PSU	C5-C1'	-3.10	1.49	1.52
32	1a	1519	MA6	C5-C4	3.07	1.47	1.40
43	2l	92	0TD	CA-C	3.04	1.54	1.50
32	2a	1207	2MG	C5-C4	2.99	1.47	1.40
54	2y	32	PSU	C5-C1'	-2.94	1.49	1.52
32	1a	966	M2G	C5-C4	2.93	1.47	1.40
32	1a	1207	2MG	C5-C4	2.85	1.46	1.40
43	1l	92	0TD	CA-C	2.85	1.54	1.50
1	2A	2251	OMG	C5-C4	2.83	1.46	1.40
32	1a	966	M2G	C2-N2	2.80	1.39	1.35
54	1y	37	MIA	C2-N3	2.78	1.36	1.32
1	2A	2503	2MA	C5-C4	2.69	1.46	1.40
54	2w	37	MIA	C2-N3	2.66	1.36	1.32
55	2x	76	M3O	C6-C5	-2.60	1.33	1.43
54	2y	37	MIA	C2-N3	2.59	1.36	1.32
55	1x	76	M3O	C5-C4	-2.56	1.34	1.40
55	1x	76	M3O	C6-C5	-2.56	1.33	1.43
54	2y	46	7MG	C4-N9	-2.54	1.35	1.38
54	1y	46	7MG	C4-N9	-2.42	1.35	1.38
1	1A	2503	2MA	C5-C4	2.40	1.45	1.40
1	1A	2605	PSU	C2-N3	-2.38	1.33	1.38
54	1y	54	5MU	C2-N3	-2.36	1.33	1.38
1	1A	1939	5MU	C2-N3	-2.35	1.33	1.38
32	2a	1498	UR3	O5'-C5'	-2.31	1.41	1.44
32	2a	516	PSU	O4'-C1'	-2.29	1.41	1.44
1	2A	2552	2MU	O5'-C5'	-2.29	1.41	1.44
54	1y	39	PSU	O5'-C5'	-2.27	1.41	1.44
55	1x	76	M3O	C5-N7	-2.27	1.31	1.39
55	2x	76	M3O	C5-N7	-2.25	1.31	1.39
32	1a	516	PSU	O4'-C1'	-2.20	1.41	1.44
1	1A	2605	PSU	O5'-C5'	-2.19	1.41	1.44
55	2x	8	4SU	C2-N3	-2.18	1.33	1.38
1	1A	1911	PSU	O4'-C1'	-2.18	1.41	1.44
32	2a	1407	5MC	O5'-C5'	-2.16	1.41	1.44
54	2w	8	4SU	C2-N3	-2.15	1.33	1.38
1	2A	2552	2MU	O4'-C1'	2.14	1.44	1.41
32	1a	527	7MG	O5'-C5'	-2.11	1.41	1.44
1	2A	2503	2MA	O5'-C5'	-2.07	1.41	1.44
32	1a	516	PSU	C2-N3	-2.06	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2605	PSU	O4'-C1'	-2.05	1.41	1.44
54	1w	8	4SU	C2-N3	-2.03	1.34	1.38
55	1x	32	5MC	O5'-C5'	-2.02	1.42	1.44

All (336) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	16.26	133.84	101.85
54	2w	39	PSU	N1-C2-N3	-10.29	120.25	128.43
54	2y	46	7MG	N3-C4-N9	9.51	139.45	126.94
54	1y	46	7MG	N3-C4-N9	9.42	139.33	126.94
55	1x	8	4SU	C2-N3-C4	9.17	128.44	115.15
54	1w	46	7MG	N3-C4-N9	9.12	138.94	126.94
1	2A	1911	PSU	N1-C2-N3	-9.00	121.28	128.43
32	1a	527	7MG	N3-C4-N9	8.89	138.64	126.94
54	2y	32	PSU	N1-C2-N3	-8.67	121.54	128.43
54	1y	32	PSU	N1-C2-N3	-8.62	121.58	128.43
54	2w	32	PSU	N1-C2-N3	-8.59	121.60	128.43
32	2a	516	PSU	N1-C2-N3	-8.45	121.71	128.43
54	2w	55	PSU	N1-C2-N3	-8.41	121.75	128.43
54	1w	55	PSU	N1-C2-N3	-8.40	121.76	128.43
1	1A	1911	PSU	N1-C2-N3	-8.31	121.82	128.43
55	1x	55	PSU	N1-C2-N3	-8.30	121.83	128.43
32	2a	527	7MG	N3-C4-N9	8.30	137.86	126.94
54	2w	54	5MU	C4-N3-C2	8.24	122.10	115.14
54	1y	39	PSU	N1-C2-N3	-8.21	121.90	128.43
55	2x	55	PSU	N1-C2-N3	-8.20	121.91	128.43
54	1y	55	PSU	N1-C2-N3	-8.19	121.92	128.43
1	1A	1917	PSU	N1-C2-N3	-8.17	121.94	128.43
54	1w	32	PSU	N1-C2-N3	-8.15	121.95	128.43
54	2y	39	PSU	N1-C2-N3	-8.12	121.98	128.43
1	1A	2605	PSU	N1-C2-N3	-8.10	121.99	128.43
54	2w	39	PSU	C4-N3-C2	8.08	121.96	115.14
54	2y	55	PSU	N1-C2-N3	-8.04	122.04	128.43
1	2A	1917	PSU	N1-C2-N3	-8.02	122.05	128.43
54	2w	46	7MG	N3-C4-N9	8.01	137.47	126.94
55	1x	54	5MU	C4-N3-C2	7.96	121.86	115.14
54	1w	39	PSU	N1-C2-N3	-7.94	122.12	128.43
1	2A	2605	PSU	N1-C2-N3	-7.92	122.13	128.43
54	1w	37	MIA	C12-C13-C14	-7.87	111.61	127.10
32	1a	516	PSU	N1-C2-N3	-7.87	122.18	128.43
54	1y	54	5MU	C4-N3-C2	7.71	121.65	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	C2-N3-C4	7.70	121.83	115.53
55	2x	54	5MU	C4-N3-C2	7.46	121.44	115.14
54	2y	54	5MU	C4-N3-C2	7.42	121.40	115.14
55	2x	8	4SU	C2-N3-C4	7.39	125.86	115.15
54	1w	54	5MU	C4-N3-C2	7.36	121.35	115.14
54	1w	55	PSU	C4-N3-C2	7.25	121.27	115.14
54	2w	32	PSU	C4-N3-C2	7.22	121.24	115.14
54	2w	55	PSU	C4-N3-C2	7.18	121.21	115.14
55	2x	76	M3O	C4'-O4'-C1'	-7.11	102.42	109.83
54	1y	55	PSU	C4-N3-C2	7.09	121.13	115.14
54	2y	32	PSU	C4-N3-C2	6.87	120.94	115.14
54	2y	55	PSU	C4-N3-C2	6.77	120.86	115.14
54	1y	39	PSU	C4-N3-C2	6.70	120.80	115.14
1	2A	1911	PSU	C4-N3-C2	6.66	120.76	115.14
54	1y	32	PSU	C4-N3-C2	6.62	120.73	115.14
54	2y	39	PSU	C4-N3-C2	6.62	120.73	115.14
1	1A	1917	PSU	C4-N3-C2	6.57	120.69	115.14
32	2a	516	PSU	C4-N3-C2	6.52	120.65	115.14
1	2A	1939	5MU	C4-N3-C2	6.51	120.64	115.14
55	1x	55	PSU	C4-N3-C2	6.43	120.57	115.14
1	1A	1911	PSU	C4-N3-C2	6.39	120.54	115.14
1	2A	1917	PSU	C4-N3-C2	6.38	120.53	115.14
1	2A	2503	2MA	C2-N3-C4	6.34	120.71	115.53
1	1A	1939	5MU	C4-N3-C2	6.33	120.49	115.14
54	1w	32	PSU	C4-N3-C2	6.32	120.47	115.14
55	2x	55	PSU	C4-N3-C2	6.28	120.44	115.14
32	1a	516	PSU	C4-N3-C2	6.23	120.40	115.14
54	1w	39	PSU	C4-N3-C2	6.18	120.36	115.14
1	1A	1915	5MU	C4-N3-C2	6.16	120.35	115.14
1	1A	2605	PSU	C4-N3-C2	6.10	120.30	115.14
1	2A	1915	5MU	C4-N3-C2	6.08	120.28	115.14
1	2A	2605	PSU	C4-N3-C2	6.04	120.24	115.14
54	2w	55	PSU	C5-C4-N3	-6.00	117.63	125.36
54	1w	55	PSU	C5-C4-N3	-5.76	117.94	125.36
54	1y	55	PSU	C5-C4-N3	-5.62	118.12	125.36
54	2w	32	PSU	C5-C4-N3	-5.62	118.13	125.36
55	1x	55	PSU	C5-C4-N3	-5.58	118.17	125.36
54	2y	55	PSU	C5-C4-N3	-5.53	118.23	125.36
55	2x	76	M3O	N3-C2-N1	-5.50	119.82	128.68
54	1y	46	7MG	C5-C4-N3	-5.49	117.31	126.47
54	2y	39	PSU	C5-C4-N3	-5.46	118.33	125.36
54	2y	46	7MG	C6-N1-C2	5.45	123.83	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	516	PSU	C5-C4-N3	-5.44	118.35	125.36
54	1y	39	PSU	C5-C4-N3	-5.43	118.37	125.36
1	2A	1917	PSU	C5-C4-N3	-5.43	118.37	125.36
55	1x	76	M3O	N3-C2-N1	-5.43	119.93	128.68
54	2y	46	7MG	C5-C4-N3	-5.42	117.43	126.47
1	1A	2251	OMG	C2-N3-C4	5.33	121.44	115.36
54	1y	32	PSU	C5-C4-N3	-5.32	118.51	125.36
55	1x	8	4SU	C5-C4-N3	-5.30	116.94	123.81
1	2A	2605	PSU	C5-C4-N3	-5.22	118.63	125.36
32	1a	527	7MG	C5-C4-N3	-5.22	117.76	126.47
54	1w	39	PSU	C5-C4-N3	-5.21	118.64	125.36
1	1A	1917	PSU	C5-C4-N3	-5.20	118.66	125.36
1	1A	1920	4OC	C2-N3-C4	5.19	121.22	116.26
54	1w	32	PSU	C5-C4-N3	-5.18	118.69	125.36
1	1A	1911	PSU	C5-C4-N3	-5.14	118.74	125.36
54	2y	32	PSU	C5-C4-N3	-5.12	118.76	125.36
1	2A	1911	PSU	C5-C4-N3	-5.06	118.84	125.36
32	2a	966	M2G	C6-N1-C2	5.06	122.21	116.18
54	2w	39	PSU	C5-C4-N3	-5.04	118.87	125.36
55	2x	55	PSU	C5-C4-N3	-5.01	118.91	125.36
54	1w	46	7MG	C5-C4-N3	-4.98	118.15	126.47
32	1a	516	PSU	C5-C4-N3	-4.96	118.97	125.36
32	2a	966	M2G	C2-N3-C4	4.94	120.88	115.28
54	1y	8	4SU	C2-N3-C4	4.92	122.29	115.15
1	2A	2251	OMG	C2-N3-C4	4.92	120.97	115.36
54	1w	55	PSU	C5-C1'-C2'	-4.90	106.58	115.32
32	1a	1207	2MG	CM2-N2-C2	-4.88	117.70	123.59
32	2a	1207	2MG	C2-N3-C4	4.87	120.81	115.28
32	1a	527	7MG	C6-N1-C2	4.83	122.93	116.06
1	2A	1920	4OC	C2-N3-C4	4.83	120.87	116.26
32	1a	966	M2G	C6-N1-C2	4.81	121.91	116.18
54	2w	8	4SU	C2-N3-C4	4.80	122.11	115.15
54	1y	46	7MG	C6-N1-C2	4.78	122.86	116.06
1	2A	1917	PSU	C5-C1'-C2'	-4.78	106.80	115.32
1	2A	1911	PSU	C5-C1'-C2'	-4.77	106.81	115.32
54	1y	46	7MG	C6-C5-C4	4.76	120.31	115.20
54	2w	46	7MG	C6-N1-C2	4.74	122.81	116.06
32	2a	527	7MG	C5-C4-N3	-4.72	118.59	126.47
32	1a	1207	2MG	C2-N3-C4	4.72	120.64	115.28
54	1w	46	7MG	C6-N1-C2	4.72	122.78	116.06
1	2A	2605	PSU	C5-C6-N1	-4.71	118.53	124.44
1	1A	2605	PSU	C5-C4-N3	-4.68	119.33	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	C6-N1-C2	4.67	122.70	116.06
54	2w	46	7MG	C5-C4-N3	-4.67	118.68	126.47
1	2A	1917	PSU	C5-C6-N1	-4.63	118.64	124.44
1	1A	2605	PSU	C5-C6-N1	-4.61	118.67	124.44
32	1a	527	7MG	C6-C5-C4	4.59	120.12	115.20
1	2A	1911	PSU	C6-N1-C2	4.59	122.63	115.32
54	2y	46	7MG	C6-C5-C4	4.57	120.10	115.20
54	1w	8	4SU	C2-N3-C4	4.54	121.73	115.15
54	2w	39	PSU	C6-N1-C2	4.47	122.44	115.32
54	1y	32	PSU	C6-N1-C2	4.45	122.41	115.32
1	1A	1911	PSU	C6-N1-C2	4.42	122.37	115.32
32	1a	966	M2G	C2-N3-C4	4.41	120.29	115.28
54	1w	39	PSU	C5-C6-N1	-4.39	118.94	124.44
32	1a	1400	5MC	C2-N3-C4	4.36	120.90	115.92
32	2a	1207	2MG	C6-C5-C4	-4.35	116.60	120.79
1	2A	2605	PSU	C6-N1-C2	4.34	122.24	115.32
54	1w	32	PSU	C5-C6-N1	-4.34	119.01	124.44
32	1a	1207	2MG	C5-C6-N1	-4.33	117.44	123.47
1	2A	1917	PSU	C6-N1-C2	4.32	122.21	115.32
1	2A	2503	2MA	C5-C6-N1	-4.31	118.36	123.10
54	1w	46	7MG	C6-C5-C4	4.31	119.83	115.20
54	1y	32	PSU	C5-C6-N1	-4.31	119.04	124.44
32	1a	1404	5MC	C2-N3-C4	4.30	120.83	115.92
32	2a	516	PSU	C6-N1-C2	4.30	122.17	115.32
1	1A	1911	PSU	C5-C6-N1	-4.29	119.07	124.44
54	2y	32	PSU	C6-N1-C2	4.28	122.15	115.32
54	1w	32	PSU	C6-N1-C2	4.28	122.15	115.32
55	1x	55	PSU	C5-C6-N1	-4.28	119.07	124.44
54	1w	39	PSU	C6-N1-C2	4.28	122.14	115.32
1	1A	2605	PSU	C6-N1-C2	4.28	122.14	115.32
54	2w	55	PSU	C6-N1-C2	4.28	122.14	115.32
55	2x	55	PSU	C6-N1-C2	4.28	122.14	115.32
32	2a	516	PSU	C5-C6-N1	-4.25	119.11	124.44
55	1x	55	PSU	C6-N1-C2	4.24	122.09	115.32
32	2a	1207	2MG	C5-C6-N1	-4.24	117.57	123.47
32	2a	1207	2MG	C6-N1-C2	4.23	122.76	115.18
55	2x	55	PSU	C5-C6-N1	-4.22	119.15	124.44
1	1A	1917	PSU	C6-N1-C2	4.21	122.04	115.32
1	1A	2251	OMG	C6-N1-C2	4.19	122.03	116.06
32	1a	966	M2G	C5-C6-N1	-4.18	117.64	123.47
1	1A	1942	5MC	C2-N3-C4	4.17	120.68	115.92
54	2w	55	PSU	C5-C6-N1	-4.15	119.24	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1407	5MC	C2-N3-C4	4.13	120.63	115.92
1	2A	2251	OMG	C6-N1-C2	4.12	121.93	116.06
54	2y	8	4SU	C2-N3-C4	4.11	121.11	115.15
32	1a	516	PSU	C5-C6-N1	-4.11	119.28	124.44
1	2A	1911	PSU	C5-C6-N1	-4.11	119.29	124.44
32	2a	966	M2G	C5-C6-N1	-4.11	117.75	123.47
54	2y	39	PSU	C6-N1-C2	4.10	121.86	115.32
32	1a	516	PSU	C6-N1-C2	4.10	121.85	115.32
54	2w	32	PSU	C6-N1-C2	4.10	121.85	115.32
32	2a	1407	5MC	C2-N3-C4	4.09	120.58	115.92
32	2a	1207	2MG	CM2-N2-C2	-4.08	118.66	123.59
32	1a	1207	2MG	C6-N1-C2	4.08	122.48	115.18
54	2w	55	PSU	C5-C1'-C2'	-4.07	108.05	115.32
54	1y	39	PSU	C6-N1-C2	4.07	121.81	115.32
54	1w	37	MIA	C2-N3-C4	4.06	120.92	115.32
54	1w	37	MIA	C15-C14-C13	-4.06	110.69	122.65
1	1A	2503	2MA	C5-C6-N1	-4.02	118.69	123.10
55	2x	32	5MC	C2-N3-C4	4.00	120.48	115.92
54	2y	55	PSU	C6-N1-C2	3.94	121.60	115.32
32	1a	1207	2MG	C6-C5-C4	-3.94	117.00	120.79
54	1w	55	PSU	C6-N1-C2	3.93	121.59	115.32
1	1A	2251	OMG	C5-C6-N1	-3.93	118.01	123.47
32	2a	1402	4OC	CM4-N4-C4	-3.92	119.56	122.95
1	2A	2251	OMG	C6-C5-C4	-3.90	117.03	120.79
32	1a	967	5MC	C2-N3-C4	3.88	120.35	115.92
32	2a	967	5MC	C2-N3-C4	3.87	120.33	115.92
1	1A	1917	PSU	C5-C6-N1	-3.86	119.60	124.44
54	1y	55	PSU	C6-N1-C2	3.84	121.45	115.32
1	1A	1962	5MC	C2-N3-C4	3.83	120.29	115.92
55	2x	8	4SU	C5-C4-N3	-3.83	118.85	123.81
32	2a	1404	5MC	C2-N3-C4	3.82	120.28	115.92
32	2a	1400	5MC	C2-N3-C4	3.77	120.22	115.92
54	1w	37	MIA	C11-S10-C2	-3.77	99.51	102.29
32	2a	527	7MG	C6-C5-C4	3.75	119.22	115.20
1	2A	2605	PSU	C5-C1'-C2'	-3.75	108.64	115.32
32	2a	1518	MA6	C4-C5-N7	-3.74	105.50	109.40
54	2y	32	PSU	C5-C6-N1	-3.71	119.79	124.44
54	1w	37	MIA	C5-C6-N1	-3.70	117.60	120.80
54	2y	55	PSU	C5-C6-N1	-3.65	119.86	124.44
54	2w	32	PSU	C5-C6-N1	-3.65	119.87	124.44
54	1y	39	PSU	O4'-C1'-C5	-3.63	104.31	109.93
54	2w	8	4SU	C5-C4-N3	-3.63	119.11	123.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	32	5MC	C2-N3-C4	3.62	120.05	115.92
32	1a	1518	MA6	C4-C5-N7	-3.60	105.64	109.40
54	1w	37	MIA	C16-C14-C13	-3.59	112.06	122.65
54	1w	32	PSU	C5-C1'-C2'	-3.58	108.93	115.32
32	1a	1207	2MG	C4-C5-N7	-3.57	105.68	109.40
32	2a	1519	MA6	C4-C5-N7	-3.56	105.69	109.40
1	2A	2251	OMG	C5-C6-N1	-3.53	118.55	123.47
54	2w	39	PSU	C5-C6-N1	-3.52	120.02	124.44
1	2A	1962	5MC	C2-N3-C4	3.51	119.93	115.92
32	1a	966	M2G	C6-C5-C4	-3.50	117.42	120.79
32	1a	1207	2MG	N2-C2-N1	3.49	120.31	116.96
43	2l	92	0TD	CSB-SB-CB	-3.46	95.04	101.85
54	2y	37	MIA	N3-C2-N1	-3.46	123.10	128.68
32	2a	1207	2MG	N2-C2-N1	3.46	120.28	116.96
54	2y	55	PSU	C5-C1'-C2'	-3.45	109.17	115.32
54	1y	39	PSU	C5-C6-N1	-3.44	120.13	124.44
32	2a	1518	MA6	N3-C2-N1	-3.42	123.17	128.68
54	1w	55	PSU	C5-C6-N1	-3.40	120.18	124.44
54	1y	55	PSU	C5-C6-N1	-3.40	120.18	124.44
1	2A	1942	5MC	C2-N3-C4	3.38	119.78	115.92
54	2w	37	MIA	N3-C2-N1	-3.37	123.24	128.68
32	2a	1518	MA6	C9-N6-C6	-3.36	109.35	119.51
54	2y	39	PSU	C5-C6-N1	-3.32	120.27	124.44
32	1a	1519	MA6	C9-N6-C6	-3.29	109.55	119.51
32	2a	1207	2MG	C4-C5-N7	-3.27	105.99	109.40
54	1y	37	MIA	N3-C2-N1	-3.27	123.41	128.68
54	2w	46	7MG	C6-C5-C4	3.27	118.71	115.20
1	1A	2251	OMG	N3-C2-N1	-3.25	122.85	127.25
55	1x	32	5MC	N4-C4-N3	3.25	121.66	117.03
55	1x	76	M3O	CA-N-CN	-3.23	117.85	122.82
1	1A	2503	2MA	C4-C5-N7	-3.22	106.04	109.40
55	1x	76	M3O	O3'-C-CA	3.22	119.30	111.43
54	2w	55	PSU	O4'-C1'-C5	3.21	114.91	109.93
54	1y	8	4SU	C5-C4-N3	-3.20	119.66	123.81
32	2a	966	M2G	C6-C5-C4	-3.17	117.74	120.79
1	1A	2605	PSU	C5-C1'-C2'	-3.16	109.68	115.32
32	1a	1519	MA6	C4-C5-N7	-3.16	106.11	109.40
32	2a	1519	MA6	N3-C2-N1	-3.12	123.64	128.68
1	1A	2251	OMG	C6-C5-C4	-3.12	117.78	120.79
1	2A	2251	OMG	N3-C2-N1	-3.11	123.04	127.25
54	2y	8	4SU	C5-C4-N3	-3.11	119.79	123.81
32	2a	1519	MA6	C9-N6-C6	-3.09	110.16	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	C9-N6-C6	-3.07	110.22	119.51
55	2x	76	M3O	O3'-C-CA	3.07	118.92	111.43
32	1a	1519	MA6	N1-C6-N6	3.02	120.24	117.06
32	1a	1518	MA6	N3-C2-N1	-3.01	123.84	128.68
1	1A	1939	5MU	C5-C6-N1	-2.98	118.93	122.15
55	1x	55	PSU	C5-C1'-C2'	-2.97	110.02	115.32
1	2A	2251	OMG	C4-C5-N7	-2.89	106.39	109.40
32	1a	1519	MA6	N3-C2-N1	-2.87	124.05	128.68
54	2w	39	PSU	C5-C1'-C2'	-2.87	110.20	115.32
1	2A	1915	5MU	C5-C6-N1	-2.83	119.08	122.15
54	2w	37	MIA	C4-C5-N7	-2.82	106.46	109.40
1	2A	1939	5MU	C5-C6-N1	-2.82	119.10	122.15
54	1y	32	PSU	C5-C1'-C2'	-2.82	110.30	115.32
1	2A	2503	2MA	C4-C5-N7	-2.82	106.47	109.40
54	1w	39	PSU	C5-C1'-C2'	-2.81	110.31	115.32
32	2a	527	7MG	C8-N7-C5	2.80	116.44	108.96
32	2a	1207	2MG	C1'-N9-C4	-2.80	121.80	126.64
1	2A	1962	5MC	C5-C6-N1	-2.79	119.13	122.15
32	1a	966	M2G	CM1-N2-C2	-2.79	118.62	121.29
32	1a	967	5MC	N4-C4-N3	2.78	121.00	117.03
32	1a	1402	4OC	CM4-N4-C4	-2.78	120.55	122.95
1	2A	1962	5MC	N4-C4-N3	2.77	120.98	117.03
54	1w	37	MIA	C2-N1-C6	2.76	122.34	117.25
1	1A	1962	5MC	N4-C4-N3	2.75	120.94	117.03
54	1w	8	4SU	C5-C4-N3	-2.72	120.29	123.81
1	1A	1917	PSU	C5-C1'-C2'	-2.70	110.49	115.32
32	2a	1407	5MC	N4-C4-N3	2.70	120.89	117.03
54	2w	46	7MG	C8-N7-C5	2.70	116.16	108.96
55	2x	32	5MC	N4-C4-N3	2.68	120.85	117.03
55	1x	76	M3O	C3'-O3'-C	-2.67	113.12	117.75
54	2y	37	MIA	C4-C5-N7	-2.67	106.62	109.40
54	1y	37	MIA	C4-C5-N7	-2.65	106.64	109.40
54	1y	46	7MG	C8-N7-C5	2.64	116.01	108.96
1	1A	1942	5MC	N4-C4-N3	2.64	120.80	117.03
32	2a	1400	5MC	C5-C6-N1	-2.64	119.30	122.15
54	1w	37	MIA	C4-C5-N7	-2.63	106.66	109.40
32	2a	966	M2G	C4-C5-N7	-2.62	106.66	109.40
54	1w	46	7MG	C8-N7-C5	2.62	115.95	108.96
32	2a	1519	MA6	N1-C6-N6	2.62	119.81	117.06
55	1x	32	5MC	C5-C6-N1	-2.61	119.33	122.15
32	1a	1404	5MC	CM5-C5-C4	-2.59	119.09	121.68
32	1a	966	M2G	C4-C5-N7	-2.59	106.70	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1404	5MC	N4-C4-N3	2.58	120.71	117.03
1	2A	1942	5MC	C5-C6-N1	-2.58	119.36	122.15
32	1a	527	7MG	C8-N7-C5	2.55	115.76	108.96
1	1A	2251	OMG	C4-C5-N7	-2.55	106.75	109.40
55	2x	55	PSU	C5-C1'-C2'	-2.54	110.79	115.32
54	2y	46	7MG	C8-N7-C5	2.53	115.72	108.96
54	1w	37	MIA	C12-N6-C6	-2.47	118.84	122.50
32	2a	967	5MC	C5-C6-N1	-2.42	119.53	122.15
54	1w	46	7MG	C5-C4-N9	-2.41	102.91	106.29
32	1a	1207	2MG	C1'-N9-C4	-2.40	122.49	126.64
32	1a	1400	5MC	C5-C6-N1	-2.35	119.61	122.15
1	1A	2552	2MU	C5-C4-N3	-2.34	118.03	123.28
32	2a	967	5MC	N4-C4-N3	2.33	120.36	117.03
54	1w	37	MIA	N3-C2-N1	-2.32	122.82	126.98
54	1y	54	5MU	C5-C6-N1	-2.32	119.64	122.15
54	2y	39	PSU	C4-C5-C1'	2.30	125.53	121.14
54	1w	54	5MU	C5-C6-N1	-2.29	119.67	122.15
32	1a	1407	5MC	C5-C6-N1	-2.29	119.67	122.15
54	2w	46	7MG	C2-N3-C4	2.29	120.35	113.94
54	2y	39	PSU	O4'-C1'-C5	-2.27	106.41	109.93
54	2y	46	7MG	C5-C4-N9	-2.26	103.12	106.29
1	1A	1942	5MC	C5-C6-N1	-2.26	119.70	122.15
55	2x	32	5MC	C5-C6-N1	-2.26	119.70	122.15
32	1a	1518	MA6	C10-N6-C6	-2.26	112.68	119.51
32	2a	1207	2MG	N3-C2-N1	-2.25	122.73	126.22
54	2y	46	7MG	C2-N3-C4	2.24	120.22	113.94
54	1y	46	7MG	C2-N3-C4	2.22	120.17	113.94
32	2a	1400	5MC	N4-C4-N3	2.21	120.18	117.03
32	2a	1518	MA6	C10-N6-C9	-2.21	108.95	116.07
32	1a	1407	5MC	N4-C4-N3	2.20	120.17	117.03
32	1a	1404	5MC	C5-C6-N1	-2.20	119.77	122.15
32	2a	1404	5MC	C5-C6-N1	-2.17	119.80	122.15
32	2a	516	PSU	O4'-C1'-C2'	2.17	108.18	104.66
55	2x	76	M3O	CA-N-CN	-2.16	119.49	122.82
32	1a	516	PSU	O4'-C1'-C2'	2.15	108.15	104.66
32	1a	1518	MA6	C10-N6-C9	-2.11	109.26	116.07
54	2y	39	PSU	C5-C1'-C2'	-2.09	111.59	115.32
1	1A	2552	2MU	O4'-C1'-N1	2.09	112.14	108.06
54	1y	46	7MG	C5-C4-N9	-2.09	103.36	106.29
55	1x	32	5MC	CM5-C5-C4	-2.09	119.59	121.68
32	2a	1404	5MC	N4-C4-N3	2.07	119.98	117.03
32	1a	967	5MC	C5-C6-N1	-2.06	119.92	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	32	PSU	C5-C1'-C2'	-2.05	111.67	115.32
32	1a	527	7MG	C2-N3-C4	2.05	119.67	113.94
32	1a	1402	4OC	C5-C4-N3	-2.01	119.80	123.17
1	2A	1917	PSU	O4'-C1'-C2'	2.01	107.92	104.66
55	1x	55	PSU	O4'-C1'-C2'	2.00	107.91	104.66
54	2w	54	5MU	C5-C6-N1	-2.00	119.98	122.15
32	2a	527	7MG	C2-N3-C4	2.00	119.54	113.94

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
54	2y	46	7MG	O4'-C4'-C5'-O5'
54	2y	46	7MG	C3'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C10
54	1y	37	MIA	C3'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	1y	46	7MG	C4'-C5'-O5'-P
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
55	2x	76	M3O	C4'-C5'-O5'-P
55	2x	76	M3O	CB-CA-N-CN
55	2x	76	M3O	OCN-CN-N-CA
43	1l	92	0TD	CG-CB-SB-CSB
55	1x	76	M3O	C4'-C5'-O5'-P
55	1x	76	M3O	OCN-CN-N-CA
55	1x	76	M3O	CA-CB-CG-SD
32	2a	1498	UR3	O4'-C4'-C5'-O5'
32	2a	1498	UR3	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
54	2y	54	5MU	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
55	2x	76	M3O	C3'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	527	7MG	O4'-C4'-C5'-O5'
54	1y	37	MIA	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
32	1a	1402	4OC	C3'-C4'-C5'-O5'
55	2x	76	M3O	N-CA-CB-CG
54	1y	46	7MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
55	1x	76	M3O	C3'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
55	2x	76	M3O	O4'-C4'-C5'-O5'
55	2x	76	M3O	C-CA-CB-CG
54	1w	46	7MG	C3'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C8
32	1a	1518	MA6	C5-C6-N6-C10
54	2y	46	7MG	C2'-C1'-N9-C4
55	1x	76	M3O	O3'-C-CA-N
54	2w	46	7MG	O4'-C1'-N9-C4
54	1y	46	7MG	C2'-C1'-N9-C8
54	2w	46	7MG	C2'-C1'-N9-C8
55	1x	76	M3O	C-CA-N-CN
32	2a	527	7MG	C4'-C5'-O5'-P
54	2w	46	7MG	O4'-C1'-N9-C8
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C4'-C5'-O5'-P
54	1y	46	7MG	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C1'-N9-C8
54	1y	55	PSU	O4'-C1'-C5-C4
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
55	1x	76	M3O	O4'-C4'-C5'-O5'
54	2y	39	PSU	C2'-C1'-C5-C6
54	1y	39	PSU	C2'-C1'-C5-C6
55	1x	76	M3O	N-CA-CB-CG
1	2A	1911	PSU	O4'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C1'-N9-C8
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	1w	46	7MG	C4'-C5'-O5'-P
55	1x	76	M3O	O-C-CA-N
32	2a	1519	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1915	5MU	2	0
1	1A	1917	PSU	1	0
1	1A	1939	5MU	2	0
1	1A	2503	2MA	1	0
1	2A	1939	5MU	2	0
1	2A	1942	5MC	1	0
1	2A	2251	OMG	2	0
1	2A	2503	2MA	2	0
1	2A	2552	2MU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2310 ligands modelled in this entry, 2306 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	$\# Z  > 2$
57	4M2	1A	3894	-	55,62,62	3.17	7 (12%)	59,90,90	2.18	12 (20%)
60	SF4	1d	501	35	0,12,12	0.00	-	-	-	-
57	4M2	2A	3673	-	55,62,62	3.13	11 (20%)	59,90,90	2.16	12 (20%)
60	SF4	2d	501	35	0,12,12	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
57	4M2	1A	3894	-	-	13/31/93/93	0/6/6/6
60	SF4	1d	501	35	-	-	0/6/5/5
57	4M2	2A	3673	-	-	7/31/93/93	0/6/6/6
60	SF4	2d	501	35	-	-	0/6/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	3894	4M2	CAN-CBI	21.06	1.56	1.34
57	2A	3673	4M2	CAN-CBI	20.83	1.56	1.34
57	2A	3673	4M2	C2-N3	4.37	1.39	1.32
57	1A	3894	4M2	CBX-CBT	-4.27	1.47	1.52
57	1A	3894	4M2	OBF-CBX	-3.98	1.35	1.41
57	1A	3894	4M2	C2-N3	3.90	1.38	1.32
57	2A	3673	4M2	CAV-CBK	2.97	1.52	1.48
57	2A	3673	4M2	CBM-CAN	-2.95	1.41	1.46
57	1A	3894	4M2	C2-N1	2.91	1.39	1.33
57	2A	3673	4M2	OBH-CCC	2.82	1.45	1.41
57	2A	3673	4M2	C5-C4	-2.70	1.34	1.40
57	2A	3673	4M2	C2-N1	2.70	1.39	1.33
57	1A	3894	4M2	CBM-CAN	-2.67	1.41	1.46
57	1A	3894	4M2	C5-C4	-2.50	1.34	1.40
57	2A	3673	4M2	CBX-CBT	-2.46	1.49	1.52
57	2A	3673	4M2	CBL-CBK	-2.17	1.32	1.34
57	2A	3673	4M2	OBF-CBX	-2.09	1.38	1.41
57	2A	3673	4M2	CBV-CBZ	-2.06	1.50	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1A	3894	4M2	CBN-OBF-CBX	-7.35	107.03	117.80
57	2A	3673	4M2	CBN-OBF-CBX	-7.25	107.18	117.80
57	2A	3673	4M2	N3-C2-N1	-7.17	117.12	128.68
57	1A	3894	4M2	N3-C2-N1	-6.65	117.96	128.68
57	1A	3894	4M2	CBW-OBH-CCC	-5.59	104.00	109.83
57	1A	3894	4M2	OBE-CBX-CBT	-5.07	97.41	105.81
57	2A	3673	4M2	CBW-OBH-CCC	-4.95	104.67	109.83
57	2A	3673	4M2	CCC-N9-C4	-4.42	119.00	126.64
57	2A	3673	4M2	CAA-OBA-CBK	-4.38	110.56	119.20
57	1A	3894	4M2	OBH-CBW-CBZ	-4.26	97.97	104.06
57	1A	3894	4M2	OBF-CBX-CBT	4.03	113.84	106.82
57	2A	3673	4M2	OBF-CBX-CBT	3.94	113.67	106.82
57	2A	3673	4M2	C4-C5-N7	-3.83	105.41	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3673	4M2	OBE-CBX-CBT	-3.75	99.59	105.81
57	1A	3894	4M2	CAA-OBA-CBK	-3.74	111.84	119.20
57	2A	3673	4M2	OBH-CBW-CBZ	-3.55	98.97	104.06
57	1A	3894	4M2	CBT-CBS-CBL	-3.39	98.78	102.08
57	1A	3894	4M2	CAC-OBC-CCB	-3.20	106.03	114.53
57	1A	3894	4M2	C4-C5-N7	-3.12	106.15	109.40
57	1A	3894	4M2	CBM-CAN-CBI	-2.86	123.72	129.35
57	1A	3894	4M2	CAE-CBR-CCA	-2.79	109.15	113.43
57	2A	3673	4M2	CBM-CAN-CBI	-2.35	124.73	129.35
57	2A	3673	4M2	OBG-CBY-OB	-2.12	104.94	109.94
57	2A	3673	4M2	CAE-CBR-CCA	-2.06	110.28	113.43

There are no chirality outliers.

