



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:37 am BST

PDB ID : 6UO1  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA (containing pseudouridine at the first position of the codon) and deacylated A-, P-, and E-site tRNAs at 2.95Å resolution  
Authors : Batool, Z.; Dobosz-Bartoszek, M.; Polikanov, Y.S.  
Deposited on : 2019-10-14  
Resolution : 2.95 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

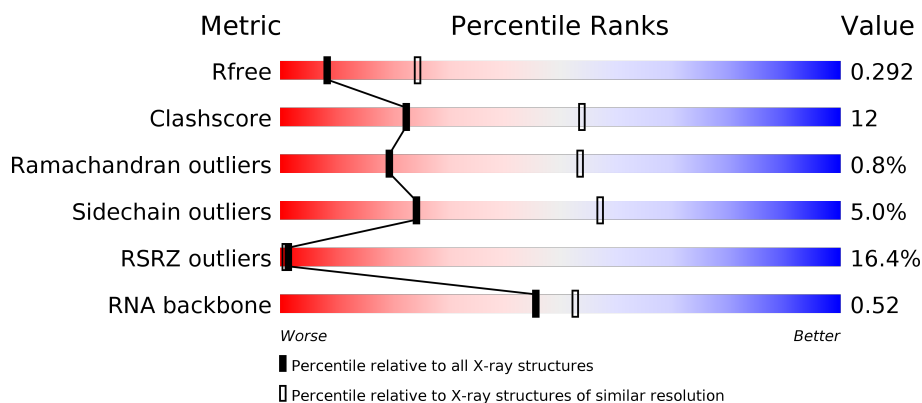
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>3%</div> <div>55%</div> <div>36%</div> <div>7%</div> <div>.</div> </div>
1	2A	2915	<div> <div>4%</div> <div>46%</div> <div>41%</div> <div>9%</div> <div>.</div> </div>
2	1B	121	<div> <div>62%</div> <div>34%</div> <div>.</div> <div>.</div> </div>
2	2B	121	<div> <div>52%</div> <div>40%</div> <div>7%</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	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3036	-	-	-	X
56	MG	1A	3098	-	-	-	X
56	MG	1A	3104	-	-	-	X
56	MG	1A	3114	-	-	-	X
56	MG	1A	3121	-	-	-	X
56	MG	1A	3123	-	-	-	X
56	MG	1A	3142	-	-	-	X
56	MG	1A	3148	-	-	-	X
56	MG	1A	3149	-	-	-	X
56	MG	1A	3190	-	-	-	X
56	MG	1A	3318	-	-	-	X
56	MG	1A	3359	-	-	-	X
56	MG	1A	3368	-	-	-	X
56	MG	1A	3377	-	-	-	X
56	MG	1A	3394	-	-	-	X
56	MG	1A	3433	-	-	-	X
56	MG	1A	3506	-	-	-	X
56	MG	1A	3513	-	-	-	X
56	MG	1a	3016	-	-	-	X
56	MG	1a	3037	-	-	-	X
56	MG	1a	3043	-	-	-	X
56	MG	1a	3053	-	-	-	X
56	MG	1a	3082	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	3092	-	-	-	X
56	MG	1a	3094	-	-	-	X
56	MG	1a	3111	-	-	-	X
56	MG	1a	3116	-	-	-	X
56	MG	1a	3122	-	-	-	X
56	MG	1a	3163	-	-	-	X
56	MG	1a	3167	-	-	-	X
56	MG	2A	3057	-	-	-	X
56	MG	2A	3092	-	-	-	X
56	MG	2A	3099	-	-	-	X
56	MG	2A	3101	-	-	-	X
56	MG	2A	3111	-	-	-	X
56	MG	2A	3142	-	-	-	X
56	MG	2A	3158	-	-	-	X
56	MG	2A	3234	-	-	-	X
56	MG	2A	3245	-	-	-	X
56	MG	2A	3315	-	-	-	X
56	MG	2A	3316	-	-	-	X
56	MG	2A	3317	-	-	-	X
56	MG	2a	3007	-	-	-	X
56	MG	2a	3017	-	-	-	X
56	MG	2a	3031	-	-	-	X
56	MG	2a	3053	-	-	-	X
56	MG	2a	3058	-	-	-	X
56	MG	2a	3059	-	-	-	X
56	MG	2a	3060	-	-	-	X
56	MG	2a	3087	-	-	-	X



## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 295398 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
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

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

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

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

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

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

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

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

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

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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	13	Total	C	N	O	P	0	0	0
			277	125	50	89	13			
53	2v	8	Total	C	N	O	P	0	0	0
			167	75	25	59	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0
			1530	685	274	498	71	2		
54	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
54	2w	69	Total	C	N	O	P	S	0	0
			1482	662	267	482	69	2		
54	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2a	183	Total	Mg	0	0
			183	183		
56	1A	680	Total	Mg	0	0
			680	680		
56	2A	351	Total	Mg	0	0
			351	351		
56	1a	238	Total	Mg	0	0
			238	238		

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

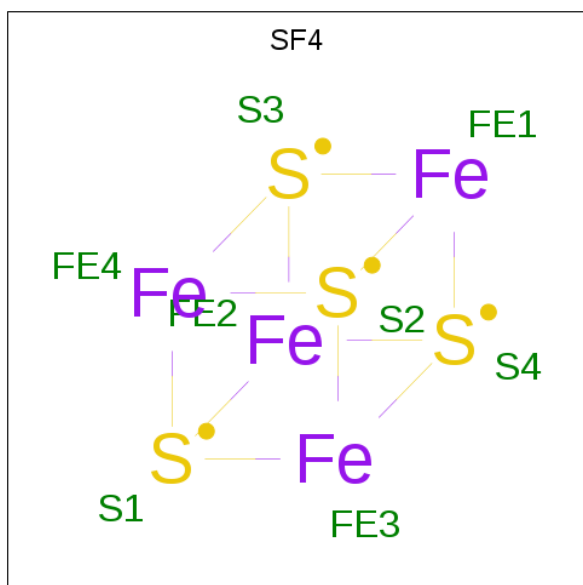
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		

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

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



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

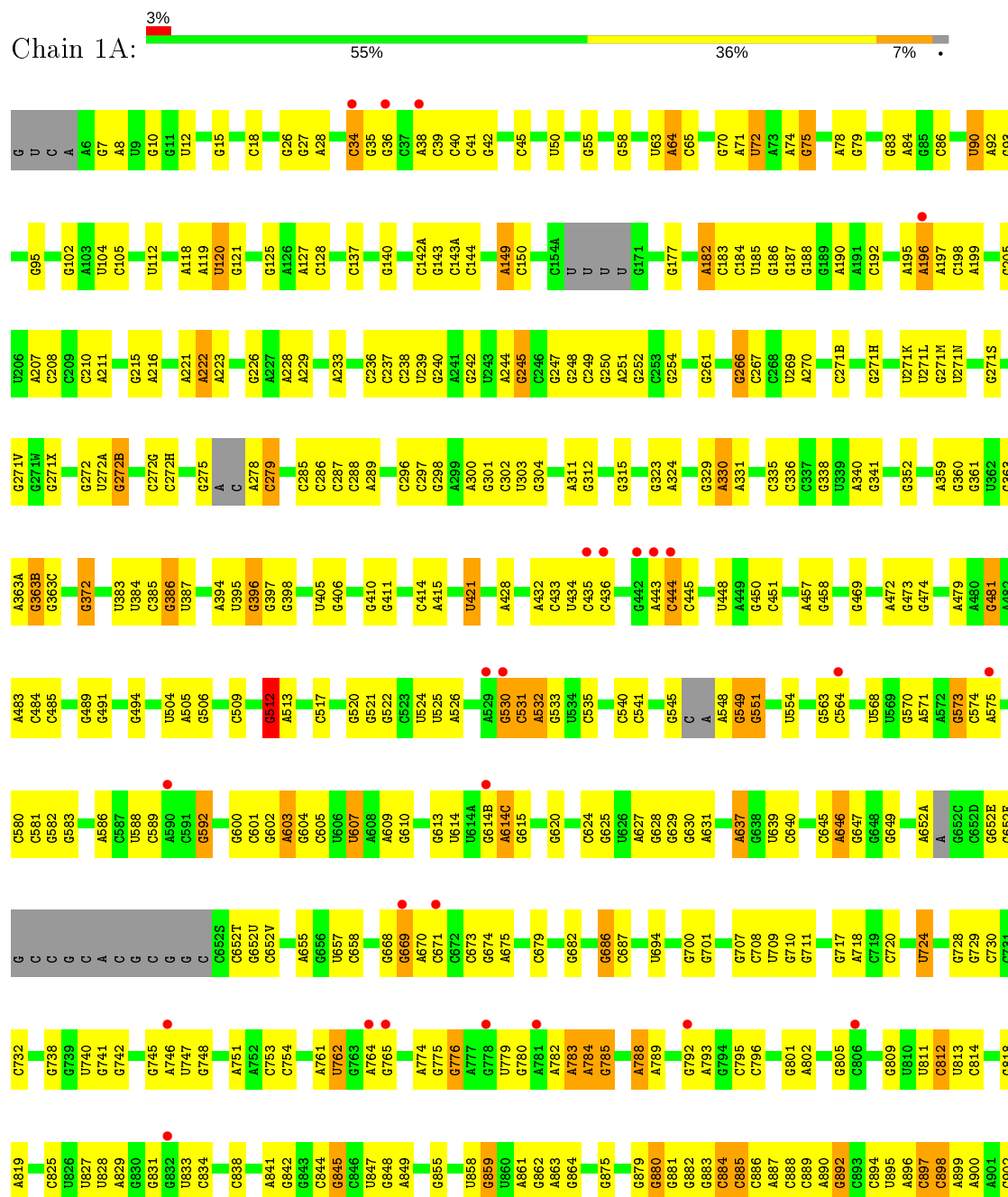
- Molecule 59 is water.

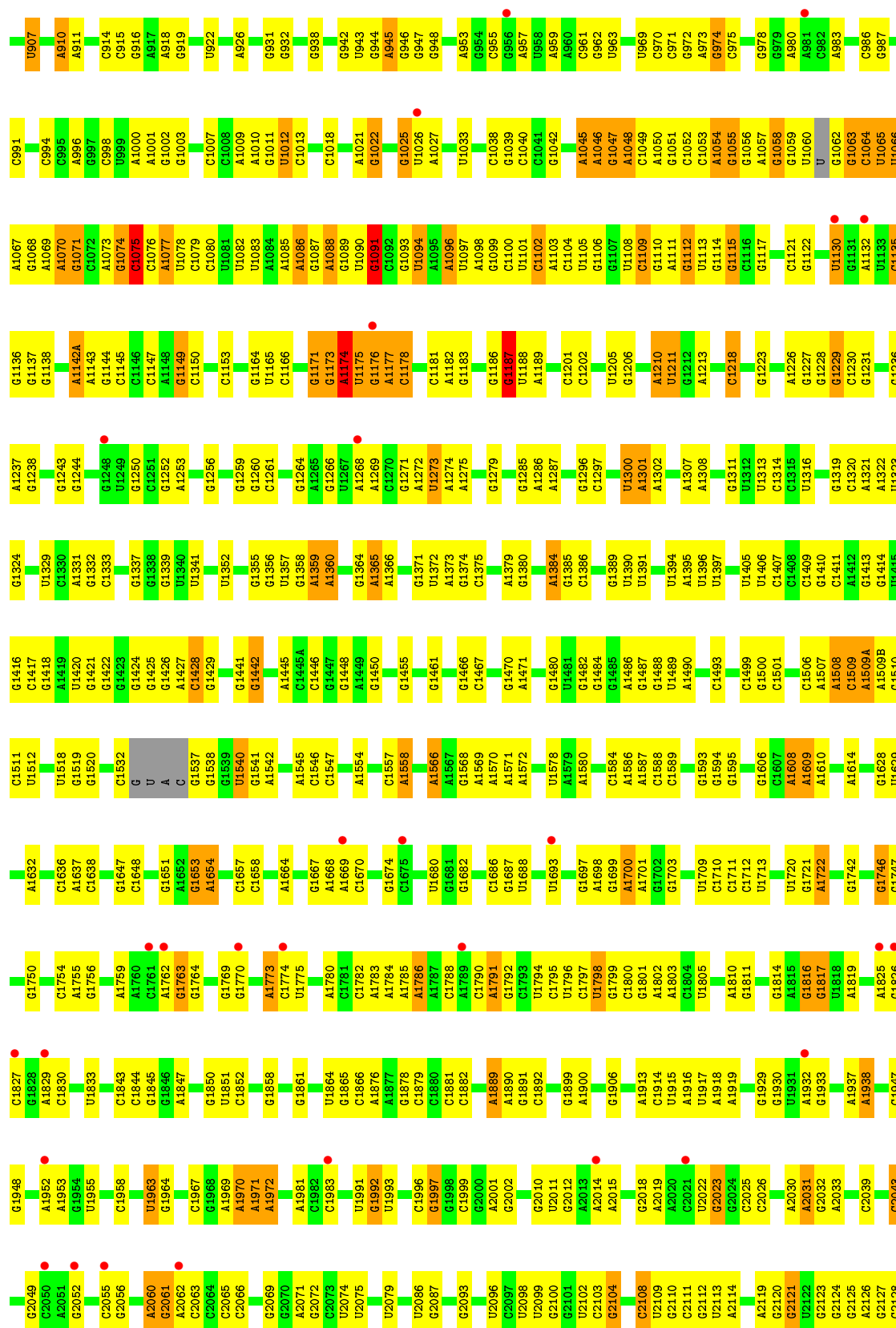
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	585	Total 585	O 585	0	0
59	1a	181	Total 181	O 181	0	0
59	2A	234	Total 234	O 234	0	0
59	2a	167	Total 167	O 167	0	0

### 3 Residue-property plots

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

#### • Molecule 1: 23S Ribosomal RNA

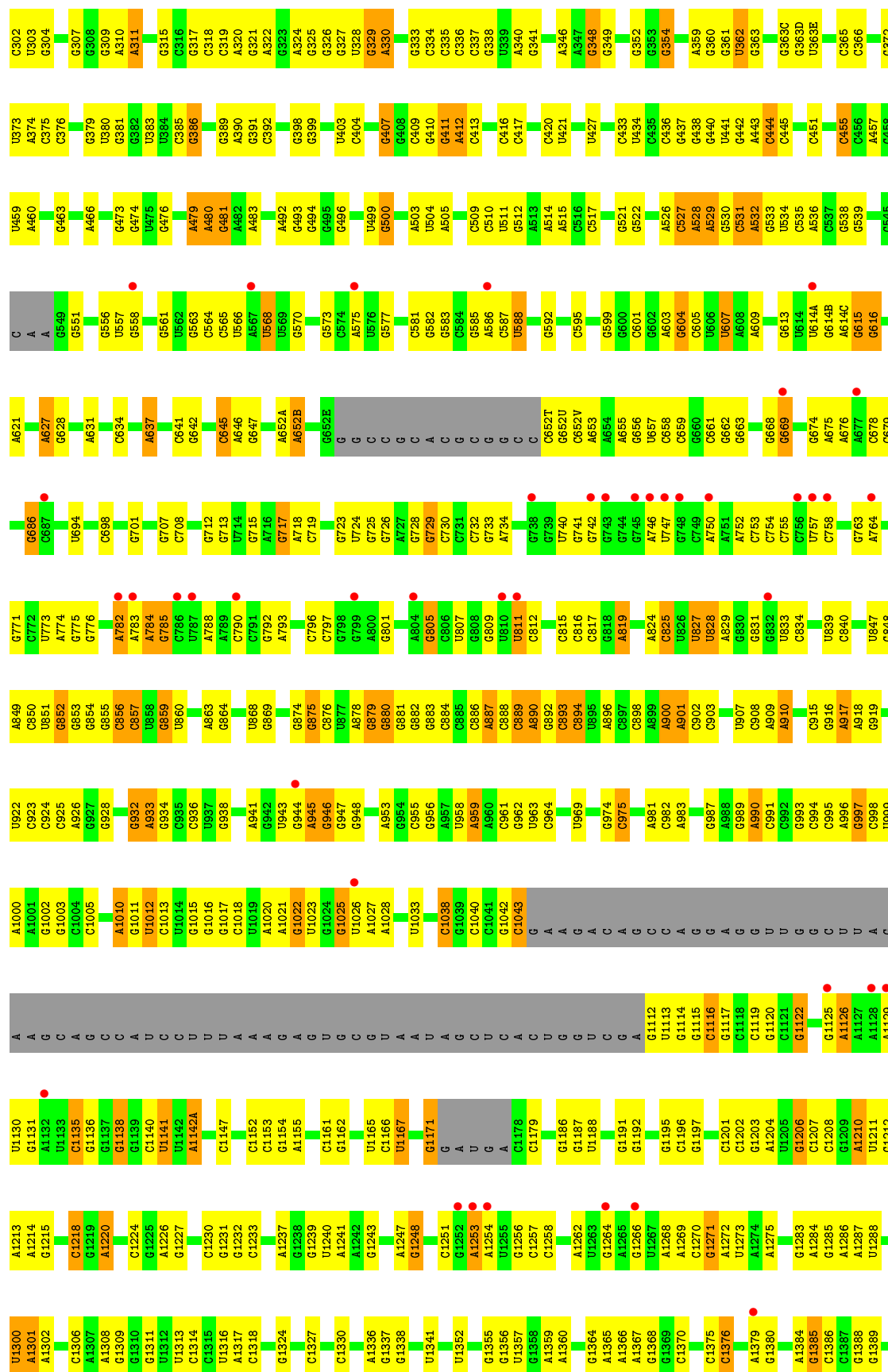




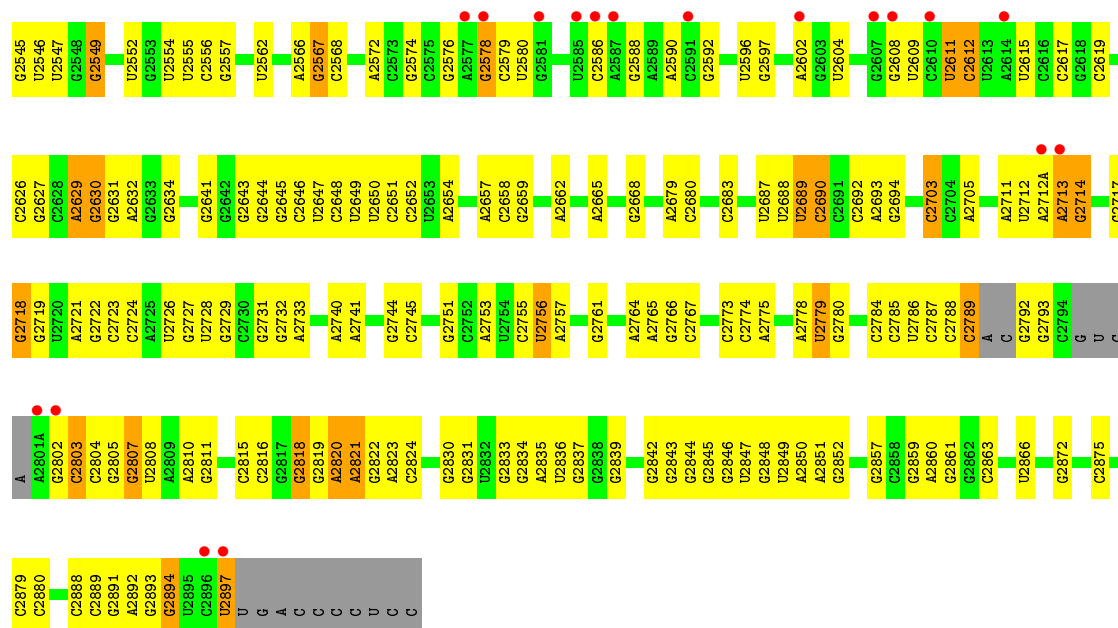


G247	U	U90	G
G248	U	A92	U
G249	U	G93	C
G250	G171	G94	A
G251	C172	G94A	A6
G252	G173	G95	G7
G253		G96	U9
	G177	G97	G10
A256	G178	G98	G11
A257	A182	G99	U12
G261	C183	G100	
	C184	G102	G15
A265	U185	A103	G16
G266	G186	U104	
C267	G187	C105	G23
	G188	C106	
A271A	G189	G107	G27
		U108	
G271F	A185	G109	G30
G271H	A196	G110	C31
G271I	A197	A111	
G271J	C198	U112	G34
G271J	A199	G113	G35
U271K		U114	G36
G271M	U205	C115	
G271N	A206	C116	C39
G271O	A207	G117	C40
G271O	C208	A118	C41
G271P	G209	A119	G42
	C210	U120	A43
G271U	A211	G121	G44
G271V	G212	G122	C45
G271V	A213		C47
	G214	G125	
G272B	G215	A126	C57
G272C	A216	A127	G58
	G217	C128	
G272G	A218		C62
G272H		G131	U63
U272J	A221		A64
G272J	A222		G68
G274		G136	C69
G275	A228	C137	G70
A276	A276	G139	A71
G277	U230	G140	U72
A278	A278	A141	A73
G279	A233		A74
C280	C234	G143	G75
	U235	C143A	C76
C286	C236	C144	
C287	C237	G145	G79
	C238		G80
C291	U239	A149	G81
	G240		G82
C296	A241	G152	G83
C297	G242	C153	A84
		G154	G85
A300	G245	C154A	C86
	C246	U157	

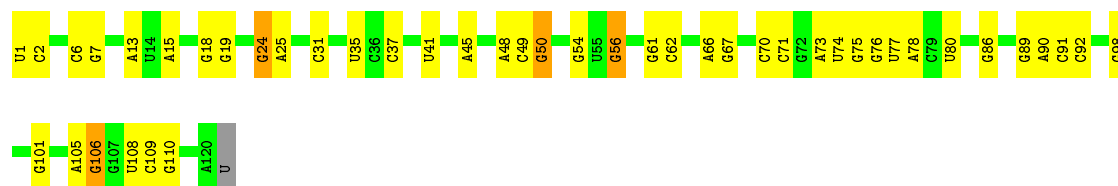




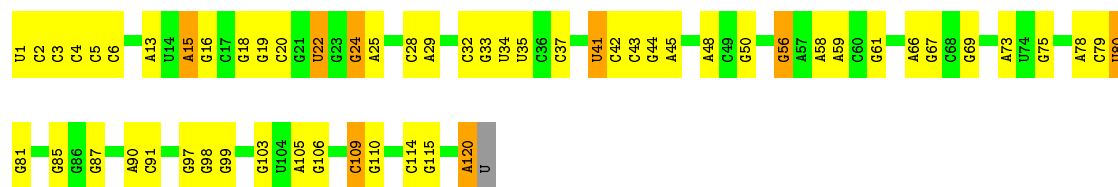
G2468	G2395	C2248	G2157	C2095	G2018	A1927	G1811	G1721	C1548	A1472	U1394
A2469	G2396	U2249	A2158	U2096	A2019	A1928	A1812	A1722	C1640	G1473	A1396
C2474	G2397	G2250	G2159	C2097	G2022	A1929	G1813	U1739	A1641		
G2475	G2399	G2251	G2160	U2098	U2022	G1930	G1814	G1740	G1642		
A2476	G2396		C2161	U2099	G2023	U1931	A1815	A1741	G1643		
G2477	A2327	C2258	G2162	G2100	G2024	G1931	G1816	G1742	C1644		
	A2328		G2163	G2101	G2025	G1935	G1817		C1557		
C2403	G2329	C2261	C2164	U2102	G2026	A1936	C1745A	C1745	A1558	G1482	C1403
C2404			G2165	G2103	G2027	A1937	A1821	C1745A	G1559	C1404	
G2405	G2334	C2264	G2166	G2104	A2030	A1938	G1827	G1746	G1560	A1490	U1405
U2406	A2335	U2265	U2167	C2105	A2031	U1939	G1828				
G2407	A2336	A2266	G2168	G2106	A2032		C1829	C1751	A1566	C1493	
G2408	G2337	A2267	A2169	C2107	G2032	C1942	A1829	C1752	A1567		
G2409	G2338	A2268	A2170	U2108	A2033	U1943	G1835	G1753	A1569	A1496	
G2486	G2339	A2269	A2171	U2109		U1944	G1835			U1497	
G2487	G2340		U2172	G2110	G2036	G1945		G1756			
A2411	A2412	A2273	A2173	G2111	G2037		C1838				
G2488	G2341	A2274	A2173	G2112	G2038	U1955	G1839	A1762	C1575	G1500	
G2489	G2342	G2275		G2113	G2039			G1764	U1576	C1501	
U2491	U2344		A2176	U2113	G2039	U1960	C1843				
	G2345	C2177	C2178	A2114	U2040	C1961	G1846	G1770	C1505	U1505	
G2494	G2345	G2278	G2179	G2115	U2041	G1962	G1847	C1771	A1507	G1421	
G2495	A2346	G2279	U2180	G2116	A2042	U1963	A1847	G1772	A1580	G1422	
	C2347		G2181	U2117	G2043	G1964	A1848		A1581	G1423	
A2492		C2283	G2182	U2118				A1773	C1582	C1509	
	G2351	C2284	C2182	A2119	G2050			C1773	A1583	A1509A	
	A2352	C2285	G2183	G2120	A2051	C1967	A1853	C1774	A1584	A1509B	
	G2353	A2286	C2184	G2121	G2052	G1968	A1854		A1586	G1426	
G2427	G2354	A2287	G2185	U2122	G2053	A1969		U1777	C1670	C1511	
C2355	C2355	A2288	G2186		A2054	A1970	G1858	U1778			
			G2187	C2055	C2055	A1971	A1859	U1779	G1674	U1514	
G2429	C2364	U2291	C2188	A2126	G2056	C1972	A1860	A1780	C1675	G1515	
U2430	G2365	C2292	U2189	C2127	G2056	A1972	G1861	G1781		C1516	
G2505	U2431	C2293	U2190	C2128	A2057	G1973	G1862	C1782	U1680	G1517	
G2506	A2432	G2293	G2190	U2129	A2058	C1974	G1862	A1783		U1518	
G2507	A2433	G2294	G2191	U2130	A2059			A1784	C1685	G1519	
G2508	A2433	G2295	G2192	G2131	A2060	A1977	G1865	A1785			
G2509	A2434	C2295	G2193	G2132	G2061			A1786	C1598	G1520	
G2510	A2435	U2296	G2193	U2132	A2061			A1786	C1599	U1523	
		G2297	G2197	G2133	A2062	C1983	A1877	A1787	G1687	G1524	
		G2297	U2197	A2134	G2066	G1984	G1878	C1788	A1689	G1525	
A2439	G2371	A2298	C2198	A2135	C2066	G1985	G1882	A1789		G1526	
G2512	G2372	G2299	U2189	A2135	G2067	A1986	G1883	C1790	U1693	A1445	A1445A
G2513	G2373	G2300	G2300	C2136	U2068			A1791		G1527	
U2514	G2373	G2300	G2300	C2136	G2068			A1791			
G2441	G2374	G2301	G2301	C2137	G2069			G1792	G1696	C1529	
G2442	G2375	G2302	G2302	C2138	G2069			G1793	C1607	C1530	
G2443	G2375	G2303	G2303	C2139	G2070			U1794	A1698	A1449	
	A2376	G2304	A2305	C2140	A2071	U1993		C1795	G1699	G1532	
		G2304		G2142				U1796	A1609	G1532	
G2446	A2377	G2305	A2224	C2142	U2074	G1987	C1894	A1700	A1610	G1533	
G2447	A2378	G2306	G2224	G2143	U2075	G1998		A1701		U	
U2448	G2379	G2308	U2232	U2144		G1998	G1899	C1702	C1612	A	
U2449	C2381	A2309	U2233	C2145	C2078	G1999	A1900	G1703	G1613	C1536	
A2450	G2382	A2310	G2234	C2146	U2079	G2001	G1906	G1703	A1614	G1461	
				G2235	G2147	A2001	G1906	G1709	G1704	C1537	
G2454	G2383	A2311		G2147				G1801	G1615	C1462	
G2455	G2384	U2312	G2236	G2148	U2086	G2002		A1802	U1706	G1539	
G2456	G2385	C2313	G2237	G2149	G2087			A1803			
U2457		C2314	G2238	G2150	G2888	A2005	A1913	A1803	U1710	U1540	
		G2315	G2238	U2150	G2888			A1803			
	A2388	G2315	G2239	G2151	U2089			A1805	C1710	G1465	
	G2389	C2316	G2239	G2152	G2090	G2010	A1915	U1805	G1541	G1467	
U2462	U2390	C2317		G2153	U2091		A1916	U1808	G1542	C1467	
G2536	G2391	G2318		G2153	G2091			U1713	G1543	C1468	
G2537	G2391	G2318		G2154	U2092	A2014	G1920	G1714	A1544	A1469	
G2538	G2392	U2243	G2242	G2154	U2092	A2015	G1921				
G2539	A2393	G2243	U2244	G2155	G2093						
G2540	G2393	A2320	U2244	G2155	G2094						
	G2394	C2321		C2156	C2094						



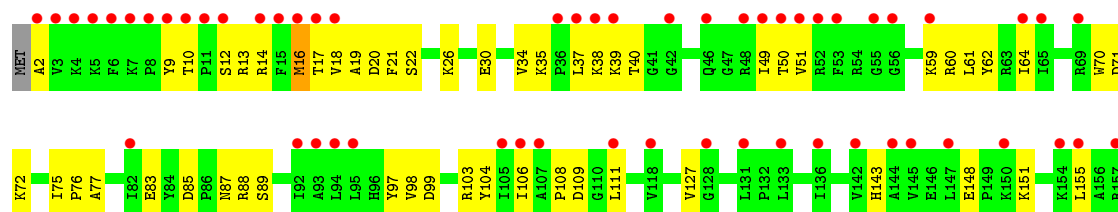
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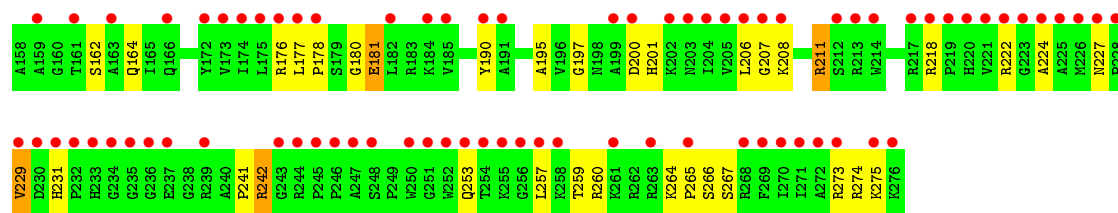


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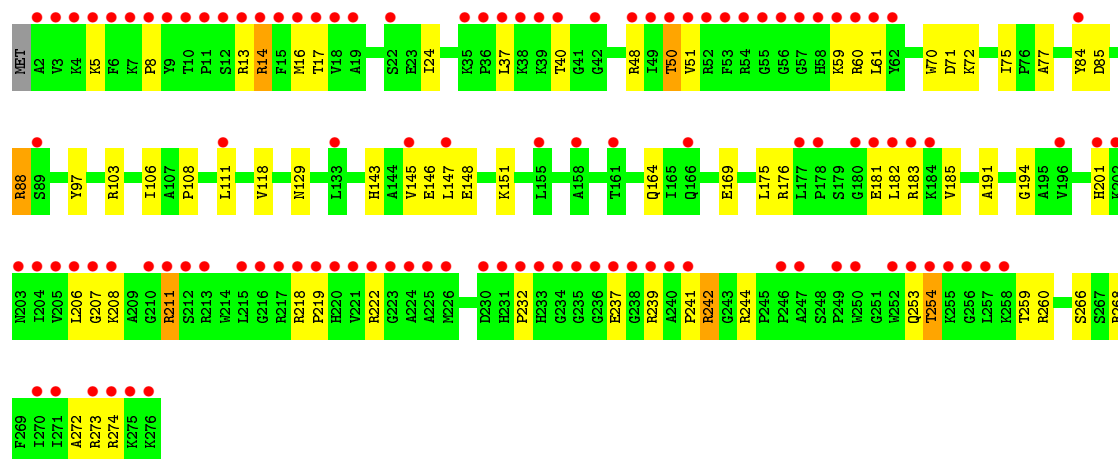
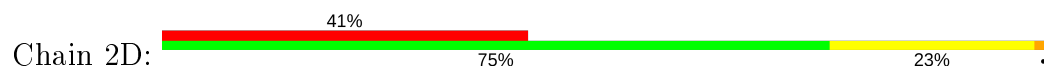


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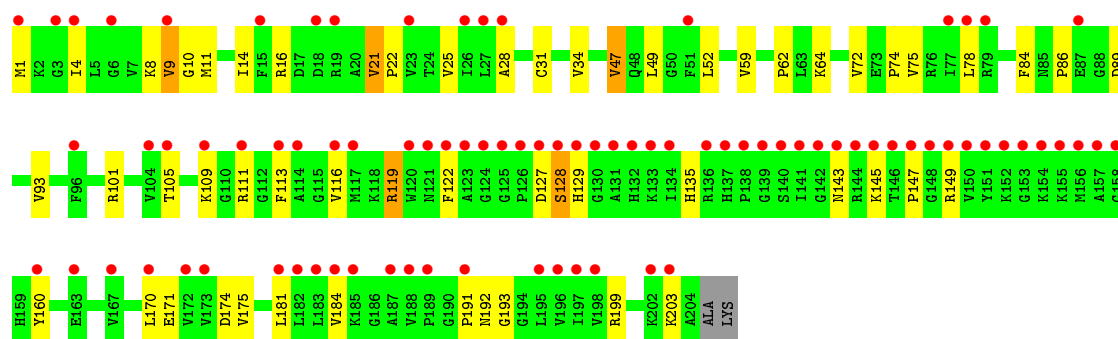
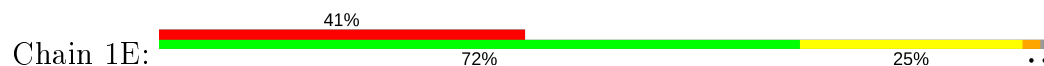




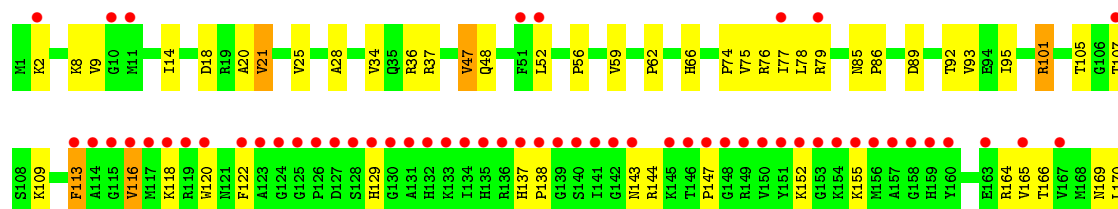
• Molecule 3: 50S ribosomal protein L2

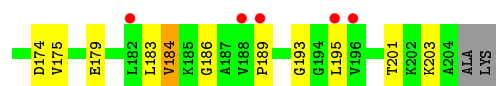


• Molecule 4: 50S ribosomal protein L3

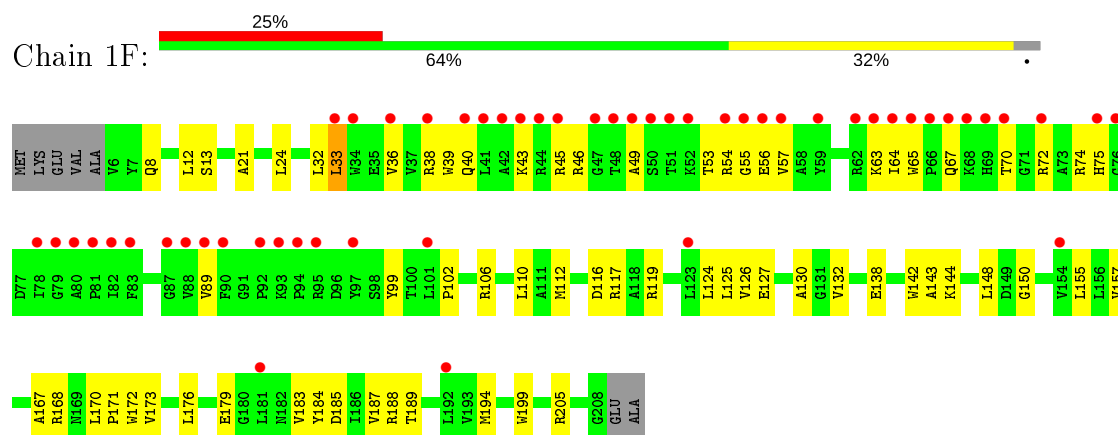


• Molecule 4: 50S ribosomal protein L3

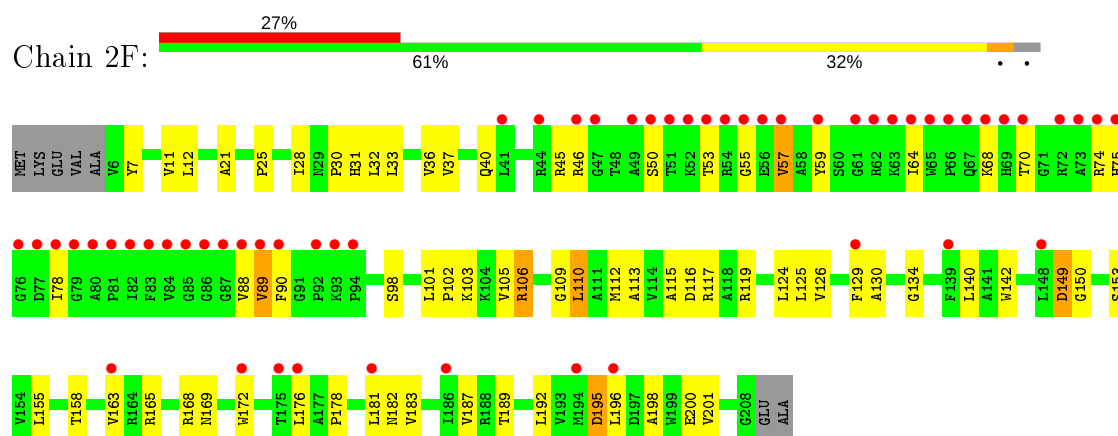




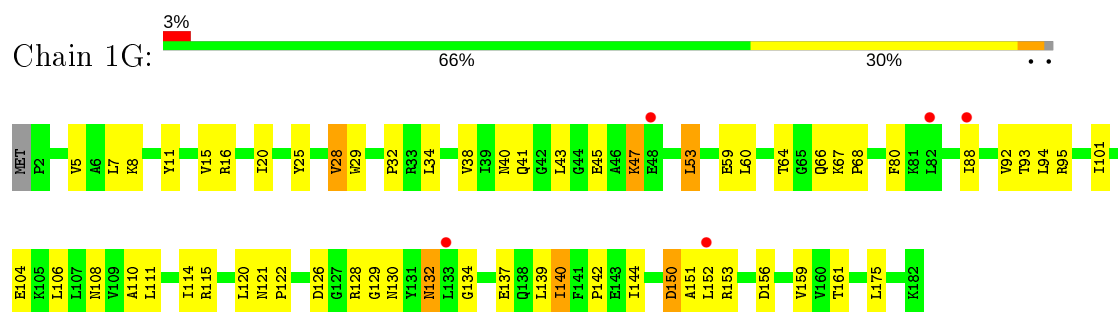
- Molecule 5: 50S ribosomal protein L4



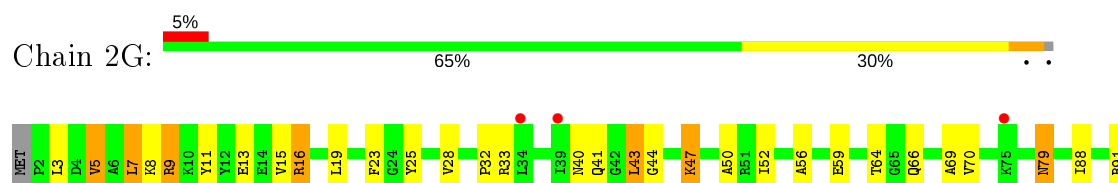
- Molecule 5: 50S ribosomal protein L4

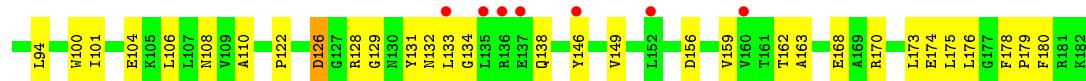


- Molecule 6: 50S ribosomal protein L5

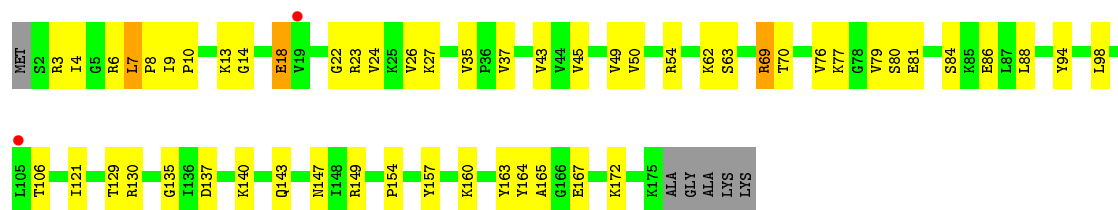


- Molecule 6: 50S ribosomal protein L5

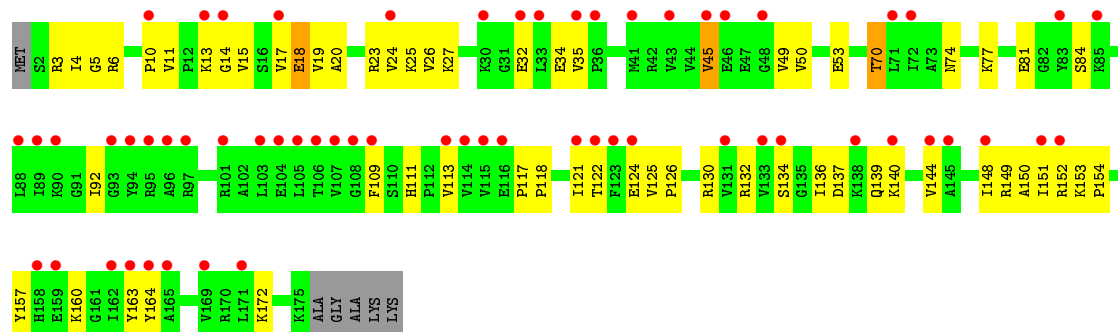




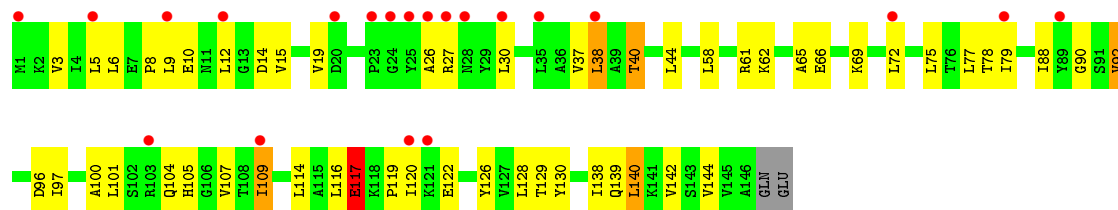
- Molecule 7: 50S ribosomal protein L6



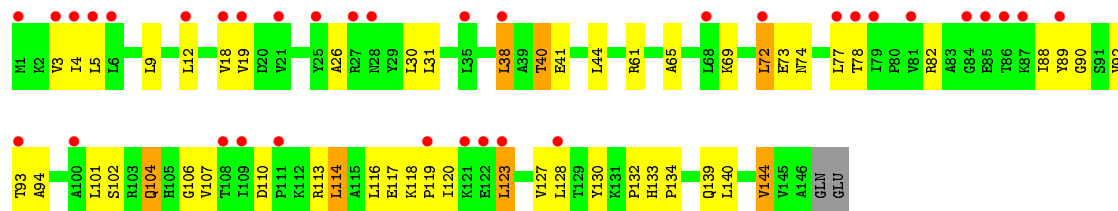
- Molecule 7: 50S ribosomal protein L6



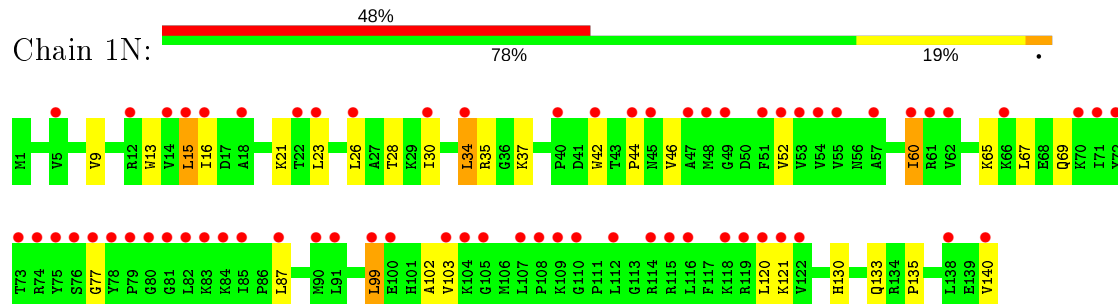
- Molecule 8: 50S ribosomal protein L9



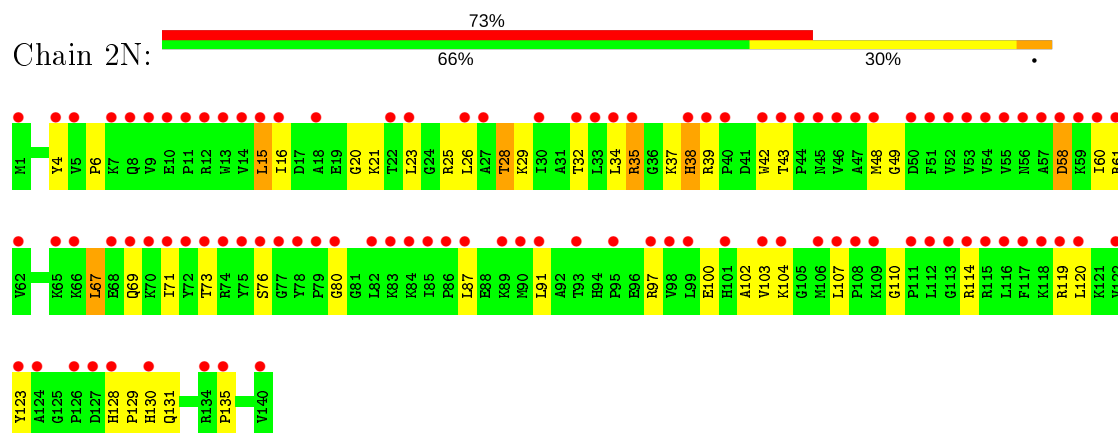
- Molecule 8: 50S ribosomal protein L9



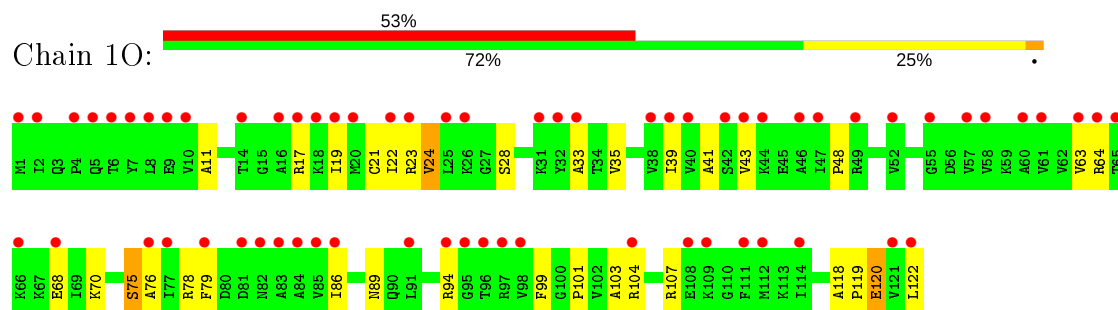
- Molecule 9: 50S ribosomal protein L13



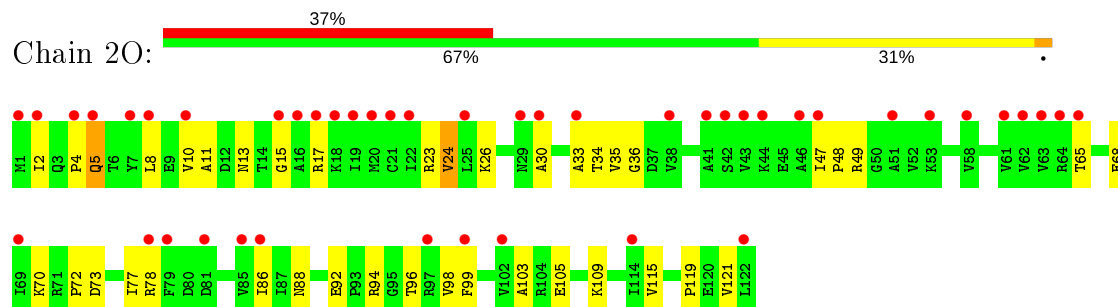
- Molecule 9: 50S ribosomal protein L13



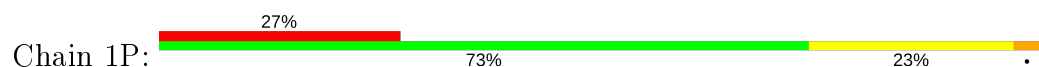
- Molecule 10: 50S ribosomal protein L14

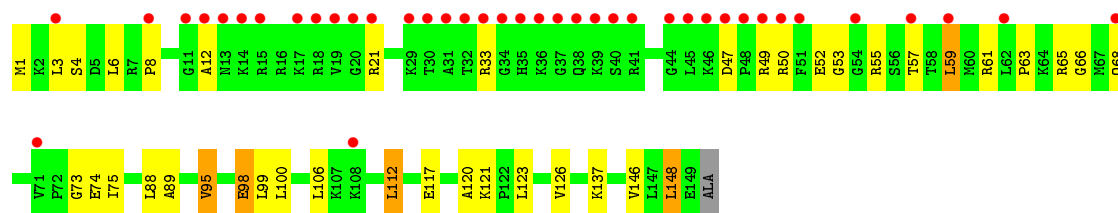


- Molecule 10: 50S ribosomal protein L14

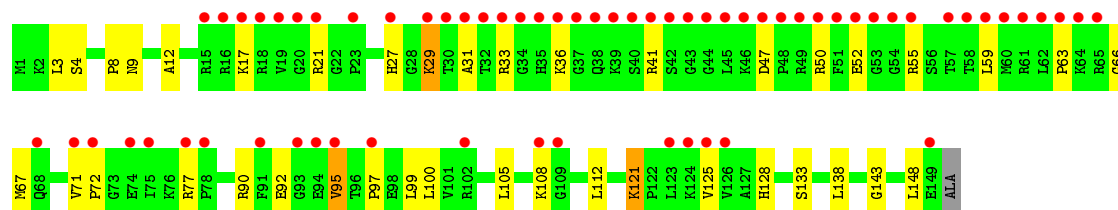
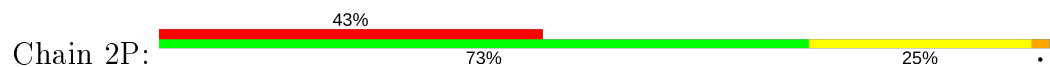


- Molecule 11: 50S ribosomal protein L15

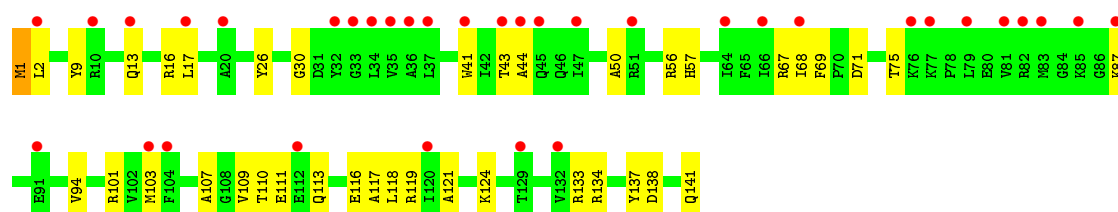
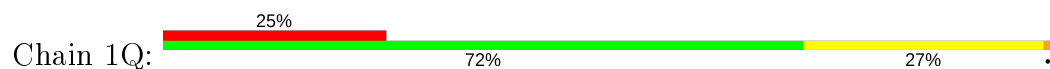




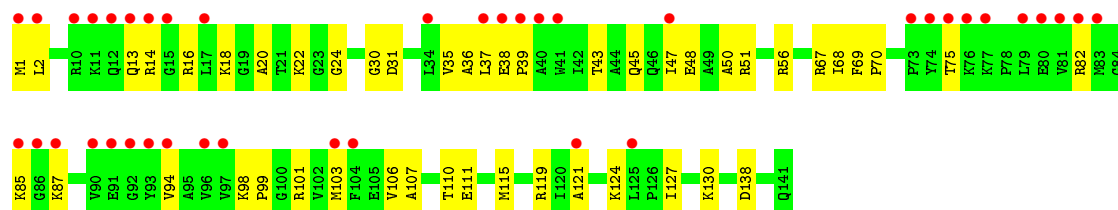
• Molecule 11: 50S ribosomal protein L15



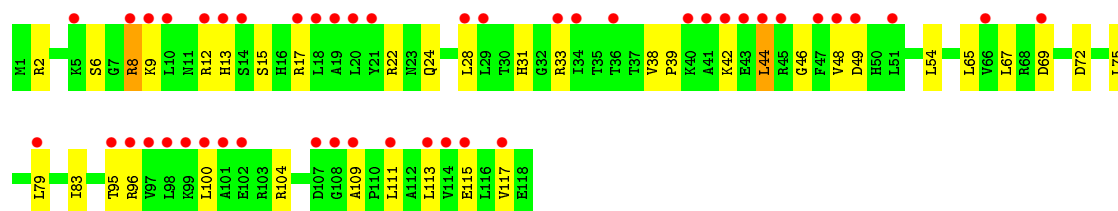
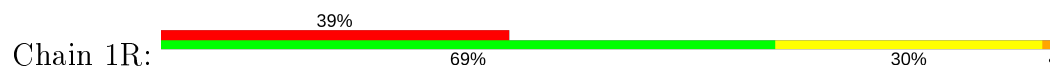
• Molecule 12: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L16

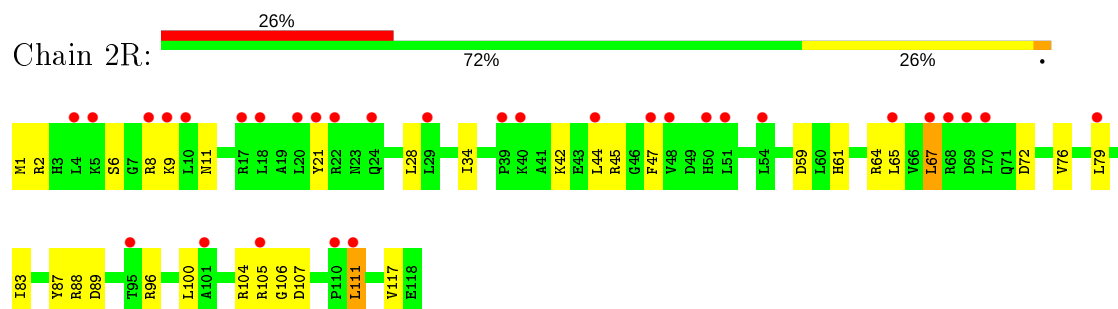


• Molecule 13: 50S ribosomal protein L17

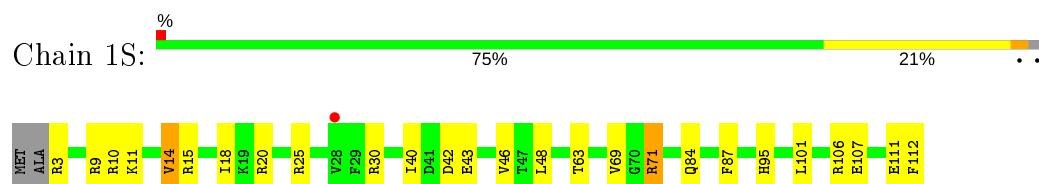




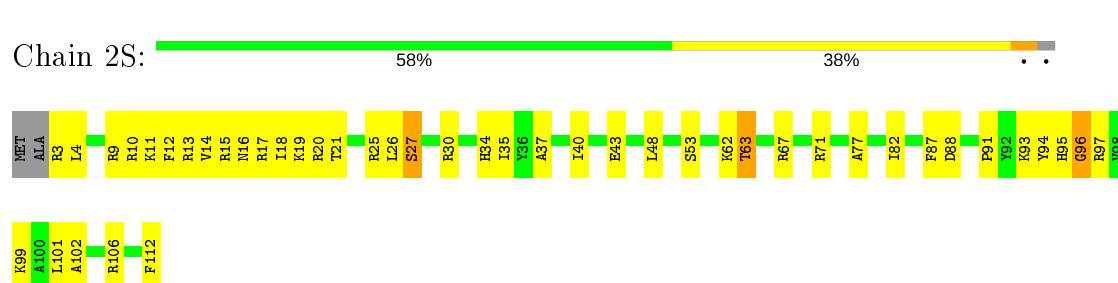
- Molecule 13: 50S ribosomal protein L17



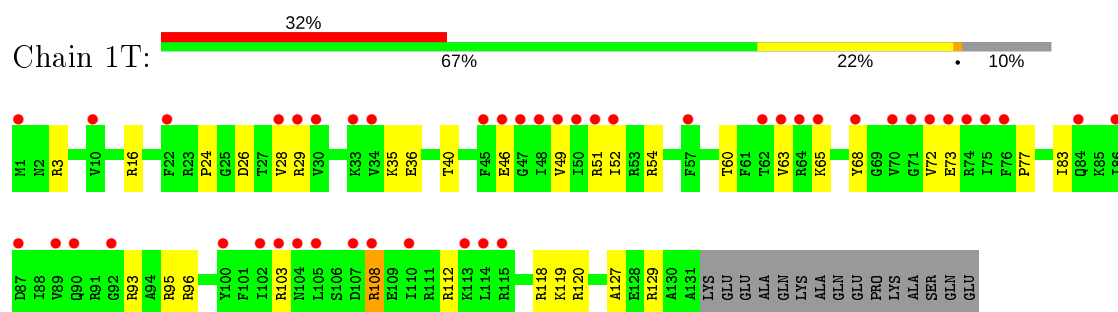
- Molecule 14: 50S ribosomal protein L18



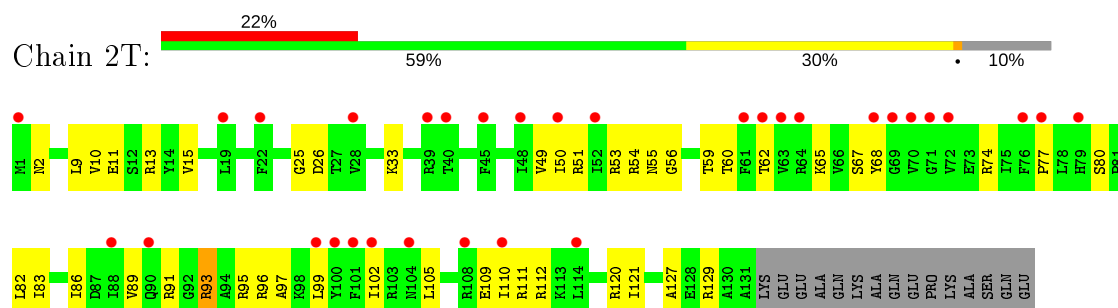
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19

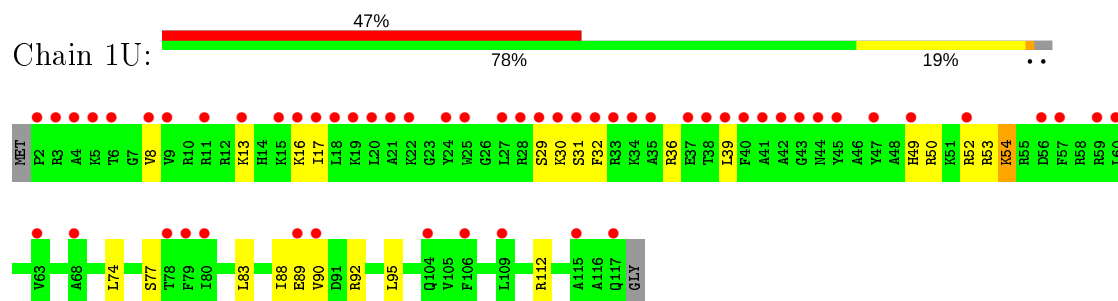


- Molecule 15: 50S ribosomal protein L19



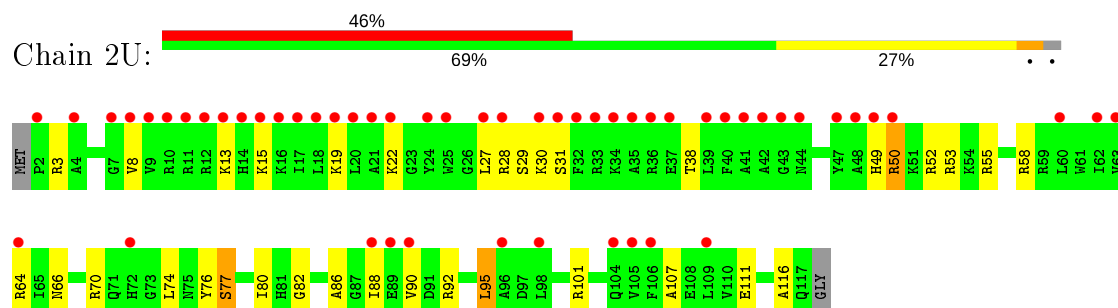
- Molecule 16: 50S ribosomal protein L20

Chain 1U:



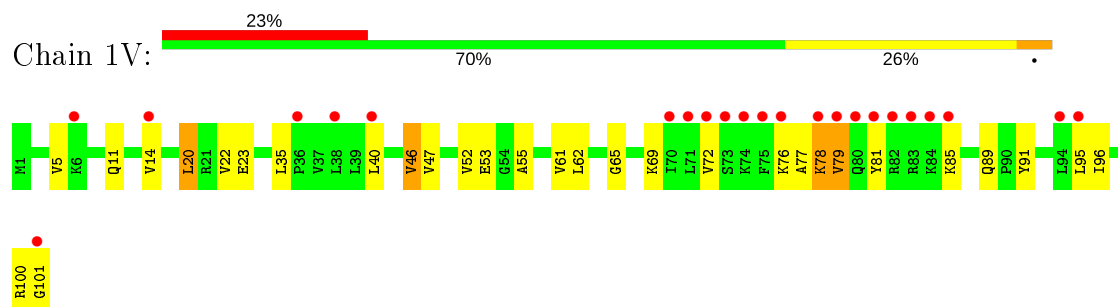
- Molecule 16: 50S ribosomal protein L20

Chain 2U:



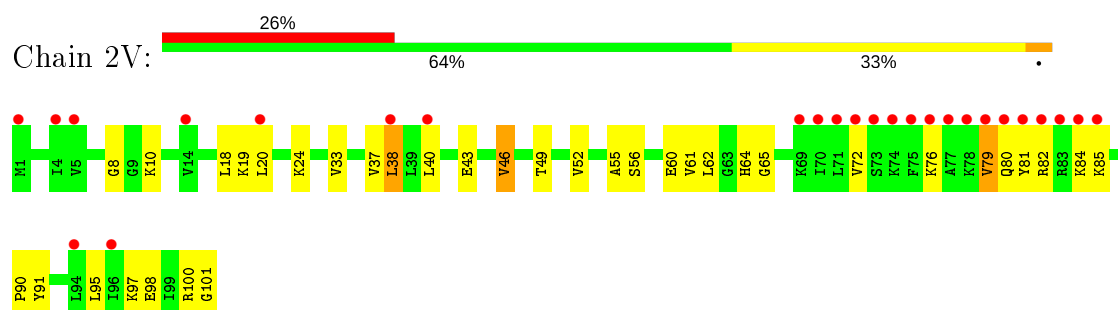
- Molecule 17: 50S ribosomal protein L21

Chain 1V:



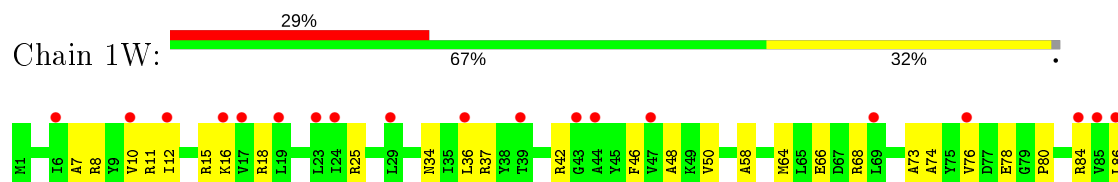
- Molecule 17: 50S ribosomal protein L21

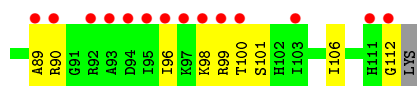
Chain 2V:



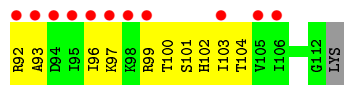
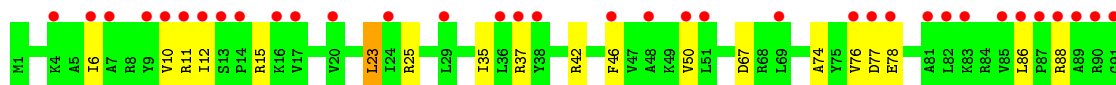
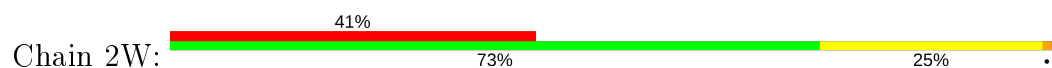
- Molecule 18: 50S ribosomal protein L22

Chain 1W:

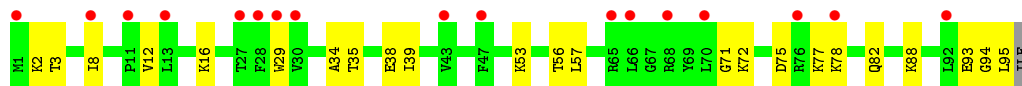
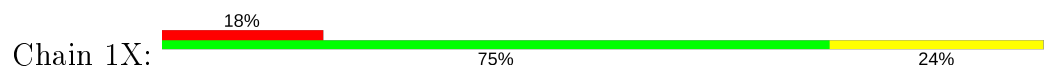




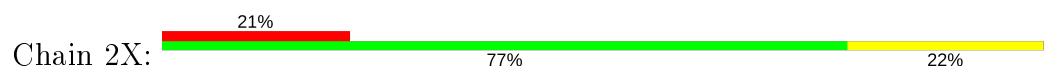
- Molecule 18: 50S ribosomal protein L22



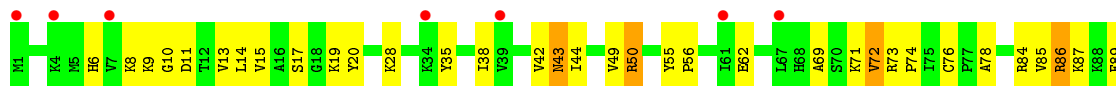
- Molecule 19: 50S ribosomal protein L23



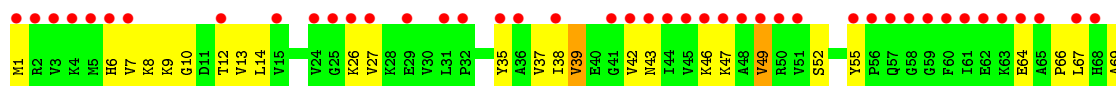
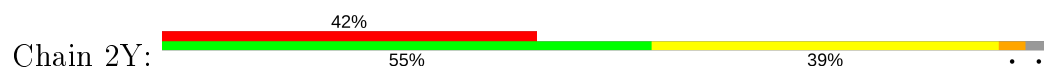
- Molecule 19: 50S ribosomal protein L23



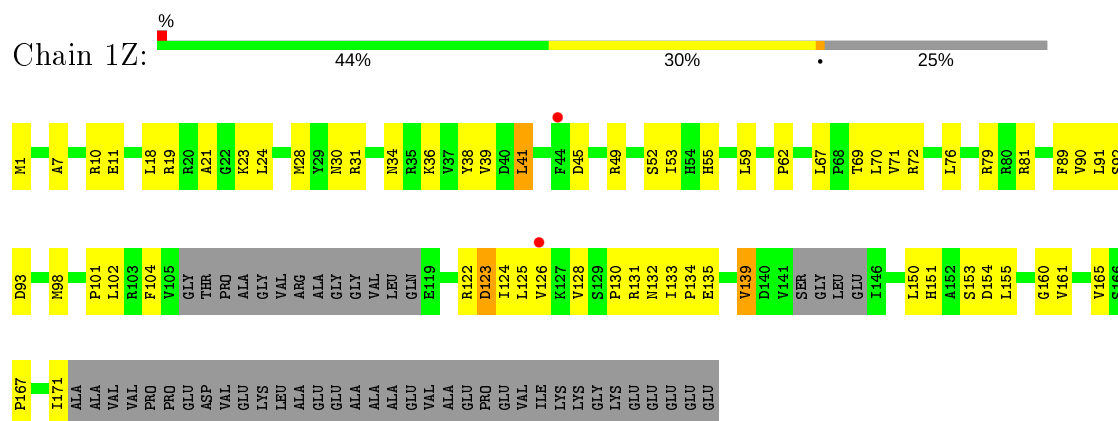
- Molecule 20: 50S ribosomal protein L24



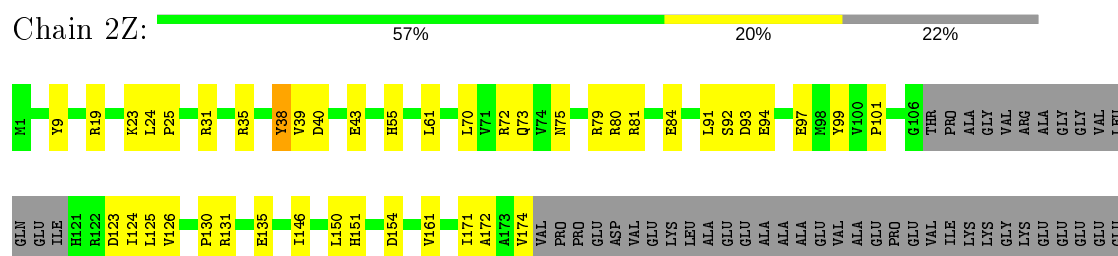
- Molecule 20: 50S ribosomal protein L24



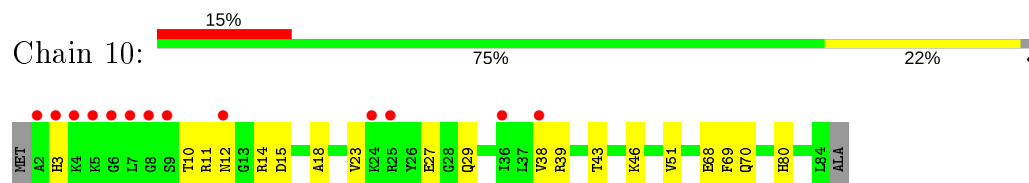
- Molecule 21: 50S ribosomal protein L25



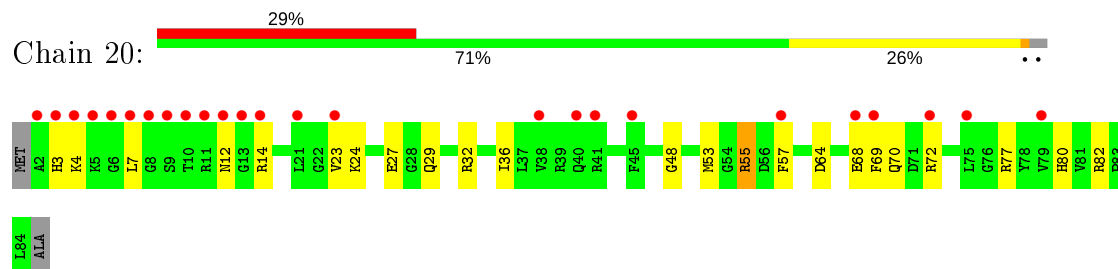
- Molecule 21: 50S ribosomal protein L25