All (20) torsion outliers are listed below:

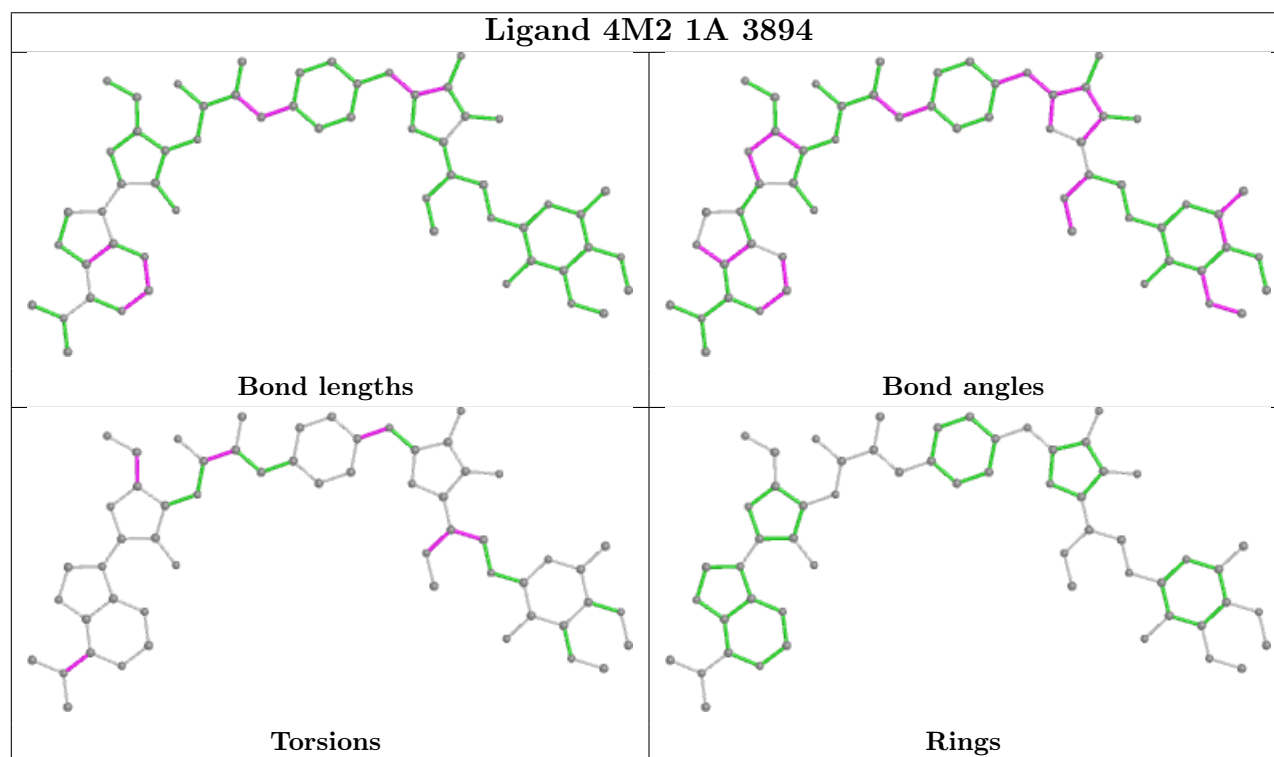
Mol	Chain	Res	Type	Atoms
57	1A	3894	4M2	C5-C6-N6-CAF
57	1A	3894	4M2	CAV-CBK-OBA-CAA
57	2A	3673	4M2	CAV-CBK-OBA-CAA
57	1A	3894	4M2	OAI-CAU-CBW-OBH
57	1A	3894	4M2	C5-C6-N6-CAG
57	1A	3894	4M2	CAN-CBI-CBJ-OAH
57	1A	3894	4M2	CAN-CBI-CBJ-NAZ
57	2A	3673	4M2	CAN-CBI-CBJ-OAH
57	2A	3673	4M2	CAN-CBI-CBJ-NAZ
57	1A	3894	4M2	OB-D-CAV-CBK-OBA
57	1A	3894	4M2	CAR-CBN-OBF-CBX
57	2A	3673	4M2	OB-D-CAV-CBK-OBA
57	1A	3894	4M2	CAD-CBI-CBJ-OAH
57	1A	3894	4M2	CAD-CBI-CBJ-NAZ
57	2A	3673	4M2	CAD-CBI-CBJ-OAH
57	2A	3673	4M2	CAD-CBI-CBJ-NAZ
57	1A	3894	4M2	CAS-CBN-OBF-CBX
57	1A	3894	4M2	CBL-CBK-OBA-CAA
57	2A	3673	4M2	CBL-CBK-OBA-CAA
57	1A	3894	4M2	OAI-CAU-CBW-CBZ

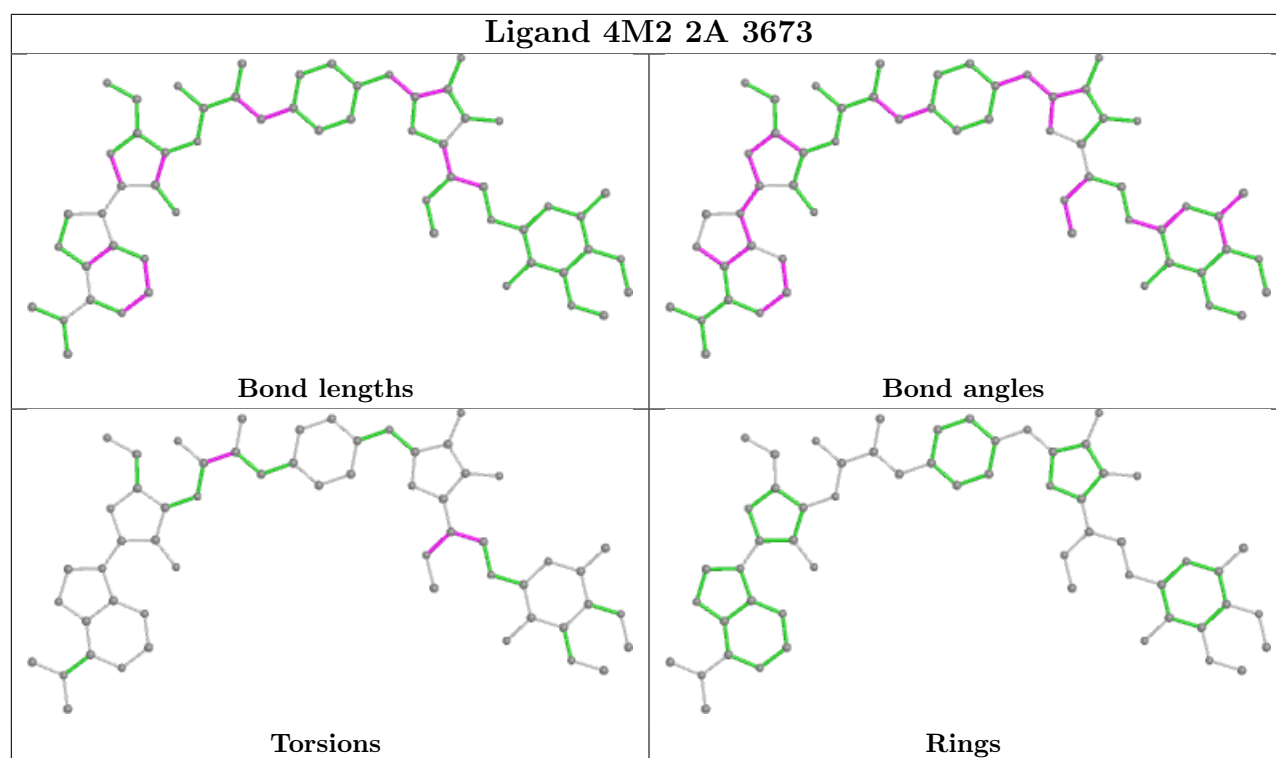
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1A	3894	4M2	5	0
57	2A	3673	4M2	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	0.27	65 (2%) 60 55	23, 42, 92, 106	0
1	2A	2789/2915 (95%)	-0.24	64 (2%) 60 55	26, 46, 90, 104	0
2	1B	120/121 (99%)	0.01	0 100 100	37, 59, 71, 89	0
2	2B	120/121 (99%)	-0.39	0 100 100	46, 66, 77, 90	0
3	1D	275/276 (99%)	0.50	3 (1%) 80 80	21, 42, 59, 79	0
3	2D	275/276 (99%)	0.38	7 (2%) 57 52	23, 44, 61, 80	0
4	1E	204/206 (99%)	0.22	0 100 100	20, 45, 65, 78	0
4	2E	204/206 (99%)	-0.04	1 (0%) 90 90	21, 49, 68, 79	0
5	1F	203/210 (96%)	0.53	5 (2%) 57 52	23, 51, 73, 89	0
5	2F	203/210 (96%)	0.42	12 (5%) 22 19	25, 56, 75, 91	0
6	1G	181/182 (99%)	0.90	16 (8%) 10 8	48, 67, 80, 92	0
6	2G	181/182 (99%)	2.31	88 (48%) 0 0	52, 71, 82, 95	0
7	1H	174/180 (96%)	0.31	1 (0%) 89 89	48, 65, 75, 82	0
7	2H	174/180 (96%)	1.63	57 (32%) 0 0	52, 70, 80, 83	0
8	1I	146/148 (98%)	0.22	0 100 100	47, 74, 83, 89	0
8	2I	146/148 (98%)	-0.24	1 (0%) 87 87	49, 74, 84, 86	0
9	1N	140/140 (100%)	0.28	0 100 100	31, 48, 69, 79	0
9	2N	140/140 (100%)	0.06	1 (0%) 87 87	36, 53, 72, 80	0
10	1O	122/122 (100%)	0.06	0 100 100	25, 38, 58, 63	0
10	2O	122/122 (100%)	0.86	10 (8%) 11 9	39, 57, 72, 76	0
11	1P	149/150 (99%)	0.24	0 100 100	23, 52, 75, 81	0
11	2P	149/150 (99%)	-0.06	1 (0%) 87 87	26, 58, 78, 83	0
12	1Q	141/141 (100%)	1.01	13 (9%) 9 7	30, 49, 64, 80	0
12	2Q	141/141 (100%)	1.28	30 (21%) 1 1	37, 54, 68, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.31	0 100 100	30, 40, 55, 67	0
13	2R	118/118 (100%)	0.17	0 100 100	32, 43, 57, 69	0
14	1S	110/112 (98%)	0.27	0 100 100	45, 59, 71, 75	0
14	2S	110/112 (98%)	-0.12	1 (0%) 84 84	52, 64, 74, 77	0
15	1T	131/146 (89%)	0.25	1 (0%) 86 86	37, 50, 73, 84	0
15	2T	131/146 (89%)	0.08	0 100 100	41, 53, 74, 84	0
16	1U	116/118 (98%)	0.31	0 100 100	26, 42, 58, 75	0
16	2U	116/118 (98%)	0.12	2 (1%) 70 67	32, 47, 62, 77	0
17	1V	101/101 (100%)	0.41	2 (1%) 65 60	29, 51, 66, 77	0
17	2V	101/101 (100%)	0.14	2 (1%) 65 60	33, 58, 70, 77	0
18	1W	112/113 (99%)	0.18	1 (0%) 84 84	25, 37, 59, 86	0
18	2W	112/113 (99%)	0.20	1 (0%) 84 84	29, 40, 61, 88	0
19	1X	95/96 (98%)	0.05	0 100 100	22, 35, 60, 84	0
19	2X	95/96 (98%)	0.65	4 (4%) 36 33	40, 60, 75, 82	0
20	1Y	107/110 (97%)	0.18	0 100 100	44, 59, 72, 85	0
20	2Y	107/110 (97%)	0.87	12 (11%) 5 3	49, 62, 75, 87	0
21	1Z	154/206 (74%)	1.57	48 (31%) 0 0	46, 71, 88, 93	0
21	2Z	160/206 (77%)	2.44	87 (54%) 0 0	52, 76, 90, 95	0
22	10	83/85 (97%)	0.81	7 (8%) 11 9	25, 36, 66, 88	0
22	20	83/85 (97%)	0.85	8 (9%) 8 6	47, 65, 77, 91	0
23	11	97/98 (98%)	0.49	3 (3%) 49 45	30, 47, 69, 79	0
23	21	97/98 (98%)	-0.03	1 (1%) 82 82	30, 51, 72, 80	0
24	12	70/72 (97%)	0.20	0 100 100	39, 56, 67, 77	0
24	22	70/72 (97%)	0.06	1 (1%) 75 73	45, 61, 69, 77	0
25	13	59/60 (98%)	0.38	0 100 100	33, 46, 68, 76	0
25	23	59/60 (98%)	0.52	3 (5%) 28 25	38, 52, 70, 79	0
26	14	69/71 (97%)	0.69	10 (14%) 2 1	47, 72, 90, 94	0
26	24	69/71 (97%)	2.97	38 (55%) 0 0	73, 86, 96, 98	0
27	15	59/60 (98%)	0.05	1 (1%) 70 67	19, 32, 51, 62	0
27	25	59/60 (98%)	0.08	0 100 100	32, 49, 66, 73	0
28	16	53/54 (98%)	0.34	1 (1%) 66 63	28, 39, 56, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.17	0 100 100	41, 58, 70, 77	0
29	17	48/49 (97%)	0.40	1 (2%) 63 58	24, 30, 58, 73	0
29	27	48/49 (97%)	1.00	6 (12%) 4 2	25, 33, 60, 75	0
30	18	64/65 (98%)	0.28	0 100 100	30, 41, 49, 58	0
30	28	64/65 (98%)	-0.28	0 100 100	35, 45, 53, 59	0
31	19	37/37 (100%)	0.53	1 (2%) 54 50	39, 49, 63, 67	0
31	29	37/37 (100%)	0.71	3 (8%) 12 9	43, 55, 65, 70	0
32	1a	1488/1521 (97%)	-0.04	24 (1%) 72 69	41, 69, 92, 105	0
32	2a	1491/1521 (98%)	-0.22	27 (1%) 68 65	45, 72, 93, 104	0
33	1b	231/256 (90%)	-0.29	0 100 100	67, 82, 90, 96	0
33	2b	231/256 (90%)	-0.32	0 100 100	70, 84, 90, 96	0
34	1c	206/239 (86%)	0.09	2 (0%) 82 82	64, 76, 85, 95	0
34	2c	206/239 (86%)	1.35	58 (28%) 0 0	68, 79, 86, 95	0
35	1d	208/209 (99%)	0.09	2 (0%) 82 82	55, 70, 80, 86	0
35	2d	208/209 (99%)	0.83	25 (12%) 4 3	58, 71, 81, 86	0
36	1e	148/162 (91%)	0.09	0 100 100	58, 70, 79, 91	0
36	2e	148/162 (91%)	0.29	5 (3%) 45 42	61, 73, 82, 90	0
37	1f	100/101 (99%)	0.27	0 100 100	54, 66, 77, 83	0
37	2f	100/101 (99%)	-0.18	0 100 100	54, 68, 77, 83	0
38	1g	155/156 (99%)	0.85	20 (12%) 3 2	63, 73, 85, 97	0
38	2g	155/156 (99%)	1.04	24 (15%) 2 1	66, 75, 87, 98	0
39	1h	137/138 (99%)	0.12	0 100 100	61, 72, 79, 85	0
39	2h	137/138 (99%)	-0.05	2 (1%) 73 70	62, 75, 81, 86	0
40	1i	127/128 (99%)	-0.12	0 100 100	49, 75, 83, 92	0
40	2i	127/128 (99%)	0.46	9 (7%) 16 12	73, 84, 92, 96	0
41	1j	97/105 (92%)	-0.30	0 100 100	45, 75, 86, 93	0
41	2j	96/105 (91%)	0.60	13 (13%) 3 2	72, 85, 93, 98	0
42	1k	114/129 (88%)	1.01	10 (8%) 10 8	46, 68, 80, 86	0
42	2k	114/129 (88%)	0.37	4 (3%) 44 40	48, 70, 81, 89	0
43	1l	121/132 (91%)	0.48	3 (2%) 57 52	44, 58, 70, 74	0
43	2l	121/132 (91%)	1.03	16 (13%) 3 2	47, 61, 72, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.49	8 (6%) 19 16	51, 67, 77, 85	0
44	2m	122/126 (96%)	2.82	75 (61%) 0 0	70, 83, 88, 92	0
45	1n	60/61 (98%)	0.31	1 (1%) 70 67	50, 62, 73, 76	0
45	2n	60/61 (98%)	2.27	31 (51%) 0 0	75, 83, 90, 93	0
46	1o	88/89 (98%)	0.38	7 (7%) 12 10	50, 68, 79, 82	0
46	2o	88/89 (98%)	0.19	2 (2%) 60 55	53, 69, 80, 83	0
47	1p	82/88 (93%)	0.21	2 (2%) 59 54	58, 70, 77, 82	0
47	2p	82/88 (93%)	0.38	2 (2%) 59 54	57, 70, 78, 84	0
48	1q	99/105 (94%)	0.74	3 (3%) 50 46	59, 71, 79, 83	0
48	2q	99/105 (94%)	1.27	25 (25%) 0 0	59, 73, 80, 83	0
49	1r	68/88 (77%)	0.82	10 (14%) 2 1	52, 64, 78, 81	0
49	2r	68/88 (77%)	-0.06	0 100 100	60, 74, 83, 87	0
50	1s	83/93 (89%)	1.20	14 (16%) 1 1	66, 75, 83, 95	0
50	2s	83/93 (89%)	2.48	47 (56%) 0 0	70, 78, 85, 96	0
51	1t	96/106 (90%)	1.44	29 (30%) 0 0	57, 70, 82, 88	0
51	2t	96/106 (90%)	0.88	13 (13%) 3 2	59, 70, 83, 85	0
52	1u	23/27 (85%)	0.61	2 (8%) 10 8	64, 70, 77, 79	0
52	2u	23/27 (85%)	2.33	14 (60%) 0 0	68, 74, 78, 81	0
53	1v	14/27 (51%)	0.80	3 (21%) 1 1	51, 71, 93, 96	0
53	2v	13/27 (48%)	0.61	0 100 100	56, 68, 87, 96	0
54	1w	67/76 (88%)	2.48	34 (50%) 0 0	62, 87, 96, 105	0
54	1y	67/76 (88%)	1.60	21 (31%) 0 0	41, 93, 98, 100	0
54	2w	66/76 (86%)	2.61	37 (56%) 0 0	66, 88, 96, 99	0
54	2y	66/76 (86%)	1.55	24 (36%) 0 0	44, 94, 99, 100	0
55	1x	71/77 (92%)	0.90	8 (11%) 5 3	25, 59, 82, 92	0
55	2x	71/77 (92%)	0.72	6 (8%) 11 8	43, 79, 90, 94	0
All	All	20875/21754 (95%)	0.32	1282 (6%) 21 18	19, 62, 88, 106	0

All (1282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	1w	20	U	12.5
22	20	2	ALA	11.9

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Mol	Chain	Res	Type	RSRZ
38	1g	82	GLY	11.6
1	1A	885	C	11.4
22	10	7	LEU	10.9
22	20	3	HIS	10.5
1	1A	884	C	10.5
22	10	2	ALA	10.4
26	24	50	VAL	10.4
1	1A	896	A	9.9
22	10	6	GLY	9.5
7	2H	45	VAL	9.4
44	2m	123	ALA	9.2
22	20	7	LEU	9.2
22	10	5	LYS	9.0
21	2Z	155	LEU	8.9
38	2g	83	ALA	8.9
26	24	49	PHE	8.9
1	1A	883	G	8.8
1	2A	896	A	8.6
54	2w	76	A	8.4
38	1g	83	ALA	8.3
6	2G	48	GLU	8.3
22	10	3	HIS	8.1
44	2m	4	ILE	8.0
54	1w	73	A	8.0
54	1w	44	G	7.9
26	24	63	TYR	7.8
26	24	56	VAL	7.7
1	1A	887	A	7.6
38	2g	81	GLY	7.6
1	2A	888	C	7.6
32	1a	1030(B)	C	7.4
1	2A	1509	C	7.4
6	2G	139	LEU	7.4
50	2s	71	LEU	7.4
54	2w	75	C	7.3
44	2m	5	ALA	7.3
44	2m	124	PRO	7.3
32	1a	1030(D)	A	7.2
6	2G	2	PRO	7.2
21	2Z	141	VAL	7.2
50	2s	69	HIS	7.2
21	2Z	144	LEU	7.1

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Mol	Chain	Res	Type	RSRZ
44	2m	90	LEU	7.1
1	1A	888	C	7.1
26	24	40	HIS	7.0
21	1Z	1	MET	7.0
38	1g	85	TYR	7.0
22	20	5	LYS	7.0
26	24	45	GLY	6.9
45	2n	35	ARG	6.9
45	2n	34	TYR	6.9
45	2n	39	LEU	6.8
26	24	57	GLU	6.8
54	2w	71	G	6.8
6	2G	140	ILE	6.8
26	24	53	GLU	6.8
38	2g	82	GLY	6.8
43	2l	64	TYR	6.7
22	20	4	LYS	6.7
6	2G	152	LEU	6.7
1	2A	884	C	6.7
1	1A	897	C	6.6
54	1w	74	C	6.6
26	24	68	ARG	6.6
1	1A	1509	C	6.6
7	2H	49	VAL	6.6
26	24	51	ASP	6.5
32	2a	1030(B)	C	6.5
1	2A	883	G	6.5
6	1G	49	ASP	6.5
1	2A	885	C	6.5
38	1g	80	VAL	6.4
38	1g	81	GLY	6.4
21	2Z	170	THR	6.4
54	2w	73	A	6.3
21	1Z	149	SER	6.3
44	1m	124	PRO	6.3
50	2s	27	GLU	6.3
7	2H	44	VAL	6.2
6	2G	157	ILE	6.2
54	1w	72	C	6.2
1	1A	1078	U	6.2
29	27	48	LYS	6.2
26	24	59	PHE	6.2

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Mol	Chain	Res	Type	RSRZ
44	2m	102	ARG	6.1
54	1w	70	G	6.1
6	2G	62	LEU	6.1
34	2c	87	LEU	6.1
7	2H	6	ARG	6.1
1	2A	886	C	6.0
21	1Z	168	GLU	6.0
44	2m	92	HIS	6.0
44	2m	78	ILE	6.0
23	1l	2	SER	6.0
6	2G	144	ILE	6.0
6	2G	146	TYR	5.9
45	2n	25	VAL	5.9
1	2A	2155	G	5.9
55	1x	47	U	5.9
7	2H	51	ARG	5.9
21	2Z	140	ASP	5.9
54	1w	76	A	5.8
54	2w	1	G	5.8
54	1w	71	G	5.8
50	2s	35	SER	5.8
21	2Z	4	ARG	5.7
22	20	6	GLY	5.7
54	2w	44	G	5.7
7	2H	13	LYS	5.7
1	1A	1064	C	5.7
1	1A	882	G	5.7
44	2m	12	ASN	5.7
6	2G	149	VAL	5.6
22	10	4	LYS	5.6
3	1D	275	LYS	5.6
44	2m	60	VAL	5.6
1	1A	898	C	5.5
44	2m	23	TYR	5.5
1	2A	887	A	5.5
1	1A	886	C	5.4
23	2l	2	SER	5.4
44	2m	66	LEU	5.4
6	2G	34	LEU	5.4
32	1a	1030(A)	G	5.4
54	2w	70	G	5.4
54	2w	74	C	5.4

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Mol	Chain	Res	Type	RSRZ
3	1D	276	LYS	5.4
6	1G	146	TYR	5.4
50	2s	13	ASP	5.3
6	2G	28	VAL	5.3
54	2w	45	U	5.3
26	24	32	TYR	5.3
6	2G	135	LEU	5.3
32	1a	1030(C)	G	5.3
29	27	46	VAL	5.3
51	1t	47	GLY	5.3
32	2a	1034	G	5.3
44	2m	7	VAL	5.3
38	2g	85	TYR	5.3
1	1A	895	U	5.3
44	2m	94	ARG	5.2
6	2G	115	ARG	5.2
21	2Z	122	ARG	5.2
7	2H	72	ILE	5.2
21	2Z	153	SER	5.2
21	2Z	147	GLY	5.2
21	2Z	50	GLN	5.2
54	2w	72	C	5.2
6	2G	136	ARG	5.2
34	2c	155	GLY	5.1
6	2G	19	LEU	5.1
55	1x	67	C	5.1
26	24	19	GLY	5.1
54	2w	14	A	5.1
32	1a	1031	G	5.1
21	2Z	139	VAL	5.1
50	1s	60	VAL	5.1
26	24	42	PHE	5.1
54	1y	35	A	5.0
54	2w	13	C	5.0
52	2u	16	GLY	5.0
44	2m	57	ARG	5.0
1	1A	1066	U	5.0
38	1g	79	ARG	4.9
6	2G	3	LEU	4.9
21	2Z	137	ILE	4.9
7	2H	35	VAL	4.9
1	1A	1508	A	4.9

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Mol	Chain	Res	Type	RSRZ
1	2A	2154	G	4.9
45	2n	38	GLY	4.9
21	2Z	151	HIS	4.9
1	1A	1057	A	4.9
21	1Z	100	VAL	4.9
50	2s	15	LEU	4.9
44	2m	77	ASN	4.9
21	2Z	161	VAL	4.8
1	1A	1081	U	4.8
21	2Z	173	ALA	4.8
54	1y	36	A	4.8
35	2d	158	ILE	4.8
44	2m	6	GLY	4.8
32	2a	1036	G	4.8
44	2m	122	LYS	4.8
34	2c	51	GLY	4.8
20	2Y	1	MET	4.8
50	2s	14	HIS	4.8
21	2Z	106	GLY	4.8
34	2c	101	LEU	4.8
6	1G	48	GLU	4.8
32	2a	1030(A)	G	4.8
21	2Z	96	VAL	4.8
38	2g	84	ASN	4.7
21	2Z	156	LYS	4.7
32	1a	1030	C	4.7
34	2c	8	ILE	4.7
21	2Z	51	ALA	4.7
54	1w	75	C	4.7
45	2n	53	LEU	4.7
54	1y	47	U	4.7
21	1Z	104	PHE	4.7
21	2Z	53	ILE	4.7
44	2m	96	LEU	4.7
32	1a	1027	C	4.7
7	2H	115	VAL	4.7
42	2k	13	GLN	4.7
40	2i	115	GLY	4.7
51	1t	95	ALA	4.7
1	1A	1087	G	4.6
6	2G	133	LEU	4.6
21	1Z	122	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
52	2u	24	ARG	4.6
34	2c	91	LEU	4.6
54	1y	45	U	4.6
44	2m	65	LYS	4.6
44	2m	87	TYR	4.6
50	2s	47	HIS	4.6
3	2D	2	ALA	4.6
44	2m	120	LYS	4.6
6	2G	181	ARG	4.6
26	24	52	THR	4.6
21	2Z	48	PHE	4.6
50	2s	80	TYR	4.6
44	2m	84	ILE	4.5
6	2G	35	GLU	4.5
50	2s	24	ALA	4.5
44	2m	76	ALA	4.5
50	2s	81	ARG	4.5
52	2u	11	GLY	4.5
5	2F	21	ALA	4.5
6	2G	37	VAL	4.5
21	1Z	152	ALA	4.5
12	2Q	63	LYS	4.5
44	2m	71	ARG	4.4
50	2s	41	VAL	4.4
7	2H	46	GLU	4.4
54	2y	53	G	4.4
29	27	47	ARG	4.4
54	2y	36	A	4.4
21	1Z	151	HIS	4.4
26	24	43	TYR	4.4
6	2G	41	GLN	4.4
50	2s	62	ILE	4.4
21	1Z	66	SER	4.4
44	2m	88	ARG	4.4
45	2n	42	ILE	4.4
52	2u	17	THR	4.4
26	24	54	GLY	4.3
45	2n	54	PRO	4.3
21	2Z	150	LEU	4.3
1	2A	881	G	4.3
38	2g	154	TYR	4.3
1	1A	881	G	4.3

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Mol	Chain	Res	Type	RSRZ
1	1A	892	G	4.3
22	10	8	GLY	4.3
21	2Z	68	PRO	4.3
21	2Z	152	ALA	4.3
41	2j	88	LEU	4.3
34	2c	124	ILE	4.3
1	1A	1058	G	4.3
1	2A	882	G	4.3
54	2y	47	U	4.3
45	2n	12	ARG	4.2
20	2Y	106	LEU	4.2
44	2m	24	GLY	4.2
1	1A	1077	A	4.2
1	2A	890	A	4.2
38	1g	156	TRP	4.2
1	1A	1097	U	4.2
1	1A	894	C	4.2
1	1A	1059	G	4.2
43	2l	28	LYS	4.2
6	2G	178	PHE	4.2
21	2Z	121	HIS	4.2
50	2s	52	TYR	4.2
54	2y	22	G	4.2
21	2Z	102	LEU	4.2
48	2q	23	VAL	4.2
44	2m	75	ALA	4.2
19	2X	92	LEU	4.2
21	1Z	170	THR	4.2
3	2D	276	LYS	4.1
44	2m	72	ALA	4.1
7	2H	82	GLY	4.1
3	2D	38	LYS	4.1
51	2t	55	ILE	4.1
54	1y	24	G	4.1
42	2k	49	GLY	4.1
21	1Z	169	GLU	4.1
21	1Z	171	ILE	4.1
1	2A	899	A	4.1
51	1t	100	ILE	4.1
1	2A	2173	A	4.1
6	2G	80	PHE	4.1
6	2G	102	PHE	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	1G	139	LEU	4.1
1	1A	1082	U	4.1
6	2G	151	ALA	4.1
45	2n	31	ARG	4.0
26	24	18	CYS	4.0
51	1t	83	ARG	4.0
52	2u	6	ARG	4.0
21	2Z	146	ILE	4.0
54	2w	4	C	4.0
35	2d	152	SER	4.0
54	2y	52	G	4.0
44	2m	61	GLU	4.0
1	1A	1176	G	4.0
36	2e	17	ALA	4.0
6	2G	138	GLN	4.0
44	2m	101	GLN	4.0
1	2A	892	G	4.0
34	2c	185	GLY	4.0
54	2w	47	U	4.0
21	2Z	91	LEU	4.0
44	2m	56	LEU	4.0
50	2s	79	THR	4.0
34	2c	49	SER	4.0
7	2H	52	VAL	4.0
6	2G	113	ARG	3.9
44	2m	15	VAL	3.9
26	24	44	THR	3.9
41	2j	65	LEU	3.9
44	2m	67	GLU	3.9
26	24	67	TYR	3.9
38	1g	155	ARG	3.9
6	2G	141	PHE	3.9
1	1A	1076	C	3.9
54	2w	6	G	3.9
21	2Z	172	ALA	3.9
31	29	37	GLY	3.9
21	1Z	137	ILE	3.9
26	24	46	GLN	3.9
21	1Z	166	SER	3.9
32	2a	1030(C)	G	3.9
54	2w	15	G	3.9
21	2Z	148	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
54	2w	23	A	3.9
54	1y	20	U	3.8
54	1w	19	G	3.8
54	2w	69	G	3.8
38	2g	80	VAL	3.8
12	2Q	33	GLY	3.8
35	2d	110	PHE	3.8
44	1m	90	LEU	3.8
44	2m	42	ALA	3.8
1	2A	2166	G	3.8
54	1y	13	C	3.8
55	2x	47	U	3.8
44	2m	93	ARG	3.7
1	1A	1080	C	3.7
38	1g	84	ASN	3.7
21	2Z	1	MET	3.7
6	2G	161	THR	3.7
1	1A	889	C	3.7
54	2y	45	U	3.7
12	1Q	60	ARG	3.7
1	1A	1084	A	3.7
54	1w	15	G	3.7
6	2G	43	LEU	3.7
21	2Z	125	LEU	3.7
54	1y	23	A	3.7
51	1t	45	GLN	3.7
12	2Q	6	ARG	3.7
32	2a	1001(A)	G	3.7
6	1G	51	ARG	3.7
29	27	1	MET	3.7
6	2G	116	ASP	3.7
32	2a	1257	U	3.7
45	2n	10	ALA	3.7
34	2c	55	VAL	3.7
7	2H	2	SER	3.7
35	2d	166	LYS	3.7
50	1s	28	LYS	3.7
21	2Z	49	ARG	3.7
21	1Z	141	VAL	3.7
7	2H	8	PRO	3.7
6	2G	155	MET	3.7
12	2Q	5	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
45	2n	37	PHE	3.6
50	1s	15	LEU	3.6
35	2d	167	GLY	3.6
38	1g	154	TYR	3.6
44	2m	8	GLU	3.6
38	2g	32	ARG	3.6
1	1A	1095	A	3.6
21	1Z	161	VAL	3.6
34	2c	184	TYR	3.6
21	1Z	156	LYS	3.6
6	2G	42	GLY	3.6
1	2A	2165	G	3.6
54	1w	1	G	3.6
21	2Z	46	LYS	3.6
50	2s	16	LEU	3.6
1	2A	897	C	3.6
21	2Z	169	GLU	3.6
50	1s	27	GLU	3.6
12	2Q	60	ARG	3.6
21	2Z	71	VAL	3.6
26	24	13	ARG	3.6
50	2s	51	VAL	3.6
35	2d	180	GLY	3.6
1	2A	889	C	3.6
12	2Q	22	LYS	3.6
21	2Z	124	ILE	3.6
21	2Z	154	ASP	3.6
32	1a	1025	U	3.6
7	2H	138	LYS	3.6
26	24	58	ARG	3.6
34	2c	189	ALA	3.6
21	2Z	126	VAL	3.6
20	2Y	55	TYR	3.6
21	2Z	162	GLU	3.6
6	2G	134	GLY	3.6
38	1g	86	GLN	3.6
44	2m	80	ARG	3.6
54	1w	5	G	3.6
54	2w	10	G	3.6
44	2m	13	LYS	3.6
34	2c	196	LEU	3.6
44	2m	64	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
21	1Z	147	GLY	3.5
6	2G	137	GLU	3.5
50	2s	32	LYS	3.5
50	2s	38	SER	3.5
21	1Z	124	ILE	3.5
26	24	15	ILE	3.5
44	2m	97	PRO	3.5
50	2s	49	ILE	3.5
25	23	26	LEU	3.5
32	1a	1001(A)	G	3.5
29	27	45	ALA	3.5
6	2G	112	PRO	3.5
26	24	55	ARG	3.5
48	2q	77	VAL	3.5
42	1k	25	TYR	3.5
1	1A	1063	G	3.5
5	2F	15	SER	3.5
19	2X	68	ARG	3.5
54	1w	10	G	3.5
54	2y	35	A	3.5
21	1Z	139	VAL	3.5
1	1A	1065	U	3.5
50	2s	12	ASP	3.5
12	2Q	20	ALA	3.5
51	1t	38	LYS	3.5
52	2u	23	PRO	3.5
6	2G	39	ILE	3.5
35	2d	176	LEU	3.5
26	24	31	ILE	3.5
7	2H	105	LEU	3.5
51	1t	80	ARG	3.5
43	1l	64	TYR	3.5
5	2F	12	LEU	3.5
34	2c	182	ILE	3.5
54	1w	3	C	3.4
1	2A	880	G	3.4
1	2A	2127	G	3.4
54	2y	19	G	3.4
51	1t	55	ILE	3.4
35	2d	160	GLN	3.4
51	2t	9	ASN	3.4
49	1r	42	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
34	2c	198	VAL	3.4
44	2m	70	LEU	3.4
6	2G	12	TYR	3.4
1	1A	1075	C	3.4
7	2H	7	LEU	3.4
21	2Z	104	PHE	3.4
34	2c	22	TRP	3.4
54	2y	59	U	3.4
6	2G	7	LEU	3.4
21	2Z	57	ILE	3.4
22	20	8	GLY	3.4
1	1A	899	A	3.4
1	2A	2153	G	3.4
26	24	35	VAL	3.4
26	14	54	GLY	3.4
48	2q	65	ILE	3.4
1	2A	2159	G	3.4
40	2i	124	GLN	3.4
21	1Z	138	GLU	3.4
48	2q	84	LEU	3.4
50	2s	84	GLY	3.4
12	2Q	104	PHE	3.3
54	1w	57	G	3.3
26	14	51	ASP	3.3
54	1w	45	U	3.3
7	2H	37	VAL	3.3
21	2Z	128	VAL	3.3
44	2m	54	VAL	3.3
1	2A	2116	G	3.3
1	2A	2157	G	3.3
6	2G	169	ALA	3.3
12	1Q	61	GLY	3.3
35	1d	167	GLY	3.3
6	2G	159	VAL	3.3
7	2H	19	VAL	3.3
38	2g	147	ALA	3.3
44	2m	68	GLY	3.3
54	1y	12	U	3.3
7	2H	41	MET	3.3
54	2w	19	G	3.3
54	2w	49	C	3.3
5	1F	15	SER	3.3

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Mol	Chain	Res	Type	RSRZ
49	1r	85	LEU	3.3
32	1a	1003	G	3.3
6	2G	179	PRO	3.3
36	2e	12	LEU	3.3
54	1w	13	C	3.3
7	2H	43	VAL	3.3
21	2Z	56	VAL	3.3
21	2Z	149	SER	3.3
40	2i	36	TYR	3.3
43	2l	39	VAL	3.3
43	2l	95	GLY	3.3
44	2m	73	GLU	3.3
1	2A	2131	G	3.3
21	2Z	24	LEU	3.3
45	2n	7	ILE	3.2
7	2H	47	GLU	3.2
6	2G	156	ASP	3.2
7	2H	36	PRO	3.2
50	2s	45	VAL	3.2
1	2A	2174	C	3.2
20	2Y	75	ILE	3.2
6	2G	29	TRP	3.2
21	2Z	99	TYR	3.2
32	2a	1030	C	3.2
48	2q	90	ILE	3.2
21	1Z	148	ASP	3.2
45	2n	50	LYS	3.2
21	2Z	55	HIS	3.2
1	1A	879	G	3.2
1	2A	2156	G	3.2
29	27	23	ARG	3.2
43	2l	69	TYR	3.2
5	2F	145	GLU	3.2
21	2Z	163	LEU	3.2
50	2s	48	THR	3.2
21	2Z	157	LEU	3.2
35	2d	188	LEU	3.2
50	2s	30	LEU	3.2
29	17	48	LYS	3.2
38	2g	115	ARG	3.2
1	2A	1719	G	3.2
1	2A	2125	G	3.2

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Mol	Chain	Res	Type	RSRZ
38	1g	153	HIS	3.1
1	2A	2167	U	3.1
32	1a	1029	C	3.1
12	1Q	79	LEU	3.1
35	2d	157	LEU	3.1
44	2m	48	LEU	3.1
44	2m	110	ARG	3.1
6	2G	15	VAL	3.1
6	2G	109	VAL	3.1
32	1a	1257	U	3.1
40	2i	109	VAL	3.1
34	2c	80	GLY	3.1
38	2g	119	ARG	3.1
20	2Y	91	GLU	3.1
51	1t	68	LYS	3.1
12	1Q	81	VAL	3.1
1	1A	271(K)	U	3.1
6	2G	51	ARG	3.1
45	2n	29	ARG	3.1
6	2G	114	ILE	3.1
7	2H	10	PRO	3.1
21	2Z	93	ASP	3.1
7	2H	123	PHE	3.1
34	2c	45	LYS	3.1
52	2u	22	ARG	3.1
50	2s	53	ASN	3.1
7	2H	9	ILE	3.1
36	2e	13	ILE	3.1
54	2w	5	G	3.1
6	2G	95	ARG	3.1
51	2t	86	ARG	3.1
34	2c	199	LYS	3.1
50	2s	28	LYS	3.1
48	2q	11	VAL	3.1
34	2c	65	ALA	3.1
21	2Z	95	PRO	3.1
21	2Z	133	ILE	3.1
1	1A	1060	U	3.1
21	2Z	145	GLU	3.1
32	1a	204	U	3.1
6	1G	76	SER	3.1
12	2Q	2	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
34	2c	50	ALA	3.1
44	2m	25	ILE	3.1
7	2H	159	GLU	3.1
21	2Z	138	GLU	3.1
51	1t	42	GLN	3.1
21	2Z	143	GLY	3.0
5	2F	20	LEU	3.0
7	2H	30	LYS	3.0
12	1Q	112	GLU	3.0
12	2Q	66	ILE	3.0
44	2m	39	ILE	3.0
54	1w	2	C	3.0
54	2w	2	C	3.0
54	2y	23	A	3.0
50	1s	18	LYS	3.0
10	2O	49	ARG	3.0
48	2q	22	LEU	3.0
47	1p	38	TYR	3.0
48	2q	42	TYR	3.0
32	2a	1035	A	3.0
54	1y	21	A	3.0
44	2m	19	LEU	3.0
1	2A	2133	G	3.0
32	2a	1033	G	3.0
51	1t	74	LYS	3.0
54	1w	69	G	3.0
51	1t	86	ARG	3.0
44	2m	74	VAL	3.0
6	2G	173	LEU	3.0
51	2t	13	LEU	3.0
54	1w	21	A	3.0
5	2F	131	GLY	3.0
6	2G	182	LYS	3.0
34	2c	158	GLY	3.0
21	2Z	59	LEU	3.0
21	2Z	70	LEU	3.0
49	1r	76	LEU	3.0
12	2Q	121	ALA	3.0
1	1A	878	A	3.0
54	2w	9	A	3.0
6	2G	58	GLN	3.0
7	2H	25	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
6	2G	176	LEU	3.0
21	1Z	39	VAL	3.0
6	2G	6	ALA	3.0
7	2H	48	GLY	3.0
50	2s	82	GLY	3.0
54	1w	25	C	3.0
1	1A	1175	U	3.0
7	2H	3	ARG	3.0
34	2c	186	PHE	3.0
44	2m	63	THR	3.0
51	1t	72	LEU	3.0
1	2A	1744	C	2.9
34	2c	57	ILE	2.9
21	1Z	121	HIS	2.9
12	1Q	59	ARG	2.9
34	2c	190	ARG	2.9
26	14	52	THR	2.9
32	1a	1032	G	2.9
54	2w	22	G	2.9
6	2G	90	LEU	2.9
36	2e	10	MET	2.9
38	1g	78	ARG	2.9
45	2n	11	LYS	2.9
54	1y	14	A	2.9
48	2q	71	PHE	2.9
1	2A	898	C	2.9
34	2c	193	TYR	2.9
52	2u	21	TYR	2.9
12	2Q	106	VAL	2.9
26	14	50	VAL	2.9
21	2Z	167	PRO	2.9
6	2G	59	GLU	2.9
50	2s	67	VAL	2.9
7	2H	128	PRO	2.9
32	1a	1002	G	2.9
1	2A	2158	A	2.9
46	1o	89	GLY	2.9
48	2q	66	SER	2.9
54	2w	21	A	2.9
21	2Z	9	TYR	2.9
40	2i	125	TYR	2.9
45	2n	30	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
38	2g	156	TRP	2.9
54	1w	4	C	2.9
7	2H	23	ARG	2.9
34	2c	13	GLY	2.9
50	2s	54	GLY	2.9
1	2A	2160	G	2.9
55	2x	46	G	2.9
7	2H	50	VAL	2.9
21	2Z	38	TYR	2.9
44	2m	17	VAL	2.9
50	2s	66	MET	2.9
12	2Q	59	ARG	2.9
38	2g	79	ARG	2.9
44	2m	9	ILE	2.9
21	1Z	136	PHE	2.9
20	2Y	63	LYS	2.9
34	2c	64	VAL	2.9
41	2j	44	VAL	2.9
52	2u	10	ARG	2.9
1	1A	1096	A	2.8
54	2y	64	A	2.8
48	2q	80	GLY	2.8
44	2m	82	MET	2.8
45	2n	27	CYS	2.8
50	2s	65	ASN	2.8
1	2A	2128	C	2.8
1	2A	2146	C	2.8
21	1Z	140	ASP	2.8
55	1x	66	C	2.8
21	1Z	165	VAL	2.8
34	2c	72	LYS	2.8
38	2g	109	ASN	2.8
6	2G	11	TYR	2.8
1	2A	2132	U	2.8
48	2q	92	ARG	2.8
1	2A	1508	A	2.8
1	2A	2126	A	2.8
1	2A	2793	G	2.8
44	2m	106	ASN	2.8
42	2k	94	ALA	2.8
54	2w	68	C	2.8
6	2G	100	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
7	2H	4	ILE	2.8
3	2D	37	LEU	2.8
12	2Q	136	ALA	2.8
32	1a	1036	G	2.8
32	1a	1531	A	2.8
54	2w	58	A	2.8
12	1Q	5	ARG	2.8
12	1Q	10	ARG	2.8
46	1o	68	ARG	2.8
9	2N	8	GLN	2.8
23	11	98	LEU	2.8
6	2G	177	GLY	2.8
12	2Q	61	GLY	2.8
43	2l	68	ALA	2.8
54	1y	27	G	2.8
54	2y	65	G	2.8
6	2G	175	LEU	2.8
26	24	9	LEU	2.8
45	2n	36	PHE	2.8
20	2Y	89	PHE	2.8
21	1Z	102	LEU	2.8
21	1Z	155	LEU	2.8
54	1w	6	G	2.8
6	1G	75	LYS	2.8
6	1G	182	LYS	2.8
41	2j	10	GLY	2.8
6	2G	118	ARG	2.8
43	2l	59	ARG	2.8
10	2O	51	ALA	2.7
6	1G	77	ILE	2.7
6	2G	154	GLY	2.7
49	1r	79	LEU	2.7
6	2G	22	ARG	2.7
41	2j	66	ARG	2.7
1	1A	1069	A	2.7
7	2H	86	GLU	2.7
32	2a	1021	G	2.7
54	1w	56	C	2.7
43	2l	40	VAL	2.7
50	2s	58	VAL	2.7
48	2q	100	LYS	2.7
12	2Q	64	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
6	2G	145	THR	2.7
50	2s	77	THR	2.7
7	2H	24	VAL	2.7
26	24	34	GLU	2.7
3	2D	4	LYS	2.7
41	2j	48	THR	2.7
7	2H	169	VAL	2.7
50	1s	21	GLU	2.7
54	2w	48	C	2.7
6	2G	23	PHE	2.7
25	23	23	LEU	2.7
45	2n	6	LEU	2.7
52	2u	14	TRP	2.7
6	2G	142	PRO	2.7
43	2l	56	ALA	2.7
6	2G	148	MET	2.7
12	2Q	19	GLY	2.7
26	14	45	GLY	2.7
50	2s	44	MET	2.7
21	2Z	171	ILE	2.7
32	2a	1224	G	2.7
28	16	28	ARG	2.7
50	2s	29	ARG	2.7
12	2Q	109	VAL	2.7
34	2c	194	GLY	2.7
38	1g	89	MET	2.7
21	1Z	125	LEU	2.7
21	2Z	89	PHE	2.7
40	2i	19	LEU	2.7
1	2A	1536	C	2.7
54	2w	3	C	2.7
54	1y	38	A	2.7
45	2n	51	GLY	2.7
1	1A	1068	G	2.7
1	2A	879	G	2.7
6	2G	60	LEU	2.7
6	1G	80	PHE	2.7
12	2Q	32	TYR	2.7
21	1Z	146	ILE	2.7
26	14	55	ARG	2.7
26	14	68	ARG	2.7
43	2l	7	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
44	2m	104	ARG	2.7
45	2n	17	LYS	2.7
41	2j	91	PRO	2.6
32	2a	1358	U	2.6
34	2c	53	ALA	2.6
1	2A	229	A	2.6
17	2V	35	LEU	2.6
49	1r	78	LEU	2.6
21	2Z	88	PHE	2.6
26	24	23	GLU	2.6
6	1G	73	ALA	2.6
25	23	51	ALA	2.6
54	2y	12	U	2.6
3	2D	275	LYS	2.6
21	2Z	76	LEU	2.6
1	2A	1507	A	2.6
54	2w	24	G	2.6
50	1s	58	VAL	2.6
1	2A	2161	C	2.6
1	2A	1847	A	2.6
21	1Z	120	ILE	2.6
34	2c	39	ILE	2.6
44	2m	95	GLY	2.6
44	2m	103	THR	2.6
38	1g	141	VAL	2.6
54	2y	6	G	2.6
12	1Q	1	MET	2.6
48	2q	74	LEU	2.6
50	1s	71	LEU	2.6
7	2H	57	ASP	2.6
48	2q	59	ILE	2.6
50	2s	43	GLU	2.6
7	2H	29	PRO	2.6
10	2O	7	TYR	2.6
12	1Q	32	TYR	2.6
34	2c	60	ALA	2.6
1	1A	890	A	2.6
21	2Z	5	LEU	2.6
44	2m	11	ARG	2.6
47	1p	19	ILE	2.6
54	1w	48	C	2.6
55	1x	68	C	2.6

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Mol	Chain	Res	Type	RSRZ
35	2d	170	VAL	2.6
46	2o	60	VAL	2.6
49	1r	40	LEU	2.6
54	2w	26	A	2.6
12	2Q	65	PHE	2.6
38	2g	77	SER	2.6
32	1a	1023	G	2.6
44	2m	91	ARG	2.6
54	1w	47	U	2.6
21	2Z	62	PRO	2.6
43	2l	94	PRO	2.6
34	2c	149	ALA	2.6
42	1k	61	ALA	2.6
50	2s	34	TRP	2.6
44	2m	111	LYS	2.6
35	2d	196	LEU	2.6
48	2q	58	GLU	2.6
21	2Z	44	PHE	2.6
1	1A	1847	A	2.6
21	2Z	101	PRO	2.5
12	2Q	53	ALA	2.5
42	1k	64	ALA	2.5
45	2n	46	GLU	2.5
54	2y	57	G	2.5
5	2F	196	LEU	2.5
12	1Q	2	LEU	2.5
42	1k	14	VAL	2.5
1	2A	2164	C	2.5
32	1a	1028	C	2.5
21	2Z	80	ARG	2.5
44	1m	2	ALA	2.5
44	2m	69	GLU	2.5
1	2A	2802	G	2.5
12	2Q	10	ARG	2.5
32	2a	1309	G	2.5
54	1y	34	G	2.5
46	2o	87	ILE	2.5
21	1Z	150	LEU	2.5
32	2a	1286	A	2.5
34	2c	23	TYR	2.5
34	2c	52	LEU	2.5
44	2m	121	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
46	1o	78	TYR	2.5
12	2Q	29	PHE	2.5
54	2y	56	C	2.5
7	2H	121	ILE	2.5
34	2c	200	ALA	2.5
50	2s	40	ILE	2.5
34	2c	21	ARG	2.5
44	2m	100	GLY	2.5
6	2G	131	TYR	2.5
34	1c	87	LEU	2.5
1	2A	878	A	2.5
38	2g	152	ALA	2.5
48	2q	60	ILE	2.5
55	2x	70	G	2.5
5	2F	140	LEU	2.5
21	1Z	163	LEU	2.5
51	1t	53	LEU	2.5
16	2U	90	VAL	2.5
1	1A	1963	U	2.5
6	2G	117	PHE	2.5
21	2Z	136	PHE	2.5
6	2G	121	ASN	2.5
21	1Z	123	ASP	2.5
12	2Q	28	ALA	2.5
26	24	5	ILE	2.5
51	1t	52	ALA	2.5
7	1H	7	LEU	2.5
32	2a	1325	C	2.5
19	2X	69	TYR	2.5
32	2a	1003	G	2.5
35	2d	20	TYR	2.5
44	2m	10	PRO	2.5
21	1Z	157	LEU	2.5
54	2y	21	A	2.5
50	1s	32	LYS	2.5
12	1Q	55	VAL	2.5
48	1q	11	VAL	2.5
41	2j	47	PHE	2.5
54	1y	56	C	2.5
1	1A	1094	U	2.4
26	14	53	GLU	2.4
44	2m	119	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
21	2Z	21	ALA	2.4
50	1s	48	THR	2.4
21	1Z	18	LEU	2.4
21	1Z	61	LEU	2.4
21	1Z	133	ILE	2.4
51	2t	62	LEU	2.4
51	2t	100	ILE	2.4
35	2d	115	ARG	2.4
5	1F	16	GLY	2.4
1	1A	1074	G	2.4
1	1A	2131	G	2.4
1	2A	2124	G	2.4
34	2c	187	ALA	2.4
54	1w	24	G	2.4
54	1y	22	G	2.4
54	1y	44	G	2.4
54	2y	5	G	2.4
54	2y	44	G	2.4
43	2l	60	LEU	2.4
46	1o	87	ILE	2.4
21	2Z	60	GLU	2.4
42	1k	92	GLU	2.4
1	2A	894	C	2.4
32	2a	1029	C	2.4
21	1Z	70	LEU	2.4
35	2d	174	LEU	2.4
45	2n	58	LYS	2.4
50	1s	61	TYR	2.4
34	2c	59	ARG	2.4
52	1u	6	ARG	2.4
53	1v	13	A	2.4
21	2Z	33	LEU	2.4
5	2F	172	TRP	2.4
6	2G	180	PHE	2.4
1	1A	1093	G	2.4
32	1a	1026	G	2.4
55	1x	70	G	2.4
36	2e	107	ARG	2.4
6	2G	106	LEU	2.4
45	1n	2	ALA	2.4
50	2s	63	THR	2.4
43	2l	100	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
51	2t	42	GLN	2.4
1	2A	1041	C	2.4
34	2c	74	GLY	2.4
38	2g	135	VAL	2.4
5	1F	14	PRO	2.4
38	2g	117	ALA	2.4
50	1s	30	LEU	2.4
54	2y	34	G	2.4
16	2U	88	ILE	2.4
35	2d	146	ILE	2.4
50	2s	23	ASN	2.4
52	2u	13	ILE	2.4
18	2W	112	GLY	2.4
38	2g	130	GLY	2.4
27	15	60	VAL	2.4
1	1A	1070	A	2.4
53	1v	14	A	2.4
1	2A	1040	C	2.4
26	24	41	PRO	2.4
40	2i	123	PRO	2.4
5	1F	21	ALA	2.4
20	2Y	90	LEU	2.4
21	1Z	69	THR	2.4
38	2g	116	ALA	2.4
44	2m	105	THR	2.4
32	1a	1024	G	2.4
54	1y	5	G	2.4
21	2Z	79	ARG	2.4
51	2t	80	ARG	2.4
1	2A	2169	A	2.3
38	1g	73	MET	2.3
34	2c	160	ALA	2.3
21	2Z	11	GLU	2.3
10	2O	52	VAL	2.3
6	1G	86	MET	2.3
45	2n	49	HIS	2.3
54	2y	51	U	2.3
6	2G	97	ASP	2.3
1	1A	893	C	2.3
7	2H	14	GLY	2.3
21	2Z	66	SER	2.3
48	2q	6	LEU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
42	1k	49	GLY	2.3
50	1s	84	GLY	2.3
54	1w	7	A	2.3
54	2w	61	C	2.3
54	2y	62	C	2.3
51	2t	83	ARG	2.3
51	1t	63	ILE	2.3
6	2G	92	VAL	2.3
26	14	59	PHE	2.3
31	29	16	VAL	2.3
21	1Z	99	TYR	2.3
34	2c	85	ARG	2.3
1	1A	2140	C	2.3
50	1s	40	ILE	2.3
54	1y	49	C	2.3
31	19	7	VAL	2.3
42	1k	42	TRP	2.3
26	24	29	PRO	2.3
52	2u	5	ASP	2.3
35	2d	130	GLY	2.3
44	2m	108	ARG	2.3
50	2s	20	LEU	2.3
21	2Z	69	THR	2.3
1	1A	2113	U	2.3
32	2a	1220	G	2.3
41	2j	50	ILE	2.3
7	2H	32	GLU	2.3
54	1w	23	A	2.3
12	2Q	56	ARG	2.3
26	24	48	ARG	2.3
44	2m	3	ARG	2.3
17	1V	101	GLY	2.3
12	2Q	37	LEU	2.3
38	2g	86	GLN	2.3
45	2n	13	THR	2.3
51	1t	32	ALA	2.3
52	2u	12	LYS	2.3
6	2G	88	ILE	2.3
34	2c	14	ILE	2.3
5	2F	132	VAL	2.3
19	2X	66	LEU	2.3
51	1t	36	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
51	2t	99	LEU	2.3
54	2w	31	A	2.3
7	2H	34	GLU	2.3
12	2Q	47	ILE	2.3
11	2P	125	VAL	2.3
21	2Z	72	ARG	2.3
42	1k	96	ARG	2.3
6	2G	49	ASP	2.3
51	1t	69	GLY	2.3
12	2Q	113	GLN	2.3
44	2m	51	ALA	2.3
55	2x	71	C	2.3
7	2H	18	GLU	2.3
42	1k	50	TYR	2.3
53	1v	12	A	2.3
35	2d	141	ARG	2.3
48	2q	27	PHE	2.3
6	1G	149	VAL	2.3
26	24	7	PRO	2.2
47	2p	48	TRP	2.2
12	2Q	112	GLU	2.2
44	2m	107	ALA	2.2
1	1A	1100	C	2.2
21	2Z	8	TYR	2.2
22	20	11	ARG	2.2
35	2d	184	LYS	2.2
40	2i	127	LYS	2.2
51	1t	79	ARG	2.2
6	2G	125	PHE	2.2
21	1Z	126	VAL	2.2
32	2a	1227	A	2.2
50	2s	11	VAL	2.2
50	2s	56	GLN	2.2
5	2F	199	TRP	2.2
51	1t	98	PRO	2.2
54	1w	12	U	2.2
17	2V	1	MET	2.2
35	2d	49	ARG	2.2
12	1Q	33	GLY	2.2
20	2Y	59	GLY	2.2
34	2c	159	GLY	2.2
1	1A	2793	G	2.2