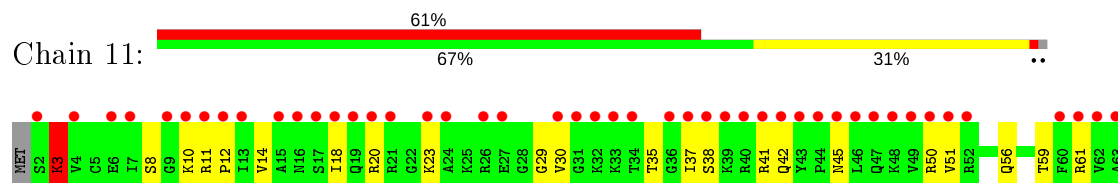
- Molecule 22: 50S ribosomal protein L27

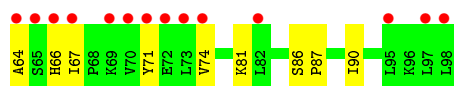


- Molecule 22: 50S ribosomal protein L27

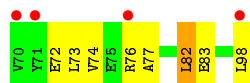
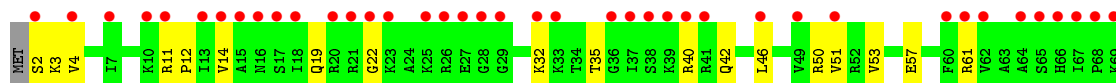
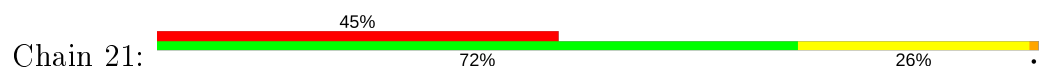


- Molecule 23: 50S ribosomal protein L28





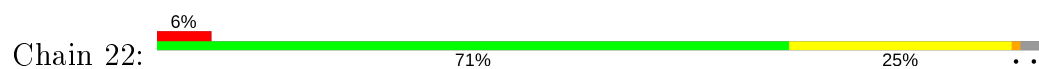
- Molecule 23: 50S ribosomal protein L28



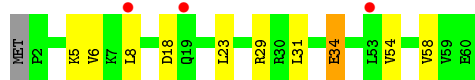
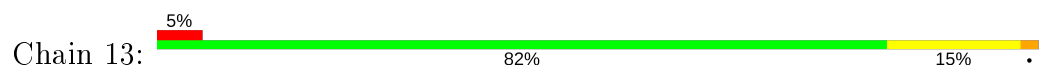
- Molecule 24: 50S ribosomal protein L29



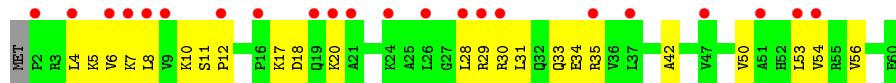
- Molecule 24: 50S ribosomal protein L29



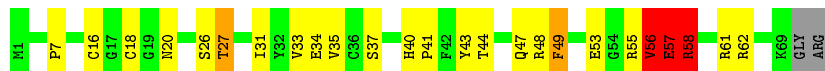
- Molecule 25: 50S ribosomal protein L30



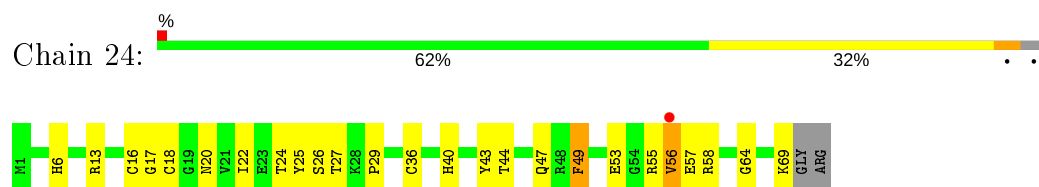
- Molecule 25: 50S ribosomal protein L30



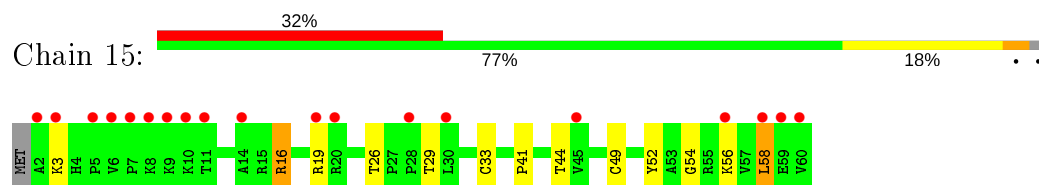
- Molecule 26: 50S ribosomal protein L31



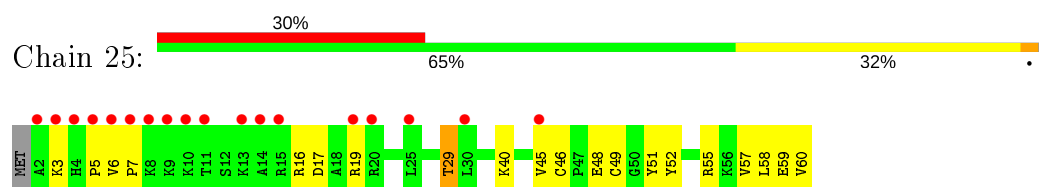
- Molecule 26: 50S ribosomal protein L31



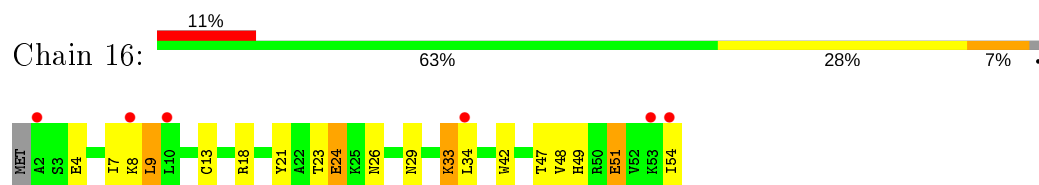
- Molecule 27: 50S ribosomal protein L32



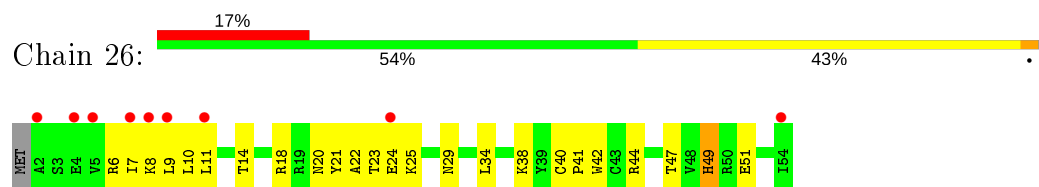
- Molecule 27: 50S ribosomal protein L32



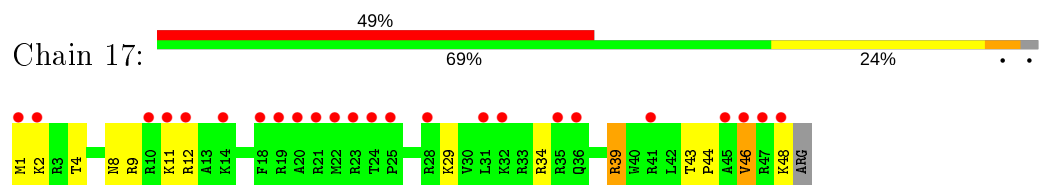
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

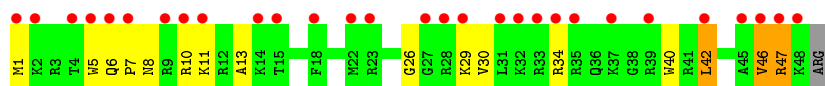


- Molecule 29: 50S ribosomal protein L34

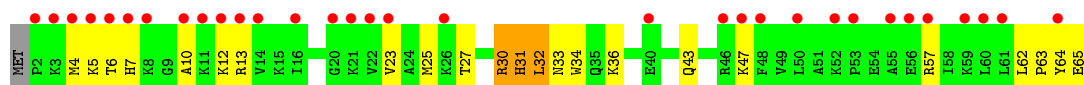


- Molecule 29: 50S ribosomal protein L34

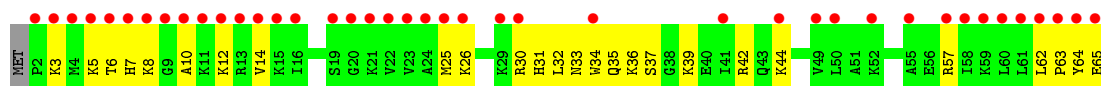




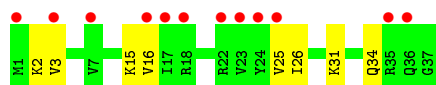
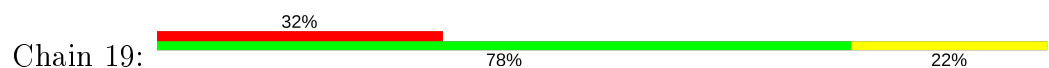
- Molecule 30: 50S ribosomal protein L35



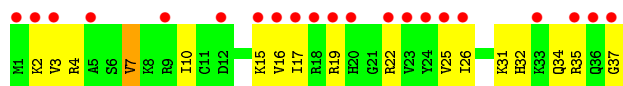
- Molecule 30: 50S ribosomal protein L35



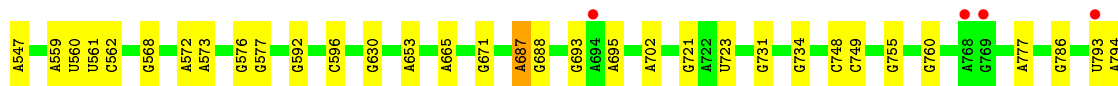
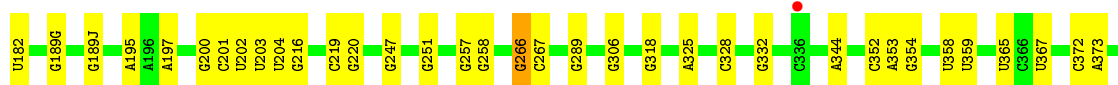
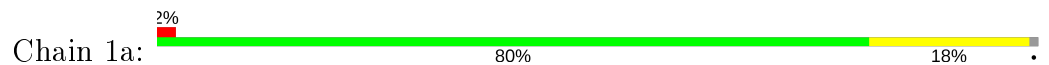
- Molecule 31: 50S ribosomal protein L36

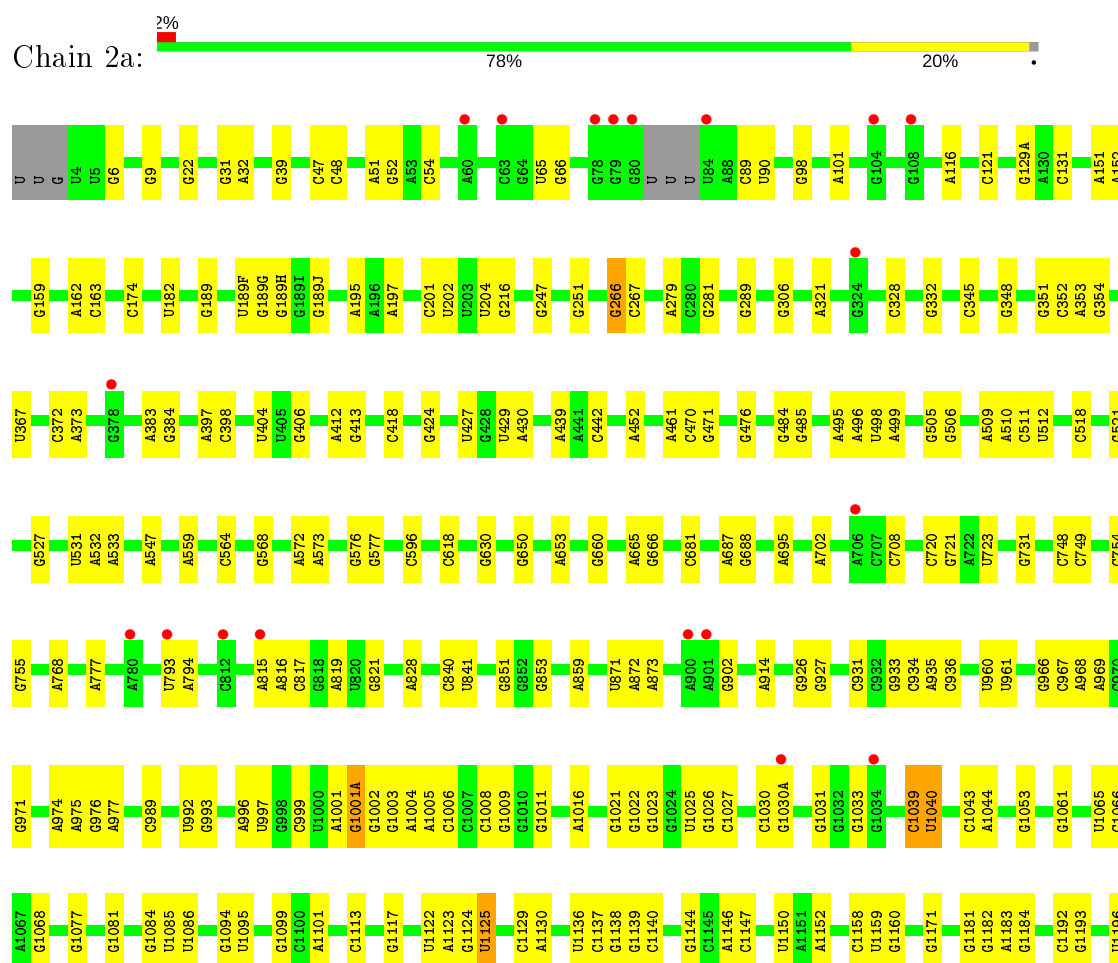
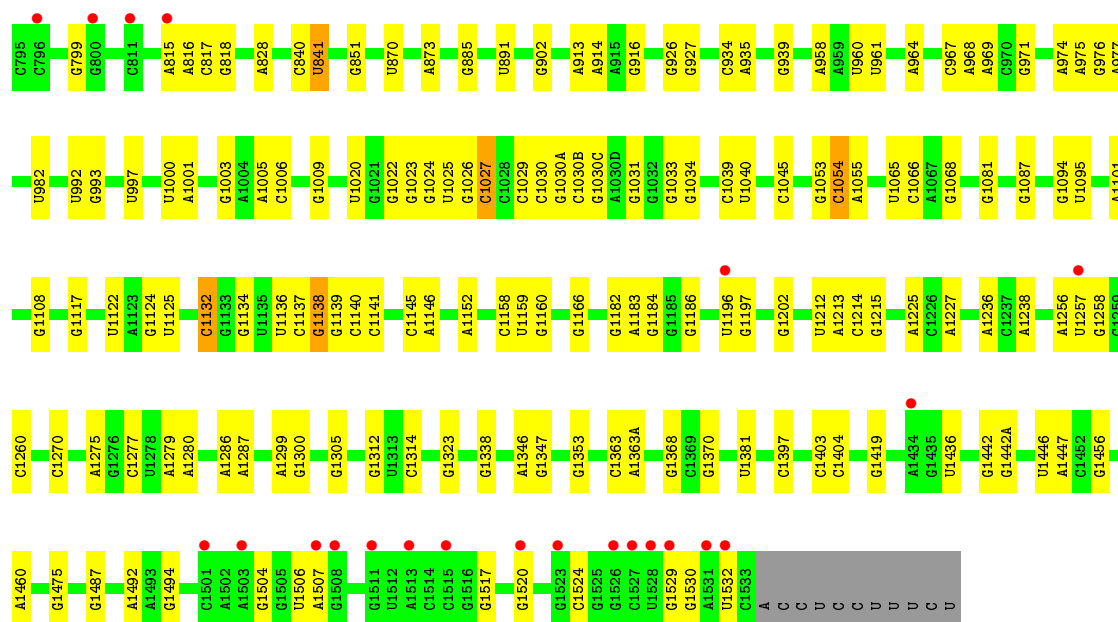


- Molecule 31: 50S ribosomal protein L36

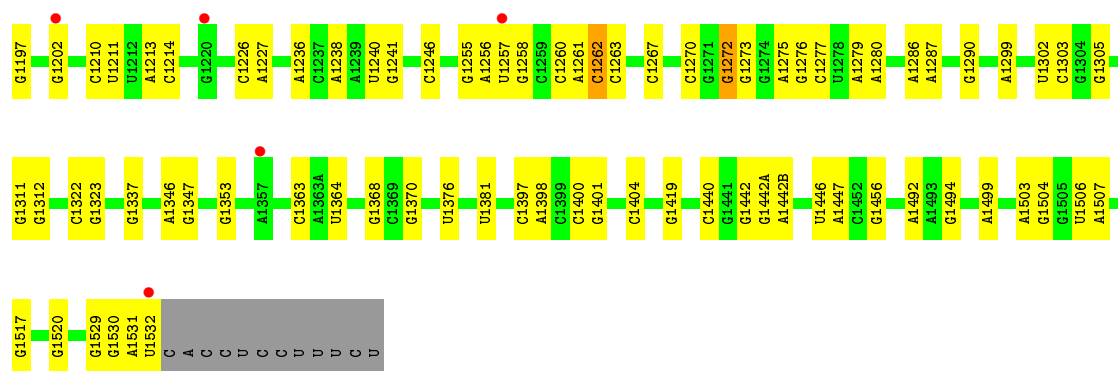


- Molecule 32: 16S Ribosomal RNA

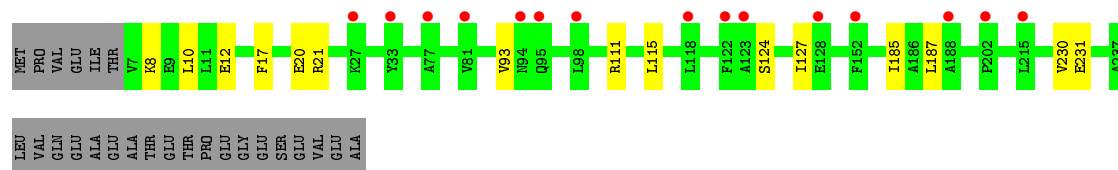
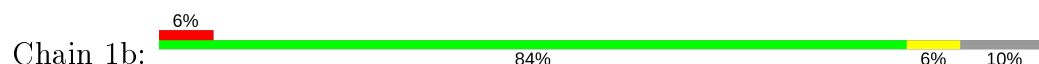




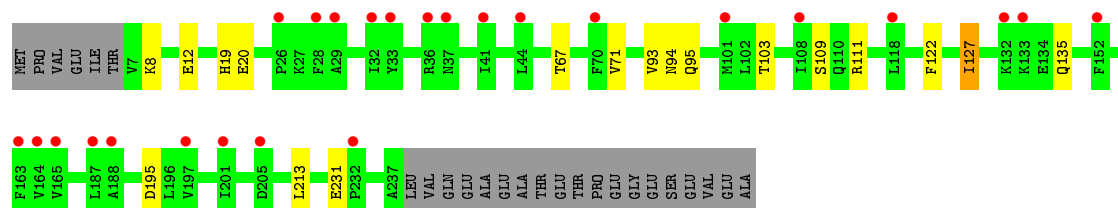
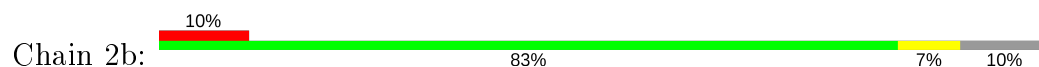




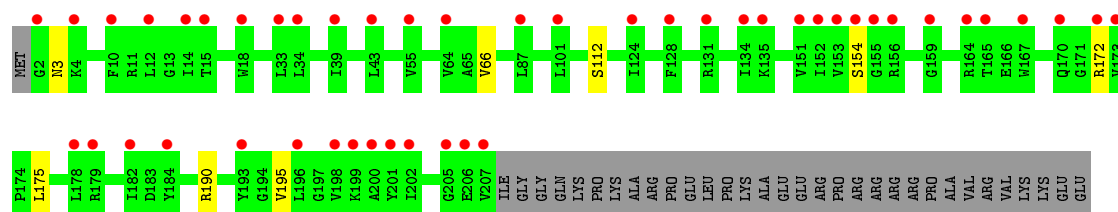
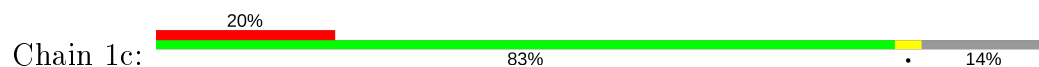
• Molecule 33: 30S ribosomal protein S2



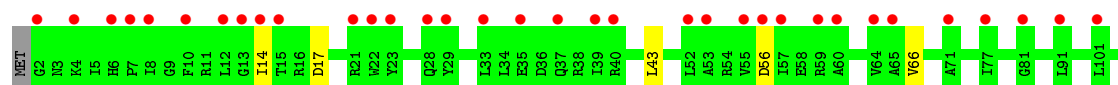
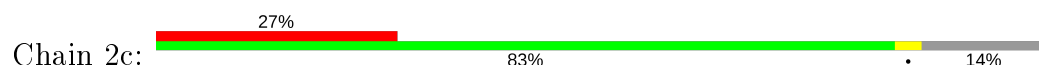
• Molecule 33: 30S ribosomal protein S2

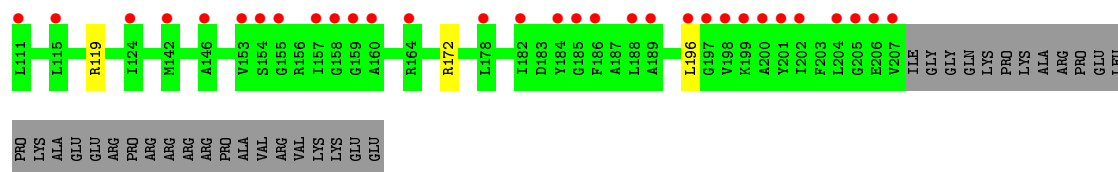


• Molecule 34: 30S ribosomal protein S3

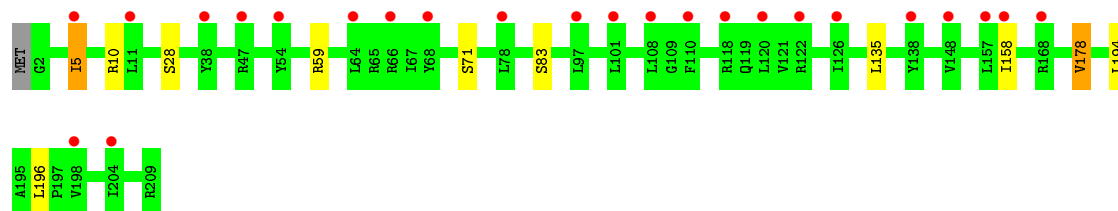


• Molecule 34: 30S ribosomal protein S3

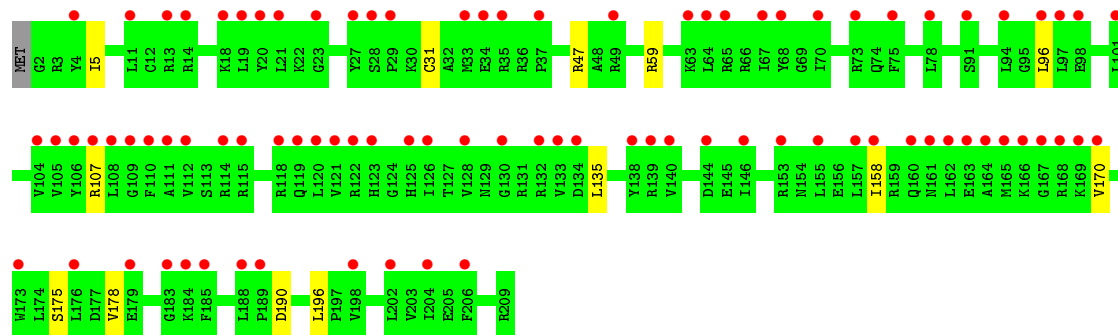
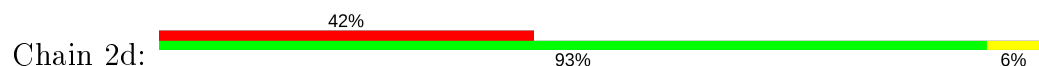




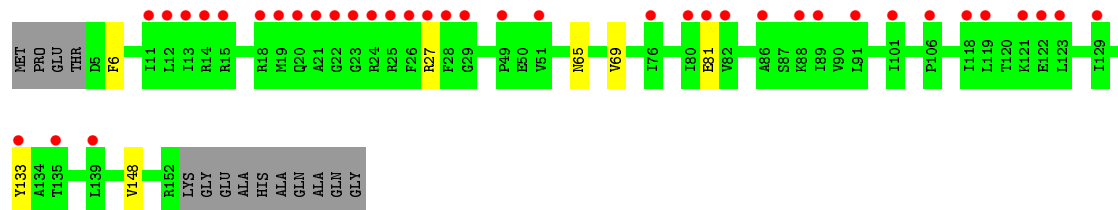
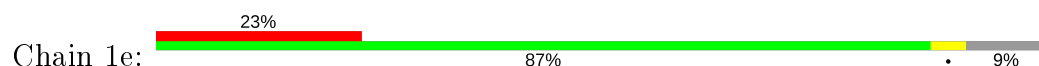
• Molecule 35: 30S ribosomal protein S4



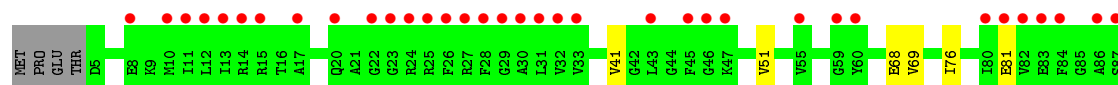
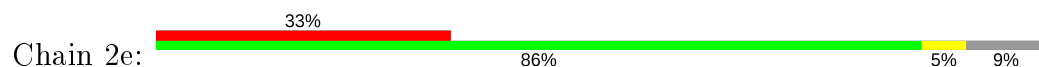
• Molecule 35: 30S ribosomal protein S4

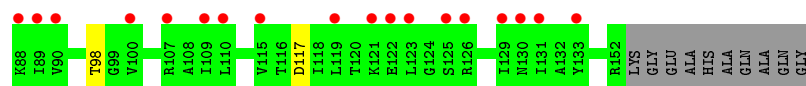


• Molecule 36: 30S ribosomal protein S5

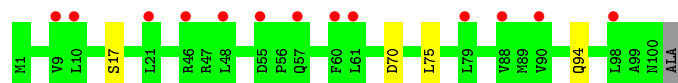


• Molecule 36: 30S ribosomal protein S5





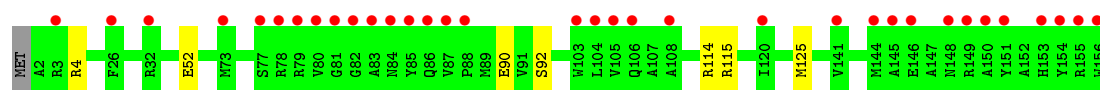
- Molecule 37: 30S ribosomal protein S6



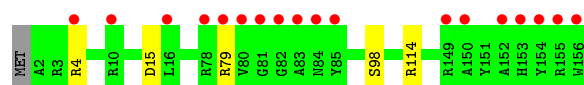
- Molecule 37: 30S ribosomal protein S6



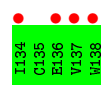
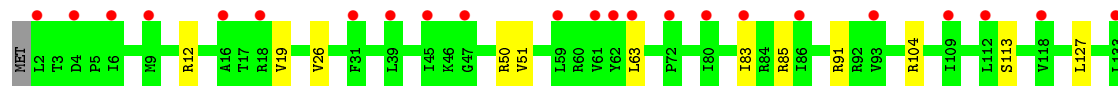
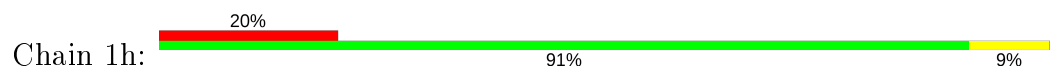
- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

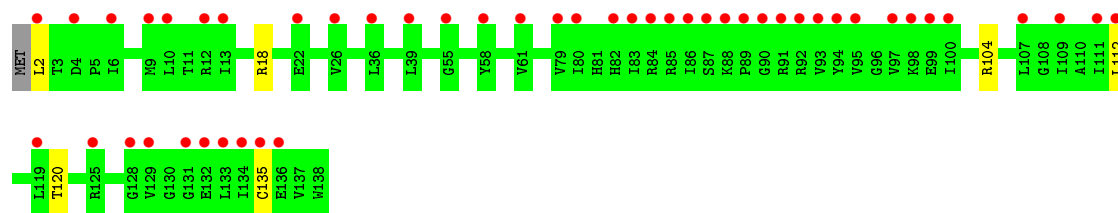


- Molecule 39: 30S ribosomal protein S8

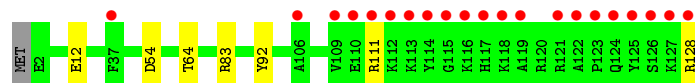
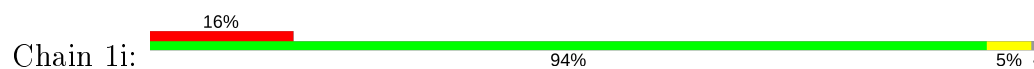


- Molecule 39: 30S ribosomal protein S8

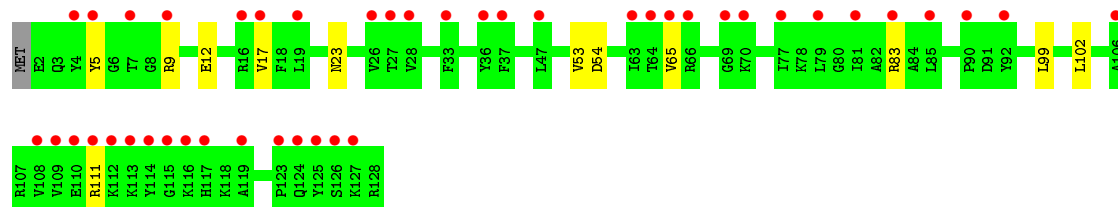
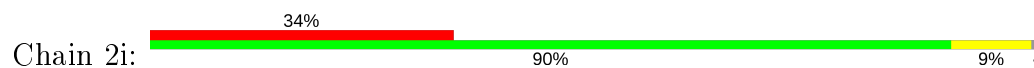




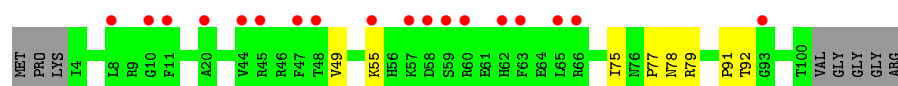
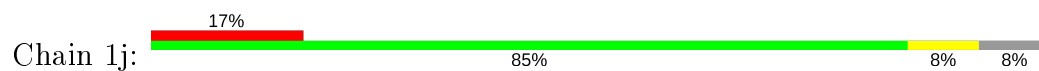
- Molecule 40: 30S ribosomal protein S9



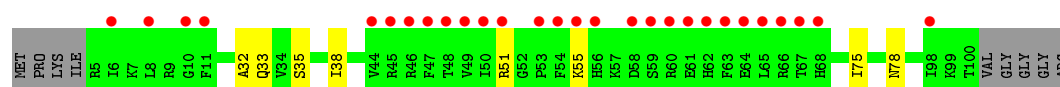
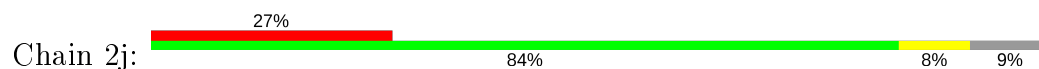
- Molecule 40: 30S ribosomal protein S9



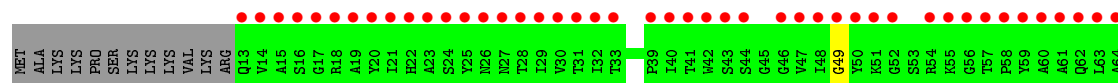
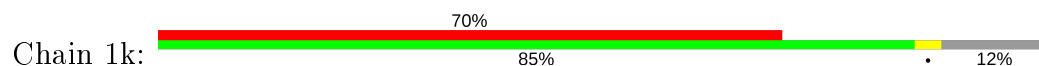
- Molecule 41: 30S ribosomal protein S10

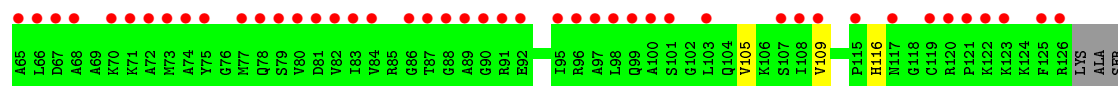


- Molecule 41: 30S ribosomal protein S10

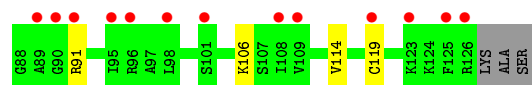
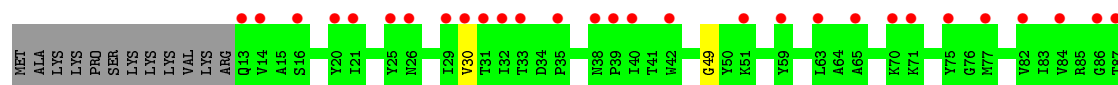
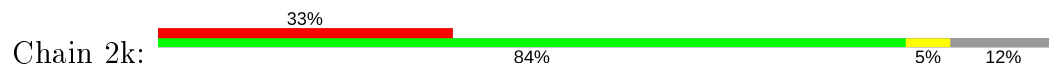


- Molecule 42: 30S ribosomal protein S11

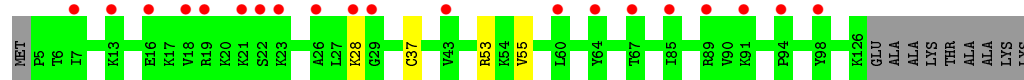
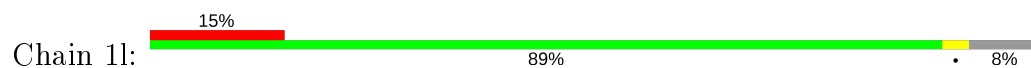




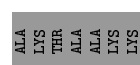
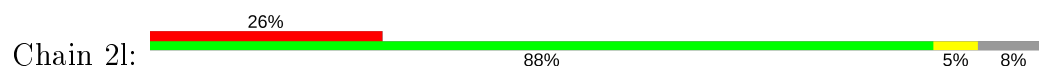
- Molecule 42: 30S ribosomal protein S11



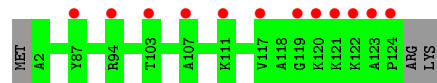
- Molecule 43: 30S ribosomal protein S12



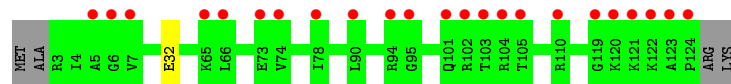
- Molecule 43: 30S ribosomal protein S12



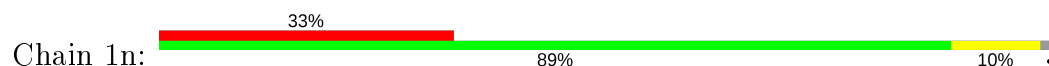
- Molecule 44: 30S ribosomal protein S13

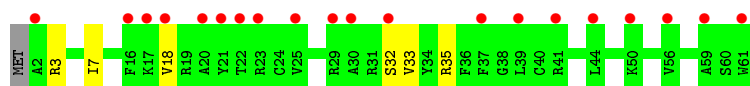


- Molecule 44: 30S ribosomal protein S13

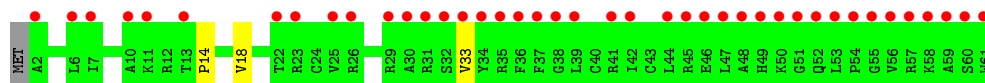


- Molecule 45: 30S ribosomal protein S14 type Z

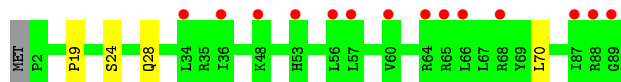




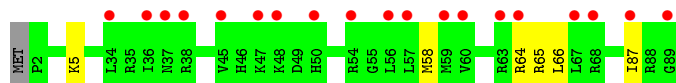
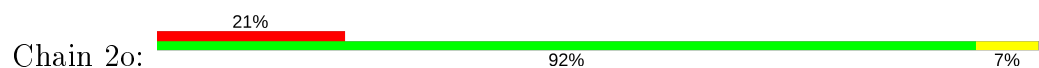
- Molecule 45: 30S ribosomal protein S14 type Z



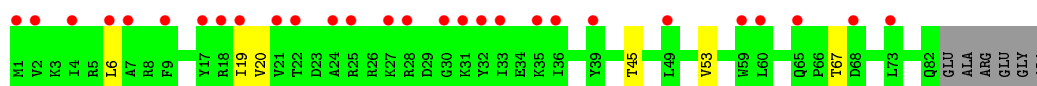
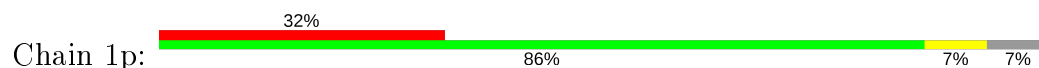
- Molecule 46: 30S ribosomal protein S15



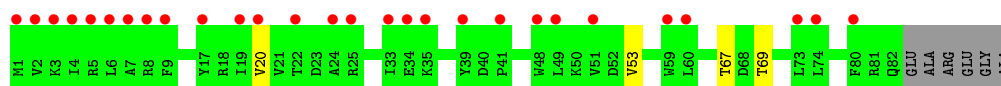
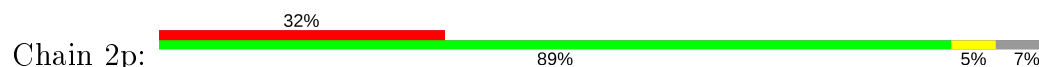
- Molecule 46: 30S ribosomal protein S15



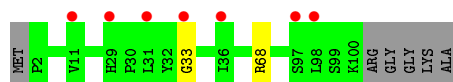
- Molecule 47: 30S ribosomal protein S16



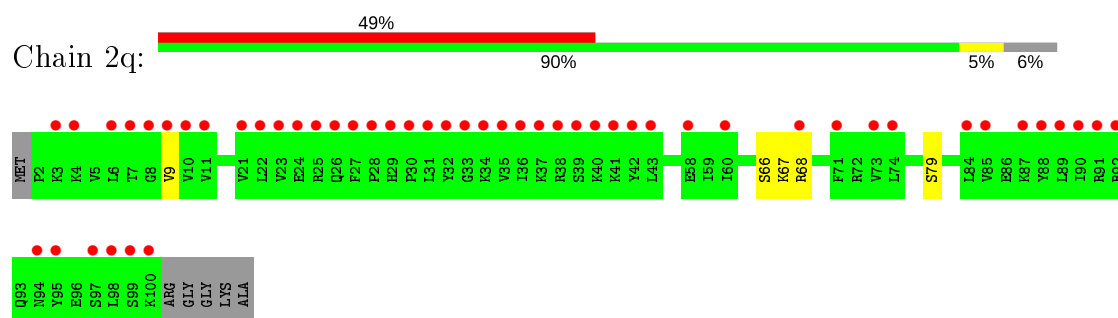
- Molecule 47: 30S ribosomal protein S16



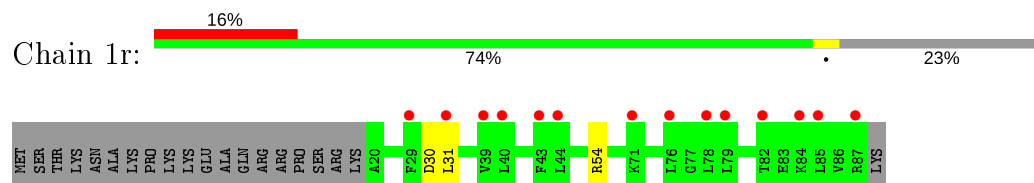
- Molecule 48: 30S ribosomal protein S17



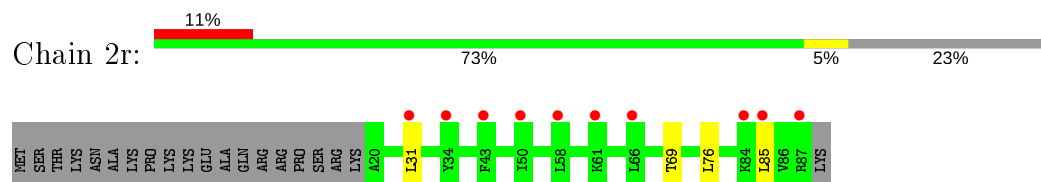
- Molecule 48: 30S ribosomal protein S17



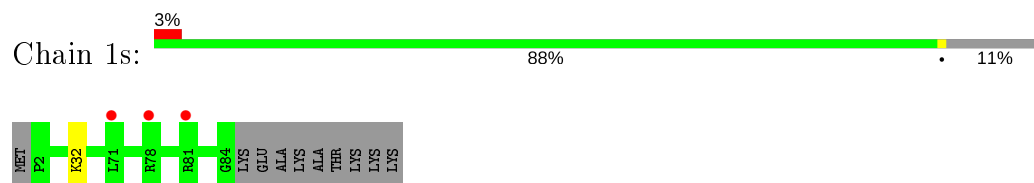
- Molecule 49: 30S ribosomal protein S18



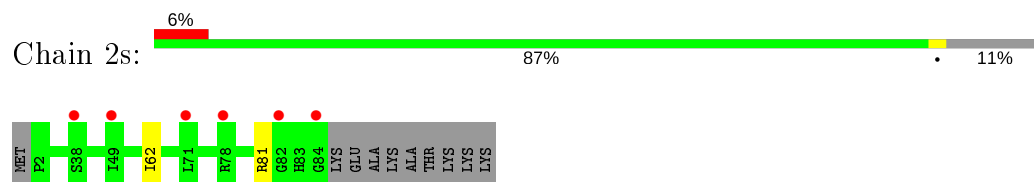
- Molecule 49: 30S ribosomal protein S18



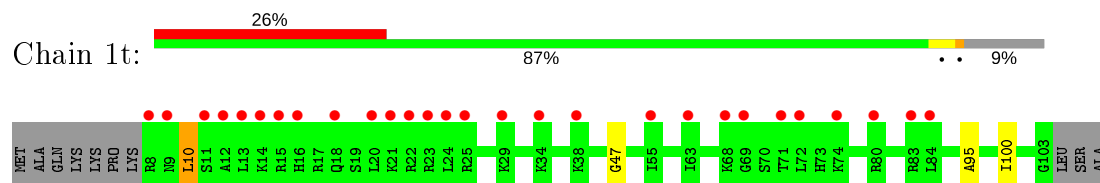
- Molecule 50: 30S ribosomal protein S19



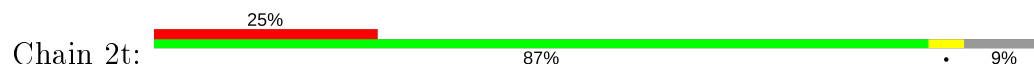
- Molecule 50: 30S ribosomal protein S19

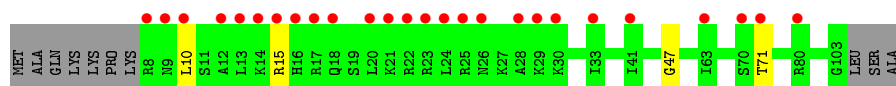


- Molecule 51: 30S ribosomal protein S20

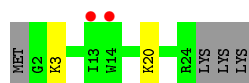
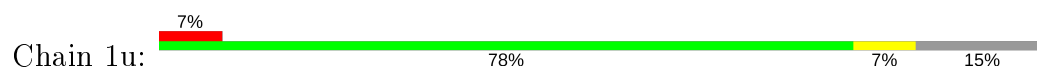


- Molecule 51: 30S ribosomal protein S20

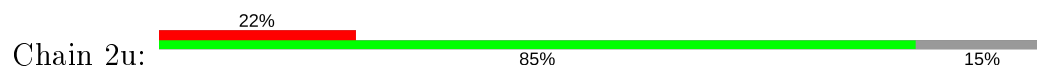




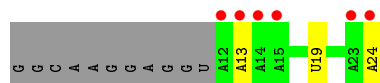
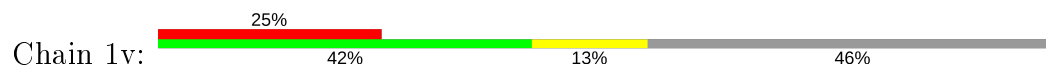
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



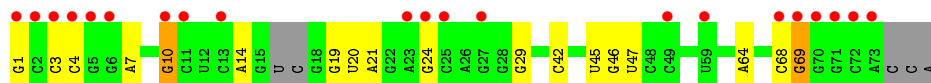
- Molecule 53: mRNA



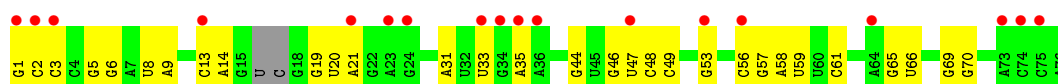
- Molecule 53: mRNA



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



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



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

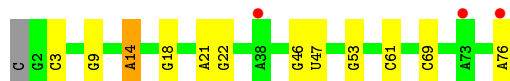
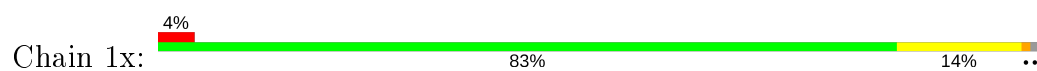




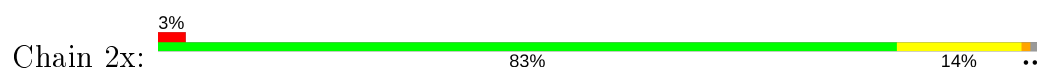
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.73Å 445.10Å 613.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	360.30 – 2.95 360.30 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (360.30-2.95) 99.7 (360.30-2.95)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.238 , 0.292 0.238 , 0.292	Depositor DCC
$R_{free}$ test set	59210 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	295398	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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, ZN, M2G, OMG, 2MU, MIA, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, 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	0.30	0/69009	0.79	27/107712 (0.0%)
1	2A	0.26	0/67293	0.79	22/105034 (0.0%)
2	1B	0.31	1/2882 (0.0%)	0.74	0/4494
2	2B	0.30	1/2879 (0.0%)	0.80	1/4487 (0.0%)
3	1D	0.28	0/2186	0.48	0/2944
3	2D	0.27	0/2186	0.48	0/2944
4	1E	0.27	0/1592	0.47	0/2149
4	2E	0.26	0/1592	0.47	0/2149
5	1F	0.27	0/1619	0.45	0/2193
5	2F	0.27	0/1615	0.43	0/2188
6	1G	0.26	0/1448	0.45	0/1957
6	2G	0.26	0/1453	0.44	0/1963
7	1H	0.28	0/1356	0.46	0/1834
7	2H	0.26	0/1356	0.45	0/1834
8	1I	0.25	0/1112	0.45	0/1514
8	2I	0.26	0/1079	0.47	0/1475
9	1N	0.27	0/1144	0.45	0/1543
9	2N	0.25	0/1144	0.43	0/1543
10	1O	0.29	0/943	0.49	0/1269
10	2O	0.28	0/943	0.49	0/1269
11	1P	0.29	0/1152	0.51	0/1533
11	2P	0.27	0/1152	0.49	0/1533
12	1Q	0.29	0/1143	0.45	0/1527
12	2Q	0.26	0/1143	0.44	0/1527
13	1R	0.25	0/982	0.45	0/1312
13	2R	0.24	0/982	0.44	0/1312
14	1S	0.26	0/883	0.42	0/1176
14	2S	0.27	0/880	0.45	0/1172
15	1T	0.26	0/1105	0.46	0/1477
15	2T	0.26	0/1097	0.46	0/1468
16	1U	0.26	0/977	0.41	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.25	0/977	0.40	0/1301
17	1V	0.30	0/782	0.51	0/1049
17	2V	0.27	0/782	0.50	0/1049
18	1W	0.28	0/897	0.45	0/1205
18	2W	0.26	0/897	0.43	0/1205
19	1X	0.29	0/764	0.50	0/1025
19	2X	0.25	0/764	0.44	0/1025
20	1Y	0.29	0/819	0.47	0/1095
20	2Y	0.28	0/819	0.47	0/1095
21	1Z	0.26	0/1267	0.46	0/1717
21	2Z	0.26	0/1299	0.47	0/1763
22	10	0.27	0/662	0.46	0/881
22	20	0.27	0/662	0.47	0/881
23	11	0.29	0/762	0.47	0/1014
23	21	0.27	0/762	0.48	0/1014
24	12	0.25	0/590	0.40	0/781
24	22	0.25	0/590	0.38	0/781
25	13	0.26	0/474	0.45	0/635
25	23	0.25	0/469	0.42	0/630
26	14	0.28	0/565	0.51	0/761
26	24	0.30	0/545	0.51	0/737
27	15	0.26	0/469	0.47	0/635
27	25	0.29	0/469	0.44	0/635
28	16	0.29	0/460	0.46	0/613
28	26	0.25	0/456	0.46	0/608
29	17	0.25	0/426	0.43	0/561
29	27	0.24	0/426	0.46	0/561
30	18	0.27	0/525	0.45	0/691
30	28	0.25	0/525	0.44	0/691
31	19	0.31	0/310	0.49	0/407
31	29	0.28	0/310	0.51	0/407
32	1a	0.26	0/35795	0.82	25/55864 (0.0%)
32	2a	0.27	2/35886 (0.0%)	0.85	31/56005 (0.1%)
33	1b	0.26	0/1881	0.46	0/2542
33	2b	0.26	0/1860	0.46	0/2518
34	1c	0.28	0/1572	0.44	0/2126
34	2c	0.25	0/1566	0.45	0/2119
35	1d	0.26	0/1685	0.43	0/2262
35	2d	0.25	0/1704	0.43	0/2284
36	1e	0.26	0/1145	0.48	0/1543
36	2e	0.27	0/1149	0.48	0/1548
37	1f	0.27	0/823	0.47	0/1115
37	2f	0.27	0/829	0.45	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.25	0/1250	0.43	0/1679
38	2g	0.25	0/1254	0.41	0/1683
39	1h	0.26	0/1108	0.45	0/1494
39	2h	0.26	0/1108	0.44	0/1494
40	1i	0.27	0/1002	0.47	0/1346
40	2i	0.26	0/997	0.49	0/1343
41	1j	0.25	0/722	0.48	0/982
41	2j	0.26	0/727	0.47	0/988
42	1k	0.25	0/844	0.44	0/1145
42	2k	0.28	0/848	0.45	0/1149
43	1l	0.27	0/937	0.48	0/1260
43	2l	0.28	0/937	0.48	0/1260
44	1m	0.26	0/969	0.46	0/1302
44	2m	0.25	0/961	0.47	0/1291
45	1n	0.28	0/501	0.42	0/664
45	2n	0.26	0/501	0.44	0/664
46	1o	0.24	0/739	0.41	0/985
46	2o	0.24	0/739	0.42	0/985
47	1p	0.25	0/697	0.46	0/939
47	2p	0.25	0/693	0.45	0/935
48	1q	0.26	0/836	0.46	0/1117
48	2q	0.26	0/836	0.46	0/1117
49	1r	0.25	0/560	0.48	0/746
49	2r	0.24	0/560	0.45	0/746
50	1s	0.25	0/667	0.50	0/900
50	2s	0.27	0/661	0.50	0/893
51	1t	0.26	0/730	0.41	0/965
51	2t	0.24	0/729	0.39	0/965
52	1u	0.23	0/203	0.43	0/266
52	2u	0.24	0/203	0.43	0/266
53	1v	0.27	0/288	0.85	0/446
53	2v	0.33	0/163	0.84	0/251
54	1w	0.46	1/1537 (0.1%)	1.06	6/2390 (0.3%)
54	1y	0.44	1/1606 (0.1%)	1.06	5/2497 (0.2%)
54	2w	0.36	0/1487	1.05	1/2311 (0.0%)
54	2y	0.50	1/1583 (0.1%)	1.15	7/2459 (0.3%)
55	1x	0.40	0/1725	1.05	9/2689 (0.3%)
55	2x	0.36	0/1725	0.99	9/2689 (0.3%)
All	All	0.28	7/316379 (0.0%)	0.74	143/473636 (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
26	24	0	1
41	2j	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	1	U	OP3-P	-10.52	1.48	1.61
54	2y	1	G	OP3-P	-10.49	1.48	1.61
54	1w	1	G	OP3-P	-10.38	1.48	1.61
2	1B	1	U	OP3-P	-10.34	1.48	1.61
54	1y	1	G	OP3-P	-10.27	1.48	1.61
32	2a	1272	G	N1-C2	-7.83	1.31	1.37
32	2a	1272	G	C6-N1	-7.12	1.34	1.39

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	N3-C2-N2	18.40	132.78	119.90
32	2a	1263	C	N1-C2-O2	17.88	129.63	118.90
32	2a	1272	G	C5-C6-O6	16.95	138.77	128.60
32	2a	1272	G	N1-C2-N2	-14.73	102.94	116.20
2	2B	80	U	O4'-C1'-N1	12.03	117.82	108.20
32	2a	1272	G	C6-N1-C2	11.72	132.13	125.10
1	2A	2136	C	N1-C2-O2	11.38	125.73	118.90
32	2a	1263	C	C2-N3-C4	11.06	125.43	119.90
1	1A	1075	C	N1-C2-O2	10.66	125.30	118.90
32	2a	1263	C	N3-C2-O2	-10.08	114.84	121.90
1	1A	1086	A	N1-C6-N6	-9.58	112.85	118.60
32	2a	1263	C	C5-C6-N1	9.55	125.77	121.00
32	2a	1272	G	C5-C6-N1	-9.50	106.75	111.50
32	2a	1272	G	N1-C6-O6	-9.08	114.45	119.90
1	1A	1187	G	O5'-P-OP2	8.73	121.18	110.70
32	1a	1034	G	C6-N1-C2	8.19	130.01	125.10
54	2y	66	U	C5-C4-O4	-8.04	121.08	125.90
1	1A	1063	G	C5-C6-O6	7.78	133.27	128.60
54	1y	56	C	N1-C2-O2	7.75	123.55	118.90
1	2A	2155	G	N3-C4-N9	7.71	130.62	126.00
32	2a	1263	C	C6-N1-C2	-7.70	117.22	120.30
32	2a	754	C	C2-N1-C1'	7.69	127.26	118.80
1	1A	1063	G	N3-C2-N2	7.51	125.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2136	C	N3-C2-O2	-7.46	116.68	121.90
1	2A	2155	G	C6-C5-N7	-7.46	125.93	130.40
55	1x	22	G	N1-C6-O6	-7.43	115.44	119.90
55	1x	46	G	C6-N1-C2	-7.39	120.67	125.10
1	1A	847	U	C2-N1-C1'	7.14	126.27	117.70
32	2a	1272	G	C4-N9-C1'	7.12	135.75	126.50
1	1A	1063	G	C6-N1-C2	7.10	129.36	125.10
32	2a	1263	C	C2-N1-C1'	7.10	126.61	118.80
1	2A	2155	G	N3-C2-N2	7.03	124.82	119.90
32	2a	754	C	N1-C2-O2	7.01	123.10	118.90
54	1y	33	U	N1-C2-O2	6.96	127.67	122.80
32	2a	1001(A)	G	N3-C4-N9	6.95	130.17	126.00
1	1A	1075	C	C2-N3-C4	6.90	123.35	119.90
1	2A	2155	G	N9-C4-C5	-6.90	102.64	105.40
54	2y	7	A	C6-N1-C2	-6.89	114.47	118.60
32	2a	1272	G	C8-N9-C1'	-6.88	118.05	127.00
32	1a	266	G	P-O3'-C3'	6.81	127.87	119.70
1	2A	2155	G	C4-C5-N7	6.79	113.52	110.80
55	2x	14	A	C4-C5-C6	6.76	120.38	117.00
54	1y	33	U	C2-N1-C1'	6.75	125.80	117.70
54	1w	4	C	C5-C4-N4	6.75	124.92	120.20
54	1y	33	U	N3-C2-O2	-6.70	117.51	122.20
55	2x	22	G	C8-N9-C1'	6.68	135.68	127.00
55	1x	22	G	C6-C5-N7	6.66	134.40	130.40
55	1x	22	G	C4-C5-C6	-6.63	114.82	118.80
1	1A	1187	G	N1-C6-O6	-6.57	115.96	119.90
1	1A	2629	A	P-O3'-C3'	6.51	127.52	119.70
1	1A	1075	C	C2-N1-C1'	6.51	125.96	118.80
1	1A	2167	U	C2-N1-C1'	6.47	125.46	117.70
55	1x	22	G	C8-N9-C1'	6.42	135.34	127.00
32	1a	1065	U	P-O3'-C3'	6.41	127.39	119.70
55	2x	22	G	N1-C6-O6	-6.35	116.09	119.90
55	1x	22	G	N3-C4-N9	-6.33	122.20	126.00
32	2a	1158	C	C2-N1-C1'	6.29	125.72	118.80
32	1a	1132	C	N1-C2-O2	6.27	122.66	118.90
32	1a	1030	C	N1-C2-O2	6.24	122.65	118.90
1	2A	2897	U	C2-N1-C1'	6.22	125.16	117.70
54	2w	47	U	C2-N1-C1'	6.16	125.09	117.70
1	1A	1091	G	N3-C4-N9	6.13	129.68	126.00
1	1A	512	G	O4'-C1'-N9	6.12	113.10	108.20
55	2x	22	G	C4-N9-C1'	-6.10	118.57	126.50
32	2a	1039	C	C5-C4-N4	-6.09	115.94	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	847	U	N1-C2-O2	6.00	127.00	122.80
1	1A	1075	C	N3-C2-O2	-5.97	117.72	121.90
32	1a	1001	A	C5-C6-N6	5.96	128.47	123.70
55	2x	46	G	N3-C2-N2	-5.95	115.73	119.90
32	1a	1065	U	OP2-P-O3'	5.92	118.22	105.20
1	1A	2134	A	P-O3'-C3'	5.91	126.80	119.70
32	2a	1263	C	C4-C5-C6	-5.88	114.46	117.40
1	2A	2136	C	C2-N1-C1'	5.85	125.24	118.80
1	2A	1313	U	C2-N1-C1'	5.85	124.72	117.70
54	2y	7	A	N3-C4-N9	5.84	132.07	127.40
32	1a	1034	G	N3-C2-N2	5.83	123.98	119.90
54	1w	4	C	N3-C4-N4	-5.81	113.93	118.00
55	1x	22	G	C4-N9-C1'	-5.79	118.98	126.50
55	2x	22	G	N3-C4-N9	-5.74	122.55	126.00
55	2x	22	G	C6-C5-N7	5.74	133.84	130.40
32	2a	754	C	C6-N1-C1'	-5.73	113.92	120.80
55	1x	14	A	C4-C5-C6	5.69	119.85	117.00
32	1a	1001	A	N1-C6-N6	-5.62	115.23	118.60
32	1a	1027	C	C6-N1-C1'	5.60	127.52	120.80
32	1a	841	U	C2-N1-C1'	5.56	124.37	117.70
32	1a	1027	C	C2-N1-C1'	-5.54	112.70	118.80
1	1A	847	U	N3-C2-O2	-5.54	118.32	122.20
54	2y	66	U	C2-N3-C4	-5.53	123.68	127.00
1	1A	1100	C	C2-N1-C1'	5.49	124.84	118.80
32	1a	748	C	P-O3'-C3'	5.49	126.28	119.70
1	1A	2167	U	N1-C2-O2	5.48	126.64	122.80
32	2a	1150	U	C5-C4-O4	5.46	129.18	125.90
32	1a	1030(B)	C	C2-N1-C1'	5.45	124.79	118.80
32	2a	1272	G	C2-N3-C4	-5.42	109.19	111.90
54	1y	56	C	C2-N3-C4	5.42	122.61	119.90
1	2A	2866	U	C2-N1-C1'	5.42	124.20	117.70
32	2a	1123	A	C5-C6-N6	5.39	128.02	123.70
1	1A	1174	A	OP1-P-O3'	5.38	117.05	105.20
32	1a	1158	C	C2-N1-C1'	5.38	124.71	118.80
1	2A	2155	G	C4-N9-C1'	5.37	133.49	126.50
1	1A	1313	U	C2-N1-C1'	5.35	124.12	117.70
32	1a	1040	U	C2-N3-C4	5.34	130.21	127.00
32	2a	1263	C	N1-C2-N3	-5.33	115.47	119.20
54	1w	64	A	N1-C6-N6	5.32	121.79	118.60
32	2a	266	G	P-O3'-C3'	5.32	126.08	119.70
54	1w	64	A	C5-C6-N6	-5.31	119.45	123.70
32	2a	1262	C	N1-C2-O2	5.31	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2134	A	OP1-P-O3'	5.30	116.85	105.20
54	2y	7	A	C5-C6-N1	5.27	120.34	117.70
54	1w	10	G	N3-C2-N2	-5.26	116.22	119.90
55	1x	14	A	C5-N7-C8	5.26	106.53	103.90
1	1A	1099	G	N3-C4-N9	5.26	129.16	126.00
1	2A	528	A	OP1-P-O3'	5.25	116.76	105.20
32	1a	266	G	OP2-P-O3'	5.25	116.74	105.20
32	1a	841	U	C5-C6-N1	5.24	125.32	122.70
32	2a	1158	C	N1-C2-O2	5.24	122.05	118.90
1	2A	2136	C	C6-N1-C1'	-5.22	114.53	120.80
32	2a	1001(A)	G	C4-N9-C1'	5.21	133.28	126.50
1	1A	1187	G	C5-C6-O6	5.18	131.71	128.60
1	2A	90	U	C2-N1-C1'	5.16	123.90	117.70
32	1a	913	A	P-O3'-C3'	5.14	125.87	119.70
32	1a	1138	G	C4-N9-C1'	5.14	133.18	126.50
1	1A	1187	G	OP1-P-OP2	-5.14	111.89	119.60
55	2x	22	G	C4-C5-C6	-5.13	115.72	118.80
1	2A	2897	U	N1-C2-O2	5.13	126.39	122.80
1	2A	847	U	C2-N1-C1'	5.11	123.83	117.70
1	1A	1063	G	C5-C6-N1	-5.10	108.95	111.50
32	1a	1158	C	N1-C2-O2	5.09	121.95	118.90
54	1w	69	G	C5-C6-O6	5.09	131.65	128.60
32	2a	1125	U	C2-N1-C1'	5.09	123.81	117.70
1	2A	2321	G	C4-N9-C1'	5.09	133.12	126.50
54	2y	22	G	C6-C5-N7	-5.09	127.35	130.40
1	2A	1644	C	N1-C2-O2	5.08	121.95	118.90
32	1a	1030	C	N3-C2-O2	-5.08	118.34	121.90
32	1a	1054	C	C2-N1-C1'	5.07	124.37	118.80
32	1a	1034	G	C5-C6-O6	5.06	131.64	128.60
32	1a	687	A	P-O3'-C3'	5.05	125.76	119.70
32	2a	1040	U	C5-C4-O4	5.05	128.93	125.90
54	2y	22	G	N1-C6-O6	5.04	122.93	119.90
55	2x	14	A	C5-C6-N1	-5.04	115.18	117.70
1	2A	228	A	P-O3'-C3'	5.02	125.73	119.70
1	2A	2155	G	C8-N9-C1'	-5.02	120.47	127.00
1	2A	2139	C	C2-N1-C1'	5.02	124.32	118.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	56	VAL	Peptide

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Mol	Chain	Res	Type	Group
41	2j	32	ALA	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31193	824	0
1	2A	60322	0	30421	1007	0
2	1B	2577	0	1305	32	0
2	2B	2575	0	1303	39	0
3	1D	2136	0	2218	73	0
3	2D	2136	0	2218	56	0
4	1E	1559	0	1618	39	0
4	2E	1559	0	1618	49	0
5	1F	1584	0	1625	52	0
5	2F	1580	0	1619	53	0
6	1G	1423	0	1436	43	0
6	2G	1428	0	1438	50	0
7	1H	1330	0	1407	34	0
7	2H	1330	0	1407	39	0
8	1I	1097	0	1140	38	0
8	2I	1064	0	1082	42	0
9	1N	1117	0	1184	21	0
9	2N	1117	0	1184	34	0
10	1O	933	0	996	25	0
10	2O	933	0	996	28	0
11	1P	1135	0	1212	42	0
11	2P	1135	0	1212	35	0
12	1Q	1122	0	1179	28	0
12	2Q	1122	0	1179	35	0
13	1R	968	0	1033	25	0
13	2R	968	0	1033	21	0
14	1S	873	0	927	21	0
14	2S	870	0	923	36	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	29	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	1V	771	0	830	19	0
17	2V	771	0	830	23	0
18	1W	886	0	940	23	0
18	2W	886	0	940	18	0
19	1X	750	0	814	16	0
19	2X	750	0	814	12	0
20	1Y	806	0	881	24	0
20	2Y	806	0	881	33	0
21	1Z	1240	0	1240	39	0
21	2Z	1271	0	1273	31	0
22	10	653	0	674	17	0
22	20	653	0	674	19	0
23	11	755	0	826	24	0
23	21	755	0	826	20	0
24	12	588	0	643	15	0
24	22	588	0	643	16	0
25	13	469	0	518	7	0
25	23	464	0	514	17	0
26	14	552	0	533	19	0
26	24	532	0	503	17	0
27	15	455	0	465	7	0
27	25	455	0	465	16	0
28	16	453	0	473	11	0
28	26	449	0	469	17	0
29	17	418	0	467	9	0
29	27	418	0	467	12	0
30	18	517	0	582	22	0
30	28	517	0	582	22	0
31	19	307	0	335	6	0
31	29	307	0	335	15	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16339	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	277	0	139	0	0
53	2v	167	0	84	0	0
54	1w	1530	0	786	0	0
54	1y	1585	0	804	0	0
54	2w	1482	0	755	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	829	0	0
55	2x	1625	0	829	0	0
56	1A	680	0	0	0	0
56	1a	238	0	0	0	0
56	2A	351	0	0	0	0
56	2a	183	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	1A	585	0	0	27	0
59	1a	181	0	0	0	0
59	2A	234	0	0	14	0
59	2a	167	0	0	0	0
All	All	295398	0	196565	2965	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 12.