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Mol	Chain	Res	Type	RSRZ
39	2h	134	ILE	2.2
32	1a	161	A	2.2
35	2d	186	LEU	2.2
43	1l	60	LEU	2.2
44	1m	96	LEU	2.2
44	1m	121	LYS	2.2
51	1t	84	LEU	2.2
49	1r	54	ARG	2.2
26	24	60	GLN	2.2
41	2j	63	PHE	2.2
48	2q	9	VAL	2.2
51	2t	41	ILE	2.2
6	2G	67	LYS	2.2
1	1A	1079	C	2.2
21	1Z	52	SER	2.2
55	1x	69	C	2.2
4	2E	52	LEU	2.2
6	2G	120	LEU	2.2
50	2s	78	ARG	2.2
10	2O	41	ALA	2.2
32	2a	1030(D)	A	2.2
26	14	32	TYR	2.2
10	2O	86	ILE	2.2
20	2Y	45	VAL	2.2
46	1o	82	ILE	2.2
10	2O	48	PRO	2.2
21	1Z	159	PRO	2.2
54	1y	48	C	2.2
54	2w	56	C	2.2
3	1D	2	ALA	2.2
1	2A	2308	G	2.2
3	2D	5	LYS	2.2
34	2c	19	GLU	2.2
55	1x	46	G	2.2
43	2l	32	PHE	2.2
7	2H	69	ARG	2.2
7	2H	107	VAL	2.2
21	2Z	131	ARG	2.2
34	2c	40	ARG	2.2
46	1o	88	ARG	2.2
48	1q	63	ARG	2.2
34	2c	188	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
49	1r	44	LEU	2.2
20	2Y	57	GLN	2.2
6	1G	46	ALA	2.2
34	2c	61	ALA	2.2
49	1r	24	ALA	2.2
5	1F	17	ARG	2.2
1	2A	2162	G	2.2
32	1a	1033	G	2.2
32	2a	1310	G	2.2
34	2c	201	TYR	2.2
41	2j	72	VAL	2.2
51	1t	75	ASN	2.2
35	1d	157	LEU	2.2
41	2j	55	LYS	2.2
54	2w	7	A	2.2
14	2S	32	LEU	2.2
6	2G	170	ARG	2.2
51	2t	8	ARG	2.2
54	1y	67	C	2.2
54	2w	11	C	2.2
42	2k	25	TYR	2.1
10	2O	19	ILE	2.1
20	2Y	24	VAL	2.1
1	2A	2115	G	2.1
6	2G	32	PRO	2.1
6	2G	33	ARG	2.1
43	2l	61	THR	2.1
24	22	37	PHE	2.1
32	2a	1322	C	2.1
1	1A	1083	U	2.1
21	1Z	128	VAL	2.1
38	1g	42	ILE	2.1
38	2g	120	ILE	2.1
48	1q	59	ILE	2.1
50	2s	60	VAL	2.1
6	1G	90	LEU	2.1
46	1o	57	LEU	2.1
38	2g	78	ARG	2.1
51	2t	77	ALA	2.1
38	1g	144	MET	2.1
26	24	10	VAL	2.1
8	2I	38	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
39	2h	83	ILE	2.1
54	1w	68	C	2.1
51	1t	81	LYS	2.1
5	2F	127	GLU	2.1
35	2d	165	MET	2.1
21	2Z	81	ARG	2.1
21	2Z	100	VAL	2.1
34	1c	190	ARG	2.1
34	2c	17	ASP	2.1
44	1m	122	LYS	2.1
44	2m	99	ARG	2.1
48	2q	19	VAL	2.1
34	2c	82	GLU	2.1
45	2n	2	ALA	2.1
7	2H	74	ASN	2.1
44	2m	62	ASN	2.1
44	2m	27	LYS	2.1
6	2G	4	ASP	2.1
31	29	12	ASP	2.1
7	2H	76	VAL	2.1
7	2H	133	VAL	2.1
17	1V	35	LEU	2.1
21	1Z	53	ILE	2.1
34	2c	43	LEU	2.1
34	2c	204	LEU	2.1
45	2n	44	LEU	2.1
35	2d	179	GLU	2.1
38	1g	151	TYR	2.1
1	2A	900	A	2.1
54	1w	58	A	2.1
54	2y	15	G	2.1
1	2A	2175	C	2.1
49	1r	25	THR	2.1
51	1t	58	LYS	2.1
52	1u	14	TRP	2.1
52	2u	4	GLY	2.1
7	2H	71	LEU	2.1
34	2c	44	GLU	2.1
41	2j	68	HIS	2.1
42	1k	63	LEU	2.1
12	2Q	68	ILE	2.1
21	1Z	167	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
44	1m	87	TYR	2.1
1	2A	2117	A	2.1
7	2H	165	ALA	2.1
32	2a	161	A	2.1
7	2H	54	ARG	2.1
26	24	24	THR	2.1
1	1A	2138	C	2.1
34	2c	56	ASP	2.1
7	2H	67	LEU	2.1
35	2d	120	LEU	2.1
43	2l	85	ILE	2.1
51	1t	49	ALA	2.1
51	1t	89	ARG	2.1
21	2Z	166	SER	2.1
1	1A	1067	A	2.1
1	1A	1088	A	2.1
6	1G	102	PHE	2.1
32	2a	250	A	2.1
32	2a	1001	A	2.1
45	2n	15	LYS	2.0
48	2q	89	LEU	2.0
43	1l	43	VAL	2.0
51	1t	90	GLN	2.0
55	1x	65	C	2.0
55	2x	68	C	2.0
6	2G	150	ASP	2.0
21	2Z	52	SER	2.0
34	2c	78	GLY	2.0
35	2d	2	GLY	2.0
40	2i	116	LYS	2.0
50	2s	6	LYS	2.0
1	2A	2114	A	2.0
1	1A	652(U)	G	2.0
10	2O	98	VAL	2.0
32	2a	1221	G	2.0
45	2n	33	VAL	2.0
7	2H	101	ARG	2.0
10	2O	22	ILE	2.0
54	1w	61	C	2.0
54	2y	49	C	2.0
6	2G	61	ALA	2.0
6	2G	73	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
15	1T	126	ALA	2.0
21	2Z	26	GLY	2.0
34	2c	28	GLN	2.0
44	1m	82	MET	2.0
51	1t	13	LEU	2.0
7	2H	124	GLU	2.0
23	11	26	ARG	2.0
32	1a	190	U	2.0
45	2n	45	ARG	2.0
48	2q	24	GLU	2.0
48	2q	73	VAL	2.0
38	1g	120	ILE	2.0
7	2H	157	TYR	2.0
1	1A	2145	C	2.0
18	1W	112	GLY	2.0
21	2Z	164	ALA	2.0
48	2q	95	TYR	2.0
55	2x	2	G	2.0
38	2g	123	GLU	2.0
47	2p	51	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	PSU	2y	55	20/21	0.55	0.38	83,99,115,129	0
54	5MU	2y	54	21/22	0.63	0.42	87,93,116,137	0
54	PSU	1y	55	20/21	0.73	0.19	82,98,110,129	0
54	4SU	2y	8	20/21	0.78	0.24	87,95,107,114	0
54	MIA	2y	37	22/30	0.80	0.25	68,80,89,112	0
54	5MU	1y	54	21/22	0.82	0.25	80,93,103,130	0
54	7MG	1y	46	24/25	0.83	0.32	81,93,105,133	0
54	7MG	2y	46	24/25	0.83	0.28	82,95,104,125	0
54	4SU	1y	8	20/21	0.84	0.23	84,90,107,112	0
54	PSU	2y	39	20/21	0.85	0.26	75,87,93,93	0
54	7MG	1w	46	24/25	0.86	0.24	71,81,95,125	0
54	PSU	2y	32	20/21	0.87	0.18	79,88,94,98	0
54	7MG	2w	46	24/25	0.87	0.38	69,93,102,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	4SU	2w	8	20/21	0.87	0.28	64,91,96,98	0
32	M2G	2a	966	25/26	0.88	0.19	45,64,88,101	0
54	MIA	2w	37	22/30	0.89	0.21	49,73,85,86	0
55	4SU	2x	8	20/21	0.89	0.19	66,80,86,89	0
54	PSU	2w	55	20/21	0.89	0.29	57,80,90,92	0
54	MIA	1y	37	22/30	0.90	0.25	74,81,87,100	0
32	2MG	2a	1207	24/25	0.90	0.20	72,87,94,98	0
54	PSU	2w	32	20/21	0.91	0.25	63,79,90,93	0
32	5MC	2a	967	21/22	0.91	0.17	60,75,80,91	0
54	PSU	1y	39	20/21	0.92	0.29	73,85,90,93	0
54	5MU	2w	54	21/22	0.92	0.20	60,71,83,85	0
55	5MU	2x	54	21/22	0.92	0.22	69,81,87,96	0
43	0TD	2l	92	10/11	0.92	0.22	50,61,67,77	0
54	PSU	1w	55	20/21	0.92	0.24	55,77,90,90	0
54	4SU	1w	8	20/21	0.92	0.20	70,77,91,94	0
43	0TD	1l	92	10/11	0.92	0.21	44,58,62,69	0
54	PSU	1y	32	20/21	0.92	0.23	75,86,94,98	0
55	PSU	2x	55	20/21	0.92	0.18	63,78,85,86	0
32	4OC	2a	1402	22/23	0.94	0.15	49,66,75,76	0
54	PSU	2w	39	20/21	0.94	0.25	63,72,81,83	0
32	MA6	2a	1519	24/25	0.94	0.19	45,65,75,82	0
32	PSU	2a	516	20/21	0.94	0.13	56,64,70,74	0
32	7MG	2a	527	24/25	0.94	0.15	53,64,78,82	0
32	MA6	2a	1518	24/25	0.95	0.23	53,67,73,75	0
32	5MC	2a	1404	21/22	0.95	0.18	52,59,71,74	0
1	5MU	2A	1915	21/22	0.95	0.19	56,63,68,75	0
55	5MC	2x	32	21/22	0.95	0.18	66,71,79,82	0
55	5MU	1x	54	21/22	0.95	0.20	52,64,69,72	0
1	4OC	2A	1920	21/23	0.95	0.21	45,51,56,64	0
1	5MU	1A	1915	21/22	0.95	0.19	50,58,65,70	0
55	M3O	2x	76	32/33	0.95	0.27	42,53,66,68	10
54	PSU	1w	32	20/21	0.96	0.17	59,74,84,92	0
54	PSU	1w	39	20/21	0.96	0.21	58,68,76,78	0
32	5MC	2a	1400	21/22	0.96	0.17	61,72,78,82	0
32	2MG	1a	1207	24/25	0.96	0.16	48,66,70,78	0
54	5MU	1w	54	21/22	0.96	0.26	51,64,74,75	0
55	PSU	1x	55	20/21	0.96	0.19	51,62,74,75	0
32	5MC	2a	1407	21/22	0.96	0.17	36,55,59,60	0
55	M3O	1x	76	32/33	0.96	0.29	21,43,53,57	10
32	UR3	2a	1498	21/22	0.96	0.20	41,54,63,70	0
55	4SU	1x	8	20/21	0.96	0.19	43,54,68,74	0
32	PSU	1a	516	20/21	0.96	0.16	53,61,67,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MC	2A	1962	21/22	0.96	0.17	34,40,48,53	0
1	PSU	2A	1911	20/21	0.96	0.16	40,51,56,58	0
54	MIA	1w	37	29/30	0.97	0.22	44,56,67,77	0
32	5MC	1a	1404	21/22	0.97	0.20	23,37,50,52	0
1	PSU	1A	1917	20/21	0.97	0.22	47,53,60,62	0
55	5MC	1x	32	21/22	0.97	0.20	35,48,56,75	0
1	PSU	1A	1911	20/21	0.97	0.20	41,47,54,55	0
1	5MC	1A	1942	21/22	0.97	0.21	38,47,55,63	0
32	4OC	1a	1402	22/23	0.97	0.18	33,44,54,59	0
1	4OC	1A	1920	21/23	0.97	0.24	38,47,52,61	0
1	5MC	2A	1942	21/22	0.97	0.18	44,47,58,74	0
32	5MC	1a	1407	21/22	0.97	0.20	27,38,45,47	0
32	5MC	1a	967	21/22	0.97	0.18	42,51,61,68	0
1	PSU	2A	1917	20/21	0.97	0.17	47,56,61,63	0
1	5MU	2A	1939	21/22	0.97	0.19	26,34,39,41	0
32	7MG	1a	527	24/25	0.97	0.14	33,43,56,62	0
32	M2G	1a	966	25/26	0.97	0.17	37,51,54,61	0
1	2MU	1A	2552	21/23	0.98	0.19	25,34,40,43	0
32	MA6	1a	1518	24/25	0.98	0.20	32,41,49,57	0
1	OMG	2A	2251	24/25	0.98	0.17	27,33,39,39	0
1	2MA	1A	2503	23/24	0.98	0.22	17,22,30,33	0
1	2MU	2A	2552	21/23	0.98	0.17	27,37,41,43	0
32	5MC	1a	1400	21/22	0.98	0.18	36,44,55,65	0
32	UR3	1a	1498	21/22	0.98	0.19	30,40,45,52	0
32	MA6	1a	1519	24/25	0.98	0.21	27,43,51,60	0
1	PSU	2A	2605	20/21	0.98	0.16	25,32,38,39	0
1	PSU	1A	2605	20/21	0.98	0.18	21,29,35,36	0
1	5MC	1A	1962	21/22	0.98	0.20	29,38,43,46	0
1	5MU	1A	1939	21/22	0.98	0.24	21,29,37,41	0
1	OMG	1A	2251	24/25	0.98	0.21	19,30,34,37	0
1	2MA	2A	2503	23/24	0.99	0.19	21,25,31,36	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3600	1/1	0.25	0.08	78,78,78,78	0
56	MG	1A	3768	1/1	0.38	0.10	61,61,61,61	0
56	MG	1A	3388	1/1	0.38	0.17	55,55,55,55	0
56	MG	1A	3799	1/1	0.41	0.15	64,64,64,64	0
56	MG	1A	3767	1/1	0.50	0.22	63,63,63,63	0
56	MG	1A	3720	1/1	0.50	0.19	66,66,66,66	0
56	MG	2A	3576	1/1	0.53	0.11	62,62,62,62	0
56	MG	2A	3280	1/1	0.54	0.11	46,46,46,46	0
56	MG	2A	3087	1/1	0.55	0.22	69,69,69,69	0
56	MG	1B	218	1/1	0.55	0.24	64,64,64,64	0
59	ZN	2n	501	1/1	0.56	0.17	152,152,152,152	0
56	MG	2f	3002	1/1	0.56	0.17	85,85,85,85	0
56	MG	1A	3235	1/1	0.56	0.19	64,64,64,64	0
56	MG	2a	1745	1/1	0.56	0.26	72,72,72,72	0
56	MG	2a	1793	1/1	0.56	0.19	86,86,86,86	0
56	MG	1a	1820	1/1	0.56	0.09	91,91,91,91	0
56	MG	2A	3548	1/1	0.57	0.11	70,70,70,70	0
56	MG	1A	3622	1/1	0.59	0.11	55,55,55,55	0
56	MG	2j	8001	1/1	0.59	0.09	76,76,76,76	0
56	MG	1F	308	1/1	0.59	0.40	63,63,63,63	0
56	MG	2A	3633	1/1	0.60	0.88	66,66,66,66	0
56	MG	1A	3575	1/1	0.61	0.18	31,31,31,31	0
56	MG	2A	3539	1/1	0.61	0.26	82,82,82,82	0
56	MG	1A	3621	1/1	0.61	0.13	56,56,56,56	0
56	MG	2A	3033	1/1	0.61	0.32	53,53,53,53	0
56	MG	2a	1798	1/1	0.62	0.17	89,89,89,89	0
56	MG	2A	3558	1/1	0.62	0.12	55,55,55,55	0
56	MG	15	105	1/1	0.62	0.24	55,55,55,55	0
56	MG	2a	1693	1/1	0.62	0.17	69,69,69,69	0
56	MG	1A	3813	1/1	0.63	0.14	63,63,63,63	0
56	MG	1A	3495	1/1	0.63	0.17	48,48,48,48	0
56	MG	1A	3838	1/1	0.64	0.18	40,40,40,40	0
56	MG	2F	302	1/1	0.64	0.16	54,54,54,54	0
56	MG	2A	3310	1/1	0.65	0.15	39,39,39,39	0
56	MG	2A	3085	1/1	0.65	0.18	56,56,56,56	0
56	MG	2a	1607	1/1	0.65	0.16	67,67,67,67	0
56	MG	2A	3591	1/1	0.65	0.16	65,65,65,65	0
56	MG	2a	1705	1/1	0.65	0.24	69,69,69,69	0
56	MG	2A	3527	1/1	0.65	0.21	60,60,60,60	0
56	MG	2a	1760	1/1	0.65	0.18	79,79,79,79	0
56	MG	1A	3342	1/1	0.66	0.61	48,48,48,48	0
56	MG	2A	3506	1/1	0.66	0.15	72,72,72,72	0
56	MG	1A	3453	1/1	0.66	0.26	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3642	1/1	0.67	0.95	57,57,57,57	0
56	MG	1y	3006	1/1	0.67	0.25	82,82,82,82	0
56	MG	1v	3001	1/1	0.67	0.15	58,58,58,58	0
56	MG	1A	3015	1/1	0.67	0.22	58,58,58,58	0
56	MG	2A	3542	1/1	0.67	0.24	67,67,67,67	0
56	MG	1A	3316	1/1	0.68	0.17	57,57,57,57	0
56	MG	1A	3686	1/1	0.68	0.24	62,62,62,62	0
56	MG	10	105	1/1	0.68	0.12	63,63,63,63	0
56	MG	2a	1623	1/1	0.69	0.28	80,80,80,80	0
56	MG	1a	1792	1/1	0.69	0.12	82,82,82,82	0
56	MG	1a	1616	1/1	0.69	0.27	68,68,68,68	0
56	MG	2A	3538	1/1	0.69	0.14	67,67,67,67	0
56	MG	2a	1657	1/1	0.69	0.20	76,76,76,76	0
56	MG	2a	1684	1/1	0.69	0.17	76,76,76,76	0
56	MG	2A	3405	1/1	0.70	0.14	39,39,39,39	0
56	MG	2A	3656	1/1	0.70	0.09	41,41,41,41	0
56	MG	2A	3532	1/1	0.70	0.17	66,66,66,66	0
56	MG	1A	3685	1/1	0.70	0.12	49,49,49,49	0
56	MG	1A	3459	1/1	0.70	0.15	42,42,42,42	0
56	MG	1A	3296	1/1	0.71	0.24	56,56,56,56	0
56	MG	1a	1828	1/1	0.71	0.17	63,63,63,63	0
56	MG	2A	3219	1/1	0.71	0.29	69,69,69,69	0
56	MG	2a	1782	1/1	0.71	0.18	90,90,90,90	0
56	MG	1A	3781	1/1	0.71	0.13	69,69,69,69	0
56	MG	2A	3316	1/1	0.71	0.12	36,36,36,36	0
56	MG	2A	3509	1/1	0.71	0.12	44,44,44,44	0
56	MG	1a	1804	1/1	0.71	0.36	61,61,61,61	0
56	MG	1A	3014	1/1	0.72	0.16	46,46,46,46	0
56	MG	2A	3072	1/1	0.72	0.17	47,47,47,47	0
59	ZN	16	101	1/1	0.72	0.36	91,91,91,91	0
56	MG	2A	3329	1/1	0.72	0.11	47,47,47,47	0
56	MG	1A	3752	1/1	0.72	0.19	62,62,62,62	0
56	MG	1A	3182	1/1	0.72	0.17	52,52,52,52	0
59	ZN	24	501	1/1	0.72	0.10	185,185,185,185	0
56	MG	2a	1726	1/1	0.72	0.12	68,68,68,68	0
56	MG	1A	3063	1/1	0.73	0.16	52,52,52,52	0
56	MG	1A	3512	1/1	0.73	0.09	66,66,66,66	0
56	MG	2a	1602	1/1	0.73	0.13	70,70,70,70	0
56	MG	2A	3516	1/1	0.73	0.09	45,45,45,45	0
56	MG	2A	3163	1/1	0.73	0.63	59,59,59,59	0
56	MG	1A	3153	1/1	0.73	0.19	52,52,52,52	0
56	MG	2a	1613	1/1	0.74	0.17	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1691	1/1	0.74	0.17	80,80,80,80	0
56	MG	1A	3423	1/1	0.74	0.11	62,62,62,62	0
56	MG	1a	1615	1/1	0.74	0.17	60,60,60,60	0
56	MG	1A	3872	1/1	0.74	0.19	50,50,50,50	0
56	MG	2B	3010	1/1	0.74	0.16	63,63,63,63	0
56	MG	1A	3640	1/1	0.74	0.40	82,82,82,82	0
56	MG	2A	3126	1/1	0.74	0.18	59,59,59,59	0
56	MG	2A	3586	1/1	0.75	0.16	64,64,64,64	0
56	MG	1A	3301	1/1	0.75	0.17	45,45,45,45	0
56	MG	1A	3696	1/1	0.75	0.22	50,50,50,50	0
56	MG	2a	1675	1/1	0.75	0.12	64,64,64,64	0
56	MG	2B	3011	1/1	0.75	0.15	72,72,72,72	0
56	MG	2a	1690	1/1	0.75	0.14	69,69,69,69	0
56	MG	2B	3009	1/1	0.75	0.16	60,60,60,60	0
56	MG	1x	103	1/1	0.75	0.18	62,62,62,62	0
56	MG	2A	3467	1/1	0.75	0.60	49,49,49,49	0
56	MG	1A	3134	1/1	0.75	0.26	56,56,56,56	0
56	MG	1a	1823	1/1	0.75	0.07	79,79,79,79	0
56	MG	1A	3104	1/1	0.75	0.24	71,71,71,71	0
56	MG	1w	3001	1/1	0.76	0.13	52,52,52,52	0
56	MG	10	103	1/1	0.76	0.14	61,61,61,61	0
56	MG	1A	3306	1/1	0.76	0.23	62,62,62,62	0
56	MG	2A	3529	1/1	0.76	0.09	73,73,73,73	0
56	MG	1A	3713	1/1	0.76	0.15	71,71,71,71	0
56	MG	1A	3233	1/1	0.76	0.17	60,60,60,60	0
56	MG	2A	3412	1/1	0.76	0.20	57,57,57,57	0
56	MG	2a	1700	1/1	0.76	0.12	57,57,57,57	0
56	MG	2A	3240	1/1	0.76	0.15	58,58,58,58	0
56	MG	1A	3905	1/1	0.76	0.30	46,46,46,46	0
56	MG	1A	3396	1/1	0.76	0.16	42,42,42,42	0
56	MG	2a	1710	1/1	0.76	0.20	65,65,65,65	0
56	MG	1a	1668	1/1	0.76	0.11	44,44,44,44	0
56	MG	2A	3545	1/1	0.76	0.33	75,75,75,75	0
56	MG	1A	3268	1/1	0.77	0.14	63,63,63,63	0
56	MG	2A	3293	1/1	0.77	0.19	47,47,47,47	0
56	MG	2B	3021	1/1	0.77	0.14	76,76,76,76	0
56	MG	2a	1686	1/1	0.77	0.12	82,82,82,82	0
56	MG	1A	3852	1/1	0.77	0.09	70,70,70,70	0
56	MG	2A	3247	1/1	0.77	0.22	61,61,61,61	0
56	MG	2A	3222	1/1	0.77	0.16	46,46,46,46	0
56	MG	2a	1699	1/1	0.77	0.14	49,49,49,49	0
56	MG	1A	3402	1/1	0.77	0.17	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3499	1/1	0.78	0.36	56,56,56,56	0
56	MG	1A	3184	1/1	0.78	0.11	59,59,59,59	0
56	MG	2A	3640	1/1	0.78	0.08	44,44,44,44	0
56	MG	1a	1746	1/1	0.78	0.12	52,52,52,52	0
56	MG	1V	204	1/1	0.78	0.22	64,64,64,64	0
56	MG	2a	1683	1/1	0.78	0.12	82,82,82,82	0
56	MG	1A	3615	1/1	0.78	0.26	34,34,34,34	0
56	MG	2a	1668	1/1	0.78	0.15	66,66,66,66	0
56	MG	2A	3587	1/1	0.78	0.16	73,73,73,73	0
56	MG	2a	1709	1/1	0.78	0.11	92,92,92,92	0
56	MG	2A	3609	1/1	0.78	0.13	64,64,64,64	0
56	MG	2A	3404	1/1	0.78	0.34	25,25,25,25	0
56	MG	2a	1649	1/1	0.78	0.11	65,65,65,65	0
56	MG	1A	3862	1/1	0.78	0.13	54,54,54,54	0
56	MG	1A	3229	1/1	0.78	0.16	56,56,56,56	0
56	MG	2a	1706	1/1	0.78	0.07	68,68,68,68	0
56	MG	1P	204	1/1	0.78	0.48	48,48,48,48	0
56	MG	2A	3468	1/1	0.78	0.20	51,51,51,51	0
56	MG	2A	3105	1/1	0.78	0.14	52,52,52,52	0
56	MG	2A	3470	1/1	0.78	0.64	53,53,53,53	0
56	MG	1a	1768	1/1	0.78	0.09	66,66,66,66	0
56	MG	2A	3357	1/1	0.79	0.14	48,48,48,48	0
56	MG	2Q	3002	1/1	0.79	0.12	52,52,52,52	0
56	MG	2A	3572	1/1	0.79	0.10	56,56,56,56	0
56	MG	1a	1667	1/1	0.79	0.35	76,76,76,76	0
56	MG	1A	3322	1/1	0.79	0.13	57,57,57,57	0
56	MG	2Z	8001	1/1	0.79	0.45	90,90,90,90	0
56	MG	1A	3773	1/1	0.79	0.24	48,48,48,48	0
56	MG	1A	3005	1/1	0.79	0.11	59,59,59,59	0
56	MG	2A	3644	1/1	0.79	0.16	63,63,63,63	0
56	MG	1A	3502	1/1	0.79	0.14	71,71,71,71	0
56	MG	1x	108	1/1	0.79	0.28	75,75,75,75	0
56	MG	2A	3397	1/1	0.79	0.13	50,50,50,50	0
56	MG	1A	3417	1/1	0.79	0.10	36,36,36,36	0
56	MG	1A	3216	1/1	0.79	0.13	65,65,65,65	0
56	MG	1a	1633	1/1	0.79	0.13	66,66,66,66	0
56	MG	2A	3670	1/1	0.79	0.23	64,64,64,64	0
56	MG	2A	3231	1/1	0.79	0.23	59,59,59,59	0
56	MG	2A	3621	1/1	0.79	0.13	70,70,70,70	0
56	MG	1a	1722	1/1	0.79	0.12	64,64,64,64	0
56	MG	2A	3342	1/1	0.79	0.16	41,41,41,41	0
56	MG	2A	3530	1/1	0.79	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3075	1/1	0.80	0.14	47,47,47,47	0
56	MG	2A	3522	1/1	0.80	0.13	52,52,52,52	0
56	MG	2A	3175	1/1	0.80	0.22	47,47,47,47	0
56	MG	2a	1651	1/1	0.80	0.28	69,69,69,69	0
56	MG	1A	3538	1/1	0.80	0.13	45,45,45,45	0
56	MG	1A	3241	1/1	0.80	0.17	50,50,50,50	0
56	MG	2a	1692	1/1	0.80	0.13	72,72,72,72	0
56	MG	2A	3244	1/1	0.80	0.19	66,66,66,66	0
56	MG	1A	3248	1/1	0.80	0.14	63,63,63,63	0
56	MG	1A	3310	1/1	0.80	0.16	52,52,52,52	0
56	MG	1A	3154	1/1	0.80	0.12	53,53,53,53	0
56	MG	2A	3236	1/1	0.80	0.14	65,65,65,65	0
56	MG	1A	3830	1/1	0.80	0.15	60,60,60,60	0
56	MG	2A	3258	1/1	0.80	0.16	61,61,61,61	0
56	MG	2A	3225	1/1	0.80	0.41	49,49,49,49	0
56	MG	1A	3198	1/1	0.80	0.23	43,43,43,43	0
56	MG	2a	1769	1/1	0.80	0.14	65,65,65,65	0
56	MG	2A	3086	1/1	0.80	0.17	51,51,51,51	0
56	MG	2A	3457	1/1	0.81	0.12	42,42,42,42	0
56	MG	1A	3294	1/1	0.81	0.25	63,63,63,63	0
56	MG	1A	3699	1/1	0.81	0.11	65,65,65,65	0
56	MG	1A	3867	1/1	0.81	0.08	76,76,76,76	0
56	MG	2A	3117	1/1	0.81	0.17	52,52,52,52	0
56	MG	1a	1698	1/1	0.81	0.36	72,72,72,72	0
56	MG	1a	1718	1/1	0.81	0.11	49,49,49,49	0
56	MG	2A	3168	1/1	0.81	0.23	59,59,59,59	0
56	MG	1A	3783	1/1	0.81	0.11	51,51,51,51	0
56	MG	2a	1677	1/1	0.81	0.19	67,67,67,67	0
56	MG	1A	3868	1/1	0.81	0.15	37,37,37,37	0
56	MG	2A	3094	1/1	0.81	0.10	50,50,50,50	0
56	MG	1a	1659	1/1	0.81	0.31	59,59,59,59	0
56	MG	2A	3588	1/1	0.81	0.11	59,59,59,59	0
56	MG	2E	305	1/1	0.81	0.16	43,43,43,43	0
56	MG	1A	3785	1/1	0.81	0.21	65,65,65,65	0
56	MG	1a	1708	1/1	0.81	0.25	60,60,60,60	0
56	MG	2a	1618	1/1	0.81	0.10	68,68,68,68	0
56	MG	2a	1680	1/1	0.81	0.15	72,72,72,72	0
56	MG	1A	3630	1/1	0.81	0.12	62,62,62,62	0
56	MG	1A	3347	1/1	0.81	0.12	46,46,46,46	0
56	MG	2A	3187	1/1	0.81	0.21	42,42,42,42	0
56	MG	2a	1655	1/1	0.81	0.14	56,56,56,56	0
56	MG	1A	3583	1/1	0.81	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3340	1/1	0.81	0.14	42,42,42,42	0
56	MG	1A	3466	1/1	0.81	0.08	64,64,64,64	0
56	MG	1A	3386	1/1	0.81	0.09	42,42,42,42	0
56	MG	2A	3104	1/1	0.81	0.16	72,72,72,72	0
56	MG	1A	3712	1/1	0.81	0.24	36,36,36,36	0
56	MG	1B	210	1/1	0.81	0.10	53,53,53,53	0
56	MG	1A	3750	1/1	0.81	0.09	51,51,51,51	0
56	MG	2R	202	1/1	0.81	0.19	58,58,58,58	0
56	MG	2a	1629	1/1	0.81	0.22	66,66,66,66	0
56	MG	1y	3004	1/1	0.81	0.28	73,73,73,73	0
56	MG	1A	3725	1/1	0.81	0.11	49,49,49,49	0
56	MG	1B	223	1/1	0.81	0.20	58,58,58,58	0
56	MG	1A	3659	1/1	0.81	0.16	41,41,41,41	0
56	MG	1A	3584	1/1	0.81	0.46	70,70,70,70	0
56	MG	12	101	1/1	0.81	0.18	54,54,54,54	0
56	MG	1A	3419	1/1	0.81	0.06	53,53,53,53	0
56	MG	1a	1641	1/1	0.81	0.12	49,49,49,49	0
56	MG	1E	306	1/1	0.81	0.14	61,61,61,61	0
56	MG	1a	1623	1/1	0.82	0.12	54,54,54,54	0
56	MG	1A	3299	1/1	0.82	0.20	41,41,41,41	0
56	MG	2A	3351	1/1	0.82	0.11	30,30,30,30	0
56	MG	2A	3226	1/1	0.82	0.50	60,60,60,60	0
56	MG	1A	3195	1/1	0.82	0.23	46,46,46,46	0
56	MG	2A	3245	1/1	0.82	0.17	46,46,46,46	0
56	MG	2A	3666	1/1	0.82	0.15	42,42,42,42	0
56	MG	1A	3247	1/1	0.82	0.14	52,52,52,52	0
56	MG	1A	3181	1/1	0.82	0.25	56,56,56,56	0
56	MG	1A	3285	1/1	0.82	0.12	57,57,57,57	0
56	MG	1a	1681	1/1	0.82	0.14	58,58,58,58	0
56	MG	2A	3121	1/1	0.82	0.11	60,60,60,60	0
56	MG	2A	3547	1/1	0.82	0.18	72,72,72,72	0
56	MG	1A	3901	1/1	0.82	0.16	36,36,36,36	0
56	MG	1A	3239	1/1	0.82	0.14	63,63,63,63	0
56	MG	1A	3244	1/1	0.82	0.34	52,52,52,52	0
56	MG	1A	3674	1/1	0.82	0.12	48,48,48,48	0
56	MG	2A	3647	1/1	0.82	0.11	46,46,46,46	0
56	MG	1a	1735	1/1	0.82	0.12	66,66,66,66	0
56	MG	2a	1648	1/1	0.82	0.13	55,55,55,55	0
56	MG	15	101	1/1	0.82	0.23	48,48,48,48	0
56	MG	1y	3001	1/1	0.82	0.09	73,73,73,73	0
56	MG	2A	3103	1/1	0.82	0.26	46,46,46,46	0
56	MG	1A	3433	1/1	0.82	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3375	1/1	0.82	0.10	47,47,47,47	0
56	MG	1A	3302	1/1	0.82	0.15	65,65,65,65	0
56	MG	2a	1788	1/1	0.82	0.19	81,81,81,81	0
56	MG	2a	1608	1/1	0.82	0.45	73,73,73,73	0
56	MG	1A	3341	1/1	0.82	0.28	68,68,68,68	0
56	MG	1A	3855	1/1	0.82	0.10	69,69,69,69	0
56	MG	2A	3179	1/1	0.82	0.23	56,56,56,56	0
56	MG	2a	1752	1/1	0.82	0.20	78,78,78,78	0
56	MG	1A	3273	1/1	0.82	0.14	59,59,59,59	0
56	MG	1a	1811	1/1	0.83	0.16	77,77,77,77	0
56	MG	2a	1746	1/1	0.83	0.11	55,55,55,55	0
56	MG	2A	3132	1/1	0.83	0.18	51,51,51,51	0
56	MG	2A	3483	1/1	0.83	0.07	77,77,77,77	0
56	MG	2F	303	1/1	0.83	0.22	53,53,53,53	0
56	MG	1A	3231	1/1	0.83	0.24	61,61,61,61	0
56	MG	2a	1732	1/1	0.83	0.09	77,77,77,77	0
56	MG	2w	3001	1/1	0.83	0.16	58,58,58,58	0
56	MG	1A	3438	1/1	0.83	0.21	40,40,40,40	0
56	MG	1a	1608	1/1	0.83	0.16	56,56,56,56	0
56	MG	1A	3531	1/1	0.83	0.15	61,61,61,61	0
56	MG	1A	3577	1/1	0.83	0.16	43,43,43,43	0
56	MG	1a	1657	1/1	0.83	0.11	50,50,50,50	0
56	MG	1a	1642	1/1	0.83	0.19	60,60,60,60	0
56	MG	2a	1763	1/1	0.83	0.10	75,75,75,75	0
56	MG	1A	3348	1/1	0.83	0.14	33,33,33,33	0
56	MG	2a	1616	1/1	0.83	0.23	64,64,64,64	0
56	MG	2A	3322	1/1	0.83	0.18	59,59,59,59	0
56	MG	1A	3845	1/1	0.83	0.13	68,68,68,68	0
56	MG	2A	3089	1/1	0.83	0.20	58,58,58,58	0
56	MG	2A	3385	1/1	0.83	0.15	61,61,61,61	0
56	MG	1A	3755	1/1	0.83	0.14	32,32,32,32	0
56	MG	1A	3520	1/1	0.83	0.16	56,56,56,56	0
56	MG	2A	3498	1/1	0.83	0.48	64,64,64,64	0
56	MG	1A	3076	1/1	0.83	0.27	66,66,66,66	0
56	MG	2A	3339	1/1	0.83	0.15	43,43,43,43	0
56	MG	1A	3827	1/1	0.83	0.16	68,68,68,68	0
56	MG	2a	1682	1/1	0.83	0.14	64,64,64,64	0
56	MG	1A	3425	1/1	0.83	0.17	52,52,52,52	0
56	MG	1A	3139	1/1	0.83	0.49	45,45,45,45	0
56	MG	2A	3305	1/1	0.83	0.17	59,59,59,59	0
56	MG	2A	3096	1/1	0.83	0.14	57,57,57,57	0
56	MG	1X	102	1/1	0.83	0.23	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3828	1/1	0.83	0.15	43,43,43,43	0
56	MG	1A	3210	1/1	0.83	0.15	45,45,45,45	0
56	MG	1A	3756	1/1	0.83	0.16	67,67,67,67	0
56	MG	2a	1604	1/1	0.83	0.18	76,76,76,76	0
56	MG	2A	3212	1/1	0.83	0.16	66,66,66,66	0
56	MG	2A	3144	1/1	0.83	0.12	49,49,49,49	0
56	MG	1A	3318	1/1	0.83	0.15	60,60,60,60	0
56	MG	2A	3638	1/1	0.83	0.07	58,58,58,58	0
56	MG	1a	1753	1/1	0.83	0.12	67,67,67,67	0
56	MG	2A	3237	1/1	0.83	0.55	63,63,63,63	0
56	MG	2A	3174	1/1	0.84	0.09	63,63,63,63	0
56	MG	1B	222	1/1	0.84	0.14	78,78,78,78	0
56	MG	1A	3173	1/1	0.84	0.21	41,41,41,41	0
56	MG	1A	3859	1/1	0.84	0.16	40,40,40,40	0
56	MG	2A	3598	1/1	0.84	0.14	65,65,65,65	0
56	MG	1A	3290	1/1	0.84	0.21	68,68,68,68	0
56	MG	1A	3745	1/1	0.84	0.10	64,64,64,64	0
56	MG	1A	3215	1/1	0.84	0.25	43,43,43,43	0
56	MG	2A	3252	1/1	0.84	0.10	59,59,59,59	0
56	MG	2A	3422	1/1	0.84	0.14	51,51,51,51	0
56	MG	2B	3015	1/1	0.84	0.19	53,53,53,53	0
56	MG	2A	3220	1/1	0.84	0.16	56,56,56,56	0
56	MG	1A	3251	1/1	0.84	0.14	47,47,47,47	0
56	MG	2a	1662	1/1	0.84	0.40	67,67,67,67	0
56	MG	1a	1658	1/1	0.84	0.15	59,59,59,59	0
56	MG	1A	3462	1/1	0.84	0.20	58,58,58,58	0
56	MG	2A	3359	1/1	0.84	0.19	50,50,50,50	0
56	MG	2A	3408	1/1	0.84	0.11	24,24,24,24	0
56	MG	2a	1601	1/1	0.84	0.11	82,82,82,82	0
56	MG	20	103	1/1	0.84	0.09	65,65,65,65	0
56	MG	1A	3550	1/1	0.84	0.20	49,49,49,49	0
56	MG	1A	3487	1/1	0.84	0.12	48,48,48,48	0
56	MG	2A	3152	1/1	0.84	0.30	50,50,50,50	0
56	MG	1A	3706	1/1	0.84	0.14	55,55,55,55	0
56	MG	1A	3861	1/1	0.84	0.15	58,58,58,58	0
56	MG	1A	3870	1/1	0.84	0.17	49,49,49,49	0
56	MG	1A	3612	1/1	0.84	0.15	43,43,43,43	0
56	MG	2a	1670	1/1	0.84	0.11	66,66,66,66	0
56	MG	2A	3191	1/1	0.84	0.45	52,52,52,52	0
58	K	1A	3931	1/1	0.84	0.19	71,71,71,71	0
56	MG	2a	1727	1/1	0.84	0.14	54,54,54,54	0
56	MG	2A	3615	1/1	0.84	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3810	1/1	0.84	0.24	63,63,63,63	0
56	MG	1A	3113	1/1	0.84	0.47	47,47,47,47	0
56	MG	1a	1790	1/1	0.84	0.23	62,62,62,62	0
56	MG	2R	201	1/1	0.84	0.35	51,51,51,51	0
56	MG	2D	301	1/1	0.84	0.22	52,52,52,52	0
56	MG	2a	1751	1/1	0.84	0.17	70,70,70,70	0
56	MG	2A	3624	1/1	0.84	0.13	52,52,52,52	0
56	MG	1A	3633	1/1	0.84	0.09	50,50,50,50	0
56	MG	2A	3070	1/1	0.84	0.20	52,52,52,52	0
56	MG	1A	3478	1/1	0.84	0.12	29,29,29,29	0
56	MG	2A	3424	1/1	0.84	0.21	36,36,36,36	0
56	MG	1a	1637	1/1	0.84	0.13	44,44,44,44	0
56	MG	1a	1688	1/1	0.84	0.20	57,57,57,57	0
56	MG	2A	3626	1/1	0.84	0.07	62,62,62,62	0
56	MG	1O	8001	1/1	0.84	0.07	63,63,63,63	0
56	MG	1A	3291	1/1	0.85	0.12	52,52,52,52	0
56	MG	1a	1786	1/1	0.85	0.10	55,55,55,55	0
56	MG	1A	3176	1/1	0.85	0.12	47,47,47,47	0
56	MG	1b	3002	1/1	0.85	0.08	85,85,85,85	0
56	MG	2A	3319	1/1	0.85	0.11	33,33,33,33	0
56	MG	2a	1776	1/1	0.85	0.07	78,78,78,78	0
56	MG	1a	1686	1/1	0.85	0.23	53,53,53,53	0
56	MG	2B	3019	1/1	0.85	0.26	44,44,44,44	0
56	MG	1a	1663	1/1	0.85	0.20	68,68,68,68	0
56	MG	1A	3669	1/1	0.85	0.25	58,58,58,58	0
56	MG	2A	3427	1/1	0.85	0.23	44,44,44,44	0
56	MG	2A	3537	1/1	0.85	0.30	53,53,53,53	0
56	MG	1A	3457	1/1	0.85	0.13	35,35,35,35	0
56	MG	1A	3412	1/1	0.85	0.13	44,44,44,44	0
56	MG	2A	3129	1/1	0.85	0.17	47,47,47,47	0
56	MG	2A	3108	1/1	0.85	0.59	37,37,37,37	0
56	MG	2A	3138	1/1	0.85	0.16	29,29,29,29	0
56	MG	2A	3426	1/1	0.85	0.14	76,76,76,76	0
56	MG	1A	3886	1/1	0.85	0.15	58,58,58,58	0
56	MG	1A	3243	1/1	0.85	0.14	66,66,66,66	0
56	MG	2a	1743	1/1	0.85	0.12	92,92,92,92	0
56	MG	2j	8002	1/1	0.85	0.17	92,92,92,92	0
56	MG	2A	3295	1/1	0.85	0.11	60,60,60,60	0
56	MG	1A	3593	1/1	0.85	0.14	38,38,38,38	0
56	MG	2A	3137	1/1	0.85	0.15	62,62,62,62	0
56	MG	2A	3448	1/1	0.85	0.09	68,68,68,68	0
56	MG	1B	220	1/1	0.85	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3741	1/1	0.85	0.10	63,63,63,63	0
56	MG	1A	3515	1/1	0.85	0.13	58,58,58,58	0
56	MG	1A	3230	1/1	0.85	0.09	55,55,55,55	0
56	MG	2A	3583	1/1	0.85	0.13	46,46,46,46	0
56	MG	20	102	1/1	0.85	0.08	61,61,61,61	0
56	MG	2A	3437	1/1	0.85	0.12	54,54,54,54	0
56	MG	1R	202	1/1	0.85	0.15	71,71,71,71	0
56	MG	1A	3232	1/1	0.85	0.12	55,55,55,55	0
56	MG	1a	1817	1/1	0.85	0.12	83,83,83,83	0
56	MG	1A	3482	1/1	0.85	0.13	35,35,35,35	0
56	MG	1a	1679	1/1	0.85	0.09	67,67,67,67	0
56	MG	2A	3206	1/1	0.85	0.18	48,48,48,48	0
56	MG	2a	1783	1/1	0.85	0.14	68,68,68,68	0
56	MG	2A	3417	1/1	0.85	0.13	54,54,54,54	0
56	MG	1A	3078	1/1	0.85	0.18	47,47,47,47	0
56	MG	1A	3190	1/1	0.85	0.14	47,47,47,47	0
56	MG	1A	3424	1/1	0.85	0.17	51,51,51,51	0
56	MG	1A	3051	1/1	0.85	0.15	58,58,58,58	0
56	MG	1A	3042	1/1	0.85	0.10	40,40,40,40	0
56	MG	2a	1605	1/1	0.85	0.36	54,54,54,54	0
56	MG	1A	3837	1/1	0.85	0.13	56,56,56,56	0
56	MG	1A	3095	1/1	0.85	0.24	56,56,56,56	0
56	MG	1a	1805	1/1	0.85	0.12	65,65,65,65	0
56	MG	1A	3677	1/1	0.85	0.11	68,68,68,68	0
56	MG	2A	3597	1/1	0.85	0.17	76,76,76,76	0
56	MG	2A	3291	1/1	0.85	0.21	50,50,50,50	0
56	MG	2a	1636	1/1	0.85	0.14	62,62,62,62	0
56	MG	1A	3560	1/1	0.85	0.20	19,19,19,19	0
56	MG	2a	1624	1/1	0.85	0.20	62,62,62,62	0
56	MG	2D	302	1/1	0.85	0.27	70,70,70,70	0
56	MG	2A	3391	1/1	0.85	0.19	51,51,51,51	0
56	MG	2A	3044	1/1	0.85	0.17	46,46,46,46	0
56	MG	2A	3344	1/1	0.85	0.16	40,40,40,40	0
56	MG	1A	3475	1/1	0.85	0.19	42,42,42,42	0
56	MG	1A	3801	1/1	0.85	0.08	43,43,43,43	0
56	MG	2a	1606	1/1	0.85	0.08	60,60,60,60	0
56	MG	2A	3462	1/1	0.85	0.30	57,57,57,57	0
56	MG	1A	3444	1/1	0.85	0.16	26,26,26,26	0
56	MG	2A	3294	1/1	0.85	0.11	54,54,54,54	0
56	MG	2A	3218	1/1	0.85	0.14	53,53,53,53	0
56	MG	1A	3676	1/1	0.85	0.12	52,52,52,52	0
56	MG	1A	3465	1/1	0.85	0.11	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3442	1/1	0.85	0.17	54,54,54,54	0
56	MG	2A	3440	1/1	0.85	0.10	60,60,60,60	0
56	MG	2A	3065	1/1	0.85	0.09	47,47,47,47	0
56	MG	2A	3482	1/1	0.85	0.34	62,62,62,62	0
56	MG	1A	3719	1/1	0.85	0.15	48,48,48,48	0
56	MG	1Q	3002	1/1	0.86	0.20	43,43,43,43	0
56	MG	1A	3812	1/1	0.86	0.11	61,61,61,61	0
56	MG	1A	3320	1/1	0.86	0.14	52,52,52,52	0
56	MG	2A	3594	1/1	0.86	0.09	41,41,41,41	0
56	MG	1A	3192	1/1	0.86	0.29	42,42,42,42	0
56	MG	1a	1830	1/1	0.86	0.12	59,59,59,59	0
56	MG	28	102	1/1	0.86	0.30	57,57,57,57	0
56	MG	2A	3102	1/1	0.86	0.99	60,60,60,60	0
56	MG	1a	1625	1/1	0.86	0.16	48,48,48,48	0
56	MG	1A	3245	1/1	0.86	0.15	48,48,48,48	0
56	MG	2a	1789	1/1	0.86	0.10	62,62,62,62	0
56	MG	2A	3536	1/1	0.86	0.09	55,55,55,55	0
56	MG	1A	3763	1/1	0.86	0.36	63,63,63,63	0
56	MG	1A	3747	1/1	0.86	0.14	30,30,30,30	0
56	MG	2A	3611	1/1	0.86	0.10	50,50,50,50	0
56	MG	1A	3568	1/1	0.86	0.16	31,31,31,31	0
56	MG	1A	3652	1/1	0.86	0.15	65,65,65,65	0
56	MG	2A	3267	1/1	0.86	0.15	53,53,53,53	0
56	MG	1A	3284	1/1	0.86	0.21	54,54,54,54	0
56	MG	2A	3180	1/1	0.86	0.38	54,54,54,54	0
56	MG	2a	1774	1/1	0.86	0.16	70,70,70,70	0
56	MG	2a	1697	1/1	0.86	0.12	64,64,64,64	0
56	MG	2A	3279	1/1	0.86	0.13	40,40,40,40	0
56	MG	2A	3213	1/1	0.86	0.08	58,58,58,58	0
56	MG	1r	3001	1/1	0.86	0.22	67,67,67,67	0
56	MG	1A	3360	1/1	0.86	0.14	52,52,52,52	0
56	MG	2A	3414	1/1	0.86	0.19	56,56,56,56	0
56	MG	1A	3726	1/1	0.86	0.12	38,38,38,38	0
56	MG	1a	1619	1/1	0.86	0.15	71,71,71,71	0
56	MG	1A	3869	1/1	0.86	0.36	52,52,52,52	0
56	MG	2r	3001	1/1	0.86	0.13	84,84,84,84	0
56	MG	2B	3003	1/1	0.86	0.09	69,69,69,69	0
56	MG	1B	221	1/1	0.86	0.08	48,48,48,48	0
56	MG	2a	1722	1/1	0.86	0.17	59,59,59,59	0
56	MG	1a	1712	1/1	0.86	0.13	61,61,61,61	0
56	MG	2a	1729	1/1	0.86	0.30	75,75,75,75	0
56	MG	2A	3486	1/1	0.86	0.16	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1665	1/1	0.86	0.22	66,66,66,66	0
56	MG	1a	1704	1/1	0.86	0.14	77,77,77,77	0
56	MG	1A	3572	1/1	0.86	0.16	41,41,41,41	0
56	MG	1B	213	1/1	0.86	0.10	49,49,49,49	0
56	MG	1a	1622	1/1	0.86	0.08	59,59,59,59	0
56	MG	1U	201	1/1	0.86	0.19	48,48,48,48	0
56	MG	1F	304	1/1	0.86	0.18	50,50,50,50	0
56	MG	1A	3795	1/1	0.86	0.12	32,32,32,32	0
56	MG	2A	3061	1/1	0.86	0.13	56,56,56,56	0
56	MG	1A	3249	1/1	0.86	0.21	69,69,69,69	0
56	MG	2A	3502	1/1	0.86	0.07	42,42,42,42	0
56	MG	2A	3557	1/1	0.86	0.10	55,55,55,55	0
56	MG	1A	3045	1/1	0.86	0.14	46,46,46,46	0
56	MG	1A	3018	1/1	0.86	0.24	53,53,53,53	0
56	MG	2A	3603	1/1	0.86	0.11	63,63,63,63	0
56	MG	1a	1611	1/1	0.86	0.16	62,62,62,62	0
56	MG	1a	1607	1/1	0.86	0.26	52,52,52,52	0
56	MG	2A	3478	1/1	0.86	0.13	52,52,52,52	0
56	MG	2Q	3001	1/1	0.86	0.09	47,47,47,47	0
56	MG	1A	3877	1/1	0.86	0.48	58,58,58,58	0
56	MG	1A	3314	1/1	0.86	0.33	68,68,68,68	0
56	MG	2A	3230	1/1	0.86	0.31	60,60,60,60	0
56	MG	1a	1673	1/1	0.86	0.22	52,52,52,52	0
56	MG	2A	3519	1/1	0.86	0.43	57,57,57,57	0
56	MG	1A	3793	1/1	0.86	0.09	38,38,38,38	0
56	MG	2A	3569	1/1	0.86	0.30	74,74,74,74	0
56	MG	1A	3498	1/1	0.87	0.21	58,58,58,58	0
56	MG	1a	1824	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3092	1/1	0.87	0.10	49,49,49,49	0
56	MG	1A	3024	1/1	0.87	0.10	57,57,57,57	0
56	MG	2A	3031	1/1	0.87	0.10	50,50,50,50	0
56	MG	1A	3398	1/1	0.87	0.18	36,36,36,36	0
56	MG	1A	3778	1/1	0.87	0.15	65,65,65,65	0
56	MG	1a	1604	1/1	0.87	0.09	64,64,64,64	0
56	MG	2B	3018	1/1	0.87	0.12	62,62,62,62	0
56	MG	2A	3552	1/1	0.87	0.10	33,33,33,33	0
56	MG	2a	1768	1/1	0.87	0.19	79,79,79,79	0
56	MG	2F	307	1/1	0.87	0.12	48,48,48,48	0
56	MG	1a	1701	1/1	0.87	0.15	50,50,50,50	0
56	MG	1A	3684	1/1	0.87	0.15	72,72,72,72	0
56	MG	2A	3592	1/1	0.87	0.10	54,54,54,54	0
56	MG	1a	1684	1/1	0.87	0.24	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1N	3001	1/1	0.87	0.28	51,51,51,51	0
56	MG	1A	3142	1/1	0.87	0.51	47,47,47,47	0
56	MG	2A	3593	1/1	0.87	0.08	54,54,54,54	0
56	MG	2A	3326	1/1	0.87	0.20	49,49,49,49	0
56	MG	2A	3571	1/1	0.87	0.17	51,51,51,51	0
56	MG	1A	3578	1/1	0.87	0.07	56,56,56,56	0
56	MG	1A	3529	1/1	0.87	0.12	60,60,60,60	0
56	MG	2A	3214	1/1	0.87	0.08	57,57,57,57	0
56	MG	1B	201	1/1	0.87	0.26	53,53,53,53	0
56	MG	1A	3022	1/1	0.87	0.12	52,52,52,52	0
56	MG	1A	3340	1/1	0.87	0.27	48,48,48,48	0
56	MG	1A	3839	1/1	0.87	0.11	61,61,61,61	0
56	MG	1A	3127	1/1	0.87	0.20	62,62,62,62	0
56	MG	1a	1656	1/1	0.87	0.21	57,57,57,57	0
56	MG	1W	3002	1/1	0.87	0.16	53,53,53,53	0
56	MG	1a	1617	1/1	0.87	0.23	71,71,71,71	0
56	MG	2A	3309	1/1	0.87	0.14	38,38,38,38	0
56	MG	1A	3589	1/1	0.87	0.20	64,64,64,64	0
56	MG	2a	1737	1/1	0.87	0.15	55,55,55,55	0
56	MG	1a	1813	1/1	0.87	0.17	65,65,65,65	0
56	MG	1A	3237	1/1	0.87	0.14	57,57,57,57	0
56	MG	1A	3279	1/1	0.87	0.18	57,57,57,57	0
56	MG	2A	3575	1/1	0.87	0.11	62,62,62,62	0
56	MG	2A	3622	1/1	0.87	0.13	48,48,48,48	0
56	MG	1A	3119	1/1	0.87	0.20	44,44,44,44	0
56	MG	1x	113	1/1	0.87	0.17	68,68,68,68	0
56	MG	1A	3194	1/1	0.87	0.15	55,55,55,55	0
56	MG	1A	3581	1/1	0.87	0.22	42,42,42,42	0
56	MG	2A	3149	1/1	0.87	0.12	41,41,41,41	0
56	MG	1a	1802	1/1	0.87	0.16	54,54,54,54	0
56	MG	2A	3413	1/1	0.87	0.07	27,27,27,27	0
56	MG	2a	1734	1/1	0.87	0.15	64,64,64,64	0
56	MG	1a	1724	1/1	0.87	0.16	46,46,46,46	0
56	MG	2A	3625	1/1	0.87	0.14	58,58,58,58	0
56	MG	1a	1835	1/1	0.87	0.15	61,61,61,61	0
56	MG	1A	3469	1/1	0.87	0.14	48,48,48,48	0
56	MG	1A	3642	1/1	0.87	0.14	42,42,42,42	0
56	MG	2a	1656	1/1	0.87	0.15	54,54,54,54	0
56	MG	1A	3399	1/1	0.87	0.14	59,59,59,59	0
56	MG	2A	3080	1/1	0.87	0.26	45,45,45,45	0
56	MG	1A	3694	1/1	0.87	0.14	27,27,27,27	0
56	MG	1A	3435	1/1	0.87	0.16	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3402	1/1	0.87	0.18	64,64,64,64	0
56	MG	1A	3646	1/1	0.87	0.08	68,68,68,68	0
56	MG	1Q	3005	1/1	0.87	0.16	58,58,58,58	0
56	MG	1A	3865	1/1	0.87	0.26	50,50,50,50	0
56	MG	2B	3005	1/1	0.87	0.12	64,64,64,64	0
56	MG	2A	3553	1/1	0.87	0.17	53,53,53,53	0
56	MG	1A	3885	1/1	0.88	0.08	64,64,64,64	0
56	MG	2A	3286	1/1	0.88	0.12	68,68,68,68	0
56	MG	2A	3093	1/1	0.88	0.12	55,55,55,55	0
56	MG	1a	1752	1/1	0.88	0.30	66,66,66,66	0
56	MG	1A	3846	1/1	0.88	0.15	39,39,39,39	0
56	MG	1a	1737	1/1	0.88	0.15	51,51,51,51	0
56	MG	1l	102	1/1	0.88	0.17	54,54,54,54	0
56	MG	1a	1819	1/1	0.88	0.12	72,72,72,72	0
56	MG	1A	3439	1/1	0.88	0.10	54,54,54,54	0
56	MG	1A	3690	1/1	0.88	0.09	48,48,48,48	0
56	MG	2A	3024	1/1	0.88	0.31	45,45,45,45	0
56	MG	1a	1761	1/1	0.88	0.20	51,51,51,51	0
56	MG	1A	3420	1/1	0.88	0.18	46,46,46,46	0
56	MG	1A	3840	1/1	0.88	0.17	65,65,65,65	0
56	MG	1A	3775	1/1	0.88	0.23	43,43,43,43	0
56	MG	1A	3672	1/1	0.88	0.08	48,48,48,48	0
56	MG	1a	1791	1/1	0.88	0.16	73,73,73,73	0
56	MG	2B	3002	1/1	0.88	0.15	67,67,67,67	0
56	MG	1A	3746	1/1	0.88	0.19	31,31,31,31	0
56	MG	2A	3513	1/1	0.88	0.12	45,45,45,45	0
56	MG	1A	3069	1/1	0.88	0.23	52,52,52,52	0
56	MG	1A	3667	1/1	0.88	0.20	51,51,51,51	0
56	MG	1A	3675	1/1	0.88	0.20	50,50,50,50	0
56	MG	2a	1678	1/1	0.88	0.65	60,60,60,60	0
56	MG	1A	3489	1/1	0.88	0.16	31,31,31,31	0
56	MG	1A	3803	1/1	0.88	0.11	65,65,65,65	0
56	MG	1V	203	1/1	0.88	0.19	59,59,59,59	0
56	MG	1a	1731	1/1	0.88	0.27	79,79,79,79	0
56	MG	1G	3001	1/1	0.88	0.14	59,59,59,59	0
56	MG	1a	1665	1/1	0.88	0.34	73,73,73,73	0
56	MG	2a	1725	1/1	0.88	0.10	58,58,58,58	0
56	MG	1a	1602	1/1	0.88	0.17	60,60,60,60	0
56	MG	2A	3501	1/1	0.88	0.07	56,56,56,56	0
56	MG	1A	3085	1/1	0.88	0.16	52,52,52,52	0
56	MG	2A	3135	1/1	0.88	0.13	36,36,36,36	0
56	MG	1A	3175	1/1	0.88	0.29	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3415	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3001	1/1	0.88	0.23	60,60,60,60	0
56	MG	1a	1750	1/1	0.88	0.11	69,69,69,69	0
56	MG	2a	1715	1/1	0.88	0.14	59,59,59,59	0
56	MG	2A	3387	1/1	0.88	0.19	33,33,33,33	0
56	MG	1a	1661	1/1	0.88	0.25	61,61,61,61	0
56	MG	1A	3780	1/1	0.88	0.14	62,62,62,62	0
56	MG	1Q	3004	1/1	0.88	0.15	56,56,56,56	0
56	MG	1A	3120	1/1	0.88	0.25	39,39,39,39	0
56	MG	2a	1625	1/1	0.88	0.11	72,72,72,72	0
56	MG	1x	107	1/1	0.88	0.23	59,59,59,59	0
56	MG	1A	3796	1/1	0.88	0.05	66,66,66,66	0
56	MG	1a	1635	1/1	0.88	0.10	62,62,62,62	0
56	MG	2a	1603	1/1	0.88	0.11	64,64,64,64	0
56	MG	1a	1703	1/1	0.88	0.19	49,49,49,49	0
56	MG	1a	1772	1/1	0.88	0.14	50,50,50,50	0
56	MG	2A	3259	1/1	0.88	0.13	35,35,35,35	0
56	MG	1A	3899	1/1	0.88	0.40	50,50,50,50	0
56	MG	1a	1747	1/1	0.88	0.15	53,53,53,53	0
56	MG	1S	8001	1/1	0.88	0.13	67,67,67,67	0
56	MG	2A	3662	1/1	0.88	0.21	61,61,61,61	0
56	MG	2A	3618	1/1	0.88	0.14	49,49,49,49	0
56	MG	2A	3271	1/1	0.88	0.12	38,38,38,38	0
56	MG	1A	3123	1/1	0.88	0.17	42,42,42,42	0
56	MG	2A	3311	1/1	0.88	0.13	36,36,36,36	0
56	MG	2p	3001	1/1	0.88	0.13	74,74,74,74	0
56	MG	2a	1673	1/1	0.88	0.22	55,55,55,55	0
56	MG	1A	3169	1/1	0.88	0.09	60,60,60,60	0
56	MG	1A	3379	1/1	0.88	0.11	48,48,48,48	0
56	MG	2a	1790	1/1	0.88	0.24	72,72,72,72	0
56	MG	13	101	1/1	0.88	0.12	46,46,46,46	0
56	MG	1A	3797	1/1	0.88	0.13	67,67,67,67	0
56	MG	1a	1787	1/1	0.88	0.19	71,71,71,71	0
56	MG	1a	1603	1/1	0.88	0.17	60,60,60,60	0
56	MG	2A	3617	1/1	0.88	0.21	64,64,64,64	0
56	MG	2A	3006	1/1	0.88	0.18	58,58,58,58	0
56	MG	2A	3173	1/1	0.88	0.16	60,60,60,60	0
56	MG	1A	3278	1/1	0.88	0.14	61,61,61,61	0
56	MG	1A	3913	1/1	0.88	0.42	54,54,54,54	0
56	MG	1A	3573	1/1	0.88	0.16	43,43,43,43	0
56	MG	2A	3112	1/1	0.88	0.10	58,58,58,58	0
56	MG	1A	3458	1/1	0.88	0.18	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3808	1/1	0.88	0.19	46,46,46,46	0
56	MG	2A	3084	1/1	0.88	0.08	59,59,59,59	0
56	MG	1x	115	1/1	0.88	0.13	57,57,57,57	0
56	MG	1A	3448	1/1	0.88	0.17	39,39,39,39	0
56	MG	2A	3635	1/1	0.88	0.14	56,56,56,56	0
56	MG	2A	3601	1/1	0.88	0.12	45,45,45,45	0
56	MG	1A	3321	1/1	0.88	0.14	48,48,48,48	0
56	MG	1A	3688	1/1	0.89	0.14	64,64,64,64	0
56	MG	1A	3334	1/1	0.89	0.17	49,49,49,49	0
56	MG	2A	3189	1/1	0.89	0.18	54,54,54,54	0
56	MG	1a	1765	1/1	0.89	0.20	51,51,51,51	0
56	MG	1a	1716	1/1	0.89	0.09	81,81,81,81	0
56	MG	2A	3122	1/1	0.89	0.16	47,47,47,47	0
56	MG	1a	1655	1/1	0.89	0.11	57,57,57,57	0
56	MG	2e	3001	1/1	0.89	0.12	71,71,71,71	0
56	MG	1A	3052	1/1	0.89	0.17	40,40,40,40	0
56	MG	1A	3254	1/1	0.89	0.10	54,54,54,54	0
56	MG	2a	1794	1/1	0.89	0.11	94,94,94,94	0
56	MG	1A	3596	1/1	0.89	0.08	51,51,51,51	0
56	MG	2A	3018	1/1	0.89	0.18	41,41,41,41	0
56	MG	2x	3002	1/1	0.89	0.40	50,50,50,50	0
56	MG	1A	3287	1/1	0.89	0.17	57,57,57,57	0
56	MG	2A	3554	1/1	0.89	0.06	45,45,45,45	0
56	MG	2A	3067	1/1	0.89	0.08	51,51,51,51	0
56	MG	2a	1773	1/1	0.89	0.11	57,57,57,57	0
56	MG	2A	3337	1/1	0.89	0.09	30,30,30,30	0
56	MG	1A	3749	1/1	0.89	0.16	39,39,39,39	0
56	MG	2A	3608	1/1	0.89	0.10	55,55,55,55	0
56	MG	1A	3060	1/1	0.89	0.17	44,44,44,44	0
56	MG	2A	3038	1/1	0.89	0.10	34,34,34,34	0