All (2965) 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	1.19	1.34
1:2A:2138:C:N4	1:2A:2153:G:H1	1.36	1.24
1:1A:1082:U:O4	1:1A:1086:A:N1	1.89	1.05
1:1A:1054:A:H61	1:1A:1105:U:H3	1.03	0.98
1:1A:765:G:H1	1:1A:812:C:HO2'	84.79	0.96
1:1A:1071:G:N2	1:1A:1091:G:N7	2.13	0.95
1:2A:2138:C:N3	1:2A:2153:G:N2	2.14	0.94
1:2A:1002:G:H1	1:2A:1038:C:H42	41.85	0.94
1:1A:882:G:H1	1:1A:894:C:H42	1.10	0.94
1:1A:1054:A:N6	1:1A:1105:U:H3	1.64	0.93
1:2A:2129:C:N4	1:2A:2159:G:H1	1.66	0.92
1:1A:2121:G:H1	1:1A:2177:C:H42	1.03	0.92
1:2A:2129:C:H42	1:2A:2159:G:H1	0.92	0.90
1:2A:880:G:N2	1:2A:898:C:O2	2.07	0.88
1:1A:2099:U:H3	1:1A:2190:G:H1	1.20	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1002:G:H1	1:2A:1038:C:N4	41.65	0.86
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.22	0.86
1:1A:2100:G:H1	1:1A:2189:U:H3	0.86	0.85
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.58	0.85
1:1A:2121:G:H1	1:1A:2177:C:N4	1.73	0.84
1:2A:2345:G:H4'	1:2A:2346:A:H5''	1.59	0.84
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.10	0.84
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.11	0.83
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	98.66	0.83
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.12	0.82
1:2A:1011:G:H1	1:2A:1018:C:H42	17.21	0.82
1:2A:2127:G:O2'	1:2A:2173:A:N3	2.13	0.82
8:2I:82:ARG:HB2	8:2I:89:TYR:HB2	1.59	0.81
1:1A:410:G:N2	1:1A:432:A:N7	40.59	0.81
1:1A:1062:G:H1	1:1A:1077:A:H61	1.27	0.80
1:2A:674:G:H1'	5:2F:74:ARG:HE	1.46	0.80
1:1A:2096:U:H3	1:1A:2193:G:H1	1.29	0.80
1:2A:309:G:N3	1:2A:329:G:O2'	2.14	0.80
3:2D:16:MET:HG2	3:2D:207:GLY:HA3	1.62	0.80
1:1A:2136:C:N3	1:1A:2155:G:C2	2.50	0.79
1:1A:1422:G:H5''	10:1O:48:PRO:HB3	99.04	0.79
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.15	0.79
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.64	0.79
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.14	0.79
1:2A:652(B):A:H61	1:2A:655:A:H1'	1.47	0.79
1:1A:2863:C:OP1	15:1T:93:ARG:NH1	2.14	0.79
1:2A:708:C:H42	1:2A:723:G:H1	1.30	0.78
1:2A:918:A:O2'	2:2B:97:G:N2	2.16	0.78
1:1A:880:G:H2'	1:1A:881:G:H8	1.48	0.78
1:2A:641:C:H42	1:2A:647:G:H1	1.32	0.78
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.17	0.78
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.17	0.78
1:2A:1532:C:N4	1:2A:1537:G:O6	2.17	0.77
1:2A:2099:U:H3	1:2A:2190:G:H1	1.32	0.77
1:1A:1053:C:H42	1:1A:1106:G:H1	1.32	0.77
1:1A:2136:C:N3	1:1A:2155:G:N2	2.32	0.77
1:2A:2078:C:N4	1:2A:2238:G:O6	2.17	0.77
1:1A:266:G:O2'	1:1A:267:C:OP2	4.81	0.77
1:2A:335:C:H4'	20:2Y:73:ARG:HD3	1.67	0.77
1:1A:2790:A:H5'	1:1A:2893:G:H21	1.49	0.77
7:1H:9:ILE:HD11	7:1H:69:ARG:HG2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1011:G:H1	1:2A:1018:C:N4	17.59	0.76
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.68	0.76
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.49	0.76
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.67	0.76
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.19	0.76
1:2A:2657:A:O3'	7:2H:160:LYS:NZ	2.17	0.76
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.17	0.75
1:1A:918:A:N3	2:1B:80:U:O2'	2.19	0.75
12:2Q:75:THR:HG21	12:2Q:87:LYS:HE3	1.69	0.75
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	1.69	0.75
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.69	0.75
1:2A:76:C:H42	1:2A:93:G:H1	26.70	0.75
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.18	0.75
1:2A:529:A:H62	1:2A:2041:U:H3	1.35	0.75
1:2A:887:A:O2'	1:2A:889:C:OP2	2.05	0.75
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.67	0.74
26:14:34:GLU:HG2	26:14:35:VAL:HG12	1.68	0.74
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.20	0.74
1:2A:1022:G:N2	1:2A:1023:U:O4	2.21	0.74
1:2A:1038:C:H42	1:2A:1117:G:H1	1.35	0.74
1:1A:335:C:H4'	20:1Y:73:ARG:HD3	1.70	0.74
1:1A:2136:C:N4	1:1A:2155:G:N1	2.35	0.74
1:1A:2682:U:OP2	59:1A:5107:HOH:O	2.05	0.74
1:1A:249:C:O2	30:18:12:LYS:NZ	2.19	0.73
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.69	0.73
1:2A:586:A:N1	1:2A:809:G:O2'	2.18	0.73
1:2A:1434:A:H61	1:2A:1558:A:H62	1.34	0.73
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.34	0.73
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.21	0.73
18:1W:34:ASN:OD1	18:1W:37:ARG:NH2	2.22	0.73
1:2A:2116:G:N2	1:2A:2162:G:OP1	2.20	0.73
1:2A:307:G:N1	1:2A:310:A:OP2	2.21	0.73
1:2A:586:A:H5'	5:2F:89:VAL:HG21	1.70	0.73
1:1A:324:A:N6	1:1A:338:G:O2'	2.20	0.73
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.71	0.73
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.22	0.73
6:2G:163:ALA:HB1	6:2G:168:GLU:HG3	1.69	0.73
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.22	0.73
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.21	0.72
1:2A:391:G:O2'	1:2A:410:G:OP1	2.07	0.72
4:2E:56:PRO:HG3	4:2E:74:PRO:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:3:ARG:HG2	7:2H:6:ARG:HE	1.53	0.72
23:11:3:LYS:HB2	23:11:61:ARG:HH12	1.54	0.72
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.72	0.72
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.22	0.72
9:2N:34:LEU:HD21	9:2N:120:LEU:HB2	1.71	0.72
1:1A:711:G:H1	1:1A:720:C:H42	1.37	0.72
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.23	0.72
1:1A:674:G:H2'	1:1A:675:A:H8	4.61	0.72
25:23:6:VAL:HG13	25:23:54:VAL:HG21	1.71	0.72
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.72	0.72
1:2A:1186:G:N7	59:2A:5121:HOH:O	54.95	0.71
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.55	0.71
20:2Y:97:ARG:NH2	20:2Y:106:LEU:O	2.24	0.71
1:1A:2347:C:HO2'	28:16:21:TYR:HH	1.39	0.71
1:1A:1002:G:H3'	1:1A:1003:G:H4'	5.30	0.71
1:1A:79:G:C6	1:1A:90:U:O2	27.81	0.71
1:1A:197:A:N6	1:1A:2430:A:O2'	2.24	0.71
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.21	0.71
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.25	0.71
1:1A:922:U:O2'	22:10:29:GLN:NE2	2.24	0.70
1:2A:1213:A:O2'	1:2A:1215:G:N7	7.49	0.70
1:2A:854:G:H2'	1:2A:855:G:H8	1.56	0.70
1:1A:2750:A:OP2	7:1H:62:LYS:NZ	2.22	0.70
7:1H:18:GLU:OE2	7:1H:27:LYS:NZ	2.24	0.70
59:2A:5060:HOH:O	23:21:19:GLN:NE2	2.23	0.70
1:2A:1218:C:OP2	16:2U:15:LYS:NZ	2.22	0.70
1:2A:1341:U:OP1	1:2A:1397:U:N3	2.25	0.70
1:2A:642:G:H21	1:2A:646:A:H2	1.37	0.70
1:1A:2142:C:N3	1:1A:2149:G:O6	2.25	0.70
1:1A:732:C:OP2	59:1A:5095:HOH:O	2.10	0.70
1:2A:2287:A:H61	1:2A:2344:U:H3	1.38	0.70
1:1A:1174:A:H4'	1:1A:1175:U:OP1	1.92	0.70
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.38	0.70
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.24	0.70
1:2A:2808:U:O2	1:2A:2892:A:N6	2.24	0.70
1:2A:2248:C:OP2	59:2A:5085:HOH:O	2.08	0.70
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.73	0.70
1:1A:1058:G:H1	1:1A:1080:C:H42	1.38	0.69
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.27	0.69
5:1F:12:LEU:HB2	5:1F:124:LEU:HD11	1.72	0.69
1:2A:2630:G:H1	1:2A:2788:C:H42	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:782:A:OP1	59:2A:5075:HOH:O	33.17	0.69
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.25	0.69
1:1A:1022:G:OP2	9:1N:65:LYS:NZ	2.25	0.69
1:1A:2136:C:N4	1:1A:2155:G:C6	2.59	0.69
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	1.74	0.69
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.25	0.69
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.25	0.69
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.74	0.69
1:1A:2012:G:OP1	18:1W:11:ARG:NH2	2.26	0.69
1:2A:2630:G:N2	1:2A:2788:C:N3	2.39	0.69
5:2F:33:LEU:HD11	5:2F:112:MET:HB3	1.74	0.69
6:2G:19:LEU:HD13	6:2G:32:PRO:HD2	1.75	0.69
1:1A:195:A:OP2	59:1A:5264:HOH:O	2.11	0.69
1:2A:1286:A:C8	1:2A:1287:A:H4'	8.54	0.69
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.74	0.69
1:1A:2141:G:O6	1:1A:2150:U:O2	2.10	0.69
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.25	0.69
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.26	0.69
1:1A:974:G:OP1	1:1A:1187:G:O2'	2.11	0.69
1:2A:1327:C:O2'	13:2R:105:ARG:NH1	2.25	0.69
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.27	0.68
1:2A:1689:A:H62	1:2A:1698:A:H2	1.41	0.68
1:2A:2129:C:N3	1:2A:2159:G:N2	2.39	0.68
2:1B:76:G:N2	2:1B:101:G:O6	2.18	0.68
1:1A:1087:G:H1	1:1A:1102:C:H42	1.41	0.68
1:1A:674:G:H2'	1:1A:675:A:C8	4.92	0.68
11:1P:89:ALA:O	11:1P:121:LYS:NZ	2.25	0.68
1:2A:2143:C:H42	1:2A:2148:G:H1	1.39	0.68
1:1A:674:G:H1'	5:1F:74:ARG:HE	1.59	0.68
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.21	0.68
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.75	0.68
1:2A:854:G:H2'	1:2A:855:G:C8	2.28	0.68
12:1Q:116:GLU:OE2	12:1Q:119:ARG:NH2	2.24	0.68
1:1A:2134:A:N3	1:1A:2159:G:O2'	2.25	0.68
26:14:58:ARG:HE	26:14:58:ARG:HA	1.59	0.68
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.75	0.68
1:2A:80:G:H1	1:2A:106:C:H42	1.40	0.68
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.77	0.67
1:1A:1426:G:O2'	1:1A:1572:A:N6	2.28	0.67
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.74	0.67
1:2A:1022:G:OP2	9:2N:69:GLN:NE2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:68:ILE:HG22	12:2Q:101:ARG:HE	1.58	0.67
25:23:12:PRO:O	25:23:20:LYS:NZ	2.27	0.67
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.30	0.67
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.27	0.67
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	1.76	0.67
4:2E:183:LEU:HD21	15:2T:10:VAL:HG11	1.76	0.67
1:1A:1053:C:N4	1:1A:1106:G:H1	1.91	0.67
17:2V:8:GLY:O	17:2V:10:LYS:NZ	2.28	0.67
8:2I:78:THR:O	8:2I:104:GLN:NE2	2.26	0.67
1:1A:1057:A:N6	1:1A:1087:G:OP2	2.28	0.67
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.27	0.67
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.76	0.67
1:1A:288:C:H2'	1:1A:289:A:H8	1.59	0.67
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.77	0.67
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.27	0.67
1:1A:2140:C:H42	1:1A:2151:G:H1	1.42	0.67
1:1A:2541:A:N7	59:1A:5523:HOH:O	2.27	0.67
1:2A:987:G:H1	1:2A:1218:C:H42	46.26	0.67
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.28	0.66
1:2A:848:G:H2'	1:2A:849:A:C8	2.31	0.66
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.76	0.66
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.77	0.66
12:1Q:26:TYR:O	12:1Q:67:ARG:NH1	2.26	0.66
1:1A:2627:G:O2'	1:1A:2781:A:N1	2.25	0.66
3:1D:75:ILE:HG21	3:1D:99:ASP:HB2	1.76	0.66
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.10	0.66
6:1G:115:ARG:NH2	6:1G:137:GLU:OE2	2.28	0.66
7:1H:77:LYS:NZ	7:1H:81:GLU:OE1	2.27	0.66
1:1A:2278:A:OP2	22:10:12:ASN:ND2	2.28	0.66
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.60	0.66
59:2A:5029:HOH:O	4:2E:76:ARG:NH1	2.29	0.66
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.29	0.66
1:1A:244:A:H4'	11:1P:74:GLU:HB2	1.78	0.66
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.69	0.66
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.29	0.66
1:1A:1918:A:N6	59:1A:5416:HOH:O	2.29	0.66
3:1D:260:ARG:NH2	3:1D:266:SER:OG	2.29	0.66
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.78	0.66
1:2A:2586:C:OP2	1:2A:2608:G:N1	2.25	0.65
1:2A:637:A:OP1	11:2P:133:SER:OG	2.12	0.65
2:1B:48:A:OP2	14:1S:30:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:70:THR:HG23	5:1F:72:ARG:H	1.61	0.65
1:1A:833:U:O2	11:1P:55:ARG:NH2	2.28	0.65
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.29	0.65
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.43	0.65
1:1A:880:G:H2'	1:1A:881:G:C8	2.31	0.65
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.78	0.65
1:2A:987:G:O2'	1:2A:1000:A:N3	2.28	0.65
1:2A:746:A:O2'	1:2A:2611:U:O2'	2.13	0.65
18:2W:12:ILE:O	18:2W:101:SER:OG	2.14	0.65
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.78	0.65
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.76	0.65
59:2A:5165:HOH:O	19:2X:44:GLU:OE1	2.15	0.65
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.30	0.65
1:1A:506:G:OP1	59:1A:5140:HOH:O	27.30	0.65
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.62	0.65
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.14	0.65
1:2A:2131:G:H1	1:2A:2158:A:H62	1.42	0.65
1:1A:1754:C:N3	1:1A:2716:U:O2'	2.29	0.65
1:2A:139:G:H2'	1:2A:140:G:N7	2.11	0.65
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.32	0.65
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.78	0.65
1:2A:307:G:H21	1:2A:330:A:H62	1.41	0.65
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.76	0.65
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.32	0.65
1:2A:392:C:H5''	1:2A:409:C:H5''	1.78	0.65
1:2A:70:G:H1	1:2A:99:U:H3	36.84	0.65
1:2A:84:A:N1	1:2A:98:G:O2'	2.26	0.65
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.78	0.65
12:2Q:39:PRO:HD3	12:2Q:99:PRO:HG3	1.79	0.65
3:1D:108:PRO:HD2	3:1D:111:LEU:HD22	1.78	0.65
1:2A:1411:C:H42	1:2A:1591:G:H1	1.45	0.65
2:2B:91:C:OP2	12:2Q:16:ARG:NH1	2.30	0.64
59:1A:5033:HOH:O	9:1N:77:GLY:O	2.15	0.64
1:1A:2121:G:N2	1:1A:2177:C:N3	2.42	0.64
1:1A:2245:U:H5''	1:1A:2246:G:H5'	1.79	0.64
1:2A:859:G:N2	1:2A:917:A:OP2	2.29	0.64
1:1A:1055:G:H1	1:1A:1104:C:H42	1.44	0.64
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.33	0.64
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	1.80	0.64
1:2A:817:C:O2'	1:2A:839:U:H5''	1.97	0.64
1:2A:839:U:OP2	1:2A:840:C:N4	6.92	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:42:C:O2	6:2G:66:GLN:NE2	2.30	0.64
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.80	0.64
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.25	0.64
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.60	0.64
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.29	0.64
1:2A:686:G:N2	1:2A:788:A:H61	1.95	0.64
11:2P:95:VAL:HA	11:2P:99:LEU:HD12	1.80	0.64
1:1A:1093:G:H3'	1:1A:1094:U:H5''	1.80	0.64
1:1A:2121:G:O6	1:1A:2176:A:N6	2.31	0.64
1:1A:955:C:OP1	12:1Q:87:LYS:NZ	2.21	0.64
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.31	0.64
6:1G:150:ASP:OD1	6:1G:150:ASP:N	2.31	0.64
1:2A:2267:A:H5''	1:2A:2268:A:H5''	1.80	0.64
21:1Z:7:ALA:HB2	21:1Z:59:LEU:HD22	1.80	0.64
1:2A:880:G:H2'	1:2A:881:G:H8	1.63	0.64
1:1A:1770:G:OP1	59:1A:5292:HOH:O	2.15	0.64
1:1A:2469:A:O2'	12:1Q:56:ARG:NH1	2.31	0.64
8:1I:78:THR:HB	8:1I:104:GLN:HE22	1.62	0.64
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.63	0.64
25:13:6:VAL:HG13	25:13:54:VAL:HG21	1.79	0.64
1:1A:2355:C:H1'	22:10:39:ARG:HH21	1.63	0.64
1:2A:1720:U:OP2	1:2A:1721:G:N2	2.30	0.64
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.29	0.64
1:2A:908:C:OP2	12:2Q:22:LYS:NZ	2.25	0.64
3:2D:164:GLN:OE1	3:2D:176:ARG:NH1	2.31	0.64
1:2A:1600:C:OP1	19:2X:58:HIS:NE2	2.30	0.64
1:2A:963:U:OP2	59:2A:5119:HOH:O	2.15	0.63
6:2G:15:VAL:HG13	6:2G:175:LEU:HD23	1.80	0.63
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.28	0.63
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.80	0.63
1:2A:2066:C:OP1	59:2A:5084:HOH:O	2.15	0.63
10:1O:63:VAL:HG23	10:1O:64:ARG:HG3	1.81	0.63
2:2B:87:G:N2	2:2B:90:A:OP2	2.29	0.63
1:2A:907:U:O2'	12:2Q:101:ARG:NH2	2.31	0.63
17:2V:40:LEU:H	17:2V:46:VAL:HG22	1.64	0.63
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.79	0.63
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.62	0.63
7:1H:149:ARG:NH2	7:1H:167:GLU:OE2	2.27	0.63
2:2B:15:A:OP2	2:2B:69:G:N2	2.31	0.63
26:14:41:PRO:HA	26:14:47:GLN:HB3	1.79	0.63
1:1A:2061:G:OP2	59:1A:5228:HOH:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:34:C:H2'	1:2A:35:G:C8	4.63	0.63
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.80	0.63
1:1A:1062:G:P	1:1A:1070:A:H1'	2.39	0.63
1:2A:271(U):G:H2'	1:2A:271(V):G:H8	1.64	0.63
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.80	0.63
1:1A:613:G:N2	1:1A:614(C):A:O2'	2.31	0.63
9:1N:34:LEU:HD21	9:1N:120:LEU:HB2	1.80	0.63
1:1A:2584:U:H2'	1:1A:2585:U:H2'	1.79	0.63
1:2A:1286:A:H8	1:2A:1287:A:H4'	8.45	0.63
2:2B:66:A:H61	2:2B:109:C:H5''	1.64	0.63
1:2A:1446:C:H42	1:2A:1465:G:H1	1.45	0.63
11:1P:50:ARG:HH21	30:18:7:HIS:HD2	1.45	0.62
1:1A:762:U:OP1	59:1A:5361:HOH:O	2.16	0.62
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.81	0.62
25:23:11:SER:HA	25:23:31:LEU:HD21	1.81	0.62
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.17	0.62
1:1A:2131:G:H5''	1:1A:2132:U:H3'	1.81	0.62
18:1W:18:ARG:HG2	18:1W:76:VAL:HB	1.81	0.62
12:2Q:48:GLU:OE2	12:2Q:51:ARG:NH1	2.30	0.62
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.14	0.62
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.35	0.62
1:2A:1788:C:OP1	3:2D:222:ARG:NH2	2.32	0.62
5:2F:134:GLY:HA3	5:2F:165:ARG:HH21	1.64	0.62
1:1A:526:A:OP1	59:1A:5245:HOH:O	2.15	0.62
1:1A:1788:C:OP1	3:1D:222:ARG:NH2	2.31	0.62
1:2A:819:A:OP2	1:2A:1187:G:N2	2.22	0.62
1:2A:925:C:H2'	1:2A:926:A:H8	1.64	0.62
7:2H:25:LYS:HE3	7:2H:27:LYS:HE2	1.81	0.62
6:1G:114:ILE:HG12	6:1G:140:ILE:HG13	1.82	0.62
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.16	0.62
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.32	0.62
1:1A:1094:U:N3	1:1A:1097:U:OP2	2.32	0.62
1:1A:137:C:N4	1:1A:226:G:O6	86.23	0.62
17:1V:23:GLU:OE1	17:1V:89:GLN:NE2	2.33	0.62
1:2A:1043:C:N4	1:2A:1112:G:O6	2.32	0.62
1:2A:1670:C:O2	4:2E:129:HIS:NE2	2.30	0.62
11:1P:63:PRO:HB2	30:18:30:ARG:HH21	1.64	0.62
1:1A:1827:C:O2'	1:1A:1970:A:N3	2.30	0.62
1:1A:687:C:H5''	29:17:2:LYS:HE2	1.80	0.62
1:2A:1218:C:H42	1:2A:1231:G:H1	1.46	0.62
1:2A:889:C:O2'	1:2A:890:A:O4'	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:55:ASN:H	15:2T:59:THR:HB	1.64	0.62
1:1A:1470:G:N2	1:1A:1520:G:OP2	2.30	0.62
6:1G:129:GLY:O	6:1G:161:THR:OG1	2.17	0.62
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.82	0.62
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.82	0.62
17:2V:80:GLN:HA	17:2V:82:ARG:HH12	1.65	0.62
59:2A:5226:HOH:O	20:2Y:94:LYS:NZ	2.33	0.62
1:1A:1670:C:O2	4:1E:129:HIS:NE2	2.27	0.62
1:2A:2114:A:N7	1:2A:2115:G:N2	2.41	0.62
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.34	0.62
3:1D:37:LEU:HD13	3:1D:62:TYR:HB2	1.82	0.62
1:1A:586:A:H5'	5:1F:89:VAL:HG21	1.81	0.62
1:2A:90:U:H1'	1:2A:92:A:C8	2.35	0.62
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.81	0.62
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.63	0.61
1:2A:379:G:N2	23:21:42:GLN:OE1	2.30	0.61
1:2A:27:G:N2	1:2A:512:G:H1'	2.15	0.61
1:1A:1082:U:N3	1:1A:1086:A:N6	2.05	0.61
1:2A:34:C:H2'	1:2A:35:G:H8	3.75	0.61
1:2A:383:U:H2'	1:2A:385:C:H5	1.65	0.61
1:2A:463:G:N2	1:2A:466:A:OP2	2.31	0.61
28:16:34:LEU:H	28:16:51:GLU:HG2	1.65	0.61
5:1F:8:GLN:HE22	5:1F:21:ALA:HA	1.65	0.61
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.65	0.61
1:2A:1962:5MC:O2'	1:2A:1964:G:OP2	2.18	0.61
4:1E:31:CYS:HB3	4:1E:49:LEU:HG	1.82	0.61
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.83	0.61
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.64	0.61
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.83	0.61
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.34	0.61
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.01	0.61
1:2A:272(G):C:H42	1:2A:363(C):G:H1	1.48	0.61
23:11:56:GLN:HB3	23:11:87:PRO:HG3	1.80	0.61
25:23:29:ARG:N	25:23:33:GLN:OE1	2.33	0.61
1:2A:1002:G:N2	1:2A:1038:C:N3	41.03	0.61
1:2A:686:G:H21	1:2A:788:A:H61	1.47	0.61
1:1A:1286:A:H2'	1:1A:1287:A:H4'	6.73	0.61
1:1A:2340:G:H2'	1:1A:2341:G:C8	2.35	0.61
1:1A:34:C:H2'	1:1A:35:G:C8	5.69	0.61
1:1A:300:A:O2'	1:1A:564:C:N3	73.38	0.61
1:2A:1042:G:H1	1:2A:1114:G:H1'	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:39:C:O2	5:2F:46:ARG:NH2	2.32	0.61
11:2P:63:PRO:HB2	30:28:30:ARG:HH21	1.65	0.61
1:1A:1176:G:H4'	1:1A:1177:A:OP1	1.99	0.60
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.36	0.60
23:21:22:GLY:O	23:21:32:LYS:NZ	2.34	0.60
1:2A:2108:C:H2'	1:2A:2109:U:H6	1.64	0.60
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.83	0.60
8:2I:133:HIS:ND1	8:2I:134:PRO:O	2.30	0.60
1:1A:987:G:O2'	1:1A:1000:A:N3	2.33	0.60
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.34	0.60
25:23:50:VAL:HB	25:23:53:LEU:HD12	1.81	0.60
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.19	0.60
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.13	0.60
1:1A:2128:C:H42	1:1A:2160:G:H1	1.49	0.60
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.81	0.60
1:2A:902:C:H2'	1:2A:903:C:H6	1.66	0.60
1:1A:793:A:OP2	1:1A:2071:A:O2'	2.18	0.60
16:1U:50:ARG:O	16:1U:54:LYS:NZ	2.34	0.60
1:2A:111:A:O2'	24:22:65:ASN:ND2	2.34	0.60
1:2A:859:G:O2'	1:2A:916:G:O6	2.16	0.60
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.34	0.60
1:1A:1007:C:OP1	9:1N:37:LYS:NZ	2.21	0.60
1:1A:298:G:N7	59:1A:5089:HOH:O	2.32	0.60
1:1A:875:G:H1	1:1A:902:C:H42	1.50	0.60
5:1F:24:LEU:HD11	5:1F:199:TRP:HH2	1.66	0.60
1:2A:1403:C:OP1	1:2A:1520:G:N2	2.35	0.60
1:2A:1423:G:H2'	1:2A:1424:G:C8	2.36	0.60
1:2A:668:G:H5'	1:2A:669:G:OP2	2.02	0.60
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.31	0.60
21:1Z:150:LEU:HG	21:1Z:151:HIS:H	1.66	0.60
1:2A:2164:C:H3'	1:2A:2165:G:O4'	2.02	0.60
1:2A:271(A):A:N7	1:2A:271(W):G:N2	2.48	0.60
1:2A:882:G:H2'	1:2A:883:G:C8	2.37	0.60
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.35	0.60
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.83	0.60
1:1A:1825:A:OP1	3:1D:231:HIS:NE2	2.35	0.60
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.20	0.60
26:24:16:CYS:SG	26:24:17:GLY:N	2.74	0.60
1:2A:1566:A:OP1	3:2D:211:ARG:NH1	2.35	0.60
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.02	0.60
1:2A:531:C:H4'	1:2A:532:A:H5''	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:29:SER:OG	16:2U:30:LYS:NZ	2.35	0.60
1:1A:7:G:H5"	9:1N:121:LYS:HE2	1.82	0.60
30:28:31:HIS:HD1	30:28:32:LEU:HD13	1.66	0.60
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.37	0.60
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.35	0.60
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.84	0.60
1:2A:2851:A:O3'	13:2R:64:ARG:NH2	2.34	0.60
1:1A:1864:U:H2'	1:1A:1865:G:C8	2.37	0.59
1:1A:79:G:O6	1:1A:90:U:C2	27.40	0.59
1:1A:973:A:OP1	1:1A:973:A:H8	1.85	0.59
17:1V:62:LEU:HD11	17:1V:95:LEU:HB2	1.84	0.59
20:1Y:17:SER:OG	20:1Y:71:LYS:NZ	2.35	0.59
1:2A:2724:C:OP1	4:2E:118:LYS:NZ	2.35	0.59
1:2A:2384:G:OP2	22:20:55:ARG:NH2	2.35	0.59
1:2A:212:G:H2'	1:2A:213:A:O4'	2.02	0.59
1:2A:2171:A:O2'	1:2A:2172:U:H5"	2.01	0.59
1:2A:2513:G:N2	4:2E:143:ASN:OD1	2.34	0.59
7:2H:149:ARG:HH21	7:2H:154:PRO:HG2	1.65	0.59
1:1A:801:G:O6	5:1F:53:THR:OG1	2.21	0.59
1:2A:2165:G:H2'	1:2A:2166:G:H5"	1.83	0.59
1:1A:7:G:H2'	1:1A:8:A:O4'	2.02	0.59
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.37	0.59
1:2A:390:A:H4'	1:2A:391:G:H5'	1.83	0.59
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.18	0.59
1:1A:740:U:H2'	1:1A:741:G:C8	2.37	0.59
1:2A:473:G:H2'	1:2A:474:G:C8	3.18	0.59
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB2	1.83	0.59
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.19	0.59
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.36	0.59
1:2A:2401:U:OP1	28:26:18:ARG:NH2	2.36	0.59
1:2A:1527:G:O2'	1:2A:1544:A:N6	2.35	0.59
1:2A:1662:C:O2'	1:2A:2687:U:OP1	2.19	0.59
1:2A:473:G:H2'	1:2A:474:G:H8	2.52	0.59
2:2B:22:U:H3	2:2B:61:G:H1	1.51	0.59
5:1F:32:LEU:HD13	5:1F:112:MET:HE1	1.85	0.59
1:1A:1252:G:N7	16:1U:36:ARG:NH1	2.49	0.59
25:23:8:LEU:HB2	25:23:28:LEU:HD13	1.85	0.59
1:2A:236:C:O2	1:2A:261:G:N2	2.29	0.59
1:2A:698:C:O2'	1:2A:734:A:N6	2.36	0.59
1:2A:82:G:H21	1:2A:104:U:H5	1.51	0.59
1:2A:910:A:N3	1:2A:2264:C:O2'	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:50:G:OP1	14:2S:63:THR:OG1	2.18	0.59
22:10:11:ARG:O	22:10:14:ARG:NH2	2.36	0.59
1:1A:1296:G:OP1	1:1A:2709:G:O2'	2.13	0.59
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.19	0.59
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.18	0.59
1:2A:2576:G:O2'	1:2A:2579:C:OP2	2.17	0.59
9:2N:42:TRP:O	16:2U:64:ARG:NE	2.27	0.59
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.84	0.59
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.76	0.59
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.36	0.59
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.35	0.59
16:2U:28:ARG:NH1	16:2U:38:THR:OG1	2.36	0.59
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.85	0.58
1:2A:1423:G:H2'	1:2A:1424:G:H8	1.68	0.58
6:2G:7:LEU:HD23	6:2G:100:TRP:HE3	1.68	0.58
8:1I:6:LEU:HD11	8:1I:37:VAL:HG23	1.84	0.58
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.84	0.58
1:2A:1155:A:H5''	16:2U:55:ARG:HH11	1.68	0.58
1:1A:2010:G:H5''	18:1W:42:ARG:HB2	1.84	0.58
1:1A:2598:A:OP1	59:1A:5143:HOH:O	2.17	0.58
1:1A:458:G:O2'	1:1A:469:G:O6	2.18	0.58
15:1T:108:ARG:HH12	15:1T:112:ARG:HD3	1.67	0.58
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	1.84	0.58
20:1Y:8:LYS:HD3	20:1Y:97:ARG:HH21	1.68	0.58
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.21	0.58
9:2N:21:LYS:HD2	9:2N:26:LEU:HD13	1.84	0.58
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.34	0.58
18:2W:6:ILE:HG12	18:2W:104:THR:HG23	1.85	0.58
1:1A:1441:G:H2'	1:1A:1442:G:H8	1.69	0.58
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.18	0.58
1:2A:1426:G:OP2	1:2A:1427:A:O2'	2.19	0.58
5:2F:165:ARG:HA	5:2F:168:ARG:HD2	1.85	0.58
1:1A:1038:C:H42	1:1A:1117:G:H1	1.50	0.58
1:1A:1181:C:H2'	1:1A:1182:A:H8	1.68	0.58
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.39	0.58
1:1A:1243:G:O2'	11:1P:4:SER:O	2.21	0.58
1:1A:2657:A:O3'	7:1H:160:LYS:NZ	2.31	0.58
1:1A:2679:A:OP2	4:1E:160:TYR:OH	2.19	0.58
1:1A:707:G:H1	1:1A:724:U:H3	1.50	0.58
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.19	0.58
8:2I:102:SER:HA	8:2I:107:VAL:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2N:4:TYR:HB2	16:2U:101:ARG:HH21	1.68	0.58
1:1A:18:C:O2'	1:1A:554:U:OP1	2.19	0.58
1:2A:375:C:H2'	1:2A:376:C:H6	1.67	0.58
1:2A:480:A:N3	1:2A:499:U:O2'	2.32	0.58
1:1A:1881:C:H2'	1:1A:1882:C:H6	1.69	0.58
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.38	0.58
1:2A:2393:A:H5''	11:2P:63:PRO:HB3	1.85	0.58
1:2A:2544:G:H2'	1:2A:2545:G:H8	1.69	0.58
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.84	0.58
20:2Y:37:VAL:HG21	20:2Y:72:VAL:HG21	1.86	0.58
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.69	0.58
14:2S:37:ALA:HB2	14:2S:101:LEU:HD11	1.85	0.58
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.37	0.58
20:2Y:83:THR:HG21	20:2Y:99:CYS:HB2	1.84	0.58
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.03	0.58
3:1D:89:SER:HB2	3:1D:201:HIS:CD2	2.39	0.58
1:2A:2146:C:O2	1:2A:2147:G:N2	2.37	0.58
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.85	0.58
10:2O:2:ILE:HG21	10:2O:8:LEU:HD11	1.86	0.58
26:14:55:ARG:N	26:14:56:VAL:HA	2.19	0.57
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.18	0.57
1:1A:784:A:OP1	59:1A:5235:HOH:O	2.17	0.57
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.69	0.57
2:2B:66:A:N6	2:2B:109:C:H5''	2.18	0.57
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.36	0.57
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.39	0.57
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.19	0.57
5:2F:149:ASP:OD1	5:2F:149:ASP:N	2.29	0.57
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.85	0.57
1:1A:1062:G:H1	1:1A:1077:A:N6	1.99	0.57
1:1A:784:A:O4'	3:1D:227:ASN:ND2	2.38	0.57
1:2A:1119:C:H2'	1:2A:1120:G:C8	3.02	0.57
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.16	0.57
6:2G:3:LEU:HD12	6:2G:8:LYS:HZ1	1.69	0.57
1:1A:1991:U:H2'	1:1A:1992:G:H5''	1.86	0.57
26:24:53:GLU:H	26:24:53:GLU:CD	2.07	0.57
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.48	0.57
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.39	0.57
8:2I:93:THR:HG22	8:2I:94:ALA:H	1.69	0.57
1:1A:2696:U:H2'	1:1A:2697:G:C8	2.40	0.57
14:1S:71:ARG:NH1	14:1S:107:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:69:THR:HG22	21:1Z:90:VAL:HG22	1.86	0.57
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.37	0.57
1:1A:1130:U:O2	4:1E:149:ARG:NH2	2.29	0.57
1:2A:2130:U:O2'	1:2A:2133:G:H4'	2.05	0.57
1:2A:380:U:H2'	1:2A:381:G:C8	2.40	0.57
10:2O:24:VAL:HG12	10:2O:33:ALA:HB2	1.86	0.57
11:2P:90:ARG:HH12	11:2P:105:LEU:HD11	1.68	0.57
1:2A:2688:U:O2'	1:2A:2721:A:N6	2.38	0.57
1:1A:1058:G:H1	1:1A:1080:C:N4	2.02	0.57
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	1.86	0.57
11:1P:126:VAL:HG12	11:1P:148:LEU:HD22	1.87	0.57
13:1R:33:ARG:HG2	13:1R:115:GLU:HB3	1.87	0.57
1:2A:1204:A:H2	1:2A:1241:A:H62	1.52	0.57
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.40	0.57
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.40	0.57
1:1A:78:A:H2'	1:1A:79:G:H8	1.69	0.57
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.87	0.57
19:1X:8:ILE:O	24:12:36:ARG:NH2	2.38	0.57
1:2A:956:G:OP2	12:2Q:14:ARG:NH1	2.28	0.57
17:2V:56:SER:H	17:2V:100:ARG:HB2	1.68	0.57
1:1A:250:G:P	30:18:13:ARG:HH22	2.28	0.57
1:1A:1085:A:O2'	1:1A:1104:C:O2'	2.22	0.57
1:1A:1171:G:OP2	1:1A:1174:A:N6	2.37	0.57
2:1B:66:A:H61	2:1B:108:U:H2'	1.70	0.57
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.85	0.57
1:2A:125:G:O6	29:27:10:ARG:NH1	2.37	0.57
1:2A:1496:A:N3	1:2A:1577:C:O2'	2.33	0.57
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.85	0.57
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.40	0.56
1:2A:2755:C:H3'	31:29:19:ARG:HH21	1.70	0.56
1:2A:723:G:H2'	1:2A:724:U:O4'	2.05	0.56
8:2I:9:LEU:HB3	8:2I:12:LEU:HD12	1.87	0.56
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.37	0.56
1:1A:1341:U:OP2	1:1A:1394:U:O2'	2.15	0.56
1:1A:2352:A:N6	1:1A:2365:G:O2'	2.37	0.56
1:1A:27:G:N2	1:1A:512:G:H1'	2.20	0.56
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.40	0.56
1:2A:372:G:N2	1:2A:373:U:O4	2.33	0.56
1:2A:375:C:H2'	1:2A:376:C:C6	2.40	0.56
1:2A:900:A:O2'	1:2A:901:A:OP1	2.20	0.56
14:2S:25:ARG:O	14:2S:40:ILE:N	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2347:C:O2'	28:16:21:TYR:OH	2.15	0.56
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.04	0.56
1:2A:272(B):G:H2'	1:2A:272(C):G:H8	1.71	0.56
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.23	0.56
1:2A:943:U:H2'	1:2A:944:G:H8	4.09	0.56
1:2A:2511:U:O2'	4:2E:138:PRO:O	2.18	0.56
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.88	0.56
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	1.88	0.56
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.87	0.56
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.52	0.56
14:2S:43:GLU:N	14:2S:43:GLU:OE1	5.08	0.56
1:1A:2689:U:H4'	1:1A:2690:C:H5'	1.88	0.56
1:1A:288:C:H2'	1:1A:289:A:C8	2.40	0.56
1:1A:841:A:H2'	1:1A:842:G:C8	2.40	0.56
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.88	0.56
24:22:11:GLU:HA	24:22:14:ARG:HB2	1.85	0.56
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.41	0.56
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.40	0.56
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.41	0.56
1:2A:83:G:H1	1:2A:102:G:HO2'	1.52	0.56
1:2A:2658:C:H5'	7:2H:160:LYS:HZ1	1.70	0.56
1:1A:1058:G:N2	1:1A:1080:C:N3	2.47	0.56
6:1G:139:LEU:HA	6:1G:144:ILE:HB	1.85	0.56
10:1O:75:SER:OG	10:1O:76:ALA:N	2.38	0.56
2:1B:37:C:O2	14:1S:95:HIS:NE2	2.38	0.56
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.40	0.56
1:2A:918:A:N3	2:2B:80:U:O2'	2.39	0.56
1:1A:942:G:O2'	1:1A:1189:A:N3	2.38	0.56
1:1A:668:G:H5'	1:1A:669:G:OP2	2.05	0.56
21:1Z:154:ASP:OD1	21:1Z:154:ASP:N	2.34	0.56
1:2A:661:C:H2'	1:2A:662:G:C8	2.39	0.56
1:2A:2224:G:OP1	3:2D:268:ARG:NE	2.38	0.56
1:1A:397:G:OP2	23:11:10:LYS:NZ	2.26	0.56
1:2A:857:C:H4'	22:20:23:VAL:HG21	1.86	0.56
1:2A:1042:G:N1	1:2A:1114:G:H1'	2.20	0.56
1:2A:1114:G:H2'	1:2A:1115:G:C8	2.40	0.56
14:2S:10:ARG:NH2	14:2S:91:PRO:O	2.36	0.56
1:1A:2402:C:O2	1:1A:2403:C:N4	2.36	0.56
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.88	0.56
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.40	0.56
1:2A:1920:4OC:HM22	1:2A:1921:G:H5'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:260:ARG:NH2	3:2D:266:SER:OG	2.39	0.56
7:2H:23:ARG:NH1	7:2H:34:GLU:OE1	2.39	0.56
1:1A:188:G:H5'	23:11:14:VAL:HG21	1.86	0.56
1:1A:1647:G:OP2	59:1A:5557:HOH:O	2.18	0.56
1:1A:414:C:H2'	1:1A:415:A:C8	2.41	0.56
1:1A:745:G:O6	1:1A:746:A:N6	2.39	0.56
1:1A:943:U:OP2	59:1A:5256:HOH:O	2.17	0.56
7:1H:88:LEU:HD22	7:1H:130:ARG:HG2	1.88	0.56
21:1Z:45:ASP:OD1	21:1Z:49:ARG:NE	2.39	0.56
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.86	0.56
1:2A:23:G:OP1	1:2A:504:U:N3	2.37	0.56
1:2A:271(K):U:H4'	1:2A:271(L):U:OP2	2.06	0.56
6:2G:131:TYR:HE2	6:2G:133:LEU:HD23	1.71	0.56
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.37	0.56
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.88	0.56
6:1G:64:THR:HB	6:1G:94:LEU:HD11	1.88	0.56
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.87	0.56
1:2A:918:A:H2	2:2B:81:G:H5'	1.71	0.56
1:1A:1355:G:H2'	1:1A:1356:G:C8	2.99	0.55
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.41	0.55
1:1A:2572:A:H62	4:1E:145:LYS:HE2	1.70	0.55
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.87	0.55
8:1I:14:ASP:OD1	8:1I:15:VAL:N	2.39	0.55
1:2A:115:C:O2'	1:2A:127:A:O2'	2.23	0.55
7:2H:70:THR:O	7:2H:74:ASN:ND2	2.35	0.55
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.21	0.55
4:1E:59:VAL:HG21	4:1E:74:PRO:HB3	1.88	0.55
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.88	0.55
1:2A:2127:G:C2	1:2A:2161:C:C2	2.94	0.55
1:2A:2313:C:H2'	1:2A:2314:C:H6	1.70	0.55
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.39	0.55
1:2A:1012:U:O4	9:2N:28:THR:HG21	2.06	0.55
12:2Q:45:GLN:N	12:2Q:45:GLN:OE1	2.39	0.55
1:1A:1183:G:O2'	25:13:29:ARG:NH1	2.39	0.55
1:1A:184:C:H2'	1:1A:185:U:C6	2.41	0.55
1:1A:2108:C:H2'	1:1A:2109:U:O4'	2.05	0.55
5:1F:167:ALA:HB1	5:1F:173:VAL:HG11	1.89	0.55
1:2A:851:U:O2'	25:23:42:ALA:O	2.22	0.55
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.42	0.55
1:2A:1129:A:O2'	1:2A:2515:C:O2'	2.25	0.55
1:2A:674:G:H2'	1:2A:675:A:H8	4.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:902:C:H2'	1:2A:903:C:C6	2.41	0.55
11:1P:52:GLU:HG2	30:18:57:ARG:HH12	1.72	0.55
1:1A:1087:G:H1	1:1A:1102:C:N4	2.03	0.55
5:1F:179:GLU:OE1	5:1F:179:GLU:N	2.36	0.55
6:1G:40:ASN:HD22	6:1G:156:ASP:HB2	1.71	0.55
8:1I:114:LEU:HD21	8:1I:128:LEU:HD13	1.87	0.55
10:1O:24:VAL:HG12	10:1O:33:ALA:HB2	1.87	0.55
26:24:24:THR:OG1	26:24:25:TYR:N	2.28	0.55
31:29:15:LYS:HB3	31:29:26:ILE:HG13	1.89	0.55
1:2A:1471:A:OP2	1:2A:1519:G:N2	2.36	0.55
1:2A:210:C:OP2	29:27:29:LYS:NZ	2.39	0.55
1:2A:2143:C:N4	1:2A:2148:G:H1	2.04	0.55
1:2A:834:C:O2	1:2A:852:G:N2	38.33	0.55
1:2A:1653:G:O6	13:2R:11:ASN:ND2	2.39	0.55
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.87	0.55
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.89	0.55
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.88	0.55
1:2A:1799:G:O2'	3:2D:181:GLU:OE2	2.21	0.55
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.88	0.55
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.41	0.55
6:2G:138:GLN:OE1	6:2G:138:GLN:N	2.36	0.55
24:12:25:VAL:HG13	24:12:57:ILE:HG23	1.87	0.55
1:1A:1889:A:H2'	1:1A:1890:A:C8	2.42	0.55
1:1A:2539:C:H4'	31:19:3:VAL:HG21	1.88	0.55
1:1A:624:C:H2'	1:1A:625:G:C8	3.31	0.55
20:1Y:13:VAL:HG12	20:1Y:74:PRO:HA	1.89	0.55
1:2A:252:G:OP1	11:2P:50:ARG:NH1	2.36	0.55
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.41	0.55
19:2X:89:ILE:HG22	19:2X:92:LEU:H	1.71	0.55
1:1A:120:U:OP2	59:1A:5572:HOH:O	2.18	0.55
1:1A:2103:C:H2'	1:1A:2104:G:C8	2.42	0.55
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.06	0.55
1:2A:2160:G:H2'	1:2A:2161:C:H5''	1.88	0.55
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.71	0.55
8:2I:3:VAL:HA	8:2I:38:LEU:HA	1.87	0.55
10:2O:13:ASN:HD21	10:2O:96:THR:H	1.55	0.55
15:2T:102:ILE:HA	15:2T:105:LEU:HG	1.89	0.55
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.42	0.55
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.06	0.55
1:1A:2429:G:O6	11:1P:61:ARG:NH2	2.33	0.55
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:101:LEU:HG	8:1I:107:VAL:HB	1.89	0.55
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.89	0.55
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.42	0.55
1:2A:1470:G:O2'	1:2A:1520:G:O6	2.20	0.55
1:2A:1779:U:OP2	1:2A:1784:A:N6	2.26	0.55
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.42	0.55
1:2A:2108:C:H2'	1:2A:2109:U:C6	2.42	0.55
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.40	0.55
1:2A:324:A:N6	1:2A:338:G:O2'	2.40	0.55
9:2N:104:LYS:HA	9:2N:107:LEU:HD12	1.89	0.55
9:2N:103:VAL:HG11	9:2N:120:LEU:HD22	1.89	0.55
1:1A:1213:A:N3	1:1A:1238:G:O2'	2.38	0.55
1:1A:1805:U:O2	3:1D:50:THR:HB	2.07	0.55
1:1A:784:A:N6	1:1A:2072:G:O2'	2.38	0.55
1:1A:2129:C:H42	1:1A:2159:G:H1	1.54	0.55
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.87	0.55
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.06	0.55
1:2A:334:C:OP1	1:2A:335:C:N4	2.40	0.55
3:2D:70:TRP:NE1	3:2D:146:GLU:OE2	2.38	0.55
9:2N:20:GLY:HA2	9:2N:61:ARG:HG3	1.89	0.55
14:2S:30:ARG:HA	14:2S:35:ILE:HA	1.89	0.55
1:1A:2629:A:H1'	1:1A:2630:G:C5'	2.36	0.55
2:1B:86:G:H1	2:1B:91:C:H42	1.55	0.55
2:2B:3:C:H2'	2:2B:4:C:C6	2.42	0.55
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	1.89	0.55
12:2Q:24:GLY:HA2	12:2Q:67:ARG:NH2	2.22	0.55
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.07	0.54
1:1A:1181:C:H2'	1:1A:1182:A:C8	2.42	0.54
1:2A:2322:A:H2'	1:2A:2323:G:O4'	2.07	0.54
21:2Z:40:ASP:HB3	21:2Z:43:GLU:HB2	1.88	0.54
30:18:23:VAL:HG13	30:18:47:LYS:HB3	1.89	0.54
1:1A:673:C:OP1	5:1F:54:ARG:NH1	2.37	0.54
12:1Q:43:THR:HG22	12:1Q:94:VAL:HG12	1.89	0.54
1:2A:2544:G:H2'	1:2A:2545:G:C8	2.42	0.54
1:2A:958:U:O2	2:2B:90:A:O2'	2.24	0.54
5:2F:28:ILE:HD13	5:2F:112:MET:HG2	1.89	0.54
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.40	0.54
1:2A:2355:C:H4'	22:20:24:LYS:HG3	1.88	0.54
31:29:2:LYS:NZ	31:29:31:LYS:O	2.37	0.54
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.43	0.54
1:2A:863:A:H2'	1:2A:864:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:928:G:H8	1:2A:928:G:O5'	1.91	0.54
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.90	0.54
1:2A:2051:A:OP1	4:2E:137:HIS:ND1	2.39	0.54
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.07	0.54
8:2I:65:ALA:O	8:2I:69:LYS:N	2.40	0.54
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.43	0.54
1:1A:272:G:O2'	1:1A:421:U:OP2	2.14	0.54
3:1D:37:LEU:HD22	3:1D:87:ASN:ND2	2.22	0.54
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.90	0.54
14:1S:25:ARG:NH2	14:1S:42:ASP:OD1	2.41	0.54
18:1W:86:LEU:HD22	18:1W:96:ILE:HD11	1.89	0.54
1:2A:83:G:N1	1:2A:102:G:O2'	2.39	0.54
1:2A:120:U:H5''	1:2A:122:G:OP2	2.07	0.54
1:2A:1791:A:H5'	3:2D:206:LEU:HD12	1.90	0.54
4:2E:8:LYS:O	4:2E:193:GLY:N	2.38	0.54
18:2W:78:GLU:OE2	18:2W:99:ARG:NH1	2.41	0.54
1:1A:1071:G:N1	1:1A:1091:G:O6	2.31	0.54
1:1A:2484:G:O2'	12:1Q:124:LYS:O	2.25	0.54
1:1A:1568:G:H5'	3:1D:60:ARG:HA	1.89	0.54
1:2A:1434:A:H2'	1:2A:1435:G:C8	2.42	0.54
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.90	0.54
1:1A:1266:G:N2	1:1A:1269:A:OP2	13.75	0.54
4:1E:34:VAL:HG12	4:1E:72:VAL:HG21	1.89	0.54
1:2A:1598:C:O3'	19:2X:35:THR:OG1	2.25	0.54
1:2A:172:C:H2'	1:2A:173:G:H8	1.72	0.54
1:2A:2001:A:H2'	1:2A:2002:G:H8	1.72	0.54
1:2A:2168:G:H2'	1:2A:2170:A:N7	2.23	0.54
1:2A:1751:C:O2'	1:2A:2861:G:O2'	2.24	0.54
1:2A:47:C:H42	1:2A:361:G:H1	42.46	0.54
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.71	0.54
1:1A:1177:A:N3	1:1A:1177:A:H2'	2.22	0.54
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.07	0.54
1:1A:530:G:N1	1:1A:2023:G:OP1	2.31	0.54
1:1A:710:G:H2'	1:1A:711:G:C8	2.43	0.54
1:1A:2303:G:O2'	6:1G:132:ASN:ND2	2.40	0.54
6:1G:43:LEU:HD23	6:1G:53:LEU:HD23	1.89	0.54
1:1A:1754:C:H5	15:1T:96:ARG:NH2	2.06	0.54
20:1Y:17:SER:HG	20:1Y:71:LYS:HZ2	1.56	0.54
1:2A:1186:G:C2	1:2A:1187:G:H1'	2.43	0.54
1:2A:2232:U:OP1	23:21:40:ARG:NH1	2.39	0.54
1:2A:245:G:O6	30:28:8:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:42:C:C6	6:2G:69:ALA:HB2	2.43	0.54
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.41	0.54
22:20:27:GLU:HB2	22:20:69:PHE:HD2	1.72	0.54
28:26:25:LYS:NZ	28:26:51:GLU:OE2	2.28	0.54
1:2A:1791:A:H3'	1:2A:1792:G:H8	1.73	0.54
1:2A:186:G:H2'	1:2A:187:G:H8	1.73	0.54
1:2A:2070:G:H2'	1:2A:2071:A:H8	1.72	0.54
1:2A:2392:A:OP2	1:2A:2422:A:N6	2.37	0.54
3:2D:72:LYS:HB3	3:2D:75:ILE:HD12	1.89	0.54
1:1A:1068:G:OP2	1:1A:1068:G:H8	3.15	0.54
1:1A:1843:C:H5''	3:1D:257:LEU:HD13	1.88	0.54
3:1D:26:LYS:HB3	3:1D:83:GLU:HG2	1.89	0.54
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.43	0.54
10:1O:64:ARG:HD2	10:1O:79:PHE:CD1	2.43	0.54
21:1Z:130:PRO:HA	21:1Z:133:ILE:HG13	1.90	0.54
21:1Z:24:LEU:HD22	21:1Z:41:LEU:HD12	1.89	0.54
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.43	0.54
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.49	0.54
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	1.88	0.54
9:2N:35:ARG:O	9:2N:42:TRP:NE1	2.39	0.54
16:2U:27:LEU:O	16:2U:31:SER:N	2.30	0.54
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.41	0.54
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.43	0.54
1:1A:848:G:H2'	1:1A:849:A:C8	2.43	0.54
7:1H:3:ARG:NH1	7:1H:4:ILE:H	2.05	0.54
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.89	0.54
10:2O:36:GLY:HA3	10:2O:109:LYS:HD2	1.89	0.54
15:2T:91:ARG:HB2	15:2T:121:ILE:HG13	1.89	0.54
23:11:18:ILE:HG12	23:11:37:ILE:HG12	1.88	0.53
1:1A:1798:U:OP2	3:1D:274:ARG:NH2	2.31	0.53
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.43	0.53
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.89	0.53
1:2A:1853:A:H2'	1:2A:1854:A:C8	2.43	0.53
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.09	0.53
8:2I:78:THR:H	8:2I:104:GLN:HE22	1.55	0.53
16:2U:82:GLY:O	16:2U:86:ALA:N	2.38	0.53
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.88	0.53
1:1A:1720:U:H3	1:1A:1742:G:H1	1.56	0.53
10:1O:11:ALA:O	10:1O:99:PHE:N	2.36	0.53
21:1Z:102:LEU:HD11	21:1Z:124:ILE:HB	1.90	0.53
1:2A:2126:A:H4'	1:2A:2127:G:OP1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2690:C:H41	1:2A:2713:A:H1'	1.72	0.53
1:2A:893:C:H2'	1:2A:894:C:C5	2.43	0.53
6:2G:41:GLN:HB3	6:2G:43:LEU:HD13	1.90	0.53
10:2O:11:ALA:O	10:2O:99:PHE:N	2.39	0.53
1:1A:1187:G:N2	1:1A:1188:U:O4	2.42	0.53
1:1A:1509(A):A:H3'	1:1A:1509(B):A:H8	1.72	0.53
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.88	0.53
16:1U:49:HIS:HA	16:1U:52:ARG:HB2	1.91	0.53
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.44	0.53
1:2A:882:G:H1	1:2A:894:C:H42	1.56	0.53
1:2A:993:G:N7	1:2A:1213:A:N6	49.37	0.53
21:2Z:75:ASN:O	21:2Z:84:GLU:N	2.35	0.53
1:1A:761:A:OP2	59:1A:5095:HOH:O	2.18	0.53
5:1F:39:TRP:O	5:1F:43:LYS:HG2	2.08	0.53
17:1V:5:VAL:HG21	17:1V:35:LEU:HD23	1.89	0.53
1:2A:1131:G:OP1	9:2N:80:GLY:N	2.38	0.53
1:2A:1230:C:H2'	1:2A:1231:G:C8	2.44	0.53
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.43	0.53
1:2A:237:C:O2	1:2A:609:A:O2'	2.26	0.53
1:2A:627:A:O4'	1:2A:637:A:N6	2.42	0.53
9:2N:69:GLN:O	9:2N:71:ILE:HG13	2.07	0.53
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.89	0.53
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.44	0.53
1:1A:1355:G:H2'	1:1A:1356:G:H8	2.36	0.53
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.35	0.53
4:1E:128:SER:OG	4:1E:129:HIS:N	2.37	0.53
7:1H:45:VAL:HG12	7:1H:50:VAL:HG22	1.89	0.53
22:20:70:GLN:HG2	22:20:72:ARG:HG3	1.91	0.53
1:2A:2145:C:O2'	1:2A:2147:G:N7	2.42	0.53
1:2A:334:C:P	1:2A:335:C:H41	2.32	0.53
1:2A:1011:G:OP1	16:2U:77:SER:OG	2.27	0.53
28:16:23:THR:OG1	28:16:24:GLU:N	2.41	0.53
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.43	0.53
1:1A:1654:A:O2'	4:1E:113:PHE:O	2.23	0.53
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.91	0.53
1:2A:1161:C:H2'	1:2A:1162:G:C8	2.44	0.53
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.73	0.53
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.08	0.53
10:2O:73:ASP:HB2	15:2T:82:LEU:HD12	1.91	0.53
26:14:40:HIS:HB3	26:14:43:TYR:HB2	1.91	0.53
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:588:U:H2'	1:1A:589:C:C6	2.44	0.53
18:1W:10:VAL:HG12	18:1W:12:ILE:HG22	1.90	0.53
1:2A:380:U:H2'	1:2A:381:G:H8	1.74	0.53
1:1A:2350:C:H42	1:1A:2367:G:H1	1.57	0.53
1:1A:601:C:O2'	1:1A:605:C:OP1	2.24	0.53
8:1I:79:ILE:HB	8:1I:144:VAL:HG12	1.91	0.53
13:1R:96:ARG:HH21	13:1R:117:VAL:HG13	1.74	0.53
1:2A:79:G:H2'	1:2A:80:G:H8	1.74	0.53
1:2A:81:G:H1	1:2A:105:C:H42	1.57	0.53
1:1A:1053:C:N3	1:1A:1106:G:N2	2.51	0.53
1:1A:709:U:H2'	1:1A:710:G:C8	2.44	0.53
1:1A:783:A:O2'	1:1A:785:G:OP1	2.17	0.53
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.91	0.53
2:1B:74:U:H1'	21:1Z:34:ASN:HD21	1.74	0.53
1:2A:1655:A:N6	1:2A:2005:A:O2'	2.42	0.53
1:2A:348:G:H2'	1:2A:349:G:C8	2.43	0.53
1:2A:675:A:H2'	1:2A:676:A:O4'	2.40	0.53
7:2H:124:GLU:HG3	7:2H:132:ARG:HB3	1.90	0.53
19:2X:11:PRO:HA	19:2X:28:PHE:HA	1.91	0.53
1:1A:1301:A:O2'	1:1A:1302:A:H3'	2.08	0.52
1:1A:1653:G:O3'	13:1R:2:ARG:HB2	2.09	0.52
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.09	0.52
1:1A:443:A:N7	5:1F:45:ARG:HG2	2.24	0.52
6:1G:67:LYS:HG2	6:1G:68:PRO:HD2	1.91	0.52
1:2A:839:U:H1'	1:2A:1191:G:H1'	1.91	0.52
1:2A:1248:G:C5	16:2U:3:ARG:HB2	2.44	0.52
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.44	0.52
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.44	0.52
1:2A:479:A:H4'	1:2A:480:A:OP1	2.08	0.52
1:2A:657:U:H2'	1:2A:658:C:C6	2.43	0.52
1:2A:833:U:H1'	11:2P:55:ARG:HH21	1.74	0.52
1:2A:918:A:C2	2:2B:81:G:H5'	2.44	0.52
11:2P:100:LEU:HD12	11:2P:112:LEU:HD21	1.91	0.52
1:1A:406:G:O6	1:1A:436:C:N4	53.52	0.52
1:2A:104:U:H5''	1:2A:105:C:H5	1.73	0.52
1:2A:2121:G:H1	1:2A:2177:C:H42	1.57	0.52
1:2A:662:G:H2'	1:2A:663:G:H8	1.74	0.52
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.09	0.52
1:1A:548:A:O2'	1:1A:549:G:OP1	2.24	0.52
4:1E:14:ILE:HG13	4:1E:21:VAL:HG13	1.90	0.52
21:1Z:126:VAL:HG13	21:1Z:161:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2285:C:OP2	28:26:6:ARG:HD3	2.10	0.52
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.74	0.52
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.41	0.52
1:2A:272(B):G:H2'	1:2A:272(C):G:C8	2.44	0.52
1:2A:514:A:N3	1:2A:581:C:O2'	2.36	0.52
1:2A:694:U:OP1	3:2D:59:LYS:NZ	2.42	0.52
10:2O:4:PRO:O	10:2O:5:GLN:HB2	2.10	0.52
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	1.91	0.52
16:2U:66:ASN:O	16:2U:70:ARG:HG3	2.08	0.52
21:2Z:171:ILE:HG12	21:2Z:172:ALA:H	1.74	0.52
1:1A:2140:C:N4	1:1A:2151:G:H1	2.05	0.52
1:1A:86:C:H4'	1:1A:104:U:H1'	1.92	0.52
1:2A:1138:G:O2'	9:2N:102:ALA:O	2.28	0.52
1:2A:725:G:N2	1:2A:732:C:O2	21.79	0.52
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.27	0.52
22:10:27:GLU:HB2	22:10:69:PHE:HD2	1.75	0.52
1:1A:2012:G:OP2	18:1W:16:LYS:NZ	2.38	0.52
1:1A:210:C:H2'	1:1A:211:A:H8	1.75	0.52
1:1A:2125:G:H22	1:1A:2172:U:P	2.32	0.52
3:1D:62:TYR:HE1	3:1D:88:ARG:HH22	1.56	0.52
1:2A:2278:A:H5''	22:20:12:ASN:HD21	1.75	0.52
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.43	0.52
1:2A:291:C:O2	1:2A:309:G:N2	48.16	0.52
1:2A:652(B):A:N6	1:2A:655:A:H1'	2.22	0.52
1:2A:675:A:N3	1:2A:2443:C:O2'	2.40	0.52
1:2A:76:C:N4	1:2A:93:G:H1	25.88	0.52
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.43	0.52
1:1A:2478:A:H5'	31:19:31:LYS:HD3	1.92	0.52
1:1A:859:G:O2'	1:1A:916:G:O6	2.27	0.52
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.23	0.52
1:2A:302:C:H42	1:2A:315:G:H1	1.58	0.52
4:2E:34:VAL:HG21	4:2E:78:LEU:HD23	1.92	0.52
2:2B:48:A:OP2	14:2S:30:ARG:NH2	2.43	0.52
16:2U:27:LEU:HA	16:2U:30:LYS:HB2	1.90	0.52
16:2U:92:ARG:HA	16:2U:95:LEU:HB2	1.92	0.52
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.92	0.52
1:1A:70:G:H5''	1:1A:112:U:O2	2.09	0.52
3:1D:164:GLN:OE1	3:1D:176:ARG:NH1	2.43	0.52
21:1Z:10:ARG:HB3	21:1Z:38:TYR:HD2	1.74	0.52
1:2A:646:A:H2'	1:2A:647:G:O4'	2.10	0.52
1:2A:652(T):C:H2'	1:2A:652(U):G:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:868:U:H3	1:2A:909:A:H61	1.58	0.52
2:2B:41:U:H5	6:2G:70:VAL:H	1.58	0.52
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	1.92	0.52
1:1A:1011:G:H1	1:1A:1018:C:H42	17.78	0.52
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.44	0.52
1:1A:694:U:OP1	3:1D:59:LYS:NZ	2.43	0.52
59:1A:5075:HOH:O	10:1O:118:ALA:O	84.01	0.52
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.44	0.52
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.23	0.52
1:2A:2494:G:OP1	22:20:3:HIS:N	2.43	0.52
26:14:26:SER:OG	26:14:27:THR:N	2.43	0.52
1:1A:1711:C:H2'	1:1A:1712:C:H6	1.75	0.52
1:1A:1773:A:H2'	1:1A:1774:C:O4'	2.10	0.52
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.44	0.52
1:1A:2712:U:H1'	1:1A:2712(A):A:C8	2.45	0.52
1:2A:1593:G:H2'	1:2A:1594:G:H8	1.74	0.52
1:2A:527:C:N4	1:2A:2779:U:OP2	2.43	0.52
17:2V:24:LYS:HG3	17:2V:64:HIS:HD2	1.75	0.52
1:1A:2137:C:H2'	1:1A:2138:C:C6	2.44	0.52
1:1A:2801(A):A:H5''	1:1A:2802:G:C8	2.45	0.52
1:1A:573:G:O2'	1:1A:574:C:H3'	2.10	0.52
7:1H:10:PRO:HA	7:1H:49:VAL:HG22	1.91	0.52
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.10	0.52
1:2A:104:U:H5''	1:2A:105:C:C5	2.45	0.52
1:2A:1203:G:OP2	1:2A:1204:A:O2'	2.18	0.52
1:2A:2562:U:H1'	10:2O:23:ARG:HE	1.75	0.52
1:2A:2705:A:O2'	1:2A:2852:G:OP1	2.18	0.52
1:2A:582:G:H2'	1:2A:583:G:C8	2.45	0.52
5:2F:7:TYR:O	5:2F:21:ALA:HA	2.10	0.52
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	1.92	0.52
1:1A:2732:G:H3'	1:1A:2733:A:O4'	2.10	0.51
3:1D:34:VAL:HB	3:1D:61:LEU:HD23	1.92	0.51
9:1N:21:LYS:NZ	9:1N:140:VAL:OXT	2.34	0.51
1:2A:2258:C:O2'	1:2A:2427:C:OP2	2.23	0.51
1:2A:251:A:C5	1:2A:252:G:H1'	2.45	0.51
1:2A:856:C:H2'	1:2A:857:C:C6	2.45	0.51
6:2G:104:GLU:O	6:2G:108:ASN:ND2	2.34	0.51
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.92	0.51
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.28	0.51
1:1A:2142:C:O2	1:1A:2149:G:N1	2.31	0.51
3:1D:38:LYS:NZ	3:1D:39:LYS:O	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.92	0.51
19:1X:72:LYS:NZ	19:1X:75:ASP:OD1	2.42	0.51
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.42	0.51
1:2A:127:A:H5''	1:2A:128:C:O4'	2.09	0.51
1:2A:1482:G:H2'	1:2A:1484:G:H8	1.75	0.51
1:2A:2299:G:H2'	1:2A:2300:G:C8	2.44	0.51
1:2A:2441:C:OP2	1:2A:2586:C:O2'	2.26	0.51
1:2A:2652:C:H42	1:2A:2668:G:H1	1.57	0.51
1:1A:2600:A:H2'	1:1A:2601:C:C6	2.45	0.51
1:1A:602:G:O2'	1:1A:655:A:N6	2.43	0.51
1:2A:570:G:H2'	1:2A:2030:A:C5	2.45	0.51
1:2A:2399:G:H2'	1:2A:2400:G:O4'	2.11	0.51
1:2A:718:A:H3'	1:2A:719:C:H6	1.75	0.51
1:1A:1187:G:OP1	17:1V:81:TYR:OH	2.26	0.51
1:1A:2447:G:N2	1:1A:2450:A:OP2	2.42	0.51
1:1A:746:A:O2'	1:1A:2611:U:O2'	2.21	0.51
1:1A:90:U:H1'	1:1A:92:A:C8	2.46	0.51
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.92	0.51
1:2A:340:A:H2'	1:2A:341:G:O4'	2.11	0.51
1:2A:724:U:H2'	1:2A:725:G:O4'	2.09	0.51
6:2G:122:PRO:HB3	6:2G:170:ARG:HH12	1.74	0.51
1:1A:1594:G:H2'	1:1A:1595:G:O4'	2.11	0.51
15:1T:16:ARG:NH2	15:1T:83:ILE:O	2.43	0.51
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.91	0.51
12:1Q:137:TYR:HB3	21:1Z:76:LEU:HD21	1.93	0.51
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.27	0.51
3:2D:37:LEU:HD23	3:2D:60:ARG:HG3	1.93	0.51
8:1I:65:ALA:O	8:1I:69:LYS:N	2.44	0.51
11:1P:106:LEU:HD22	11:1P:112:LEU:HG	1.92	0.51
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.10	0.51
1:2A:1227:G:OP1	16:2U:13:LYS:NZ	2.32	0.51
1:2A:79:G:H2'	1:2A:80:G:C8	2.46	0.51
1:1A:2711:A:H5''	1:1A:2712:U:H5''	1.92	0.51
2:1B:50:G:OP1	14:1S:63:THR:OG1	2.24	0.51
1:1A:780:G:OP1	3:1D:218:ARG:NH2	2.44	0.51
3:1D:26:LYS:NZ	3:1D:30:GLU:OE1	2.40	0.51
14:1S:15:ARG:HD3	14:1S:25:ARG:HH11	1.76	0.51
19:1X:56:THR:HB	19:1X:77:LYS:HE2	1.91	0.51
23:21:3:LYS:H	23:21:61:ARG:HH12	1.58	0.51
1:2A:1468:C:H42	1:2A:1524:G:H1	1.59	0.51
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2443:C:OP1	5:2F:68:LYS:HD3	2.11	0.51
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.11	0.51
8:2I:77:LEU:HD23	8:2I:78:THR:N	2.26	0.51
12:2Q:47:ILE:HD12	12:2Q:70:PRO:HD3	1.93	0.51
1:1A:2820:A:O2'	1:1A:2821:A:OP1	2.27	0.51
1:1A:78:A:H2'	1:1A:79:G:C8	2.46	0.51
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.43	0.51
8:1I:77:LEU:HD21	8:1I:100:ALA:HB1	1.92	0.51
13:1R:22:ARG:HG2	13:1R:69:ASP:HB3	1.91	0.51
15:1T:46:GLU:H	15:1T:65:LYS:HZ3	1.59	0.51
1:2A:1154:G:OP2	16:2U:58:ARG:NE	2.36	0.51
1:2A:1226:A:OP1	17:2V:84:LYS:NZ	2.23	0.51
1:2A:2643:G:H2'	1:2A:2644:G:O4'	2.11	0.51
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	1.92	0.51
22:10:23:VAL:HG22	22:10:38:VAL:HG22	1.92	0.51
1:1A:2602:A:C8	22:10:3:His:HE1	2.27	0.51
28:16:8:LYS:HD3	30:18:34:TRP:CD2	2.46	0.51
1:1A:1173:G:H22	1:1A:1177:A:P	2.34	0.51
1:1A:300:A:OP1	20:1Y:86:ARG:NH2	2.44	0.51
1:1A:833:U:H2'	1:1A:834:C:C6	2.61	0.51
1:1A:728:G:H5''	3:1D:13:ARG:HH21	1.75	0.51
28:26:40:CYS:O	28:26:44:ARG:N	2.44	0.51
1:2A:86:C:O2'	1:2A:104:U:O2'	2.28	0.51
1:2A:118:A:H5'	1:2A:119:A:H8	1.75	0.51
1:2A:1436:G:H1	1:2A:1556:C:H42	1.59	0.51
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.46	0.51
1:2A:1568:G:H5'	3:2D:60:ARG:HA	1.92	0.51
6:2G:50:ALA:HB1	6:2G:52:ILE:H	1.75	0.51
1:1A:1201:C:H2'	1:1A:1202:C:H6	1.76	0.51
1:1A:1480:G:H1	1:1A:1511:C:H42	1.59	0.51
1:1A:210:C:H2'	1:1A:211:A:C8	2.46	0.51
1:1A:991:C:O2'	17:1V:85:LYS:NZ	2.43	0.51
6:1G:111:LEU:HD22	6:1G:120:LEU:HD21	1.93	0.51
11:1P:65:ARG:HG2	11:1P:66:GLY:H	1.75	0.51
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.41	0.51
3:2D:5:LYS:HG2	3:2D:17:THR:HG22	1.92	0.51
18:2W:25:ARG:NH2	18:2W:74:ALA:O	2.25	0.51
1:1A:910:A:N3	1:1A:2264:C:O2'	2.41	0.50
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.76	0.50
4:1E:109:LYS:O	4:1E:111:ARG:NH1	2.45	0.50
1:2A:890:A:H2'	1:2A:892:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:122:THR:HB	7:2H:134:SER:HB2	1.92	0.50
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.08	0.50
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.51	0.50
22:20:27:GLU:HG3	22:20:68:GLU:HA	1.93	0.50
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.93	0.50
1:2A:2298:A:H62	1:2A:2318:G:H8	1.58	0.50
1:2A:253:C:OP2	30:28:5:LYS:NZ	2.37	0.50
1:2A:2552:2MU:OP2	59:2A:5151:HOH:O	2.19	0.50
1:2A:588:U:H1'	5:2F:90:PHE:HB3	1.92	0.50
23:11:11:ARG:HG3	23:11:12:PRO:HD2	1.93	0.50
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.46	0.50
8:1I:75:LEU:HD22	8:1I:105:HIS:HD2	1.76	0.50
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.45	0.50
1:2A:2538:C:H2'	1:2A:2539:C:H6	1.76	0.50
1:2A:712:G:H2'	1:2A:713:G:O4'	2.11	0.50
1:2A:774:A:N3	1:2A:774:A:H2'	2.27	0.50
24:12:38:GLN:HG3	24:12:43:GLN:HB2	1.93	0.50
1:1A:2336:A:H61	22:10:43:THR:HG22	1.75	0.50
5:1F:117:ARG:NH2	11:1P:1:MET:O	2.37	0.50
23:21:73:LEU:HD21	23:21:98:LEU:HD23	1.93	0.50
1:2A:108:U:H2'	1:2A:109:G:C8	2.47	0.50
1:2A:256:A:H2'	1:2A:257:A:H8	1.76	0.50
1:2A:320:A:H4'	1:2A:322:A:C8	2.47	0.50
1:2A:922:U:O2'	22:20:29:GLN:NE2	2.44	0.50
8:2I:41:GLU:HA	8:2I:44:LEU:HB2	1.93	0.50
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	1.94	0.50
1:1A:1064:C:N3	1:1A:1074:G:O6	2.45	0.50
1:1A:1448:G:H5''	1:1A:1542:A:OP2	2.11	0.50
1:1A:2061:G:H2'	1:1A:2501:C:O2'	2.12	0.50
1:1A:1138:G:O2'	9:1N:102:ALA:O	2.29	0.50
1:2A:1434:A:H61	1:2A:1558:A:N6	2.07	0.50
1:2A:144:C:H2'	1:2A:145:G:H8	1.77	0.50
1:2A:1592:C:H2'	1:2A:1593:G:C8	2.46	0.50
1:2A:526:A:O2'	1:2A:2043:C:O2	2.20	0.50
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.93	0.50
1:1A:1065:U:H5''	1:1A:1066:U:OP2	2.10	0.50
1:1A:1983:C:H4'	1:1A:2606:C:H4'	1.94	0.50
1:1A:657:U:H2'	1:1A:658:C:C6	2.47	0.50
8:1I:5:LEU:HD11	8:1I:19:VAL:HG22	1.93	0.50
1:2A:2351:G:O2'	1:2A:2352:A:O5'	2.29	0.50
1:2A:1662:C:H1'	1:2A:2687:U:H5''	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:557:U:H2'	1:2A:558:G:H8	1.76	0.50
1:2A:2785:C:O2'	4:2E:66:HIS:ND1	2.41	0.50
14:2S:34:HIS:ND1	14:2S:53:SER:OG	2.44	0.50
14:2S:94:TYR:CZ	14:2S:99:LYS:HG3	2.46	0.50
1:1A:1230:C:H2'	1:1A:1231:G:C8	2.46	0.50
1:1A:568:U:O5'	1:1A:945:A:N6	2.45	0.50
5:1F:126:VAL:HG11	5:1F:142:TRP:HH2	1.77	0.50
1:2A:1119:C:H2'	1:2A:1120:G:H8	2.24	0.50
1:2A:1674:G:H1	1:2A:1990:C:H42	1.59	0.50
1:2A:2001:A:OP1	13:2R:9:LYS:NZ	2.45	0.50
4:2E:77:ILE:HG12	4:2E:195:LEU:HD22	1.94	0.50
1:1A:242:G:C8	30:18:5:LYS:HG2	2.47	0.50
1:1A:2547:U:O2	10:1O:23:ARG:NH2	2.44	0.50
1:1A:600:G:N2	1:1A:605:C:O3'	2.44	0.50
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	1.93	0.50
5:1F:125:LEU:HD21	5:1F:199:TRP:CD2	2.47	0.50
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.12	0.50
1:2A:2393:A:H2'	1:2A:2394:C:O4'	2.11	0.50
5:2F:40:GLN:HE22	5:2F:183:VAL:H	1.60	0.50
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.33	0.50
1:1A:1680:U:O2'	1:1A:1763:G:N7	2.39	0.50
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.76	0.50
1:1A:711:G:H1	1:1A:720:C:N4	2.08	0.50
1:1A:884:C:H42	1:1A:892:G:H1	1.60	0.50
1:1A:92:A:H2'	1:1A:93:G:H8	1.77	0.50
1:2A:1364:G:C8	23:21:3:LYS:HD2	2.47	0.50
28:26:8:LYS:HG2	30:28:34:TRP:CD1	2.47	0.50
1:2A:1138:G:C6	1:2A:1140:C:H1'	6.41	0.50
1:2A:2233:U:H2'	1:2A:2234:G:C8	2.47	0.50
1:2A:532:A:N6	1:2A:1206:G:O2'	62.58	0.50
1:2A:2482:G:O6	12:2Q:124:LYS:NZ	2.44	0.50
17:2V:18:LEU:HD22	17:2V:20:LEU:HD23	1.93	0.50
18:2W:10:VAL:HG12	18:2W:12:ILE:HG22	1.94	0.50
1:1A:1007:C:N3	1:1A:1022:G:O6	16.77	0.49
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.47	0.49
1:1A:2235:G:H2'	1:1A:2236:C:C6	2.46	0.49
1:1A:2534:A:N7	59:1A:5496:HOH:O	2.32	0.49
59:1A:5034:HOH:O	15:1T:103:ARG:NH1	2.45	0.49
16:1U:88:ILE:HG22	16:1U:90:VAL:HG23	1.94	0.49
30:28:62:LEU:HB3	30:28:65:GLU:HG3	1.92	0.49
1:2A:1689:A:OP2	1:2A:1698:A:N6	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1999:C:H5''	1:2A:2723:C:O2'	2.12	0.49
1:2A:557:U:H2'	1:2A:558:G:C8	2.47	0.49
1:2A:815:C:H2'	1:2A:816:C:H6	1.77	0.49
5:2F:117:ARG:NH2	5:2F:189:THR:O	2.36	0.49
8:2I:77:LEU:HD12	8:2I:101:LEU:HD13	1.93	0.49
6:1G:66:GLN:HE21	6:1G:92:VAL:HG23	1.77	0.49
13:1R:96:ARG:NH2	13:1R:117:VAL:HG13	2.27	0.49
1:1A:1223:G:O6	17:1V:69:LYS:NZ	2.45	0.49
21:1Z:91:LEU:HD23	21:1Z:130:PRO:HB3	1.95	0.49
23:21:83:GLU:N	23:21:83:GLU:OE1	2.45	0.49
28:26:23:THR:OG1	28:26:24:GLU:N	2.43	0.49
1:2A:1003:G:O2'	1:2A:1010:A:N1	2.38	0.49
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.77	0.49
1:2A:2232:U:P	23:21:40:ARG:HH12	2.34	0.49
1:2A:2619:C:OP1	4:2E:152:LYS:HE3	2.12	0.49
1:2A:2756:U:OP2	31:29:19:ARG:NH2	2.45	0.49
1:2A:2816:C:O2	1:2A:2830:G:N2	2.37	0.49
2:2B:42:C:N4	6:2G:91:ARG:HH12	2.09	0.49
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.45	0.49
6:2G:25:TYR:CZ	6:2G:32:PRO:HD3	2.47	0.49
8:2I:110:ASP:OD2	8:2I:113:ARG:N	2.44	0.49
19:2X:31:HIS:HB3	19:2X:34:ALA:HB2	1.94	0.49
20:2Y:37:VAL:N	20:2Y:67:LEU:O	2.38	0.49
31:19:16:VAL:HG22	31:19:25:VAL:HG22	1.95	0.49
1:1A:1038:C:N4	1:1A:1117:G:H1	2.10	0.49
1:1A:1668:A:H4'	1:1A:1669:A:O5'	2.12	0.49
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.45	0.49
1:1A:271(B):C:H42	1:1A:271(V):G:H1	1.59	0.49
1:1A:524:U:H2'	1:1A:525:U:C6	2.47	0.49
1:1A:571:A:O2'	17:1V:78:LYS:HE2	2.11	0.49
1:2A:239:U:H2'	1:2A:240:G:O4'	2.12	0.49
1:2A:2689:U:H4'	1:2A:2690:C:O5'	2.13	0.49
3:2D:8:PRO:HB3	3:2D:14:ARG:HB3	1.94	0.49
1:1A:1057:A:C2	1:1A:1058:G:H1'	2.47	0.49
1:1A:1499:C:H2'	1:1A:1500:G:C8	2.47	0.49
1:1A:652(U):G:H2'	1:1A:652(V):C:C6	2.47	0.49
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.45	0.49
13:1R:33:ARG:HH21	13:1R:113:LEU:HD22	1.76	0.49
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	1.93	0.49
18:1W:68:ARG:NH1	18:1W:112:GLY:H	2.09	0.49
26:24:40:HIS:O	26:24:44:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1792:G:H2'	1:2A:1793:C:C6	2.47	0.49
1:2A:2286:A:OP1	28:26:29:ASN:ND2	2.45	0.49
1:2A:2786:U:H2'	1:2A:2787:C:C6	2.48	0.49
1:2A:35:G:H2'	1:2A:36:G:O4'	2.11	0.49
1:2A:455:C:N4	1:2A:476:G:O6	19.89	0.49
9:2N:39:ARG:HE	9:2N:48:MET:HG2	1.76	0.49
21:2Z:126:VAL:HG13	21:2Z:161:VAL:HG23	1.95	0.49
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.95	0.49
31:19:2:LYS:NZ	31:19:31:LYS:O	2.46	0.49
1:1A:1826:G:H4'	3:1D:242:ARG:CZ	2.43	0.49
1:1A:36:G:N3	1:1A:450:G:O2'	2.45	0.49
1:1A:41:C:H2'	1:1A:42:G:O4'	2.12	0.49
1:1A:829:A:N7	1:1A:2247:A:O2'	2.42	0.49
3:1D:16:MET:HG3	3:1D:207:GLY:HA3	1.95	0.49
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.95	0.49
1:2A:2155:G:C5	1:2A:2156:G:H1'	2.48	0.49
1:2A:1669:A:O2'	1:2A:2549:G:OP1	2.24	0.49
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.44	0.49
1:1A:1055:G:H1	1:1A:1104:C:N4	2.10	0.49
1:1A:1056:G:H5''	1:1A:1057:A:O4'	2.12	0.49
1:1A:272(G):C:N3	1:1A:363(C):G:N2	2.45	0.49
1:1A:971:C:H2'	1:1A:972:G:O4'	2.12	0.49
3:1D:16:MET:HE1	3:1D:208:LYS:HE2	1.93	0.49
5:1F:155:LEU:HD11	5:1F:176:LEU:HD12	1.94	0.49
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	1.94	0.49
21:1Z:21:ALA:O	21:1Z:23:LYS:NZ	2.45	0.49
12:2Q:85:LYS:HE2	22:20:7:LEU:HB2	1.94	0.49
26:24:57:GLU:CB	26:24:58:ARG:HD2	2.42	0.49
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.23	0.49
1:2A:1685:C:H2'	1:2A:1686:C:H6	1.78	0.49
1:2A:2114:A:N6	1:2A:2119:A:N7	2.61	0.49
1:2A:708:C:N4	1:2A:723:G:H1	2.04	0.49
1:2A:784:A:H5'	1:2A:785:G:OP1	2.13	0.49
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.95	0.49
7:2H:3:ARG:HH11	7:2H:4:ILE:H	1.60	0.49
13:2R:79:LEU:HA	13:2R:83:ILE:HD12	1.94	0.49
1:1A:919:G:N2	1:1A:2269:A:OP2	2.45	0.49
1:1A:2470:G:O6	1:1A:2476:A:O2'	2.26	0.49
5:1F:39:TRP:NE1	5:1F:99:TYR:O	2.44	0.49
10:1O:64:ARG:HD3	10:1O:101:PRO:O	2.13	0.49
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:645:C:H5''	1:2A:646:A:OP2	2.13	0.49
1:2A:742:G:H1	1:2A:755:C:H42	1.61	0.49
3:2D:71:ASP:CB	3:2D:103:ARG:HH12	2.25	0.49
4:2E:101:ARG:HB3	4:2E:201:THR:HG21	1.95	0.49
5:2F:64:ILE:HD11	5:2F:75:HIS:HB2	1.95	0.49
6:2G:173:LEU:HB3	6:2G:178:PHE:CD2	2.47	0.49
7:2H:11:VAL:HG13	7:2H:15:VAL:HG13	1.93	0.49
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.13	0.49
26:14:7:PRO:HB2	26:14:27:THR:HG21	1.95	0.49
1:1A:1833:U:O2'	1:1A:1969:A:N1	2.34	0.49
1:1A:472:A:H2'	1:1A:473:G:O4'	4.50	0.49
4:1E:127:ASP:HA	4:1E:135:HIS:HD1	1.77	0.49
8:1I:72:LEU:HD22	8:1I:140:LEU:HD21	1.93	0.49
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	1.93	0.49
1:1A:2405:G:H5''	11:1P:75:ILE:HG21	1.95	0.49
1:2A:1612:C:O2'	29:27:5:TRP:O	2.25	0.49
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.31	0.49
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.27	0.49
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.46	0.49
3:2D:175:LEU:HD12	3:2D:185:VAL:HG21	1.95	0.49
7:2H:150:ALA:HA	7:2H:153:LYS:HG2	1.95	0.49
8:2I:101:LEU:HG	8:2I:107:VAL:HB	1.95	0.49
1:1A:2593:U:H2'	1:1A:2594:C:C6	2.47	0.49
1:1A:628:G:H2'	1:1A:629:G:C8	2.48	0.49
1:2A:122:G:OP1	1:2A:149:A:O2'	2.31	0.49
1:2A:1550:C:OP1	1:2A:1720:U:O2'	2.25	0.49
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.31	0.49
1:2A:361:G:O2'	1:2A:362:U:H5'	2.13	0.49
1:2A:718:A:H3'	1:2A:719:C:C6	2.47	0.49
1:1A:1205:U:H2'	1:1A:1206:G:C8	5.30	0.49
1:1A:1321:A:H2'	1:1A:1322:A:C8	2.48	0.49
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.48	0.49
1:1A:252:G:OP1	11:1P:50:ARG:NH1	2.31	0.49
1:1A:2543:G:H2'	1:1A:2544:G:C8	2.48	0.49
1:1A:2629:A:H1'	1:1A:2630:G:H5''	1.95	0.49
1:1A:473:G:H2'	1:1A:474:G:C8	3.25	0.49
15:1T:35:LYS:HG3	15:1T:40:THR:HG22	1.94	0.49
25:23:6:VAL:HG12	25:23:28:LEU:HD11	1.94	0.49
1:2A:1116:C:N4	1:2A:1117:G:O6	2.45	0.49
1:2A:1641:A:H2'	1:2A:1642:G:O4'	2.13	0.49
1:2A:1791:A:H3'	1:2A:1792:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2050:C:N4	1:2A:2051:A:N1	2.60	0.49
1:2A:2405:G:O2'	1:2A:2406:U:OP1	2.27	0.49
1:2A:62:C:H42	1:2A:93:G:H1	1.61	0.49
2:2B:18:G:H2'	2:2B:19:G:H8	1.77	0.49
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.13	0.49
1:1A:1653:G:H3'	13:1R:2:ARG:HD3	1.95	0.48
1:1A:1711:C:H2'	1:1A:1712:C:C6	2.47	0.48
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.48	0.48
1:1A:831:G:N2	11:1P:53:GLY:O	2.46	0.48
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.48	0.48
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.48	0.48
1:2A:2313:C:H2'	1:2A:2314:C:C6	2.47	0.48
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.12	0.48
11:2P:92:GLU:OE2	11:2P:121:LYS:NZ	2.31	0.48
1:2A:2845:G:H5''	15:2T:54:ARG:O	2.13	0.48
24:12:25:VAL:HG11	24:12:61:LEU:HD21	1.94	0.48
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.95	0.48
1:2A:1356:G:H2'	1:2A:1357:U:O4'	2.12	0.48
1:2A:154(A):C:H42	1:2A:171:G:H1	1.62	0.48
1:2A:2295:C:H41	14:2S:13:ARG:NH1	2.11	0.48
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.28	0.48
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.95	0.48
7:2H:17:VAL:HG22	7:2H:26:VAL:HG13	1.95	0.48
8:2I:93:THR:HG23	8:2I:119:PRO:HG3	1.94	0.48
14:2S:12:PHE:O	14:2S:16:ASN:ND2	2.46	0.48
5:1F:110:LEU:HA	5:1F:183:VAL:HG12	1.95	0.48
14:1S:106:ARG:HG3	14:1S:112:PHE:CE2	2.48	0.48
16:1U:29:SER:OG	16:1U:30:LYS:NZ	2.43	0.48
19:1X:94:GLY:N	19:1X:95:LEU:HB2	2.28	0.48
28:26:34:LEU:H	28:26:51:GLU:HG2	1.76	0.48
1:2A:1207:C:H2'	1:2A:1208:C:C6	2.48	0.48
1:2A:2018:G:H2'	1:2A:2019:A:O4'	2.12	0.48
1:2A:2343:C:O2'	1:2A:2373:G:O2'	2.24	0.48
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.13	0.48
1:2A:2376:A:H3'	1:2A:2377:A:H8	1.78	0.48
9:2N:35:ARG:HB3	9:2N:37:LYS:HG3	1.94	0.48
1:2A:997:G:H5''	16:2U:92:ARG:HH12	1.79	0.48
1:1A:2263:C:N4	22:10:15:ASP:OD1	2.44	0.48
1:1A:1002:G:H3'	1:1A:1003:G:C4'	4.86	0.48
1:1A:143(A):C:H2'	1:1A:144:C:H6	1.78	0.48
1:1A:1471:A:OP2	1:1A:1519:G:N1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2124:G:H1	1:1A:2174:C:H42	1.60	0.48
1:1A:2162:G:H1'	1:1A:2173:A:H1'	1.96	0.48
1:1A:270:A:OP2	1:1A:271(X):G:N2	2.41	0.48
1:1A:301:G:H1'	1:1A:302:C:C6	2.49	0.48
1:1A:639:U:H2'	1:1A:640:C:C6	2.48	0.48
2:1B:45:A:O4'	6:1G:95:ARG:NH1	2.47	0.48
12:1Q:109:VAL:HG12	12:1Q:113:GLN:HB3	1.94	0.48
1:2A:1745:C:H2'	1:2A:1745(A):C:O4'	2.14	0.48
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.46	0.48
1:2A:411:G:OP2	1:2A:2406:U:O2'	2.31	0.48
1:2A:747:U:O2	1:2A:2014:A:H1'	2.13	0.48
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.47	0.48
12:2Q:20:ALA:HB2	21:2Z:79:ARG:HG2	1.95	0.48
24:12:51:ARG:O	24:12:55:ARG:HG3	2.13	0.48
1:1A:1182:A:H2'	1:1A:1183:G:C8	2.49	0.48
1:1A:1509(A):A:H3'	1:1A:1509(B):A:C8	2.48	0.48
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.78	0.48
29:27:34:ARG:HE	29:27:42:LEU:HA	1.78	0.48
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.12	0.48
1:2A:2370:G:C6	1:2A:2371:G:C6	3.02	0.48
1:2A:2659:G:N2	1:2A:2662:A:OP2	2.46	0.48
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.46	0.48
1:2A:848:G:H2'	1:2A:849:A:H8	1.76	0.48
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.44	0.48
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.13	0.48
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.28	0.48
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.31	0.48
1:1A:582:G:H2'	1:1A:583:G:C8	2.49	0.48
1:1A:624:C:O2'	1:1A:657:U:OP1	2.30	0.48
1:1A:784:A:H5'	1:1A:785:G:OP1	2.13	0.48
1:1A:879:G:O5'	1:1A:879:G:H8	1.97	0.48
10:1O:19:ILE:HG22	10:1O:43:VAL:HA	1.95	0.48
1:2A:1324:G:H1	1:2A:1330:C:H42	1.62	0.48
1:2A:171:G:H2'	1:2A:172:C:C6	2.49	0.48
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.47	0.48
1:2A:510:C:H2'	1:2A:511:U:O4'	2.14	0.48
1:2A:652(A):A:H2'	1:2A:652(A):A:N3	2.27	0.48
2:2B:105:A:H2'	2:2B:106:G:O4'	2.14	0.48
1:2A:297:C:H5''	20:2Y:87:LYS:HG3	1.95	0.48
21:2Z:24:LEU:HD12	21:2Z:25:PRO:HD2	1.94	0.48
25:13:18:ASP:OD1	25:13:18:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.49	0.48
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.48	0.48
1:1A:1850:G:H1	1:1A:1892:C:H42	1.61	0.48
1:1A:196:A:N3	1:1A:196:A:H2'	2.29	0.48
1:1A:188:G:H1	1:1A:208:C:H42	1.61	0.48
1:1A:2299:G:H2'	1:1A:2300:G:H8	1.78	0.48
1:1A:2660:A:H2'	1:1A:2661:G:O4'	2.14	0.48
1:1A:2735:G:H2'	1:1A:2736:G:C8	2.49	0.48
1:1A:279:C:H42	1:1A:361:G:H1	1.61	0.48
2:1B:74:U:H2'	2:1B:75:G:O4'	2.13	0.48
1:2A:2127:G:C6	1:2A:2161:C:C4	3.02	0.48
1:2A:256:A:H2'	1:2A:257:A:C8	2.49	0.48
1:2A:329:G:N7	20:2Y:71:LYS:NZ	2.59	0.48
1:2A:113:G:O2'	1:2A:354:G:H5'	47.29	0.48
1:2A:740:U:H2'	1:2A:741:G:C8	2.49	0.48
6:2G:15:VAL:HG21	6:2G:176:LEU:HD23	1.94	0.48
6:2G:44:GLY:O	6:2G:47:LYS:HG3	2.14	0.48
21:2Z:92:SER:O	21:2Z:130:PRO:HG2	2.13	0.48
1:1A:1047:G:HO2'	1:1A:1048:A:H8	1.61	0.48
1:1A:1112:G:H2'	1:1A:1113:U:C6	2.48	0.48
1:1A:1418:G:O2'	1:1A:1580:A:N6	2.44	0.48
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.14	0.48
1:1A:2633:G:H2'	1:1A:2634:G:O4'	2.13	0.48
1:1A:2867:G:OP2	15:1T:119:LYS:NZ	2.32	0.48
1:1A:897:C:H2'	1:1A:898:C:C6	2.49	0.48
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.48	0.48
15:1T:49:VAL:HG12	15:1T:63:VAL:HG22	1.94	0.48
21:1Z:67:LEU:HB3	21:1Z:90:VAL:HG13	1.96	0.48
1:2A:1364:G:OP1	23:21:2:SER:HA	2.14	0.48
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.14	0.48
1:2A:1860:G:H2'	1:2A:1861:G:H8	1.79	0.48
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.13	0.48
1:2A:824:A:H2'	1:2A:825:C:O4'	2.14	0.48
2:2B:106:G:H5'	21:2Z:31:ARG:HG2	1.96	0.48
18:2W:77:ASP:HB2	18:2W:102:HIS:HB2	1.95	0.48
1:1A:1358:G:O2'	1:1A:1373:A:N6	2.47	0.48
1:1A:747:U:O2	1:1A:2014:A:H1'	2.14	0.48
1:1A:483:A:O3'	20:1Y:50:ARG:HA	2.14	0.48
12:1Q:2:LEU:HD22	12:1Q:69:PHE:CE1	2.49	0.48
1:2A:1614:A:P	1:2A:1614:A:H8	2.35	0.48
1:2A:2820:A:C8	4:2E:109:LYS:HE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:140:LEU:HD12	5:2F:140:LEU:H	1.79	0.48
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.13	0.48
1:1A:383:U:H2'	1:1A:385:C:H5	1.78	0.48
14:1S:69:VAL:HG13	14:1S:101:LEU:HG	1.96	0.48
25:23:6:VAL:N	25:23:35:ARG:O	2.39	0.48
1:2A:336:C:H2'	1:2A:337:C:C6	2.66	0.48
3:2D:242:ARG:HG2	3:2D:242:ARG:H	1.39	0.48
7:2H:149:ARG:HD3	7:2H:164:TYR:CE2	2.49	0.48
14:2S:26:LEU:HD22	14:2S:87:PHE:HD1	1.79	0.48
24:12:18:PRO:O	24:12:22:GLU:HG3	2.14	0.47
1:1A:1062:G:H1'	1:1A:1088:A:C8	2.49	0.47
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.30	0.47
1:1A:700:G:O2'	1:1A:1632:A:N3	2.43	0.47
1:1A:302:C:H42	1:1A:315:G:H1	1.62	0.47
17:1V:77:ALA:O	17:1V:79:VAL:N	2.47	0.47
20:1Y:8:LYS:HD3	20:1Y:97:ARG:NH2	2.28	0.47
21:1Z:55:HIS:HE1	21:1Z:135:GLU:HG3	1.78	0.47
23:21:50:ARG:HD2	23:21:57:GLU:OE2	2.14	0.47
27:25:16:ARG:HG3	27:25:17:ASP:N	2.29	0.47
1:2A:1016:G:H2'	1:2A:1017:G:O4'	2.15	0.47
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.95	0.47
23:11:12:PRO:HB2	23:11:41:ARG:HH21	1.79	0.47
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.14	0.47
1:1A:1999:C:H5''	1:1A:2723:C:O2'	2.15	0.47
1:1A:682:G:O6	1:1A:708:C:N4	67.97	0.47
6:1G:47:LYS:HD3	6:1G:80:PHE:O	2.13	0.47
7:1H:86:GLU:HB2	7:1H:165:ALA:HB2	1.96	0.47
8:1I:109:ILE:HD12	8:1I:109:ILE:HA	1.66	0.47
12:1Q:75:THR:HG21	12:1Q:87:LYS:HE2	1.95	0.47
18:1W:11:ARG:C	18:1W:11:ARG:HH11	2.18	0.47
1:2A:1472:A:H2'	1:2A:1473:G:O4'	2.14	0.47
1:2A:783:A:H8	1:2A:1778:U:O2'	1.97	0.47
1:2A:1814:G:OP1	3:2D:40:THR:OG1	2.24	0.47
1:2A:827:U:O2'	1:2A:2068:U:C2	2.63	0.47
1:2A:459:U:H2'	1:2A:460:A:H8	1.79	0.47
1:2A:536:A:H5'	16:2U:53:ARG:HD2	1.96	0.47
1:2A:946:G:H2'	1:2A:947:G:C8	2.49	0.47
1:2A:773:U:O2'	3:2D:48:ARG:HD3	2.14	0.47
8:2I:88:ILE:HG22	8:2I:90:GLY:N	2.28	0.47
1:2A:1262:A:OP2	18:2W:97:LYS:NZ	2.48	0.47
19:2X:65:ARG:HB2	19:2X:70:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1720:U:H2'	1:1A:1721:G:O4'	2.15	0.47
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.14	0.47
12:1Q:50:ALA:HB1	12:1Q:121:ALA:HB1	1.96	0.47
14:1S:25:ARG:HH21	14:1S:40:ILE:HG21	1.79	0.47
1:2A:1021:A:H62	1:2A:1141:U:H3	1.61	0.47
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.14	0.47
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.14	0.47
1:2A:907:U:H4'	12:2Q:101:ARG:HH22	1.79	0.47
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.12	0.47
10:2O:88:ASN:HD21	10:2O:92:GLU:HB2	1.80	0.47
18:2W:76:VAL:HG22	18:2W:103:ILE:HG23	1.96	0.47
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.95	0.47
1:1A:1628:G:H2'	1:1A:1629:U:C6	2.50	0.47
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.49	0.47
1:1A:287:C:H2'	1:1A:288:C:H6	1.78	0.47
1:1A:222:A:H5''	1:1A:421:U:OP1	2.14	0.47
4:1E:16:ARG:NH1	4:1E:171:GLU:OE2	2.42	0.47
1:1A:2296:U:OP2	14:1S:9:ARG:NH2	2.47	0.47
12:1Q:138:ASP:OD2	21:1Z:81:ARG:NH1	2.48	0.47
1:2A:1202:C:H42	1:2A:1243:G:H1	1.62	0.47
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.50	0.47
1:2A:1637:A:H4'	1:2A:2711:A:O2'	2.14	0.47
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.14	0.47
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.96	0.47
1:1A:1410:G:H2'	1:1A:1411:C:C6	3.02	0.47
1:1A:628:G:H2'	1:1A:629:G:H8	1.78	0.47
1:1A:884:C:C4	1:1A:885:C:H1'	2.49	0.47
1:1A:252:G:P	11:1P:50:ARG:HH12	2.36	0.47
11:1P:68:GLN:OE1	30:18:12:LYS:HG2	2.15	0.47
25:23:50:VAL:O	25:23:54:VAL:HG12	2.15	0.47
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.14	0.47
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.49	0.47
1:2A:917:A:H5'	1:2A:918:A:OP2	2.15	0.47
1:2A:2786:U:O2'	4:2E:62:PRO:O	2.23	0.47
17:2V:37:VAL:O	17:2V:52:VAL:HG22	2.14	0.47
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.15	0.47
1:1A:1046:A:N6	1:1A:1211:U:O2	142.09	0.47
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.49	0.47
1:1A:795:C:H2'	1:1A:796:C:C6	2.50	0.47
1:1A:812:C:H5''	1:1A:1250:G:O2'	2.14	0.47
1:1A:784:A:C5	3:1D:229:VAL:HG21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:101:PRO:HA	21:1Z:123:ASP:HA	1.96	0.47
24:22:1:MET:HG3	24:22:52:ASP:OD2	2.14	0.47
1:2A:104:U:H3'	1:2A:105:C:H6	1.80	0.47
1:2A:962:G:H4'	1:2A:2496:C:O2'	2.14	0.47
1:2A:2807:G:N2	1:2A:2893:G:O6	2.46	0.47
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.37	0.47
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	1.95	0.47
6:2G:131:TYR:CE2	6:2G:133:LEU:HD23	2.50	0.47
13:2R:42:LYS:HB3	13:2R:45:ARG:HH21	1.78	0.47
1:2A:480:A:O2'	20:2Y:46:LYS:O	2.22	0.47
27:15:49:CYS:O	27:15:56:LYS:HE3	2.15	0.47
1:1A:1186:G:C2	1:1A:1187:G:H1'	2.50	0.47
1:1A:1466:G:HO2'	1:1A:1546:C:HO2'	1.61	0.47
1:1A:581:C:OP1	16:1U:31:SER:OG	2.31	0.47
1:1A:603:A:O4'	1:1A:655:A:N6	2.47	0.47
1:1A:686:G:N2	1:1A:788:A:H61	2.12	0.47
1:1A:728:G:H4'	3:1D:13:ARG:HE	1.79	0.47
9:1N:16:ILE:HG21	9:1N:26:LEU:HD11	1.97	0.47
18:1W:80:PRO:O	18:1W:100:THR:OG1	2.32	0.47
1:2A:2096:U:H3	1:2A:2193:G:H1	1.61	0.47
4:2E:116:VAL:HG21	4:2E:138:PRO:HB3	1.96	0.47
8:2I:26:ALA:HA	8:2I:30:LEU:HB2	1.95	0.47
8:2I:5:LEU:H	8:2I:5:LEU:HD12	1.78	0.47
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.15	0.47
17:2V:55:ALA:HA	17:2V:101:GLY:H	1.80	0.47
12:2Q:138:ASP:OD2	21:2Z:81:ARG:NH1	2.48	0.47
26:14:40:HIS:O	26:14:44:THR:HG22	2.14	0.47
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.15	0.47
1:1A:2532:G:O2'	1:1A:2657:A:N1	2.42	0.47
1:1A:540:C:H2'	1:1A:541:C:C6	2.50	0.47
1:1A:883:G:H2'	1:1A:884:C:C5	2.50	0.47
16:1U:112:ARG:HD2	17:1V:47:VAL:HG11	1.97	0.47
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.50	0.47
1:2A:2382:G:H21	30:28:42:ARG:CZ	2.28	0.47
1:2A:30:G:H2'	1:2A:31:C:C6	2.50	0.47
6:2G:11:TYR:OH	6:2G:16:ARG:NH1	2.47	0.47
21:2Z:55:HIS:CE1	21:2Z:135:GLU:HG3	2.50	0.47
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.49	0.47
1:1A:2171:A:O2'	1:1A:2172:U:H5"	2.14	0.47
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.49	0.47
1:1A:2404:C:OP2	59:1A:5126:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:287:C:H2'	1:1A:288:C:C6	2.49	0.47
1:1A:192:C:O2'	1:1A:802:A:N3	2.40	0.47
1:1A:811:U:H2'	11:1P:21:ARG:HA	1.96	0.47
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.15	0.47
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.96	0.47
1:1A:444:C:H4'	5:1F:49:ALA:HB2	1.97	0.47
1:2A:1152:C:H2'	1:2A:1153:C:H6	1.80	0.47
1:2A:1308:A:H2'	1:2A:1309:G:O4'	2.15	0.47
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.79	0.47
1:2A:1971:A:H5'	1:2A:1972:A:H5''	1.97	0.47
1:2A:2166:G:H5'	1:2A:2167:U:OP2	2.15	0.47
1:2A:271(F):C:H2'	1:2A:271(G):C:C6	2.50	0.47
1:2A:538:G:H2'	1:2A:539:G:H8	1.80	0.47
3:2D:273:ARG:HG2	3:2D:274:ARG:H	1.79	0.47
9:2N:123:TYR:CZ	9:2N:129:PRO:HD2	2.49	0.47
16:2U:19:LYS:HA	16:2U:22:LYS:HG3	1.95	0.47
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.29	0.47
1:1A:1060:U:H3	1:1A:1062:G:HO2'	1.61	0.47
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.49	0.47
1:1A:779:U:OP1	3:1D:49:ILE:HG13	2.15	0.47
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.28	0.47
4:1E:1:MET:HE3	4:1E:199:ARG:HB3	1.97	0.47
9:1N:103:VAL:HG11	9:1N:120:LEU:HD22	1.96	0.47
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.49	0.47
1:1A:2393:A:H5''	11:1P:63:PRO:HB3	1.97	0.47
21:1Z:155:LEU:HD12	21:1Z:155:LEU:HA	1.75	0.47
28:26:11:LEU:HD12	28:26:21:TYR:HB2	1.96	0.47
1:2A:108:U:H2'	1:2A:109:G:H8	1.80	0.47
1:2A:154(A):C:N4	1:2A:171:G:H1	2.12	0.47
1:2A:2098:U:H2'	1:2A:2099:U:O4'	2.14	0.47
1:2A:850:C:H5''	25:23:18:ASP:HB2	1.97	0.47
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.48	0.47
1:1A:1409:C:H2'	1:1A:1410:G:C8	2.50	0.47
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.29	0.47
1:1A:247:G:H4'	1:1A:386:G:C5	2.50	0.47
1:1A:2695:C:H2'	1:1A:2696:U:C6	2.50	0.47
1:1A:2633:G:H5''	1:1A:2812:G:H5'	1.97	0.47
2:1B:18:G:H2'	2:1B:19:G:C8	2.49	0.47
9:1N:23:LEU:HA	9:1N:60:ILE:HD11	1.96	0.47
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.50	0.47
1:2A:1449:A:H2	1:2A:1529:G:H1'	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.50	0.47
1:2A:286:C:H2'	1:2A:287:C:C6	2.50	0.47
1:2A:348:G:H2'	1:2A:349:G:H8	1.80	0.47
1:2A:879:G:H2'	1:2A:879:G:N3	2.30	0.47
14:2S:62:LYS:HD3	14:2S:97:ARG:HD2	1.97	0.47
15:2T:26:ASP:O	15:2T:49:VAL:HG22	2.15	0.47
15:2T:83:ILE:HD13	15:2T:86:ILE:HD11	1.96	0.47
1:1A:72:U:H5'	24:12:61:LEU:HD12	1.98	0.46
1:1A:1424:G:H2'	1:1A:1425:G:O4'	2.15	0.46
1:1A:1709:U:H2'	1:1A:1710:C:C6	2.51	0.46
1:1A:1971:A:H5'	1:1A:1972:A:H5''	1.95	0.46
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.15	0.46
1:1A:2136:C:C2	1:1A:2155:G:N2	2.83	0.46
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.39	0.46
5:1F:179:GLU:O	5:1F:205:ARG:NH2	2.48	0.46
8:1I:69:LYS:HG3	8:1I:138:ILE:HG12	1.97	0.46
9:1N:121:LYS:HD3	9:1N:130:HIS:CE1	2.49	0.46
15:1T:26:ASP:OD1	15:1T:120:ARG:NH2	2.46	0.46
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	1.97	0.46
26:24:40:HIS:HB3	26:24:43:TYR:HD2	1.80	0.46
1:2A:140:G:H1'	1:2A:141:A:H2	1.79	0.46
1:2A:1448:G:H5''	1:2A:1542:A:OP1	2.14	0.46
1:2A:2408:U:H2'	1:2A:2409:G:H8	1.80	0.46
1:2A:43:A:H61	1:2A:434:U:H3	1.62	0.46
1:2A:90:U:H1'	1:2A:92:A:N7	2.30	0.46
2:2B:18:G:H2'	2:2B:19:G:C8	2.49	0.46
4:2E:2:LYS:HB2	4:2E:95:ILE:HD12	1.97	0.46
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.15	0.46
1:2A:2658:C:P	7:2H:160:LYS:HZ3	2.38	0.46
1:2A:389:G:N2	11:2P:71:VAL:O	2.38	0.46
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HB3	1.97	0.46
1:2A:1649:G:O2'	13:2R:107:ASP:OD2	2.27	0.46
1:1A:1259:G:H2'	1:1A:1260:G:C8	2.49	0.46
5:1F:53:THR:HG22	5:1F:56:GLU:HG3	1.97	0.46
16:1U:83:LEU:HG	16:1U:88:ILE:HB	1.97	0.46
24:22:35:LEU:HD12	24:22:53:LEU:HD12	1.98	0.46
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.15	0.46
1:2A:2089:U:H2'	1:2A:2090:G:C8	2.50	0.46
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.51	0.46
8:2I:140:LEU:HA	8:2I:140:LEU:HD23	1.74	0.46
21:2Z:24:LEU:N	21:2Z:39:VAL:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:58:ALA:O	24:12:62:THR:OG1	2.27	0.46
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.50	0.46
1:1A:1947:C:H2'	1:1A:1948:G:C8	2.50	0.46
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.15	0.46
1:1A:26:G:C6	1:1A:27:G:N1	2.83	0.46
1:1A:2726:U:O2'	1:1A:2727:G:H8	1.98	0.46
8:1I:140:LEU:HD23	8:1I:140:LEU:HA	1.79	0.46
1:1A:907:U:O2'	12:1Q:101:ARG:NH2	2.48	0.46
20:1Y:28:LYS:N	20:1Y:38:ILE:O	2.43	0.46
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.25	0.46
1:2A:2773:C:OP1	4:2E:166:THR:OG1	2.29	0.46
1:2A:521:G:H2'	1:2A:522:G:H8	1.80	0.46
10:2O:77:ILE:HB	15:2T:74:ARG:HH11	1.80	0.46
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.48	0.46
1:1A:1002:G:C5	1:1A:1003:G:H1'	4.38	0.46
1:1A:1441:G:H2'	1:1A:1442:G:C8	2.49	0.46
1:1A:2396:G:H2'	1:1A:2397:G:H8	1.81	0.46
1:1A:2893:G:H5''	1:1A:2894:G:O4'	2.15	0.46
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.50	0.46
3:1D:76:PRO:HG2	3:1D:98:VAL:HG21	1.98	0.46
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.50	0.46
17:1V:65:GLY:HA3	17:1V:91:TYR:CZ	2.50	0.46
28:26:10:LEU:HD23	28:26:22:ALA:HB2	1.96	0.46
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.51	0.46
1:2A:172:C:H2'	1:2A:173:G:C8	2.48	0.46
1:2A:1800:C:H3'	3:2D:147:LEU:HD22	1.96	0.46
1:2A:1945:G:O6	1:2A:1960:A:N6	2.48	0.46
1:2A:581:C:H2'	1:2A:582:G:C8	2.51	0.46
5:2F:110:LEU:HD21	5:2F:181:LEU:HD23	1.96	0.46
14:2S:15:ARG:O	14:2S:19:LYS:HG3	2.15	0.46
28:16:26:ASN:HB3	28:16:29:ASN:HB2	1.97	0.46
30:18:63:PRO:HG2	30:18:64:TYR:CE2	2.51	0.46
1:1A:222:A:H3'	1:1A:421:U:H5'	1.97	0.46
1:1A:2235:G:H2'	1:1A:2236:C:H6	1.78	0.46
1:1A:2298:A:H2'	1:1A:2299:G:O4'	2.16	0.46
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.15	0.46
1:1A:521:G:H2'	1:1A:522:G:C8	2.51	0.46
7:1H:24:VAL:HG11	7:1H:43:VAL:HG11	1.98	0.46
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.50	0.46
1:2A:2539:C:H4'	31:29:35:ARG:HH21	1.80	0.46
1:2A:1660:C:H2'	1:2A:1661:G:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2842:G:H1	1:2A:2875:C:H42	1.63	0.46
1:2A:427:U:OP1	3:2D:13:ARG:NH1	84.04	0.46
1:2A:652(U):G:H2'	1:2A:652(V):C:O4'	2.15	0.46
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.15	0.46
3:2D:182:LEU:HB2	3:2D:272:ALA:H	1.79	0.46
8:2I:102:SER:O	8:2I:106:GLY:HA2	2.16	0.46
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.15	0.46
1:1A:1614:A:H8	1:1A:1614:A:P	2.39	0.46
1:1A:2391:G:O6	1:1A:2425:A:H8	1.99	0.46
1:1A:671:C:OP2	11:1P:33:ARG:NH2	2.45	0.46
2:1B:6:C:H2'	2:1B:7:G:O4'	2.16	0.46
2:1B:90:A:C5	2:1B:91:C:H1'	2.50	0.46
13:1R:33:ARG:HG2	13:1R:115:GLU:CB	2.45	0.46
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	1.97	0.46
20:1Y:44:ILE:HG23	20:1Y:62:GLU:HB3	1.97	0.46
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.34	0.46
1:2A:1790:C:H2'	1:2A:1791:A:C4	2.50	0.46
1:2A:1861:G:C2	1:2A:1862:G:C8	3.04	0.46
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.40	0.46
2:2B:98:G:H2'	2:2B:99:G:O4'	2.16	0.46
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.98	0.46
9:2N:49:GLY:O	9:2N:119:ARG:NH1	2.48	0.46
1:1A:149:A:H2'	1:1A:150:C:C6	2.91	0.46
1:1A:1540:U:H2'	1:1A:1541:G:O4'	2.15	0.46
1:1A:1307:A:N6	1:1A:1606:G:O2'	2.49	0.46
1:1A:1963:U:H4'	1:1A:1964:G:OP1	2.16	0.46
1:1A:2129:C:N4	1:1A:2159:G:H1	2.13	0.46
7:1H:76:VAL:O	7:1H:80:SER:OG	2.26	0.46
13:1R:44:LEU:HA	13:1R:44:LEU:HD23	1.83	0.46
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	1.97	0.46
20:1Y:55:TYR:N	20:1Y:56:PRO:HD3	2.30	0.46
1:2A:1685:C:H2'	1:2A:1686:C:C6	2.51	0.46
1:2A:271(J):C:O2'	1:2A:271(K):U:OP2	2.27	0.46
1:2A:275:G:H2'	1:2A:276:A:O4'	2.16	0.46
1:2A:6:A:O2'	9:2N:130:HIS:ND1	2.48	0.46
1:2A:2641:G:H5''	9:2N:76:SER:HB3	1.97	0.46
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.49	0.46
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.16	0.46
1:1A:251:A:C5	1:1A:252:G:H1'	2.50	0.46
1:1A:549:G:H2'	1:1A:551:G:O4'	2.15	0.46
1:1A:631:A:OP1	11:1P:65:ARG:NE	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:64:ILE:HD11	5:1F:75:HIS:HB2	1.98	0.46
8:1I:77:LEU:HD13	8:1I:97:ILE:HG23	1.98	0.46
16:1U:89:GLU:O	17:1V:11:GLN:NE2	2.46	0.46
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.51	0.46
1:2A:1171:G:H22	1:2A:1179:C:N4	2.13	0.46
1:2A:1201:C:H2'	1:2A:1202:C:C6	2.50	0.46
1:2A:1777:U:H2'	1:2A:1778:U:C6	2.51	0.46
1:2A:2299:G:N1	1:2A:2318:G:N7	2.64	0.46
1:2A:266:G:H2'	1:2A:266:G:N3	3.09	0.46
1:2A:31:C:H5''	1:2A:1239:G:OP1	2.16	0.46
3:2D:232:PRO:HB3	3:2D:244:ARG:NH2	2.31	0.46
5:2F:158:THR:HB	5:2F:195:ASP:HB3	1.98	0.46
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.98	0.46
1:2A:2265:U:H4'	12:2Q:13:GLN:HE22	1.81	0.46
1:1A:1039:G:H2'	1:1A:1040:C:C6	2.51	0.46
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.16	0.46
1:1A:2420:C:H5'	28:16:54:ILE:HD11	1.98	0.46
1:1A:360:G:H2'	1:1A:361:G:C8	2.51	0.46
1:1A:629:G:H2'	1:1A:630:G:O4'	2.88	0.46
5:1F:116:ASP:OD2	11:1P:1:MET:N	2.41	0.46
14:1S:87:PHE:HB2	14:1S:112:PHE:CD1	2.51	0.46
29:27:13:ALA:HB2	29:27:46:VAL:HG11	1.98	0.46
1:2A:300:A:O2'	1:2A:318:C:O2	2.33	0.46
1:2A:438:G:H2'	1:2A:440:G:C8	2.51	0.46
1:2A:947:G:H2'	1:2A:948:G:H8	1.79	0.46
10:2O:105:GLU:OE1	10:2O:105:GLU:N	2.44	0.46
1:2A:997:G:H5''	16:2U:92:ARG:NH1	2.30	0.46
19:2X:58:HIS:CE1	19:2X:77:LYS:HD2	2.50	0.46
23:11:50:ARG:HG3	23:11:59:THR:HG22	1.97	0.46
1:1A:1186:G:H2'	1:1A:1187:G:O4'	2.16	0.46
1:1A:1311:G:N7	29:17:9:ARG:NH2	2.59	0.46
1:1A:190:A:N3	1:1A:679:C:O2'	2.42	0.46
1:1A:2577:A:H2'	1:1A:2614:A:N6	2.31	0.46
2:1B:24:G:N7	2:1B:56:G:H2'	2.30	0.46
13:1R:100:LEU:HD11	13:1R:113:LEU:HD23	1.98	0.46
1:2A:686:G:H8	29:27:6:GLN:O	1.99	0.46
2:2B:24:G:N7	2:2B:56:G:H2'	2.31	0.46
6:2G:33:ARG:NH2	6:2G:162:THR:HG21	2.31	0.46
9:2N:23:LEU:HA	9:2N:60:ILE:HD11	1.98	0.46
1:2A:252:G:P	11:2P:50:ARG:HH22	2.39	0.46
1:1A:1826:G:OP1	3:1D:224:ALA:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1916:A:H2'	1:1A:1917:PSU:H6	1.80	0.45
1:1A:2014:A:H2'	1:1A:2015:A:C8	2.51	0.45
1:1A:748:G:C8	18:1W:89:ALA:HB1	2.51	0.45
4:1E:170:LEU:HB3	4:1E:184:VAL:HG22	1.97	0.45
4:1E:9:VAL:HG22	4:1E:25:VAL:HB	1.97	0.45
1:1A:2060:A:H62	5:1F:74:ARG:HH12	1.64	0.45
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.51	0.45
9:1N:15:LEU:HB2	9:1N:135:PRO:HB2	1.98	0.45
1:2A:1015:G:H1	1:2A:1147:C:H42	1.63	0.45
1:2A:1529:G:O6	1:2A:1530:C:N4	2.49	0.45
1:2A:1688:U:H2'	1:2A:1698:A:N6	2.31	0.45
1:2A:1703:G:H2'	1:2A:1704:G:C8	2.51	0.45
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.81	0.45
1:2A:2185:C:H2'	1:2A:2186:G:O4'	2.15	0.45
1:2A:2238:G:N3	1:2A:2238:G:H2'	2.31	0.45
1:2A:2287:A:O2'	1:2A:2288:A:H5''	2.15	0.45
1:2A:2390:U:P	30:28:35:GLN:HE22	2.39	0.45
1:2A:2396:G:C2	1:2A:2421:G:C6	3.04	0.45
1:2A:2538:C:H2'	1:2A:2539:C:C6	2.49	0.45
1:2A:492:A:H2'	1:2A:493:G:O4'	2.16	0.45
1:2A:674:G:H2'	1:2A:675:A:C8	5.05	0.45
1:2A:987:G:H1	1:2A:1218:C:N4	45.94	0.45
7:2H:77:LYS:NZ	7:2H:81:GLU:OE1	2.30	0.45
1:2A:1653:G:H3'	13:2R:2:ARG:HB2	1.98	0.45
1:1A:1144:G:C6	1:1A:1145:C:N4	3.18	0.45
1:1A:1174:A:H1'	1:1A:1175:U:H5''	1.98	0.45
1:1A:2128:C:N4	1:1A:2160:G:H1	2.14	0.45
1:1A:2807:G:N2	1:1A:2893:G:O6	2.48	0.45
1:1A:609:A:H2'	1:1A:610:G:O4'	2.28	0.45
1:1A:2875:C:H5''	15:1T:3:ARG:HH22	1.81	0.45
27:25:40:LYS:HD3	27:25:46:CYS:HB2	1.97	0.45
28:26:40:CYS:SG	28:26:42:TRP:HB2	2.55	0.45
1:2A:1152:C:H2'	1:2A:1153:C:C6	2.50	0.45
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.98	0.45
1:2A:764:A:N1	1:2A:1789:A:O2'	2.43	0.45
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.51	0.45
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	1.98	0.45
7:2H:19:VAL:HG13	7:2H:24:VAL:HG12	1.98	0.45
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HG22	1.98	0.45
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.97	0.45
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1365:A:P	23:11:41:ARG:HH22	2.40	0.45
1:1A:1047:G:O2'	1:1A:1048:A:H8	1.99	0.45
1:1A:1145:C:O2	1:1A:1147:C:N4	8.20	0.45
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.50	0.45
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.49	0.45
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.51	0.45
1:1A:396:G:H1'	23:11:42:GLN:HB3	1.99	0.45
26:24:36:CYS:O	26:24:40:HIS:HB2	2.17	0.45
27:25:52:TYR:O	27:25:55:ARG:HG2	2.16	0.45
28:26:38:LYS:HB2	28:26:49:HIS:CD2	2.51	0.45
30:28:34:TRP:CG	30:28:35:GLN:N	2.83	0.45
1:2A:1388:G:H2'	1:2A:1389:G:H8	1.81	0.45
1:2A:2167:U:H3'	1:2A:2168:G:H21	1.81	0.45
1:2A:247:G:H4'	1:2A:386:G:C5	2.51	0.45
1:2A:2515:C:H2'	1:2A:2516:G:C8	2.52	0.45
1:2A:947:G:H2'	1:2A:948:G:C8	2.51	0.45
1:2A:94(A):G:H2'	1:2A:95:G:O4'	2.16	0.45
2:2B:58:A:H2'	2:2B:59:A:O4'	2.16	0.45
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	1.98	0.45
4:2E:105:THR:HG21	4:2E:164:ARG:CZ	2.47	0.45
1:2A:321:G:C4	5:2F:165:ARG:HD2	2.51	0.45
8:2I:77:LEU:HD23	8:2I:104:GLN:HE22	1.79	0.45
21:2Z:97:GLU:HA	21:2Z:126:VAL:O	2.17	0.45
1:1A:1227:G:OP1	16:1U:13:LYS:NZ	2.37	0.45
1:1A:1500:G:H2'	1:1A:1501:C:C6	2.52	0.45
1:1A:2160:G:C6	1:1A:2161:C:N4	2.84	0.45
4:1E:10:GLY:HA2	4:1E:192:ASN:OD1	2.15	0.45
13:1R:33:ARG:HH22	27:15:58:LEU:HB3	1.80	0.45
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.50	0.45
1:2A:1416:G:O2'	1:2A:1417:C:OP2	2.25	0.45
1:2A:1713:U:H2'	1:2A:1714:G:H8	1.80	0.45
1:2A:981:A:HO2'	1:2A:2036:C:HO2'	1.58	0.45
1:2A:2651:C:H2'	1:2A:2652:C:C6	2.51	0.45
1:2A:2731:G:OP1	4:2E:169:ASN:ND2	2.48	0.45
1:2A:365:C:H2'	1:2A:366:C:O4'	2.17	0.45
4:2E:34:VAL:HG22	4:2E:48:GLN:HG2	1.98	0.45
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.97	0.45
7:2H:109:PHE:C	7:2H:111:HIS:H	2.19	0.45
7:2H:157:TYR:CD1	7:2H:172:LYS:HG3	2.51	0.45
12:2Q:43:THR:HA	12:2Q:94:VAL:HG12	1.98	0.45
1:1A:1466:G:H2'	1:1A:1547:C:N4	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1508:A:O2'	1:1A:1509:C:OP1	2.26	0.45
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.48	0.45
1:1A:535:C:O3'	16:1U:53:ARG:NH1	2.48	0.45
1:1A:592:G:O2'	30:18:4:MET:HG3	2.17	0.45
1:1A:863:A:H2'	1:1A:864:G:C8	2.52	0.45
1:1A:2305:A:H5''	6:1G:134:GLY:HA3	1.98	0.45
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.60	0.45
27:25:45:VAL:HG21	27:25:57:VAL:HG11	1.99	0.45
1:2A:1971:A:C4	3:2D:241:PRO:HD3	2.52	0.45
1:2A:2242:G:H2'	1:2A:2243:U:O4'	2.15	0.45
1:2A:271(U):G:H2'	1:2A:271(V):G:C8	2.47	0.45
1:2A:320:A:H4'	1:2A:322:A:N7	2.31	0.45
1:2A:466:A:OP1	29:27:34:ARG:NH1	2.49	0.45
1:2A:732:C:H2'	1:2A:733:G:O4'	2.17	0.45
20:2Y:12:THR:HA	20:2Y:26:LYS:HA	1.97	0.45
24:12:3:LEU:O	24:12:7:ARG:HG3	2.17	0.45
24:12:51:ARG:HD3	24:12:55:ARG:NH1	2.31	0.45
1:1A:1357:U:H2'	1:1A:1358:G:O4'	2.17	0.45
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.16	0.45
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.52	0.45
1:1A:2060:A:N6	5:1F:74:ARG:HH12	2.15	0.45
1:1A:484:C:H2'	1:1A:485:C:C6	2.52	0.45
1:1A:586:A:N1	1:1A:809:G:O2'	2.48	0.45
13:1R:72:ASP:HB3	13:1R:75:LEU:HB3	1.98	0.45
12:2Q:82:ARG:HD2	22:20:4:LYS:HE3	1.99	0.45
28:26:11:LEU:N	28:26:21:TYR:O	2.48	0.45
1:2A:585:G:H2'	1:2A:1251:C:H42	1.82	0.45
1:2A:2152:G:H2'	1:2A:2153:G:O4'	2.17	0.45
1:2A:2236:C:H2'	1:2A:2237:G:O4'	2.17	0.45
1:2A:249:C:O2	30:28:12:LYS:NZ	2.31	0.45
1:2A:2692:C:O2	1:2A:2847:U:O2'	2.29	0.45
1:2A:2848:G:C8	15:2T:97:ALA:HB2	2.51	0.45
1:2A:441:U:H2'	1:2A:442:G:C8	2.51	0.45
1:2A:615:G:H2'	1:2A:616:G:C8	2.51	0.45
6:2G:3:LEU:HD12	6:2G:8:LYS:NZ	2.31	0.45
6:2G:56:ALA:HA	6:2G:59:GLU:HG2	1.99	0.45
7:2H:152:ARG:HD3	7:2H:152:ARG:HA	1.66	0.45
1:1A:1442:G:H2'	1:1A:1442:G:N3	2.78	0.45
1:1A:1537:G:H2'	1:1A:1538:G:H8	1.82	0.45
1:1A:1446:C:O2'	1:1A:1545:A:O2'	2.33	0.45
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2300:G:H2'	1:1A:2301:C:C6	2.52	0.45
1:1A:254:G:H4'	1:1A:384:U:H5'	1.99	0.45
1:1A:2691:C:O3'	1:1A:2871:C:H4'	2.17	0.45
1:1A:2845:G:H5''	15:1T:54:ARG:O	2.16	0.45
1:1A:340:A:H2'	1:1A:341:G:O4'	2.17	0.45
1:1A:40:C:H2'	1:1A:41:C:C6	2.51	0.45
1:1A:700:G:H2'	1:1A:701:G:C8	2.51	0.45
1:1A:875:G:H1	1:1A:902:C:N4	2.15	0.45
16:1U:17:ILE:HG13	16:1U:32:PHE:HE1	1.82	0.45
1:2A:1112:G:H2'	1:2A:1113:U:O4'	2.17	0.45
1:2A:2731:G:H5''	4:2E:203:LYS:HE3	1.99	0.45
5:2F:196:LEU:O	5:2F:200:GLU:N	2.49	0.45
6:2G:11:TYR:CZ	6:2G:16:ARG:HG3	2.52	0.45
9:2N:4:TYR:CZ	9:2N:6:PRO:HA	2.51	0.45
11:2P:97:PRO:HG2	11:2P:128:HIS:HE1	1.80	0.45
14:2S:15:ARG:O	14:2S:19:LYS:N	2.38	0.45
1:2A:2875:C:O2'	15:2T:2:ASN:OD1	2.35	0.45
16:2U:76:TYR:O	16:2U:80:ILE:HG12	2.17	0.45
1:1A:2336:A:H61	22:10:43:THR:CG2	2.30	0.45
1:1A:858:U:O2	1:1A:2268:A:H2'	2.16	0.45
2:1B:61:G:H2'	2:1B:62:C:C6	2.51	0.45
3:1D:109:ASP:N	3:1D:195:ALA:O	2.44	0.45
18:1W:73:ALA:HB3	18:1W:106:ILE:HB	1.99	0.45
1:2A:1510:G:H2'	1:2A:1511:C:C6	2.52	0.45
1:2A:1821:A:OP1	3:2D:201:HIS:NE2	2.39	0.45
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.51	0.45
1:2A:515:A:H1'	1:2A:581:C:H1'	1.98	0.45
6:2G:16:ARG:HH21	6:2G:28:VAL:HB	1.81	0.45
8:2I:116:LEU:HD11	8:2I:119:PRO:HA	1.99	0.45
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.82	0.45
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.17	0.45
16:2U:90:VAL:HG22	17:2V:38:LEU:HB3	1.99	0.45
1:1A:1058:G:N1	1:1A:1080:C:N4	2.55	0.45
1:1A:104:U:H3'	1:1A:105:C:H6	1.81	0.45
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.52	0.45
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.32	0.45
1:1A:236:C:H2'	1:1A:237:C:C6	2.52	0.45
1:1A:2682:U:H5'	4:1E:11:MET:O	2.17	0.45
1:1A:862:G:H2'	1:1A:863:A:O4'	2.16	0.45
1:2A:118:A:H5'	1:2A:119:A:C8	2.51	0.45
1:2A:1442:G:H2'	1:2A:1442:G:N3	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1394:U:H4'	1:2A:1603:A:H4'	1.99	0.45
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.50	0.45
1:2A:2293:C:H2'	1:2A:2294:C:C6	2.51	0.45
2:2B:37:C:O2	14:2S:95:HIS:NE2	2.49	0.45
8:2I:102:SER:HA	8:2I:107:VAL:H	1.80	0.45
8:2I:73:GLU:OE2	8:2I:139:GLN:N	2.47	0.45
10:2O:86:ILE:HG22	10:2O:94:ARG:HD3	1.97	0.45
1:2A:1614:A:N1	18:2W:93:ALA:HB2	2.32	0.45
21:2Z:35:ARG:HD2	21:2Z:35:ARG:HA	1.78	0.45
22:10:68:GLU:HB3	22:10:80:HIS:HB2	1.99	0.45
1:1A:271(H):G:H4'	23:11:81:LYS:HG2	1.99	0.45
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.99	0.45
1:1A:1653:G:N2	59:1A:5103:HOH:O	2.48	0.45
1:1A:34:C:H2'	1:1A:35:G:H8	4.93	0.45
1:1A:649:G:N7	59:1A:5297:HOH:O	2.48	0.45
1:1A:881:G:N2	1:1A:897:C:O2	2.50	0.45
1:1A:910:A:N1	1:1A:2277:G:H1'	2.32	0.45
6:1G:59:GLU:CD	6:1G:153:ARG:HH21	2.20	0.45
8:1I:8:PRO:HD3	8:1I:15:VAL:HB	1.98	0.45
17:1V:20:LEU:HD13	17:1V:22:VAL:HG13	1.99	0.45
19:1X:35:THR:O	19:1X:39:ILE:HG13	2.17	0.45
26:24:18:CYS:SG	26:24:20:ASN:HB2	2.57	0.45
1:2A:1269:A:H2'	1:2A:1270:C:C6	2.52	0.45
1:2A:1422:G:O3'	10:2O:49:ARG:NH1	99.00	0.45
1:2A:197:A:N6	1:2A:2430:A:H2'	2.31	0.45
1:2A:2095:C:H2'	1:2A:2096:U:O4'	2.17	0.45
1:2A:2590:A:H5''	3:2D:239:ARG:HG3	1.98	0.45
1:2A:2717:G:H2'	1:2A:2718:G:O4'	2.16	0.45
1:2A:828:U:H2'	1:2A:829:A:C8	2.52	0.45
7:2H:27:LYS:NZ	7:2H:32:GLU:HB2	2.31	0.45
20:2Y:14:LEU:HB2	20:2Y:75:ILE:HD11	1.98	0.45
1:1A:1721:G:H3'	1:1A:1722:A:H5''	1.99	0.44
1:1A:2114:A:N6	1:1A:2119:A:H62	2.15	0.44
5:1F:40:GLN:NE2	5:1F:183:VAL:HG22	2.32	0.44
8:1I:130:TYR:O	8:1I:138:ILE:N	2.50	0.44
1:2A:1027:A:C6	1:2A:1126:A:C4	3.05	0.44
1:2A:104:U:H3'	1:2A:105:C:C6	2.52	0.44
1:2A:1434:A:H2'	1:2A:1435:G:H8	1.81	0.44
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.81	0.44
1:2A:2340:G:H2'	1:2A:2341:G:H8	1.83	0.44
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:661:C:H2'	1:2A:662:G:H8	1.82	0.44
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.97	0.44
7:2H:24:VAL:HG22	7:2H:35:VAL:HB	1.99	0.44
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.16	0.44
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD23	1.98	0.44
26:14:18:CYS:SG	26:14:20:ASN:HB2	2.56	0.44
1:1A:570:G:H2'	1:1A:2030:A:C5	2.52	0.44
1:1A:335:C:H2'	1:1A:336:C:H6	1.82	0.44
3:1D:260:ARG:NH1	3:1D:267:SER:OG	2.48	0.44
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.55	0.44
19:1X:34:ALA:O	19:1X:77:LYS:NZ	2.48	0.44
1:2A:1846:G:H1	1:2A:1894:C:H42	1.64	0.44
1:2A:398:G:H2'	1:2A:399:G:C8	2.52	0.44
1:2A:892:G:H2'	1:2A:893:C:H4'	1.99	0.44
1:2A:932:G:H4'	1:2A:933:A:O5'	2.17	0.44
4:2E:48:GLN:HE21	4:2E:78:LEU:HB3	1.83	0.44
6:2G:129:GLY:HA3	6:2G:163:ALA:O	2.18	0.44
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.16	0.44
1:2A:2295:C:H5	14:2S:13:ARG:HH12	1.65	0.44
29:17:8:ASN:HB3	29:17:11:LYS:HB3	1.99	0.44
1:1A:1055:G:H2'	1:1A:1056:G:O4'	2.17	0.44
1:1A:1389:G:H2'	1:1A:1390:U:O4'	2.18	0.44
1:1A:2563:U:H4'	10:1O:28:SER:HA	2.00	0.44
1:1A:38:A:H2'	1:1A:39:C:C6	2.52	0.44
1:1A:674:G:O2'	5:1F:67:GLN:NE2	2.47	0.44
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.52	0.44
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	2.00	0.44
6:1G:126:ASP:N	6:1G:130:ASN:O	2.49	0.44
12:1Q:134:ARG:NE	21:1Z:122:ARG:HE	2.15	0.44
23:21:11:ARG:HG3	23:21:12:PRO:HD2	2.00	0.44
1:2A:1614:A:N6	18:2W:92:ARG:O	2.50	0.44
1:2A:2103:C:H1'	1:2A:2187:G:N2	2.33	0.44
1:2A:197:A:O2'	1:2A:2244:U:OP1	2.27	0.44
1:2A:2629:A:H1'	1:2A:2630:G:H5''	1.99	0.44
1:2A:2745:C:O2'	7:2H:139:GLN:O	2.35	0.44
1:2A:601:C:O2	1:2A:605:C:H4'	2.17	0.44
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.99	0.44
6:2G:40:ASN:HD22	6:2G:156:ASP:HB2	1.82	0.44
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	2.00	0.44
12:2Q:37:LEU:HD11	12:2Q:130:LYS:HB2	1.99	0.44
20:2Y:12:THR:OG1	20:2Y:26:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:62:ARG:HD3	26:14:62:ARG:HA	1.47	0.44
30:18:6:THR:HG23	30:18:64:TYR:HD2	1.83	0.44
1:1A:207:A:H2'	1:1A:208:C:O4'	2.17	0.44
1:1A:2365:G:O6	30:18:43:GLN:NE2	2.50	0.44
1:1A:2512:C:H4'	4:1E:122:PHE:CE2	2.52	0.44
1:1A:387:U:P	23:11:20:ARG:HH12	2.40	0.44
1:1A:944:G:O6	1:1A:1337:G:H8	82.81	0.44
4:1E:1:MET:O	4:1E:84:PHE:HB2	2.17	0.44
5:1F:155:LEU:HB2	5:1F:189:THR:HG21	1.99	0.44
6:1G:41:GLN:HG3	6:1G:60:LEU:HD21	1.98	0.44
8:1I:72:LEU:HD23	8:1I:72:LEU:HA	1.82	0.44
11:1P:126:VAL:HA	11:1P:146:VAL:HB	1.98	0.44
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.17	0.44
1:2A:2186:G:H2'	1:2A:2187:G:H8	1.83	0.44
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.17	0.44
1:2A:2722:G:H2'	1:2A:2723:C:C6	2.53	0.44
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.18	0.44
1:2A:82:G:H5''	1:2A:296:C:H5'	1.99	0.44
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	1.98	0.44
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.83	0.44
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.38	0.44
1:1A:127:A:H5''	1:1A:128:C:C6	2.52	0.44
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.83	0.44
1:1A:1713:U:H3	1:1A:1746:G:H1	1.65	0.44
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.18	0.44
1:1A:2319:G:N2	14:1S:3:ARG:HA	2.33	0.44
1:1A:2853:C:H2'	1:1A:2854:G:H8	1.83	0.44
1:1A:603:A:N1	1:1A:625:G:O2'	2.44	0.44
1:1A:717:G:H2'	1:1A:718:A:O4'	2.18	0.44
1:1A:729:G:H2'	1:1A:1775:U:H1'	1.99	0.44
3:1D:35:LYS:HD3	3:1D:64:ILE:HD11	1.98	0.44
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.52	0.44
5:1F:36:VAL:HG12	5:1F:40:GLN:HE21	1.83	0.44
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.66	0.44
16:1U:50:ARG:HH12	17:1V:72:VAL:HA	1.83	0.44
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.52	0.44
22:20:68:GLU:OE1	22:20:82:ARG:HD3	2.17	0.44
28:26:41:PRO:O	28:26:44:ARG:HG3	2.18	0.44
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.53	0.44
1:2A:1598:C:H2'	1:2A:1599:C:C6	2.52	0.44
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:444:C:H2'	1:2A:445:C:H6	1.82	0.44
1:2A:707:G:H1	1:2A:724:U:H3	1.64	0.44
1:2A:827:U:H4'	1:2A:828:U:C6	2.53	0.44
1:2A:923:C:H2'	1:2A:924:C:H6	1.82	0.44
2:2B:6:C:H42	2:2B:115:G:H1	1.64	0.44
5:2F:12:LEU:HB2	5:2F:124:LEU:HD11	1.99	0.44
9:2N:67:LEU:HA	9:2N:87:LEU:HD23	2.00	0.44
26:14:16:CYS:HA	26:14:33:VAL:O	2.17	0.44
27:15:52:TYR:C	27:15:54:GLY:H	2.21	0.44
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.17	0.44
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.53	0.44
1:1A:1790:C:H5''	1:1A:1791:A:OP1	2.18	0.44
1:1A:1891:G:H2'	1:1A:1892:C:C6	2.53	0.44
1:1A:1915:5MU:H73	1:1A:1916:A:N6	2.32	0.44
1:1A:1914:C:H2'	1:1A:1915:5MU:O4'	2.18	0.44
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.52	0.44
1:1A:79:G:C6	1:1A:90:U:C2	28.56	0.44
10:1O:119:PRO:HB2	15:1T:68:TYR:CD2	2.53	0.44
10:1O:86:ILE:HG22	10:1O:94:ARG:HD3	2.00	0.44
1:1A:2319:G:H22	14:1S:3:ARG:HA	1.83	0.44
27:25:59:GLU:HG2	27:25:60:VAL:N	2.32	0.44
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	2.00	0.44
1:2A:136:G:H2'	1:2A:137:C:C6	2.52	0.44
1:2A:2305:A:H5''	6:2G:134:GLY:HA3	2.00	0.44
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.51	0.44
1:2A:717:G:H2'	1:2A:718:A:O4'	2.17	0.44
3:2D:118:VAL:N	3:2D:129:ASN:OD1	2.44	0.44
24:12:22:GLU:HG2	24:12:64:LEU:HD11	2.00	0.44
3:1D:180:GLY:HA3	3:1D:275:LYS:HG2	1.99	0.44
5:1F:13:SER:HB2	5:1F:127:GLU:OE1	2.18	0.44
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.99	0.44
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.50	0.44
22:20:53:MET:HG2	22:20:57:PHE:HA	2.00	0.44
1:2A:1023:U:O2'	1:2A:1122:G:H5'	2.18	0.44
1:2A:1287:A:C5	1:2A:1288:U:C4	3.06	0.44
1:2A:1388:G:H2'	1:2A:1389:G:C8	2.52	0.44
1:2A:1505:C:H2'	1:2A:1506:C:H6	1.82	0.44
1:2A:1497:U:N3	1:2A:1578:U:O5'	2.50	0.44
1:2A:16:G:H5''	27:25:17:ASP:HB2	1.98	0.44
1:2A:182:A:N3	1:2A:433:C:O2'	2.41	0.44
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2527:C:H2'	1:2A:2528:U:O4'	2.17	0.44
1:2A:855:G:H1	1:2A:922:U:H3	1.66	0.44
1:2A:995:C:P	16:2U:53:ARG:HH21	2.41	0.44
2:2B:24:G:H5'	2:2B:25:A:N7	2.33	0.44
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.52	0.44
25:13:5:LYS:NZ	25:13:34:GLU:OE2	2.51	0.44
1:1A:1390:U:H2'	1:1A:1391:U:C6	3.49	0.44
1:1A:1413:G:H2'	1:1A:1414:G:O4'	2.18	0.44
1:1A:2437:U:O2'	1:1A:2438:U:H5'	2.18	0.44
1:1A:2478:A:O2'	1:1A:2536:G:N2	2.51	0.44
1:1A:2756:U:H3	1:1A:2758:A:H62	1.65	0.44
1:1A:28:A:H1'	1:1A:513:A:C2	2.53	0.44
1:1A:753:C:H2'	1:1A:754:C:H6	1.83	0.44
4:1E:119:ARG:HA	4:1E:160:TYR:CD2	2.52	0.44
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.98	0.44
6:1G:5:VAL:HG11	6:1G:101:ILE:HG12	2.00	0.44
10:1O:78:ARG:NH2	15:1T:73:GLU:OE1	2.38	0.44
1:2A:1311:G:OP1	26:24:56:VAL:HG21	162.86	0.44
30:28:26:LYS:HB2	30:28:44:LYS:O	2.18	0.44
1:2A:834:C:H5'	30:28:57:ARG:HH11	1.83	0.44
1:2A:1166:C:H2'	1:2A:1167:U:C6	2.52	0.44
1:2A:2138:C:N4	1:2A:2153:G:N1	2.18	0.44
1:2A:2166:G:H2'	1:2A:2167:U:C6	2.52	0.44
1:2A:2261:C:H1'	1:2A:2388:A:N3	2.33	0.44
1:2A:627:A:H4'	1:2A:628:G:H5'	1.99	0.44
2:2B:33:G:C6	2:2B:34:U:C4	3.06	0.44
5:2F:155:LEU:HD11	5:2F:176:LEU:HD12	1.99	0.44
14:2S:67:ARG:HD3	14:2S:71:ARG:HH12	1.81	0.44
15:2T:77:PRO:HB2	15:2T:80:SER:HB2	1.98	0.44
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.53	0.44
21:2Z:93:ASP:OD1	21:2Z:94:GLU:N	2.50	0.44
1:1A:1374:G:H2'	1:1A:1375:C:C6	2.52	0.44
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.18	0.44
1:1A:1814:G:OP1	3:1D:40:THR:OG1	2.29	0.44
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	2.00	0.44
1:1A:239:U:H2'	1:1A:240:G:O4'	2.18	0.44
1:1A:2774:C:H2'	1:1A:2775:A:O4'	2.17	0.44
1:1A:360:G:H2'	1:1A:361:G:H8	1.83	0.44
1:1A:531:C:H4'	1:1A:532:A:H5"	1.99	0.44
1:1A:987:G:H1	1:1A:1218:C:H42	45.99	0.44
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.99	0.44
11:1P:120:ALA:HB2	11:1P:137:LYS:HB3	2.00	0.44
13:1R:79:LEU:HA	13:1R:83:ILE:HB	1.99	0.44
10:1O:104:ARG:NH2	15:1T:36:GLU:OE2	2.45	0.44
1:2A:1827:C:OP2	3:2D:222:ARG:NH1	2.50	0.44
1:2A:2366:A:H2'	1:2A:2367:G:O4'	2.18	0.44
1:2A:2728:U:H5'	10:2O:70:LYS:NZ	2.33	0.44
1:2A:412:A:N6	1:2A:2412:A:O4'	2.51	0.44
4:2E:79:ARG:HD3	4:2E:79:ARG:HA	1.86	0.44
5:2F:28:ILE:O	5:2F:30:PRO:HD3	2.18	0.44
7:2H:125:VAL:HG13	7:2H:130:ARG:O	2.17	0.44
11:2P:138:LEU:HG	11:2P:143:GLY:HA3	2.00	0.44
14:2S:11:LYS:HG3	14:2S:91:PRO:HD3	1.99	0.44
1:1A:2220:G:H2'	1:1A:2221:G:H8	1.83	0.43
1:1A:2366:A:H2'	1:1A:2367:G:O4'	2.18	0.43
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.18	0.43
1:1A:588:U:O4	1:1A:670:A:H1'	2.18	0.43
7:1H:157:TYR:CE1	7:1H:172:LYS:HG3	2.53	0.43
8:1I:62:LYS:O	8:1I:66:GLU:HG2	2.17	0.43
1:2A:1161:C:H2'	1:2A:1162:G:H8	1.83	0.43
1:2A:2319:G:N2	14:2S:3:ARG:HA	2.33	0.43
1:2A:242:G:C8	30:28:3:LYS:HG3	2.53	0.43
7:2H:18:GLU:HG3	7:2H:25:LYS:O	2.17	0.43
8:2I:114:LEU:HD21	8:2I:128:LEU:HD13	2.00	0.43
9:2N:25:ARG:O	9:2N:29:LYS:HE2	2.18	0.43
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	1.99	0.43
11:2P:90:ARG:NH1	11:2P:105:LEU:HD11	2.33	0.43
11:2P:8:PRO:HB2	11:2P:12:ALA:HB3	1.99	0.43
24:12:25:VAL:HG12	24:12:29:LYS:HD2	2.00	0.43
26:14:56:VAL:HG23	26:14:57:GLU:H	1.83	0.43
28:16:7:ILE:HG13	28:16:9:LEU:HD23	2.00	0.43
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.53	0.43
1:1A:1384:A:N3	1:1A:1405:U:H1'	2.33	0.43
1:1A:1784:A:H4'	1:1A:1785:A:O5'	2.18	0.43
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.53	0.43
1:1A:710:G:H2'	1:1A:711:G:H8	1.83	0.43
1:1A:774:A:N3	1:1A:774:A:H2'	2.34	0.43
1:1A:884:C:C5	1:1A:885:C:H1'	2.53	0.43
5:1F:38:ARG:NH1	5:1F:99:TYR:OH	2.50	0.43
7:1H:3:ARG:HG2	7:1H:6:ARG:HE	1.83	0.43
7:1H:26:VAL:HG12	7:1H:79:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:88:ILE:HG22	8:1I:90:GLY:H	1.82	0.43
11:1P:8:PRO:HB2	11:1P:12:ALA:HB3	2.01	0.43
20:1Y:76:CYS:HA	20:1Y:106:LEU:HD22	2.00	0.43
25:23:7:LYS:O	25:23:54:VAL:HG23	2.18	0.43
1:2A:2351:G:O6	30:28:39:LYS:HG3	2.17	0.43
1:2A:1815:A:OP1	1:2A:1815:A:H8	2.00	0.43
1:2A:2579:C:H2'	1:2A:2580:U:O4'	2.17	0.43
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.00	0.43
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.35	0.43
1:2A:981:A:N1	1:2A:2027:G:O2'	2.43	0.43
5:2F:37:VAL:HG22	5:2F:183:VAL:HG23	2.00	0.43
6:2G:126:ASP:HB3	6:2G:128:ARG:H	1.83	0.43
12:2Q:56:ARG:HD2	12:2Q:56:ARG:HA	1.71	0.43
1:1A:1228:G:H2'	1:1A:1229:G:O4'	2.18	0.43
1:1A:1791:A:H5'	3:1D:206:LEU:HD12	1.99	0.43
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.48	0.43
11:1P:95:VAL:HA	11:1P:99:LEU:HD12	2.01	0.43
24:22:64:LEU:O	24:22:68:ARG:HG3	2.18	0.43
28:26:6:ARG:HH21	28:26:24:GLU:HG3	1.83	0.43
1:2A:1113:U:H2'	1:2A:1114:G:H8	1.82	0.43
1:2A:2774:C:H2'	1:2A:2775:A:O4'	2.18	0.43
1:2A:480:A:OP2	20:2Y:47:LYS:HE3	2.17	0.43
1:2A:68:G:H2'	1:2A:69:C:O4'	2.19	0.43
15:2T:127:ALA:C	15:2T:129:ARG:H	2.20	0.43
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.99	0.43
20:2Y:79:CYS:SG	20:2Y:81:LYS:HD2	2.59	0.43
28:16:33:LYS:HA	28:16:33:LYS:HD2	1.62	0.43
1:1A:1149:G:H2'	1:1A:1150:C:C6	2.53	0.43
1:1A:1323:U:H2'	1:1A:1324:G:H5'	2.00	0.43
1:1A:1878:G:H2'	1:1A:1879:C:C6	2.53	0.43
1:1A:2018:G:H2'	1:1A:2019:A:O4'	2.18	0.43
1:1A:2299:G:N2	1:1A:2318:G:H1'	2.33	0.43
1:1A:266:G:HO2'	1:1A:267:C:P	3.41	0.43
1:1A:899:A:HO2'	1:1A:900:A:H8	1.64	0.43
2:1B:91:C:OP2	12:1Q:16:ARG:NH1	2.51	0.43
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.54	0.43
6:1G:16:ARG:NH2	6:1G:28:VAL:O	2.48	0.43
6:1G:67:LYS:HB3	6:1G:67:LYS:HE2	1.90	0.43
8:1I:61:ARG:HA	8:1I:61:ARG:HD3	1.77	0.43
14:1S:11:LYS:O	14:1S:15:ARG:HG3	2.18	0.43
1:2A:272(I):U:H3'	1:2A:272(J):C:H5''	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:946:G:H2'	1:2A:947:G:H8	1.82	0.43
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	2.01	0.43
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.53	0.43
1:1A:1331:A:C6	1:1A:1333:C:C2	3.05	0.43
1:1A:1969:A:N6	59:1A:5071:HOH:O	63.45	0.43
1:1A:195:A:H5''	1:1A:196:A:OP2	2.18	0.43
1:1A:397:G:H2'	1:1A:398:G:H8	1.84	0.43
3:1D:20:ASP:N	3:1D:20:ASP:OD1	2.44	0.43
5:1F:33:LEU:HB3	11:1P:6:LEU:HD21	2.00	0.43
17:1V:40:LEU:HB2	17:1V:46:VAL:HG22	2.00	0.43
23:21:51:VAL:HG11	23:21:74:VAL:HG21	2.01	0.43
26:24:26:SER:OG	26:24:27:THR:N	2.51	0.43
1:2A:839:U:O2'	1:2A:1191:G:N3	2.51	0.43
1:2A:152:G:H2'	1:2A:153:C:C6	2.53	0.43
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.54	0.43
1:2A:1865:G:N2	1:2A:1877:A:OP2	2.46	0.43
1:2A:311:A:C6	1:2A:328:U:C4	3.06	0.43
1:2A:754:C:H2'	1:2A:755:C:C6	2.52	0.43
2:2B:19:G:H2'	2:2B:20:C:O4'	2.18	0.43
5:2F:109:GLY:O	5:2F:113:ALA:N	2.50	0.43
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.99	0.43
8:2I:38:LEU:HD11	8:2I:40:THR:HG23	2.00	0.43
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.18	0.43
1:1A:1754:C:H2'	1:1A:1755:A:O4'	2.19	0.43
1:1A:1759:A:H1'	1:1A:2711:A:C2	2.54	0.43
2:1B:70:C:H2'	2:1B:71:C:H6	1.83	0.43
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.53	0.43
18:1W:84:ARG:O	18:1W:96:ILE:N	2.50	0.43
26:24:13:ARG:HA	26:24:22:ILE:O	2.19	0.43
1:2A:565:C:H4'	1:2A:1253:A:C6	2.54	0.43
1:2A:1355:G:H2'	1:2A:1356:G:O4'	2.26	0.43
1:2A:2166:G:H2'	1:2A:2167:U:H6	1.82	0.43
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.19	0.43
1:2A:300:A:H1'	1:2A:319:C:H1'	2.00	0.43
1:2A:436:C:H2'	1:2A:437:G:H8	1.83	0.43
5:2F:129:PHE:CG	5:2F:163:VAL:HG11	2.54	0.43
1:2A:1142(A):A:H4'	9:2N:25:ARG:NH2	2.34	0.43
15:2T:33:LYS:HB3	15:2T:82:LEU:HD22	1.99	0.43
20:2Y:35:TYR:CE2	20:2Y:69:ALA:HB3	2.54	0.43
1:1A:1341:U:OP1	1:1A:1397:U:N3	2.47	0.43
1:1A:1409:C:H2'	1:1A:1410:G:H8	1.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1819:A:H2'	3:1D:178:PRO:HB2	2.01	0.43
1:1A:2723:C:OP1	1:1A:2820:A:H8	2.01	0.43
1:1A:957:A:N1	1:1A:2458:G:H4'	2.34	0.43
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.99	0.43
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.53	0.43
10:1O:17:ARG:HD3	10:1O:17:ARG:HA	1.76	0.43
14:1S:43:GLU:OE1	14:1S:43:GLU:N	4.97	0.43
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.34	0.43
27:25:16:ARG:HG3	27:25:17:ASP:H	1.84	0.43
1:2A:1196:C:H2'	1:2A:1197:G:C8	2.53	0.43
1:2A:1230:C:H2'	1:2A:1231:G:H8	1.82	0.43
1:2A:1574:C:H2'	1:2A:1575:C:H6	1.84	0.43
1:2A:1710:C:H5'	1:2A:2859:G:H1'	2.00	0.43
1:2A:186:G:H2'	1:2A:187:G:C8	2.53	0.43
1:2A:1942:5MC:HM53	1:2A:1943:U:C2	2.53	0.43
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.60	0.43
1:2A:325:G:H2'	1:2A:326:G:O4'	2.19	0.43
1:2A:479:A:H1'	1:2A:481:G:H5''	2.01	0.43
1:2A:599:G:H4'	5:2F:31:HIS:HD2	1.83	0.43
14:2S:93:LYS:HZ2	14:2S:95:HIS:HB2	1.83	0.43
1:1A:1359:A:H2	1:1A:1372:U:O4	2.01	0.43
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.54	0.43
1:1A:2262:U:H4'	1:1A:2328:A:C2	2.54	0.43
1:1A:2703:C:H2'	1:1A:2704:C:H6	1.84	0.43
1:1A:272:G:N7	1:1A:421:U:H2'	2.33	0.43
1:1A:286:C:H2'	1:1A:287:C:C6	2.53	0.43
1:1A:776:G:N7	1:1A:793:A:O2'	2.45	0.43
4:1E:4:ILE:HD13	4:1E:28:ALA:HB1	2.00	0.43
12:1Q:118:LEU:HA	12:1Q:118:LEU:HD23	1.87	0.43
16:1U:16:LYS:HE2	16:1U:16:LYS:HB3	1.72	0.43
1:2A:1207:C:H2'	1:2A:1208:C:H6	1.82	0.43
1:2A:1567:A:OP2	3:2D:84:TYR:OH	2.24	0.43
1:2A:1752:C:H2'	1:2A:1753:G:C8	2.54	0.43
1:2A:860:U:C2	1:2A:2268:A:C8	3.06	0.43
1:2A:975:C:OP1	59:2A:5194:HOH:O	2.21	0.43
2:2B:78:A:H2'	2:2B:79:C:O4'	2.19	0.43
5:2F:7:TYR:HE1	5:2F:119:ARG:HG2	1.84	0.43
8:2I:88:ILE:HG22	8:2I:90:GLY:H	1.84	0.43
1:2A:587:C:H42	11:2P:33:ARG:HD2	1.83	0.43
12:2Q:130:LYS:HB3	12:2Q:130:LYS:HE2	1.78	0.43
6:1G:142:PRO:HB2	26:14:31:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:687:C:H1'	29:17:4:THR:HG22	2.01	0.43
1:1A:1051:G:H2'	1:1A:1052:C:O4'	2.18	0.43
1:1A:1137:G:H2'	1:1A:1138:G:C8	2.54	0.43
1:1A:2135:A:N6	1:1A:2156:G:O2'	2.47	0.43
1:1A:2369:A:H2'	1:1A:2370:G:H8	1.84	0.43
1:1A:1783:A:H5'	1:1A:2608:G:H4'	2.01	0.43
1:1A:2886:G:H2'	1:1A:2887:U:C6	2.53	0.43
1:1A:637:A:H2'	11:1P:117:GLU:OE1	2.19	0.43
1:1A:978:G:C2	1:1A:986:C:C2	3.07	0.43
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.25	0.43
5:1F:144:LYS:HE2	5:1F:144:LYS:HB3	1.69	0.43
5:1F:183:VAL:O	5:1F:187:VAL:HG23	2.18	0.43
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.37	0.43
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.19	0.43
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG13	2.01	0.43
31:29:3:VAL:HA	31:29:35:ARG:O	2.19	0.43
1:2A:944:G:N2	1:2A:1338:G:N7	82.35	0.43
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.18	0.43
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.17	0.43
1:2A:195:A:H5''	1:2A:196:A:O5'	2.18	0.43
1:2A:2094:G:H2'	1:2A:2095:C:O4'	2.19	0.43
1:2A:2179:C:H2'	1:2A:2180:U:O4'	2.19	0.43
1:2A:41:C:H2'	1:2A:42:G:C8	2.54	0.43
1:2A:568:U:H5'	1:2A:945:A:N1	2.33	0.43
1:2A:631:A:H1'	11:2P:66:GLY:HA2	2.01	0.43
1:2A:733:G:N2	1:2A:734:A:N7	2.66	0.43
6:2G:44:GLY:N	6:2G:88:ILE:O	2.51	0.43
1:1A:1082:U:C4	1:1A:1086:A:N1	2.77	0.43
1:1A:1285:G:C5	1:1A:1329:U:C4	3.07	0.43
1:1A:1332:G:HO2'	1:1A:1609:A:H2	1.65	0.43
1:1A:143(A):C:H2'	1:1A:144:C:C6	2.54	0.43
1:1A:2079:U:O3'	23:11:35:THR:OG1	2.28	0.43
1:1A:303:U:H2'	1:1A:304:G:H8	1.84	0.43
1:1A:34:C:H5''	1:1A:35:G:OP2	2.19	0.43
1:1A:397:G:H5''	23:11:45:ASN:HB2	2.01	0.43
1:1A:962:G:H2'	1:1A:963:U:C6	2.54	0.43
11:1P:57:THR:O	11:1P:61:ARG:HG3	2.19	0.43
21:1Z:125:LEU:HB3	21:1Z:165:VAL:HG13	2.01	0.43
18:2W:37:ARG:NH1	27:25:48:GLU:OE2	2.52	0.43
29:27:47:ARG:HA	29:27:47:ARG:HD3	1.78	0.43
1:2A:2420:C:P	30:28:33:ASN:H	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:116:C:H2'	1:2A:117:G:O4'	2.19	0.43
1:2A:300:A:H3'	20:2Y:84:ARG:NH2	2.33	0.43
1:2A:729:G:O2'	1:2A:763:G:H4'	2.19	0.43
5:2F:115:ALA:O	5:2F:119:ARG:HG3	2.19	0.43
6:2G:23:PHE:HB2	6:2G:25:TYR:CE2	2.54	0.43
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.19	0.43
13:2R:21:TYR:HB3	13:2R:47:PHE:CD2	2.53	0.43
6:1G:108:ASN:O	26:14:37:SER:N	2.52	0.42
1:1A:1201:C:H2'	1:1A:1202:C:C6	2.53	0.42
1:1A:1638:C:H5''	1:1A:2710:C:O2'	2.19	0.42
1:1A:414:C:H4'	1:1A:1879:C:O2	2.18	0.42
1:1A:620:G:N3	1:1A:620:G:H5'	2.33	0.42
1:1A:825:C:H4'	1:1A:2428:G:N7	2.34	0.42
4:1E:109:LYS:HG3	4:1E:191:PRO:HD3	2.01	0.42
8:1I:78:THR:O	8:1I:104:GLN:NE2	2.52	0.42
11:1P:6:LEU:HA	11:1P:6:LEU:HD23	1.80	0.42
13:1R:49:ASP:OD1	13:1R:95:THR:HG23	2.19	0.42
21:1Z:128:VAL:HG23	21:1Z:160:GLY:O	2.18	0.42
2:1B:92:C:H5''	21:1Z:79:ARG:NH1	2.34	0.42
1:2A:188:G:H5'	23:21:14:VAL:HG21	2.00	0.42
25:23:6:VAL:HG22	25:23:56:VAL:HG22	2.00	0.42
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.19	0.42
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.50	0.42
6:2G:9:ARG:NE	6:2G:13:GLU:OE2	2.46	0.42
14:2S:87:PHE:HB2	14:2S:112:PHE:CE1	2.54	0.42
4:2E:18:ASP:HB3	15:2T:82:LEU:HD21	2.00	0.42
20:2Y:39:VAL:HB	20:2Y:42:VAL:HB	2.01	0.42
1:1A:1001:A:H2'	1:1A:1002:G:O4'	2.18	0.42
1:1A:1074:G:C6	1:1A:1075:C:H1'	2.53	0.42
1:1A:1010:A:H1'	1:1A:1153:C:H1'	2.02	0.42
1:1A:1486:A:H2'	1:1A:1487:G:H8	1.82	0.42
1:1A:195:A:H61	1:1A:198:C:H3'	1.84	0.42
1:1A:2075:U:H1'	1:1A:2597:G:H21	1.84	0.42
1:1A:813:U:H2'	1:1A:814:C:C6	2.54	0.42
3:1D:108:PRO:HG2	3:1D:111:LEU:HB2	2.00	0.42
4:1E:8:LYS:O	4:1E:193:GLY:N	2.44	0.42
11:1P:88:LEU:HD22	11:1P:95:VAL:HG21	2.00	0.42
13:1R:104:ARG:HD2	13:1R:109:ALA:HB3	2.01	0.42
21:1Z:153:SER:HA	21:1Z:167:PRO:HB3	2.01	0.42
24:22:1:MET:N	24:22:52:ASP:OD1	2.47	0.42
1:2A:1232:G:H2'	1:2A:1233:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1774:C:OP1	59:2A:5081:HOH:O	2.21	0.42
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.54	0.42
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.55	0.42
1:2A:413:C:H42	1:2A:2410:G:H1	1.65	0.42
7:2H:15:VAL:HG23	7:2H:27:LYS:O	2.19	0.42
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.54	0.42
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.19	0.42
28:16:47:THR:O	28:16:49:HIS:ND1	2.46	0.42
1:1A:1012:U:O4	9:1N:28:THR:HG21	2.19	0.42
1:1A:2533:A:H2'	1:1A:2534:A:O4'	2.19	0.42
10:1O:39:ILE:HD12	10:1O:41:ALA:HB2	2.02	0.42
10:1O:70:LYS:HE2	10:1O:70:LYS:HB3	1.75	0.42
16:1U:17:ILE:HG23	16:1U:39:LEU:HD12	2.02	0.42
18:1W:36:LEU:HD13	18:1W:48:ALA:HA	2.00	0.42
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.19	0.42
1:2A:1838:C:H4'	1:2A:1839:G:C8	2.54	0.42
1:2A:57:C:H2'	1:2A:58:G:O4'	2.18	0.42
1:2A:875:G:H3'	1:2A:876:C:H6	1.84	0.42
1:2A:991:C:OP2	1:2A:1186:G:H5'	2.19	0.42
8:2I:5:LEU:HD23	8:2I:9:LEU:HD13	2.01	0.42
8:2I:72:LEU:C	8:2I:74:ASN:H	2.22	0.42
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.26	0.42
1:2A:1288:U:O4	13:2R:106:GLY:HA3	2.19	0.42
20:2Y:52:SER:OG	20:2Y:55:TYR:HB2	2.19	0.42
20:2Y:7:VAL:HG11	20:2Y:27:VAL:HG21	2.01	0.42
21:2Z:150:LEU:HG	21:2Z:151:HIS:H	1.84	0.42
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.54	0.42
1:1A:1176:G:N2	1:1A:1178:C:OP1	2.51	0.42
1:1A:1566:A:OP1	3:1D:211:ARG:NH1	2.51	0.42
1:1A:1682:G:OP1	1:1A:1699:G:N1	2.52	0.42
1:1A:1981:A:OP1	59:1A:5313:HOH:O	2.22	0.42
1:1A:526:A:O2'	1:1A:2043:C:O2	2.34	0.42
1:1A:2123:G:H2'	1:1A:2124:G:C8	2.54	0.42
1:1A:2572:A:O5'	1:1A:2574:G:H4'	2.20	0.42
1:1A:624:C:H2'	1:1A:625:G:H8	2.67	0.42
5:1F:33:LEU:HD13	5:1F:112:MET:HE3	2.01	0.42
59:1A:5032:HOH:O	6:1G:45:GLU:OE2	2.21	0.42
1:1A:494:G:OP1	18:1W:8:ARG:HD3	2.20	0.42
21:1Z:104:PHE:HD1	21:1Z:139:VAL:HG11	1.83	0.42
21:1Z:93:ASP:HB2	21:1Z:131:ARG:HH22	1.85	0.42
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1375:C:H2'	1:2A:1376:C:H6	1.85	0.42
1:2A:1713:U:H2'	1:2A:1714:G:C8	2.54	0.42
1:2A:184:C:H2'	1:2A:185:U:C6	2.54	0.42
1:2A:2269:A:OP1	59:2A:5110:HOH:O	2.21	0.42
1:2A:754:C:H2'	1:2A:755:C:H6	1.85	0.42
1:2A:807:U:H4'	1:2A:2446:G:OP1	2.18	0.42
1:2A:815:C:H2'	1:2A:816:C:C6	2.54	0.42
1:2A:863:A:H2'	1:2A:864:G:H8	1.84	0.42
1:2A:969:U:OP1	25:23:17:LYS:HB3	2.20	0.42
3:2D:24:ILE:HD11	3:2D:84:TYR:HB2	2.00	0.42
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	2.00	0.42
13:2R:28:LEU:HD13	13:2R:34:ILE:HG12	2.01	0.42
17:2V:18:LEU:HD23	17:2V:19:LYS:N	2.34	0.42
17:2V:24:LYS:HD3	17:2V:90:PRO:HB3	2.01	0.42
21:2Z:146:ILE:HA	21:2Z:174:VAL:O	2.20	0.42
29:17:12:ARG:HH21	29:17:44:PRO:HB3	1.83	0.42
1:1A:1339:G:H5'	19:1X:16:LYS:HD3	2.02	0.42
1:1A:2853:C:H2'	1:1A:2854:G:C8	2.54	0.42
6:1G:5:VAL:HG23	6:1G:8:LYS:H	1.84	0.42
1:1A:2748:A:H5'	7:1H:4:ILE:HD12	2.00	0.42
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.20	0.42
22:20:48:GLY:HA3	22:20:80:HIS:ND1	2.34	0.42
1:2A:2615:U:C2	27:25:7:PRO:HA	2.55	0.42
31:29:17:ILE:HA	31:29:17:ILE:HD12	1.83	0.42
31:29:7:VAL:HG12	31:29:34:GLN:HB3	2.01	0.42
1:2A:195:A:H2'	1:2A:198:C:H41	1.85	0.42
1:2A:2078:C:C4	1:2A:2079:U:C4	3.07	0.42
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.54	0.42
1:2A:500:G:N1	1:2A:503:A:OP2	2.52	0.42
2:2B:4:C:H2'	2:2B:5:C:H6	1.85	0.42
4:2E:170:LEU:HB3	4:2E:184:VAL:CG2	2.49	0.42
6:2G:174:GLU:HB2	6:2G:180:PHE:HE2	1.84	0.42
6:2G:8:LYS:HE2	6:2G:8:LYS:HB3	1.81	0.42
16:2U:86:ALA:HB2	16:2U:116:ALA:HB2	2.00	0.42
1:1A:1114:G:H2'	1:1A:1115:G:O4'	2.20	0.42
1:1A:1488:G:H2'	1:1A:1489:U:O4'	2.19	0.42
1:1A:121:G:H4'	1:1A:149:A:H5'	2.01	0.42
1:1A:2071:A:H2'	1:1A:2072:G:C8	2.54	0.42
1:1A:2100:G:N2	1:1A:2189:U:O2	2.49	0.42
1:1A:2626:C:H2'	1:1A:2627:G:C8	2.55	0.42
6:1G:7:LEU:HD13	6:1G:104:GLU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:94:TYR:HA	7:1H:106:THR:O	2.20	0.42
18:1W:7:ALA:HB2	18:1W:50:VAL:HG22	2.01	0.42
21:1Z:53:ILE:HG22	21:1Z:71:VAL:HG12	2.01	0.42
1:2A:2383:G:OP2	30:28:37:SER:HB2	2.20	0.42
1:2A:115:C:HO2'	1:2A:127:A:HO2'	1.56	0.42
1:2A:1192:G:OP2	11:2P:17:LYS:NZ	2.38	0.42
1:2A:1283:G:O2'	1:2A:1285:G:N7	2.40	0.42
1:2A:1317:A:H2'	1:2A:1318:C:C6	2.55	0.42
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.53	0.42
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.35	0.42
1:2A:828:U:H4'	1:2A:831:G:N1	2.34	0.42
5:2F:57:VAL:HG13	5:2F:59:TYR:H	1.85	0.42
4:2E:20:ALA:N	10:2O:72:PRO:O	2.53	0.42
11:2P:27:HIS:O	11:2P:31:ALA:HA	2.19	0.42
1:2A:2294:C:OP1	14:2S:10:ARG:HD2	2.20	0.42
10:2O:119:PRO:HB2	15:2T:68:TYR:CE2	2.54	0.42
16:2U:49:HIS:HA	16:2U:52:ARG:HB3	2.01	0.42
21:2Z:97:GLU:HB3	21:2Z:125:LEU:HD11	2.02	0.42
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.67	0.42
1:1A:1003:G:O2'	1:1A:1010:A:N1	2.39	0.42
1:1A:142(A):C:H2'	1:1A:143:G:O4'	2.20	0.42
1:1A:1697:G:OP2	1:1A:1698:A:O2'	2.24	0.42
1:1A:434:U:H2'	1:1A:435:C:O4'	7.84	0.42
1:1A:861:A:H2'	1:1A:862:G:O4'	2.20	0.42
1:1A:918:A:H5''	2:1B:98:G:O2'	2.20	0.42
7:1H:143:GLN:HG3	7:1H:147:ASN:HD21	1.84	0.42
8:1I:3:VAL:HA	8:1I:38:LEU:HA	2.01	0.42
1:2A:30:G:O2'	1:2A:1214:A:N3	2.51	0.42
1:2A:1858:G:OP2	1:2A:1858:G:H8	2.02	0.42
1:2A:1935:G:H1'	1:2A:1964:G:N2	2.34	0.42
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.34	0.42
1:2A:2863:C:OP1	15:2T:93:ARG:NH1	2.52	0.42
1:2A:728:G:H5''	3:2D:13:ARG:NH2	2.35	0.42
6:2G:79:ASN:OD1	6:2G:79:ASN:N	2.45	0.42
1:2A:2376:A:H2'	14:2S:106:ARG:HH22	1.84	0.42
1:1A:104:U:H3'	1:1A:105:C:C6	2.55	0.42
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.20	0.42
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.55	0.42
1:1A:2300:G:H2'	1:1A:2301:C:H6	1.83	0.42
1:1A:2471:C:H2'	1:1A:2472:G:O4'	2.20	0.42
1:1A:2552:2MU:O5'	1:1A:2552:2MU:H6	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:818:G:H4'	1:1A:838:C:O3'	2.20	0.42
1:1A:969:U:H2'	1:1A:970:C:C6	2.54	0.42
6:1G:121:ASN:HA	6:1G:122:PRO:HD3	1.95	0.42
7:1H:121:ILE:HD13	7:1H:135:GLY:HA3	2.01	0.42
8:1I:88:ILE:HG22	8:1I:90:GLY:N	2.35	0.42
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.19	0.42
1:2A:1115:G:H2'	1:2A:1116:C:O4'	2.19	0.42
1:2A:1341:U:O4'	19:2X:57:LEU:HD23	2.19	0.42
1:2A:1810:A:H2'	1:2A:1811:G:O4'	2.20	0.42
1:2A:2295:C:OP1	14:2S:10:ARG:NH1	2.51	0.42
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.35	0.42
1:2A:2784:C:H2'	1:2A:2785:C:C6	2.54	0.42
1:2A:291:C:N3	1:2A:309:G:N1	50.92	0.42
1:2A:436:C:H2'	1:2A:437:G:C8	2.55	0.42
4:2E:120:TRP:CG	4:2E:155:LYS:HB3	2.55	0.42
25:13:8:LEU:HD22	25:13:23:LEU:HD23	2.02	0.42
1:1A:1260:G:C6	1:1A:1261:C:C4	3.08	0.42
1:1A:1274:A:N3	1:1A:1297:C:H1'	2.35	0.42
1:1A:1651:G:H4'	13:1R:39:PRO:HG2	2.01	0.42
1:1A:2854:G:H2'	1:1A:2855:C:C6	2.55	0.42
1:1A:330:A:H8	1:1A:1210:A:C4	2.38	0.42
1:1A:312:G:H4'	1:1A:331:A:C2	2.55	0.42
1:1A:751:A:H5'	18:1W:90:ARG:HA	2.02	0.42
2:1B:18:G:H2'	2:1B:19:G:H8	1.85	0.42
5:1F:8:GLN:NE2	5:1F:21:ALA:HA	2.34	0.42
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	2.02	0.42
13:1R:8:ARG:HH22	13:1R:42:LYS:HD2	1.84	0.42
21:1Z:98:MET:O	21:1Z:125:LEU:HA	2.20	0.42
1:2A:1028:A:H61	1:2A:1125:G:H2'	1.83	0.42
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.55	0.42
1:2A:1703:G:H2'	1:2A:1704:G:H8	1.85	0.42
1:2A:1741:A:H2'	1:2A:1742:G:O4'	2.20	0.42
1:2A:2031:A:N3	1:2A:2455:G:O2'	2.46	0.42
1:2A:2128:C:H2'	1:2A:2129:C:O4'	2.19	0.42
1:2A:2576:G:H3'	1:2A:2576:G:N3	2.35	0.42
1:2A:444:C:H2'	1:2A:445:C:C6	2.55	0.42
1:2A:604:G:OP2	11:2P:90:ARG:NH2	2.53	0.42
1:2A:757:U:H2'	1:2A:758:C:O4'	2.20	0.42
1:2A:901:A:H2'	1:2A:902:C:O4'	2.19	0.42
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	2.01	0.42
8:2I:130:TYR:O	8:2I:132:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	2.01	0.42
12:2Q:2:LEU:HD12	12:2Q:69:PHE:HE1	1.85	0.42
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.54	0.42
18:2W:23:LEU:HD12	18:2W:23:LEU:HA	1.87	0.42
1:1A:2277:G:OP1	22:10:10:THR:HG21	2.19	0.42
1:1A:2244:U:H2'	1:1A:2245:U:O4'	2.19	0.42
1:1A:2260:C:H2'	1:1A:2261:C:C6	2.55	0.42
1:1A:2808:U:H5''	1:1A:2891:G:O6	2.19	0.42
1:1A:296:C:H2'	1:1A:297:C:C6	2.54	0.42
1:1A:646:A:H2'	1:1A:647:G:O4'	2.20	0.42
8:1I:40:THR:O	8:1I:44:LEU:N	2.53	0.42
14:1S:46:VAL:HG12	14:1S:48:LEU:HD12	2.01	0.42
21:1Z:52:SER:OG	21:1Z:53:ILE:N	2.52	0.42
29:27:8:ASN:HB3	29:27:11:LYS:HB3	2.02	0.42
31:29:10:ILE:HD12	31:29:32:HIS:CG	2.55	0.42
1:2A:1131:G:C8	1:2A:2025:C:H4'	2.55	0.42
1:2A:1576:U:H2'	1:2A:1577:C:C6	2.55	0.42
1:2A:2101:G:C6	1:2A:2102:U:C4	3.07	0.42
1:2A:2197:U:O2'	1:2A:2198:A:H2'	2.20	0.42
1:2A:2023:G:H5'	1:2A:2617:C:H4'	2.01	0.42
1:2A:2893:G:H5''	1:2A:2894:G:O4'	2.19	0.42
1:2A:531:C:OP1	1:2A:561:G:N1	2.47	0.42
1:2A:300:A:O2'	1:2A:564:C:N3	73.24	0.42
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.55	0.42
9:2N:15:LEU:HG	9:2N:16:ILE:N	2.35	0.42
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.55	0.42
26:14:61:ARG:HG3	26:14:62:ARG:N	2.34	0.41
1:1A:182:A:OP2	1:1A:182:A:H8	2.02	0.41
1:1A:2025:C:H2'	1:1A:2026:C:C6	2.55	0.41
1:1A:2405:G:O2'	1:1A:2406:U:OP1	2.31	0.41
1:1A:2561:A:H2'	1:1A:2562:U:O4'	2.20	0.41
1:1A:394:A:N6	1:1A:395:U:O4	2.53	0.41
1:1A:709:U:H2'	1:1A:710:G:H8	1.85	0.41
3:1D:72:LYS:HE3	3:1D:75:ILE:HD12	2.01	0.41
4:1E:203:LYS:HD3	4:1E:203:LYS:HA	1.79	0.41
6:1G:67:LYS:HE3	6:1G:68:PRO:O	2.21	0.41
7:1H:23:ARG:HB2	7:1H:23:ARG:HE	1.69	0.41
7:1H:3:ARG:HE	7:1H:54:ARG:HH12	1.68	0.41
7:1H:3:ARG:HE	7:1H:54:ARG:NH1	2.18	0.41
8:1I:117:GLU:H	8:1I:117:GLU:HG2	1.63	0.41
11:1P:121:LYS:O	11:1P:123:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:47:ASP:OD2	11:1P:49:ARG:NH2	2.51	0.41
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.19	0.41
1:1A:998:C:P	16:1U:92:ARG:HH22	2.43	0.41
24:22:11:GLU:HG3	24:22:11:GLU:H	1.37	0.41
24:22:63:VAL:HA	24:22:66:GLU:OE1	2.20	0.41
26:24:49:PHE:HD1	26:24:49:PHE:HA	1.67	0.41
29:27:26:GLY:O	29:27:30:VAL:HG23	2.20	0.41
1:2A:1227:G:OP1	16:2U:13:LYS:HG2	2.20	0.41
1:2A:1422:G:H5''	10:2O:48:PRO:CB	99.45	0.41
1:2A:251:A:C4	1:2A:252:G:H1'	2.55	0.41
1:2A:2632:A:H61	1:2A:2786:U:H3	1.68	0.41
1:2A:330:A:H2	1:2A:1210:A:O2'	2.03	0.41
1:2A:656:G:H2'	1:2A:657:U:O4'	2.20	0.41
1:2A:69:C:H2'	1:2A:70:G:C8	2.55	0.41
5:2F:195:ASP:O	5:2F:198:ALA:N	2.50	0.41
13:2R:104:ARG:HG3	13:2R:111:LEU:HD11	2.02	0.41
15:2T:50:ILE:HA	15:2T:99:LEU:HD12	2.01	0.41
20:2Y:67:LEU:HD23	20:2Y:67:LEU:HA	1.89	0.41
29:17:34:ARG:NH2	29:17:39:ARG:HG2	2.34	0.41
1:1A:1142(A):A:O2'	1:1A:1143:A:H3'	2.20	0.41
1:1A:2682:U:O2	4:1E:22:PRO:HB3	2.20	0.41
1:1A:433:C:H2'	1:1A:434:U:C6	2.90	0.41
1:1A:614:U:H5'	1:1A:614(C):A:N6	2.35	0.41
2:1B:86:G:H1	2:1B:91:C:N4	2.17	0.41
4:1E:64:LYS:HB2	4:1E:64:LYS:HE3	1.68	0.41
12:1Q:68:ILE:HG23	12:1Q:103:MET:HA	2.02	0.41
19:1X:88:LYS:HE3	19:1X:93:GLU:OE1	2.20	0.41
1:2A:1011:G:N2	1:2A:1018:C:N3	20.09	0.41
1:2A:1449:A:H8	1:2A:1449:A:OP2	2.03	0.41
1:2A:1517:G:C6	1:2A:1518:U:C4	3.08	0.41
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.19	0.41
1:2A:1973:G:H2'	1:2A:1974:C:C6	2.55	0.41
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	2.02	0.41
1:2A:875:G:H3'	1:2A:876:C:C6	2.55	0.41
3:2D:143:HIS:ND1	3:2D:194:GLY:O	2.35	0.41
15:2T:51:ARG:HG2	15:2T:62:THR:HB	2.02	0.41
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.21	0.41
1:1A:2123:G:H2'	1:1A:2124:G:H8	1.86	0.41
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.20	0.41
1:1A:647:G:H8	1:1A:647:G:O5'	2.04	0.41
1:1A:753:C:H2'	1:1A:754:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:109:ASP:HB2	3:1D:197:GLY:HA2	2.01	0.41
4:1E:143:ASN:HD22	4:1E:147:PRO:CD	2.33	0.41
12:1Q:57:HIS:CD2	12:1Q:117:ALA:HB2	2.56	0.41
13:1R:13:HIS:HE1	13:1R:15:SER:OG	2.04	0.41
23:21:72:GLU:O	23:21:76:ARG:HG3	2.21	0.41
23:21:77:ALA:O	23:21:82:LEU:HD11	2.19	0.41
24:22:52:ASP:O	24:22:56:GLN:HG3	2.20	0.41
1:2A:1125:G:H5'	31:29:37:GLY:HA2	2.02	0.41
1:2A:1301:A:O2'	1:2A:1302:A:H3'	2.19	0.41
1:2A:1530:C:H6	1:2A:1530:C:H2'	1.67	0.41
1:2A:1791:A:C6	1:2A:1829:A:H5'	2.55	0.41
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.55	0.41
1:2A:2502:G:H5''	1:2A:2503:2MA:H5''	2.02	0.41
1:2A:459:U:H4'	29:27:40:TRP:CZ3	2.55	0.41
1:2A:801:G:O6	5:2F:53:THR:OG1	2.37	0.41
5:2F:126:VAL:HG11	5:2F:142:TRP:CH2	2.56	0.41
6:2G:146:TYR:O	6:2G:149:VAL:HG12	2.20	0.41
9:2N:91:LEU:HD23	9:2N:91:LEU:HA	1.93	0.41
11:2P:47:ASP:OD1	11:2P:47:ASP:N	4.20	0.41
14:2S:20:ARG:HD2	14:2S:20:ARG:HA	1.87	0.41
21:2Z:79:ARG:HD2	21:2Z:80:ARG:HH12	1.85	0.41
21:2Z:93:ASP:CB	21:2Z:131:ARG:HH22	2.33	0.41
23:11:23:LYS:HB3	23:11:29:GLY:HA3	2.02	0.41
1:1A:1510:G:H2'	1:1A:1511:C:C6	2.56	0.41
1:1A:2099:U:H2'	1:1A:2100:G:C8	2.56	0.41
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.85	0.41
1:1A:2146:C:H5''	1:1A:2147:G:C5	2.55	0.41
1:1A:2813:A:H2'	1:1A:2814:C:O4'	2.20	0.41
1:1A:36:G:H4'	1:1A:451:C:C2	2.55	0.41
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.53	0.41
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.26	0.41
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.53	0.41
8:1I:10:GLU:O	8:1I:12:LEU:HG	2.20	0.41
1:1A:1022:G:P	9:1N:69:GLN:HE22	2.44	0.41
12:1Q:17:LEU:HD21	12:1Q:41:TRP:HE1	1.86	0.41
12:1Q:71:ASP:OD1	12:1Q:71:ASP:N	2.44	0.41
1:2A:990:A:C6	1:2A:1186:G:H1'	2.55	0.41
1:2A:1685:C:H42	1:2A:1703:G:H1	1.68	0.41
1:2A:1805:U:O2	3:2D:50:THR:HB	2.20	0.41
1:2A:184:C:H1'	1:2A:217:G:H1'	2.01	0.41
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:852:G:H2'	1:2A:853:G:C8	2.56	0.41
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.55	0.41
7:2H:10:PRO:HA	7:2H:49:VAL:HG22	2.03	0.41
8:2I:61:ARG:HD3	8:2I:61:ARG:HA	1.79	0.41
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.21	0.41
20:2Y:43:ASN:O	20:2Y:64:GLU:HA	2.20	0.41
23:11:86:SER:O	23:11:90:ILE:HG13	2.20	0.41
26:14:48:ARG:HD3	26:14:48:ARG:HA	1.88	0.41
1:1A:1657:C:H2'	1:1A:1658:C:C6	2.56	0.41
1:1A:2185:C:H2'	1:1A:2186:G:O4'	2.21	0.41
3:1D:18:VAL:HG12	3:1D:211:ARG:NH1	2.35	0.41
4:1E:143:ASN:HD22	4:1E:147:PRO:HD2	1.85	0.41
4:1E:49:LEU:O	4:1E:78:LEU:HA	2.20	0.41
7:1H:22:GLY:HA2	7:1H:37:VAL:O	2.19	0.41
15:1T:127:ALA:C	15:1T:129:ARG:H	2.24	0.41
24:22:35:LEU:HA	24:22:35:LEU:HD23	1.84	0.41
29:27:5:TRP:CZ2	29:27:7:PRO:HB3	2.55	0.41
1:2A:1002:G:C5	1:2A:1003:G:H8	3.93	0.41
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.21	0.41
1:2A:1496:A:OP2	1:2A:1496:A:H8	2.04	0.41
1:2A:1541:G:H8	1:2A:1542:A:H2'	1.85	0.41
1:2A:1667:G:OP2	1:2A:1667:G:H8	2.03	0.41
1:2A:2181:G:H5'	1:2A:2182:G:OP2	2.20	0.41
1:2A:1889:A:N1	1:2A:2234:G:H1'	2.35	0.41
1:2A:324:A:H2'	1:2A:325:G:O4'	2.19	0.41
1:2A:41:C:H2'	1:2A:42:G:H8	1.85	0.41
1:2A:599:G:H5'	11:2P:9:ASN:ND2	2.35	0.41
1:2A:729:G:OP2	3:2D:13:ARG:NH2	2.51	0.41
1:2A:196:A:O2'	1:2A:805:G:O6	2.32	0.41
7:2H:121:ILE:HD13	7:2H:121:ILE:HA	1.95	0.41
13:2R:88:ARG:NH1	13:2R:89:ASP:OD2	2.53	0.41
14:2S:3:ARG:HD3	14:2S:4:LEU:N	2.35	0.41
30:18:63:PRO:HG2	30:18:64:TYR:CD2	2.56	0.41
1:1A:186:G:H2'	1:1A:187:G:H8	1.86	0.41
1:1A:2340:G:H2'	1:1A:2341:G:H8	1.82	0.41
3:1D:264:LYS:HA	3:1D:265:PRO:HD3	1.97	0.41
9:1N:67:LEU:HA	9:1N:87:LEU:HD22	2.02	0.41
9:1N:99:LEU:HD23	9:1N:99:LEU:HA	1.87	0.41
18:1W:11:ARG:HH21	18:1W:98:LYS:HG2	1.84	0.41
21:1Z:7:ALA:O	21:1Z:62:PRO:HD3	2.20	0.41
22:20:32:ARG:HA	22:20:64:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1547:C:H2'	1:2A:1548:C:C6	2.55	0.41
1:2A:1791:A:N6	1:2A:1828:G:O2'	2.43	0.41
1:2A:1985:G:H2'	1:2A:1986:A:H8	1.85	0.41
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.55	0.41
1:2A:2126:A:H62	1:2A:2163:C:H5'	1.86	0.41
1:2A:2369:A:H2'	1:2A:2370:G:H8	1.85	0.41
1:2A:2468:G:OP1	12:2Q:119:ARG:NH2	2.33	0.41
1:2A:2250:G:C8	1:2A:2496:C:H5''	2.55	0.41
1:2A:2788:C:H2'	1:2A:2789:C:H5	1.86	0.41
59:2A:5027:HOH:O	2:2B:120:A:OP2	2.22	0.41
5:2F:181:LEU:HA	5:2F:181:LEU:HD12	1.91	0.41
7:2H:3:ARG:CZ	7:2H:5:GLY:H	2.34	0.41
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	2.02	0.41
12:2Q:75:THR:HG21	12:2Q:87:LYS:CE	2.46	0.41
1:2A:2378:A:H2'	14:2S:21:THR:HG21	2.02	0.41
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.20	0.41
21:2Z:92:SER:OG	21:2Z:94:GLU:OE1	2.38	0.41
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.92	0.41
29:17:46:VAL:HG13	29:17:48:LYS:NZ	2.36	0.41
1:1A:1049:C:H2'	1:1A:1050:A:H8	1.85	0.41
1:1A:26:G:O3'	1:1A:1260:G:H4'	2.21	0.41
1:1A:1499:C:H2'	1:1A:1500:G:H8	1.86	0.41
1:1A:1971:A:C4	3:1D:241:PRO:HD3	2.56	0.41
1:1A:444:C:H2'	1:1A:445:C:H6	1.85	0.41
2:1B:48:A:H2'	2:1B:49:C:C6	2.55	0.41
3:1D:72:LYS:HB3	3:1D:72:LYS:HE3	1.95	0.41
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.38	0.41
23:21:53:VAL:HG22	23:21:74:VAL:HG13	2.02	0.41
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.56	0.41
1:2A:2489:G:C6	1:2A:2490:G:N1	2.88	0.41
1:2A:2803:C:H5''	1:2A:2804:C:OP2	2.20	0.41
1:2A:750:A:OP1	1:2A:1615:C:N4	2.50	0.41
1:2A:783:A:H4'	1:2A:2588:G:H4'	2.02	0.41
1:2A:796:C:H2'	1:2A:797:C:C6	2.55	0.41
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.20	0.41
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.55	0.41
1:2A:2852:G:P	13:2R:64:ARG:HH22	2.44	0.41
21:2Z:93:ASP:HB3	21:2Z:131:ARG:HH22	1.85	0.41
1:1A:1364:G:N7	23:11:3:LYS:HD2	2.36	0.41
24:12:50:ILE:O	24:12:54:LYS:HG3	2.19	0.41
1:1A:1045:A:H5'	1:1A:1046:A:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1273:U:H4'	1:1A:1275:A:OP2	2.21	0.41
1:1A:2001:A:OP1	13:1R:9:LYS:NZ	2.45	0.41
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.55	0.41
1:1A:2151:G:C2	1:1A:2152:G:C6	3.09	0.41
1:1A:863:A:H2'	1:1A:864:G:H8	1.85	0.41
2:1B:91:C:OP1	12:1Q:16:ARG:HG3	2.21	0.41
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	2.03	0.41
20:1Y:19:LYS:HE3	20:1Y:20:TYR:CE2	2.56	0.41
1:1A:297:C:H5''	20:1Y:87:LYS:HG3	2.02	0.41
21:1Z:7:ALA:HA	21:1Z:39:VAL:HG12	2.03	0.41
25:23:4:LEU:HD23	25:23:4:LEU:HA	1.92	0.41
6:2G:3:LEU:HD13	26:24:25:TYR:CE2	2.56	0.41
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.20	0.41
1:2A:1525:G:H2'	1:2A:1526:G:C8	2.56	0.41
1:2A:1882:C:H2'	1:2A:1883:G:O4'	2.21	0.41
1:2A:2301:C:H2'	1:2A:2302:G:H8	1.86	0.41
1:2A:2432:A:C6	1:2A:2433:A:C6	3.09	0.41
1:2A:2572:A:H2'	4:2E:144:ARG:HD3	2.02	0.41
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.54	0.41
1:2A:641:C:N4	1:2A:647:G:H1	2.10	0.41
1:2A:729:G:O5'	3:2D:208:LYS:NZ	2.48	0.41
1:2A:746:A:H2'	1:2A:2612:C:H5''	2.02	0.41
1:2A:882:G:H1	1:2A:894:C:N4	2.19	0.41
2:2B:114:C:H2'	2:2B:115:G:C8	2.55	0.41
2:2B:28:C:H2'	2:2B:29:A:O4'	2.20	0.41
1:2A:2680:C:H5'	4:2E:189:PRO:HA	2.02	0.41
5:2F:36:VAL:HB	5:2F:183:VAL:HG21	2.03	0.41
7:2H:117:PRO:HA	7:2H:118:PRO:HD3	1.91	0.41
8:2I:77:LEU:HD23	8:2I:78:THR:H	1.84	0.41
12:2Q:50:ALA:HB1	12:2Q:121:ALA:HB1	2.02	0.41
20:2Y:38:ILE:HD13	20:2Y:66:PRO:HA	2.02	0.41
27:15:41:PRO:O	27:15:44:THR:OG1	2.39	0.41
1:1A:1082:U:H3	1:1A:1086:A:H61	0.49	0.41
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.21	0.41
1:1A:1300:U:H4'	1:1A:1301:A:C5'	2.46	0.41
1:1A:1511:C:H2'	1:1A:1512:U:O4'	2.21	0.41
1:1A:2011:U:H2'	1:1A:2012:G:O4'	2.19	0.41
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.56	0.41
1:1A:963:U:H1'	1:1A:2250:G:O6	2.20	0.41
1:1A:27:G:C2	1:1A:512:G:N3	2.89	0.41
1:1A:884:C:H6	1:1A:884:C:O5'	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:862:G:O2'	2:1B:78:A:N3	2.50	0.41
3:1D:9:TYR:CD1	3:1D:10:THR:HG23	2.56	0.41
8:1I:27:ARG:HD3	23:11:71:TYR:CE2	2.55	0.41
1:2A:177:G:H3'	1:2A:178:G:H8	1.86	0.41
1:2A:1771:C:O2'	1:2A:1786:A:O4'	2.36	0.41
1:2A:265:A:H1'	1:2A:266:G:O4'	2.21	0.41
1:2A:1654:A:O4'	1:2A:2823:A:H5'	2.20	0.41
1:2A:296:C:H2'	1:2A:297:C:C6	2.56	0.41
1:2A:303:U:H2'	1:2A:304:G:C8	2.55	0.41
1:2A:319:C:H2'	1:2A:320:A:O4'	2.21	0.41
1:2A:658:C:H2'	1:2A:659:C:C6	2.56	0.41
1:2A:7:G:H2'	1:2A:8:A:C8	2.55	0.41
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.20	0.41
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.20	0.41
1:1A:238:C:H2'	1:1A:239:U:O4'	2.20	0.41
1:1A:479:A:N3	1:1A:481:G:H5''	2.35	0.41
2:1B:66:A:H61	2:1B:109:C:H5''	1.85	0.41
3:1D:148:GLU:O	3:1D:151:LYS:HB2	2.21	0.41
1:1A:1803:A:H4'	3:1D:259:THR:HG23	2.02	0.41
3:1D:273:ARG:HG2	3:1D:274:ARG:H	1.86	0.41
1:1A:1952:A:N3	10:1O:22:ILE:HD12	2.35	0.41
12:1Q:1:MET:HG3	12:1Q:44:ALA:HB1	2.03	0.41
1:2A:2466:C:OP1	31:29:4:ARG:HB2	2.21	0.41
1:2A:1186:G:H2'	1:2A:1187:G:O4'	2.21	0.41
1:2A:1270:C:H2'	1:2A:1271:G:C8	6.63	0.41
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.21	0.41
1:2A:964:C:O2'	1:2A:2273:A:N3	2.37	0.41
1:2A:2284:C:P	28:26:6:ARG:HG3	2.61	0.41
1:2A:2354:G:H21	22:20:36:ILE:HD12	1.85	0.41
1:2A:2462:U:H2'	1:2A:2463:C:C6	2.56	0.41
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.50	0.41
1:2A:2596:U:H2'	1:2A:2597:G:O4'	2.20	0.41
1:2A:2689:U:P	1:2A:2719:G:H22	2.44	0.41
1:2A:2740:A:C6	1:2A:2741:A:C6	3.08	0.41
1:2A:535:C:H2'	1:2A:536:A:C8	2.56	0.41
1:2A:70:G:O4'	1:2A:73:A:H1'	2.21	0.41
1:2A:2679:A:H4'	4:2E:165:VAL:HG11	2.02	0.41
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	2.02	0.41
10:2O:17:ARG:HA	10:2O:17:ARG:HD3	1.53	0.41
17:2V:40:LEU:HD11	17:2V:101:GLY:HA3	2.03	0.41
16:2U:86:ALA:O	17:2V:49:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:65:GLY:HA3	17:2V:91:TYR:CZ	2.56	0.41
1:1A:1366:A:P	23:11:3:LYS:HZ3	2.44	0.41
1:1A:1066:U:H2'	1:1A:1068:G:OP2	2.21	0.41
1:1A:2138:C:C2	1:1A:2154:G:C2	3.09	0.41
1:1A:2183:C:HO2'	1:1A:2184:G:P	2.43	0.41
1:1A:2351:G:HO2'	1:1A:2352:A:H8	1.69	0.41
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.36	0.41
1:1A:92:A:H2'	1:1A:93:G:C8	2.55	0.41
1:1A:947:G:H2'	1:1A:948:G:C8	2.57	0.41
3:1D:19:ALA:HB3	3:1D:21:PHE:CE1	2.56	0.41
1:1A:2820:A:C8	4:1E:109:LYS:HE3	2.55	0.41
5:1F:40:GLN:HE22	5:1F:183:VAL:H	1.69	0.41
6:1G:151:ALA:HB3	6:1G:153:ARG:NH1	2.36	0.41
9:1N:133:GLN:N	9:1N:133:GLN:OE1	2.54	0.41
9:1N:30:ILE:HG23	9:1N:52:VAL:HG11	2.02	0.41
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.21	0.41
1:2A:76:C:O3'	24:22:59:ARG:HG2	2.21	0.41
1:2A:1257:C:H2'	1:2A:1258:C:C6	2.56	0.41
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.56	0.41
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.51	0.41
1:2A:959:A:N3	1:2A:2457:U:O2'	2.51	0.41
1:2A:2729:G:O2'	4:2E:186:GLY:HA3	2.21	0.41
6:2G:5:VAL:HG23	6:2G:8:LYS:HB2	2.02	0.41
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.20	0.41
1:2A:2723:C:H4'	13:2R:1:MET:HE3	2.02	0.41
30:18:31:HIS:ND1	30:18:32:LEU:HD13	2.36	0.40
1:1A:1259:G:H2'	1:1A:1260:G:H8	1.87	0.40
1:1A:182:A:H2'	1:1A:183:C:O4'	2.21	0.40
1:1A:2168:G:N1	1:1A:2171:A:C8	2.89	0.40
1:1A:2552:2MU:H2'	1:1A:2554:U:OP2	2.21	0.40
1:1A:741:G:H2'	1:1A:742:G:O4'	2.46	0.40
2:1B:89:G:C6	2:1B:90:A:C6	3.09	0.40
3:1D:148:GLU:OE1	3:1D:151:LYS:NZ	2.40	0.40
3:1D:155:LEU:HD23	3:1D:177:LEU:HD22	2.02	0.40
8:1I:122:GLU:HB2	8:1I:126:TYR:OH	2.21	0.40
21:1Z:30:ASN:HA	21:1Z:89:PHE:CE1	2.56	0.40
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.56	0.40
1:2A:1154:G:H8	1:2A:1154:G:O5'	2.04	0.40
1:2A:177:G:H3'	1:2A:178:G:C8	2.57	0.40
1:2A:218:A:C2	1:2A:235:U:H4'	2.56	0.40
1:2A:2291:U:O2'	1:2A:2374:C:O2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2556:C:H2'	1:2A:2557:G:O4'	2.21	0.40
1:2A:271(V):G:H2'	1:2A:271(W):G:O4'	2.21	0.40
1:2A:2786:U:H2'	1:2A:2787:C:H6	1.84	0.40
1:2A:407:G:H1	1:2A:420:C:H42	1.69	0.40
1:2A:533:G:H2'	1:2A:534:U:O4'	2.21	0.40
1:2A:852:G:H2'	1:2A:853:G:O4'	2.57	0.40
3:2D:145:VAL:HG22	3:2D:191:ALA:HB1	2.02	0.40
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.54	0.40
1:2A:443:A:N7	5:2F:45:ARG:HG2	2.36	0.40
8:2I:3:VAL:O	8:2I:18:VAL:HA	2.21	0.40
8:2I:94:ALA:HB2	8:2I:114:LEU:HD22	2.02	0.40
10:2O:68:GLU:CB	10:2O:78:ARG:HB2	2.52	0.40
1:2A:2414:G:N2	11:2P:67:MET:SD	2.89	0.40
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.54	0.40
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.21	0.40
1:1A:1844:C:H2'	1:1A:1845:G:H8	1.86	0.40
1:1A:2260:C:H2'	1:1A:2261:C:H6	1.86	0.40
1:1A:2752:C:OP2	7:1H:4:ILE:HD11	2.21	0.40
1:1A:520:G:H2'	1:1A:521:G:C8	2.56	0.40
2:1B:66:A:N6	2:1B:108:U:H2'	2.35	0.40
6:1G:152:LEU:HD23	6:1G:152:LEU:HA	1.90	0.40
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.21	0.40
6:1G:59:GLU:HB2	6:1G:144:ILE:HD12	2.02	0.40
26:24:69:LYS:HA	26:24:69:LYS:HD2	1.94	0.40
28:26:47:THR:HB	28:26:49:HIS:HE1	1.87	0.40
1:2A:1515:G:H2'	1:2A:1516:C:C6	2.57	0.40
1:2A:1605:C:H2'	1:2A:1606:G:O4'	2.22	0.40
1:2A:1770:G:H2'	1:2A:1771:C:O4'	2.21	0.40
1:2A:2338:G:H2'	1:2A:2339:G:C8	2.55	0.40
1:2A:2647:U:H2'	1:2A:2648:C:H6	1.86	0.40
1:2A:2732:G:OP1	4:2E:203:LYS:NZ	2.52	0.40
1:2A:2792:G:C6	1:2A:2805:G:C2	3.09	0.40
1:2A:2843:G:H2'	1:2A:2844:G:H8	1.86	0.40
1:2A:300:A:H8	1:2A:300:A:O5'	3.01	0.40
1:2A:359:A:H2'	1:2A:360:G:O4'	2.22	0.40
1:2A:416:C:H2'	1:2A:417:C:O4'	2.21	0.40
2:2B:16:G:C6	2:2B:69:G:C2	3.09	0.40
3:2D:254:THR:OG1	3:2D:254:THR:O	2.33	0.40
5:2F:183:VAL:O	5:2F:187:VAL:HG23	2.22	0.40
5:2F:155:LEU:HB3	5:2F:192:LEU:HG	2.04	0.40
15:2T:25:GLY:N	15:2T:99:LEU:HD11	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:46:LYS:HB2	20:2Y:46:LYS:HE3	1.90	0.40
1:1A:75:G:H4'	24:12:55:ARG:NH1	2.37	0.40
26:14:49:PHE:HD1	26:14:49:PHE:HA	1.75	0.40
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.56	0.40
1:1A:1792:G:O2'	1:1A:1830:C:OP1	2.33	0.40
1:1A:2590:A:H2'	1:1A:2591:C:C6	2.57	0.40
1:1A:272(A):U:HO2'	1:1A:272(B):G:P	2.42	0.40
1:1A:372:G:H3'	23:11:66:HIS:CE1	2.56	0.40
1:1A:489:G:H2'	1:1A:491:G:O4'	2.22	0.40
1:1A:962:G:H4'	1:1A:2496:C:O2'	2.21	0.40
5:1F:184:TYR:HE1	11:1P:3:LEU:HD21	1.86	0.40
7:1H:3:ARG:HA	7:1H:3:ARG:HD2	1.85	0.40
11:1P:98:GLU:HG3	11:1P:99:LEU:N	2.37	0.40
1:1A:910:A:C5	12:1Q:13:GLN:HG3	2.56	0.40
19:1X:3:THR:HG21	24:12:29:LYS:HD3	2.03	0.40
1:2A:98:G:H5''	24:22:3:LEU:HG	2.03	0.40
1:2A:1479:G:H5''	1:2A:1560:G:H4'	2.03	0.40
1:2A:1500:G:H2'	1:2A:1501:C:H6	1.86	0.40
1:2A:1613:G:C2	1:2A:1619:G:C5	3.09	0.40
1:2A:1792:G:H2'	1:2A:1793:C:H6	1.85	0.40
1:2A:2111:C:OP2	1:2A:2111:C:H2'	2.20	0.40
1:2A:2546:U:H5''	1:2A:2547:U:H5'	2.04	0.40
1:2A:2690:C:N4	1:2A:2713:A:H1'	2.35	0.40
1:2A:2850:A:H2	13:2R:61:HIS:CG	2.38	0.40
1:2A:601:C:O2'	1:2A:605:C:H5''	2.21	0.40
1:2A:678:C:H2'	1:2A:679:C:C6	2.56	0.40
1:2A:998:C:H2'	1:2A:999:U:O4'	2.21	0.40
8:2I:123:LEU:HD22	8:2I:144:VAL:HG23	2.02	0.40
11:2P:112:LEU:HD23	11:2P:112:LEU:HA	1.87	0.40
18:2W:88:ARG:HA	18:2W:88:ARG:HD2	1.94	0.40
1:1A:1021:A:N3	1:1A:1021:A:H3'	2.37	0.40
1:1A:1541:G:H3'	1:1A:1542:A:H2'	2.03	0.40
1:1A:1608:A:H1'	1:1A:1610:A:OP2	2.21	0.40
1:1A:1952:A:C6	1:1A:1953:A:N1	2.89	0.40
1:1A:2337:G:C2	1:1A:2338:G:C8	3.09	0.40
1:1A:2360:A:O5'	1:1A:2360:A:H8	2.04	0.40
1:1A:245:G:O5'	11:1P:73:GLY:HA2	2.21	0.40
1:1A:359:A:H2'	1:1A:360:G:O4'	2.22	0.40
1:1A:675:A:OP1	5:1F:63:LYS:NZ	2.48	0.40
4:1E:89:ASP:OD1	4:1E:89:ASP:N	2.54	0.40
5:1F:157:VAL:HB	5:1F:194:MET:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:89:PHE:HA	20:1Y:94:LYS:O	2.20	0.40
1:2A:2056:G:N2	27:25:5:PRO:HA	2.36	0.40
1:2A:1388:G:H4'	1:2A:1525:G:O2'	2.20	0.40
1:2A:196:A:N3	1:2A:196:A:H2'	2.35	0.40
1:2A:2303:G:O2'	6:2G:132:ASN:ND2	2.42	0.40
1:2A:2378:A:H8	1:2A:2378:A:O5'	2.05	0.40
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.21	0.40
1:2A:511:U:O4	1:2A:512:G:N1	2.54	0.40
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	2.04	0.40
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.55	0.40
23:11:51:VAL:HG11	23:11:74:VAL:HG21	2.03	0.40
26:14:58:ARG:HE	26:14:58:ARG:CA	2.32	0.40
1:1A:1121:C:H2'	1:1A:1122:G:O4'	2.21	0.40
1:1A:1279:G:H4'	13:1R:31:HIS:CD2	2.57	0.40
1:1A:1557:C:H5''	1:1A:1558:A:OP2	2.20	0.40
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.57	0.40
1:1A:210:C:OP2	29:17:29:LYS:NZ	2.34	0.40
1:1A:2256:G:H2'	1:1A:2257:U:O4'	2.22	0.40
1:1A:580:C:H2'	1:1A:581:C:C6	2.57	0.40
1:1A:65:C:H5'	19:1X:71:GLY:HA3	2.04	0.40
1:1A:844:C:C2'	1:1A:845:G:H5'	2.51	0.40
8:1I:26:ALA:HA	8:1I:30:LEU:HB2	2.04	0.40
8:1I:77:LEU:HD12	8:1I:101:LEU:HD13	2.04	0.40
10:1O:120:GLU:HB2	15:1T:68:TYR:CD2	2.57	0.40
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.62	0.40
1:2A:1482:G:H1	1:2A:1506:C:H42	1.69	0.40
1:2A:1500:G:H2'	1:2A:1501:C:C6	2.57	0.40
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.21	0.40
1:2A:1860:G:H2'	1:2A:1861:G:C8	2.54	0.40
1:2A:1936:A:H2	1:2A:1962:5MC:O2	2.04	0.40
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.20	0.40
1:2A:2484:G:C2	1:2A:2485:G:C8	3.09	0.40
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.56	0.40
1:2A:2822:G:O2'	1:2A:2824:C:OP2	2.29	0.40
1:2A:373:U:H2'	1:2A:374:A:C8	2.57	0.40
13:2R:87:TYR:OH	13:2R:117:VAL:O	2.30	0.40
14:2S:95:HIS:CG	14:2S:96:GLY:N	2.90	0.40
16:2U:88:ILE:HG22	16:2U:90:VAL:HG23	2.04	0.40
21:2Z:101:PRO:HA	21:2Z:123:ASP:HA	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	34	69
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	29	64
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	15	48
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	64
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	15	48
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25	60
6	2G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	25	60
7	1H	172/180 (96%)	159 (92%)	13 (8%)	0	100	100
7	2H	172/180 (96%)	162 (94%)	8 (5%)	2 (1%)	13	43
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	22	56
8	2I	144/148 (97%)	127 (88%)	16 (11%)	1 (1%)	22	56
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	53
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	11	39
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	51
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	53
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	4	20
17	2V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	15	48
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	131 (88%)	16 (11%)	1 (1%)	22	56
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100	100
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	46
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	7
26	24	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	7
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	6	28
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	23 (10%)	4 (2%)	9	34
33	2b	229/256 (90%)	205 (90%)	20 (9%)	4 (2%)	9	34
34	1c	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	64
34	2c	204/239 (85%)	192 (94%)	10 (5%)	2 (1%)	15	48
35	1d	206/209 (99%)	200 (97%)	4 (2%)	2 (1%)	15	48
35	2d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	64
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	11	39
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	11	39
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	7	30
38	2g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	22	56
39	1h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	22	56
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	1i	125/128 (98%)	116 (93%)	7 (6%)	2 (2%)	9	36
40	2i	125/128 (98%)	113 (90%)	10 (8%)	2 (2%)	9	36
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	6
41	2j	94/105 (90%)	83 (88%)	7 (7%)	4 (4%)	2	12
42	1k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	33
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	33
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	110 (91%)	11 (9%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	10 (8%)	0	100	100
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	34
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13	43
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	41
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	48
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	15	48
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	13	43
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	12
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	29
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11370/12128 (94%)	10654 (94%)	629 (6%)	87 (1%)	19	53