56	MG	2A	3510	1/1	0.89	0.14	35,35,35,35	0
56	MG	1a	1796	1/1	0.89	0.11	80,80,80,80	0
56	MG	2A	3215	1/1	0.89	0.13	53,53,53,53	0
56	MG	1A	3563	1/1	0.89	0.18	30,30,30,30	0
56	MG	1A	3405	1/1	0.89	0.15	62,62,62,62	0
56	MG	1A	3639	1/1	0.89	0.17	61,61,61,61	0
56	MG	2a	1721	1/1	0.89	0.13	54,54,54,54	0
56	MG	2a	1791	1/1	0.89	0.09	75,75,75,75	0
56	MG	2A	3120	1/1	0.89	0.19	57,57,57,57	0
56	MG	1a	1618	1/1	0.89	0.21	48,48,48,48	0
56	MG	1A	3056	1/1	0.89	0.11	43,43,43,43	0
56	MG	2a	1661	1/1	0.89	0.28	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3364	1/1	0.89	0.12	35,35,35,35	0
56	MG	2A	3419	1/1	0.89	0.15	41,41,41,41	0
56	MG	2A	3455	1/1	0.89	0.12	34,34,34,34	0
56	MG	1a	1719	1/1	0.89	0.12	62,62,62,62	0
56	MG	2A	3667	1/1	0.89	0.08	43,43,43,43	0
56	MG	2A	3435	1/1	0.89	0.15	34,34,34,34	0
56	MG	1A	3730	1/1	0.89	0.10	58,58,58,58	0
56	MG	1A	3391	1/1	0.89	0.16	30,30,30,30	0
56	MG	2A	3157	1/1	0.89	0.21	55,55,55,55	0
56	MG	2a	1780	1/1	0.89	0.14	69,69,69,69	0
56	MG	2a	1674	1/1	0.89	0.13	62,62,62,62	0
56	MG	2A	3578	1/1	0.89	0.11	62,62,62,62	0
56	MG	1a	1720	1/1	0.89	0.11	57,57,57,57	0
56	MG	1A	3036	1/1	0.89	0.12	54,54,54,54	0
56	MG	1A	3758	1/1	0.89	0.13	33,33,33,33	0
56	MG	2A	3043	1/1	0.89	0.16	44,44,44,44	0
56	MG	2V	3002	1/1	0.89	0.11	50,50,50,50	0
56	MG	1A	3900	1/1	0.89	0.34	35,35,35,35	0
56	MG	2A	3116	1/1	0.89	0.10	67,67,67,67	0
56	MG	1a	1749	1/1	0.89	0.22	56,56,56,56	0
56	MG	1y	3002	1/1	0.89	0.45	72,72,72,72	0
56	MG	2A	3336	1/1	0.89	0.10	47,47,47,47	0
56	MG	2A	3076	1/1	0.89	0.28	60,60,60,60	0
56	MG	1l	101	1/1	0.89	0.16	44,44,44,44	0
56	MG	2A	3429	1/1	0.89	0.20	34,34,34,34	0
56	MG	2A	3335	1/1	0.89	0.16	35,35,35,35	0
56	MG	1A	3313	1/1	0.89	0.10	56,56,56,56	0
56	MG	1A	3557	1/1	0.89	0.17	22,22,22,22	0
56	MG	1A	3200	1/1	0.89	0.12	48,48,48,48	0
56	MG	1A	3893	1/1	0.89	0.14	71,71,71,71	0
56	MG	2a	1611	1/1	0.89	0.16	68,68,68,68	0
56	MG	2A	3543	1/1	0.89	0.14	48,48,48,48	0
56	MG	1A	3863	1/1	0.89	0.23	56,56,56,56	0
56	MG	2a	1681	1/1	0.89	0.13	84,84,84,84	0
56	MG	2A	3471	1/1	0.89	0.08	53,53,53,53	0
56	MG	1A	3847	1/1	0.89	0.15	51,51,51,51	0
56	MG	1a	1669	1/1	0.89	0.14	49,49,49,49	0
56	MG	1A	3236	1/1	0.89	0.15	58,58,58,58	0
56	MG	1A	3643	1/1	0.89	0.11	55,55,55,55	0
56	MG	2A	3239	1/1	0.89	0.94	61,61,61,61	0
56	MG	2A	3324	1/1	0.89	0.07	47,47,47,47	0
56	MG	1a	1626	1/1	0.89	0.30	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3919	1/1	0.89	0.32	46,46,46,46	0
56	MG	2A	3300	1/1	0.89	0.23	54,54,54,54	0
56	MG	15	106	1/1	0.89	0.09	55,55,55,55	0
56	MG	1a	1770	1/1	0.89	0.25	44,44,44,44	0
56	MG	1a	1694	1/1	0.89	0.13	55,55,55,55	0
56	MG	1A	3440	1/1	0.89	0.14	61,61,61,61	0
56	MG	1A	3227	1/1	0.89	0.12	63,63,63,63	0
56	MG	2a	1749	1/1	0.89	0.11	59,59,59,59	0
56	MG	2A	3194	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	3455	1/1	0.89	0.14	25,25,25,25	0
56	MG	1a	1785	1/1	0.89	0.17	71,71,71,71	0
56	MG	1a	1800	1/1	0.89	0.15	56,56,56,56	0
56	MG	2a	1626	1/1	0.89	0.13	63,63,63,63	0
56	MG	2A	3551	1/1	0.89	0.07	70,70,70,70	0
56	MG	1a	1640	1/1	0.89	0.15	47,47,47,47	0
56	MG	1W	3001	1/1	0.89	0.15	48,48,48,48	0
56	MG	1a	1674	1/1	0.89	0.31	59,59,59,59	0
56	MG	2E	301	1/1	0.89	0.20	34,34,34,34	0
56	MG	2a	1797	1/1	0.89	0.18	67,67,67,67	0
56	MG	2a	1764	1/1	0.89	0.15	67,67,67,67	0
56	MG	1A	3196	1/1	0.89	0.12	61,61,61,61	0
56	MG	2A	3650	1/1	0.89	0.07	54,54,54,54	0
56	MG	1a	1728	1/1	0.89	0.16	67,67,67,67	0
56	MG	1A	3170	1/1	0.89	0.28	64,64,64,64	0
56	MG	2A	3325	1/1	0.89	0.16	45,45,45,45	0
56	MG	1a	1745	1/1	0.89	0.13	81,81,81,81	0
56	MG	1A	3093	1/1	0.89	0.13	59,59,59,59	0
56	MG	1A	3189	1/1	0.90	0.16	47,47,47,47	0
56	MG	1a	1740	1/1	0.90	0.12	60,60,60,60	0
56	MG	1a	1727	1/1	0.90	0.24	64,64,64,64	0
56	MG	1A	3112	1/1	0.90	0.15	44,44,44,44	0
56	MG	1y	3007	1/1	0.90	0.09	79,79,79,79	0
56	MG	1D	308	1/1	0.90	0.45	51,51,51,51	0
56	MG	2a	1676	1/1	0.90	0.12	58,58,58,58	0
56	MG	1E	308	1/1	0.90	0.15	49,49,49,49	0
56	MG	1A	3395	1/1	0.90	0.07	58,58,58,58	0
56	MG	1c	3001	1/1	0.90	0.22	61,61,61,61	0
56	MG	2A	3057	1/1	0.90	0.12	54,54,54,54	0
56	MG	2A	3134	1/1	0.90	0.23	54,54,54,54	0
56	MG	2a	1612	1/1	0.90	0.18	66,66,66,66	0
56	MG	1a	1778	1/1	0.90	0.14	65,65,65,65	0
56	MG	2A	3454	1/1	0.90	0.36	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	ZN	14	501	1/1	0.90	0.10	90,90,90,90	0
56	MG	1A	3410	1/1	0.90	0.12	43,43,43,43	0
56	MG	1A	3802	1/1	0.90	0.10	56,56,56,56	0
56	MG	2A	3198	1/1	0.90	0.18	52,52,52,52	0
56	MG	2a	1615	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	3834	1/1	0.90	0.09	60,60,60,60	0
56	MG	1A	3871	1/1	0.90	0.20	69,69,69,69	0
56	MG	1A	3363	1/1	0.90	0.08	49,49,49,49	0
56	MG	1A	3604	1/1	0.90	0.22	32,32,32,32	0
56	MG	2A	3561	1/1	0.90	0.17	47,47,47,47	0
56	MG	1A	3623	1/1	0.90	0.12	59,59,59,59	0
56	MG	1A	3338	1/1	0.90	0.09	47,47,47,47	0
56	MG	2a	1643	1/1	0.90	0.22	60,60,60,60	0
56	MG	2A	3567	1/1	0.90	0.15	41,41,41,41	0
56	MG	1A	3634	1/1	0.90	0.14	57,57,57,57	0
56	MG	2A	3403	1/1	0.90	0.08	62,62,62,62	0
56	MG	2A	3193	1/1	0.90	0.13	48,48,48,48	0
56	MG	1A	3058	1/1	0.90	0.12	53,53,53,53	0
56	MG	1A	3250	1/1	0.90	0.32	57,57,57,57	0
56	MG	1A	3150	1/1	0.90	0.20	55,55,55,55	0
56	MG	1a	1806	1/1	0.90	0.10	58,58,58,58	0
56	MG	2a	1617	1/1	0.90	0.17	51,51,51,51	0
56	MG	1Z	303	1/1	0.90	0.17	59,59,59,59	0
56	MG	19	503	1/1	0.90	0.12	37,37,37,37	0
56	MG	2A	3347	1/1	0.90	0.09	31,31,31,31	0
56	MG	1G	3003	1/1	0.90	0.11	50,50,50,50	0
56	MG	2a	1685	1/1	0.90	0.22	62,62,62,62	0
56	MG	2A	3431	1/1	0.90	0.14	58,58,58,58	0
56	MG	2A	3016	1/1	0.90	0.12	38,38,38,38	0
56	MG	1A	3860	1/1	0.90	0.13	58,58,58,58	0
56	MG	2A	3570	1/1	0.90	0.34	43,43,43,43	0
56	MG	2A	3099	1/1	0.90	0.26	50,50,50,50	0
56	MG	1a	1683	1/1	0.90	0.13	64,64,64,64	0
56	MG	2A	3306	1/1	0.90	0.10	43,43,43,43	0
56	MG	1A	3009	1/1	0.90	0.23	44,44,44,44	0
56	MG	1A	3722	1/1	0.90	0.10	46,46,46,46	0
56	MG	2a	1796	1/1	0.90	0.12	64,64,64,64	0
56	MG	1a	1797	1/1	0.90	0.17	51,51,51,51	0
56	MG	2a	1733	1/1	0.90	0.12	78,78,78,78	0
56	MG	2A	3046	1/1	0.90	0.17	50,50,50,50	0
56	MG	1B	205	1/1	0.90	0.16	43,43,43,43	0
56	MG	1l	8001	1/1	0.90	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3211	1/1	0.90	0.09	48,48,48,48	0
56	MG	1A	3836	1/1	0.90	0.11	48,48,48,48	0
56	MG	1a	1672	1/1	0.90	0.21	55,55,55,55	0
56	MG	1A	3213	1/1	0.90	0.13	55,55,55,55	0
56	MG	2A	3620	1/1	0.90	0.46	47,47,47,47	0
56	MG	1A	3130	1/1	0.90	0.18	40,40,40,40	0
56	MG	2a	1632	1/1	0.90	0.16	63,63,63,63	0
56	MG	2A	3606	1/1	0.90	0.13	58,58,58,58	0
56	MG	2A	3148	1/1	0.90	0.12	59,59,59,59	0
56	MG	1A	3349	1/1	0.90	0.13	43,43,43,43	0
56	MG	1A	3599	1/1	0.90	0.09	46,46,46,46	0
56	MG	1a	1706	1/1	0.90	0.12	72,72,72,72	0
56	MG	1A	3144	1/1	0.90	0.14	51,51,51,51	0
56	MG	2V	3001	1/1	0.90	0.47	62,62,62,62	0
56	MG	1A	3856	1/1	0.90	0.12	41,41,41,41	0
56	MG	1A	3102	1/1	0.90	0.28	58,58,58,58	0
56	MG	1a	1812	1/1	0.90	0.09	58,58,58,58	0
56	MG	2A	3297	1/1	0.90	0.33	52,52,52,52	0
56	MG	1A	3317	1/1	0.90	0.52	43,43,43,43	0
56	MG	1a	1609	1/1	0.90	0.16	56,56,56,56	0
56	MG	2A	3338	1/1	0.90	0.11	48,48,48,48	0
56	MG	1A	3281	1/1	0.90	0.17	52,52,52,52	0
56	MG	2A	3318	1/1	0.90	0.14	48,48,48,48	0
56	MG	1A	3408	1/1	0.90	0.17	36,36,36,36	0
56	MG	2A	3535	1/1	0.90	0.12	58,58,58,58	0
56	MG	1A	3206	1/1	0.90	0.33	40,40,40,40	0
56	MG	2A	3614	1/1	0.90	0.23	71,71,71,71	0
56	MG	1A	3381	1/1	0.90	0.08	47,47,47,47	0
56	MG	2A	3147	1/1	0.90	0.15	55,55,55,55	0
56	MG	2A	3396	1/1	0.90	0.13	53,53,53,53	0
56	MG	1x	114	1/1	0.90	0.14	68,68,68,68	0
56	MG	2A	3048	1/1	0.90	0.18	46,46,46,46	0
56	MG	2a	1614	1/1	0.90	0.29	58,58,58,58	0
56	MG	2A	3643	1/1	0.90	0.19	65,65,65,65	0
56	MG	1A	3613	1/1	0.90	0.12	34,34,34,34	0
56	MG	1A	3908	1/1	0.90	0.26	43,43,43,43	0
56	MG	2A	3223	1/1	0.90	0.11	56,56,56,56	0
56	MG	2w	3002	1/1	0.90	0.14	75,75,75,75	0
56	MG	2A	3634	1/1	0.90	0.17	62,62,62,62	0
56	MG	1a	1709	1/1	0.90	0.12	62,62,62,62	0
56	MG	2a	1688	1/1	0.90	0.09	65,65,65,65	0
56	MG	1a	1754	1/1	0.90	0.20	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3771	1/1	0.90	0.11	63,63,63,63	0
56	MG	2A	3283	1/1	0.90	0.14	41,41,41,41	0
56	MG	2A	3370	1/1	0.90	0.14	64,64,64,64	0
56	MG	1A	3701	1/1	0.90	0.10	58,58,58,58	0
56	MG	2A	3068	1/1	0.90	0.12	47,47,47,47	0
56	MG	2A	3480	1/1	0.90	0.12	53,53,53,53	0
56	MG	1a	1666	1/1	0.90	0.20	46,46,46,46	0
56	MG	1a	1821	1/1	0.91	0.21	72,72,72,72	0
56	MG	1A	3825	1/1	0.91	0.12	64,64,64,64	0
56	MG	2a	1785	1/1	0.91	0.15	58,58,58,58	0
56	MG	2A	3410	1/1	0.91	0.16	46,46,46,46	0
56	MG	2a	1628	1/1	0.91	0.15	66,66,66,66	0
56	MG	1A	3806	1/1	0.91	0.08	67,67,67,67	0
56	MG	2A	3119	1/1	0.91	0.10	54,54,54,54	0
56	MG	2A	3651	1/1	0.91	0.13	55,55,55,55	0
56	MG	2A	3203	1/1	0.91	0.27	42,42,42,42	0
56	MG	2A	3073	1/1	0.91	0.27	53,53,53,53	0
56	MG	1A	3734	1/1	0.91	0.14	58,58,58,58	0
56	MG	1E	302	1/1	0.91	0.30	35,35,35,35	0
56	MG	1x	104	1/1	0.91	0.59	54,54,54,54	0
56	MG	1A	3277	1/1	0.91	0.18	49,49,49,49	0
56	MG	2A	3115	1/1	0.91	0.06	62,62,62,62	0
56	MG	2A	3113	1/1	0.91	0.13	46,46,46,46	0
56	MG	1A	3843	1/1	0.91	0.30	47,47,47,47	0
56	MG	1a	1675	1/1	0.91	0.08	41,41,41,41	0
56	MG	2A	3584	1/1	0.91	0.13	70,70,70,70	0
56	MG	1A	3777	1/1	0.91	0.09	43,43,43,43	0
56	MG	2A	3071	1/1	0.91	0.08	34,34,34,34	0
56	MG	2O	201	1/1	0.91	0.22	54,54,54,54	0
56	MG	1A	3355	1/1	0.91	0.23	51,51,51,51	0
56	MG	2A	3406	1/1	0.91	0.20	58,58,58,58	0
56	MG	2A	3287	1/1	0.91	0.18	47,47,47,47	0
56	MG	1A	3499	1/1	0.91	0.15	49,49,49,49	0
56	MG	2a	1641	1/1	0.91	0.14	55,55,55,55	0
56	MG	2a	1792	1/1	0.91	0.23	76,76,76,76	0
56	MG	1A	3644	1/1	0.91	0.09	51,51,51,51	0
56	MG	1A	3536	1/1	0.91	0.17	24,24,24,24	0
56	MG	1A	3043	1/1	0.91	0.14	34,34,34,34	0
56	MG	2A	3276	1/1	0.91	0.10	31,31,31,31	0
56	MG	2A	3465	1/1	0.91	0.10	55,55,55,55	0
56	MG	2A	3158	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	3582	1/1	0.91	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3311	1/1	0.91	0.10	54,54,54,54	0
56	MG	2A	3166	1/1	0.91	0.11	45,45,45,45	0
56	MG	2A	3407	1/1	0.91	0.23	58,58,58,58	0
56	MG	2A	3472	1/1	0.91	0.14	48,48,48,48	0
56	MG	1A	3429	1/1	0.91	0.17	49,49,49,49	0
56	MG	2A	3330	1/1	0.91	0.17	35,35,35,35	0
56	MG	2A	3035	1/1	0.91	0.11	45,45,45,45	0
56	MG	2B	3007	1/1	0.91	0.18	74,74,74,74	0
56	MG	1a	1644	1/1	0.91	0.20	48,48,48,48	0
56	MG	1a	1793	1/1	0.91	0.12	74,74,74,74	0
56	MG	1A	3788	1/1	0.91	0.17	61,61,61,61	0
56	MG	2A	3296	1/1	0.91	0.20	42,42,42,42	0
56	MG	1f	3001	1/1	0.91	0.12	42,42,42,42	0
56	MG	1A	3516	1/1	0.91	0.09	65,65,65,65	0
56	MG	1Z	302	1/1	0.91	0.18	48,48,48,48	0
56	MG	1a	1725	1/1	0.91	0.11	63,63,63,63	0
56	MG	2a	1716	1/1	0.91	0.22	69,69,69,69	0
56	MG	2A	3447	1/1	0.91	0.13	41,41,41,41	0
56	MG	2t	3001	1/1	0.91	0.06	57,57,57,57	0
56	MG	1A	3140	1/1	0.91	0.57	47,47,47,47	0
56	MG	2A	3365	1/1	0.91	0.18	55,55,55,55	0
56	MG	2a	1609	1/1	0.91	0.09	47,47,47,47	0
56	MG	1A	3687	1/1	0.91	0.08	63,63,63,63	0
56	MG	2A	3224	1/1	0.91	0.08	49,49,49,49	0
56	MG	2a	1738	1/1	0.91	0.29	70,70,70,70	0
56	MG	1A	3135	1/1	0.91	0.24	30,30,30,30	0
56	MG	2A	3153	1/1	0.91	0.28	59,59,59,59	0
56	MG	1A	3483	1/1	0.91	0.17	27,27,27,27	0
56	MG	2A	3379	1/1	0.91	0.10	40,40,40,40	0
56	MG	1A	3662	1/1	0.91	0.19	45,45,45,45	0
56	MG	1A	3651	1/1	0.91	0.11	62,62,62,62	0
56	MG	1A	3089	1/1	0.91	0.22	54,54,54,54	0
56	MG	1A	3776	1/1	0.91	0.14	48,48,48,48	0
56	MG	2B	3012	1/1	0.91	0.10	65,65,65,65	0
56	MG	2A	3081	1/1	0.91	0.09	45,45,45,45	0
56	MG	2a	1627	1/1	0.91	0.09	61,61,61,61	0
56	MG	2A	3208	1/1	0.91	0.08	52,52,52,52	0
56	MG	1A	3234	1/1	0.91	0.19	50,50,50,50	0
56	MG	1A	3826	1/1	0.91	0.14	55,55,55,55	0
56	MG	1A	3081	1/1	0.91	0.41	35,35,35,35	0
56	MG	1d	502	1/1	0.91	0.38	58,58,58,58	0
56	MG	2A	3170	1/1	0.91	0.20	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3110	1/1	0.91	0.14	31,31,31,31	0
56	MG	2A	3077	1/1	0.91	0.15	51,51,51,51	0
56	MG	2A	3250	1/1	0.91	0.13	45,45,45,45	0
56	MG	1A	3637	1/1	0.91	0.13	54,54,54,54	0
56	MG	1A	3476	1/1	0.91	0.25	36,36,36,36	0
56	MG	2a	1767	1/1	0.91	0.17	55,55,55,55	0
56	MG	1A	3111	1/1	0.91	0.11	45,45,45,45	0
56	MG	2A	3619	1/1	0.91	0.33	45,45,45,45	0
56	MG	1A	3874	1/1	0.91	0.21	27,27,27,27	0
56	MG	2A	3490	1/1	0.91	0.20	73,73,73,73	0
56	MG	1A	3152	1/1	0.91	0.15	43,43,43,43	0
56	MG	1A	3535	1/1	0.91	0.11	40,40,40,40	0
56	MG	2a	1640	1/1	0.91	0.16	48,48,48,48	0
56	MG	1A	3743	1/1	0.91	0.27	52,52,52,52	0
56	MG	2G	3001	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3614	1/1	0.91	0.17	23,23,23,23	0
56	MG	1a	1699	1/1	0.91	0.19	68,68,68,68	0
56	MG	1A	3754	1/1	0.91	0.22	26,26,26,26	0
56	MG	2a	1698	1/1	0.91	0.14	64,64,64,64	0
56	MG	2A	3133	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3617	1/1	0.91	0.07	41,41,41,41	0
56	MG	1a	1601	1/1	0.91	0.10	68,68,68,68	0
56	MG	1a	1741	1/1	0.91	0.12	47,47,47,47	0
56	MG	1A	3681	1/1	0.91	0.16	37,37,37,37	0
56	MG	1x	111	1/1	0.91	0.12	55,55,55,55	0
56	MG	2A	3420	1/1	0.91	0.17	60,60,60,60	0
56	MG	2a	1759	1/1	0.91	0.11	75,75,75,75	0
56	MG	2A	3492	1/1	0.91	0.12	49,49,49,49	0
56	MG	1A	3059	1/1	0.91	0.13	66,66,66,66	0
56	MG	2a	1772	1/1	0.91	0.10	76,76,76,76	0
56	MG	2a	1658	1/1	0.91	0.12	81,81,81,81	0
56	MG	2A	3623	1/1	0.91	0.59	49,49,49,49	0
56	MG	1a	1685	1/1	0.91	0.23	57,57,57,57	0
56	MG	1a	1629	1/1	0.91	0.14	69,69,69,69	0
56	MG	1A	3540	1/1	0.91	0.19	55,55,55,55	0
56	MG	1A	3337	1/1	0.91	0.39	34,34,34,34	0
56	MG	1A	3732	1/1	0.91	0.13	55,55,55,55	0
56	MG	1A	3385	1/1	0.91	0.06	68,68,68,68	0
56	MG	2d	502	1/1	0.91	0.09	64,64,64,64	0
56	MG	1A	3357	1/1	0.91	0.21	60,60,60,60	0
56	MG	2A	3411	1/1	0.91	0.20	56,56,56,56	0
56	MG	1A	3888	1/1	0.91	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3484	1/1	0.91	0.16	46,46,46,46	0
56	MG	2A	3495	1/1	0.91	0.16	53,53,53,53	0
56	MG	1A	3606	1/1	0.91	0.12	62,62,62,62	0
56	MG	1A	3128	1/1	0.91	0.11	47,47,47,47	0
56	MG	1A	3295	1/1	0.91	0.20	49,49,49,49	0
56	MG	2A	3186	1/1	0.91	0.16	51,51,51,51	0
56	MG	1A	3267	1/1	0.91	0.19	63,63,63,63	0
56	MG	1A	3256	1/1	0.91	0.11	53,53,53,53	0
56	MG	2a	1766	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3626	1/1	0.91	0.07	44,44,44,44	0
56	MG	2A	3101	1/1	0.91	0.28	58,58,58,58	0
56	MG	2A	3001	1/1	0.91	0.29	63,63,63,63	0
56	MG	2A	3514	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3041	1/1	0.91	0.08	43,43,43,43	0
56	MG	2a	1787	1/1	0.91	0.14	62,62,62,62	0
56	MG	1A	3854	1/1	0.91	0.13	67,67,67,67	0
56	MG	1A	3463	1/1	0.91	0.18	57,57,57,57	0
56	MG	1A	3671	1/1	0.92	0.18	40,40,40,40	0
56	MG	1A	3702	1/1	0.92	0.18	26,26,26,26	0
56	MG	1A	3447	1/1	0.92	0.21	20,20,20,20	0
56	MG	2A	3304	1/1	0.92	0.12	48,48,48,48	0
56	MG	2A	3655	1/1	0.92	0.28	42,42,42,42	0
56	MG	2A	3484	1/1	0.92	0.27	56,56,56,56	0
56	MG	2A	3312	1/1	0.92	0.18	46,46,46,46	0
56	MG	1A	3219	1/1	0.92	0.19	57,57,57,57	0
56	MG	1a	1628	1/1	0.92	0.27	43,43,43,43	0
56	MG	2A	3627	1/1	0.92	0.08	51,51,51,51	0
56	MG	1A	3252	1/1	0.92	0.46	47,47,47,47	0
56	MG	1A	3629	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	1771	1/1	0.92	0.16	53,53,53,53	0
56	MG	1a	1707	1/1	0.92	0.26	49,49,49,49	0
56	MG	2A	3139	1/1	0.92	0.14	47,47,47,47	0
56	MG	2A	3433	1/1	0.92	0.12	37,37,37,37	0
56	MG	1a	1678	1/1	0.92	0.08	54,54,54,54	0
56	MG	1Y	502	1/1	0.92	0.23	60,60,60,60	0
56	MG	1A	3013	1/1	0.92	0.21	33,33,33,33	0
56	MG	2a	1778	1/1	0.92	0.23	78,78,78,78	0
56	MG	1A	3769	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3474	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3437	1/1	0.92	0.15	24,24,24,24	0
56	MG	1A	3270	1/1	0.92	0.16	48,48,48,48	0
56	MG	2a	1659	1/1	0.92	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3697	1/1	0.92	0.27	64,64,64,64	0
56	MG	2E	303	1/1	0.92	0.10	51,51,51,51	0
56	MG	1B	216	1/1	0.92	0.14	58,58,58,58	0
56	MG	1A	3850	1/1	0.92	0.12	54,54,54,54	0
56	MG	2a	1744	1/1	0.92	0.23	56,56,56,56	0
56	MG	2A	3146	1/1	0.92	0.09	47,47,47,47	0
56	MG	2A	3160	1/1	0.92	0.07	36,36,36,36	0
56	MG	1A	3255	1/1	0.92	0.28	44,44,44,44	0
56	MG	2a	1679	1/1	0.92	0.15	66,66,66,66	0
56	MG	1A	3661	1/1	0.92	0.11	51,51,51,51	0
56	MG	2A	3540	1/1	0.92	0.07	63,63,63,63	0
56	MG	1D	301	1/1	0.92	0.23	40,40,40,40	0
56	MG	2A	3320	1/1	0.92	0.13	40,40,40,40	0
59	ZN	29	501	1/1	0.92	0.09	64,64,64,64	0
56	MG	2D	304	1/1	0.92	0.54	38,38,38,38	0
56	MG	1A	3853	1/1	0.92	0.12	37,37,37,37	0
56	MG	2a	1638	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3585	1/1	0.92	0.14	34,34,34,34	0
56	MG	1A	3292	1/1	0.92	0.13	33,33,33,33	0
56	MG	2A	3095	1/1	0.92	0.74	65,65,65,65	0
56	MG	2A	3657	1/1	0.92	0.22	58,58,58,58	0
56	MG	1A	3376	1/1	0.92	0.21	51,51,51,51	0
56	MG	1A	3485	1/1	0.92	0.28	51,51,51,51	0
56	MG	2B	3020	1/1	0.92	0.10	66,66,66,66	0
56	MG	1a	1680	1/1	0.92	0.15	48,48,48,48	0
56	MG	1A	3377	1/1	0.92	0.16	42,42,42,42	0
56	MG	2A	3573	1/1	0.92	0.06	49,49,49,49	0
56	MG	1b	3001	1/1	0.92	0.27	68,68,68,68	0
56	MG	1B	202	1/1	0.92	0.17	61,61,61,61	0
56	MG	1a	1612	1/1	0.92	0.15	56,56,56,56	0
56	MG	1a	1794	1/1	0.92	0.13	54,54,54,54	0
56	MG	2a	1786	1/1	0.92	0.14	64,64,64,64	0
56	MG	2A	3669	1/1	0.92	0.13	47,47,47,47	0
56	MG	2A	3302	1/1	0.92	0.10	58,58,58,58	0
56	MG	2A	3496	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3394	1/1	0.92	0.18	43,43,43,43	0
56	MG	2A	3505	1/1	0.92	0.09	55,55,55,55	0
56	MG	2B	3008	1/1	0.92	0.21	61,61,61,61	0
56	MG	2A	3363	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3798	1/1	0.92	0.14	27,27,27,27	0
56	MG	2A	3415	1/1	0.92	0.15	59,59,59,59	0
56	MG	2A	3508	1/1	0.92	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3653	1/1	0.92	0.08	49,49,49,49	0
56	MG	2A	3436	1/1	0.92	0.15	45,45,45,45	0
56	MG	1A	3635	1/1	0.92	0.20	66,66,66,66	0
56	MG	1t	3001	1/1	0.92	0.13	49,49,49,49	0
56	MG	1A	3300	1/1	0.92	0.09	24,24,24,24	0
56	MG	1a	1762	1/1	0.92	0.18	64,64,64,64	0
56	MG	1A	3207	1/1	0.92	0.15	50,50,50,50	0
56	MG	1A	3663	1/1	0.92	0.12	43,43,43,43	0
56	MG	1W	3004	1/1	0.92	0.11	41,41,41,41	0
56	MG	2A	3416	1/1	0.92	0.18	44,44,44,44	0
56	MG	1A	3416	1/1	0.92	0.12	25,25,25,25	0
56	MG	1A	3491	1/1	0.92	0.12	46,46,46,46	0
56	MG	1A	3016	1/1	0.92	0.07	39,39,39,39	0
56	MG	2l	202	1/1	0.92	0.12	54,54,54,54	0
56	MG	2A	3055	1/1	0.92	0.11	47,47,47,47	0
56	MG	1A	3655	1/1	0.92	0.15	28,28,28,28	0
56	MG	1A	3654	1/1	0.92	0.12	27,27,27,27	0
56	MG	1A	3319	1/1	0.92	0.33	51,51,51,51	0
56	MG	2a	1669	1/1	0.92	0.16	67,67,67,67	0
56	MG	2A	3167	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3332	1/1	0.92	0.18	50,50,50,50	0
56	MG	1x	106	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	3167	1/1	0.92	0.21	50,50,50,50	0
56	MG	1a	1654	1/1	0.92	0.24	46,46,46,46	0
56	MG	2A	3390	1/1	0.92	0.09	39,39,39,39	0
56	MG	2a	1703	1/1	0.92	0.10	76,76,76,76	0
56	MG	2A	3114	1/1	0.92	0.14	49,49,49,49	0
56	MG	1A	3305	1/1	0.92	0.14	55,55,55,55	0
56	MG	1A	3488	1/1	0.92	0.23	32,32,32,32	0
56	MG	1a	1714	1/1	0.92	0.23	61,61,61,61	0
56	MG	2A	3255	1/1	0.92	0.15	36,36,36,36	0
56	MG	1a	1726	1/1	0.92	0.10	87,87,87,87	0
56	MG	1A	3587	1/1	0.92	0.10	40,40,40,40	0
56	MG	1A	3618	1/1	0.92	0.16	29,29,29,29	0
56	MG	1A	3807	1/1	0.92	0.14	63,63,63,63	0
56	MG	2a	1639	1/1	0.92	0.13	54,54,54,54	0
56	MG	2a	1731	1/1	0.92	0.16	87,87,87,87	0
56	MG	2a	1801	1/1	0.92	0.13	82,82,82,82	0
56	MG	1a	1815	1/1	0.92	0.22	74,74,74,74	0
56	MG	1A	3067	1/1	0.92	0.58	42,42,42,42	0
56	MG	2A	3493	1/1	0.92	0.10	59,59,59,59	0
56	MG	2A	3284	1/1	0.92	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3249	1/1	0.92	0.13	43,43,43,43	0
56	MG	1A	3698	1/1	0.92	0.29	65,65,65,65	0
56	MG	1A	3500	1/1	0.92	0.16	62,62,62,62	0
56	MG	1A	3790	1/1	0.92	0.09	48,48,48,48	0
56	MG	2A	3246	1/1	0.92	0.15	55,55,55,55	0
56	MG	2a	1622	1/1	0.92	0.11	42,42,42,42	0
56	MG	2A	3671	1/1	0.92	0.20	44,44,44,44	0
56	MG	1A	3571	1/1	0.92	0.21	33,33,33,33	0
56	MG	2A	3017	1/1	0.92	0.15	42,42,42,42	0
56	MG	2A	3376	1/1	0.92	0.06	51,51,51,51	0
56	MG	2A	3328	1/1	0.92	0.11	48,48,48,48	0
56	MG	2a	1702	1/1	0.92	0.20	64,64,64,64	0
56	MG	1A	3607	1/1	0.92	0.09	48,48,48,48	0
56	MG	1A	3542	1/1	0.92	0.19	33,33,33,33	0
56	MG	20	101	1/1	0.92	0.44	68,68,68,68	0
56	MG	1A	3204	1/1	0.92	0.08	38,38,38,38	0
56	MG	2A	3289	1/1	0.92	0.17	56,56,56,56	0
56	MG	2a	1748	1/1	0.92	0.13	59,59,59,59	0
56	MG	2A	3131	1/1	0.92	0.18	55,55,55,55	0
56	MG	2a	1664	1/1	0.92	0.11	60,60,60,60	0
56	MG	2A	3345	1/1	0.92	0.16	31,31,31,31	0
56	MG	2A	3274	1/1	0.92	0.12	47,47,47,47	0
56	MG	1a	1809	1/1	0.92	0.09	40,40,40,40	0
56	MG	1A	3017	1/1	0.92	0.15	53,53,53,53	0
56	MG	1A	3926	1/1	0.92	0.25	44,44,44,44	0
56	MG	2A	3034	1/1	0.92	0.12	34,34,34,34	0
56	MG	1A	3048	1/1	0.92	0.16	32,32,32,32	0
56	MG	1A	3166	1/1	0.92	0.24	65,65,65,65	0
56	MG	2A	3196	1/1	0.92	0.30	47,47,47,47	0
56	MG	2A	3564	1/1	0.92	0.36	62,62,62,62	0
56	MG	1a	1825	1/1	0.92	0.11	69,69,69,69	0
56	MG	2A	3636	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3652	1/1	0.92	0.26	54,54,54,54	0
56	MG	2A	3645	1/1	0.92	0.08	45,45,45,45	0
56	MG	1A	3359	1/1	0.92	0.14	22,22,22,22	0
56	MG	1a	1650	1/1	0.92	0.23	57,57,57,57	0
56	MG	1A	3344	1/1	0.92	0.26	40,40,40,40	0
56	MG	2a	1756	1/1	0.92	0.14	78,78,78,78	0
56	MG	1A	3137	1/1	0.92	0.27	45,45,45,45	0
59	ZN	15	104	1/1	0.92	0.29	81,81,81,81	0
56	MG	1A	3099	1/1	0.92	0.13	44,44,44,44	0
56	MG	1x	105	1/1	0.93	0.19	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3272	1/1	0.93	0.22	39,39,39,39	0
56	MG	2a	1621	1/1	0.93	0.08	80,80,80,80	0
56	MG	1A	3335	1/1	0.93	0.19	63,63,63,63	0
56	MG	2V	3003	1/1	0.93	0.53	57,57,57,57	0
56	MG	2T	3001	1/1	0.93	0.18	45,45,45,45	0
56	MG	1A	3842	1/1	0.93	0.17	56,56,56,56	0
56	MG	2a	1646	1/1	0.93	0.22	68,68,68,68	0
56	MG	1A	3282	1/1	0.93	0.25	58,58,58,58	0
56	MG	19	502	1/1	0.93	0.17	49,49,49,49	0
56	MG	2a	1647	1/1	0.93	0.10	68,68,68,68	0
56	MG	15	103	1/1	0.93	0.24	40,40,40,40	0
56	MG	1A	3221	1/1	0.93	0.27	30,30,30,30	0
56	MG	1A	3757	1/1	0.93	0.12	23,23,23,23	0
56	MG	2O	202	1/1	0.93	0.13	52,52,52,52	0
56	MG	1w	3004	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3131	1/1	0.93	0.28	40,40,40,40	0
56	MG	1a	1621	1/1	0.93	0.12	70,70,70,70	0
56	MG	2A	3500	1/1	0.93	0.29	35,35,35,35	0
56	MG	2A	3580	1/1	0.93	0.09	56,56,56,56	0
56	MG	1A	3764	1/1	0.93	0.12	47,47,47,47	0
56	MG	2A	3596	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3514	1/1	0.93	0.26	66,66,66,66	0
56	MG	2A	3069	1/1	0.93	0.11	52,52,52,52	0
56	MG	1A	3823	1/1	0.93	0.12	67,67,67,67	0
56	MG	2A	3082	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	3430	1/1	0.93	0.17	47,47,47,47	0
56	MG	1A	3849	1/1	0.93	0.07	46,46,46,46	0
56	MG	1m	3001	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	3143	1/1	0.93	0.18	48,48,48,48	0
56	MG	2A	3130	1/1	0.93	0.14	66,66,66,66	0
56	MG	2A	3323	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3647	1/1	0.93	0.09	59,59,59,59	0
56	MG	1A	3464	1/1	0.93	0.10	57,57,57,57	0
56	MG	1a	1693	1/1	0.93	0.16	44,44,44,44	0
56	MG	2A	3181	1/1	0.93	0.17	55,55,55,55	0
56	MG	1A	3875	1/1	0.93	0.13	22,22,22,22	0
56	MG	2A	3409	1/1	0.93	0.14	54,54,54,54	0
56	MG	2A	3568	1/1	0.93	0.28	54,54,54,54	0
56	MG	1A	3804	1/1	0.93	0.19	61,61,61,61	0
56	MG	2a	1653	1/1	0.93	0.13	62,62,62,62	0
56	MG	1A	3924	1/1	0.93	0.13	49,49,49,49	0
56	MG	1a	1687	1/1	0.93	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1O	8003	1/1	0.93	0.22	54,54,54,54	0
56	MG	1A	3658	1/1	0.93	0.15	52,52,52,52	0
56	MG	1a	1822	1/1	0.93	0.16	65,65,65,65	0
56	MG	1A	3682	1/1	0.93	0.18	47,47,47,47	0
56	MG	1A	3289	1/1	0.93	0.31	44,44,44,44	0
56	MG	1A	3524	1/1	0.93	0.14	32,32,32,32	0
56	MG	1A	3714	1/1	0.93	0.14	56,56,56,56	0
56	MG	2A	3430	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3554	1/1	0.93	0.12	42,42,42,42	0
56	MG	2A	3637	1/1	0.93	0.15	52,52,52,52	0
56	MG	2Q	3003	1/1	0.93	0.28	48,48,48,48	0
56	MG	2A	3632	1/1	0.93	0.05	57,57,57,57	0
56	MG	1A	3761	1/1	0.93	0.15	71,71,71,71	0
56	MG	1A	3691	1/1	0.93	0.11	60,60,60,60	0
56	MG	2A	3256	1/1	0.93	0.12	57,57,57,57	0
56	MG	1A	3441	1/1	0.93	0.13	50,50,50,50	0
56	MG	1A	3472	1/1	0.93	0.10	37,37,37,37	0
56	MG	1A	3811	1/1	0.93	0.15	46,46,46,46	0
56	MG	2I	101	1/1	0.93	0.91	49,49,49,49	0
56	MG	1a	1729	1/1	0.93	0.22	67,67,67,67	0
56	MG	2x	3003	1/1	0.93	0.06	72,72,72,72	0
56	MG	2A	3559	1/1	0.93	0.10	64,64,64,64	0
56	MG	2a	1620	1/1	0.93	0.20	55,55,55,55	0
56	MG	1A	3100	1/1	0.93	0.20	55,55,55,55	0
56	MG	1A	3217	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3848	1/1	0.93	0.19	66,66,66,66	0
56	MG	1B	203	1/1	0.93	0.17	33,33,33,33	0
56	MG	2A	3124	1/1	0.93	0.21	50,50,50,50	0
56	MG	1A	3805	1/1	0.93	0.16	52,52,52,52	0
56	MG	1a	1803	1/1	0.93	0.28	69,69,69,69	0
56	MG	2A	3378	1/1	0.93	0.11	40,40,40,40	0
56	MG	2a	1666	1/1	0.93	0.13	63,63,63,63	0
56	MG	2a	1784	1/1	0.93	0.28	87,87,87,87	0
56	MG	2A	3672	1/1	0.93	0.14	68,68,68,68	0
56	MG	1A	3293	1/1	0.93	0.20	60,60,60,60	0
56	MG	1A	3779	1/1	0.93	0.18	70,70,70,70	0
56	MG	1A	3053	1/1	0.93	0.15	48,48,48,48	0
56	MG	1a	1606	1/1	0.93	0.23	57,57,57,57	0
56	MG	2A	3005	1/1	0.93	0.14	50,50,50,50	0
56	MG	1A	3280	1/1	0.93	0.21	44,44,44,44	0
56	MG	1Q	3003	1/1	0.93	0.17	41,41,41,41	0
56	MG	1A	3601	1/1	0.93	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3666	1/1	0.93	0.19	45,45,45,45	0
56	MG	2A	3169	1/1	0.93	0.19	41,41,41,41	0
56	MG	1A	3114	1/1	0.93	0.26	41,41,41,41	0
56	MG	2A	3401	1/1	0.93	0.19	61,61,61,61	0
56	MG	2A	3353	1/1	0.93	0.17	47,47,47,47	0
56	MG	2A	3123	1/1	0.93	0.52	52,52,52,52	0
56	MG	2A	3143	1/1	0.93	0.21	56,56,56,56	0
56	MG	1A	3275	1/1	0.93	0.14	48,48,48,48	0
56	MG	2A	3109	1/1	0.93	0.08	40,40,40,40	0
56	MG	1A	3598	1/1	0.93	0.16	61,61,61,61	0
56	MG	2A	3566	1/1	0.93	0.22	45,45,45,45	0
56	MG	2A	3307	1/1	0.93	0.12	30,30,30,30	0
56	MG	2A	3079	1/1	0.93	0.11	42,42,42,42	0
56	MG	2A	3164	1/1	0.93	0.60	40,40,40,40	0
56	MG	2A	3037	1/1	0.93	0.11	51,51,51,51	0
56	MG	2a	1761	1/1	0.93	0.11	71,71,71,71	0
56	MG	1A	3133	1/1	0.93	0.12	52,52,52,52	0
56	MG	2a	1750	1/1	0.93	0.22	66,66,66,66	0
56	MG	2a	1707	1/1	0.93	0.15	43,43,43,43	0
56	MG	1A	3083	1/1	0.93	0.16	37,37,37,37	0
56	MG	1A	3262	1/1	0.93	0.33	31,31,31,31	0
56	MG	2A	3479	1/1	0.93	0.08	53,53,53,53	0
56	MG	1A	3361	1/1	0.93	0.20	55,55,55,55	0
56	MG	1A	3203	1/1	0.93	0.23	45,45,45,45	0
56	MG	1a	1648	1/1	0.93	0.12	48,48,48,48	0
56	MG	2A	3178	1/1	0.93	0.13	41,41,41,41	0
56	MG	2A	3200	1/1	0.93	0.09	56,56,56,56	0
56	MG	2A	3475	1/1	0.93	0.08	41,41,41,41	0
56	MG	1a	1638	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3528	1/1	0.93	0.15	34,34,34,34	0
56	MG	2A	3260	1/1	0.93	0.17	30,30,30,30	0
56	MG	1B	206	1/1	0.93	0.18	44,44,44,44	0
56	MG	2A	3464	1/1	0.93	0.07	59,59,59,59	0
56	MG	1A	3413	1/1	0.93	0.07	62,62,62,62	0
56	MG	2A	3613	1/1	0.93	0.32	56,56,56,56	0
56	MG	1A	3220	1/1	0.93	0.21	31,31,31,31	0
56	MG	2A	3563	1/1	0.93	0.10	60,60,60,60	0
56	MG	2A	3059	1/1	0.93	0.08	66,66,66,66	0
56	MG	1a	1775	1/1	0.93	0.24	58,58,58,58	0
56	MG	1A	3645	1/1	0.93	0.09	58,58,58,58	0
56	MG	2B	3017	1/1	0.93	0.18	59,59,59,59	0
56	MG	2A	3589	1/1	0.93	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3209	1/1	0.93	0.15	55,55,55,55	0
56	MG	1A	3632	1/1	0.93	0.31	40,40,40,40	0
56	MG	1F	305	1/1	0.93	0.14	36,36,36,36	0
56	MG	1A	3454	1/1	0.93	0.16	24,24,24,24	0
56	MG	1a	1733	1/1	0.93	0.16	51,51,51,51	0
56	MG	2A	3091	1/1	0.93	0.14	45,45,45,45	0
56	MG	2A	3453	1/1	0.93	0.15	32,32,32,32	0
56	MG	2A	3285	1/1	0.93	0.13	47,47,47,47	0
56	MG	1A	3061	1/1	0.93	0.20	38,38,38,38	0
56	MG	1X	103	1/1	0.93	0.19	38,38,38,38	0
56	MG	2A	3612	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3787	1/1	0.93	0.14	62,62,62,62	0
56	MG	2A	3380	1/1	0.93	0.12	35,35,35,35	0
56	MG	2A	3469	1/1	0.93	0.26	43,43,43,43	0
56	MG	1A	3354	1/1	0.93	0.11	42,42,42,42	0
56	MG	2A	3585	1/1	0.93	0.08	36,36,36,36	0
56	MG	2A	3315	1/1	0.93	0.13	39,39,39,39	0
56	MG	1a	1798	1/1	0.93	0.10	67,67,67,67	0
56	MG	1A	3378	1/1	0.93	0.11	45,45,45,45	0
56	MG	2A	3520	1/1	0.93	0.08	64,64,64,64	0
56	MG	1A	3303	1/1	0.93	0.26	28,28,28,28	0
56	MG	2a	1635	1/1	0.93	0.18	61,61,61,61	0
56	MG	1A	3197	1/1	0.93	0.17	44,44,44,44	0
56	MG	1A	3678	1/1	0.93	0.08	46,46,46,46	0
56	MG	2A	3176	1/1	0.93	0.20	37,37,37,37	0
56	MG	2A	3183	1/1	0.93	0.13	29,29,29,29	0
56	MG	2A	3439	1/1	0.93	0.16	39,39,39,39	0
56	MG	2A	3549	1/1	0.93	0.16	56,56,56,56	0
56	MG	16	102	1/1	0.93	0.24	41,41,41,41	0
56	MG	2A	3270	1/1	0.93	0.08	53,53,53,53	0
56	MG	1A	3323	1/1	0.93	0.23	55,55,55,55	0
56	MG	1a	1723	1/1	0.93	0.10	61,61,61,61	0
56	MG	2A	3604	1/1	0.93	0.08	47,47,47,47	0
56	MG	1A	3141	1/1	0.93	0.55	44,44,44,44	0
56	MG	1A	3648	1/1	0.93	0.19	69,69,69,69	0
56	MG	1a	1744	1/1	0.93	0.12	63,63,63,63	0
56	MG	2A	3521	1/1	0.93	0.16	56,56,56,56	0
56	MG	2a	1720	1/1	0.93	0.13	76,76,76,76	0
56	MG	1A	3208	1/1	0.94	0.47	42,42,42,42	0
56	MG	1F	301	1/1	0.94	0.21	49,49,49,49	0
56	MG	2A	3190	1/1	0.94	0.26	37,37,37,37	0
56	MG	1A	3031	1/1	0.94	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1713	1/1	0.94	0.19	52,52,52,52	0
56	MG	1A	3566	1/1	0.94	0.18	32,32,32,32	0
56	MG	1A	3821	1/1	0.94	0.16	60,60,60,60	0
56	MG	1A	3298	1/1	0.94	0.23	53,53,53,53	0
56	MG	1A	3080	1/1	0.94	0.34	41,41,41,41	0
56	MG	1A	3744	1/1	0.94	0.09	40,40,40,40	0
56	MG	1a	1748	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3387	1/1	0.94	0.16	18,18,18,18	0
56	MG	1a	1711	1/1	0.94	0.19	68,68,68,68	0
56	MG	1X	101	1/1	0.94	0.17	38,38,38,38	0
56	MG	2a	1777	1/1	0.94	0.12	53,53,53,53	0
56	MG	2A	3159	1/1	0.94	0.27	44,44,44,44	0
57	4M2	2A	3673	57/57	0.94	0.29	26,50,69,76	0
56	MG	1V	201	1/1	0.94	0.21	55,55,55,55	0
56	MG	2A	3333	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3486	1/1	0.94	0.23	27,27,27,27	0
56	MG	2A	3523	1/1	0.94	0.12	44,44,44,44	0
56	MG	1A	3627	1/1	0.94	0.18	66,66,66,66	0
56	MG	2a	1741	1/1	0.94	0.13	65,65,65,65	0
56	MG	1A	3162	1/1	0.94	0.23	39,39,39,39	0
56	MG	1a	1739	1/1	0.94	0.15	70,70,70,70	0
56	MG	2A	3438	1/1	0.94	0.08	36,36,36,36	0
56	MG	1A	3925	1/1	0.94	0.30	44,44,44,44	0
56	MG	1A	3565	1/1	0.94	0.20	29,29,29,29	0
56	MG	1A	3715	1/1	0.94	0.17	69,69,69,69	0
56	MG	1E	307	1/1	0.94	0.18	36,36,36,36	0
56	MG	1A	3532	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3541	1/1	0.94	0.08	58,58,58,58	0
56	MG	2A	3393	1/1	0.94	0.20	51,51,51,51	0
56	MG	1T	202	1/1	0.94	0.14	43,43,43,43	0
56	MG	2a	1730	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3333	1/1	0.94	0.17	40,40,40,40	0
56	MG	2A	3199	1/1	0.94	0.39	60,60,60,60	0
56	MG	2A	3555	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3423	1/1	0.94	0.11	34,34,34,34	0
56	MG	2A	3616	1/1	0.94	0.11	69,69,69,69	0
56	MG	2A	3574	1/1	0.94	0.05	52,52,52,52	0
56	MG	1A	3312	1/1	0.94	0.34	60,60,60,60	0
56	MG	25	503	1/1	0.94	0.93	49,49,49,49	0
56	MG	1A	3404	1/1	0.94	0.13	52,52,52,52	0
56	MG	1a	1632	1/1	0.94	0.10	78,78,78,78	0
56	MG	1A	3185	1/1	0.94	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1682	1/1	0.94	0.19	43,43,43,43	0
56	MG	1A	3409	1/1	0.94	0.14	33,33,33,33	0
56	MG	1A	3510	1/1	0.94	0.17	52,52,52,52	0
56	MG	1a	1764	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3844	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3724	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3507	1/1	0.94	0.11	57,57,57,57	0
56	MG	2A	3372	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3608	1/1	0.94	0.15	60,60,60,60	0
56	MG	1A	3562	1/1	0.94	0.16	29,29,29,29	0
56	MG	1A	3567	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3343	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3308	1/1	0.94	0.10	42,42,42,42	0
56	MG	25	502	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3770	1/1	0.94	0.08	63,63,63,63	0
56	MG	1U	202	1/1	0.94	0.47	40,40,40,40	0
56	MG	2V	3004	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3759	1/1	0.94	0.23	43,43,43,43	0
56	MG	1A	3226	1/1	0.94	0.23	57,57,57,57	0
56	MG	2A	3078	1/1	0.94	0.18	51,51,51,51	0
56	MG	1A	3336	1/1	0.94	0.21	28,28,28,28	0
56	MG	1A	3087	1/1	0.94	0.20	63,63,63,63	0
56	MG	1A	3329	1/1	0.94	0.09	54,54,54,54	0
56	MG	2A	3054	1/1	0.94	0.17	50,50,50,50	0
56	MG	1a	1643	1/1	0.94	0.28	61,61,61,61	0
56	MG	2A	3377	1/1	0.94	0.11	41,41,41,41	0
56	MG	2A	3301	1/1	0.94	0.14	45,45,45,45	0
56	MG	1a	1789	1/1	0.94	0.15	75,75,75,75	0
56	MG	1a	1769	1/1	0.94	0.26	58,58,58,58	0
56	MG	1A	3003	1/1	0.94	0.28	32,32,32,32	0
56	MG	1D	307	1/1	0.94	0.21	40,40,40,40	0
56	MG	1A	3214	1/1	0.94	0.14	54,54,54,54	0
56	MG	2A	3004	1/1	0.94	0.20	50,50,50,50	0
56	MG	1A	3817	1/1	0.94	0.24	54,54,54,54	0
56	MG	1A	3422	1/1	0.94	0.20	45,45,45,45	0
56	MG	2A	3373	1/1	0.94	0.15	54,54,54,54	0
56	MG	1A	3636	1/1	0.94	0.20	51,51,51,51	0
56	MG	1A	3858	1/1	0.94	0.18	45,45,45,45	0
56	MG	2A	3517	1/1	0.94	0.17	46,46,46,46	0
56	MG	2A	3444	1/1	0.94	0.07	45,45,45,45	0
56	MG	2a	1717	1/1	0.94	0.07	63,63,63,63	0
56	MG	1A	3782	1/1	0.94	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3259	1/1	0.94	0.20	37,37,37,37	0
56	MG	1A	3497	1/1	0.94	0.12	26,26,26,26	0
56	MG	2A	3028	1/1	0.94	0.33	40,40,40,40	0
56	MG	2A	3216	1/1	0.94	0.19	57,57,57,57	0
56	MG	1A	3035	1/1	0.94	0.28	41,41,41,41	0
56	MG	1A	3309	1/1	0.94	0.24	66,66,66,66	0
56	MG	1A	3411	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3679	1/1	0.94	0.15	61,61,61,61	0
56	MG	1A	3921	1/1	0.94	0.24	38,38,38,38	0
56	MG	1A	3094	1/1	0.94	0.13	41,41,41,41	0
56	MG	1A	3556	1/1	0.94	0.25	62,62,62,62	0
56	MG	1A	3044	1/1	0.94	0.12	22,22,22,22	0
56	MG	23	101	1/1	0.94	0.42	62,62,62,62	0
56	MG	1A	3110	1/1	0.94	0.29	38,38,38,38	0
56	MG	2A	3050	1/1	0.94	0.15	55,55,55,55	0
56	MG	2A	3349	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	3693	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3116	1/1	0.94	0.71	51,51,51,51	0
56	MG	1A	3383	1/1	0.94	0.13	31,31,31,31	0
56	MG	1w	3002	1/1	0.94	0.06	37,37,37,37	0
56	MG	1N	3006	1/1	0.94	0.17	44,44,44,44	0
56	MG	1D	305	1/1	0.94	0.18	38,38,38,38	0
59	ZN	2Y	501	1/1	0.94	0.07	85,85,85,85	0
56	MG	2A	3045	1/1	0.94	0.11	38,38,38,38	0
56	MG	2A	3272	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3151	1/1	0.94	0.23	44,44,44,44	0
56	MG	2A	3192	1/1	0.94	0.08	46,46,46,46	0
56	MG	2A	3025	1/1	0.94	0.76	60,60,60,60	0
56	MG	2A	3022	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	3545	1/1	0.94	0.21	49,49,49,49	0
56	MG	2a	1765	1/1	0.94	0.16	61,61,61,61	0
56	MG	2A	3481	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3172	1/1	0.94	0.23	41,41,41,41	0
56	MG	2A	3487	1/1	0.94	0.25	58,58,58,58	0
56	MG	2a	1747	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3388	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3002	1/1	0.94	0.16	32,32,32,32	0
56	MG	2A	3142	1/1	0.94	0.13	44,44,44,44	0
56	MG	2A	3221	1/1	0.94	0.15	35,35,35,35	0
56	MG	2A	3066	1/1	0.94	0.08	39,39,39,39	0
56	MG	1a	1627	1/1	0.94	0.10	42,42,42,42	0
56	MG	1a	1636	1/1	0.94	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1690	1/1	0.94	0.16	35,35,35,35	0
56	MG	1A	3315	1/1	0.94	0.16	46,46,46,46	0
56	MG	2A	3515	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3534	1/1	0.94	0.09	40,40,40,40	0
56	MG	2A	3381	1/1	0.94	0.09	48,48,48,48	0
56	MG	1A	3530	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3709	1/1	0.94	0.15	50,50,50,50	0
56	MG	1A	3356	1/1	0.94	0.16	26,26,26,26	0
56	MG	1A	3090	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3304	1/1	0.94	0.11	39,39,39,39	0
56	MG	1y	3003	1/1	0.94	0.24	59,59,59,59	0
56	MG	1A	3814	1/1	0.94	0.12	39,39,39,39	0
56	MG	2a	1719	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3891	1/1	0.94	0.15	57,57,57,57	0
56	MG	2A	3556	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3006	1/1	0.94	0.14	42,42,42,42	0
56	MG	1A	3307	1/1	0.94	0.24	33,33,33,33	0
56	MG	2A	3451	1/1	0.94	0.13	39,39,39,39	0
56	MG	1x	109	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3168	1/1	0.94	0.09	44,44,44,44	0
56	MG	2g	8001	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3086	1/1	0.94	0.15	51,51,51,51	0
56	MG	2U	201	1/1	0.94	0.28	44,44,44,44	0
56	MG	2A	3654	1/1	0.94	0.10	46,46,46,46	0
56	MG	1A	3555	1/1	0.94	0.25	40,40,40,40	0
56	MG	2A	3145	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3235	1/1	0.94	0.13	53,53,53,53	0
56	MG	2a	1663	1/1	0.94	0.22	55,55,55,55	0
56	MG	1A	3887	1/1	0.94	0.13	27,27,27,27	0
56	MG	2A	3456	1/1	0.94	0.21	39,39,39,39	0
56	MG	2A	3434	1/1	0.94	0.12	34,34,34,34	0
56	MG	2a	1671	1/1	0.94	0.10	86,86,86,86	0
56	MG	1A	3199	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3421	1/1	0.94	0.13	36,36,36,36	0
56	MG	2A	3217	1/1	0.94	0.11	68,68,68,68	0
56	MG	1A	3161	1/1	0.94	0.16	32,32,32,32	0
56	MG	2A	3432	1/1	0.94	0.07	54,54,54,54	0
56	MG	2a	1795	1/1	0.94	0.20	76,76,76,76	0
56	MG	2A	3346	1/1	0.94	0.07	45,45,45,45	0
56	MG	2A	3023	1/1	0.94	0.36	43,43,43,43	0
56	MG	2A	3452	1/1	0.94	0.17	40,40,40,40	0
56	MG	1a	1795	1/1	0.94	0.19	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3711	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3032	1/1	0.94	0.20	47,47,47,47	0
56	MG	1A	3224	1/1	0.94	0.17	32,32,32,32	0