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
33	1b	17	PHE
35	1d	5	ILE
40	1i	54	ASP
5	2F	130	ALA
33	2b	127	ILE
40	2i	54	ASP
42	2k	106	LYS
5	1F	130	ALA
26	14	53	GLU
26	14	58	ARG
38	1g	114	ARG
42	1k	49	GLY
47	1p	53	VAL
51	1t	95	ALA
5	2F	89	VAL
6	2G	47	LYS
14	2S	96	GLY
35	2d	5	ILE
36	2e	98	THR
41	2j	33	GLN
41	2j	75	ILE

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Mol	Chain	Res	Type
47	2p	53	VAL
17	1V	53	GLU
17	1V	78	LYS
17	1V	100	ARG
21	1Z	134	PRO
23	1l	3	LYS
33	1b	20	GLU
36	1e	6	PHE
38	1g	52	GLU
40	1i	12	GLU
41	1j	55	LYS
51	1t	10	LEU
4	2E	113	PHE
10	2O	5	GLN
15	2T	56	GLY
26	24	47	GLN
26	24	55	ARG
33	2b	95	GLN
40	2i	12	GLU
41	2j	78	ASN
48	2q	68	ARG
51	2t	10	LEU
51	2t	47	GLY
4	1E	52	LEU
8	1I	117	GLU
20	1Y	78	ALA
26	14	57	GLU
41	1j	78	ASN
51	1t	47	GLY
4	2E	52	LEU
7	2H	92	ILE
7	2H	126	PRO
33	2b	20	GLU
36	2e	69	VAL
42	2k	49	GLY
50	2s	81	ARG
3	1D	127	VAL
26	14	56	VAL
38	1g	4	ARG
41	1j	79	ARG
46	1o	19	PRO
8	2I	104	GLN

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Mol	Chain	Res	Type
11	2P	36	LYS
29	27	47	ARG
41	2j	55	LYS
51	1t	100	ILE
11	2P	29	LYS
26	24	29	PRO
38	2g	4	ARG
45	2n	14	PRO
34	1c	66	VAL
36	1e	69	VAL
34	2c	66	VAL
41	1j	77	PRO
42	1k	105	VAL
39	1h	83	ILE
41	1j	91	PRO
48	1q	33	GLY
34	2c	14	ILE
33	1b	231	GLU
35	1d	178	VAL
41	1j	75	ILE
33	2b	231	GLU
33	1b	124	SER
26	24	64	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	207 (96%)	8 (4%)	34	66
3	2D	215/218 (99%)	205 (95%)	10 (5%)	26	59
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25	58
4	2E	164/166 (99%)	155 (94%)	9 (6%)	21	53
5	1F	160/166 (96%)	155 (97%)	5 (3%)	40	71
5	2F	159/166 (96%)	148 (93%)	11 (7%)	15	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	1G	143/156 (92%)	137 (96%)	6 (4%)	30	63
6	2G	143/156 (92%)	135 (94%)	8 (6%)	21	53
7	1H	144/148 (97%)	136 (94%)	8 (6%)	21	53
7	2H	144/148 (97%)	138 (96%)	6 (4%)	30	63
8	1I	113/124 (91%)	104 (92%)	9 (8%)	12	37
8	2I	105/124 (85%)	97 (92%)	8 (8%)	13	39
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19	50
9	2N	118/119 (99%)	110 (93%)	8 (7%)	16	45
10	1O	100/100 (100%)	94 (94%)	6 (6%)	19	50
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31	64
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29	62
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29	62
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	59	82
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	27	61
13	1R	101/101 (100%)	93 (92%)	8 (8%)	12	37
13	2R	101/101 (100%)	93 (92%)	8 (8%)	12	37
14	1S	86/88 (98%)	84 (98%)	2 (2%)	50	78
14	2S	85/88 (97%)	82 (96%)	3 (4%)	36	68
15	1T	115/127 (91%)	111 (96%)	4 (4%)	36	68
15	2T	113/127 (89%)	108 (96%)	5 (4%)	28	62
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	54
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	54
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18	48
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18	48
18	1W	90/92 (98%)	88 (98%)	2 (2%)	52	79
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	62
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	65
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	16
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	19	50
21	1Z	135/179 (75%)	127 (94%)	8 (6%)	19	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	52	79
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	71
23	11	80/83 (96%)	77 (96%)	3 (4%)	33	66
23	21	80/83 (96%)	78 (98%)	2 (2%)	47	76
24	12	65/67 (97%)	63 (97%)	2 (3%)	40	71
24	22	65/67 (97%)	64 (98%)	1 (2%)	65	85
25	13	51/52 (98%)	49 (96%)	2 (4%)	32	65
25	23	50/52 (96%)	49 (98%)	1 (2%)	55	80
26	14	59/63 (94%)	54 (92%)	5 (8%)	10	34
26	24	53/63 (84%)	52 (98%)	1 (2%)	57	81
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	26
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	50
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	15
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	26
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	27
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	41
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	53
30	28	54/55 (98%)	53 (98%)	1 (2%)	57	81
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	73
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	50
33	1b	192/220 (87%)	181 (94%)	11 (6%)	20	52
33	2b	187/220 (85%)	172 (92%)	15 (8%)	12	37
34	1c	142/188 (76%)	135 (95%)	7 (5%)	25	58
34	2c	140/188 (74%)	134 (96%)	6 (4%)	29	62
35	1d	169/181 (93%)	158 (94%)	11 (6%)	17	46
35	2d	173/181 (96%)	161 (93%)	12 (7%)	15	44
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28	62
36	2e	114/123 (93%)	108 (95%)	6 (5%)	22	55
37	1f	84/90 (93%)	80 (95%)	4 (5%)	25	59
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	1g	119/127 (94%)	115 (97%)	4 (3%)	37	69
38	2g	120/127 (94%)	116 (97%)	4 (3%)	38	70
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	28
39	2h	114/119 (96%)	108 (95%)	6 (5%)	22	55
40	1i	90/99 (91%)	85 (94%)	5 (6%)	21	53
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	22
41	1j	66/92 (72%)	64 (97%)	2 (3%)	41	72
41	2j	69/92 (75%)	66 (96%)	3 (4%)	29	62
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49	77
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25	59
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	63
43	2l	96/108 (89%)	90 (94%)	6 (6%)	18	48
44	1m	93/101 (92%)	93 (100%)	0	100	100
44	2m	92/101 (91%)	91 (99%)	1 (1%)	73	89
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	19
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	64
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33	66
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13	39
47	1p	69/74 (93%)	64 (93%)	5 (7%)	14	42
47	2p	68/74 (92%)	65 (96%)	3 (4%)	28	62
48	1q	94/97 (97%)	93 (99%)	1 (1%)	73	89
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29	62
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	56
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	45
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67	86
50	2s	67/80 (84%)	66 (98%)	1 (2%)	65	85
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	86
51	2t	70/82 (85%)	68 (97%)	2 (3%)	42	73
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	22
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8839 (95%)	464 (5%)	24	57

All (464) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	16	MET
3	1D	22	SER
3	1D	106	ILE
3	1D	162	SER
3	1D	181	GLU
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
4	1E	9	VAL
4	1E	21	VAL
4	1E	47	VAL
4	1E	75	VAL
4	1E	116	VAL
4	1E	119	ARG
4	1E	128	SER
4	1E	181	LEU
5	1F	33	LEU
5	1F	57	VAL
5	1F	106	ARG
5	1F	168	ARG
5	1F	170	LEU
6	1G	28	VAL
6	1G	53	LEU
6	1G	132	ASN
6	1G	140	ILE
6	1G	150	ASP
6	1G	159	VAL
7	1H	7	LEU
7	1H	18	GLU
7	1H	63	SER
7	1H	69	ARG
7	1H	70	THR
7	1H	84	SER
7	1H	98	LEU
7	1H	129	THR
8	1I	9	LEU
8	1I	38	LEU
8	1I	40	THR
8	1I	58	LEU
8	1I	92	VAL
8	1I	96	ASP
8	1I	109	ILE

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Mol	Chain	Res	Type
8	1I	117	GLU
8	1I	140	LEU
9	1N	9	VAL
9	1N	15	LEU
9	1N	34	LEU
9	1N	35	ARG
9	1N	46	VAL
9	1N	60	ILE
9	1N	99	LEU
10	1O	21	CYS
10	1O	24	VAL
10	1O	75	SER
10	1O	89	ASN
10	1O	107	ARG
10	1O	120	GLU
11	1P	59	LEU
11	1P	95	VAL
11	1P	98	GLU
11	1P	112	LEU
11	1P	148	LEU
12	1Q	1	MET
12	1Q	110	THR
13	1R	6	SER
13	1R	8	ARG
13	1R	24	GLN
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	111	LEU
14	1S	14	VAL
14	1S	71	ARG
15	1T	28	VAL
15	1T	51	ARG
15	1T	108	ARG
15	1T	118	ARG
16	1U	8	VAL
16	1U	54	LYS
16	1U	74	LEU
16	1U	77	SER
16	1U	95	LEU
17	1V	20	LEU