56	MG	2A	3074	1/1	0.94	0.14	50,50,50,50	0
56	MG	2A	3400	1/1	0.94	0.09	58,58,58,58	0
56	MG	1A	3507	1/1	0.94	0.10	60,60,60,60	0
56	MG	1A	3597	1/1	0.94	0.13	45,45,45,45	0
56	MG	2A	3491	1/1	0.94	0.09	51,51,51,51	0
56	MG	1a	1696	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3784	1/1	0.94	0.13	45,45,45,45	0
56	MG	2A	3477	1/1	0.94	0.17	41,41,41,41	0
56	MG	1A	3070	1/1	0.94	0.29	60,60,60,60	0
56	MG	1A	3883	1/1	0.94	0.27	33,33,33,33	0
56	MG	1A	3579	1/1	0.94	0.16	27,27,27,27	0
56	MG	2A	3610	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3228	1/1	0.94	0.26	51,51,51,51	0
56	MG	2A	3184	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3721	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	3620	1/1	0.94	0.21	43,43,43,43	0
56	MG	2A	3646	1/1	0.94	0.19	72,72,72,72	0
56	MG	2A	3106	1/1	0.94	0.14	55,55,55,55	0
56	MG	1A	3523	1/1	0.94	0.21	33,33,33,33	0
56	MG	1A	3105	1/1	0.94	0.21	39,39,39,39	0
56	MG	2A	3398	1/1	0.94	0.08	56,56,56,56	0
56	MG	1a	1613	1/1	0.94	0.30	47,47,47,47	0
56	MG	2a	1654	1/1	0.94	0.23	69,69,69,69	0
56	MG	1A	3546	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3526	1/1	0.94	0.09	64,64,64,64	0
56	MG	2A	3665	1/1	0.95	0.20	53,53,53,53	0
56	MG	2A	3466	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3400	1/1	0.95	0.11	35,35,35,35	0
56	MG	1A	3146	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	3163	1/1	0.95	0.25	43,43,43,43	0
56	MG	2a	1714	1/1	0.95	0.14	56,56,56,56	0
56	MG	2A	3019	1/1	0.95	0.11	47,47,47,47	0
56	MG	1a	1743	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3326	1/1	0.95	0.16	44,44,44,44	0
56	MG	1A	3263	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3328	1/1	0.95	0.26	61,61,61,61	0
56	MG	2l	201	1/1	0.95	0.42	77,77,77,77	0
56	MG	1A	3603	1/1	0.95	0.24	54,54,54,54	0
56	MG	1A	3616	1/1	0.95	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3929	1/1	0.95	0.36	39,39,39,39	0
56	MG	2A	3364	1/1	0.95	0.10	65,65,65,65	0
56	MG	1A	3008	1/1	0.95	0.13	29,29,29,29	0
56	MG	1A	3456	1/1	0.95	0.13	23,23,23,23	0
56	MG	2a	1633	1/1	0.95	0.15	71,71,71,71	0
56	MG	1A	3040	1/1	0.95	0.21	38,38,38,38	0
56	MG	1a	1799	1/1	0.95	0.07	46,46,46,46	0
56	MG	1A	3164	1/1	0.95	0.17	53,53,53,53	0
56	MG	2A	3639	1/1	0.95	0.07	53,53,53,53	0
56	MG	1A	3366	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3365	1/1	0.95	0.17	45,45,45,45	0
56	MG	2A	3027	1/1	0.95	0.46	45,45,45,45	0
56	MG	1A	3895	1/1	0.95	0.17	39,39,39,39	0
56	MG	1A	3269	1/1	0.95	0.22	57,57,57,57	0
56	MG	1A	3879	1/1	0.95	0.20	34,34,34,34	0
56	MG	1A	3881	1/1	0.95	0.15	46,46,46,46	0
56	MG	1a	1715	1/1	0.95	0.14	62,62,62,62	0
56	MG	1A	3576	1/1	0.95	0.22	24,24,24,24	0
56	MG	1A	3071	1/1	0.95	0.18	27,27,27,27	0
56	MG	2A	3051	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3151	1/1	0.95	0.23	36,36,36,36	0
56	MG	2A	3233	1/1	0.95	0.15	48,48,48,48	0
56	MG	1A	3421	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3508	1/1	0.95	0.11	41,41,41,41	0
56	MG	1A	3889	1/1	0.95	0.11	40,40,40,40	0
56	MG	2F	301	1/1	0.95	0.30	47,47,47,47	0
56	MG	1A	3077	1/1	0.95	0.25	47,47,47,47	0
56	MG	1a	1784	1/1	0.95	0.08	45,45,45,45	0
56	MG	2a	1704	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3050	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3062	1/1	0.95	0.09	41,41,41,41	0
56	MG	2A	3278	1/1	0.95	0.08	38,38,38,38	0
56	MG	2I	103	1/1	0.95	0.10	45,45,45,45	0
56	MG	1a	1691	1/1	0.95	0.15	47,47,47,47	0
56	MG	1a	1742	1/1	0.95	0.12	20,20,20,20	0
56	MG	2A	3524	1/1	0.95	0.11	46,46,46,46	0
56	MG	18	101	1/1	0.95	0.25	37,37,37,37	0
56	MG	1a	1801	1/1	0.95	0.21	59,59,59,59	0
56	MG	1a	1757	1/1	0.95	0.11	57,57,57,57	0
56	MG	2A	3238	1/1	0.95	0.53	46,46,46,46	0
56	MG	15	102	1/1	0.95	0.18	39,39,39,39	0
56	MG	1A	3592	1/1	0.95	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3370	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3664	1/1	0.95	0.16	50,50,50,50	0
56	MG	1A	3362	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3205	1/1	0.95	0.56	41,41,41,41	0
56	MG	1A	3449	1/1	0.95	0.13	27,27,27,27	0
56	MG	1A	3020	1/1	0.95	0.08	40,40,40,40	0
56	MG	1A	3611	1/1	0.95	0.16	22,22,22,22	0
56	MG	1A	3866	1/1	0.95	0.13	63,63,63,63	0
56	MG	2A	3383	1/1	0.95	0.21	40,40,40,40	0
56	MG	1U	204	1/1	0.95	0.43	55,55,55,55	0
56	MG	1x	102	1/1	0.95	0.14	40,40,40,40	0
56	MG	2N	8001	1/1	0.95	0.08	53,53,53,53	0
56	MG	2A	3450	1/1	0.95	0.07	34,34,34,34	0
56	MG	2A	3204	1/1	0.95	0.23	55,55,55,55	0
56	MG	1A	3026	1/1	0.95	0.14	43,43,43,43	0
56	MG	2A	3546	1/1	0.95	0.07	66,66,66,66	0
56	MG	2A	3497	1/1	0.95	0.05	54,54,54,54	0
56	MG	1l	8002	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3492	1/1	0.95	0.09	40,40,40,40	0
56	MG	1T	201	1/1	0.95	0.11	62,62,62,62	0
56	MG	1A	3631	1/1	0.95	0.14	36,36,36,36	0
56	MG	2A	3265	1/1	0.95	0.22	52,52,52,52	0
56	MG	2a	1724	1/1	0.95	0.15	77,77,77,77	0
56	MG	2A	3188	1/1	0.95	0.33	59,59,59,59	0
56	MG	2A	3030	1/1	0.95	0.89	48,48,48,48	0
56	MG	2A	3428	1/1	0.95	0.17	65,65,65,65	0
56	MG	2A	3021	1/1	0.95	0.20	29,29,29,29	0
56	MG	2A	3036	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3753	1/1	0.95	0.16	33,33,33,33	0
56	MG	2E	306	1/1	0.95	0.16	39,39,39,39	0
56	MG	10	102	1/1	0.95	0.25	47,47,47,47	0
56	MG	2a	1718	1/1	0.95	0.11	71,71,71,71	0
56	MG	2a	1712	1/1	0.95	0.13	58,58,58,58	0
56	MG	1A	3107	1/1	0.95	0.12	24,24,24,24	0
56	MG	1A	3680	1/1	0.95	0.15	54,54,54,54	0
56	MG	1A	3331	1/1	0.95	0.14	37,37,37,37	0
56	MG	2a	1742	1/1	0.95	0.06	70,70,70,70	0
56	MG	1A	3274	1/1	0.95	0.35	49,49,49,49	0
56	MG	2A	3602	1/1	0.95	0.08	38,38,38,38	0
56	MG	2A	3058	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3286	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3707	1/1	0.95	0.23	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3314	1/1	0.95	0.20	55,55,55,55	0
56	MG	1A	3451	1/1	0.95	0.12	21,21,21,21	0
58	K	2A	3243	1/1	0.95	0.18	65,65,65,65	0
56	MG	1w	3005	1/1	0.95	0.07	65,65,65,65	0
56	MG	1A	3733	1/1	0.95	0.28	48,48,48,48	0
56	MG	2a	1740	1/1	0.95	0.16	66,66,66,66	0
56	MG	1A	3118	1/1	0.95	0.54	50,50,50,50	0
56	MG	2A	3399	1/1	0.95	0.14	45,45,45,45	0
56	MG	1a	1610	1/1	0.95	0.26	59,59,59,59	0
56	MG	1X	104	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3470	1/1	0.95	0.18	58,58,58,58	0
56	MG	2q	202	1/1	0.95	0.05	59,59,59,59	0
56	MG	1a	1653	1/1	0.95	0.28	50,50,50,50	0
56	MG	2A	3418	1/1	0.95	0.20	51,51,51,51	0
56	MG	2A	3458	1/1	0.95	0.15	45,45,45,45	0
56	MG	2a	1667	1/1	0.95	0.13	57,57,57,57	0
56	MG	2A	3232	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3115	1/1	0.95	0.26	46,46,46,46	0
56	MG	1A	3574	1/1	0.95	0.19	47,47,47,47	0
56	MG	1A	3223	1/1	0.95	0.30	36,36,36,36	0
56	MG	1A	3774	1/1	0.95	0.10	61,61,61,61	0
56	MG	1O	8002	1/1	0.95	0.15	63,63,63,63	0
56	MG	1A	3191	1/1	0.95	0.15	27,27,27,27	0
56	MG	1A	3479	1/1	0.95	0.10	53,53,53,53	0
56	MG	1x	112	1/1	0.95	0.08	61,61,61,61	0
56	MG	1A	3818	1/1	0.95	0.14	24,24,24,24	0
56	MG	1A	3171	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3543	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3088	1/1	0.95	0.20	38,38,38,38	0
56	MG	2a	1696	1/1	0.95	0.13	66,66,66,66	0
56	MG	1a	1702	1/1	0.95	0.06	67,67,67,67	0
56	MG	2A	3512	1/1	0.95	0.07	62,62,62,62	0
56	MG	1A	3004	1/1	0.95	0.12	47,47,47,47	0
56	MG	1w	3003	1/1	0.95	0.15	50,50,50,50	0
56	MG	2a	1779	1/1	0.95	0.11	54,54,54,54	0
56	MG	2l	102	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3242	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3205	1/1	0.95	0.20	46,46,46,46	0
56	MG	2A	3389	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3240	1/1	0.95	0.18	55,55,55,55	0
56	MG	1A	3258	1/1	0.95	0.28	29,29,29,29	0
56	MG	1U	203	1/1	0.95	0.59	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3007	1/1	0.95	0.18	29,29,29,29	0
56	MG	1A	3149	1/1	0.95	0.62	50,50,50,50	0
56	MG	2B	3004	1/1	0.95	0.21	50,50,50,50	0
56	MG	1A	3264	1/1	0.95	0.15	53,53,53,53	0
56	MG	1a	1651	1/1	0.95	0.36	56,56,56,56	0
56	MG	2A	3384	1/1	0.95	0.11	52,52,52,52	0
56	MG	2A	3111	1/1	0.95	0.05	51,51,51,51	0
56	MG	2A	3118	1/1	0.95	0.17	33,33,33,33	0
56	MG	1A	3819	1/1	0.95	0.14	43,43,43,43	0
56	MG	2a	1689	1/1	0.95	0.11	51,51,51,51	0
56	MG	2A	3107	1/1	0.95	0.25	42,42,42,42	0
56	MG	1A	3297	1/1	0.95	0.16	62,62,62,62	0
56	MG	1A	3700	1/1	0.95	0.13	71,71,71,71	0
56	MG	1A	3037	1/1	0.95	0.12	32,32,32,32	0
56	MG	2A	3136	1/1	0.95	0.19	53,53,53,53	0
56	MG	2E	302	1/1	0.95	0.10	39,39,39,39	0
56	MG	2A	3014	1/1	0.95	0.29	41,41,41,41	0
56	MG	2a	1781	1/1	0.95	0.26	64,64,64,64	0
56	MG	2a	1650	1/1	0.95	0.17	39,39,39,39	0
57	4M2	1A	3894	57/57	0.95	0.27	21,37,55,60	0
56	MG	1A	3505	1/1	0.95	0.18	55,55,55,55	0
56	MG	1A	3815	1/1	0.95	0.19	31,31,31,31	0
56	MG	1A	3242	1/1	0.95	0.06	83,83,83,83	0
56	MG	1A	3266	1/1	0.95	0.37	50,50,50,50	0
56	MG	1A	3165	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	3610	1/1	0.95	0.15	30,30,30,30	0
56	MG	1A	3923	1/1	0.95	0.35	43,43,43,43	0
56	MG	1A	3569	1/1	0.95	0.15	38,38,38,38	0
56	MG	1G	3005	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3072	1/1	0.95	0.19	35,35,35,35	0
56	MG	1a	1605	1/1	0.95	0.15	71,71,71,71	0
56	MG	2A	3012	1/1	0.95	0.16	43,43,43,43	0
56	MG	1E	305	1/1	0.95	0.17	26,26,26,26	0
56	MG	1G	3002	1/1	0.95	0.11	34,34,34,34	0
56	MG	2A	3127	1/1	0.95	0.19	47,47,47,47	0
56	MG	2a	1753	1/1	0.95	0.12	72,72,72,72	0
56	MG	2A	3327	1/1	0.95	0.15	35,35,35,35	0
56	MG	1A	3101	1/1	0.95	0.10	61,61,61,61	0
56	MG	1A	3178	1/1	0.95	0.26	38,38,38,38	0
56	MG	1a	1760	1/1	0.95	0.18	59,59,59,59	0
56	MG	2A	3607	1/1	0.95	0.31	40,40,40,40	0
56	MG	2a	1637	1/1	0.95	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3339	1/1	0.95	0.20	32,32,32,32	0
56	MG	2a	1694	1/1	0.95	0.15	62,62,62,62	0
56	MG	2A	3209	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3631	1/1	0.95	0.06	56,56,56,56	0
56	MG	2A	3047	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3025	1/1	0.95	0.38	34,34,34,34	0
56	MG	1A	3665	1/1	0.95	0.13	59,59,59,59	0
56	MG	1A	3890	1/1	0.95	0.17	42,42,42,42	0
56	MG	2A	3003	1/1	0.95	0.20	31,31,31,31	0
56	MG	2A	3489	1/1	0.95	0.21	50,50,50,50	0
56	MG	2a	1634	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3431	1/1	0.95	0.14	34,34,34,34	0
56	MG	2a	1800	1/1	0.95	0.23	51,51,51,51	0
56	MG	1a	1664	1/1	0.95	0.30	56,56,56,56	0
56	MG	1A	3138	1/1	0.95	0.54	36,36,36,36	0
56	MG	1A	3600	1/1	0.95	0.13	38,38,38,38	0
56	MG	1a	1732	1/1	0.95	0.20	60,60,60,60	0
56	MG	1A	3564	1/1	0.95	0.18	52,52,52,52	0
56	MG	2B	3016	1/1	0.95	0.32	61,61,61,61	0
56	MG	2A	3266	1/1	0.95	0.12	33,33,33,33	0
56	MG	1A	3401	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3276	1/1	0.95	0.24	47,47,47,47	0
56	MG	1a	1700	1/1	0.95	0.20	57,57,57,57	0
56	MG	1a	1766	1/1	0.95	0.07	48,48,48,48	0
56	MG	2a	1755	1/1	0.95	0.12	67,67,67,67	0
56	MG	2A	3264	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3624	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3689	1/1	0.95	0.24	53,53,53,53	0
56	MG	1a	1751	1/1	0.95	0.12	65,65,65,65	0
56	MG	2A	3605	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3740	1/1	0.95	0.13	34,34,34,34	0
56	MG	1A	3064	1/1	0.95	0.33	38,38,38,38	0
56	MG	2A	3261	1/1	0.95	0.13	27,27,27,27	0
56	MG	2A	3449	1/1	0.95	0.15	33,33,33,33	0
56	MG	1a	1774	1/1	0.95	0.15	81,81,81,81	0
56	MG	1A	3653	1/1	0.95	0.16	31,31,31,31	0
56	MG	1a	1833	1/1	0.95	0.19	40,40,40,40	0
56	MG	1a	1692	1/1	0.95	0.13	45,45,45,45	0
56	MG	1P	203	1/1	0.95	0.17	30,30,30,30	0
56	MG	1A	3851	1/1	0.95	0.10	50,50,50,50	0
56	MG	1a	1776	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3915	1/1	0.95	0.24	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3426	1/1	0.95	0.11	53,53,53,53	0
56	MG	2A	3658	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3518	1/1	0.95	0.10	57,57,57,57	0
56	MG	1A	3079	1/1	0.95	0.17	38,38,38,38	0
56	MG	1a	1807	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3473	1/1	0.95	0.09	47,47,47,47	0
56	MG	2a	1799	1/1	0.95	0.09	43,43,43,43	0
56	MG	1a	1710	1/1	0.95	0.20	51,51,51,51	0
56	MG	10	106	1/1	0.95	0.06	56,56,56,56	0
56	MG	2A	3263	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3158	1/1	0.95	0.15	39,39,39,39	0
56	MG	1A	3519	1/1	0.96	0.10	51,51,51,51	0
56	MG	2A	3371	1/1	0.96	0.08	44,44,44,44	0
56	MG	2A	3227	1/1	0.96	0.12	42,42,42,42	0
56	MG	1a	1782	1/1	0.96	0.14	60,60,60,60	0
56	MG	1A	3129	1/1	0.96	0.27	41,41,41,41	0
56	MG	1A	3075	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3717	1/1	0.96	0.10	56,56,56,56	0
56	MG	2A	3354	1/1	0.96	0.18	35,35,35,35	0
56	MG	2A	3269	1/1	0.96	0.09	49,49,49,49	0
56	MG	17	101	1/1	0.96	0.13	55,55,55,55	0
56	MG	1a	1780	1/1	0.96	0.15	74,74,74,74	0
56	MG	2a	1630	1/1	0.96	0.26	62,62,62,62	0
56	MG	1A	3656	1/1	0.96	0.15	38,38,38,38	0
56	MG	2A	3360	1/1	0.96	0.07	54,54,54,54	0
56	MG	2A	3008	1/1	0.96	0.12	42,42,42,42	0
56	MG	2a	1672	1/1	0.96	0.07	64,64,64,64	0
56	MG	2B	3014	1/1	0.96	0.12	68,68,68,68	0
56	MG	1A	3533	1/1	0.96	0.10	55,55,55,55	0
56	MG	2A	3172	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3414	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3019	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3126	1/1	0.96	0.12	36,36,36,36	0
56	MG	2A	3628	1/1	0.96	0.05	49,49,49,49	0
56	MG	2A	3298	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	3903	1/1	0.96	0.31	39,39,39,39	0
56	MG	1a	1671	1/1	0.96	0.23	48,48,48,48	0
56	MG	1F	307	1/1	0.96	0.15	43,43,43,43	0
56	MG	2A	3262	1/1	0.96	0.07	56,56,56,56	0
56	MG	1G	3004	1/1	0.96	0.15	51,51,51,51	0
56	MG	1A	3742	1/1	0.96	0.17	54,54,54,54	0
56	MG	2A	3446	1/1	0.96	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3476	1/1	0.96	0.04	53,53,53,53	0
56	MG	1a	1781	1/1	0.96	0.08	76,76,76,76	0
56	MG	2A	3098	1/1	0.96	0.12	32,32,32,32	0
56	MG	1A	3703	1/1	0.96	0.16	60,60,60,60	0
56	MG	1A	3122	1/1	0.96	0.21	51,51,51,51	0
56	MG	2A	3544	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3054	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3207	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	3739	1/1	0.96	0.41	43,43,43,43	0
56	MG	2A	3392	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3670	1/1	0.96	0.07	66,66,66,66	0
56	MG	2A	3248	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3382	1/1	0.96	0.08	54,54,54,54	0
56	MG	1A	3434	1/1	0.96	0.18	25,25,25,25	0
56	MG	2a	1758	1/1	0.96	0.11	59,59,59,59	0
56	MG	2A	3241	1/1	0.96	0.30	45,45,45,45	0
56	MG	2A	3550	1/1	0.96	0.10	62,62,62,62	0
56	MG	1a	1826	1/1	0.96	0.12	66,66,66,66	0
56	MG	1A	3660	1/1	0.96	0.14	54,54,54,54	0
56	MG	1e	3001	1/1	0.96	0.13	71,71,71,71	0
56	MG	1A	3390	1/1	0.96	0.09	64,64,64,64	0
56	MG	2A	3251	1/1	0.96	0.06	52,52,52,52	0
56	MG	2A	3350	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3692	1/1	0.96	0.22	52,52,52,52	0
56	MG	1A	3371	1/1	0.96	0.12	49,49,49,49	0
56	MG	2A	3518	1/1	0.96	0.12	55,55,55,55	0
56	MG	1A	3436	1/1	0.96	0.19	40,40,40,40	0
56	MG	1a	1631	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3467	1/1	0.96	0.15	41,41,41,41	0
56	MG	2a	1723	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3427	1/1	0.96	0.12	45,45,45,45	0
56	MG	2a	1652	1/1	0.96	0.11	57,57,57,57	0
56	MG	2A	3254	1/1	0.96	0.14	57,57,57,57	0
56	MG	1A	3911	1/1	0.96	0.17	31,31,31,31	0
56	MG	1a	1705	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3660	1/1	0.96	0.16	31,31,31,31	0
56	MG	2A	3100	1/1	0.96	0.11	52,52,52,52	0
59	ZN	1Y	501	1/1	0.96	0.18	71,71,71,71	0
56	MG	2A	3648	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3503	1/1	0.96	0.24	57,57,57,57	0
56	MG	1B	207	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3907	1/1	0.96	0.20	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3789	1/1	0.96	0.16	56,56,56,56	0
56	MG	1A	3728	1/1	0.96	0.16	40,40,40,40	0
56	MG	2X	3001	1/1	0.96	0.28	63,63,63,63	0
56	MG	1A	3271	1/1	0.96	0.16	33,33,33,33	0
56	MG	1A	3324	1/1	0.96	0.18	53,53,53,53	0
56	MG	1a	1755	1/1	0.96	0.19	44,44,44,44	0
56	MG	1A	3522	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3225	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3156	1/1	0.96	0.33	50,50,50,50	0
56	MG	1A	3481	1/1	0.96	0.17	45,45,45,45	0
56	MG	1a	1614	1/1	0.96	0.16	59,59,59,59	0
56	MG	2a	1770	1/1	0.96	0.12	67,67,67,67	0
56	MG	2A	3063	1/1	0.96	0.10	48,48,48,48	0
56	MG	1A	3428	1/1	0.96	0.16	39,39,39,39	0
56	MG	1a	1730	1/1	0.96	0.12	63,63,63,63	0
56	MG	1a	1647	1/1	0.96	0.14	49,49,49,49	0
56	MG	1A	3496	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3257	1/1	0.96	0.58	48,48,48,48	0
56	MG	1A	3384	1/1	0.96	0.22	41,41,41,41	0
56	MG	1A	3445	1/1	0.96	0.12	26,26,26,26	0
56	MG	2w	3003	1/1	0.96	0.07	58,58,58,58	0
56	MG	1B	215	1/1	0.96	0.09	26,26,26,26	0
56	MG	2A	3425	1/1	0.96	0.17	54,54,54,54	0
56	MG	1A	3117	1/1	0.96	0.23	44,44,44,44	0
56	MG	1A	3800	1/1	0.96	0.34	46,46,46,46	0
56	MG	1A	3084	1/1	0.96	0.16	60,60,60,60	0
56	MG	1A	3393	1/1	0.96	0.12	52,52,52,52	0
56	MG	1a	1759	1/1	0.96	0.12	48,48,48,48	0
56	MG	1A	3452	1/1	0.96	0.18	26,26,26,26	0
56	MG	1A	3705	1/1	0.96	0.15	32,32,32,32	0
56	MG	2A	3577	1/1	0.96	0.18	42,42,42,42	0
56	MG	2A	3015	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	3074	1/1	0.96	0.19	40,40,40,40	0
56	MG	1A	3473	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	3418	1/1	0.96	0.09	54,54,54,54	0
56	MG	2A	3083	1/1	0.96	0.36	41,41,41,41	0
56	MG	2B	3013	1/1	0.96	0.13	54,54,54,54	0
56	MG	2a	1754	1/1	0.96	0.16	73,73,73,73	0
56	MG	1A	3308	1/1	0.96	0.27	39,39,39,39	0
56	MG	1A	3898	1/1	0.96	0.35	31,31,31,31	0
56	MG	2A	3161	1/1	0.96	0.16	53,53,53,53	0
56	MG	1A	3212	1/1	0.96	0.25	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1818	1/1	0.96	0.16	64,64,64,64	0
56	MG	16	103	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3548	1/1	0.96	0.16	54,54,54,54	0
56	MG	2a	1631	1/1	0.96	0.20	65,65,65,65	0
56	MG	1a	1808	1/1	0.96	0.20	58,58,58,58	0
56	MG	10	101	1/1	0.96	0.07	45,45,45,45	0
56	MG	2a	1775	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3238	1/1	0.96	0.21	31,31,31,31	0
56	MG	1A	3736	1/1	0.96	0.28	49,49,49,49	0
56	MG	2A	3443	1/1	0.96	0.12	29,29,29,29	0
56	MG	2B	3001	1/1	0.96	0.13	59,59,59,59	0
56	MG	2A	3273	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3082	1/1	0.96	0.52	42,42,42,42	0
56	MG	2A	3663	1/1	0.96	0.16	35,35,35,35	0
56	MG	1A	3201	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3032	1/1	0.96	0.12	44,44,44,44	0
56	MG	1a	1734	1/1	0.96	0.07	53,53,53,53	0
56	MG	1A	3906	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3527	1/1	0.96	0.08	69,69,69,69	0
56	MG	2A	3362	1/1	0.96	0.12	54,54,54,54	0
56	MG	2a	1711	1/1	0.96	0.22	69,69,69,69	0
56	MG	1B	217	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3023	1/1	0.96	0.20	42,42,42,42	0
56	MG	10	104	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3128	1/1	0.96	0.20	33,33,33,33	0
56	MG	1a	1756	1/1	0.96	0.09	40,40,40,40	0
56	MG	1A	3580	1/1	0.96	0.21	36,36,36,36	0
56	MG	1D	303	1/1	0.96	0.32	49,49,49,49	0
56	MG	1A	3765	1/1	0.96	0.28	66,66,66,66	0
56	MG	2B	3006	1/1	0.96	0.13	59,59,59,59	0
56	MG	1A	3748	1/1	0.96	0.17	33,33,33,33	0
56	MG	1P	202	1/1	0.96	0.08	51,51,51,51	0
56	MG	1A	3878	1/1	0.96	0.18	43,43,43,43	0
56	MG	1A	3188	1/1	0.96	0.24	28,28,28,28	0
56	MG	2D	303	1/1	0.96	0.12	36,36,36,36	0
56	MG	1a	1660	1/1	0.96	0.26	56,56,56,56	0
56	MG	1g	3001	1/1	0.96	0.17	54,54,54,54	0
56	MG	1a	1777	1/1	0.96	0.08	57,57,57,57	0
56	MG	2A	3299	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3824	1/1	0.96	0.17	53,53,53,53	0
56	MG	1x	110	1/1	0.96	0.17	57,57,57,57	0
56	MG	2v	3001	1/1	0.96	0.18	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1x	101	1/1	0.96	0.14	55,55,55,55	0
56	MG	2A	3367	1/1	0.96	0.20	34,34,34,34	0
56	MG	1A	3346	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3345	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	3125	1/1	0.96	0.17	34,34,34,34	0
56	MG	2A	3257	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3928	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3352	1/1	0.96	0.09	56,56,56,56	0
56	MG	2A	3382	1/1	0.96	0.25	42,42,42,42	0
56	MG	1A	3174	1/1	0.96	0.19	39,39,39,39	0
56	MG	2A	3026	1/1	0.96	0.44	41,41,41,41	0
56	MG	1A	3570	1/1	0.96	0.23	31,31,31,31	0
56	MG	2A	3331	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3673	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3202	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3605	1/1	0.96	0.15	45,45,45,45	0
56	MG	2A	3042	1/1	0.96	0.09	48,48,48,48	0
56	MG	1N	3003	1/1	0.96	0.14	40,40,40,40	0
56	MG	2A	3009	1/1	0.96	0.13	45,45,45,45	0
56	MG	1N	3002	1/1	0.96	0.25	45,45,45,45	0
56	MG	2A	3010	1/1	0.96	0.08	34,34,34,34	0
56	MG	1A	3528	1/1	0.96	0.06	53,53,53,53	0
56	MG	2F	305	1/1	0.96	0.34	51,51,51,51	0
56	MG	2A	3565	1/1	0.96	0.18	34,34,34,34	0
56	MG	1A	3327	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3352	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3526	1/1	0.96	0.17	52,52,52,52	0
56	MG	2A	3332	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3480	1/1	0.96	0.17	36,36,36,36	0
56	MG	1B	225	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3407	1/1	0.96	0.12	38,38,38,38	0
56	MG	2a	1642	1/1	0.96	0.24	61,61,61,61	0
56	MG	2A	3060	1/1	0.96	0.14	49,49,49,49	0
56	MG	2A	3488	1/1	0.96	0.16	53,53,53,53	0
56	MG	1a	1645	1/1	0.96	0.29	63,63,63,63	0
56	MG	1A	3375	1/1	0.96	0.14	31,31,31,31	0
56	MG	2a	1757	1/1	0.96	0.14	71,71,71,71	0
56	MG	2A	3355	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	3718	1/1	0.96	0.14	23,23,23,23	0
56	MG	1A	3353	1/1	0.96	0.20	46,46,46,46	0
56	MG	1A	3265	1/1	0.96	0.23	41,41,41,41	0
56	MG	1a	1697	1/1	0.96	0.31	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3162	1/1	0.96	0.20	45,45,45,45	0
56	MG	1A	3461	1/1	0.96	0.21	23,23,23,23	0
56	MG	1A	3876	1/1	0.96	0.51	46,46,46,46	0
56	MG	2A	3268	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3920	1/1	0.96	0.45	34,34,34,34	0
56	MG	1A	3065	1/1	0.96	0.19	29,29,29,29	0
56	MG	1A	3910	1/1	0.96	0.57	38,38,38,38	0
56	MG	2A	3374	1/1	0.96	0.06	39,39,39,39	0
56	MG	2A	3011	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3253	1/1	0.96	0.23	33,33,33,33	0
56	MG	2A	3253	1/1	0.96	0.16	48,48,48,48	0
56	MG	2A	3288	1/1	0.96	0.07	29,29,29,29	0
56	MG	1A	3762	1/1	0.96	0.16	68,68,68,68	0
56	MG	2A	3341	1/1	0.96	0.14	51,51,51,51	0
56	MG	2A	3053	1/1	0.96	0.13	45,45,45,45	0
56	MG	1B	209	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3108	1/1	0.96	0.30	36,36,36,36	0
56	MG	1A	3864	1/1	0.96	0.23	38,38,38,38	0
56	MG	2A	3394	1/1	0.96	0.08	51,51,51,51	0
56	MG	1A	3471	1/1	0.96	0.17	28,28,28,28	0
56	MG	1A	3786	1/1	0.96	0.12	59,59,59,59	0
56	MG	2A	3445	1/1	0.96	0.05	57,57,57,57	0
56	MG	2A	3641	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3397	1/1	0.97	0.14	17,17,17,17	0
56	MG	1B	211	1/1	0.97	0.13	43,43,43,43	0
56	MG	2A	3197	1/1	0.97	0.10	42,42,42,42	0
56	MG	1a	1662	1/1	0.97	0.12	25,25,25,25	0
56	MG	2a	1802	1/1	0.97	0.12	55,55,55,55	0
56	MG	2A	3177	1/1	0.97	0.14	40,40,40,40	0
56	MG	1a	1814	1/1	0.97	0.23	50,50,50,50	0
56	MG	2A	3494	1/1	0.97	0.12	39,39,39,39	0
56	MG	2A	3534	1/1	0.97	0.08	73,73,73,73	0
56	MG	1A	3145	1/1	0.97	0.25	37,37,37,37	0
56	MG	1A	3708	1/1	0.97	0.21	55,55,55,55	0
56	MG	1R	201	1/1	0.97	0.09	45,45,45,45	0
56	MG	2A	3630	1/1	0.97	0.07	53,53,53,53	0
56	MG	1A	3511	1/1	0.97	0.08	52,52,52,52	0
56	MG	2A	3386	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3477	1/1	0.97	0.15	18,18,18,18	0
56	MG	2a	1619	1/1	0.97	0.14	40,40,40,40	0
56	MG	2A	3368	1/1	0.97	0.10	44,44,44,44	0
56	MG	1A	3260	1/1	0.97	0.54	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1634	1/1	0.97	0.23	45,45,45,45	0
56	MG	1A	3343	1/1	0.97	0.16	34,34,34,34	0
56	MG	2a	1762	1/1	0.97	0.22	64,64,64,64	0
56	MG	1A	3559	1/1	0.97	0.19	40,40,40,40	0
56	MG	1a	1829	1/1	0.97	0.07	83,83,83,83	0
56	MG	1A	3103	1/1	0.97	0.48	44,44,44,44	0
56	MG	1A	3884	1/1	0.97	0.16	40,40,40,40	0
56	MG	1A	3816	1/1	0.97	0.15	25,25,25,25	0
56	MG	2a	1736	1/1	0.97	0.11	66,66,66,66	0
56	MG	1B	212	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3124	1/1	0.97	0.43	46,46,46,46	0
56	MG	2A	3459	1/1	0.97	0.16	37,37,37,37	0
56	MG	1a	1677	1/1	0.97	0.19	51,51,51,51	0
56	MG	1A	3373	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3330	1/1	0.97	0.22	39,39,39,39	0
56	MG	2A	3007	1/1	0.97	0.14	34,34,34,34	0
56	MG	2A	3154	1/1	0.97	0.08	49,49,49,49	0
56	MG	2A	3090	1/1	0.97	0.30	37,37,37,37	0
56	MG	1A	3288	1/1	0.97	0.20	42,42,42,42	0
56	MG	2A	3052	1/1	0.97	0.28	58,58,58,58	0
56	MG	1n	502	1/1	0.97	0.09	42,42,42,42	0
56	MG	1A	3325	1/1	0.97	0.25	43,43,43,43	0
56	MG	2A	3056	1/1	0.97	0.11	23,23,23,23	0
56	MG	2F	306	1/1	0.97	0.26	49,49,49,49	0
56	MG	1A	3136	1/1	0.97	0.45	36,36,36,36	0
56	MG	1A	3193	1/1	0.97	0.48	40,40,40,40	0
56	MG	1Y	503	1/1	0.97	0.10	56,56,56,56	0
56	MG	1F	302	1/1	0.97	0.28	32,32,32,32	0
56	MG	1a	1816	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3160	1/1	0.97	0.19	24,24,24,24	0
56	MG	1A	3474	1/1	0.97	0.17	26,26,26,26	0
56	MG	1A	3727	1/1	0.97	0.08	39,39,39,39	0
56	MG	2A	3581	1/1	0.97	0.11	50,50,50,50	0
56	MG	1B	214	1/1	0.97	0.16	41,41,41,41	0
56	MG	1I	3001	1/1	0.97	0.22	65,65,65,65	0
56	MG	2A	3040	1/1	0.97	0.18	36,36,36,36	0
56	MG	1A	3766	1/1	0.97	0.12	31,31,31,31	0
56	MG	1A	3027	1/1	0.97	0.21	35,35,35,35	0
56	MG	1A	3389	1/1	0.97	0.17	23,23,23,23	0
56	MG	1A	3731	1/1	0.97	0.32	52,52,52,52	0
56	MG	1A	3549	1/1	0.97	0.13	40,40,40,40	0
56	MG	1a	1771	1/1	0.97	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3831	1/1	0.97	0.18	23,23,23,23	0
56	MG	2a	1708	1/1	0.97	0.10	61,61,61,61	0
56	MG	1A	3594	1/1	0.97	0.13	52,52,52,52	0
56	MG	2A	3282	1/1	0.97	0.28	52,52,52,52	0
56	MG	1A	3832	1/1	0.97	0.09	23,23,23,23	0
56	MG	1a	1652	1/1	0.97	0.18	63,63,63,63	0
56	MG	2A	3229	1/1	0.97	0.21	41,41,41,41	0
56	MG	1A	3057	1/1	0.97	0.21	43,43,43,43	0
56	MG	1A	3591	1/1	0.97	0.04	69,69,69,69	0
56	MG	1D	304	1/1	0.97	0.12	22,22,22,22	0
56	MG	1A	3493	1/1	0.97	0.12	53,53,53,53	0
56	MG	2A	3649	1/1	0.97	0.09	43,43,43,43	0
56	MG	1A	3561	1/1	0.97	0.18	43,43,43,43	0
56	MG	1A	3187	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3504	1/1	0.97	0.12	47,47,47,47	0
56	MG	1F	303	1/1	0.97	0.33	41,41,41,41	0
56	MG	1y	3005	1/1	0.97	0.07	78,78,78,78	0
56	MG	2A	3460	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3539	1/1	0.97	0.17	17,17,17,17	0
56	MG	1A	3841	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3628	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3350	1/1	0.97	0.20	40,40,40,40	0
56	MG	1A	3147	1/1	0.97	0.28	36,36,36,36	0
59	ZN	26	501	1/1	0.97	0.18	63,63,63,63	0
56	MG	1A	3501	1/1	0.97	0.33	62,62,62,62	0
56	MG	1A	3148	1/1	0.97	0.36	35,35,35,35	0
56	MG	1A	3857	1/1	0.97	0.10	25,25,25,25	0
56	MG	1A	3132	1/1	0.97	0.17	17,17,17,17	0
56	MG	1A	3261	1/1	0.97	0.22	36,36,36,36	0
56	MG	1a	1810	1/1	0.97	0.07	60,60,60,60	0
60	SF4	2d	501	8/8	0.97	0.14	58,71,79,93	0
56	MG	1A	3553	1/1	0.97	0.05	44,44,44,44	0
56	MG	2A	3292	1/1	0.97	0.16	28,28,28,28	0
56	MG	2A	3125	1/1	0.97	0.08	40,40,40,40	0
56	MG	1A	3106	1/1	0.97	0.32	47,47,47,47	0
56	MG	2A	3156	1/1	0.97	0.07	50,50,50,50	0
56	MG	1D	306	1/1	0.97	0.30	36,36,36,36	0
56	MG	1A	3904	1/1	0.97	0.19	27,27,27,27	0
56	MG	1A	3625	1/1	0.97	0.35	55,55,55,55	0
56	MG	1A	3011	1/1	0.97	0.41	32,32,32,32	0
56	MG	1A	3046	1/1	0.97	0.18	28,28,28,28	0
56	MG	2A	3195	1/1	0.97	0.22	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1E	301	1/1	0.97	0.24	43,43,43,43	0
56	MG	2A	3511	1/1	0.97	0.11	46,46,46,46	0
56	MG	1a	1783	1/1	0.97	0.13	58,58,58,58	0
56	MG	1A	3012	1/1	0.97	0.27	33,33,33,33	0
56	MG	1A	3039	1/1	0.97	0.20	49,49,49,49	0
56	MG	2A	3485	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3159	1/1	0.97	0.18	29,29,29,29	0
56	MG	1a	1676	1/1	0.97	0.29	53,53,53,53	0
56	MG	2A	3664	1/1	0.97	0.44	37,37,37,37	0
56	MG	1A	3729	1/1	0.97	0.10	47,47,47,47	0
56	MG	2A	3290	1/1	0.97	0.08	37,37,37,37	0
56	MG	1A	3547	1/1	0.97	0.25	55,55,55,55	0
56	MG	2A	3234	1/1	0.97	0.16	56,56,56,56	0
56	MG	1A	3098	1/1	0.97	0.22	24,24,24,24	0
56	MG	1A	3096	1/1	0.97	0.40	52,52,52,52	0
56	MG	1A	3657	1/1	0.97	0.10	35,35,35,35	0
56	MG	2A	3321	1/1	0.97	0.20	51,51,51,51	0
56	MG	1a	1624	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3650	1/1	0.97	0.13	38,38,38,38	0
56	MG	1A	3380	1/1	0.97	0.17	26,26,26,26	0
56	MG	2A	3150	1/1	0.97	0.17	54,54,54,54	0
56	MG	1A	3792	1/1	0.97	0.34	34,34,34,34	0
56	MG	1A	3218	1/1	0.97	0.12	44,44,44,44	0
56	MG	2A	3533	1/1	0.97	0.14	57,57,57,57	0
56	MG	1A	3791	1/1	0.97	0.41	34,34,34,34	0
56	MG	2f	3001	1/1	0.97	0.15	47,47,47,47	0
56	MG	1D	309	1/1	0.97	0.46	28,28,28,28	0
56	MG	27	101	1/1	0.97	0.45	46,46,46,46	0
56	MG	1A	3179	1/1	0.97	0.24	26,26,26,26	0
56	MG	1N	3005	1/1	0.97	0.16	40,40,40,40	0
56	MG	2A	3629	1/1	0.97	0.19	49,49,49,49	0
56	MG	1A	3055	1/1	0.97	0.16	45,45,45,45	0
56	MG	2E	304	1/1	0.97	0.06	40,40,40,40	0
56	MG	2A	3595	1/1	0.97	0.14	52,52,52,52	0
56	MG	1A	3751	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3525	1/1	0.97	0.15	24,24,24,24	0
56	MG	1A	3029	1/1	0.97	0.41	40,40,40,40	0
56	MG	1A	3716	1/1	0.97	0.11	60,60,60,60	0
56	MG	1A	3641	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	3351	1/1	0.97	0.14	55,55,55,55	0
56	MG	2A	3228	1/1	0.97	0.07	42,42,42,42	0
56	MG	1Z	301	1/1	0.97	0.37	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3735	1/1	0.97	0.14	52,52,52,52	0
56	MG	1a	1738	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	3049	1/1	0.97	0.19	42,42,42,42	0
56	MG	1E	303	1/1	0.97	0.34	48,48,48,48	0
56	MG	2A	3275	1/1	0.97	0.08	43,43,43,43	0
56	MG	2A	3277	1/1	0.97	0.21	51,51,51,51	0
56	MG	1a	1788	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3586	1/1	0.97	0.14	27,27,27,27	0
56	MG	1A	3494	1/1	0.97	0.16	34,34,34,34	0
56	MG	2A	3361	1/1	0.97	0.12	19,19,19,19	0
56	MG	1a	1831	1/1	0.97	0.16	61,61,61,61	0
56	MG	1A	3028	1/1	0.97	0.30	19,19,19,19	0
56	MG	1a	1713	1/1	0.97	0.13	34,34,34,34	0
56	MG	2A	3442	1/1	0.97	0.16	48,48,48,48	0
56	MG	1A	3619	1/1	0.97	0.16	44,44,44,44	0
56	MG	1a	1779	1/1	0.97	0.18	52,52,52,52	0
56	MG	1A	3392	1/1	0.97	0.09	31,31,31,31	0
56	MG	2A	3334	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3121	1/1	0.97	0.16	38,38,38,38	0
56	MG	2v	3002	1/1	0.97	0.14	60,60,60,60	0
56	MG	2x	3001	1/1	0.97	0.08	49,49,49,49	0
56	MG	2a	1739	1/1	0.97	0.17	64,64,64,64	0
56	MG	1A	3177	1/1	0.97	0.61	52,52,52,52	0
56	MG	2a	1687	1/1	0.97	0.28	50,50,50,50	0
56	MG	2A	3097	1/1	0.97	0.31	42,42,42,42	0
56	MG	1A	3820	1/1	0.97	0.10	52,52,52,52	0
56	MG	1A	3283	1/1	0.97	0.37	44,44,44,44	0
56	MG	1A	3551	1/1	0.97	0.09	35,35,35,35	0
56	MG	2A	3531	1/1	0.97	0.12	50,50,50,50	0
56	MG	2A	3659	1/1	0.97	0.12	44,44,44,44	0
56	MG	2P	201	1/1	0.97	0.30	57,57,57,57	0
56	MG	1A	3246	1/1	0.97	0.34	40,40,40,40	0
56	MG	2a	1610	1/1	0.97	0.32	53,53,53,53	0
56	MG	1A	3909	1/1	0.97	0.27	42,42,42,42	0
56	MG	1A	3833	1/1	0.97	0.07	66,66,66,66	0
56	MG	2A	3185	1/1	0.97	0.30	50,50,50,50	0
56	MG	1A	3927	1/1	0.97	0.36	40,40,40,40	0
56	MG	2A	3281	1/1	0.97	0.13	25,25,25,25	0
56	MG	2A	3020	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3021	1/1	0.97	0.16	17,17,17,17	0
56	MG	2A	3210	1/1	0.97	0.12	58,58,58,58	0
56	MG	1B	224	1/1	0.97	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3661	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3902	1/1	0.98	0.12	40,40,40,40	0
56	MG	1V	202	1/1	0.98	0.16	44,44,44,44	0
56	MG	1A	3930	1/1	0.98	0.30	41,41,41,41	0
56	MG	2a	1660	1/1	0.98	0.20	52,52,52,52	0
56	MG	2A	3590	1/1	0.98	0.09	49,49,49,49	0
56	MG	1A	3835	1/1	0.98	0.16	36,36,36,36	0
56	MG	1A	3683	1/1	0.98	0.09	53,53,53,53	0
56	MG	1s	3001	1/1	0.98	0.05	57,57,57,57	0
56	MG	2E	307	1/1	0.98	0.16	47,47,47,47	0
56	MG	1B	204	1/1	0.98	0.16	42,42,42,42	0
56	MG	1A	3157	1/1	0.98	0.16	41,41,41,41	0
56	MG	2A	3155	1/1	0.98	0.49	46,46,46,46	0
56	MG	1A	3738	1/1	0.98	0.28	39,39,39,39	0
56	MG	1F	306	1/1	0.98	0.09	46,46,46,46	0
56	MG	1A	3450	1/1	0.98	0.13	36,36,36,36	0
56	MG	1A	3183	1/1	0.98	0.40	36,36,36,36	0
56	MG	1A	3922	1/1	0.98	0.11	41,41,41,41	0
56	MG	2A	3303	1/1	0.98	0.11	33,33,33,33	0
56	MG	2A	3092	1/1	0.98	0.15	36,36,36,36	0
56	MG	1a	1620	1/1	0.98	0.14	37,37,37,37	0
56	MG	1A	3202	1/1	0.98	0.14	46,46,46,46	0
56	MG	1A	3882	1/1	0.98	0.17	41,41,41,41	0
56	MG	1N	3004	1/1	0.98	0.12	41,41,41,41	0
60	SF4	1d	501	8/8	0.98	0.18	51,62,75,79	0
56	MG	2A	3560	1/1	0.98	0.12	52,52,52,52	0
56	MG	1A	3506	1/1	0.98	0.15	53,53,53,53	0
56	MG	2A	3356	1/1	0.98	0.09	22,22,22,22	0
56	MG	1A	3918	1/1	0.98	0.29	39,39,39,39	0
56	MG	2a	1695	1/1	0.98	0.15	66,66,66,66	0
56	MG	1A	3822	1/1	0.98	0.18	56,56,56,56	0
56	MG	2A	3441	1/1	0.98	0.13	37,37,37,37	0
56	MG	1A	3809	1/1	0.98	0.14	50,50,50,50	0
56	MG	1A	3517	1/1	0.98	0.10	51,51,51,51	0
56	MG	1A	3406	1/1	0.98	0.17	27,27,27,27	0
56	MG	1A	3062	1/1	0.98	0.12	31,31,31,31	0
56	MG	2A	3463	1/1	0.98	0.08	37,37,37,37	0
56	MG	1A	3211	1/1	0.98	0.29	44,44,44,44	0
56	MG	2A	3668	1/1	0.98	0.17	41,41,41,41	0
56	MG	2A	3165	1/1	0.98	0.27	31,31,31,31	0
56	MG	1A	3374	1/1	0.98	0.18	32,32,32,32	0
56	MG	1A	3010	1/1	0.98	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3034	1/1	0.98	0.52	44,44,44,44	0
56	MG	1a	1827	1/1	0.98	0.14	60,60,60,60	0
56	MG	1Q	3001	1/1	0.98	0.15	36,36,36,36	0
56	MG	1A	3372	1/1	0.98	0.17	41,41,41,41	0
56	MG	1A	3880	1/1	0.98	0.19	23,23,23,23	0
56	MG	2q	201	1/1	0.98	0.49	80,80,80,80	0
56	MG	1A	3917	1/1	0.98	0.29	32,32,32,32	0
56	MG	1A	3595	1/1	0.98	0.14	48,48,48,48	0
56	MG	2A	3064	1/1	0.98	0.10	50,50,50,50	0
56	MG	1A	3468	1/1	0.98	0.12	30,30,30,30	0
56	MG	1A	3504	1/1	0.98	0.08	13,13,13,13	0
56	MG	2A	3182	1/1	0.98	0.18	39,39,39,39	0
56	MG	1A	3723	1/1	0.98	0.07	58,58,58,58	0
56	MG	1a	1763	1/1	0.98	0.14	49,49,49,49	0
56	MG	2a	1645	1/1	0.98	0.17	47,47,47,47	0
56	MG	1a	1670	1/1	0.98	0.06	56,56,56,56	0
56	MG	1A	3038	1/1	0.98	0.26	33,33,33,33	0
56	MG	1A	3109	1/1	0.98	0.19	28,28,28,28	0
56	MG	1P	201	1/1	0.98	0.36	26,26,26,26	0
56	MG	1a	1773	1/1	0.98	0.13	44,44,44,44	0
56	MG	1A	3668	1/1	0.98	0.17	45,45,45,45	0
56	MG	1A	3704	1/1	0.98	0.20	26,26,26,26	0
56	MG	1A	3892	1/1	0.98	0.28	34,34,34,34	0
56	MG	1A	3794	1/1	0.98	0.12	21,21,21,21	0
56	MG	1A	3710	1/1	0.98	0.04	45,45,45,45	0
56	MG	1a	1717	1/1	0.98	0.08	60,60,60,60	0
56	MG	1a	1630	1/1	0.98	0.13	27,27,27,27	0
56	MG	1A	3368	1/1	0.98	0.21	37,37,37,37	0
56	MG	1a	1646	1/1	0.98	0.08	52,52,52,52	0
56	MG	1A	3609	1/1	0.98	0.17	31,31,31,31	0
56	MG	2A	3141	1/1	0.98	0.11	49,49,49,49	0
56	MG	1A	3649	1/1	0.98	0.07	67,67,67,67	0
56	MG	1A	3638	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3897	1/1	0.98	0.31	30,30,30,30	0
56	MG	1A	3446	1/1	0.98	0.14	26,26,26,26	0
56	MG	2A	3599	1/1	0.98	0.17	52,52,52,52	0
56	MG	1A	3097	1/1	0.98	0.19	26,26,26,26	0
56	MG	2a	1701	1/1	0.98	0.05	55,55,55,55	0
56	MG	28	101	1/1	0.98	0.12	57,57,57,57	0
56	MG	2A	3369	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3091	1/1	0.98	0.21	42,42,42,42	0
56	MG	1A	3186	1/1	0.98	0.51	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1735	1/1	0.98	0.12	56,56,56,56	0
56	MG	1B	208	1/1	0.98	0.13	56,56,56,56	0
56	MG	2A	3503	1/1	0.98	0.11	51,51,51,51	0
56	MG	1A	3537	1/1	0.98	0.19	28,28,28,28	0
56	MG	2A	3317	1/1	0.98	0.11	31,31,31,31	0
56	MG	1a	1736	1/1	0.98	0.17	58,58,58,58	0
56	MG	2A	3461	1/1	0.98	0.08	47,47,47,47	0
56	MG	1A	3914	1/1	0.98	0.19	37,37,37,37	0
56	MG	1A	3180	1/1	0.98	0.14	40,40,40,40	0
56	MG	2A	3171	1/1	0.98	0.22	47,47,47,47	0
56	MG	1A	3552	1/1	0.98	0.15	20,20,20,20	0
56	MG	1A	3829	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3590	1/1	0.98	0.17	24,24,24,24	0
56	MG	1A	3558	1/1	0.98	0.19	43,43,43,43	0
56	MG	2A	3313	1/1	0.98	0.10	54,54,54,54	0
56	MG	1A	3521	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3760	1/1	0.98	0.11	19,19,19,19	0
56	MG	1A	3088	1/1	0.98	0.20	22,22,22,22	0
56	MG	1A	3737	1/1	0.98	0.20	40,40,40,40	0
56	MG	1a	1639	1/1	0.98	0.12	43,43,43,43	0
56	MG	2A	3395	1/1	0.98	0.07	56,56,56,56	0
56	MG	1B	219	1/1	0.98	0.14	49,49,49,49	0
56	MG	1A	3460	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3033	1/1	0.98	0.18	20,20,20,20	0
56	MG	1A	3513	1/1	0.98	0.13	25,25,25,25	0
56	MG	2A	3582	1/1	0.98	0.12	34,34,34,34	0
56	MG	1A	3073	1/1	0.98	0.56	51,51,51,51	0
56	MG	1A	3367	1/1	0.98	0.18	13,13,13,13	0
56	MG	2A	3541	1/1	0.98	0.06	53,53,53,53	0
56	MG	1A	3916	1/1	0.98	0.21	41,41,41,41	0
56	MG	1A	3588	1/1	0.98	0.14	55,55,55,55	0
56	MG	2A	3366	1/1	0.98	0.16	52,52,52,52	0
56	MG	1A	3066	1/1	0.98	0.20	17,17,17,17	0
56	MG	2A	3039	1/1	0.98	0.09	37,37,37,37	0
56	MG	12	102	1/1	0.98	0.16	49,49,49,49	0
56	MG	1A	3222	1/1	0.98	0.45	38,38,38,38	0
56	MG	1a	1767	1/1	0.98	0.10	50,50,50,50	0
56	MG	1A	3358	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3140	1/1	0.98	0.24	37,37,37,37	0
56	MG	1A	3068	1/1	0.98	0.15	17,17,17,17	0
56	MG	2A	3013	1/1	0.98	0.14	33,33,33,33	0
56	MG	2A	3041	1/1	0.98	0.19	29,29,29,29	0

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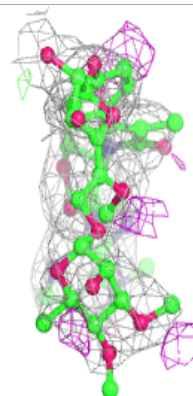
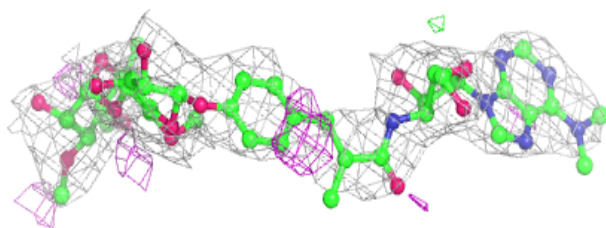
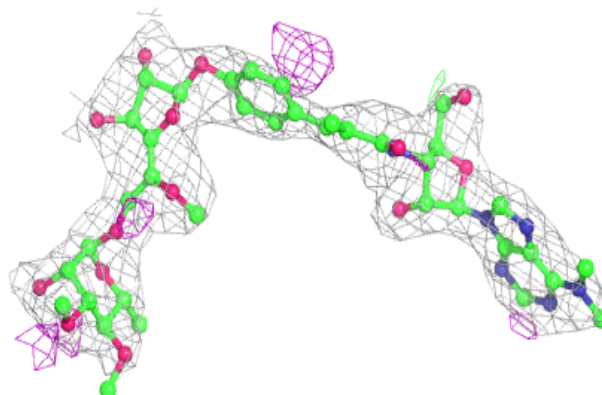
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3896	1/1	0.98	0.70	41,41,41,41	0
56	MG	2A	3579	1/1	0.98	0.09	51,51,51,51	0
56	MG	1A	3695	1/1	0.98	0.19	45,45,45,45	0
56	MG	2A	3201	1/1	0.98	0.16	42,42,42,42	0
56	MG	1A	3369	1/1	0.98	0.21	37,37,37,37	0
56	MG	2A	3049	1/1	0.99	0.04	41,41,41,41	0
59	ZN	1n	501	1/1	0.99	0.16	56,56,56,56	0
56	MG	2a	1644	1/1	0.99	0.11	61,61,61,61	0
56	MG	2A	3002	1/1	0.99	0.13	29,29,29,29	0
56	MG	1W	3003	1/1	0.99	0.26	34,34,34,34	0
56	MG	1A	3443	1/1	0.99	0.19	31,31,31,31	0
56	MG	1A	3490	1/1	0.99	0.10	9,9,9,9	0
56	MG	1A	3047	1/1	0.99	0.16	28,28,28,28	0
56	MG	1E	304	1/1	0.99	0.17	23,23,23,23	0
59	ZN	25	501	1/1	0.99	0.18	54,54,54,54	0
59	ZN	19	501	1/1	0.99	0.20	42,42,42,42	0
56	MG	2A	3358	1/1	0.99	0.08	35,35,35,35	0
56	MG	1A	3873	1/1	0.99	0.14	13,13,13,13	0
56	MG	1a	1758	1/1	0.99	0.13	29,29,29,29	0
56	MG	1A	3155	1/1	0.99	0.26	36,36,36,36	0
56	MG	2A	3348	1/1	0.99	0.07	54,54,54,54	0
56	MG	2a	1728	1/1	0.99	0.10	75,75,75,75	0
56	MG	1A	3602	1/1	0.99	0.18	33,33,33,33	0
56	MG	1a	1834	1/1	0.99	0.28	57,57,57,57	0
56	MG	1A	3432	1/1	0.99	0.14	29,29,29,29	0
56	MG	1A	3525	1/1	0.99	0.18	23,23,23,23	0
56	MG	2A	3562	1/1	0.99	0.14	34,34,34,34	0
56	MG	1a	1689	1/1	0.99	0.18	39,39,39,39	0
56	MG	1a	1832	1/1	0.99	0.09	37,37,37,37	0
56	MG	1A	3030	1/1	0.99	0.17	36,36,36,36	0
56	MG	1D	302	1/1	0.99	0.20	32,32,32,32	0
56	MG	2F	304	1/1	0.99	0.07	39,39,39,39	0
56	MG	1a	1695	1/1	0.99	0.22	42,42,42,42	0
56	MG	1A	3509	1/1	0.99	0.17	48,48,48,48	0
56	MG	1A	3544	1/1	0.99	0.22	35,35,35,35	0
56	MG	2A	3029	1/1	0.99	0.10	26,26,26,26	0
56	MG	1A	3772	1/1	0.99	0.13	33,33,33,33	0
56	MG	1A	3912	1/1	0.99	0.31	37,37,37,37	0
56	MG	1a	1649	1/1	0.99	0.34	58,58,58,58	0
56	MG	1a	1721	1/1	0.99	0.18	47,47,47,47	0
56	MG	1A	3403	1/1	0.99	0.13	15,15,15,15	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