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Mol	Chain	Res	Type
17	1V	46	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	79	VAL
18	1W	66	GLU
18	1W	101	SER
20	1Y	11	ASP
20	1Y	14	LEU
20	1Y	43	ASN
20	1Y	50	ARG
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	86	ARG
20	1Y	90	LEU
20	1Y	91	GLU
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	1	MET
21	1Z	18	LEU
21	1Z	28	MET
21	1Z	41	LEU
21	1Z	70	LEU
21	1Z	123	ASP
21	1Z	139	VAL
21	1Z	171	ILE
23	11	3	LYS
23	11	30	VAL
23	11	38	SER
24	12	17	SER
24	12	52	ASP
25	13	34	GLU
25	13	58	VAL
26	14	27	THR
26	14	49	PHE
26	14	56	VAL
26	14	57	GLU
26	14	58	ARG
27	15	16	ARG
27	15	26	THR
27	15	29	THR
27	15	33	CYS
27	15	58	LEU

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Mol	Chain	Res	Type
28	16	4	GLU
28	16	9	LEU
28	16	13	CYS
28	16	24	GLU
28	16	33	LYS
28	16	48	VAL
28	16	51	GLU
29	17	1	MET
29	17	39	ARG
29	17	43	THR
29	17	46	VAL
30	18	30	ARG
30	18	31	HIS
30	18	32	LEU
31	19	26	ILE
33	1b	8	LYS
33	1b	10	LEU
33	1b	12	GLU
33	1b	21	ARG
33	1b	93	VAL
33	1b	111	ARG
33	1b	115	LEU
33	1b	127	ILE
33	1b	185	ILE
33	1b	187	LEU
33	1b	230	VAL
34	1c	3	ASN
34	1c	112	SER
34	1c	154	SER
34	1c	172	ARG
34	1c	175	LEU
34	1c	190	ARG
34	1c	195	VAL
35	1d	5	ILE
35	1d	10	ARG
35	1d	28	SER
35	1d	59	ARG
35	1d	71	SER
35	1d	83	SER
35	1d	135	LEU
35	1d	158	ILE
35	1d	178	VAL

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Mol	Chain	Res	Type
35	1d	194	LEU
35	1d	196	LEU
36	1e	27	ARG
36	1e	65	ASN
36	1e	81	GLU
36	1e	133	TYR
36	1e	148	VAL
37	1f	17	SER
37	1f	70	ASP
37	1f	75	LEU
37	1f	94	GLN
38	1g	90	GLU
38	1g	92	SER
38	1g	115	ARG
38	1g	125	MET
39	1h	12	ARG
39	1h	19	VAL
39	1h	26	VAL
39	1h	50	ARG
39	1h	51	VAL
39	1h	63	LEU
39	1h	85	ARG
39	1h	91	ARG
39	1h	104	ARG
39	1h	113	SER
39	1h	127	LEU
40	1i	64	THR
40	1i	83	ARG
40	1i	92	TYR
40	1i	111	ARG
40	1i	128	ARG
41	1j	49	VAL
41	1j	92	THR
42	1k	109	VAL
42	1k	116	HIS
43	1l	28	LYS
43	1l	37	CYS
43	1l	53	ARG
43	1l	55	VAL
45	1n	3	ARG
45	1n	7	ILE
45	1n	18	VAL

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Mol	Chain	Res	Type
45	1n	32	SER
45	1n	33	VAL
45	1n	35	ARG
46	1o	24	SER
46	1o	28	GLN
46	1o	70	LEU
47	1p	6	LEU
47	1p	19	ILE
47	1p	20	VAL
47	1p	45	THR
47	1p	67	THR
48	1q	68	ARG
49	1r	30	ASP
49	1r	31	LEU
49	1r	54	ARG
50	1s	32	LYS
51	1t	10	LEU
52	1u	3	LYS
52	1u	20	LYS
3	2D	14	ARG
3	2D	50	THR
3	2D	61	LEU
3	2D	88	ARG
3	2D	106	ILE
3	2D	169	GLU
3	2D	211	ARG
3	2D	237	GLU
3	2D	242	ARG
3	2D	254	THR
4	2E	21	VAL
4	2E	47	VAL
4	2E	75	VAL
4	2E	89	ASP
4	2E	92	THR
4	2E	101	ARG
4	2E	107	THR
4	2E	116	VAL
4	2E	184	VAL
5	2F	50	SER
5	2F	57	VAL
5	2F	70	THR
5	2F	88	VAL

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Mol	Chain	Res	Type
5	2F	98	SER
5	2F	106	ARG
5	2F	110	LEU
5	2F	149	ASP
5	2F	153	SER
5	2F	195	ASP
5	2F	201	VAL
6	2G	5	VAL
6	2G	7	LEU
6	2G	9	ARG
6	2G	16	ARG
6	2G	43	LEU
6	2G	79	ASN
6	2G	126	ASP
6	2G	159	VAL
7	2H	18	GLU
7	2H	45	VAL
7	2H	53	GLU
7	2H	70	THR
7	2H	84	SER
7	2H	136	ILE
8	2I	31	LEU
8	2I	38	LEU
8	2I	40	THR
8	2I	72	LEU
8	2I	114	LEU
8	2I	123	LEU
8	2I	127	VAL
8	2I	144	VAL
9	2N	15	LEU
9	2N	28	THR
9	2N	35	ARG
9	2N	38	HIS
9	2N	43	THR
9	2N	58	ASP
9	2N	67	LEU
9	2N	73	THR
10	2O	10	VAL
10	2O	24	VAL
10	2O	65	THR
10	2O	98	VAL
11	2P	3	LEU

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Mol	Chain	Res	Type
11	2P	4	SER
11	2P	95	VAL
11	2P	121	LYS
11	2P	148	LEU
12	2Q	1	MET
12	2Q	31	ASP
12	2Q	35	VAL
12	2Q	106	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	44	LEU
13	2R	59	ASP
13	2R	65	LEU
13	2R	67	LEU
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU
14	2S	27	SER
14	2S	48	LEU
14	2S	63	THR
15	2T	13	ARG
15	2T	89	VAL
15	2T	93	ARG
15	2T	96	ARG
15	2T	111	ARG
16	2U	8	VAL
16	2U	50	ARG
16	2U	74	LEU
16	2U	77	SER
16	2U	95	LEU
17	2V	33	VAL
17	2V	38	LEU
17	2V	46	VAL
17	2V	61	VAL
17	2V	79	VAL
18	2W	23	LEU
18	2W	35	ILE
18	2W	67	ASP
18	2W	100	THR
19	2X	14	SER
19	2X	30	VAL
19	2X	62	LYS

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Mol	Chain	Res	Type
20	2Y	1	MET
20	2Y	39	VAL
20	2Y	49	VAL
20	2Y	90	LEU
20	2Y	99	CYS
21	2Z	38	TYR
21	2Z	70	LEU
21	2Z	91	LEU
22	20	14	ARG
22	20	55	ARG
23	21	4	VAL
23	21	82	LEU
24	22	11	GLU
25	23	30	ARG
26	24	49	PHE
27	25	6	VAL
27	25	29	THR
27	25	58	LEU
28	26	7	ILE
28	26	9	LEU
28	26	14	THR
28	26	20	ASN
28	26	49	HIS
29	27	1	MET
29	27	42	LEU
29	27	46	VAL
30	28	14	VAL
31	29	7	VAL
31	29	22	ARG
33	2b	8	LYS
33	2b	12	GLU
33	2b	19	HIS
33	2b	67	THR
33	2b	71	VAL
33	2b	93	VAL
33	2b	94	ASN
33	2b	103	THR
33	2b	109	SER
33	2b	111	ARG
33	2b	122	PHE
33	2b	127	ILE
33	2b	135	GLN

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Mol	Chain	Res	Type
33	2b	195	ASP
33	2b	213	LEU
34	2c	17	ASP
34	2c	43	LEU
34	2c	56	ASP
34	2c	119	ARG
34	2c	172	ARG
34	2c	196	LEU
35	2d	31	CYS
35	2d	47	ARG
35	2d	59	ARG
35	2d	96	LEU
35	2d	107	ARG
35	2d	135	LEU
35	2d	158	ILE
35	2d	170	VAL
35	2d	175	SER
35	2d	178	VAL
35	2d	190	ASP
35	2d	196	LEU
36	2e	41	VAL
36	2e	51	VAL
36	2e	68	GLU
36	2e	76	ILE
36	2e	81	GLU
36	2e	117	ASP
37	2f	31	GLU
37	2f	72	VAL
37	2f	75	LEU
37	2f	94	GLN
38	2g	15	ASP
38	2g	79	ARG
38	2g	98	SER
38	2g	114	ARG
39	2h	2	LEU
39	2h	18	ARG
39	2h	104	ARG
39	2h	112	LEU
39	2h	120	THR
39	2h	135	CYS
40	2i	5	TYR
40	2i	9	ARG

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Mol	Chain	Res	Type
40	2i	17	VAL
40	2i	23	ASN
40	2i	53	VAL
40	2i	65	VAL
40	2i	83	ARG
40	2i	99	LEU
40	2i	102	LEU
40	2i	111	ARG
41	2j	35	SER
41	2j	38	ILE
41	2j	51	ARG
42	2k	30	VAL
42	2k	91	ARG
42	2k	114	VAL
42	2k	119	CYS
43	2l	6	THR
43	2l	27	LEU
43	2l	33	ARG
43	2l	73	GLU
43	2l	83	VAL
43	2l	112	ASP
44	2m	32	GLU
45	2n	18	VAL
45	2n	33	VAL
46	2o	5	LYS
46	2o	58	MET
46	2o	64	ARG
46	2o	65	ARG
46	2o	66	LEU
46	2o	87	ILE
47	2p	20	VAL
47	2p	67	THR
47	2p	69	THR
48	2q	9	VAL
48	2q	66	SER
48	2q	67	LYS
48	2q	79	SER
49	2r	31	LEU
49	2r	69	THR
49	2r	76	LEU
49	2r	85	LEU
50	2s	62	ILE

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Mol	Chain	Res	Type
51	2t	15	ARG
51	2t	71	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
5	1F	8	GLN
5	1F	40	GLN
5	1F	69	HIS
6	1G	58	GLN
6	1G	132	ASN
7	1H	147	ASN
8	1I	11	ASN
8	1I	74	ASN
10	1O	5	GLN
13	1R	13	HIS
16	1U	94	ASN
17	1V	64	HIS
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	32	HIS
21	1Z	34	ASN
21	1Z	55	HIS
22	10	3	HIS
22	10	29	GLN
24	12	65	ASN
33	1b	94	ASN
34	1c	6	HIS
34	1c	98	ASN
34	1c	162	GLN
34	1c	176	HIS
35	1d	42	GLN
35	1d	43	HIS
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	161	ASN
36	1e	78	HIS
38	1g	13	GLN
38	1g	28	ASN
38	1g	51	GLN

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Mol	Chain	Res	Type
38	1g	148	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	58	HIS
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
44	1m	77	ASN
46	1o	46	HIS
48	1q	26	GLN
49	1r	63	GLN
50	1s	83	HIS
3	2D	115	GLN
5	2F	69	HIS
5	2F	75	HIS
6	2G	41	GLN
10	2O	5	GLN
13	2R	13	HIS
15	2T	58	ASN
15	2T	79	HIS
16	2U	94	ASN
21	2Z	32	HIS
21	2Z	55	HIS
21	2Z	73	GLN
22	20	12	ASN
24	22	65	ASN
28	26	20	ASN
30	28	35	GLN
33	2b	37	ASN
33	2b	94	ASN
33	2b	212	GLN
34	2c	37	GLN
34	2c	102	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	129	ASN
36	2e	65	ASN
38	2g	28	ASN
38	2g	37	ASN
38	2g	51	GLN
38	2g	64	GLN

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Mol	Chain	Res	Type
38	2g	68	ASN
38	2g	148	ASN
40	2i	31	GLN
40	2i	58	HIS
41	2j	33	GLN
41	2j	56	HIS
42	2k	116	HIS
44	2m	77	ASN
46	2o	53	HIS
46	2o	62	GLN
47	2p	16	HIS
50	2s	69	HIS
50	2s	83	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2860/2915 (98%)	474 (16%)	22 (0%)
1	2A	2788/2915 (95%)	531 (19%)	22 (0%)
2	1B	119/121 (98%)	14 (11%)	0
2	2B	118/121 (97%)	17 (14%)	0
32	1a	1494/1521 (98%)	279 (18%)	0
32	2a	1498/1521 (98%)	311 (20%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	7/24 (29%)	3 (42%)	0
54	1w	68/76 (89%)	15 (22%)	0
54	1y	71/76 (93%)	27 (38%)	0
54	2w	65/76 (85%)	18 (27%)	0
54	2y	69/76 (90%)	24 (34%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	10 (13%)	0
All	All	9319/9620 (96%)	1736 (18%)	44 (0%)

All (1736) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C

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Mol	Chain	Res	Type
1	1A	50	U
1	1A	55	G
1	1A	58	G
1	1A	63	U
1	1A	64	A
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	83	G
1	1A	84	A
1	1A	95	G
1	1A	102	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	140	G
1	1A	149	A
1	1A	177	G
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	223	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	245	G
1	1A	248	G
1	1A	261	G
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(S)	G
1	1A	272(B)	G

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Mol	Chain	Res	Type
1	1A	272(H)	C
1	1A	275	G
1	1A	279	C
1	1A	285	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	372	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	421	U
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	512	G
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	551	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	614(C)	A
1	1A	615	G

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Mol	Chain	Res	Type
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	724	U
1	1A	730	C
1	1A	738	G
1	1A	762	U
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	788	A
1	1A	789	A
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	845	G
1	1A	855	G
1	1A	859	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	889	C
1	1A	890	A
1	1A	892	G
1	1A	895	U

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Mol	Chain	Res	Type
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	914	C
1	1A	915	C
1	1A	926	A
1	1A	931	G
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	980	A
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1025	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1042	G
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	1059	G
1	1A	1063	G
1	1A	1064	C
1	1A	1066	U
1	1A	1070	A
1	1A	1071	G

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Mol	Chain	Res	Type
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	1083	U
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1094	U
1	1A	1096	A
1	1A	1098	A
1	1A	1101	U
1	1A	1102	C
1	1A	1103	A
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1130	U
1	1A	1132	A
1	1A	1135	C
1	1A	1136	G
1	1A	1142(A)	A
1	1A	1149	G
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	1187	G
1	1A	1211	U
1	1A	1218	C
1	1A	1229	G
1	1A	1236	G
1	1A	1237	A
1	1A	1244	G

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Mol	Chain	Res	Type
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1308	A
1	1A	1314	C
1	1A	1316	U
1	1A	1319	G
1	1A	1320	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1429	G
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C
1	1A	1482	G
1	1A	1484	G
1	1A	1490	A
1	1A	1493	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1540	U
1	1A	1554	A

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Mol	Chain	Res	Type
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1667	G
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1746	G
1	1A	1747	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1786	A
1	1A	1791	A
1	1A	1798	U
1	1A	1800	C
1	1A	1801	G
1	1A	1802	A
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1847	A
1	1A	1858	G
1	1A	1861	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A

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Mol	Chain	Res	Type
1	1A	1919	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2049	G
1	1A	2052	G
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2063	C
1	1A	2069	G
1	1A	2093	G
1	1A	2098	U
1	1A	2102	U
1	1A	2104	G
1	1A	2108	C
1	1A	2110	G
1	1A	2112	G
1	1A	2113	U
1	1A	2120	G
1	1A	2121	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U

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Mol	Chain	Res	Type
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	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2166	G
1	1A	2168	G
1	1A	2170	A
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2178	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
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	2268	A
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2294	C
1	1A	2296	U
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
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	2384	G
1	1A	2385	C
1	1A	2391	G
1	1A	2406	U
1	1A	2410	G
1	1A	2423	U
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2438	U
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2535	G
1	1A	2537	U

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Mol	Chain	Res	Type
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2585	U
1	1A	2586	C
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	2641	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2732	G
1	1A	2733	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A
1	1A	2791	C
1	1A	2792	G
1	1A	2793	G
1	1A	2802	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2834	G
1	1A	2835	A
1	1A	2839	G

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Mol	Chain	Res	Type
1	1A	2858	C
1	1A	2872	G
1	1A	2873	A
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	13	A
2	1B	15	A
2	1B	24	G
2	1B	25	A
2	1B	35	U
2	1B	41	U
2	1B	50	G
2	1B	54	G
2	1B	56	G
2	1B	67	G
2	1B	73	A
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	46	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	69	G
32	1a	70	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	129(A)	G
32	1a	131	C

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Mol	Chain	Res	Type
32	1a	144	G
32	1a	153	C
32	1a	159	G
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(G)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	200	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	219	C
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	257	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	306	G
32	1a	318	G
32	1a	325	A
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	358	U
32	1a	359	U
32	1a	365	U
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A

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Mol	Chain	Res	Type
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	419	C
32	1a	422	C
32	1a	423	G
32	1a	428	G
32	1a	429	U
32	1a	430	A
32	1a	434	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	474	G
32	1a	480	U
32	1a	482	A
32	1a	484	G
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	519	C
32	1a	522	C
32	1a	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	702	A
32	1a	721	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	749	C
32	1a	755	G
32	1a	760	G
32	1a	777	A
32	1a	786	G
32	1a	793	U
32	1a	794	A
32	1a	799	G
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	818	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	873	A
32	1a	885	G
32	1a	891	U
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	934	C
32	1a	935	A
32	1a	939	G
32	1a	958	A
32	1a	960	U
32	1a	961	U
32	1a	964	A
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
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	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1045	C
32	1a	1053	G
32	1a	1054	C
32	1a	1055	A
32	1a	1066	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1068	G
32	1a	1081	G
32	1a	1087	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1117	G
32	1a	1122	U
32	1a	1124	G
32	1a	1125	U
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1145	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1160	G
32	1a	1166	G
32	1a	1182	G
32	1a	1183	A
32	1a	1184	G
32	1a	1186	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1215	G
32	1a	1225	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U

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Mol	Chain	Res	Type
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1277	C
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1305	G
32	1a	1312	G
32	1a	1314	C
32	1a	1323	G
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1368	G
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C
32	1a	1403	C
32	1a	1404	5MC
32	1a	1419	G
32	1a	1436	U
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1460	A
32	1a	1475	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A

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Mol	Chain	Res	Type
32	1a	1517	G
32	1a	1520	G
32	1a	1524	C
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	19	PSU
53	1v	24	A
54	1w	3	C
54	1w	7	A
54	1w	10	G
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	29	G
54	1w	42	C
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	68	C
54	1w	69	G
55	1x	3	C
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	21	A
55	1x	47	U
55	1x	53	G
55	1x	61	C
55	1x	69	C
55	1x	76	A
54	1y	2	C
54	1y	3	C
54	1y	5	G
54	1y	6	G
54	1y	8	4SU
54	1y	9	A
54	1y	13	C
54	1y	14	A

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Mol	Chain	Res	Type
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	31	A
54	1y	35	A
54	1y	44	G
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	53	G
54	1y	57	G
54	1y	58	A
54	1y	59	U
54	1y	61	C
54	1y	65	G
54	1y	66	U
54	1y	69	G
54	1y	70	G
1	2A	10	G
1	2A	12	U
1	2A	15	G
1	2A	16	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	104	U
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G

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Mol	Chain	Res	Type
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	267	C
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	271(O)	C
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	280	C
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	346	A
1	2A	348	G
1	2A	352	G
1	2A	354	G
1	2A	362	U
1	2A	363	G
1	2A	363(D)	G
1	2A	363(E)	U
1	2A	386	G

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Mol	Chain	Res	Type
1	2A	403	U
1	2A	404	C
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	444	C
1	2A	451	C
1	2A	455	C
1	2A	457	A
1	2A	479	A
1	2A	480	A
1	2A	481	G
1	2A	494	G
1	2A	496	G
1	2A	500	G
1	2A	505	A
1	2A	509	C
1	2A	527	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	551	G
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	592	G
1	2A	595	C
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	613	G
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A

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Mol	Chain	Res	Type
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	715	G
1	2A	717	G
1	2A	726	G
1	2A	729	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	825	C
1	2A	827	U
1	2A	828	U
1	2A	852	G
1	2A	857	C
1	2A	859	G
1	2A	869	G
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

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Mol	Chain	Res	Type
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	919	G
1	2A	932	G
1	2A	933	A
1	2A	934	G
1	2A	936	C
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	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	989	G
1	2A	990	A
1	2A	996	A
1	2A	997	G
1	2A	1005	C
1	2A	1010	A
1	2A	1012	U
1	2A	1013	C
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1040	C

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Mol	Chain	Res	Type
1	2A	1043	C
1	2A	1116	C
1	2A	1122	G
1	2A	1126	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1138	G
1	2A	1141	U
1	2A	1142(A)	A
1	2A	1167	U
1	2A	1171	G
1	2A	1195	G
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1218	C
1	2A	1220	A
1	2A	1224	C
1	2A	1237	A
1	2A	1247	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1275	A
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1306	C
1	2A	1314	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	1376	C
1	2A	1384	A

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Mol	Chain	Res	Type
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1402	C
1	2A	1403	C
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	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1541	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A

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Mol	Chain	Res	Type
1	2A	1582	C
1	2A	1584	C
1	2A	1586	A
1	2A	1589	C
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1622	G
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1663	C
1	2A	1664	A
1	2A	1667	G
1	2A	1674	G
1	2A	1680	U
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1706	U
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1745(A)	C
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	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1808	U
1	2A	1812	A
1	2A	1816	G

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Mol	Chain	Res	Type
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1967	C
1	2A	1969	A
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1983	C
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2036	C
1	2A	2037	G
1	2A	2043	C
1	2A	2052	G
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G

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Mol	Chain	Res	Type
1	2A	2092	U
1	2A	2093	G
1	2A	2099	U
1	2A	2102	U
1	2A	2106	G
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2113	U
1	2A	2114	A
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2141	G
1	2A	2143	C
1	2A	2144	U
1	2A	2146	C
1	2A	2150	U
1	2A	2153	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2160	G
1	2A	2161	C
1	2A	2162	G

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Mol	Chain	Res	Type
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2178	C
1	2A	2181	G
1	2A	2182	G
1	2A	2185	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2239	G
1	2A	2248	C
1	2A	2268	A
1	2A	2273	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2285	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2310	A
1	2A	2311	A
1	2A	2316	C
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2344	U

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Mol	Chain	Res	Type
1	2A	2346	A
1	2A	2347	C
1	2A	2352	A
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2422	A
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	2447	G
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2480	C
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2530	A
1	2A	2536	G
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G

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Mol	Chain	Res	Type
1	2A	2578	G
1	2A	2592	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2654	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	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2751	G
1	2A	2757	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2779	U
1	2A	2780	G
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2810	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G

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Mol	Chain	Res	Type
1	2A	2879	C
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	13	A
2	2B	15	A
2	2B	22	U
2	2B	24	G
2	2B	32	C
2	2B	35	U
2	2B	41	U
2	2B	44	G
2	2B	45	A
2	2B	56	G
2	2B	67	G
2	2B	73	A
2	2B	85	G
2	2B	109	C
2	2B	110	G
2	2B	120	A
32	2a	6	G
32	2a	9	G
32	2a	22	G
32	2a	31	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	54	C
32	2a	65	U
32	2a	66	G
32	2a	89	C
32	2a	90	U
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C

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Mol	Chain	Res	Type
32	2a	151	A
32	2a	152	A
32	2a	159	G
32	2a	162	A
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189	G
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	189(H)	G
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	281	G
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	348	G
32	2a	351	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	383	A
32	2a	384	G
32	2a	397	A
32	2a	398	C

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Mol	Chain	Res	Type
32	2a	404	U
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	418	C
32	2a	424	G
32	2a	427	U
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	484	G
32	2a	485	G
32	2a	495	A
32	2a	496	A
32	2a	498	U
32	2a	499	A
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	512	U
32	2a	518	C
32	2a	521	G
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
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G

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Mol	Chain	Res	Type
32	2a	596	C
32	2a	618	C
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	660	G
32	2a	665	A
32	2a	666	G
32	2a	681	C
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	708	C
32	2a	720	C
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	748	C
32	2a	749	C
32	2a	755	G
32	2a	768	A
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	819	A
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	871	U
32	2a	872	A
32	2a	873	A
32	2a	902	G
32	2a	914	A
32	2a	926	G

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Mol	Chain	Res	Type
32	2a	927	G
32	2a	931	C
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	936	C
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	967	5MC
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1001	A
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	1011	G
32	2a	1016	A
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1030	C
32	2a	1030(A)	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1031	G
32	2a	1033	G
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1044	A
32	2a	1053	G
32	2a	1061	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1084	G
32	2a	1085	U
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1099	G
32	2a	1101	A
32	2a	1113	C
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1144	G
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1159	U
32	2a	1160	G
32	2a	1171	G
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A

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Mol	Chain	Res	Type
32	2a	1184	G
32	2a	1192	C
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1210	C
32	2a	1211	U
32	2a	1213	A
32	2a	1214	C
32	2a	1226	C
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1262	C
32	2a	1267	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1275	A
32	2a	1276	G
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1290	G
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1311	G
32	2a	1312	G

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Mol	Chain	Res	Type
32	2a	1322	C
32	2a	1323	G
32	2a	1337	G
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1376	U
32	2a	1381	U
32	2a	1397	C
32	2a	1398	A
32	2a	1400	5MC
32	2a	1401	G
32	2a	1404	5MC
32	2a	1419	G
32	2a	1440	C
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	19	PSU
53	2v	22	U
53	2v	23	A
54	2w	3	C

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Mol	Chain	Res	Type
54	2w	8	4SU
54	2w	9	A
54	2w	10	G
54	2w	11	C
54	2w	14	A
54	2w	19	G
54	2w	24	G
54	2w	25	C
54	2w	34	G
54	2w	41	C
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	61	C
54	2w	63	G
54	2w	68	C
54	2w	69	G
55	2x	9	G
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	43	A
55	2x	47	U
55	2x	48	C
55	2x	61	C
55	2x	69	C
55	2x	76	A
54	2y	13	C
54	2y	15	G
54	2y	19	G
54	2y	23	A
54	2y	27	G
54	2y	34	G
54	2y	36	A
54	2y	40	C
54	2y	43	C
54	2y	45	U
54	2y	46	7MG
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU

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Mol	Chain	Res	Type
54	2y	56	C
54	2y	57	G
54	2y	59	U
54	2y	61	C
54	2y	62	C
54	2y	65	G
54	2y	69	G
54	2y	70	G
54	2y	72	C

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	266	G
1	1A	278	A
1	1A	895	U
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1175	U
1	1A	1210	A
1	1A	1442	G
1	1A	1508	A
1	1A	1653	G
1	1A	1992	G
1	1A	2111	C
1	1A	2126	A
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2601	C
1	1A	2629	A
1	1A	2689	U
1	2A	195	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A

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Mol	Chain	Res	Type
1	2A	752	A
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2156	G
1	2A	2351	G
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	$\# Z  > 2$
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.65	4 (22%)
32	M2G	2a	966	32	20,27,28	1.41	3 (15%)	22,40,43	2.12	5 (22%)
55	PSU	2x	55	55	17,21,22	1.50	2 (11%)	20,30,33	3.11	6 (30%)
43	0TD	1l	92	43	4,9,10	3.08	1 (25%)	3,11,13	9.13	1 (33%)
54	5MU	1y	54	54	15,22,23	1.04	1 (6%)	16,32,35	1.72	2 (12%)
54	PSU	2w	32	54	17,21,22	1.58	2 (11%)	20,30,33	3.16	6 (30%)
55	4SU	1x	8	55,56	14,21,22	1.44	2 (14%)	15,30,33	2.13	2 (13%)
54	PSU	1w	32	54	17,21,22	1.55	2 (11%)	20,30,33	3.12	6 (30%)
1	5MC	2A	1962	1	15,22,23	1.30	1 (6%)	19,32,35	1.39	3 (15%)
32	MA6	2a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.60	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	5MC	1a	967	32	15,22,23	1.27	1 (6%)	19,32,35	1.31	3 (15%)
54	MIA	2y	37	54,32	18,24,32	1.13	2 (11%)	18,35,47	1.22	2 (11%)
54	4SU	1y	8	54	14,21,22	1.28	1 (7%)	15,30,33	1.41	2 (13%)
53	PSU	2v	19	54,56,53	17,21,22	1.68	2 (11%)	20,30,33	3.41	6 (30%)
55	4SU	2x	8	55,56	14,21,22	1.27	2 (14%)	15,30,33	2.21	2 (13%)
32	2MG	1a	1207	32	19,26,27	1.21	2 (10%)	21,38,41	2.21	8 (38%)
54	5MU	2y	54	54	15,22,23	1.07	1 (6%)	16,32,35	1.92	2 (12%)
32	4OC	2a	1402	32,56	16,23,24	0.58	0	17,32,35	1.39	1 (5%)
32	7MG	2a	527	32	22,26,27	1.76	4 (18%)	28,39,42	2.77	9 (32%)
54	MIA	1w	37	54	24,31,32	2.27	3 (12%)	26,44,47	2.54	10 (38%)
1	2MU	1A	2552	1,56	14,22,24	0.88	0	14,31,36	0.84	1 (7%)
54	MIA	2w	37	54	20,27,32	1.84	2 (10%)	22,39,47	1.87	7 (31%)
54	PSU	2y	55	54	17,21,22	1.50	3 (17%)	20,30,33	3.13	7 (35%)
54	4SU	2y	8	54,56	14,21,22	1.33	1 (7%)	15,30,33	1.26	2 (13%)
54	PSU	1w	55	54	17,21,22	1.46	2 (11%)	20,30,33	3.40	6 (30%)
54	PSU	2w	39	54	17,21,22	1.40	2 (11%)	20,30,33	2.85	6 (30%)
1	5MU	1A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	1.83	2 (12%)
54	PSU	2y	32	54	17,21,22	1.47	3 (17%)	20,30,33	3.09	6 (30%)
1	2MU	2A	2552	1,56	14,22,24	0.89	0	14,31,36	0.81	1 (7%)
54	7MG	2w	46	54	22,26,27	1.79	4 (18%)	28,39,42	2.73	9 (32%)
54	5MU	1w	54	54	15,22,23	1.04	2 (13%)	16,32,35	2.28	1 (6%)
1	5MU	2A	1939	1	15,22,23	1.08	1 (6%)	16,32,35	1.80	2 (12%)
54	7MG	2y	46	54	22,26,27	1.85	4 (18%)	28,39,42	3.07	10 (35%)
1	OMG	2A	2251	1,55	18,26,27	1.16	2 (11%)	20,38,41	2.05	6 (30%)
55	5MU	1x	54	55	15,22,23	1.09	1 (6%)	16,32,35	1.91	1 (6%)
32	M2G	1a	966	32	20,27,28	1.40	3 (15%)	22,40,43	2.18	5 (22%)
54	7MG	1y	46	54	22,26,27	1.85	4 (18%)	28,39,42	3.04	10 (35%)
1	5MC	1A	1962	1	15,22,23	1.36	1 (6%)	19,32,35	1.30	3 (15%)
32	MA6	1a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.72	6 (33%)
32	5MC	2a	1407	32,56	15,22,23	1.33	1 (6%)	19,32,35	1.29	2 (10%)
1	PSU	1A	2605	1	17,21,22	1.46	2 (11%)	20,30,33	3.11	6 (30%)
1	PSU	1A	1911	1	17,21,22	1.61	3 (17%)	20,30,33	3.11	6 (30%)
54	PSU	2w	55	54	17,21,22	1.48	2 (11%)	20,30,33	3.45	7 (35%)
54	PSU	1y	39	54	17,21,22	1.48	2 (11%)	20,30,33	2.96	5 (25%)
54	4SU	2w	8	54	14,21,22	1.31	1 (7%)	15,30,33	1.40	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	2MG	2a	1207	32,56	19,26,27	1.25	2 (10%)	21,38,41	2.13	6 (28%)
32	5MC	1a	1407	32	15,22,23	1.30	1 (6%)	19,32,35	1.32	3 (15%)
1	5MC	1A	1942	1	15,22,23	1.23	1 (6%)	19,32,35	1.39	3 (15%)
1	PSU	2A	2605	1	17,21,22	1.56	3 (17%)	20,30,33	3.18	6 (30%)
43	0TD	2l	92	43	4,9,10	3.09	1 (25%)	3,11,13	10.39	1 (33%)
1	2MA	1A	2503	1,56	17,25,26	1.37	2 (11%)	19,37,40	2.07	3 (15%)
32	5MC	1a	1404	32	15,22,23	1.34	1 (6%)	19,32,35	1.33	3 (15%)
32	5MC	1a	1400	32	15,22,23	1.30	1 (6%)	19,32,35	1.40	3 (15%)
32	PSU	1a	516	32	17,21,22	1.51	3 (17%)	20,30,33	3.20	5 (25%)
1	2MA	2A	2503	1	17,25,26	1.29	2 (11%)	19,37,40	2.07	3 (15%)
1	5MU	1A	1939	1	15,22,23	1.12	2 (13%)	16,32,35	1.89	2 (12%)
32	UR3	1a	1498	32	14,22,23	0.71	0	15,32,35	0.63	0
1	4OC	2A	1920	1	15,22,24	0.64	0	17,31,35	1.46	2 (11%)
1	PSU	1A	1917	1	17,21,22	1.54	2 (11%)	20,30,33	3.06	6 (30%)
54	MIA	1y	37	54	18,24,32	1.12	2 (11%)	18,35,47	1.19	2 (11%)
53	PSU	1v	19	54,53	17,21,22	1.46	3 (17%)	20,30,33	3.56	6 (30%)
32	5MC	2a	967	32	15,22,23	1.33	1 (6%)	19,32,35	1.34	3 (15%)
32	5MC	2a	1404	32	15,22,23	1.27	1 (6%)	19,32,35	1.49	4 (21%)
32	5MC	2a	1400	32	15,22,23	1.35	1 (6%)	19,32,35	1.46	2 (10%)
32	4OC	1a	1402	32	16,23,24	0.63	0	17,32,35	1.16	1 (5%)
54	PSU	2y	39	54	17,21,22	1.47	2 (11%)	20,30,33	3.36	7 (35%)
55	PSU	1x	55	55	17,21,22	1.61	2 (11%)	20,30,33	3.09	6 (30%)
54	PSU	1w	39	54	17,21,22	1.51	2 (11%)	20,30,33	2.82	5 (25%)
1	4OC	1A	1920	1	15,22,24	0.69	0	17,31,35	1.43	2 (11%)
55	5MC	1x	32	55	15,22,23	1.31	1 (6%)	19,32,35	1.33	3 (15%)
1	PSU	2A	1911	1	17,21,22	1.57	2 (11%)	20,30,33	3.15	6 (30%)
32	MA6	2a	1518	32	19,26,27	0.98	1 (5%)	18,38,41	1.68	4 (22%)
1	PSU	2A	1917	1	17,21,22	1.55	2 (11%)	20,30,33	3.09	6 (30%)
54	PSU	1y	55	54	17,21,22	1.53	3 (17%)	20,30,33	3.09	7 (35%)
32	UR3	2a	1498	32	14,22,23	0.80	1 (7%)	15,32,35	0.72	0
54	5MU	2w	54	54	15,22,23	1.09	2 (13%)	16,32,35	2.04	2 (12%)
55	5MC	2x	32	55	15,22,23	1.37	1 (6%)	19,32,35	1.33	3 (15%)
55	5MU	2x	54	55	15,22,23	1.07	1 (6%)	16,32,35	1.80	2 (12%)
54	PSU	1y	32	54	17,21,22	1.54	2 (11%)	20,30,33	3.22	6 (30%)
1	5MC	2A	1942	1	15,22,23	1.30	1 (6%)	19,32,35	1.47	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	7MG	1a	527	32,56	22,26,27	1.81	4 (18%)	28,39,42	2.76	8 (28%)
1	5MU	2A	1915	1	15,22,23	1.11	1 (6%)	16,32,35	1.81	2 (12%)
54	4SU	1w	8	54	14,21,22	1.28	1 (7%)	15,30,33	1.50	2 (13%)
54	7MG	1w	46	54	22,26,27	1.80	4 (18%)	28,39,42	2.77	9 (32%)
1	OMG	1A	2251	1,55,56	18,26,27	1.23	2 (11%)	20,38,41	2.12	6 (30%)
32	PSU	2a	516	32	17,21,22	1.57	3 (17%)	20,30,33	3.16	7 (35%)

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
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
55	PSU	2x	55	55	-	1/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
54	5MU	1y	54	54	-	0/5/25/26	0/2/2/2
54	PSU	2w	32	54	-	1/7/25/26	0/2/2/2
55	4SU	1x	8	55,56	-	0/5/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	2/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	5/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
54	MIA	2y	37	54,32	-	2/3/25/34	0/3/3/3
54	4SU	1y	8	54	-	2/5/25/26	0/2/2/2
53	PSU	2v	19	54,56,53	-	2/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	1/5/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
54	5MU	2y	54	54	-	0/5/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
32	7MG	2a	527	32	-	3/7/37/38	0/3/3/3
54	MIA	1w	37	54	-	2/11/33/34	0/3/3/3
1	2MU	1A	2552	1,56	-	0/7/27/28	0/2/2/2
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
54	PSU	2y	55	54	-	5/7/25/26	0/2/2/2
54	4SU	2y	8	54,56	-	1/5/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1915	1	-	1/5/25/26	0/2/2/2
54	PSU	2y	32	54	-	1/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/7/27/28	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	2/5/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/5/25/26	0/2/2/2
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
55	5MU	1x	54	55	-	0/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
1	5MC	1A	1962	1	-	2/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
32	5MC	2a	1407	32,56	-	0/5/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/5/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	2/5/27/28	0/3/3/3
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
1	2MA	1A	2503	1,56	-	2/3/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
32	PSU	1a	516	32	-	1/7/25/26	0/2/2/2
1	2MA	2A	2503	1	-	1/3/25/26	0/3/3/3
1	5MU	1A	1939	1	-	0/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	2/3/25/34	0/3/3/3
53	PSU	1v	19	54,53	-	3/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	2/5/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	4/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	0/7/27/30	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
54	PSU	1y	32	54	-	2/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
54	7MG	1w	46	54	-	0/7/37/38	0/3/3/3
1	OMG	1A	2251	1,55,56	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.24	1.53	1.32
54	1w	37	MIA	C2-S10	-7.02	1.69	1.75
54	2w	37	MIA	C2-S10	-6.89	1.69	1.75
43	2l	92	0TD	CB-SB	-5.91	1.69	1.84
43	1l	92	0TD	CB-SB	-5.88	1.69	1.84
32	1a	527	7MG	C6-C5	5.13	1.48	1.41
54	1w	46	7MG	C6-C5	5.07	1.48	1.41
54	2w	46	7MG	C6-C5	5.05	1.48	1.41
32	2a	527	7MG	C6-C5	4.97	1.48	1.41
54	1y	46	7MG	C6-C5	4.91	1.48	1.41
54	2y	46	7MG	C5-C4	4.88	1.48	1.39
55	2x	32	5MC	C5-C4	4.87	1.48	1.41
54	1y	46	7MG	C5-C4	4.79	1.48	1.39
32	1a	1404	5MC	C5-C4	4.79	1.48	1.41
32	2a	967	5MC	C5-C4	4.78	1.48	1.41
32	2a	1400	5MC	C5-C4	4.77	1.48	1.41
1	1A	1962	5MC	C5-C4	4.77	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	32	5MC	C5-C4	4.72	1.48	1.41
55	1x	55	PSU	C5-C1'	-4.72	1.48	1.52
32	2a	1407	5MC	C5-C4	4.72	1.48	1.41
1	1A	2503	2MA	C6-C5	4.66	1.48	1.41
1	2A	1942	5MC	C5-C4	4.59	1.48	1.41
32	1a	1400	5MC	C5-C4	4.58	1.48	1.41
1	2A	1962	5MC	C5-C4	4.57	1.48	1.41
32	1a	967	5MC	C5-C4	4.56	1.48	1.41
32	1a	1407	5MC	C5-C4	4.55	1.48	1.41
1	1A	1911	PSU	C5-C1'	-4.54	1.48	1.52
32	2a	1404	5MC	C5-C4	4.53	1.48	1.41
54	2y	46	7MG	C6-C5	4.53	1.47	1.41
54	1w	46	7MG	C5-C4	4.52	1.48	1.39
54	2w	46	7MG	C5-C4	4.50	1.48	1.39
1	1A	1942	5MC	C5-C4	4.42	1.48	1.41
32	1a	527	7MG	C5-C4	4.42	1.47	1.39
53	2v	19	PSU	C5-C1'	-4.42	1.48	1.52
1	2A	2503	2MA	C6-C5	4.39	1.48	1.41
1	2A	1911	PSU	C5-C1'	-4.35	1.48	1.52
32	2a	527	7MG	C5-C4	4.32	1.47	1.39
54	1y	32	PSU	C5-C1'	-4.31	1.48	1.52
32	2a	1207	2MG	C6-C5	4.26	1.48	1.41
54	1w	32	PSU	C5-C1'	-4.23	1.48	1.52
1	2A	2605	PSU	C5-C1'	-4.23	1.48	1.52
32	2a	516	PSU	C5-C1'	-4.21	1.48	1.52
54	1y	55	PSU	C5-C1'	-4.18	1.48	1.52
1	1A	2251	OMG	C6-C5	4.15	1.48	1.41
32	2a	966	M2G	C6-C5	4.15	1.48	1.41
54	2w	32	PSU	C5-C1'	-4.14	1.48	1.52
54	2y	8	4SU	C4-S4	-4.14	1.59	1.67
1	2A	1917	PSU	C5-C1'	-4.12	1.48	1.52
54	2w	8	4SU	C4-S4	-4.09	1.60	1.67
54	2w	39	PSU	C4-C5	4.08	1.50	1.41
32	1a	966	M2G	C6-C5	4.07	1.48	1.41
55	1x	8	4SU	C4-S4	-4.07	1.60	1.67
32	1a	1207	2MG	C6-C5	4.03	1.48	1.41
54	1w	8	4SU	C4-S4	-3.98	1.60	1.67
54	2y	55	PSU	C5-C1'	-3.94	1.48	1.52
55	2x	8	4SU	C4-S4	-3.90	1.60	1.67
53	2v	19	PSU	C4-C5	3.89	1.49	1.41
54	1y	39	PSU	C4-C5	3.85	1.49	1.41
1	2A	2251	OMG	C6-C5	3.85	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1917	PSU	C5-C1'	-3.84	1.49	1.52
54	1y	8	4SU	C4-S4	-3.81	1.60	1.67
54	2y	39	PSU	C5-C1'	-3.77	1.49	1.52
54	2y	46	7MG	C5-N7	-3.76	1.33	1.39
54	2w	55	PSU	C4-C5	3.75	1.49	1.41
1	1A	2605	PSU	C5-C1'	-3.72	1.49	1.52
54	2w	32	PSU	C4-C5	3.70	1.49	1.41
55	2x	55	PSU	C5-C1'	-3.70	1.49	1.52
53	1v	19	PSU	C5-C1'	-3.67	1.49	1.52
55	2x	55	PSU	C4-C5	3.66	1.49	1.41
54	1w	39	PSU	C4-C5	3.65	1.49	1.41
54	1w	39	PSU	C5-C1'	-3.63	1.49	1.52
54	1w	55	PSU	C5-C1'	-3.63	1.49	1.52
32	1a	516	PSU	C4-C5	3.61	1.49	1.41
32	1a	966	M2G	C2-N2	3.58	1.40	1.34
1	2A	1915	5MU	C4-C5	3.57	1.49	1.41
54	2w	55	PSU	C5-C1'	-3.56	1.49	1.52
32	1a	516	PSU	C5-C1'	-3.56	1.49	1.52
54	2y	32	PSU	C5-C1'	-3.55	1.49	1.52
54	1y	46	7MG	C5-N7	-3.48	1.33	1.39
1	2A	1917	PSU	C4-C5	3.47	1.48	1.41
1	1A	1917	PSU	C4-C5	3.47	1.48	1.41
32	2a	516	PSU	C4-C5	3.47	1.48	1.41
32	2a	966	M2G	C2-N2	3.46	1.40	1.34
54	2y	32	PSU	C4-C5	3.44	1.48	1.41
54	1y	39	PSU	C5-C1'	-3.43	1.49	1.52
32	1a	527	7MG	C5-N7	-3.43	1.34	1.39
54	2y	39	PSU	C4-C5	3.42	1.48	1.41
32	2a	527	7MG	C5-N7	-3.40	1.34	1.39
1	1A	1915	5MU	C4-C5	3.39	1.48	1.41
55	1x	54	5MU	C4-C5	3.38	1.48	1.41
55	2x	54	5MU	C4-C5	3.37	1.48	1.41
54	1y	54	5MU	C4-C5	3.37	1.48	1.41
1	1A	1939	5MU	C4-C5	3.36	1.48	1.41
54	2w	54	5MU	C4-C5	3.36	1.48	1.41
54	1w	46	7MG	C5-N7	-3.36	1.34	1.39
54	1w	32	PSU	C4-C5	3.34	1.48	1.41
1	2A	1939	5MU	C4-C5	3.31	1.48	1.41
54	1y	32	PSU	C4-C5	3.30	1.48	1.41
1	2A	2605	PSU	C4-C5	3.30	1.48	1.41
54	1w	55	PSU	C4-C5	3.30	1.48	1.41
54	2y	54	5MU	C4-C5	3.28	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	55	PSU	C4-C5	3.26	1.48	1.41
1	2A	1911	PSU	C4-C5	3.24	1.48	1.41
54	2y	55	PSU	C4-C5	3.23	1.48	1.41
54	1w	54	5MU	C4-C5	3.22	1.48	1.41
1	1A	1911	PSU	C4-C5	3.19	1.48	1.41
54	2w	46	7MG	C5-N7	-3.17	1.34	1.39
55	1x	55	PSU	C4-C5	3.12	1.48	1.41
55	1x	8	4SU	C2-N3	-3.11	1.32	1.38
1	1A	2605	PSU	C4-C5	3.10	1.48	1.41
53	1v	19	PSU	C4-C5	3.09	1.48	1.41
54	2y	37	MIA	C2-N3	2.73	1.36	1.32
54	1y	37	MIA	C5-C4	2.71	1.48	1.40
54	1w	37	MIA	C5-C4	2.70	1.48	1.40
54	1y	37	MIA	C2-N3	2.68	1.36	1.32
54	2y	37	MIA	C5-C4	2.67	1.48	1.40
54	2w	37	MIA	C5-C4	2.65	1.47	1.40
32	2a	1519	MA6	C5-C4	2.61	1.47	1.40
32	1a	1519	MA6	C5-C4	2.60	1.47	1.40
32	2a	1518	MA6	C5-C4	2.57	1.47	1.40
32	2a	966	M2G	C5-C4	2.56	1.47	1.40
32	2a	1207	2MG	C5-C4	2.56	1.47	1.40
32	1a	1518	MA6	C5-C4	2.54	1.47	1.40
1	1A	2251	OMG	C5-C4	2.48	1.47	1.40
1	2A	2251	OMG	C5-C4	2.45	1.47	1.40
32	1a	1207	2MG	C5-C4	2.38	1.47	1.40
1	1A	2503	2MA	C5-C4	2.37	1.47	1.40
54	2w	46	7MG	C4-N9	-2.35	1.33	1.38
32	1a	966	M2G	C5-C4	2.35	1.47	1.40
32	2a	1498	UR3	C4-N3	2.31	1.41	1.38
32	1a	527	7MG	C4-N9	-2.30	1.34	1.38
1	2A	2503	2MA	C5-C4	2.27	1.46	1.40
32	2a	527	7MG	C4-N9	-2.26	1.34	1.38
55	2x	8	4SU	C2-N3	-2.25	1.33	1.38
54	2w	39	PSU	C5-C1'	-2.22	1.50	1.52
54	1w	46	7MG	C4-N9	-2.20	1.34	1.38
54	2y	32	PSU	O4'-C1'	-2.18	1.41	1.44
1	1A	1939	5MU	C2-N3	-2.16	1.33	1.38
53	1v	19	PSU	C2-N3	-2.14	1.33	1.38
32	2a	516	PSU	O4'-C1'	-2.13	1.41	1.44
54	1y	55	PSU	O4'-C1'	-2.09	1.41	1.44
54	1y	46	7MG	C4-N3	2.08	1.36	1.34
1	1A	1911	PSU	C2-N3	-2.06	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	54	5MU	C2-N3	-2.04	1.34	1.38
54	2y	55	PSU	C2-N3	-2.02	1.34	1.38
54	1w	54	5MU	C2-N3	-2.02	1.34	1.38
32	1a	516	PSU	O4'-C1'	-2.01	1.41	1.44
1	2A	2605	PSU	C2-N3	-2.00	1.34	1.38
54	2y	46	7MG	C4-N3	2.00	1.36	1.34

All (365) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-17.95	66.54	101.85
43	1l	92	0TD	CSB-SB-CB	-15.74	70.90	101.85
54	2y	46	7MG	N3-C4-N9	10.22	140.03	126.91
54	1y	46	7MG	N3-C4-N9	10.18	139.99	126.91
53	1v	19	PSU	N1-C2-N3	-9.84	120.61	128.43
54	1w	46	7MG	N3-C4-N9	9.19	138.72	126.91
32	1a	527	7MG	N3-C4-N9	9.05	138.53	126.91
54	2y	39	PSU	N1-C2-N3	-9.03	121.25	128.43
32	2a	527	7MG	N3-C4-N9	9.01	138.49	126.91
53	1v	19	PSU	C4-N3-C2	9.00	122.74	115.14
1	1A	2605	PSU	N1-C2-N3	-8.89	121.36	128.43
32	1a	516	PSU	N1-C2-N3	-8.78	121.45	128.43
54	2w	46	7MG	N3-C4-N9	8.76	138.16	126.91
54	1w	54	5MU	C4-N3-C2	8.72	122.50	115.14
32	2a	516	PSU	N1-C2-N3	-8.65	121.55	128.43
54	2y	55	PSU	N1-C2-N3	-8.57	121.62	128.43
1	2A	2605	PSU	N1-C2-N3	-8.52	121.66	128.43
54	2y	32	PSU	N1-C2-N3	-8.49	121.68	128.43
53	2v	19	PSU	N1-C2-N3	-8.48	121.69	128.43
54	1y	32	PSU	N1-C2-N3	-8.41	121.74	128.43
54	2w	32	PSU	N1-C2-N3	-8.34	121.80	128.43
54	1w	55	PSU	N1-C2-N3	-8.32	121.81	128.43
1	2A	1911	PSU	N1-C2-N3	-8.32	121.82	128.43
54	1w	32	PSU	N1-C2-N3	-8.31	121.82	128.43
55	2x	55	PSU	N1-C2-N3	-8.30	121.83	128.43
1	1A	1917	PSU	N1-C2-N3	-8.25	121.87	128.43
54	2w	55	PSU	N1-C2-N3	-8.19	121.92	128.43
1	1A	1911	PSU	N1-C2-N3	-8.18	121.92	128.43
54	1y	55	PSU	N1-C2-N3	-8.11	121.98	128.43
55	1x	55	PSU	N1-C2-N3	-7.97	122.09	128.43
54	1y	39	PSU	N1-C2-N3	-7.97	122.09	128.43
54	2w	39	PSU	N1-C2-N3	-7.95	122.11	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1917	PSU	N1-C2-N3	-7.90	122.15	128.43
54	1w	37	MIA	C12-C13-C14	-7.80	111.96	127.14
54	1w	39	PSU	N1-C2-N3	-7.73	122.28	128.43
54	2w	54	5MU	C4-N3-C2	7.51	121.49	115.14
32	1a	516	PSU	C4-N3-C2	7.46	121.44	115.14
55	2x	8	4SU	C2-N3-C4	7.36	125.82	115.15
54	2y	39	PSU	C4-N3-C2	7.31	121.32	115.14
55	1x	54	5MU	C4-N3-C2	7.21	121.23	115.14
53	2v	19	PSU	C4-N3-C2	7.20	121.22	115.14
55	1x	8	4SU	C2-N3-C4	7.09	125.44	115.15
54	1w	55	PSU	C4-N3-C2	7.08	121.12	115.14
54	2y	32	PSU	C4-N3-C2	7.05	121.09	115.14
32	2a	516	PSU	C4-N3-C2	7.04	121.08	115.14
54	2w	55	PSU	C4-N3-C2	7.01	121.06	115.14
54	2w	32	PSU	C4-N3-C2	6.88	120.95	115.14
54	2y	54	5MU	C4-N3-C2	6.85	120.93	115.14
54	1w	32	PSU	C4-N3-C2	6.84	120.91	115.14
54	2y	55	PSU	C4-N3-C2	6.84	120.91	115.14
1	1A	1915	5MU	C4-N3-C2	6.75	120.84	115.14
54	1y	55	PSU	C4-N3-C2	6.71	120.81	115.14
1	1A	1917	PSU	C4-N3-C2	6.69	120.79	115.14
1	2A	1917	PSU	C4-N3-C2	6.66	120.77	115.14
1	2A	1911	PSU	C4-N3-C2	6.66	120.77	115.14
1	1A	2605	PSU	C4-N3-C2	6.66	120.76	115.14
1	2A	1915	5MU	C4-N3-C2	6.60	120.72	115.14
1	1A	2503	2MA	C2-N3-C4	6.59	120.88	115.52
54	1y	32	PSU	C4-N3-C2	6.59	120.70	115.14
55	2x	55	PSU	C4-N3-C2	6.52	120.65	115.14
1	2A	2503	2MA	C2-N3-C4	6.40	120.72	115.52
55	2x	54	5MU	C4-N3-C2	6.39	120.54	115.14
55	1x	55	PSU	C4-N3-C2	6.39	120.53	115.14
1	2A	2605	PSU	C4-N3-C2	6.33	120.48	115.14
54	2w	55	PSU	C5-C1'-C2'	-6.29	104.10	115.32
54	1w	55	PSU	C5-C1'-C2'	-6.21	104.25	115.32
1	1A	1911	PSU	C4-N3-C2	6.20	120.38	115.14
54	1y	39	PSU	C4-N3-C2	6.15	120.33	115.14
54	1y	54	5MU	C4-N3-C2	6.08	120.27	115.14
1	2A	1939	5MU	C4-N3-C2	6.03	120.24	115.14
1	1A	1939	5MU	C4-N3-C2	6.03	120.23	115.14
53	2v	19	PSU	C5-C4-N3	-5.81	117.88	125.36
54	2y	46	7MG	C5-C4-N3	-5.77	117.06	126.49
53	1v	19	PSU	C5-C4-N3	-5.74	117.97	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2v	19	PSU	C5-C1'-C2'	-5.66	105.22	115.32
54	1y	46	7MG	C5-C4-N3	-5.65	117.27	126.49
54	1y	55	PSU	C5-C4-N3	-5.63	118.10	125.36
54	2w	55	PSU	C5-C4-N3	-5.62	118.11	125.36
32	1a	516	PSU	C5-C4-N3	-5.59	118.16	125.36
54	2w	46	7MG	N7-C8-N9	-5.55	95.44	103.38
55	1x	55	PSU	C5-C4-N3	-5.55	118.21	125.36
1	2A	1917	PSU	C5-C4-N3	-5.54	118.22	125.36
54	2y	32	PSU	C5-C4-N3	-5.50	118.27	125.36
32	2a	527	7MG	N7-C8-N9	-5.50	95.51	103.38
54	1w	55	PSU	C5-C4-N3	-5.50	118.28	125.36
32	2a	516	PSU	C5-C4-N3	-5.46	118.33	125.36
54	1w	32	PSU	C5-C4-N3	-5.45	118.33	125.36
54	2y	46	7MG	C6-N1-C2	5.39	124.50	115.93
54	2w	32	PSU	C5-C4-N3	-5.39	118.41	125.36
1	2A	1911	PSU	C5-C4-N3	-5.37	118.44	125.36
32	1a	527	7MG	C5-C4-N3	-5.36	117.73	126.49
54	2y	39	PSU	C5-C4-N3	-5.34	118.49	125.36
54	1y	32	PSU	C5-C4-N3	-5.32	118.50	125.36
1	1A	1917	PSU	C5-C4-N3	-5.32	118.51	125.36
54	1y	39	PSU	C5-C4-N3	-5.31	118.52	125.36
55	2x	55	PSU	C5-C4-N3	-5.31	118.52	125.36
32	2a	966	M2G	C6-N1-C2	5.27	122.45	116.18
54	2y	55	PSU	C5-C4-N3	-5.24	118.61	125.36
54	1y	46	7MG	C6-N1-C2	5.23	124.24	115.93
54	1w	46	7MG	N7-C8-N9	-5.23	95.90	103.38
32	1a	966	M2G	C6-N1-C2	5.22	122.39	116.18
1	1A	2251	OMG	C2-N3-C4	5.20	121.29	115.36
32	1a	527	7MG	N7-C8-N9	-5.19	95.95	103.38
54	1w	46	7MG	C5-C4-N3	-5.18	118.03	126.49
32	2a	527	7MG	C5-C4-N3	-5.14	118.09	126.49
1	1A	1911	PSU	C5-C4-N3	-5.09	118.80	125.36
32	1a	966	M2G	C2-N3-C4	5.08	121.05	115.28
54	1w	39	PSU	C4-N3-C2	5.06	119.41	115.14
54	2y	46	7MG	C6-C5-C4	5.01	120.58	115.20
1	2A	2251	OMG	C2-N3-C4	4.98	121.04	115.36
54	2w	39	PSU	C4-N3-C2	4.97	119.33	115.14
1	2A	2605	PSU	C5-C4-N3	-4.91	119.04	125.36
54	1w	39	PSU	C5-C4-N3	-4.86	119.10	125.36
1	2A	2503	2MA	C5-C6-N1	-4.83	117.99	123.06
32	2a	1207	2MG	C2-N3-C4	4.82	120.75	115.28
32	2a	966	M2G	C2-N3-C4	4.82	120.75	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	N7-C8-N9	-4.80	96.51	103.38
1	1A	2605	PSU	C5-C4-N3	-4.79	119.19	125.36
54	2w	46	7MG	C6-N1-C2	4.78	123.52	115.93
1	1A	2503	2MA	C5-C6-N1	-4.74	118.09	123.06
32	1a	1207	2MG	C2-N3-C4	4.71	120.63	115.28
54	2w	46	7MG	C5-C4-N3	-4.69	118.83	126.49
1	2A	1920	4OC	C2-N3-C4	4.66	121.07	116.34
1	1A	1911	PSU	C5-C6-N1	-4.65	118.73	124.44
32	2a	1400	5MC	C2-N3-C4	4.61	121.59	116.02
54	2w	39	PSU	C6-N1-C2	4.60	122.95	115.36
32	2a	1402	4OC	CM4-N4-C4	-4.56	119.05	122.97
32	2a	527	7MG	C6-N1-C2	4.54	123.14	115.93
54	1y	46	7MG	C6-C5-C4	4.49	120.02	115.20
54	1w	8	4SU	C2-N3-C4	4.45	121.60	115.15
54	2y	46	7MG	N7-C8-N9	-4.45	97.02	103.38
55	1x	55	PSU	C5-C6-N1	-4.44	118.98	124.44
54	1w	39	PSU	C6-N1-C2	4.43	122.67	115.36
54	2w	39	PSU	C5-C4-N3	-4.41	119.68	125.36
54	1y	32	PSU	C5-C6-N1	-4.38	119.05	124.44
54	1w	39	PSU	C5-C6-N1	-4.38	119.06	124.44
1	2A	2605	PSU	C5-C6-N1	-4.37	119.07	124.44
54	2w	37	MIA	C2-N3-C4	4.34	121.31	115.32
32	1a	527	7MG	C6-C5-C4	4.33	119.85	115.20
1	1A	1920	4OC	C2-N3-C4	4.33	120.73	116.34
1	2A	2605	PSU	C6-N1-C2	4.32	122.48	115.36
55	2x	55	PSU	C5-C6-N1	-4.30	119.16	124.44
1	1A	1911	PSU	C6-N1-C2	4.28	122.43	115.36
32	1a	527	7MG	C6-N1-C2	4.27	122.72	115.93
32	1a	1207	2MG	C5-C6-N1	-4.25	117.61	123.43
32	1a	1207	2MG	C6-N1-C2	4.25	122.79	115.18
54	2w	8	4SU	C2-N3-C4	4.23	121.28	115.15
1	2A	1911	PSU	C5-C6-N1	-4.23	119.24	124.44
54	2y	39	PSU	C5-C6-N1	-4.23	119.25	124.44
54	2w	39	PSU	C5-C6-N1	-4.22	119.25	124.44
1	2A	2605	PSU	C5-C1'-C2'	-4.21	107.81	115.32
55	2x	55	PSU	C6-N1-C2	4.20	122.29	115.36
54	1w	46	7MG	C6-N1-C2	4.20	122.61	115.93
1	2A	1917	PSU	C5-C6-N1	-4.18	119.30	124.44
54	1y	32	PSU	C6-N1-C2	4.16	122.22	115.36
54	1y	39	PSU	C6-N1-C2	4.16	122.22	115.36
32	2a	1207	2MG	C5-C6-N1	-4.15	117.76	123.43
54	2y	39	PSU	C6-N1-C2	4.14	122.20	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	55	PSU	C6-N1-C2	4.14	122.19	115.36
54	1y	32	PSU	C5-C1'-C2'	-4.13	107.94	115.32
54	1w	46	7MG	C6-C5-C4	4.13	119.63	115.20
1	1A	2605	PSU	C6-N1-C2	4.12	122.16	115.36
32	2a	527	7MG	C6-C5-C4	4.10	119.61	115.20
53	2v	19	PSU	C6-N1-C2	4.10	122.12	115.36
54	1w	37	MIA	C15-C14-C13	-4.09	110.81	122.65
54	1y	39	PSU	C5-C6-N1	-4.09	119.41	124.44
54	1y	55	PSU	C5-C6-N1	-4.09	119.42	124.44
32	2a	966	M2G	C5-C6-N1	-4.08	117.84	123.43
1	2A	1911	PSU	C6-N1-C2	4.07	122.08	115.36
32	1a	966	M2G	C6-C5-C4	-4.06	116.93	120.80
54	1w	37	MIA	C2-N3-C4	4.05	120.90	115.32
32	2a	516	PSU	C6-N1-C2	4.03	122.02	115.36
54	2y	55	PSU	C5-C6-N1	-4.01	119.51	124.44
53	2v	19	PSU	C5-C6-N1	-3.98	119.54	124.44
1	1A	1917	PSU	C6-N1-C2	3.98	121.92	115.36
54	1y	8	4SU	C2-N3-C4	3.97	120.91	115.15
32	2a	1207	2MG	C6-N1-C2	3.97	122.29	115.18
54	2y	46	7MG	C5-C6-N1	-3.97	114.99	123.14
55	1x	55	PSU	C6-N1-C2	3.96	121.89	115.36
54	2w	32	PSU	C6-N1-C2	3.96	121.89	115.36
32	1a	516	PSU	C6-N1-C2	3.95	121.88	115.36
54	1w	32	PSU	C6-N1-C2	3.93	121.85	115.36
1	2A	1917	PSU	C6-N1-C2	3.93	121.84	115.36
1	1A	2251	OMG	C5-C6-N1	-3.92	118.07	123.43
32	2a	516	PSU	C5-C6-N1	-3.92	119.62	124.44
54	2w	55	PSU	C6-N1-C2	3.92	121.82	115.36
54	1w	32	PSU	C5-C6-N1	-3.90	119.64	124.44
54	1y	55	PSU	C6-N1-C2	3.88	121.76	115.36
54	1w	37	MIA	C16-C14-C13	-3.87	111.45	122.65
54	2y	32	PSU	C6-N1-C2	3.87	121.74	115.36
32	1a	966	M2G	C5-C6-N1	-3.86	118.15	123.43
54	1w	37	MIA	C5-C6-N1	-3.85	117.61	120.81
55	2x	8	4SU	C5-C4-N3	-3.85	118.68	123.83
54	2w	55	PSU	C5-C6-N1	-3.84	119.72	124.44
53	1v	19	PSU	C6-N1-C2	3.83	121.68	115.36
1	2A	2251	OMG	C6-N1-C2	3.80	121.97	115.93
1	1A	2251	OMG	C6-N1-C2	3.80	121.97	115.93
55	2x	32	5MC	C2-N3-C4	3.80	120.60	116.02
54	1y	46	7MG	C5-C6-N1	-3.80	115.34	123.14
1	2A	2251	OMG	C5-C6-N1	-3.79	118.25	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1911	PSU	C5-C1'-C2'	-3.78	108.58	115.32
1	1A	1917	PSU	C5-C6-N1	-3.77	119.80	124.44
54	1w	55	PSU	C6-N1-C2	3.76	121.57	115.36
1	1A	2605	PSU	C5-C6-N1	-3.76	119.82	124.44
32	2a	1404	5MC	C2-N3-C4	3.76	120.56	116.02
32	1a	1407	5MC	C2-N3-C4	3.73	120.52	116.02
32	2a	1407	5MC	C2-N3-C4	3.73	120.52	116.02
32	2a	1207	2MG	C6-C5-C4	-3.73	117.24	120.80
32	1a	967	5MC	C2-N3-C4	3.72	120.51	116.02
54	2w	46	7MG	C5-C6-N1	-3.71	115.52	123.14
55	1x	8	4SU	C5-C4-N3	-3.70	118.88	123.83
32	2a	967	5MC	C2-N3-C4	3.69	120.47	116.02
54	2w	32	PSU	C5-C6-N1	-3.69	119.90	124.44
32	2a	527	7MG	C5-C6-N1	-3.68	115.58	123.14
54	2y	8	4SU	C2-N3-C4	3.67	120.47	115.15
1	1A	1911	PSU	C5-C1'-C2'	-3.66	108.78	115.32
1	1A	1942	5MC	C2-N3-C4	3.65	120.43	116.02
55	1x	32	5MC	C2-N3-C4	3.64	120.41	116.02
54	2w	46	7MG	C6-C5-C4	3.64	119.10	115.20
53	1v	19	PSU	C5-C6-N1	-3.62	119.99	124.44
54	2w	32	PSU	C5-C1'-C2'	-3.61	108.87	115.32
1	2A	1962	5MC	C2-N3-C4	3.61	120.37	116.02
32	1a	527	7MG	C5-C6-N1	-3.60	115.74	123.14
54	2y	32	PSU	C5-C6-N1	-3.60	120.02	124.44
32	1a	1207	2MG	C6-C5-C4	-3.58	117.38	120.80
54	2y	39	PSU	C5-C1'-C2'	-3.57	108.96	115.32
32	2a	966	M2G	C6-C5-C4	-3.56	117.40	120.80
32	1a	1402	4OC	CM4-N4-C4	-3.55	119.91	122.97
54	1w	46	7MG	C5-C6-N1	-3.53	115.88	123.14
32	1a	1404	5MC	C2-N3-C4	3.53	120.28	116.02
54	2w	37	MIA	C5-C6-N1	-3.52	117.89	120.81
1	2A	1917	PSU	C5-C1'-C2'	-3.52	109.05	115.32
54	1w	55	PSU	C5-C6-N1	-3.51	120.13	124.44
32	2a	1518	MA6	C9-N6-C6	-3.49	108.94	119.51
32	1a	1400	5MC	C2-N3-C4	3.48	120.22	116.02
1	1A	1962	5MC	C2-N3-C4	3.47	120.21	116.02
32	2a	1518	MA6	C4-C5-N7	-3.47	105.78	109.40
54	2w	37	MIA	C12-N6-C6	-3.46	119.89	122.87
32	1a	516	PSU	C5-C6-N1	-3.46	120.19	124.44
32	2a	1518	MA6	N3-C2-N1	-3.40	123.36	128.68
32	1a	1518	MA6	C9-N6-C6	-3.40	109.23	119.51
32	1a	1518	MA6	N3-C2-N1	-3.38	123.40	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1519	MA6	C4-C5-N7	-3.35	105.91	109.40
1	1A	1939	5MU	C5-C6-N1	-3.34	118.60	122.19
1	1A	2251	OMG	C6-C5-C4	-3.29	117.66	120.80
32	1a	1519	MA6	N1-C6-N6	3.25	120.48	117.06
54	1y	37	MIA	N3-C2-N1	-3.24	123.62	128.68
1	2A	1942	5MC	C2-N3-C4	3.23	119.92	116.02
32	1a	1518	MA6	C4-C5-N7	-3.21	106.05	109.40
32	2a	1519	MA6	C9-N6-C6	-3.21	109.79	119.51
1	2A	2251	OMG	C6-C5-C4	-3.19	117.75	120.80
1	2A	2251	OMG	N3-C2-N1	-3.18	122.97	127.22
54	2y	37	MIA	N3-C2-N1	-3.17	123.73	128.68
55	1x	55	PSU	C5-C1'-C2'	-3.15	109.70	115.32
1	2A	1939	5MU	C5-C6-N1	-3.15	118.80	122.19
54	1w	37	MIA	C11-S10-C2	-3.14	99.92	102.27
1	1A	2251	OMG	N3-C2-N1	-3.14	123.04	127.22
32	1a	1519	MA6	C4-C5-N7	-3.12	106.15	109.40
54	1w	32	PSU	C5-C1'-C2'	-3.06	109.86	115.32
54	1y	8	4SU	C5-C4-N3	-3.06	119.74	123.83
32	1a	1519	MA6	N3-C2-N1	-3.03	123.94	128.68
32	2a	1519	MA6	N3-C2-N1	-3.02	123.95	128.68
32	1a	1519	MA6	C9-N6-C6	-3.01	110.40	119.51
1	2A	1962	5MC	N4-C4-N3	2.96	121.21	117.03
54	1w	8	4SU	C5-C4-N3	-2.95	119.88	123.83
1	1A	2605	PSU	C5-C1'-C2'	-2.93	110.10	115.32
54	1w	37	MIA	C2-N1-C6	2.87	122.33	117.19
54	1y	55	PSU	C5-C1'-C2'	-2.86	110.22	115.32
32	2a	1404	5MC	N4-C4-N3	2.85	121.07	117.03
32	2a	1207	2MG	C4-C5-N7	-2.85	106.43	109.40
54	2w	8	4SU	C5-C4-N3	-2.84	120.03	123.83
54	2w	55	PSU	O4'-C1'-C5	2.82	114.30	109.93
54	2y	37	MIA	C4-C5-N7	-2.82	106.46	109.40
32	2a	527	7MG	C8-N7-C5	2.81	116.24	108.94
32	1a	1207	2MG	C4-C5-N7	-2.81	106.47	109.40
32	1a	1207	2MG	CM2-N2-C2	-2.77	120.24	123.59
54	2w	37	MIA	C4-C5-N7	-2.76	106.53	109.40
1	2A	1942	5MC	N4-C4-N3	2.76	120.93	117.03
32	1a	527	7MG	C8-N7-C5	2.74	116.06	108.94
32	1a	966	M2G	C4-C5-N7	-2.73	106.55	109.40
1	1A	1942	5MC	N4-C4-N3	2.71	120.87	117.03
54	1w	37	MIA	C4-C5-N7	-2.70	106.58	109.40
54	1w	46	7MG	C8-N7-C5	2.68	115.92	108.94
1	2A	1942	5MC	C5-C6-N1	-2.67	119.31	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	46	7MG	C8-N7-C5	2.67	115.89	108.94
54	1y	37	MIA	C4-C5-N7	-2.66	106.62	109.40
53	1v	19	PSU	C5-C1'-C2'	-2.65	110.59	115.32
32	1a	1400	5MC	N4-C4-N3	2.65	120.78	117.03
54	1y	46	7MG	C5-C4-N9	-2.64	102.74	106.44
1	1A	2251	OMG	C4-C5-N7	-2.61	106.68	109.40
1	1A	1917	PSU	C5-C1'-C2'	-2.61	110.67	115.32
32	1a	1407	5MC	N4-C4-N3	2.59	120.70	117.03
54	2w	37	MIA	C2-N1-C6	2.59	121.82	117.19
1	1A	2503	2MA	C4-C5-N7	-2.58	106.71	109.40
54	1y	46	7MG	C8-N7-C5	2.58	115.64	108.94
54	1w	37	MIA	C12-N6-C6	-2.57	118.74	122.55
32	2a	1400	5MC	N4-C4-N3	2.56	120.64	117.03
1	2A	2503	2MA	C4-C5-N7	-2.55	106.74	109.40
54	2y	55	PSU	C5-C1'-C2'	-2.55	110.77	115.32
54	2y	8	4SU	C5-C4-N3	-2.54	120.43	123.83
54	2y	46	7MG	C5-C4-N9	-2.53	102.90	106.44
54	1y	54	5MU	C5-C6-N1	-2.53	119.47	122.19
1	1A	1962	5MC	C5-C6-N1	-2.52	119.47	122.19
32	1a	1404	5MC	N4-C4-N3	2.52	120.60	117.03
32	2a	1407	5MC	N4-C4-N3	2.52	120.59	117.03
55	1x	32	5MC	N4-C4-N3	2.51	120.58	117.03
54	2y	46	7MG	C8-N7-C5	2.51	115.46	108.94
54	2w	37	MIA	C11-S10-C2	-2.50	100.40	102.27
32	1a	1404	5MC	C5-C6-N1	-2.49	119.51	122.19
32	1a	967	5MC	N4-C4-N3	2.46	120.52	117.03
54	2w	46	7MG	C5-C4-N9	-2.46	102.99	106.44
32	1a	1400	5MC	C5-C6-N1	-2.45	119.55	122.19
32	2a	1404	5MC	CM5-C5-C4	-2.45	119.24	121.72
55	2x	55	PSU	C5-C1'-C2'	-2.44	110.96	115.32
32	1a	1518	MA6	N1-C6-N6	2.44	119.62	117.06
32	2a	1207	2MG	CM2-N2-C2	-2.42	120.67	123.59
32	2a	966	M2G	C4-C5-N7	-2.40	106.90	109.40
1	1A	1920	4OC	N4-C4-N3	2.39	120.27	116.49
32	1a	1518	MA6	C10-N6-C9	-2.38	108.47	116.12
1	1A	1962	5MC	N4-C4-N3	2.37	120.38	117.03
32	1a	1207	2MG	N2-C2-N3	2.35	119.22	116.96
55	2x	32	5MC	N4-C4-N3	2.34	120.34	117.03
54	1y	46	7MG	C2-N3-C4	2.33	120.34	113.89
32	2a	967	5MC	N4-C4-N3	2.33	120.33	117.03
54	2y	46	7MG	C2-N3-C4	2.33	120.32	113.89
54	2y	54	5MU	C5-C6-N1	-2.30	119.72	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	527	7MG	C2-N3-C4	2.28	120.19	113.89
54	1w	46	7MG	C5-C4-N9	-2.27	103.26	106.44
32	2a	1518	MA6	C10-N6-C9	-2.27	108.81	116.12
55	2x	54	5MU	C5-C6-N1	-2.26	119.76	122.19
1	1A	1942	5MC	C5-C6-N1	-2.25	119.77	122.19
54	2w	54	5MU	C5-C6-N1	-2.25	119.77	122.19
55	1x	32	5MC	C5-C6-N1	-2.25	119.77	122.19
1	2A	1942	5MC	CM5-C5-C4	-2.25	119.44	121.72
1	2A	1915	5MU	C5-C6-N1	-2.25	119.77	122.19
54	1y	46	7MG	N2-C2-N3	2.24	120.74	117.25
32	2a	1404	5MC	C5-C6-N1	-2.22	119.80	122.19
54	2w	39	PSU	O4'-C1'-C5	2.21	113.35	109.93
54	2y	39	PSU	O4'-C1'-C5	2.20	113.33	109.93
54	1w	46	7MG	C2-N3-C4	2.19	119.95	113.89
32	2a	527	7MG	C2-N3-C4	2.18	119.93	113.89
54	2w	37	MIA	N3-C2-N1	-2.18	122.98	126.98
32	2a	967	5MC	C5-C6-N1	-2.18	119.85	122.19
32	2a	527	7MG	C5-C4-N9	-2.16	103.41	106.44
32	2a	1519	MA6	N1-C6-N6	2.16	119.33	117.06
32	1a	1207	2MG	N3-C2-N1	-2.16	122.81	126.23
1	2A	1962	5MC	C5-C6-N1	-2.16	119.87	122.19
32	1a	967	5MC	C5-C6-N1	-2.16	119.87	122.19
1	2A	1920	4OC	N4-C4-N3	2.15	119.90	116.49
32	1a	1518	MA6	C10-N6-C6	-2.13	113.06	119.51
54	1w	37	MIA	N3-C2-N1	-2.13	123.06	126.98
54	2y	32	PSU	O4'-C1'-C2'	2.13	108.11	104.66
32	2a	1519	MA6	C10-N6-C6	-2.12	113.08	119.51
55	2x	32	5MC	C5-C6-N1	-2.11	119.92	122.19
54	1y	55	PSU	O4'-C1'-C2'	2.10	108.06	104.66
1	1A	1915	5MU	C5-C6-N1	-2.09	119.94	122.19
54	2w	46	7MG	C2-N3-C4	2.06	119.60	113.89
32	2a	516	PSU	O4'-C1'-C2'	2.06	108.00	104.66
54	2y	46	7MG	C4-N9-C1'	2.04	131.44	126.60
1	2A	2251	OMG	C4-C5-N7	-2.03	107.28	109.40
1	1A	2552	2MU	C5-C4-N3	-2.02	118.86	123.31
32	2a	516	PSU	C5-C1'-C2'	-2.02	111.71	115.32
32	1a	1407	5MC	C5-C6-N1	-2.02	120.02	122.19
1	2A	2552	2MU	C5-C4-N3	-2.01	118.88	123.31
54	2y	55	PSU	O4'-C1'-C2'	2.01	107.92	104.66

There are no chirality outliers.