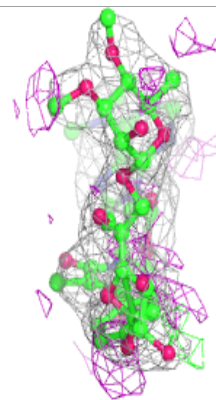
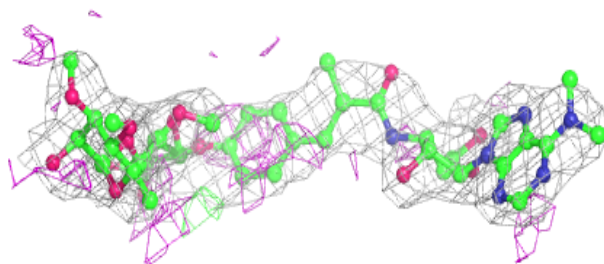
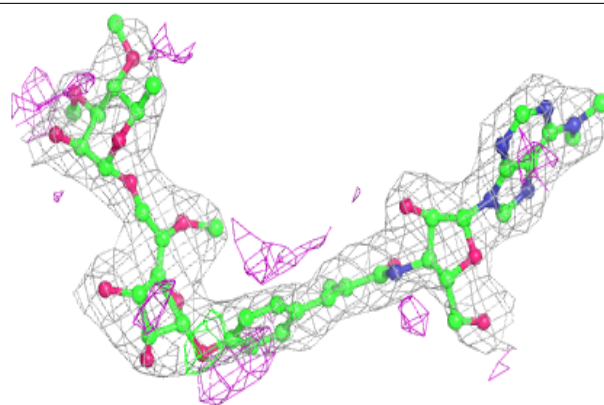
**Electron density around 4M2 2A 3673:**

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



**Electron density around 4M2 1A 3894:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.