All (85) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
32	1a	967	5MC	O4'-C4'-C5'-O5'
55	2x	8	4SU	C2'-C1'-N1-C6
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	2w	37	MIA	N1-C6-N6-C12
54	2y	55	PSU	C2'-C1'-C5-C4
54	2y	55	PSU	O4'-C1'-C5-C4
54	2y	55	PSU	C2'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6
54	2y	46	7MG	C2'-C1'-N9-C8
54	2y	46	7MG	C2'-C1'-N9-C4
54	1y	46	7MG	C4'-C5'-O5'-P
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
32	1a	1518	MA6	C5-C6-N6-C10
32	2a	1207	2MG	N1-C2-N2-CM2
54	1y	37	MIA	O4'-C4'-C5'-O5'
54	1y	37	MIA	C3'-C4'-C5'-O5'
53	1v	19	PSU	O4'-C4'-C5'-O5'
32	2a	967	5MC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C2'-C1'-N1-C6
32	2a	1518	MA6	C5-C6-N6-C10
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
32	2a	967	5MC	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	8	4SU	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
53	1v	19	PSU	C3'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	1y	46	7MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
53	2v	19	PSU	O4'-C4'-C5'-O5'
54	1y	32	PSU	O4'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C9
54	1w	54	5MU	O4'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	1404	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
54	1y	46	7MG	C2'-C1'-N9-C8
54	2y	37	MIA	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
32	1a	1518	MA6	C5-C6-N6-C9
1	1A	2503	2MA	C4'-C5'-O5'-P
32	2a	1400	5MC	C4'-C5'-O5'-P
55	2x	55	PSU	O4'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	2y	8	4SU	C4'-C5'-O5'-P
54	1w	37	MIA	N6-C12-C13-C14
32	1a	1402	4OC	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
54	1y	55	PSU	O4'-C1'-C5-C4
54	2y	55	PSU	C3'-C4'-C5'-O5'
54	2y	32	PSU	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C1'-N9-C8
54	2w	32	PSU	C2'-C1'-C5-C6
32	1a	516	PSU	C2'-C1'-C5-C6
53	2v	19	PSU	C3'-C4'-C5'-O5'
54	1w	54	5MU	C3'-C4'-C5'-O5'
54	1y	32	PSU	C3'-C4'-C5'-O5'
1	1A	1915	5MU	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	2503	2MA	O4'-C4'-C5'-O5'
53	1v	19	PSU	C4'-C5'-O5'-P
32	1a	527	7MG	C4'-C5'-O5'-P

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1962	5MC	2	0
1	1A	2552	2MU	2	0
1	1A	1915	5MU	2	0
1	2A	2552	2MU	2	0
1	2A	1939	5MU	1	0
1	2A	2251	OMG	1	0
1	2A	2503	2MA	2	0
1	2A	1920	4OC	1	0
1	1A	1917	PSU	1	0
1	2A	1942	5MC	1	0
1	2A	1915	5MU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1466 ligands modelled in this entry, 1464 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	SF4	1d	501	35	0,12,12	0.00	-	-		
58	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
58	SF4	1d	501	35	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	2d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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%)	0.51	88 (3%) 49 32	67, 83, 117, 127	0
1	2A	2789/2915 (95%)	0.33	106 (3%) 40 26	79, 94, 115, 128	0
2	1B	120/121 (99%)	0.15	0 100 100	77, 89, 99, 110	0
2	2B	120/121 (99%)	-0.20	0 100 100	96, 106, 115, 119	0
3	1D	275/276 (99%)	2.13	132 (48%) 0 0	71, 84, 93, 110	0
3	2D	275/276 (99%)	1.87	112 (40%) 0 0	78, 89, 98, 106	0
4	1E	204/206 (99%)	1.87	85 (41%) 0 0	70, 85, 96, 106	0
4	2E	204/206 (99%)	1.43	62 (30%) 0 0	82, 92, 100, 104	0
5	1F	203/210 (96%)	1.22	53 (26%) 0 0	72, 87, 101, 111	0
5	2F	203/210 (96%)	1.42	57 (28%) 0 0	82, 96, 105, 111	0
6	1G	181/182 (99%)	0.18	5 (2%) 53 36	77, 95, 104, 116	0
6	2G	181/182 (99%)	0.17	10 (5%) 25 15	97, 106, 113, 116	0
7	1H	174/180 (96%)	0.26	2 (1%) 80 65	81, 90, 98, 104	0
7	2H	174/180 (96%)	1.77	61 (35%) 0 0	95, 106, 112, 115	0
8	1I	146/148 (98%)	0.55	21 (14%) 2 1	86, 101, 107, 111	0
8	2I	146/148 (98%)	1.16	35 (23%) 0 0	92, 109, 117, 126	0
9	1N	140/140 (100%)	2.05	67 (47%) 0 0	74, 86, 97, 103	0
9	2N	140/140 (100%)	3.26	102 (72%) 0 0	82, 96, 104, 115	0
10	1O	122/122 (100%)	2.25	65 (53%) 0 0	73, 84, 92, 100	0
10	2O	122/122 (100%)	1.78	45 (36%) 0 0	82, 92, 99, 106	0
11	1P	149/150 (99%)	1.29	40 (26%) 0 0	67, 87, 100, 108	0
11	2P	149/150 (99%)	1.88	65 (43%) 0 0	81, 98, 111, 116	0
12	1Q	141/141 (100%)	1.36	35 (24%) 0 0	76, 86, 94, 105	0
12	2Q	141/141 (100%)	1.36	40 (28%) 0 0	85, 97, 105, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	1.62	46 (38%)	0	0	72, 83, 95, 97	0
13	2R	118/118 (100%)	1.44	31 (26%)	0	0	82, 90, 97, 99	0
14	1S	110/112 (98%)	0.16	1 (0%)	84	71	80, 89, 94, 102	0
14	2S	110/112 (98%)	-0.14	0	100	100	92, 99, 104, 108	0
15	1T	131/146 (89%)	1.46	46 (35%)	0	0	78, 87, 99, 107	0
15	2T	131/146 (89%)	1.19	32 (24%)	0	0	83, 93, 104, 108	0
16	1U	116/118 (98%)	1.94	56 (48%)	0	0	71, 83, 92, 104	0
16	2U	116/118 (98%)	1.84	54 (46%)	0	0	81, 95, 105, 111	0
17	1V	101/101 (100%)	1.20	23 (22%)	0	0	72, 86, 95, 99	0
17	2V	101/101 (100%)	1.38	26 (25%)	0	0	88, 99, 106, 109	0
18	1W	112/113 (99%)	1.52	33 (29%)	0	0	72, 82, 93, 111	0
18	2W	112/113 (99%)	1.90	46 (41%)	0	0	80, 90, 100, 112	0
19	1X	95/96 (98%)	1.13	17 (17%)	1	1	71, 84, 96, 108	0
19	2X	95/96 (98%)	1.24	20 (21%)	1	0	87, 97, 105, 111	0
20	1Y	107/110 (97%)	0.81	7 (6%)	18	11	79, 89, 102, 106	0
20	2Y	107/110 (97%)	1.95	46 (42%)	0	0	92, 99, 108, 114	0
21	1Z	154/206 (74%)	0.13	2 (1%)	77	61	85, 96, 110, 116	0
21	2Z	160/206 (77%)	-0.23	0	100	100	95, 105, 112, 120	0
22	10	83/85 (97%)	1.70	13 (15%)	2	1	75, 85, 101, 110	0
22	20	83/85 (97%)	2.11	25 (30%)	0	0	90, 97, 109, 113	0
23	11	97/98 (98%)	2.76	60 (61%)	0	0	75, 86, 102, 108	0
23	21	97/98 (98%)	1.66	44 (45%)	0	0	81, 92, 103, 107	0
24	12	70/72 (97%)	0.65	6 (8%)	10	6	80, 89, 97, 104	0
24	22	70/72 (97%)	0.19	4 (5%)	23	14	90, 100, 106, 110	0
25	13	59/60 (98%)	0.76	3 (5%)	28	17	75, 85, 94, 97	0
25	23	59/60 (98%)	1.53	22 (37%)	0	0	91, 97, 106, 110	0
26	14	69/71 (97%)	-0.38	0	100	100	91, 102, 113, 117	0
26	24	69/71 (97%)	-0.51	1 (1%)	75	59	98, 110, 116, 121	0
27	15	59/60 (98%)	1.76	19 (32%)	0	0	74, 82, 93, 98	0
27	25	59/60 (98%)	1.60	18 (30%)	0	0	79, 88, 99, 105	0
28	16	53/54 (98%)	0.78	6 (11%)	5	3	76, 85, 92, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.87	9 (16%)	1	1	88, 95, 102, 105	0
29	17	48/49 (97%)	2.53	24 (50%)	0	0	73, 79, 94, 102	0
29	27	48/49 (97%)	2.92	29 (60%)	0	0	80, 86, 97, 107	0
30	18	64/65 (98%)	2.01	32 (50%)	0	0	72, 82, 88, 91	0
30	28	64/65 (98%)	2.68	41 (64%)	0	0	84, 92, 99, 100	0
31	19	37/37 (100%)	1.26	12 (32%)	0	0	78, 84, 92, 94	0
31	29	37/37 (100%)	2.47	21 (56%)	0	0	93, 101, 105, 110	0
32	1a	1488/1521 (97%)	0.11	28 (1%)	66	49	80, 97, 114, 122	0
32	2a	1491/1521 (98%)	-0.01	24 (1%)	72	55	89, 105, 116, 125	0
33	1b	231/256 (90%)	0.29	15 (6%)	18	11	92, 103, 111, 120	0
33	2b	231/256 (90%)	0.30	25 (10%)	5	3	96, 109, 115, 120	0
34	1c	206/239 (86%)	1.02	47 (22%)	0	0	89, 99, 106, 109	0
34	2c	206/239 (86%)	1.44	65 (31%)	0	0	97, 107, 111, 114	0
35	1d	208/209 (99%)	0.57	24 (11%)	4	3	87, 97, 105, 115	0
35	2d	208/209 (99%)	1.79	88 (42%)	0	0	91, 102, 111, 116	0
36	1e	148/162 (91%)	1.19	38 (25%)	0	0	86, 95, 101, 106	0
36	2e	148/162 (91%)	1.28	53 (35%)	0	0	93, 103, 110, 111	0
37	1f	100/101 (99%)	0.60	13 (13%)	3	2	89, 98, 104, 108	0
37	2f	100/101 (99%)	-0.13	2 (2%)	65	48	91, 99, 105, 110	0
38	1g	155/156 (99%)	1.08	34 (21%)	0	0	91, 98, 109, 112	0
38	2g	155/156 (99%)	0.50	18 (11%)	4	2	94, 104, 111, 114	0
39	1h	137/138 (99%)	0.96	27 (19%)	1	0	88, 97, 103, 108	0
39	2h	137/138 (99%)	1.59	48 (35%)	0	0	94, 104, 109, 116	0
40	1i	127/128 (99%)	0.47	21 (16%)	1	1	88, 99, 106, 110	0
40	2i	127/128 (99%)	1.30	44 (34%)	0	0	93, 107, 113, 115	0
41	1j	97/105 (92%)	0.58	18 (18%)	1	0	86, 102, 109, 116	0
41	2j	96/105 (91%)	1.50	28 (29%)	0	0	98, 109, 114, 117	0
42	1k	114/129 (88%)	3.55	90 (78%)	0	0	89, 99, 106, 111	0
42	2k	114/129 (88%)	1.79	42 (36%)	0	0	91, 101, 107, 110	0
43	1l	121/132 (91%)	0.82	20 (16%)	1	1	83, 91, 98, 103	0
43	2l	121/132 (91%)	1.17	34 (28%)	0	0	91, 100, 106, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.52	12 (9%) 7 4	86, 99, 107, 117	0
44	2m	122/126 (96%)	0.97	23 (18%) 1 0	97, 107, 115, 120	0
45	1n	60/61 (98%)	1.56	20 (33%) 0 0	88, 95, 101, 102	0
45	2n	60/61 (98%)	3.52	41 (68%) 0 0	96, 108, 113, 115	0
46	1o	88/89 (98%)	0.71	14 (15%) 1 1	83, 96, 104, 109	0
46	2o	88/89 (98%)	0.94	19 (21%) 0 0	94, 102, 109, 111	0
47	1p	82/88 (93%)	1.37	28 (34%) 0 0	92, 100, 106, 108	0
47	2p	82/88 (93%)	1.55	28 (34%) 0 0	90, 99, 104, 109	0
48	1q	99/105 (94%)	0.52	7 (7%) 16 9	88, 97, 103, 107	0
48	2q	99/105 (94%)	2.11	51 (51%) 0 0	91, 99, 107, 111	0
49	1r	68/88 (77%)	1.20	14 (20%) 1 0	88, 97, 104, 106	0
49	2r	68/88 (77%)	0.65	10 (14%) 2 1	91, 101, 106, 111	0
50	1s	83/93 (89%)	0.03	3 (3%) 42 28	93, 99, 106, 113	0
50	2s	83/93 (89%)	0.17	6 (7%) 15 8	102, 107, 112, 114	0
51	1t	96/106 (90%)	1.08	28 (29%) 0 0	90, 100, 105, 108	0
51	2t	96/106 (90%)	1.36	26 (27%) 0 0	91, 99, 107, 111	0
52	1u	23/27 (85%)	0.89	2 (8%) 10 6	93, 98, 101, 102	0
52	2u	23/27 (85%)	1.53	6 (26%) 0 0	102, 106, 109, 112	0
53	1v	12/24 (50%)	2.46	6 (50%) 0 0	88, 98, 119, 119	0
53	2v	7/24 (29%)	0.77	2 (28%) 0 0	100, 103, 118, 118	0
54	1w	64/76 (84%)	1.63	21 (32%) 0 0	94, 117, 124, 127	0
54	1y	67/76 (88%)	1.27	18 (26%) 0 0	83, 120, 124, 126	0
54	2w	62/76 (81%)	0.53	6 (9%) 7 4	107, 122, 127, 130	0
54	2y	66/76 (86%)	0.59	9 (13%) 3 1	97, 119, 123, 126	0
55	1x	72/77 (93%)	0.24	3 (4%) 36 23	85, 97, 110, 112	0
55	2x	72/77 (93%)	-0.12	2 (2%) 53 36	95, 108, 115, 119	0
All	All	20862/21748 (95%)	0.82	3414 (16%) 1 1	67, 96, 113, 130	0

All (3414) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	18.6
22	10	6	GLY	15.7

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Mol	Chain	Res	Type	RSRZ
22	20	7	LEU	14.7
44	2m	124	PRO	14.2
44	1m	123	ALA	13.8
22	20	5	LYS	13.7
22	20	4	LYS	13.4
38	1g	85	TYR	13.4
44	2m	123	ALA	13.0
22	10	7	LEU	12.9
31	29	37	GLY	12.8
22	10	4	LYS	12.1
23	11	2	SER	11.8
44	2m	121	LYS	11.3
45	2n	34	TYR	11.2
9	2N	8	GLN	11.2
3	2D	2	ALA	11.2
45	2n	25	VAL	11.1
38	1g	84	ASN	11.1
8	2I	123	LEU	11.0
22	10	5	LYS	10.7
29	27	47	ARG	10.4
27	15	2	ALA	10.4
22	20	3	HIS	10.3
22	20	2	ALA	10.1
22	10	3	HIS	10.1
42	2k	13	GLN	9.9
45	2n	39	LEU	9.8
40	2i	125	TYR	9.6
45	2n	38	GLY	9.5
44	2m	120	LYS	9.4
8	2I	89	TYR	9.4
41	2j	47	PHE	9.3
45	2n	37	PHE	9.2
3	2D	276	LYS	9.1
9	2N	44	PRO	9.1
10	2O	1	MET	9.0
43	2I	64	TYR	9.0
11	2P	45	LEU	9.0
22	20	6	GLY	8.9
22	20	8	GLY	8.8
38	2g	82	GLY	8.7
39	2h	133	LEU	8.7
4	2E	132	HIS	8.6

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Mol	Chain	Res	Type	RSRZ
3	1D	275	LYS	8.6
5	2F	82	ILE	8.6
5	2F	89	VAL	8.6
41	2j	62	HIS	8.6
3	1D	276	LYS	8.5
3	2D	55	GLY	8.4
29	27	48	LYS	8.4
22	10	8	GLY	8.3
3	2D	215	LEU	8.3
23	11	36	GLY	8.2
4	1E	141	ILE	8.2
35	2d	108	LEU	8.1
42	1k	50	TYR	8.0
42	1k	42	TRP	8.0
42	1k	75	TYR	8.0
9	2N	45	ASN	7.9
3	2D	38	LYS	7.9
9	2N	9	VAL	7.8
23	21	2	SER	7.8
7	2H	107	VAL	7.8
44	1m	120	LYS	7.8
31	29	16	VAL	7.8
13	2R	69	ASP	7.7
43	2l	18	VAL	7.7
5	2F	83	PHE	7.7
40	1i	115	GLY	7.7
9	2N	43	THR	7.7
22	20	11	ARG	7.7
41	2j	59	SER	7.6
45	2n	35	ARG	7.6
17	1V	73	SER	7.6
29	17	46	VAL	7.6
42	2k	89	ALA	7.5
42	1k	25	TYR	7.5
5	2F	57	VAL	7.5
27	15	60	VAL	7.5
5	1F	89	VAL	7.4
34	2c	198	VAL	7.4
5	2F	56	GLU	7.4
22	10	2	ALA	7.4
29	17	1	MET	7.3
8	2I	109	ILE	7.3

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Mol	Chain	Res	Type	RSRZ
12	1Q	33	GLY	7.3
5	2F	90	PHE	7.3
27	25	2	ALA	7.2
27	25	6	VAL	7.2
52	2u	14	TRP	7.2
8	2I	85	GLU	7.1
18	2W	92	ARG	7.1
45	2n	2	ALA	7.1
23	11	21	ARG	7.0
30	28	2	PRO	7.0
17	1V	84	LYS	7.0
9	2N	73	THR	7.0
20	2Y	35	TYR	7.0
7	2H	115	VAL	6.9
5	2F	62	ARG	6.9
48	2q	37	LYS	6.9
42	1k	30	VAL	6.9
27	25	3	LYS	6.9
9	2N	83	LYS	6.9
9	2N	116	LEU	6.9
51	1t	14	LYS	6.9
8	2I	84	GLY	6.8
17	2V	74	LYS	6.8
3	2D	4	LYS	6.8
45	2n	44	LEU	6.8
7	2H	94	TYR	6.8
47	1p	7	ALA	6.8
39	2h	83	ILE	6.8
51	2t	9	ASN	6.7
34	1c	201	TYR	6.7
18	2W	85	VAL	6.7
5	2F	78	ILE	6.7
12	2Q	103	MET	6.7
38	1g	151	TYR	6.7
48	2q	38	ARG	6.7
22	20	9	SER	6.7
47	1p	1	MET	6.7
23	11	41	ARG	6.7
38	1g	156	TRP	6.6
47	2p	1	MET	6.6
41	2j	65	LEU	6.6
42	1k	123	LYS	6.6

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Mol	Chain	Res	Type	RSRZ
23	21	39	LYS	6.6
30	28	7	HIS	6.6
4	2E	141	ILE	6.6
44	2m	102	ARG	6.6
4	1E	151	TYR	6.6
29	17	48	LYS	6.6
39	2h	111	ILE	6.6
4	2E	134	ILE	6.6
51	2t	18	GLN	6.5
29	27	1	MET	6.5
13	2R	68	ARG	6.5
44	1m	122	LYS	6.5
39	2h	112	LEU	6.5
9	2N	10	GLU	6.5
20	2Y	55	TYR	6.5
53	1v	24	A	6.5
30	28	16	ILE	6.5
38	1g	153	HIS	6.5
35	2d	37	PRO	6.5
9	2N	23	LEU	6.4
4	2E	150	VAL	6.4
3	1D	15	PHE	6.4
29	27	46	VAL	6.4
54	1w	71	G	6.4
48	2q	30	PRO	6.4
5	2F	76	GLY	6.4
9	2N	51	PHE	6.4
9	2N	75	TYR	6.4
51	2t	24	LEU	6.3
20	2Y	1	MET	6.3
23	11	46	LEU	6.3
20	2Y	42	VAL	6.3
30	28	22	VAL	6.3
12	2Q	85	LYS	6.3
44	2m	122	LYS	6.3
17	2V	75	PHE	6.3
3	2D	39	LYS	6.3
42	1k	49	GLY	6.3
30	28	61	LEU	6.3
48	2q	100	LYS	6.3
41	2j	63	PHE	6.3
9	1N	54	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
42	1k	18	ARG	6.3
3	2D	6	PHE	6.3
9	2N	76	SER	6.3
41	2j	58	ASP	6.2
11	2P	38	GLN	6.2
9	2N	84	LYS	6.2
23	11	23	LYS	6.2
7	2H	103	LEU	6.2
54	2w	73	A	6.2
4	2E	133	LYS	6.2
11	2P	51	PHE	6.2
27	25	7	PRO	6.2
30	18	7	HIS	6.2
18	2W	86	LEU	6.2
42	1k	83	ILE	6.2
4	2E	137	HIS	6.2
9	2N	74	ARG	6.1
41	2j	55	LYS	6.1
38	1g	86	GLN	6.1
5	2F	69	HIS	6.1
17	1V	38	LEU	6.1
23	11	47	GLN	6.1
42	1k	87	THR	6.1
43	1l	64	TYR	6.1
4	1E	143	ASN	6.1
42	1k	14	VAL	6.1
7	2H	13	LYS	6.1
35	2d	68	TYR	6.1
45	2n	42	ILE	6.1
9	1N	72	TYR	6.1
5	2F	80	ALA	6.1
51	1t	18	GLN	6.1
3	2D	5	LYS	6.0
3	2D	221	VAL	6.0
11	2P	35	HIS	6.0
3	2D	207	GLY	6.0
16	1U	4	ALA	6.0
51	2t	23	ARG	6.0
3	1D	5	LYS	5.9
3	2D	217	ARG	5.9
19	2X	33	LYS	5.9
19	2X	68	ARG	5.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
51	2t	21	LYS	5.9
8	2I	122	GLU	5.9
11	2P	46	LYS	5.9
29	17	47	ARG	5.9
8	2I	121	LYS	5.9
34	2c	155	GLY	5.9
35	2d	146	ILE	5.9
46	2o	87	ILE	5.9
27	25	4	HIS	5.9
42	1k	77	MET	5.9
1	2A	2897	U	5.9
5	2F	81	PRO	5.8
38	2g	156	TRP	5.8
3	2D	273	ARG	5.8
9	2N	11	PRO	5.8
3	2D	202	LYS	5.8
29	17	36	GLN	5.8
43	2l	26	ALA	5.8
7	2H	159	GLU	5.8
48	2q	32	TYR	5.8
51	1t	9	ASN	5.8
23	21	61	ARG	5.8
54	1w	72	C	5.8
45	2n	53	LEU	5.8
51	1t	8	ARG	5.7
51	2t	22	ARG	5.7
29	17	45	ALA	5.7
51	1t	20	LEU	5.7
5	1F	50	SER	5.7
23	11	97	LEU	5.7
4	2E	131	ALA	5.7
3	1D	222	ARG	5.7
53	1v	13	A	5.7
3	2D	15	PHE	5.7
9	2N	104	LYS	5.7
3	2D	51	VAL	5.7
8	2I	3	VAL	5.7
9	2N	122	VAL	5.7
29	27	2	LYS	5.7
42	1k	60	ALA	5.6
5	2F	79	GLY	5.6
3	1D	204	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
47	2p	8	ARG	5.6
22	20	10	THR	5.6
3	1D	263	ARG	5.6
40	1i	113	LYS	5.6
44	2m	119	GLY	5.6
22	20	12	ASN	5.6
36	1e	24	ARG	5.6
8	2I	87	LYS	5.6
16	2U	20	LEU	5.6
44	1m	121	LYS	5.6
29	27	18	PHE	5.6
45	2n	61	TRP	5.6
13	2R	70	LEU	5.6
45	2n	23	ARG	5.5
40	2i	127	LYS	5.5
11	2P	95	VAL	5.5
36	2e	22	GLY	5.5
38	1g	79	ARG	5.5
42	1k	13	GLN	5.5
39	2h	91	ARG	5.5
4	1E	123	ALA	5.5
39	2h	131	GLY	5.5
51	2t	13	LEU	5.5
42	1k	16	SER	5.5
42	1k	126	ARG	5.5
11	2P	125	VAL	5.5
18	2W	94	ASP	5.5
42	1k	92	GLU	5.5
4	1E	140	SER	5.5
9	2N	82	LEU	5.5
5	2F	64	ILE	5.5
36	2e	31	LEU	5.4
27	15	3	LYS	5.4
42	1k	28	THR	5.4
4	2E	157	ALA	5.4
12	2Q	12	GLN	5.4
30	28	64	TYR	5.4
40	1i	125	TYR	5.4
5	2F	72	ARG	5.4
8	1I	27	ARG	5.4
16	2U	47	TYR	5.4
3	1D	202	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
27	15	7	PRO	5.4
39	2h	2	LEU	5.4
11	2P	42	SER	5.4
48	2q	7	THR	5.4
11	2P	21	ARG	5.4
11	2P	47	ASP	5.4
12	2Q	34	LEU	5.4
23	11	49	VAL	5.4
4	2E	151	TYR	5.4
41	1j	60	ARG	5.4
54	1w	10	G	5.4
3	1D	39	LYS	5.4
36	2e	88	LYS	5.4
13	2R	21	TYR	5.4
34	2c	14	ILE	5.3
8	2I	111	PRO	5.3
5	1F	92	PRO	5.3
43	2l	5	PRO	5.3
9	2N	120	LEU	5.3
11	2P	30	THR	5.3
35	2d	165	MET	5.3
4	2E	130	GLY	5.3
11	2P	20	GLY	5.3
30	28	10	ALA	5.3
49	1r	78	LEU	5.3
39	1h	61	VAL	5.3
42	1k	47	VAL	5.3
5	1F	52	LYS	5.3
9	2N	119	ARG	5.3
39	2h	92	ARG	5.3
18	1W	95	ILE	5.3
3	2D	203	ASN	5.2
35	2d	167	GLY	5.2
16	1U	40	PHE	5.2
34	1c	179	ARG	5.2
43	1l	18	VAL	5.2
16	1U	5	LYS	5.2
42	2k	59	TYR	5.2
4	2E	149	ARG	5.2
17	2V	83	ARG	5.2
17	1V	74	LYS	5.2
33	2b	165	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
3	2D	257	LEU	5.2
9	1N	48	MET	5.2
10	2O	41	ALA	5.2
40	1i	126	SER	5.2
35	2d	168	ARG	5.2
38	2g	81	GLY	5.2
3	2D	59	LYS	5.2
10	2O	19	ILE	5.2
11	1P	15	ARG	5.2
16	2U	8	VAL	5.2
18	2W	90	ARG	5.2
4	1E	149	ARG	5.1
42	1k	73	MET	5.1
30	28	62	LEU	5.1
47	2p	74	LEU	5.1
38	2g	83	ALA	5.1
42	1k	15	ALA	5.1
48	2q	87	LYS	5.1
43	2l	7	ILE	5.1
41	2j	67	THR	5.1
34	2c	201	TYR	5.1
20	1Y	1	MET	5.1
3	1D	203	ASN	5.1
49	1r	87	ARG	5.1
4	2E	129	HIS	5.1
34	2c	60	ALA	5.1
3	1D	182	LEU	5.1
36	2e	84	PHE	5.1
42	1k	100	ALA	5.1
3	1D	273	ARG	5.1
15	1T	46	GLU	5.1
11	2P	37	GLY	5.1
19	2X	92	LEU	5.1
38	1g	154	TYR	5.1
3	2D	206	LEU	5.0
20	2Y	29	GLU	5.0
41	2j	61	GLU	5.0
1	2A	2132	U	5.0
34	2c	160	ALA	5.0
38	1g	77	SER	5.0
30	28	63	PRO	5.0
5	2F	172	TRP	5.0

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Mol	Chain	Res	Type	RSRZ
23	11	7	ILE	5.0
42	1k	120	ARG	5.0
3	1D	227	ASN	5.0
48	2q	29	HIS	5.0
7	2H	48	GLY	5.0
4	1E	154	LYS	5.0
42	1k	70	LYS	5.0
10	1O	1	MET	5.0
38	2g	154	TYR	5.0
29	17	2	LYS	5.0
35	2d	35	ARG	5.0
9	2N	140	VAL	5.0
9	2N	70	LYS	5.0
10	1O	79	PHE	5.0
42	1k	57	THR	5.0
38	1g	80	VAL	5.0
5	1F	69	HIS	5.0
34	1c	12	LEU	5.0
52	1u	14	TRP	5.0
3	1D	11	PRO	5.0
5	1F	90	PHE	5.0
34	2c	154	SER	5.0
16	2U	13	LYS	5.0
35	2d	20	TYR	4.9
5	2F	41	LEU	4.9
3	1D	219	PRO	4.9
23	11	26	ARG	4.9
42	1k	89	ALA	4.9
39	2h	134	ILE	4.9
35	2d	160	GLN	4.9
38	2g	153	HIS	4.9
44	2m	101	GLN	4.9
9	1N	107	LEU	4.9
51	2t	20	LEU	4.9
39	2h	85	ARG	4.9
5	1F	88	VAL	4.9
8	2I	19	VAL	4.9
16	2U	43	GLY	4.9
35	2d	107	ARG	4.9
11	1P	40	SER	4.9
42	1k	81	ASP	4.9
10	2O	2	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
4	1E	122	PHE	4.9
36	2e	45	PHE	4.9
3	1D	176	ARG	4.9
4	2E	127	ASP	4.9
16	2U	36	ARG	4.9
34	2c	2	GLY	4.9
36	1e	23	GLY	4.9
9	2N	117	PHE	4.9
11	1P	45	LEU	4.9
3	2D	16	MET	4.9
11	2P	149	GLU	4.9
40	2i	4	TYR	4.9
48	2q	42	TYR	4.9
48	2q	11	VAL	4.8
33	2b	187	LEU	4.8
36	2e	13	ILE	4.8
48	2q	31	LEU	4.8
10	1O	82	ASN	4.8
23	11	70	VAL	4.8
27	25	9	LYS	4.8
4	1E	132	HIS	4.8
9	2N	26	LEU	4.8
3	2D	216	GLY	4.8
12	2Q	15	GLY	4.8
15	2T	69	GLY	4.8
42	1k	29	ILE	4.8
15	1T	72	VAL	4.8
38	1g	82	GLY	4.8
5	1F	48	THR	4.8
48	2q	22	LEU	4.8
12	2Q	87	LYS	4.8
23	11	67	ILE	4.8
42	1k	80	VAL	4.8
45	2n	33	VAL	4.8
18	2W	82	LEU	4.8
36	1e	89	ILE	4.8
42	2k	108	ILE	4.8
47	2p	17	TYR	4.8
9	2N	77	GLY	4.8
35	2d	184	LYS	4.8
42	2k	32	ILE	4.8
9	1N	109	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
10	1O	97	ARG	4.8
30	28	21	LYS	4.8
19	2X	69	TYR	4.8
4	1E	1	MET	4.7
42	1k	56	GLY	4.7
23	11	60	PHE	4.7
41	2j	11	PHE	4.7
5	1F	93	LYS	4.7
28	26	54	ILE	4.7
51	2t	14	LYS	4.7
11	1P	49	ARG	4.7
11	2P	54	GLY	4.7
54	1w	73	A	4.7
47	2p	59	TRP	4.7
35	2d	104	VAL	4.7
35	2d	185	PHE	4.7
17	2V	73	SER	4.7
39	2h	119	LEU	4.7
7	2H	148	ILE	4.7
48	2q	90	ILE	4.7
45	1n	23	ARG	4.7
4	1E	158	GLY	4.7
27	25	10	LYS	4.7
45	1n	50	LYS	4.7
18	2W	93	ALA	4.7
41	2j	98	ILE	4.7
31	29	15	LYS	4.7
54	1y	1	G	4.7
5	2F	65	TRP	4.7
9	2N	13	TRP	4.7
42	1k	63	LEU	4.7
45	2n	26	ARG	4.7
51	2t	25	ARG	4.7
23	21	38	SER	4.7
3	2D	9	TYR	4.7
3	1D	221	VAL	4.7
3	2D	54	ARG	4.7
35	1d	118	ARG	4.7
35	2d	64	LEU	4.7
3	2D	8	PRO	4.7
12	2Q	73	PRO	4.7
13	2R	10	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
18	1W	69	LEU	4.7
42	1k	98	LEU	4.7
5	2F	77	ASP	4.7
31	29	17	ILE	4.7
42	1k	108	ILE	4.7
3	1D	243	GLY	4.7
4	1E	124	GLY	4.7
47	1p	25	ARG	4.7
3	2D	84	TYR	4.7
10	1O	7	TYR	4.7
9	2N	99	LEU	4.7
6	2G	137	GLU	4.7
35	2d	162	LEU	4.7
3	2D	204	ILE	4.7
9	1N	85	ILE	4.7
39	2h	100	ILE	4.7
9	1N	119	ARG	4.7
7	2H	123	PHE	4.6
35	2d	140	VAL	4.6
9	1N	116	LEU	4.6
11	1P	3	LEU	4.6
40	2i	115	GLY	4.6
47	1p	36	ILE	4.6
36	1e	88	LYS	4.6
42	1k	82	VAL	4.6
38	1g	78	ARG	4.6
4	2E	128	SER	4.6
7	2H	105	LEU	4.6
20	2Y	50	ARG	4.6
4	2E	126	PRO	4.6
3	1D	233	HIS	4.6
54	1w	70	G	4.6
4	1E	195	LEU	4.6
11	2P	62	LEU	4.6
19	2X	70	LEU	4.6
30	28	25	MET	4.6
3	2D	208	LYS	4.6
11	2P	39	LYS	4.6
42	1k	122	LYS	4.6
3	1D	206	LEU	4.6
23	11	24	ALA	4.6
10	1O	122	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
15	1T	28	VAL	4.6
7	2H	90	LYS	4.6
29	17	14	LYS	4.6
30	28	59	LYS	4.6
3	1D	268	ARG	4.6
41	2j	60	ARG	4.6
4	2E	10	GLY	4.6
33	1b	77	ALA	4.6
42	1k	20	TYR	4.6
29	27	14	LYS	4.6
3	1D	205	VAL	4.5
4	2E	142	GLY	4.6
11	2P	123	LEU	4.5
34	2c	52	LEU	4.5
41	2j	66	ARG	4.5
20	2Y	48	ALA	4.5
34	2c	184	TYR	4.5
1	2A	2896	C	4.5
41	2j	54	PHE	4.5
49	2r	84	LYS	4.5
23	11	62	VAL	4.5
12	1Q	41	TRP	4.5
42	2k	126	ARG	4.5
36	2e	90	VAL	4.5
49	1r	40	LEU	4.5
8	1I	1	MET	4.5
11	2P	18	ARG	4.5
20	2Y	45	VAL	4.5
49	2r	85	LEU	4.5
11	2P	29	LYS	4.5
31	29	1	MET	4.5
41	2j	50	ILE	4.5
34	1c	164	ARG	4.5
35	2d	122	ARG	4.5
42	1k	78	GLN	4.5
1	1A	2145	C	4.5
4	1E	147	PRO	4.5
12	2Q	80	GLU	4.5
4	1E	125	GLY	4.5
9	1N	75	TYR	4.5
45	2n	47	LEU	4.5
34	2c	8	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
9	2N	109	LYS	4.5
11	2P	36	LYS	4.5
16	1U	32	PHE	4.5
35	1d	110	PHE	4.5
5	2F	87	GLY	4.5
4	1E	129	HIS	4.5
9	2N	72	TYR	4.5
19	2X	13	LEU	4.5
41	2j	56	HIS	4.5
1	1A	529	A	4.5
40	2i	65	VAL	4.5
9	2N	12	ARG	4.5
11	2P	33	ARG	4.5
15	1T	64	ARG	4.5
3	2D	219	PRO	4.5
3	1D	16	MET	4.5
5	2F	49	ALA	4.5
19	1X	29	TRP	4.5
16	2U	40	PHE	4.5
4	1E	139	GLY	4.5
9	2N	61	ARG	4.5
47	2p	4	ILE	4.5
27	15	5	PRO	4.5
36	1e	22	GLY	4.5
27	25	19	ARG	4.5
10	1O	10	VAL	4.5
16	2U	33	ARG	4.4
7	2H	114	VAL	4.4
48	2q	23	VAL	4.4
10	1O	5	GLN	4.4
11	2P	59	LEU	4.4
47	2p	6	LEU	4.4
10	2O	7	TYR	4.4
19	2X	18	TYR	4.4
3	2D	14	ARG	4.4
11	1P	108	LYS	4.4
22	20	13	GLY	4.4
13	1R	10	LEU	4.4
13	1R	42	LYS	4.4
45	2n	7	ILE	4.4
5	1F	83	PHE	4.4
13	1R	20	LEU	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	1w	1	G	4.4
12	1Q	85	LYS	4.4
45	1n	25	VAL	4.4
3	2D	52	ARG	4.4
16	1U	25	TRP	4.4
5	2F	75	HIS	4.4
11	1P	48	PRO	4.4
45	2n	41	ARG	4.4
23	11	34	THR	4.4
23	11	42	GLN	4.4
48	2q	27	PHE	4.4
36	1e	81	GLU	4.4
28	26	7	ILE	4.4
15	1T	45	PHE	4.4
20	1Y	4	LYS	4.4
9	2N	60	ILE	4.4
30	28	12	LYS	4.4
47	2p	9	PHE	4.4
18	2W	81	ALA	4.4
27	25	11	THR	4.4
42	1k	43	SER	4.4
15	2T	99	LEU	4.4
3	2D	236	GLY	4.4
20	2Y	4	LYS	4.4
30	28	5	LYS	4.4
16	1U	28	ARG	4.3
7	2H	133	VAL	4.3
36	1e	82	VAL	4.3
5	2F	73	ALA	4.3
18	1W	90	ARG	4.3
28	26	2	ALA	4.3
45	2n	29	ARG	4.3
7	2H	116	GLU	4.3
54	2w	72	C	4.3
37	1f	48	LEU	4.3
11	1P	11	GLY	4.3
32	1a	1511	G	4.3
32	2a	78	G	4.3
10	1O	44	LYS	4.3
23	11	98	LEU	4.3
48	2q	21	VAL	4.3
3	1D	53	PHE	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
12	1Q	76	LYS	4.3
5	2F	61	GLY	4.3
45	2n	22	THR	4.3
16	1U	37	GLU	4.3
27	25	8	LYS	4.3
45	2n	36	PHE	4.3
42	2k	119	CYS	4.3
30	18	50	LEU	4.3
41	2j	10	GLY	4.3
3	1D	254	THR	4.3
7	2H	145	ALA	4.3
12	1Q	82	ARG	4.3
16	2U	39	LEU	4.3
7	2H	35	VAL	4.3
23	11	4	VAL	4.3
34	1c	87	LEU	4.3
17	1V	81	TYR	4.3
5	2F	50	SER	4.3
3	1D	257	LEU	4.3
34	2c	13	GLY	4.3
34	2c	196	LEU	4.3
9	2N	48	MET	4.3
45	2n	49	HIS	4.3
10	1O	63	VAL	4.3
30	28	15	LYS	4.3
12	2Q	38	GLU	4.2
3	1D	226	MET	4.2
40	1i	114	TYR	4.2
23	11	50	ARG	4.2
3	2D	223	GLY	4.2
11	2P	50	ARG	4.2
12	2Q	11	LYS	4.2
43	2l	32	PHE	4.2
45	2n	56	VAL	4.2
18	2W	103	ILE	4.2
39	2h	94	TYR	4.2
29	27	15	THR	4.2
30	18	5	LYS	4.2
33	2b	37	ASN	4.2
4	1E	156	MET	4.2
9	2N	5	VAL	4.2
9	2N	108	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
9	2N	111	PRO	4.2
3	1D	225	ALA	4.2
18	1W	112	GLY	4.2
54	1y	2	C	4.2
40	2i	64	THR	4.2
3	2D	18	VAL	4.2
5	2F	88	VAL	4.2
47	2p	19	ILE	4.2
35	2d	164	ALA	4.2
42	1k	74	ALA	4.2
6	2G	133	LEU	4.2
9	1N	82	LEU	4.2
9	1N	120	LEU	4.2
16	1U	27	LEU	4.2
46	2o	67	LEU	4.2
23	2l	14	VAL	4.2
38	1g	87	VAL	4.2
7	2H	89	ILE	4.2
39	2h	136	GLU	4.2
42	1k	96	ARG	4.2
45	2n	30	ALA	4.2
35	2d	19	LEU	4.2
1	1A	2146	C	4.2
3	2D	17	THR	4.2
39	2h	86	ILE	4.2
42	1k	54	ARG	4.2
42	2k	25	TYR	4.2
11	1P	39	LYS	4.2
17	2V	72	VAL	4.2
20	2Y	7	VAL	4.2
18	2W	99	ARG	4.2
42	1k	91	ARG	4.2
4	1E	142	GLY	4.2
46	1o	56	LEU	4.2
17	1V	75	PHE	4.2
54	1y	24	G	4.2
34	2c	40	ARG	4.2
5	1F	51	THR	4.2
10	1O	65	THR	4.2
30	28	3	LYS	4.2
12	2Q	79	LEU	4.1
34	2c	204	LEU	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
45	2n	52	GLN	4.1
7	2H	152	ARG	4.1
12	2Q	81	VAL	4.1
48	2q	39	SER	4.1
7	2H	151	ILE	4.1
51	2t	26	ASN	4.1
9	2N	7	LYS	4.1
7	2H	88	LEU	4.1
34	1c	196	LEU	4.1
3	2D	13	ARG	4.1
3	2D	211	ARG	4.1
10	1O	81	ASP	4.1
40	2i	109	VAL	4.1
16	2U	88	ILE	4.1
8	1I	23	PRO	4.1
34	1c	193	TYR	4.1
36	2e	12	LEU	4.1
4	1E	155	LYS	4.1
9	2N	54	VAL	4.1
15	2T	48	ILE	4.1
35	2d	67	ILE	4.1
54	2w	71	G	4.1
3	2D	53	PHE	4.1
11	1P	38	GLN	4.1
15	1T	89	VAL	4.1
30	18	23	VAL	4.1
34	2c	207	VAL	4.1
23	11	11	ARG	4.1
3	2D	7	LYS	4.1
18	2W	89	ALA	4.1
4	2E	135	HIS	4.1
16	1U	117	GLN	4.1
40	2i	114	TYR	4.1
9	1N	122	VAL	4.1
17	2V	5	VAL	4.1
11	2P	52	GLU	4.1
12	2Q	41	TRP	4.1
51	1t	11	SER	4.1
10	1O	46	ALA	4.1
13	1R	100	LEU	4.1
36	1e	21	ALA	4.1
45	2n	6	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
4	1E	3	GLY	4.1
4	1E	116	VAL	4.1
39	2h	90	GLY	4.1
39	2h	93	VAL	4.1
36	2e	89	ILE	4.1
17	2V	71	LEU	4.1
54	1y	56	C	4.1
1	2A	586	A	4.1
54	2w	31	A	4.1
3	1D	37	LEU	4.1
27	25	13	LYS	4.1
34	2c	199	LYS	4.1
34	2c	197	GLY	4.1
34	1c	33	LEU	4.1
44	2m	90	LEU	4.1
11	2P	15	ARG	4.0
18	1W	97	LYS	4.1
3	1D	9	TYR	4.0
9	2N	46	VAL	4.0
11	2P	64	LYS	4.0
17	1V	78	LYS	4.0
17	2V	1	MET	4.0
41	2j	51	ARG	4.0
23	11	63	ALA	4.0
42	1k	17	GLY	4.0
10	2O	47	ILE	4.0
13	1R	21	TYR	4.0
23	11	95	LEU	4.0
10	1O	114	ILE	4.0
9	2N	34	LEU	4.0
43	2l	10	LEU	4.0
30	28	4	MET	4.0
12	1Q	81	VAL	4.0
41	2j	46	ARG	4.0
47	2p	5	ARG	4.0
1	2A	2801(A)	A	4.0
3	1D	166	GLN	4.0
30	28	60	LEU	4.0
11	1P	51	PHE	4.0
1	1A	614(B)	G	4.0
38	1g	81	GLY	4.0
30	28	14	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
51	2t	70	SER	4.0
9	2N	85	ILE	4.0
42	2k	71	LYS	4.0
43	2l	28	LYS	4.0
12	2Q	104	PHE	4.0
38	1g	145	ALA	4.0
43	2l	15	ARG	4.0
54	1w	3	C	4.0
10	1O	85	VAL	4.0
42	1k	26	ASN	4.0
20	2Y	63	LYS	4.0
51	1t	21	LYS	4.0
36	2e	10	MET	4.0
4	1E	145	LYS	4.0
9	2N	50	ASP	4.0
11	2P	124	LYS	4.0
12	1Q	68	ILE	4.0
18	2W	95	ILE	4.0
20	2Y	61	ILE	4.0
5	1F	72	ARG	4.0
40	2i	36	TYR	4.0
9	1N	53	VAL	3.9
16	1U	2	PRO	3.9
9	1N	30	ILE	3.9
31	29	36	GLN	3.9
54	2y	53	G	3.9
20	2Y	25	GLY	3.9
31	29	24	TYR	3.9
9	2N	90	MET	3.9
39	2h	9	MET	3.9
51	2t	29	LYS	3.9
20	2Y	32	PRO	3.9
35	2d	70	ILE	3.9
3	1D	155	LEU	3.9
16	2U	18	LEU	3.9
19	2X	66	LEU	3.9
34	2c	10	PHE	3.9
48	2q	4	LYS	3.9
3	2D	226	MET	3.9
54	1y	33	U	3.9
47	1p	21	VAL	3.9
47	2p	20	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
10	2O	18	LYS	3.9
1	1A	2506	U	3.9
54	1y	34	G	3.9
9	2N	52	VAL	3.9
16	2U	63	VAL	3.9
11	1P	44	GLY	3.9
17	2V	94	LEU	3.9
37	1f	61	LEU	3.9
42	1k	66	LEU	3.9
42	1k	86	GLY	3.9
39	2h	87	SER	3.9
42	1k	44	SER	3.9
17	2V	78	LYS	3.9
5	2F	66	PRO	3.9
40	2i	110	GLU	3.9
42	1k	31	THR	3.9
1	2A	229	A	3.9
19	1X	68	ARG	3.9
43	1l	22	SER	3.9
3	2D	270	ILE	3.9
11	1P	19	VAL	3.9
28	16	54	ILE	3.9
33	2b	108	ILE	3.9
35	2d	98	GLU	3.9
39	2h	6	ILE	3.9
42	2k	14	VAL	3.9
39	2h	10	LEU	3.9
41	2j	48	THR	3.9
42	2k	91	ARG	3.9
9	1N	47	ALA	3.9
4	1E	134	ILE	3.9
9	1N	52	VAL	3.9
10	1O	86	ILE	3.9
15	1T	57	PHE	3.9
9	1N	84	LYS	3.9
17	2V	20	LEU	3.9
23	11	44	PRO	3.9
45	2n	45	ARG	3.9
11	1P	35	HIS	3.9
23	11	37	ILE	3.9
23	21	37	ILE	3.9
13	2R	17	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
25	23	26	LEU	3.9
29	27	9	ARG	3.9
51	2t	28	ALA	3.9
4	2E	140	SER	3.9
7	2H	41	MET	3.9
7	2H	85	LYS	3.8
17	2V	76	LYS	3.8
32	2a	84	U	3.8
11	2P	65	ARG	3.8
13	1R	17	ARG	3.8
36	1e	28	PHE	3.8
47	2p	73	LEU	3.8
42	1k	51	LYS	3.8
9	1N	61	ARG	3.8
4	2E	115	GLY	3.8
11	2P	43	GLY	3.8
3	1D	175	LEU	3.8
10	2O	8	LEU	3.8
34	2c	178	LEU	3.8
3	2D	184	LYS	3.8
42	1k	61	ALA	3.8
44	2m	103	THR	3.8
3	2D	201	HIS	3.8
34	1c	170	GLN	3.8
9	2N	16	ILE	3.8
10	1O	22	ILE	3.8
16	2U	17	ILE	3.8
38	2g	80	VAL	3.8
39	2h	13	ILE	3.8
3	2D	61	LEU	3.8
5	2F	181	LEU	3.8
15	1T	105	LEU	3.8
16	1U	20	LEU	3.8
35	1d	157	LEU	3.8
23	21	15	ALA	3.8
29	27	33	ARG	3.8
3	2D	250	TRP	3.8
37	1f	57	GLN	3.8
9	1N	71	ILE	3.8
22	10	9	SER	3.8
36	2e	129	ILE	3.8
4	1E	152	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
43	2l	27	LEU	3.8
45	2n	50	LYS	3.8
17	1V	83	ARG	3.8
23	1l	20	ARG	3.8
36	1e	18	ARG	3.8
39	2h	84	ARG	3.8
8	1l	120	ILE	3.8
18	2W	46	PHE	3.8
23	2l	13	ILE	3.8
39	2h	132	GLU	3.8
3	1D	244	ARG	3.8
4	2E	138	PRO	3.8
3	1D	253	GLN	3.8
9	1N	45	ASN	3.8
20	2Y	3	VAL	3.8
25	23	9	VAL	3.8
54	1y	36	A	3.8
16	1U	17	ILE	3.8
20	2Y	64	GLU	3.8
30	18	8	LYS	3.8
40	1i	119	ALA	3.8
43	2l	29	GLY	3.8
1	1A	2141	G	3.8
3	1D	271	ILE	3.8
7	2H	169	VAL	3.8
20	2Y	43	ASN	3.8
41	1j	58	ASP	3.8
51	2t	8	ARG	3.8
3	1D	248	SER	3.8
3	1D	261	LYS	3.8
4	1E	153	GLY	3.8
9	2N	69	GLN	3.8
44	2m	95	GLY	3.8
39	2h	99	GLU	3.8
9	2N	103	VAL	3.8
42	1k	40	ILE	3.8
9	2N	112	LEU	3.8
13	2R	29	LEU	3.8
15	1T	114	LEU	3.8
22	10	12	ASN	3.8
3	2D	275	LYS	3.8
16	1U	24	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
32	2a	1202	G	3.8
53	1v	12	A	3.8
53	1v	15	A	3.8
3	2D	11	PRO	3.8
3	2D	232	PRO	3.8
5	1F	80	ALA	3.8
13	1R	12	ARG	3.8
18	1W	93	ALA	3.8
29	27	23	ARG	3.8
3	1D	49	ILE	3.8
10	1O	98	VAL	3.8
33	2b	201	ILE	3.8
35	2d	112	VAL	3.8
3	1D	4	LYS	3.7
10	1O	18	LYS	3.7
27	15	9	LYS	3.7
3	2D	220	HIS	3.7
4	1E	137	HIS	3.7
8	1I	28	ASN	3.7
35	2d	4	TYR	3.7
5	2F	74	ARG	3.7
36	1e	14	ARG	3.7
47	1p	59	TRP	3.7
51	2t	12	ALA	3.7
20	2Y	24	VAL	3.7
38	1g	141	VAL	3.7
1	1A	1026	U	3.7
19	1X	92	LEU	3.7
35	2d	188	LEU	3.7
34	1c	155	GLY	3.7
8	2I	100	ALA	3.7
12	2Q	77	LYS	3.7
34	1c	167	TRP	3.7
4	2E	122	PHE	3.7
8	2I	35	LEU	3.7
10	1O	19	ILE	3.7
10	1O	40	VAL	3.7
40	2i	26	VAL	3.7
29	27	42	LEU	3.7
36	1e	19	MET	3.7
5	1F	95	ARG	3.7
12	2Q	82	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
16	2U	14	HIS	3.7
51	2t	17	ARG	3.7
44	2m	6	GLY	3.7
42	2k	35	PRO	3.7
3	1D	252	TRP	3.7
9	1N	51	PHE	3.7
6	2G	34	LEU	3.7
17	2V	82	ARG	3.7
29	27	35	ARG	3.7
9	1N	105	GLY	3.7
3	1D	232	PRO	3.7
10	1O	52	VAL	3.7
22	20	14	ARG	3.7
7	2H	138	LYS	3.7
16	1U	21	ALA	3.7
47	2p	39	TYR	3.7
3	1D	133	LEU	3.7
39	2h	95	VAL	3.7
49	1r	76	LEU	3.7
4	1E	131	ALA	3.7
34	2c	65	ALA	3.7
33	2b	32	ILE	3.7
12	1Q	83	MET	3.7
9	1N	49	GLY	3.7
23	11	33	LYS	3.7
23	11	39	LYS	3.7
35	2d	166	LYS	3.7
42	1k	71	LYS	3.7
43	1l	28	LYS	3.7
43	2l	19	ARG	3.7
3	1D	144	ALA	3.7
5	1F	49	ALA	3.7
23	11	71	TYR	3.7
4	1E	150	VAL	3.7
12	1Q	37	LEU	3.7
34	1c	153	VAL	3.7
35	2d	133	VAL	3.7
36	2e	109	ILE	3.7
42	1k	103	LEU	3.7
31	29	12	ASP	3.7
44	2m	110	ARG	3.7
30	18	2	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
42	2k	75	TYR	3.7
43	1l	98	TYR	3.7
42	1k	67	ASP	3.6
50	2s	38	SER	3.7
7	2H	108	GLY	3.6
45	1n	59	ALA	3.6
10	1O	58	VAL	3.6
42	1k	59	TYR	3.6
30	28	29	LYS	3.6
3	1D	251	GLY	3.6
9	2N	93	THR	3.6
12	2Q	10	ARG	3.6
39	2h	135	CYS	3.6
17	2V	80	GLN	3.6
40	2i	124	GLN	3.6
12	2Q	40	ALA	3.6
11	1P	17	LYS	3.6
23	11	48	LYS	3.6
40	1i	127	LYS	3.6
4	2E	189	PRO	3.6
7	2H	45	VAL	3.6
9	2N	14	VAL	3.6
9	2N	30	ILE	3.6
9	2N	98	VAL	3.6
10	1O	2	ILE	3.6
16	1U	47	TYR	3.6
34	2c	39	ILE	3.6
48	2q	98	LEU	3.6
51	1t	24	LEU	3.6
5	2F	51	THR	3.6
3	1D	38	LYS	3.6
18	2W	98	LYS	3.6
7	2H	24	VAL	3.6
13	1R	48	VAL	3.6
18	2W	6	ILE	3.6
39	1h	109	ILE	3.6
4	1E	117	MET	3.6
39	2h	22	GLU	3.6
4	1E	113	PHE	3.6
10	2O	17	ARG	3.6
33	2b	188	ALA	3.6
45	2n	57	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
54	1w	2	C	3.6
3	2D	271	ILE	3.6
33	1b	215	LEU	3.6
36	1e	13	ILE	3.6
39	1h	133	LEU	3.6
42	1k	21	ILE	3.6
3	1D	223	GLY	3.6
52	2u	17	THR	3.6
5	1F	62	ARG	3.6
3	1D	111	LEU	3.6
4	2E	116	VAL	3.6
41	2j	6	ILE	3.6
9	1N	70	LYS	3.6
4	1E	128	SER	3.6
11	2P	58	THR	3.6
5	2F	63	LYS	3.6
20	2Y	67	LEU	3.6
23	21	27	GLU	3.6
42	2k	90	GLY	3.6
32	1a	1508	G	3.6
38	1g	155	ARG	3.6
52	2u	22	ARG	3.6
23	11	38	SER	3.6
4	2E	155	LYS	3.6
54	1y	35	A	3.6
8	2I	79	ILE	3.6
12	2Q	91	GLU	3.6
15	2T	110	ILE	3.6
42	1k	95	ILE	3.6
9	2N	114	ARG	3.6
45	1n	37	PHE	3.6
34	1c	199	LYS	3.6
18	1W	86	LEU	3.6
9	2N	97	ARG	3.6
11	2P	49	ARG	3.6
10	1O	33	ALA	3.5
12	2Q	121	ALA	3.5
29	17	24	THR	3.5
35	1d	108	LEU	3.5
35	2d	130	GLY	3.5
47	2p	24	ALA	3.5
48	2q	8	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
3	1D	17	THR	3.5
48	2q	36	ILE	3.5
3	2D	233	HIS	3.5
9	1N	108	PRO	3.5
10	1O	4	PRO	3.5
17	1V	76	LYS	3.5
35	2d	134	ASP	3.5
10	2O	79	PHE	3.5
20	2Y	5	MET	3.5
35	2d	163	GLU	3.5
35	2d	23	GLY	3.5
45	2n	31	ARG	3.5
16	2U	16	LYS	3.5
18	2W	97	LYS	3.5
33	2b	133	LYS	3.5
9	1N	79	PRO	3.5
43	1l	94	PRO	3.5
43	2l	98	TYR	3.5
23	2l	26	ARG	3.5
7	2H	30	LYS	3.5
10	2O	33	ALA	3.5
33	1b	118	LEU	3.5
16	2U	90	VAL	3.5
18	2W	96	ILE	3.5
35	1d	148	VAL	3.5
22	20	45	PHE	3.5
18	2W	38	TYR	3.5
43	1l	19	ARG	3.5
9	2N	15	LEU	3.5
13	1R	51	LEU	3.5
5	1F	56	GLU	3.5
7	2H	10	PRO	3.5
12	2Q	14	ARG	3.5
40	1i	111	ARG	3.5
30	28	50	LEU	3.5
23	11	18	ILE	3.5
16	2U	25	TRP	3.5
11	1P	36	LYS	3.5
3	1D	8	PRO	3.5
34	2c	15	THR	3.5
40	2i	27	THR	3.5
3	1D	247	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
31	29	23	VAL	3.5
3	1D	213	ARG	3.5
3	1D	214	TRP	3.5
3	1D	250	TRP	3.5
15	1T	87	ASP	3.5
41	1j	59	SER	3.5
8	2I	86	THR	3.5
29	27	7	PRO	3.5
4	2E	114	ALA	3.5
13	1R	41	ALA	3.5
16	1U	42	ALA	3.5
20	2Y	106	LEU	3.5
39	1h	2	LEU	3.5
3	2D	253	GLN	3.5
5	1F	78	ILE	3.5
4	2E	136	ARG	3.5
11	2P	19	VAL	3.5
12	2Q	94	VAL	3.5
18	2W	105	VAL	3.5
35	2d	114	ARG	3.5
46	2o	60	VAL	3.5
11	2P	97	PRO	3.5
34	2c	158	GLY	3.5
35	2d	183	GLY	3.5
3	2D	58	HIS	3.5
9	1N	73	THR	3.5
49	1r	82	THR	3.5
23	11	32	LYS	3.5
34	2c	101	LEU	3.5
40	2i	92	TYR	3.5
36	1e	25	ARG	3.5
1	1A	2578	G	3.5
5	2F	68	LYS	3.4
27	25	5	PRO	3.4
8	2I	1	MET	3.4
20	2Y	2	ARG	3.4
24	12	69	ARG	3.4
5	1F	67	GLN	3.4
10	1O	38	VAL	3.4
12	2Q	96	VAL	3.4
3	1D	200	ASP	3.4
3	1D	255	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
44	1m	119	GLY	3.4
9	2N	38	HIS	3.4
9	1N	60	ILE	3.4
25	23	21	ALA	3.4
15	2T	72	VAL	3.4
42	1k	55	LYS	3.4
54	1w	4	C	3.4
1	2A	2585	U	3.4
4	1E	163	GLU	3.4
18	1W	92	ARG	3.4
23	11	17	SER	3.4
43	2l	22	SER	3.4
19	1X	13	LEU	3.4
25	23	8	LEU	3.4
41	1j	65	LEU	3.4
9	2N	57	ALA	3.4
3	1D	18	VAL	3.4
23	11	16	ASN	3.4
35	1d	5	ILE	3.4
5	1F	44	ARG	3.4
35	2d	115	ARG	3.4
36	1e	139	LEU	3.4
38	1g	88	PRO	3.4
7	2H	96	ALA	3.4
10	2O	114	ILE	3.4
23	21	10	LYS	3.4
39	1h	86	ILE	3.4
46	2o	48	LYS	3.4
20	2Y	51	VAL	3.4
33	2b	197	VAL	3.4
3	1D	42	GLY	3.4
11	2P	44	GLY	3.4
23	21	28	GLY	3.4
42	1k	125	PHE	3.4
43	1l	89	ARG	3.4
49	2r	87	ARG	3.4
11	2P	72	PRO	3.4
12	2Q	17	LEU	3.4
27	15	8	LYS	3.4
30	28	11	LYS	3.4
34	2c	4	LYS	3.4
48	2q	40	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
34	2c	37	GLN	3.4
15	2T	102	ILE	3.4
38	1g	73	MET	3.4
7	2H	113	VAL	3.4
15	2T	70	VAL	3.4
31	29	25	VAL	3.4
9	1N	74	ARG	3.4
11	1P	30	THR	3.4
30	18	46	ARG	3.4
44	1m	103	THR	3.4
48	2q	95	TYR	3.4
28	26	8	LYS	3.4
39	2h	88	LYS	3.4
3	2D	37	LEU	3.4
9	2N	107	LEU	3.4
41	1j	8	LEU	3.4
15	2T	1	MET	3.4
16	2U	10	ARG	3.4
29	27	22	MET	3.4
9	2N	78	TYR	3.4
54	1w	23	A	3.4
4	2E	2	LYS	3.4
3	2D	182	LEU	3.4
12	2Q	37	LEU	3.4
20	2Y	105	ALA	3.4
4	1E	133	LYS	3.4
16	1U	34	LYS	3.4
35	2d	169	LYS	3.4
47	2p	35	LYS	3.4
25	23	30	ARG	3.4
20	2Y	47	LYS	3.4
5	1F	75	HIS	3.4
9	2N	113	GLY	3.4
23	21	41	ARG	3.3
35	2d	118	ARG	3.3
23	21	33	LYS	3.3
30	18	61	LEU	3.3
3	2D	224	ALA	3.3
4	1E	4	ILE	3.3
4	2E	156	MET	3.3
23	11	64	ALA	3.3
34	2c	200	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
36	1e	86	ALA	3.3
29	17	10	ARG	3.3
44	2m	104	ARG	3.3
5	2F	70	THR	3.3
27	15	10	LYS	3.3
4	1E	120	TRP	3.3
5	2F	84	VAL	3.3
9	1N	140	VAL	3.3
10	1O	16	ALA	3.3
12	1Q	66	ILE	3.3
30	28	58	ILE	3.3
30	18	14	VAL	3.3
37	1f	88	VAL	3.3
42	1k	65	ALA	3.3
40	2i	9	ARG	3.3
9	2N	65	LYS	3.3
30	18	59	LYS	3.3
11	1P	32	THR	3.3
3	2D	49	ILE	3.3
7	2H	121	ILE	3.3
4	2E	167	VAL	3.3
9	2N	79	PRO	3.3
16	1U	35	ALA	3.3
28	26	5	VAL	3.3
32	1a	1531	A	3.3
42	1k	68	ALA	3.3
11	2P	60	MET	3.3
39	1h	9	MET	3.3
3	2D	89	SER	3.3
29	27	37	LYS	3.3
11	2P	94	GLU	3.3
5	1F	79	GLY	3.3
3	2D	145	VAL	3.3
5	2F	52	LYS	3.3
10	2O	99	PHE	3.3
11	2P	78	PRO	3.3
17	2V	14	VAL	3.3
20	2Y	65	ALA	3.3
42	2k	96	ARG	3.3
43	2l	31	PRO	3.3
10	1O	8	LEU	3.3
47	1p	6	LEU	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	1D	184	LYS	3.3
10	1O	17	ARG	3.3
3	1D	2	ALA	3.3
3	2D	40	THR	3.3
10	1O	47	ILE	3.3
16	2U	28	ARG	3.3
22	20	41	ARG	3.3
29	27	4	THR	3.3
30	18	11	LYS	3.3
19	2X	28	PHE	3.3
5	1F	81	PRO	3.3
7	2H	36	PRO	3.3
10	2O	81	ASP	3.3
13	1R	98	LEU	3.3
15	2T	114	LEU	3.3
17	2V	81	TYR	3.3
7	2H	95	ARG	3.3
18	2W	11	ARG	3.3
23	21	18	ILE	3.3
42	1k	23	ALA	3.3
42	2k	95	ILE	3.3
3	1D	10	THR	3.3
36	2e	55	VAL	3.3
1	2A	2155	G	3.3
3	2D	181	GLU	3.3
15	1T	65	LYS	3.3
19	2X	63	LYS	3.3
32	1a	1503	A	3.3
32	2a	60	A	3.3
42	1k	90	GLY	3.3
23	11	13	ILE	3.3
11	2P	126	VAL	3.3
28	26	4	GLU	3.3
40	2i	112	LYS	3.3
23	11	73	LEU	3.3
3	1D	51	VAL	3.3
3	1D	272	ALA	3.3
7	2H	144	VAL	3.3
13	1R	97	VAL	3.3
23	21	62	VAL	3.3
5	2F	53	THR	3.3
9	2N	40	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
38	2g	78	ARG	3.3
5	1F	87	GLY	3.3
18	1W	43	GLY	3.3
3	1D	270	ILE	3.2
20	2Y	60	PHE	3.2
30	18	64	TYR	3.2
9	1N	118	LYS	3.2
16	1U	22	LYS	3.2
33	2b	41	ILE	3.2
41	1j	55	LYS	3.2
46	2o	47	LYS	3.2
16	2U	11	ARG	3.2
47	1p	28	ARG	3.2
42	2k	31	THR	3.2
4	1E	182	LEU	3.2
13	2R	4	LEU	3.2
19	1X	66	LEU	3.2
27	25	30	LEU	3.2
38	1g	103	TRP	3.2
48	1q	98	LEU	3.2
11	2P	75	ILE	3.2
18	2W	76	VAL	3.2
51	1t	83	ARG	3.2
3	1D	178	PRO	3.2
5	2F	93	LYS	3.2
3	2D	239	ARG	3.2
16	2U	44	ASN	3.2
18	1W	99	ARG	3.2
42	1k	64	ALA	3.2
3	1D	246	PRO	3.2
9	1N	44	PRO	3.2
9	2N	1	MET	3.2
11	2P	23	PRO	3.2
31	29	33	LYS	3.2
3	2D	56	GLY	3.2
3	2D	210	GLY	3.2
3	2D	235	GLY	3.2
3	1D	231	HIS	3.2
29	17	23	ARG	3.2
5	1F	64	ILE	3.2
3	2D	158	ALA	3.2
10	2O	43	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
16	2U	9	VAL	3.2
17	1V	14	VAL	3.2
42	1k	72	ALA	3.2
42	2k	20	TYR	3.2
45	1n	30	ALA	3.2
4	1E	202	LYS	3.2
1	1A	2505	G	3.2
42	1k	58	PRO	3.2
42	1k	121	PRO	3.2
16	2U	98	LEU	3.2
23	21	76	ARG	3.2
41	1j	45	ARG	3.2
7	2H	162	ILE	3.2
34	2c	202	ILE	3.2
44	2m	78	ILE	3.2
51	1t	16	HIS	3.2
4	2E	154	LYS	3.2
5	1F	97	TYR	3.2
10	1O	42	SER	3.2
30	18	52	LYS	3.2
34	1c	4	LYS	3.2
40	1i	109	VAL	3.2
47	1p	39	TYR	3.2
34	2c	205	GLY	3.2
40	2i	90	PRO	3.2
11	2P	55	ARG	3.2
16	1U	33	ARG	3.2
49	1r	43	PHE	3.2
35	2d	126	ILE	3.2
10	1O	84	ALA	3.2
10	2O	42	SER	3.2
10	2O	5	GLN	3.2
10	2O	21	CYS	3.2
11	1P	50	ARG	3.2
31	29	9	ARG	3.2
3	2D	177	LEU	3.2
11	1P	59	LEU	3.2
23	11	12	PRO	3.2
23	21	68	PRO	3.2
33	2b	44	LEU	3.2
35	2d	157	LEU	3.2
44	2m	66	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	2R	9	LYS	3.2
1	2A	1783	A	3.2
3	2D	161	THR	3.2
16	2U	72	HIS	3.2
35	2d	34	GLU	3.2
35	2d	111	ALA	3.2
12	2Q	13	GLN	3.2
36	2e	133	TYR	3.2
20	2Y	41	GLY	3.2
3	2D	249	PRO	3.2
18	2W	14	PRO	3.2
34	1c	101	LEU	3.2
47	1p	35	LYS	3.2
5	2F	186	ILE	3.2
30	18	16	ILE	3.2
31	29	26	ILE	3.2
1	2A	2506	U	3.2
10	1O	83	ALA	3.2
10	2O	58	VAL	3.2
13	2R	50	HIS	3.2
17	1V	79	VAL	3.2
27	15	20	ARG	3.2
41	1j	62	HIS	3.2
7	2H	14	GLY	3.2
13	1R	40	LYS	3.2
18	2W	13	SER	3.2
42	1k	27	ASN	3.2
42	1k	117	ASN	3.2
12	1Q	34	LEU	3.2
30	18	53	PRO	3.2
40	2i	123	PRO	3.2
15	2T	50	ILE	3.1
10	1O	26	LYS	3.1
20	2Y	36	ALA	3.1
1	2A	2505	G	3.1
3	1D	147	LEU	3.1
5	1F	33	LEU	3.1
16	2U	31	SER	3.1
34	2c	23	TYR	3.1
23	11	82	LEU	3.1
33	2b	101	MET	3.1
3	1D	7	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
4	1E	26	ILE	3.1
34	2c	21	ARG	3.1
20	2Y	46	LYS	3.1
51	2t	41	ILE	3.1
7	2H	131	VAL	3.1
30	18	22	VAL	3.1
4	1E	78	LEU	3.1
13	2R	51	LEU	3.1
15	2T	104	ASN	3.1
19	2X	95	LEU	3.1
36	1e	119	LEU	3.1
53	1v	14	A	3.1
5	1F	66	PRO	3.1
35	2d	73	ARG	3.1
45	1n	17	LYS	3.1
34	2c	77	ILE	3.1
3	1D	3	VAL	3.1
34	2c	64	VAL	3.1
41	2j	49	VAL	3.1
4	1E	148	GLY	3.1
30	28	9	GLY	3.1
42	1k	19	ALA	3.1
47	2p	22	THR	3.1
4	2E	195	LEU	3.1
5	1F	41	LEU	3.1
3	1D	52	ARG	3.1
3	2D	274	ARG	3.1
9	1N	78	TYR	3.1
10	1O	108	GLU	3.1
11	2P	41	ARG	3.1
9	2N	58	ASP	3.1
36	1e	26	PHE	3.1
42	2k	70	LYS	3.1
9	2N	95	PRO	3.1
8	1I	79	ILE	3.1
30	28	23	VAL	3.1
23	11	19	GLN	3.1
25	23	19	GLN	3.1
3	2D	147	LEU	3.1
4	2E	146	THR	3.1
7	2H	33	LEU	3.1
7	2H	122	THR	3.1

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Mol	Chain	Res	Type	RSRZ
9	1N	26	LEU	3.1
9	2N	22	THR	3.1
9	2N	39	ARG	3.1
12	1Q	10	ARG	3.1
36	2e	27	ARG	3.1
35	2d	106	TYR	3.1
23	11	65	SER	3.1
16	1U	80	ILE	3.1
4	1E	130	GLY	3.1
1	1A	2576	G	3.1
15	1T	90	GLN	3.1
29	27	45	ALA	3.1
36	2e	29	GLY	3.1
42	2k	65	ALA	3.1
47	2p	48	TRP	3.1
48	2q	26	GLN	3.1
9	2N	59	LYS	3.1
1	1A	1983	C	3.1
15	1T	29	ARG	3.1
16	2U	37	GLU	3.1
48	2q	91	ARG	3.1
5	1F	123	LEU	3.1
36	2e	43	LEU	3.1
45	2n	13	THR	3.1
47	1p	73	LEU	3.1
7	2H	163	TYR	3.1
36	2e	26	PHE	3.1
18	1W	94	ASP	3.1
39	2h	89	PRO	3.1
42	1k	24	SER	3.1
1	1A	2062	A	3.1
3	1D	229	VAL	3.1
9	1N	77	GLY	3.1
13	1R	114	VAL	3.1
42	1k	88	GLY	3.1
47	1p	24	ALA	3.1
55	1x	76	A	3.1
8	2I	27	ARG	3.1
3	2D	111	LEU	3.1
13	2R	20	LEU	3.1
54	1w	25	C	3.1
54	1y	3	C	3.1

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Mol	Chain	Res	Type	RSRZ
12	1Q	47	ILE	3.1
34	2c	157	ILE	3.1
42	1k	101	SER	3.1
48	1q	36	ILE	3.1
20	2Y	59	GLY	3.1
5	1F	40	GLN	3.1
23	11	61	ARG	3.1
27	25	45	VAL	3.1
1	1A	781	A	3.1
35	1d	78	LEU	3.1
40	2i	85	LEU	3.1
11	2P	27	HIS	3.1
3	1D	190	TYR	3.1
41	1j	57	LYS	3.1
47	2p	3	LYS	3.1
3	1D	14	ARG	3.1
3	1D	245	PRO	3.1
11	2P	109	GLY	3.1
34	1c	134	ILE	3.1
38	2g	4	ARG	3.1
45	1n	29	ARG	3.1
45	2n	32	SER	3.1
46	2o	68	ARG	3.1
35	2d	110	PHE	3.1
48	2q	6	LEU	3.1
10	1O	64	ARG	3.1
38	2g	79	ARG	3.1
3	2D	246	PRO	3.1
4	2E	124	GLY	3.1
23	11	45	ASN	3.1
27	15	11	THR	3.1
5	2F	67	GLN	3.1
25	23	47	VAL	3.0
47	1p	65	GLN	3.1
42	1k	97	ALA	3.0
23	11	69	LYS	3.0
3	1D	269	PHE	3.0
6	2G	152	LEU	3.0
16	2U	12	ARG	3.0
54	2y	23	A	3.0
40	1i	110	GLU	3.0
8	1I	109	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
16	1U	45	TYR	3.0
44	1m	87	TYR	3.0
9	2N	55	VAL	3.0
11	1P	31	ALA	3.0
16	2U	22	LYS	3.0
23	11	10	LYS	3.0
54	2y	18	G	3.0
4	1E	19	ARG	3.0
18	1W	23	LEU	3.0
43	2l	33	ARG	3.0
37	2f	89	MET	3.0
30	18	3	LYS	3.0
40	2i	63	ILE	3.0
5	2F	92	PRO	3.0
20	1Y	7	VAL	3.0
25	23	54	VAL	3.0
36	2e	32	VAL	3.0
3	2D	247	ALA	3.0
7	2H	165	ALA	3.0
30	18	55	ALA	3.0
19	2X	60	ARG	3.0
32	1a	1529	G	3.0
3	2D	237	GLU	3.0
3	1D	258	LYS	3.0
4	1E	127	ASP	3.0
11	1P	46	LYS	3.0
17	2V	84	LYS	3.0
29	17	11	LYS	3.0
35	2d	33	MET	3.0
42	1k	99	GLN	3.0
1	1A	2142	C	3.0
1	2A	756	C	3.0
16	2U	2	PRO	3.0
35	2d	170	VAL	3.0
35	2d	189	PRO	3.0
36	2e	82	VAL	3.0
42	1k	109	VAL	3.0
13	2R	101	ALA	3.0
44	2m	5	ALA	3.0
28	26	11	LEU	3.0
35	2d	94	LEU	3.0
4	2E	145	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
9	2N	89	LYS	3.0
40	1i	112	LYS	3.0
15	2T	71	GLY	3.0
18	1W	111	HIS	3.0
4	2E	160	TYR	3.0
9	2N	35	ARG	3.0
9	2N	86	PRO	3.0
15	2T	100	TYR	3.0
27	25	20	ARG	3.0
48	2q	35	VAL	3.0
1	2A	6	A	3.0
3	1D	208	LYS	3.0
9	1N	76	SER	3.0
13	1R	44	LEU	3.0
16	1U	15	LYS	3.0
16	2U	32	PHE	3.0
41	1j	47	PHE	3.0
4	2E	158	GLY	3.0
38	1g	106	GLN	3.0
11	2P	102	ARG	3.0
52	2u	13	ILE	3.0
15	1T	34	VAL	3.0
30	28	52	LYS	3.0
31	29	2	LYS	3.0
33	2b	33	TYR	3.0
36	1e	51	VAL	3.0
38	2g	84	ASN	3.0
43	2l	16	GLU	3.0
43	2l	21	LYS	3.0
51	2t	30	LYS	3.0
4	1E	183	LEU	3.0
34	2c	12	LEU	3.0
35	2d	120	LEU	3.0
47	2p	49	LEU	3.0
4	2E	153	GLY	3.0
19	1X	76	ARG	3.0
4	2E	159	HIS	3.0
9	2N	130	HIS	3.0
17	1V	72	VAL	3.0
3	1D	265	PRO	3.0
3	2D	62	TYR	3.0
11	1P	12	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
23	11	15	ALA	3.0
28	16	2	ALA	3.0
18	1W	19	LEU	3.0
1	2A	2591	C	3.0
1	2A	1128	A	3.0
1	2A	2051	A	3.0
7	2H	93	GLY	3.0
32	2a	815	A	3.0
42	1k	62	GLN	3.0
46	1o	36	ILE	3.0
51	1t	55	ILE	3.0
37	1f	60	PHE	3.0
47	1p	32	TYR	3.0
1	1A	444	C	3.0
23	21	11	ARG	3.0
34	2c	59	ARG	3.0
34	2c	81	GLY	3.0
7	2H	106	THR	3.0
34	1c	135	LYS	3.0
3	1D	106	ILE	3.0
10	2O	63	VAL	3.0
15	2T	63	VAL	3.0
17	2V	79	VAL	3.0
4	1E	144	ARG	2.9
8	2I	68	LEU	2.9
19	2X	73	ARG	2.9
47	1p	31	LYS	2.9
49	1r	71	LYS	2.9
3	2D	254	THR	2.9
32	1a	800	G	2.9
3	1D	92	ILE	2.9
10	1O	68	GLU	2.9
1	1A	764	A	2.9
1	2A	2577	A	2.9
32	2a	1357	A	2.9
9	1N	14	VAL	2.9
25	23	51	ALA	2.9
13	2R	54	LEU	2.9
16	1U	18	LEU	2.9
16	1U	43	GLY	2.9
34	1c	39	ILE	2.9
1	1A	1248	G	2.9

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Mol	Chain	Res	Type	RSRZ
1	2A	2509	G	2.9
9	1N	83	LYS	2.9
13	2R	5	LYS	2.9
18	2W	17	VAL	2.9
27	25	15	ARG	2.9
4	1E	15	PHE	2.9
5	2F	55	GLY	2.9
9	2N	33	LEU	2.9
17	2V	38	LEU	2.9
24	12	53	LEU	2.9
25	23	4	LEU	2.9
30	18	60	LEU	2.9
35	1d	101	LEU	2.9
17	1V	80	GLN	2.9
36	1e	20	GLN	2.9
1	2A	2610	C	2.9
36	1e	129	ILE	2.9
47	1p	4	ILE	2.9
12	2Q	76	LYS	2.9
23	21	21	ARG	2.9
9	1N	55	VAL	2.9
9	1N	62	VAL	2.9
41	2j	44	VAL	2.9
20	2Y	6	HIS	2.9
34	2c	33	LEU	2.9
35	2d	155	LEU	2.9
35	2d	176	LEU	2.9
18	2W	87	PRO	2.9
55	1x	73	A	2.9
27	15	59	GLU	2.9
4	2E	118	LYS	2.9
11	1P	33	ARG	2.9
13	2R	105	ARG	2.9
7	2H	17	VAL	2.9
42	2k	87	THR	2.9
35	2d	75	PHE	2.9
12	2Q	125	LEU	2.9
20	2Y	58	GLY	2.9
23	21	22	GLY	2.9
34	2c	115	LEU	2.9
4	1E	138	PRO	2.9
9	2N	101	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
25	23	20	LYS	2.9
32	1a	1507	A	2.9
33	2b	132	LYS	2.9
3	1D	218	ARG	2.9
4	1E	136	ARG	2.9
11	1P	71	VAL	2.9
36	2e	119	LEU	2.9
47	1p	60	LEU	2.9
50	2s	71	LEU	2.9
30	28	8	LYS	2.9
38	1g	148	ASN	2.9
16	1U	9	VAL	2.9
34	1c	198	VAL	2.9
3	2D	57	GLY	2.9
10	2O	20	MET	2.9
1	1A	2896	C	2.9
11	2P	17	LYS	2.9
12	2Q	2	LEU	2.9
13	1R	79	LEU	2.9
23	21	64	ALA	2.9
38	2g	152	ALA	2.9
1	1A	1130	U	2.9
9	1N	115	ARG	2.9
35	1d	168	ARG	2.9
36	1e	15	ARG	2.9
41	2j	53	PRO	2.9
49	2r	34	TYR	2.9
1	2A	804	A	2.9
34	2c	124	ILE	2.9
5	1F	55	GLY	2.9
12	2Q	90	VAL	2.9
13	1R	9	LYS	2.9
40	2i	113	LYS	2.9
54	2y	22	G	2.9
47	2p	2	VAL	2.9
9	2N	115	ARG	2.9
16	2U	60	LEU	2.9
40	2i	19	LEU	2.9
45	1n	44	LEU	2.9
1	1A	34	C	2.9
16	1U	6	THR	2.9
33	1b	95	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
10	2O	22	ILE	2.9
46	1o	87	ILE	2.9
4	2E	51	PHE	2.9
15	2T	22	PHE	2.9
1	2A	1763	G	2.9
11	2P	77	ARG	2.9
16	2U	7	GLY	2.9
32	1a	162	A	2.9
35	2d	198	VAL	2.9
4	1E	114	ALA	2.9
9	1N	15	LEU	2.9
9	1N	57	ALA	2.9
23	21	98	LEU	2.9
27	25	25	LEU	2.9
29	17	31	LEU	2.9
40	2i	79	LEU	2.9
43	1l	26	ALA	2.9
48	2q	43	LEU	2.9
36	2e	87	SER	2.8
46	1o	48	LYS	2.8
3	1D	105	ILE	2.8
20	2Y	38	ILE	2.8
35	2d	144	ASP	2.8
3	1D	177	LEU	2.8
9	1N	91	LEU	2.8
30	18	4	MET	2.8
32	1a	1513	A	2.8
53	1v	23	A	2.8
9	1N	104	LYS	2.8
11	1P	29	LYS	2.8
23	21	65	SER	2.8
1	2A	2055	C	2.8
42	2k	39	PRO	2.8
5	1F	54	ARG	2.8
5	1F	82	ILE	2.8
9	1N	114	ARG	2.8
10	1O	77	ILE	2.8
9	2N	127	ASP	2.8
12	1Q	32	TYR	2.8
15	1T	115	ARG	2.8
35	2d	49	ARG	2.8
20	2Y	15	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
40	2i	108	VAL	2.8
16	1U	109	LEU	2.8
13	2R	39	PRO	2.8
9	1N	12	ARG	2.8
15	1T	62	THR	2.8
34	2c	35	GLU	2.8
36	1e	27	ARG	2.8
42	1k	41	THR	2.8
15	2T	61	PHE	2.8
18	2W	10	VAL	2.8
3	2D	133	LEU	2.8
3	2D	155	LEU	2.8
5	2F	176	LEU	2.8
20	1Y	67	LEU	2.8
38	1g	144	MET	2.8
48	2q	24	GLU	2.8
19	2X	76	ARG	2.8
35	1d	47	ARG	2.8
46	2o	38	ARG	2.8
3	1D	220	HIS	2.8
34	1c	165	THR	2.8
36	1e	11	ILE	2.8
42	1k	32	ILE	2.8
1	2A	2578	G	2.8
24	12	37	PHE	2.8
3	2D	205	VAL	2.8
27	15	6	VAL	2.8
46	1o	60	VAL	2.8
8	2I	72	LEU	2.8
27	15	58	LEU	2.8
34	2c	28	GLN	2.8
32	2a	1257	U	2.8
3	1D	228	PRO	2.8
4	2E	147	PRO	2.8
42	2k	123	LYS	2.8
49	2r	61	LYS	2.8
1	2A	687	C	2.8
33	2b	163	PHE	2.8
37	1f	55	ASP	2.8
4	1E	188	VAL	2.8
13	1R	66	VAL	2.8
4	1E	79	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
5	1F	38	ARG	2.8
23	11	40	ARG	2.8
29	17	12	ARG	2.8
50	1s	81	ARG	2.8
9	1N	66	LYS	2.8
15	1T	33	LYS	2.8
35	2d	158	ILE	2.8
39	2h	80	ILE	2.8
40	2i	81	ILE	2.8
42	1k	115	PRO	2.8
15	2T	40	THR	2.8
1	1A	2551	C	2.8
9	2N	68	GLU	2.8
9	2N	87	LEU	2.8
13	1R	29	LEU	2.8
23	21	46	LEU	2.8
28	16	34	LEU	2.8
35	2d	121	VAL	2.8
36	1e	123	LEU	2.8
29	17	20	ALA	2.8
42	2k	51	LYS	2.8
45	2n	59	ALA	2.8
9	2N	106	MET	2.8
32	2a	79	G	2.8
54	1w	24	G	2.8
4	1E	126	PRO	2.8
4	2E	139	GLY	2.8
9	2N	126	PRO	2.8
3	1D	173	VAL	2.8
4	2E	107	THR	2.8
10	2O	38	VAL	2.8
10	2O	97	ARG	2.8
34	2c	6	HIS	2.8
36	2e	33	VAL	2.8
18	1W	16	LYS	2.8
29	27	29	LYS	2.8
48	2q	88	TYR	2.8
9	2N	18	ALA	2.8
54	1w	13	C	2.8
7	2H	101	ARG	2.8
16	1U	79	PHE	2.8
8	1I	20	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
22	20	68	GLU	2.8
38	1g	32	ARG	2.8
44	1m	94	ARG	2.8
48	2q	58	GLU	2.8
9	1N	138	LEU	2.8
10	2O	25	LEU	2.8
18	1W	29	LEU	2.8
36	2e	123	LEU	2.8
51	2t	71	THR	2.8
16	1U	68	ALA	2.8
1	2A	1129	A	2.7
1	2A	2059	A	2.7
29	17	22	MET	2.7
42	2k	38	ASN	2.7
54	1y	73	A	2.7
5	1F	47	GLY	2.7
11	1P	41	ARG	2.7
31	29	19	ARG	2.7
34	1c	152	ILE	2.7
42	2k	125	PHE	2.7
45	2n	58	LYS	2.7
1	1A	2509	G	2.7
11	2P	63	PRO	2.7
25	23	16	PRO	2.7
11	1P	47	ASP	2.7
3	1D	145	VAL	2.7
3	2D	12	SER	2.7
39	2h	4	ASP	2.7
4	1E	104	VAL	2.7
4	2E	196	VAL	2.7
29	27	31	LEU	2.7
48	2q	9	VAL	2.7
12	1Q	36	ALA	2.7
12	2Q	93	TYR	2.7
16	2U	41	ALA	2.7
23	21	71	TYR	2.7
1	1A	2579	C	2.7
15	1T	108	ARG	2.7
29	27	10	ARG	2.7
45	2n	55	GLY	2.7
51	1t	29	LYS	2.7
33	1b	122	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
39	1h	45	ILE	2.7
3	2D	231	HIS	2.7
13	1R	18	LEU	2.7
31	19	25	VAL	2.7
48	2q	10	VAL	2.7
29	27	6	GLN	2.7
4	1E	157	ALA	2.7
11	2P	31	ALA	2.7
13	1R	109	ALA	2.7
36	2e	30	ALA	2.7
5	1F	63	LYS	2.7
13	1R	95	THR	2.7
31	29	18	ARG	2.7
1	1A	1761	C	2.7
16	1U	44	ASN	2.7
23	21	60	PHE	2.7
32	1a	815	A	2.7
33	2b	152	PHE	2.7
41	1j	63	PHE	2.7
24	22	60	LEU	2.7
31	19	3	VAL	2.7
35	2d	96	LEU	2.7
51	1t	13	LEU	2.7
13	2R	40	LYS	2.7
12	1Q	51	ARG	2.7
32	2a	1030(A)	G	2.7
39	2h	58	TYR	2.7
4	2E	117	MET	2.7
39	2h	128	GLY	2.7
46	2o	89	GLY	2.7
4	1E	96	PHE	2.7
19	1X	28	PHE	2.7
19	2X	80	ILE	2.7
1	2A	196	A	2.7
1	2A	2058	A	2.7
5	2F	196	LEU	2.7
8	1I	38	LEU	2.7
18	2W	4	LYS	2.7
27	15	45	VAL	2.7
48	2q	84	LEU	2.7
40	1i	117	HIS	2.7
42	1k	46	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	1252	G	2.7
20	1Y	61	ILE	2.7
31	19	17	ILE	2.7
34	1c	182	ILE	2.7
35	2d	204	ILE	2.7
3	1D	59	LYS	2.7
8	2I	12	LEU	2.7
9	1N	99	LEU	2.7
10	2O	4	PRO	2.7
10	2O	85	VAL	2.7
13	2R	44	LEU	2.7
13	2R	65	LEU	2.7
16	1U	39	LEU	2.7
36	2e	24	ARG	2.7
17	2V	77	ALA	2.7
11	1P	13	ASN	2.7
12	1Q	120	ILE	2.7
34	1c	202	ILE	2.7
1	1A	2603	G	2.7
33	1b	98	LEU	2.7
36	2e	100	VAL	2.7
1	2A	2057	A	2.7
29	27	5	TRP	2.7
29	27	32	LYS	2.7
45	1n	32	SER	2.7
13	1R	47	PHE	2.7
19	1X	1	MET	2.7
36	1e	133	TYR	2.7
48	2q	71	PHE	2.7
10	2O	78	ARG	2.7
11	1P	18	ARG	2.7
19	1X	8	ILE	2.7
29	17	21	ARG	2.7
41	1j	48	THR	2.7
47	1p	19	ILE	2.7
1	2A	1656	C	2.7
3	2D	196	VAL	2.7
17	1V	71	LEU	2.7
9	2N	135	PRO	2.7
11	2P	71	VAL	2.7
22	20	79	VAL	2.7
23	11	30	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
30	18	40	GLU	2.7
37	1f	9	VAL	2.7
39	1h	4	ASP	2.7
45	2n	54	PRO	2.7
9	2N	47	ALA	2.7
15	1T	71	GLY	2.7
40	2i	119	ALA	2.7
15	1T	22	PHE	2.7
29	27	34	ARG	2.7
42	1k	48	ILE	2.7
3	1D	230	ASP	2.7
4	1E	184	VAL	2.7
18	2W	36	LEU	2.7
19	1X	70	LEU	2.7
35	2d	179	GLU	2.7
36	1e	135	THR	2.7
46	2o	37	ASN	2.7
25	23	24	LYS	2.7
30	18	21	LYS	2.7
43	2l	20	LYS	2.7
51	1t	34	LYS	2.7
5	2F	47	GLY	2.7
36	2e	59	GLY	2.7
16	2U	21	ALA	2.7
3	1D	48	ARG	2.7
13	2R	22	ARG	2.7
7	2H	134	SER	2.6
12	1Q	103	MET	2.6
9	1N	16	ILE	2.6
15	1T	52	ILE	2.6
15	1T	100	TYR	2.6
35	1d	126	ILE	2.6
13	1R	99	LYS	2.6
18	1W	98	LYS	2.6
34	2c	188	LEU	2.6
35	1d	11	LEU	2.6
14	1S	28	VAL	2.6
23	21	70	VAL	2.6
43	2l	8	ASN	2.6
5	2F	86	GLY	2.6
50	2s	84	GLY	2.6
3	1D	93	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
38	1g	83	ALA	2.6
45	1n	2	ALA	2.6
54	1w	68	C	2.6
4	2E	119	ARG	2.6
30	28	30	ARG	2.6
45	1n	41	ARG	2.6
20	2Y	68	HIS	2.6
1	2A	1125	G	2.6
4	2E	11	MET	2.6
10	2O	44	LYS	2.6
16	2U	34	LYS	2.6
18	2W	78	GLU	2.6
20	2Y	26	LYS	2.6
32	2a	104	G	2.6
43	2l	85	ILE	2.6
54	1w	69	G	2.6
20	2Y	57	GLN	2.6
32	1a	768	A	2.6
45	1n	21	TYR	2.6
17	1V	95	LEU	2.6
33	2b	118	LEU	2.6
3	1D	185	VAL	2.6
4	1E	173	VAL	2.6
7	1H	19	VAL	2.6
9	2N	62	VAL	2.6
10	1O	121	VAL	2.6
20	2Y	49	VAL	2.6
42	2k	84	VAL	2.6
48	2q	73	VAL	2.6
18	2W	91	GLY	2.6
3	2D	60	ARG	2.6
5	1F	94	PRO	2.6
37	1f	46	ARG	2.6
1	1A	806	C	2.6
32	1a	1501	C	2.6
38	2g	150	ALA	2.6
20	1Y	34	LYS	2.6
28	16	53	LYS	2.6
7	2H	72	ILE	2.6
9	1N	90	MET	2.6
1	2A	1264	G	2.6
15	1T	68	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
53	2v	22	U	2.6
32	1a	769	G	2.6
46	1o	57	LEU	2.6
51	2t	10	LEU	2.6
54	1w	6	G	2.6
4	2E	148	GLY	2.6
12	2Q	86	GLY	2.6
15	1T	49	VAL	2.6
30	28	49	VAL	2.6
33	2b	164	VAL	2.6
34	1c	207	VAL	2.6
47	1p	2	VAL	2.6
51	1t	25	ARG	2.6
54	1y	23	A	2.6
4	1E	146	THR	2.6
4	1E	191	PRO	2.6
12	2Q	39	PRO	2.6
16	1U	38	THR	2.6
33	1b	188	ALA	2.6
36	2e	17	ALA	2.6
7	2H	104	GLU	2.6
43	1l	16	GLU	2.6
17	2V	4	ILE	2.6
4	1E	181	LEU	2.6
48	1q	97	SER	2.6
48	2q	68	ARG	2.6
3	1D	56	GLY	2.6
31	19	16	VAL	2.6
34	1c	55	VAL	2.6
48	2q	41	LYS	2.6
49	1r	84	LYS	2.6
51	1t	68	LYS	2.6
19	1X	11	PRO	2.6
34	1c	206	GLU	2.6
1	2A	2146	C	2.6
18	2W	106	ILE	2.6
8	1I	72	LEU	2.6
12	1Q	79	LEU	2.6
47	2p	60	LEU	2.6
10	2O	61	VAL	2.6
18	1W	76	VAL	2.6
40	2i	5	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
51	1t	38	LYS	2.6
7	2H	32	GLU	2.6
16	2U	4	ALA	2.6
31	29	5	ALA	2.6
34	1c	10	PHE	2.6
42	2k	33	THR	2.6
54	2y	35	A	2.6
1	1A	2511	U	2.6
3	1D	236	GLY	2.6
8	2I	77	LEU	2.6
9	1N	112	LEU	2.6
11	1P	62	LEU	2.6
16	1U	16	LYS	2.6
16	1U	104	GLN	2.6
30	28	41	ILE	2.6
8	2I	81	VAL	2.6
33	1b	81	VAL	2.6
39	1h	62	TYR	2.6
28	26	24	GLU	2.6
44	2m	73	GLU	2.6
3	1D	6	PHE	2.6
12	1Q	104	PHE	2.6
15	1T	104	ASN	2.6
33	2b	232	PRO	2.6
40	2i	106	ALA	2.6
3	1D	161	THR	2.6
46	1o	65	ARG	2.6
46	1o	88	ARG	2.6
46	2o	54	ARG	2.6
1	1A	1770	G	2.6
3	1D	46	GLN	2.6
52	1u	13	ILE	2.6
1	1A	435	C	2.6
8	2I	6	LEU	2.6
10	1O	95	GLY	2.6
23	11	9	GLY	2.6
34	2c	185	GLY	2.6
39	1h	59	LEU	2.6
7	2H	164	TYR	2.6
10	1O	57	VAL	2.6
13	1R	69	ASP	2.6
31	19	7	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
48	2q	85	VAL	2.6
16	1U	57	PHE	2.6
10	1O	31	LYS	2.6
11	1P	8	PRO	2.6
11	2P	16	ARG	2.6
30	28	24	ALA	2.6
31	29	35	ARG	2.6
49	2r	43	PHE	2.6
15	1T	110	ILE	2.6
18	1W	96	ILE	2.6
20	2Y	12	THR	2.6
1	2A	1253	A	2.6
8	1I	9	LEU	2.6
8	1I	35	LEU	2.6
10	2O	122	LEU	2.6
34	2c	159	GLY	2.6
35	2d	11	LEU	2.6
48	2q	33	GLY	2.6
1	1A	1176	G	2.6
1	1A	2498	C	2.6
4	1E	87	GLU	2.6
32	2a	108	G	2.6
23	1I	51	VAL	2.6
39	2h	129	VAL	2.6
5	1F	68	LYS	2.6
30	18	47	LYS	2.6
36	2e	15	ARG	2.6
51	2t	15	ARG	2.6
34	2c	189	ALA	2.6
3	2D	252	TRP	2.6
33	1b	94	ASN	2.6
12	1Q	13	GLN	2.5
3	2D	50	THR	2.5
42	2k	40	ILE	2.5
13	1R	115	GLU	2.5
35	2d	97	LEU	2.5
3	2D	3	VAL	2.5
3	2D	230	ASP	2.5
31	29	22	ARG	2.5
40	2i	66	ARG	2.5
43	1l	91	LYS	2.5
54	2w	40	C	2.5

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Mol	Chain	Res	Type	RSRZ
1	2A	2802	G	2.5
12	1Q	44	ALA	2.5
15	2T	45	PHE	2.5
42	1k	107	SER	2.5
4	2E	143	ASN	2.5
9	2N	42	TRP	2.5
3	1D	65	ILE	2.5
13	1R	34	ILE	2.5
43	1l	85	ILE	2.5
50	2s	49	ILE	2.5
8	2I	128	LEU	2.5
3	1D	217	ARG	2.5
3	2D	255	LYS	2.5
10	1O	109	LYS	2.5
11	1P	57	THR	2.5
12	2Q	75	THR	2.5
35	2d	202	LEU	2.5
11	1P	21	ARG	2.5
16	1U	59	ARG	2.5
32	1a	1196	U	2.5
32	2a	1532	U	2.5
34	2c	142	MET	2.5
40	1i	121	ARG	2.5
43	2l	23	LYS	2.5
16	1U	90	VAL	2.5
31	19	23	VAL	2.5
46	2o	63	ARG	2.5
48	2q	92	ARG	2.5
32	1a	1527	C	2.5
54	1w	49	C	2.5
34	1c	154	SER	2.5
54	1w	5	G	2.5
3	1D	174	ILE	2.5
3	2D	256	GLY	2.5
12	1Q	91	GLU	2.5
34	2c	206	GLU	2.5
11	1P	14	LYS	2.5
39	1h	6	ILE	2.5
3	2D	213	ARG	2.5
16	2U	64	ARG	2.5
38	2g	16	LEU	2.5
39	2h	12	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
46	2o	34	LEU	2.5
52	2u	10	ARG	2.5
4	1E	105	THR	2.5
32	1a	1528	U	2.5
43	1l	67	THR	2.5
13	1R	13	HIS	2.5
13	1R	49	ASP	2.5
1	1A	2575	C	2.5
10	1O	111	PHE	2.5
1	2A	1847	A	2.5
10	1O	60	ALA	2.5
23	11	43	TYR	2.5
15	1T	73	GLU	2.5
30	28	44	LYS	2.5
36	2e	83	GLU	2.5
39	1h	72	PRO	2.5
1	2A	743	G	2.5
1	2A	2052	G	2.5
3	1D	64	ILE	2.5
3	2D	222	ARG	2.5
13	1R	33	ARG	2.5
18	2W	37	ARG	2.5
39	2h	55	GLY	2.5
47	1p	33	ILE	2.5
47	2p	33	ILE	2.5
4	2E	120	TRP	2.5
15	1T	10	VAL	2.5
16	1U	8	VAL	2.5
19	1X	30	VAL	2.5
39	2h	82	HIS	2.5
51	1t	71	THR	2.5
5	2F	129	PHE	2.5
15	2T	76	PHE	2.5
1	1A	436	C	2.5
3	1D	199	ALA	2.5
8	1I	121	LYS	2.5
16	2U	35	ALA	2.5
27	15	56	LYS	2.5
38	1g	146	GLU	2.5
1	1A	1932	A	2.5
1	2A	1254	A	2.5
1	2A	1379	A	2.5

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Mol	Chain	Res	Type	RSRZ
3	2D	218	ARG	2.5
5	2F	54	ARG	2.5
9	2N	91	LEU	2.5
12	1Q	2	LEU	2.5
27	15	30	LEU	2.5
35	1d	120	LEU	2.5
46	2o	57	LEU	2.5
1	1A	2513	G	2.5
10	1O	43	VAL	2.5
34	2c	153	VAL	2.5
39	1h	118	VAL	2.5
8	2I	108	THR	2.5
10	1O	96	THR	2.5
16	2U	15	LYS	2.5
23	21	69	LYS	2.5
10	1O	94	ARG	2.5
22	10	25	ARG	2.5
4	1E	6	GLY	2.5
10	2O	15	GLY	2.5
45	2n	60	SER	2.5
48	1q	33	GLY	2.5
1	2A	1785	A	2.5
10	1O	39	ILE	2.5
15	1T	75	ILE	2.5
17	2V	96	ILE	2.5
6	1G	82	LEU	2.5
1	2A	810	U	2.5
12	2Q	97	VAL	2.5
23	21	23	LYS	2.5
36	2e	115	VAL	2.5
20	2Y	62	GLU	2.5
22	20	69	PHE	2.5
13	1R	45	ARG	2.5
41	2j	45	ARG	2.5
47	2p	25	ARG	2.5
9	2N	80	GLY	2.5
34	1c	184	TYR	2.5
8	2I	5	LEU	2.5
16	2U	62	ILE	2.5
46	2o	56	LEU	2.5
51	2t	33	ILE	2.5
16	2U	19	LYS	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
51	1t	74	LYS	2.5
55	2x	76	A	2.5
3	1D	142	VAL	2.5
18	2W	20	VAL	2.5
25	23	29	ARG	2.5
1	2A	748	G	2.5
1	2A	799	G	2.5
3	1D	256	GLY	2.5
11	2P	68	GLN	2.5
13	1R	36	THR	2.5
32	1a	1520	G	2.5
34	2c	53	ALA	2.5
38	1g	150	ALA	2.5
40	2i	69	GLY	2.5
8	1I	25	TYR	2.5
15	2T	52	ILE	2.5
34	1c	124	ILE	2.5
36	1e	121	LYS	2.5
42	2k	29	ILE	2.5
5	1F	154	VAL	2.5
5	2F	46	ARG	2.5
7	2H	43	VAL	2.5
19	2X	59	VAL	2.5
24	22	1	MET	2.5
41	1j	66	ARG	2.5
13	1R	5	LYS	2.5
22	10	24	LYS	2.5
1	2A	1835	G	2.5
5	1F	101	LEU	2.5
17	1V	40	LEU	2.5
33	1b	33	TYR	2.5
35	1d	54	TYR	2.5
48	2q	89	LEU	2.5
51	2t	63	ILE	2.5
54	1y	75	C	2.4
1	2A	1026	U	2.4
16	1U	106	PHE	2.4
40	2i	17	VAL	2.4
43	2l	11	VAL	2.4
46	2o	59	MET	2.4
47	2p	80	PHE	2.4
1	2A	1780	A	2.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2713	A	2.4
18	2W	83	LYS	2.4
11	2P	57	THR	2.4
18	1W	24	ILE	2.4
18	1W	100	THR	2.4
18	2W	12	ILE	2.4
34	1c	14	ILE	2.4
37	1f	98	LEU	2.4
39	1h	80	ILE	2.4
39	1h	83	ILE	2.4
52	2u	6	ARG	2.4
17	1V	36	PRO	2.4
10	2O	102	VAL	2.4
18	1W	17	VAL	2.4
15	1T	1	MET	2.4
30	28	26	LYS	2.4
36	2e	130	ASN	2.4
4	1E	187	ALA	2.4
9	1N	18	ALA	2.4
10	2O	16	ALA	2.4
27	25	14	ALA	2.4
1	2A	1787	A	2.4
12	1Q	112	GLU	2.4
35	1d	122	ARG	2.4
36	2e	107	ARG	2.4
39	1h	18	ARG	2.4
25	13	53	LEU	2.4
5	2F	59	TYR	2.4
4	2E	152	LYS	2.4
16	1U	13	LYS	2.4
16	2U	30	LYS	2.4
29	17	25	PRO	2.4
33	1b	202	PRO	2.4
42	2k	82	VAL	2.4
48	1q	11	VAL	2.4
48	2q	99	SER	2.4
32	1a	1526	G	2.4
11	1P	68	GLN	2.4
10	1O	49	ARG	2.4
16	1U	41	ALA	2.4
40	1i	106	ALA	2.4
45	2n	10	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
13	1R	43	GLU	2.4
4	1E	197	ILE	2.4
24	12	24	LEU	2.4
54	2y	21	A	2.4
3	1D	36	PRO	2.4
16	2U	24	TYR	2.4
34	2c	29	TYR	2.4
15	1T	70	VAL	2.4
18	1W	10	VAL	2.4
26	24	56	VAL	2.4
4	1E	121	ASN	2.4
50	2s	82	GLY	2.4
16	2U	50	ARG	2.4
23	11	52	ARG	2.4
32	1a	811	C	2.4
32	1a	1523	G	2.4
32	2a	80	G	2.4
54	1y	53	G	2.4
6	2G	75	LYS	2.4
40	1i	116	LYS	2.4
24	22	35	LEU	2.4
35	2d	123	HIS	2.4
36	1e	91	LEU	2.4
36	2e	110	LEU	2.4
41	2j	68	HIS	2.4
42	2k	63	LEU	2.4
46	1o	34	LEU	2.4
1	2A	2587	A	2.4
15	2T	77	PRO	2.4
20	2Y	27	VAL	2.4
39	1h	138	TRP	2.4
43	2l	39	VAL	2.4
3	2D	42	GLY	2.4
9	1N	80	GLY	2.4
10	2O	64	ARG	2.4
17	1V	101	GLY	2.4
33	2b	205	ASP	2.4
34	1c	172	ARG	2.4
35	2d	139	ARG	2.4
46	2o	64	ARG	2.4
12	1Q	77	LYS	2.4
36	2e	47	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
43	2l	91	LYS	2.4
16	1U	115	ALA	2.4
18	2W	48	ALA	2.4
1	1A	442	G	2.4
1	1A	530	G	2.4
1	2A	2602	A	2.4
4	1E	167	VAL	2.4
22	10	38	VAL	2.4
39	2h	97	VAL	2.4
44	2m	105	THR	2.4
51	1t	23	ARG	2.4
19	2X	2	LYS	2.4
19	2X	77	LYS	2.4
3	2D	212	SER	2.4
10	1O	20	MET	2.4
3	1D	224	ALA	2.4
9	2N	124	ALA	2.4
1	2A	1657	C	2.4
1	2A	1675	C	2.4
20	2Y	44	ILE	2.4
34	1c	43	LEU	2.4
35	1d	97	LEU	2.4
1	2A	1764	G	2.4
19	1X	43	VAL	2.4
23	1l	27	GLU	2.4
34	1c	2	GLY	2.4
35	1d	198	VAL	2.4
42	2k	86	GLY	2.4
43	2l	25	PRO	2.4
48	2q	28	PRO	2.4
8	2I	93	THR	2.4
9	2N	32	THR	2.4
32	1a	1257	U	2.4
1	1A	2614	A	2.4
1	2A	1784	A	2.4
34	2c	56	ASP	2.4
3	2D	19	ALA	2.4
3	2D	225	ALA	2.4
1	2A	758	C	2.4
6	1G	133	LEU	2.4
10	1O	91	LEU	2.4
28	16	10	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
35	1d	204	ILE	2.4
41	2j	8	LEU	2.4
49	2r	66	LEU	2.4
30	28	13	ARG	2.4
35	2d	132	ARG	2.4
36	2e	14	ARG	2.4
4	2E	163	GLU	2.4
15	1T	63	VAL	2.4
16	1U	63	VAL	2.4
36	1e	49	PRO	2.4
38	2g	85	TYR	2.4
1	1A	2052	G	2.4
9	1N	22	THR	2.4
10	1O	6	THR	2.4
30	18	6	THR	2.4
54	2y	63	G	2.4
1	1A	590	A	2.4
1	1A	2602	A	2.4
16	2U	109	LEU	2.4
22	20	72	ARG	2.4
23	21	7	ILE	2.4
23	21	25	LYS	2.4
29	17	32	LYS	2.4
30	28	57	ARG	2.4
35	2d	14	ARG	2.4
36	2e	11	ILE	2.4
36	2e	121	LYS	2.4
38	2g	149	ARG	2.4
40	2i	16	ARG	2.4
51	1t	22	ARG	2.4
1	2A	790	C	2.4
11	2P	93	GLY	2.3
30	28	65	GLU	2.3
33	1b	152	PHE	2.3
18	1W	47	VAL	2.3
41	1j	93	GLY	2.3
31	19	36	GLN	2.3
35	1d	38	TYR	2.3
5	1F	43	LYS	2.3
16	1U	78	THR	2.3
5	1F	34	TRP	2.3
11	2P	40	SER	2.3

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Mol	Chain	Res	Type	RSRZ
19	1X	65	ARG	2.3
31	19	22	ARG	2.3
40	2i	83	ARG	2.3
54	2y	34	G	2.3
1	1A	2014	A	2.3
13	1R	113	LEU	2.3
35	2d	28	SER	2.3
35	2d	78	LEU	2.3
36	1e	12	LEU	2.3
37	1f	21	LEU	2.3
39	1h	134	ILE	2.3
54	1y	64	A	2.3
36	2e	81	GLU	2.3
1	1A	671	C	2.3
1	1A	1827	C	2.3
1	2A	208	C	2.3
10	1O	55	GLY	2.3
11	2P	34	GLY	2.3
32	1a	336	C	2.3
8	2I	18	VAL	2.3
43	2I	55	VAL	2.3
5	1F	59	TYR	2.3
28	16	8	LYS	2.3
30	18	26	LYS	2.3
3	1D	239	ARG	2.3
51	2t	80	ARG	2.3
7	1H	105	LEU	2.3
1	2A	832	G	2.3
10	2O	69	ILE	2.3
15	2T	88	ILE	2.3
17	1V	70	ILE	2.3
25	13	8	LEU	2.3
34	2c	91	LEU	2.3
35	1d	64	LEU	2.3
39	2h	36	LEU	2.3
34	2c	22	TRP	2.3
43	2I	62	SER	2.3
1	2A	207	A	2.3
1	2A	1132	A	2.3
1	2A	2015	A	2.3
1	2A	2712(A)	A	2.3
3	1D	55	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
15	1T	92	GLY	2.3
29	27	27	GLY	2.3
41	1j	11	PHE	2.3
43	1l	29	GLY	2.3
1	1A	2055	C	2.3
13	2R	48	VAL	2.3
40	2i	117	HIS	2.3
44	2m	74	VAL	2.3
32	1a	793	U	2.3
38	2g	155	ARG	2.3
40	1i	128	ARG	2.3
40	2i	111	ARG	2.3
4	2E	123	ALA	2.3
10	2O	30	ALA	2.3
18	1W	44	ALA	2.3
8	1I	30	LEU	2.3
10	2O	65	THR	2.3
18	1W	39	THR	2.3
22	20	21	LEU	2.3
36	1e	118	ILE	2.3
39	1h	136	GLU	2.3
42	2k	98	LEU	2.3
3	2D	22	SER	2.3
9	2N	118	LYS	2.3
30	28	34	TRP	2.3
1	1A	575	A	2.3
1	1A	2572	A	2.3
1	2A	1266	G	2.3
1	2A	2062	A	2.3
1	2A	2581	G	2.3
22	20	40	GLN	2.3
23	21	4	VAL	2.3
31	29	3	VAL	2.3
54	1y	74	C	2.3
35	2d	138	TYR	2.3
23	11	6	GLU	2.3
23	11	72	GLU	2.3
34	1c	200	ALA	2.3
4	2E	52	LEU	2.3
18	2W	29	LEU	2.3
36	1e	76	ILE	2.3
37	1f	10	LEU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
49	1r	85	LEU	2.3
10	1O	14	THR	2.3
17	2V	69	LYS	2.3
11	1P	34	GLY	2.3
42	2k	26	ASN	2.3
5	1F	45	ARG	2.3
3	1D	118	VAL	2.3
10	1O	61	VAL	2.3
10	2O	62	VAL	2.3
22	20	38	VAL	2.3
23	21	49	VAL	2.3
1	1A	443	A	2.3
1	1A	1669	A	2.3
16	1U	49	HIS	2.3
32	2a	900	A	2.3
46	2o	50	HIS	2.3
54	2y	36	A	2.3
4	1E	189	PRO	2.3
7	2H	83	TYR	2.3
12	2Q	74	TYR	2.3
8	1I	12	LEU	2.3
17	1V	6	LYS	2.3
38	1g	108	ALA	2.3
44	2m	65	LYS	2.3
47	1p	17	TYR	2.3
9	2N	71	ILE	2.3
18	1W	6	ILE	2.3
37	1f	79	LEU	2.3
3	1D	157	ARG	2.3
29	27	39	ARG	2.3
35	2d	109	GLY	2.3
45	2n	51	GLY	2.3
47	1p	18	ARG	2.3
16	1U	29	SER	2.3
15	2T	90	GLN	2.3
35	2d	128	VAL	2.3
37	2f	6	VAL	2.3
23	21	66	HIS	2.3
45	2n	46	GLU	2.3
1	2A	669	G	2.3
32	2a	780	A	2.3
3	1D	131	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
7	2H	171	LEU	2.3
8	1I	24	GLY	2.3
8	2I	4	ILE	2.3
23	2I	67	ILE	2.3
39	2h	107	LEU	2.3
35	2d	13	ARG	2.3
46	1o	68	ARG	2.3
5	2F	139	PHE	2.3
7	2H	109	PHE	2.3
47	1p	9	PHE	2.3
40	1i	124	GLN	2.3
16	2U	105	VAL	2.3
13	1R	102	GLU	2.3
40	1i	118	LYS	2.3
45	2n	11	LYS	2.3
48	2q	3	LYS	2.3
1	2A	2586	C	2.3
1	1A	1132	A	2.3
1	1A	2577	A	2.3
1	2A	2014	A	2.3
6	2G	135	LEU	2.3
8	1I	89	TYR	2.3
10	1O	32	TYR	2.3
10	1O	104	ARG	2.3
16	1U	52	ARG	2.3
18	2W	51	LEU	2.3
25	23	28	LEU	2.3
39	1h	112	LEU	2.3
45	1n	20	ALA	2.3
32	2a	706	A	2.3
45	1n	39	LEU	2.3
46	1o	64	ARG	2.3
46	1o	66	LEU	2.3
48	1q	31	LEU	2.3
50	1s	78	ARG	2.3
15	1T	102	ILE	2.3
54	1y	21	A	2.3
1	1A	1826	G	2.3
40	2i	33	PHE	2.3
45	1n	16	PHE	2.3
9	2N	66	LYS	2.3
47	1p	27	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
48	2q	34	LYS	2.3
9	1N	103	VAL	2.3
43	1l	43	VAL	2.3
48	2q	94	ASN	2.3
13	1R	14	SER	2.3
5	2F	44	ARG	2.3
17	1V	82	ARG	2.3
47	1p	68	ASP	2.3
1	1A	1675	C	2.3
9	1N	81	GLY	2.3
9	1N	87	LEU	2.3
12	1Q	17	LEU	2.3
12	1Q	20	ALA	2.3
17	2V	40	LEU	2.3
18	1W	36	LEU	2.3
49	2r	58	LEU	2.3
36	2e	80	ILE	2.3
40	2i	77	ILE	2.3
1	2A	782	A	2.3
1	2A	1829	A	2.3
15	1T	113	LYS	2.3
18	2W	16	LYS	2.3
35	2d	63	LYS	2.3
1	2A	242	G	2.3
1	2A	2607	G	2.3
19	2X	81	VAL	2.2
39	2h	79	VAL	2.2
15	2T	39	ARG	2.2
35	2d	125	HIS	2.2
42	1k	22	HIS	2.2
48	1q	29	HIS	2.2
36	2e	46	GLY	2.2
41	1j	20	ALA	2.2
15	1T	50	ILE	2.2
36	2e	60	TYR	2.2
39	1h	31	PHE	2.2
42	2k	21	ILE	2.2
6	1G	48	GLU	2.2
11	2P	74	GLU	2.2
1	2A	2176	A	2.2
30	18	57	ARG	2.2
31	19	35	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
35	2d	105	VAL	2.2
42	2k	109	VAL	2.2
3	2D	10	THR	2.2
30	18	12	LYS	2.2
7	2H	71	LEU	2.2
8	1I	5	LEU	2.2
16	2U	48	ALA	2.2
6	1G	88	ILE	2.2
3	1D	172	TYR	2.2
4	1E	160	TYR	2.2
9	1N	42	TRP	2.2
38	1g	26	PHE	2.2
4	1E	9	VAL	2.2
4	1E	198	VAL	2.2
38	1g	149	ARG	2.2
50	2s	78	ARG	2.2
1	2A	1655	A	2.2
1	2A	1762	A	2.2
7	2H	140	LYS	2.2
25	23	7	LYS	2.2
33	1b	27	LYS	2.2
44	1m	111	LYS	2.2
1	1A	2553	G	2.2
5	2F	94	PRO	2.2
13	1R	111	LEU	2.2
32	2a	793	U	2.2
41	1j	10	GLY	2.2
54	1y	47	U	2.2
22	10	36	ILE	2.2
33	1b	123	ALA	2.2
40	1i	122	ALA	2.2
46	1o	53	HIS	2.2
51	2t	16	HIS	2.2
6	2G	39	ILE	2.2
49	1r	29	PHE	2.2
15	2T	68	TYR	2.2
33	2b	36	ARG	2.2
1	1A	1774	C	2.2
1	2A	786	C	2.2
15	2T	28	VAL	2.2
39	2h	26	VAL	2.2
1	1A	1789	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	764	A	2.2
1	2A	1969	A	2.2
1	1A	1693	U	2.2
1	1A	2554	U	2.2
9	1N	110	GLY	2.2
3	1D	237	GLU	2.2
5	1F	181	LEU	2.2
5	2F	175	THR	2.2
7	2H	124	GLU	2.2
10	1O	25	LEU	2.2
36	2e	23	GLY	2.2
16	2U	89	GLU	2.2
40	2i	47	LEU	2.2
27	15	28	PRO	2.2
34	2c	182	ILE	2.2
35	1d	158	ILE	2.2
36	2e	28	PHE	2.2
42	2k	77	MET	2.2
46	2o	36	ILE	2.2
1	1A	956	G	2.2
3	2D	258	LYS	2.2
4	1E	185	LYS	2.2
10	2O	53	LYS	2.2
12	1Q	132	VAL	2.2
13	1R	107	ASP	2.2
1	2A	783	A	2.2
13	2R	67	LEU	2.2
16	1U	56	ASP	2.2
33	1b	128	GLU	2.2
46	1o	89	GLY	2.2
10	2O	51	ALA	2.2
13	1R	8	ARG	2.2
13	1R	96	ARG	2.2
19	1X	27	THR	2.2
42	1k	33	THR	2.2
51	1t	84	LEU	2.2
4	1E	109	LYS	2.2
12	2Q	83	MET	2.2
15	2T	79	HIS	2.2
35	2d	29	PRO	2.2
42	1k	39	PRO	2.2
16	2U	104	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
44	1m	117	VAL	2.2
1	1A	2501	C	2.2
3	1D	235	GLY	2.2
11	2P	53	GLY	2.2
30	18	20	GLY	2.2
32	1a	796	C	2.2
36	1e	29	GLY	2.2
36	1e	122	GLU	2.2
47	1p	30	GLY	2.2
54	1y	13	C	2.2
15	1T	74	ARG	2.2
15	2T	64	ARG	2.2
16	1U	3	ARG	2.2
16	1U	30	LYS	2.2
23	21	40	ARG	2.2
38	1g	3	ARG	2.2
40	2i	70	LYS	2.2
3	1D	50	THR	2.2
12	1Q	43	THR	2.2
1	2A	2054	A	2.2
3	2D	178	PRO	2.2
5	1F	70	THR	2.2
36	2e	125	SER	2.2
25	23	2	PRO	2.2
39	2h	109	ILE	2.2
8	2I	25	TYR	2.2
1	1A	832	G	2.2
1	2A	2116	G	2.2
1	2A	2608	G	2.2
3	1D	150	LYS	2.2
3	2D	180	GLY	2.2
11	1P	20	GLY	2.2
11	2P	108	LYS	2.2
15	2T	108	ARG	2.2
17	1V	85	LYS	2.2
23	21	20	ARG	2.2
29	17	35	ARG	2.2
34	1c	156	ARG	2.2
39	2h	125	ARG	2.2
42	2k	42	TRP	2.2
43	1l	13	LYS	2.2
51	1t	15	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
9	1N	23	LEU	2.2
34	2c	111	LEU	2.2
5	2F	194	MET	2.2
8	2I	78	THR	2.2
13	2R	110	PRO	2.2
35	2d	91	SER	2.2
36	1e	106	PRO	2.2
42	2k	16	SER	2.2
45	1n	22	THR	2.2
5	2F	163	VAL	2.2
30	18	56	GLU	2.2
34	2c	55	VAL	2.2
36	2e	122	GLU	2.2
39	2h	98	LYS	2.2
42	2k	30	VAL	2.2
11	1P	37	GLY	2.2
16	1U	11	ARG	2.2
30	28	20	GLY	2.2
34	1c	131	ARG	2.2
36	2e	126	ARG	2.2
1	1A	564	C	2.2
18	2W	77	ASP	2.2
22	20	75	LEU	2.2
35	2d	21	LEU	2.2
45	1n	61	TRP	2.2
35	2d	161	ASN	2.2
54	1w	11	C	2.2
10	2O	86	ILE	2.2
44	1m	107	ALA	2.2
45	2n	48	ALA	2.2
10	1O	112	MET	2.2
30	28	19	SER	2.2
47	1p	22	THR	2.2
4	1E	172	VAL	2.2
4	2E	79	ARG	2.2
29	27	11	LYS	2.2
1	1A	2590	A	2.2
5	1F	57	VAL	2.2
12	1Q	35	VAL	2.2
13	1R	117	VAL	2.2
32	2a	901	A	2.2
34	1c	205	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
35	1d	68	TYR	2.2
45	1n	18	VAL	2.2
43	2l	14	GLY	2.1
15	2T	101	PHE	2.1
22	20	57	PHE	2.1
25	23	37	LEU	2.1
34	2c	186	PHE	2.1
38	1g	104	LEU	2.1
49	2r	31	LEU	2.1
51	1t	72	LEU	2.1
1	1A	2612	C	2.1
1	2A	2507	C	2.1
8	1I	26	ALA	2.1
10	1O	76	ALA	2.1
12	1Q	45	GLN	2.1
16	2U	96	ALA	2.1
17	2V	70	ILE	2.1
1	1A	778	G	2.1
1	1A	792	G	2.1
1	2A	2131	G	2.1
3	1D	12	SER	2.1
9	1N	40	PRO	2.1
35	2d	18	LYS	2.1
43	1l	21	LYS	2.1
54	1w	27	G	2.1
7	2H	158	HIS	2.1
29	17	41	ARG	2.1
31	19	18	ARG	2.1
31	29	20	HIS	2.1
42	1k	79	SER	2.1
13	2R	95	THR	2.1
51	1t	80	ARG	2.1
3	2D	234	GLY	2.1
9	2N	53	VAL	2.1
15	1T	30	VAL	2.1
23	11	31	GLY	2.1
23	21	29	GLY	2.1
25	23	6	VAL	2.1
42	1k	84	VAL	2.1
9	2N	123	TYR	2.1
1	1A	1829	A	2.1
18	2W	69	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	1D	159	ALA	2.1
4	1E	203	LYS	2.1
15	1T	86	ILE	2.1
24	22	41	ILE	2.1
27	15	14	ALA	2.1
30	18	10	ALA	2.1
34	2c	146	ALA	2.1
1	1A	2143	C	2.1
3	1D	69	ARG	2.1
7	2H	46	GLU	2.1
11	2P	61	ARG	2.1
18	1W	84	ARG	2.1
29	17	28	ARG	2.1
32	1a	1515	C	2.1
32	2a	812	C	2.1
47	2p	41	PRO	2.1
1	1A	2446	G	2.1
1	2A	745	G	2.1
12	1Q	129	THR	2.1
13	1R	108	GLY	2.1
23	11	74	VAL	2.1
30	28	6	THR	2.1
34	1c	159	GLY	2.1
39	2h	61	VAL	2.1
3	1D	95	LEU	2.1
4	2E	182	LEU	2.1
10	1O	66	LYS	2.1
1	2A	750	A	2.1
15	1T	76	PHE	2.1
33	2b	28	PHE	2.1
39	1h	39	LEU	2.1
40	2i	37	PHE	2.1
43	1l	23	LYS	2.1
43	2l	84	LEU	2.1
1	2A	614(A)	U	2.1
1	2A	757	U	2.1
3	2D	166	GLN	2.1
36	2e	20	GLN	2.1
53	2v	23	A	2.1
47	2p	7	ALA	2.1
3	1D	128	GLY	2.1
4	2E	125	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	2E	165	VAL	2.1
9	2N	128	HIS	2.1
16	1U	31	SER	2.1
23	2I	17	SER	2.1
1	2A	742	G	2.1
23	2I	32	LYS	2.1
4	1E	170	LEU	2.1
9	2N	134	ARG	2.1
13	2R	8	ARG	2.1
15	1T	103	ARG	2.1
16	2U	106	PHE	2.1
20	2Y	31	LEU	2.1
35	1d	138	TYR	2.1
25	23	35	ARG	2.1
35	1d	66	ARG	2.1
35	2d	206	PHE	2.1
40	1i	37	PHE	2.1
47	1p	49	LEU	2.1
49	1r	31	LEU	2.1
1	2A	747	U	2.1
15	1T	48	ILE	2.1
16	1U	89	GLU	2.1
44	2m	94	ARG	2.1
1	1A	2439	A	2.1
1	2A	677	A	2.1
1	2A	2614	A	2.1
3	1D	191	ALA	2.1
3	2D	240	ALA	2.1
4	2E	77	ILE	2.1
33	2b	29	ALA	2.1
43	1l	7	ILE	2.1
43	2l	100	ILE	2.1
48	2q	60	ILE	2.1
11	1P	54	GLY	2.1
32	2a	63	C	2.1
35	2d	173	TRP	2.1
34	1c	64	VAL	2.1
34	1c	173	VAL	2.1
39	1h	93	VAL	2.1
39	1h	137	VAL	2.1
15	2T	62	THR	2.1
4	1E	51	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
11	2P	91	PHE	2.1
13	2R	111	LEU	2.1
19	1X	47	PHE	2.1
29	17	19	ARG	2.1
31	19	24	TYR	2.1
35	2d	153	ARG	2.1
41	2j	64	GLU	2.1
48	2q	74	LEU	2.1
32	2a	324	G	2.1
3	1D	82	ILE	2.1
18	1W	103	ILE	2.1
32	1a	1532	U	2.1
38	1g	120	ILE	2.1
51	1t	63	ILE	2.1
1	1A	746	A	2.1
1	1A	1762	A	2.1
1	2A	1977	A	2.1
12	1Q	87	LYS	2.1
19	1X	78	LYS	2.1
40	2i	116	LYS	2.1
4	1E	23	VAL	2.1
23	21	51	VAL	2.1
37	1f	90	VAL	2.1
38	1g	105	VAL	2.1
3	1D	212	SER	2.1
3	2D	183	ARG	2.1
23	11	66	HIS	2.1
11	2P	32	THR	2.1
29	17	18	PHE	2.1
47	2p	34	GLU	2.1
4	1E	18	ASP	2.1
18	2W	9	TYR	2.1
1	1A	2449	U	2.1
3	1D	107	ALA	2.1
16	2U	42	ALA	2.1
18	1W	89	ALA	2.1
18	2W	24	ILE	2.1
34	2c	71	ALA	2.1
39	1h	16	ALA	2.1
1	1A	2447	G	2.1
1	2A	189	G	2.1
3	1D	207	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	567	A	2.1
1	2A	746	A	2.1
4	1E	111	ARG	2.1
4	1E	196	VAL	2.1
7	2H	97	ARG	2.1
8	1I	103	ARG	2.1
47	2p	51	VAL	2.1
55	1x	38	A	2.1
9	1N	100	GLU	2.1
16	2U	49	HIS	2.1
34	1c	18	TRP	2.1
4	1E	27	LEU	2.1
40	2i	126	SER	2.1
43	1l	60	LEU	2.1
17	2V	85	LYS	2.1
35	2d	27	TYR	2.1
4	1E	28	ALA	2.1
5	1F	42	ALA	2.1
36	2e	86	ALA	2.1
43	2l	56	ALA	2.1
5	2F	85	GLY	2.1
39	1h	47	GLY	2.1
42	1k	52	GLY	2.1
1	1A	36	G	2.1
1	1A	2147	G	2.1
36	2e	25	ARG	2.1
22	20	23	VAL	2.1
33	2b	26	PRO	2.1
41	1j	44	VAL	2.1
45	1n	56	VAL	2.1
1	1A	196	A	2.1
1	1A	2050	C	2.1
1	2A	575	A	2.1
9	1N	34	LEU	2.1
9	1N	121	LYS	2.1
13	1R	28	LEU	2.1
13	2R	79	LEU	2.1
15	2T	19	LEU	2.1
34	1c	128	PHE	2.1
15	1T	84	GLN	2.1
48	2q	97	SER	2.1
6	2G	146	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
30	28	55	ALA	2.1
34	1c	15	THR	2.1
34	2c	57	ILE	2.1
49	2r	50	ILE	2.1
1	1A	2144	U	2.1
1	2A	1778	U	2.1
54	1w	59	U	2.1
15	1T	47	GLY	2.1
23	21	36	GLY	2.1
30	18	13	ARG	2.1
35	2d	65	ARG	2.1
3	2D	241	PRO	2.1
20	1Y	39	VAL	2.1
34	1c	151	VAL	2.1
1	2A	944	G	2.1
32	2a	378	G	2.1
13	2R	18	LEU	2.0
16	1U	60	LEU	2.0
16	2U	27	LEU	2.0
24	12	10	LEU	2.0
30	18	48	PHE	2.1
33	2b	70	PHE	2.1
1	1A	1952	A	2.0
1	1A	2021	C	2.0
32	1a	694	A	2.0
35	2d	119	GLN	2.0
3	1D	136	ILE	2.0
6	2G	136	ARG	2.0
9	2N	27	ALA	2.0
15	1T	51	ARG	2.0
18	2W	7	ALA	2.0
27	15	19	ARG	2.0
40	2i	7	THR	2.0
48	2q	25	ARG	2.0
12	2Q	92	GLY	2.0
51	1t	69	GLY	2.0
3	2D	35	LYS	2.0
4	2E	188	VAL	2.0
8	2I	119	PRO	2.0
10	2O	10	VAL	2.0
18	2W	50	VAL	2.0
31	19	1	MET	2.0

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Mol	Chain	Res	Type	RSRZ
10	2O	29	ASN	2.0
40	1i	123	PRO	2.0
3	1D	94	LEU	2.0
4	2E	113	PHE	2.0
5	2F	148	LEU	2.0
25	23	53	LEU	2.0
35	2d	101	LEU	2.0
49	1r	44	LEU	2.0
49	1r	79	LEU	2.0
1	1A	765	G	2.0
1	2A	558	G	2.0
1	2A	738	G	2.0
10	1O	23	ARG	2.0
32	2a	1034	G	2.0
1	1A	38	A	2.0
4	1E	77	ILE	2.0
5	1F	65	TRP	2.0
18	1W	12	ILE	2.0
19	2X	89	ILE	2.0
24	12	50	ILE	2.0
32	1a	1434	A	2.0
36	1e	80	ILE	2.0
38	2g	10	ARG	2.0
1	2A	787	U	2.0
1	2A	811	U	2.0
3	1D	154	LYS	2.0
5	1F	76	GLY	2.0
10	1O	9	GLU	2.0
16	1U	19	LYS	2.0
54	2w	47	U	2.0
5	1F	36	VAL	2.0
21	1Z	126	VAL	2.0
42	1k	119	CYS	2.0
44	2m	7	VAL	2.0
46	2o	45	VAL	2.0
3	2D	36	PRO	2.0
5	1F	192	LEU	2.0
17	1V	94	LEU	2.0
23	21	16	ASN	2.0
25	13	19	GLN	2.0
28	26	9	LEU	2.0
34	1c	34	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
50	1s	71	LEU	2.0
18	2W	88	ARG	2.0
34	2c	164	ARG	2.0
12	1Q	64	ILE	2.0
15	1T	107	ASP	2.0
13	1R	19	ALA	2.0
13	1R	101	ALA	2.0
1	1A	669	G	2.0
1	1A	2499	C	2.0
1	2A	2050	C	2.0
42	2k	101	SER	2.0
51	1t	12	ALA	2.0
9	2N	4	TYR	2.0
32	2a	1220	G	2.0
55	2x	70	G	2.0
6	2G	160	VAL	2.0
8	2I	21	VAL	2.0
49	1r	39	VAL	2.0
3	2D	48	ARG	2.0
13	2R	47	PHE	2.0
9	2N	56	ASN	2.0
11	2P	48	PRO	2.0
21	1Z	44	PHE	2.0
13	2R	24	GLN	2.0
29	27	28	ARG	2.0
34	1c	178	LEU	2.0
39	1h	63	LEU	2.0
12	2Q	47	ILE	2.0
3	1D	163	ALA	2.0
3	1D	234	GLY	2.0
3	2D	238	GLY	2.0
36	1e	101	ILE	2.0
36	2e	8	GLU	2.0
36	2e	131	ILE	2.0
10	2O	46	ALA	2.0
43	2I	68	ALA	2.0
1	1A	981	A	2.0
1	1A	1268	A	2.0
1	1A	1825	A	2.0
9	1N	5	VAL	2.0
18	1W	85	VAL	2.0
20	2Y	72	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
40	2i	28	VAL	2.0
12	2Q	1	MET	2.0
6	1G	152	LEU	2.0
8	2I	38	LEU	2.0
20	2Y	56	PRO	2.0
25	23	12	PRO	2.0
34	2c	7	PRO	2.0
39	2h	39	LEU	2.0
43	2l	71	PRO	2.0
8	2I	28	ASN	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( $\text{\AA}^2$ )	Q<0.9
54	5MU	2y	54	21/22	0.66	0.34	101,120,137,154	0
54	PSU	2w	55	20/21	0.68	0.16	105,120,127,131	0
54	PSU	2w	39	20/21	0.72	0.40	115,123,126,127	0
54	4SU	2w	8	20/21	0.75	0.16	122,126,137,146	0
54	PSU	2y	55	20/21	0.76	0.39	114,121,139,154	0
54	PSU	1y	55	20/21	0.76	0.35	119,126,131,138	0
54	4SU	1y	8	20/21	0.77	0.15	115,120,127,132	0
54	4SU	2y	8	20/21	0.77	0.13	115,120,129,132	0
54	PSU	1w	55	20/21	0.80	0.21	102,112,115,117	0
54	7MG	2y	46	24/25	0.81	0.36	114,121,128,137	0
54	PSU	2y	32	20/21	0.82	0.37	109,122,134,138	0
54	PSU	2y	39	20/21	0.82	0.33	110,119,130,143	0
54	PSU	1y	39	20/21	0.82	0.36	107,116,137,143	0
54	4SU	1w	8	20/21	0.82	0.22	112,119,134,134	0
54	MIA	2y	37	22/30	0.84	0.29	107,116,130,143	0
54	7MG	2w	46	24/25	0.85	0.15	113,122,129,141	0
54	MIA	2w	37	25/30	0.85	0.19	91,115,118,133	0
32	5MC	2a	1400	21/22	0.86	0.33	87,108,118,120	0
53	PSU	2v	19	20/21	0.86	0.18	105,112,119,120	0
54	7MG	1w	46	24/25	0.86	0.17	105,115,124,133	0
54	5MU	2w	54	21/22	0.88	0.13	103,113,118,121	0
55	PSU	2x	55	20/21	0.89	0.11	106,112,122,123	0
54	5MU	1y	54	21/22	0.89	0.25	114,120,132,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	7MG	1y	46	24/25	0.89	0.26	109,119,125,130	0
54	PSU	1w	32	20/21	0.90	0.24	90,101,108,117	0
54	PSU	1y	32	20/21	0.90	0.29	105,113,128,129	0
54	MIA	1w	37	29/30	0.90	0.26	78,99,107,108	0
32	2MG	2a	1207	24/25	0.90	0.16	100,107,116,125	0
32	PSU	2a	516	20/21	0.90	0.16	92,103,111,114	0
54	MIA	1y	37	22/30	0.91	0.24	108,117,123,134	0
32	5MC	2a	967	21/22	0.91	0.16	99,102,110,118	0
32	5MC	2a	1404	21/22	0.91	0.17	84,99,105,110	0
55	4SU	2x	8	20/21	0.91	0.11	97,110,116,120	0
54	PSU	2w	32	20/21	0.91	0.29	108,114,123,126	0
54	PSU	1w	39	20/21	0.91	0.29	97,105,119,120	0
43	0TD	1l	92	10/11	0.93	0.22	88,91,97,113	0
55	4SU	1x	8	20/21	0.93	0.15	93,100,106,110	0
53	PSU	1v	19	20/21	0.93	0.14	79,95,102,102	0
55	5MC	2x	32	21/22	0.93	0.22	99,105,110,112	0
1	PSU	1A	2605	20/21	0.93	0.28	66,79,85,86	0
1	5MU	1A	1915	21/22	0.93	0.17	82,100,104,110	0
32	4OC	2a	1402	22/23	0.93	0.17	97,104,109,114	0
32	7MG	2a	527	24/25	0.93	0.18	89,95,101,112	0
43	0TD	2l	92	10/11	0.94	0.15	95,101,103,110	0
32	PSU	1a	516	20/21	0.94	0.17	84,92,98,104	0
1	PSU	2A	1911	20/21	0.94	0.14	86,98,105,106	0
1	PSU	2A	1917	20/21	0.94	0.13	86,103,108,111	0
1	4OC	2A	1920	21/23	0.94	0.15	89,98,103,108	0
32	UR3	2a	1498	21/22	0.94	0.24	88,98,102,106	0
1	5MC	2A	1962	21/22	0.94	0.17	77,89,95,99	0
32	MA6	2a	1519	24/25	0.94	0.30	86,99,103,105	0
55	5MU	2x	54	21/22	0.94	0.13	103,111,114,124	0
54	5MU	1w	54	21/22	0.94	0.25	104,108,117,119	0
1	5MU	2A	1915	21/22	0.94	0.13	101,107,111,116	0
1	PSU	1A	1911	20/21	0.94	0.18	70,90,95,100	0
32	5MC	1a	1407	21/22	0.94	0.23	76,88,93,97	0
32	4OC	1a	1402	22/23	0.94	0.26	82,92,98,100	0
32	M2G	2a	966	25/26	0.95	0.19	93,99,106,113	0
1	PSU	1A	1917	20/21	0.95	0.18	83,90,95,96	0
1	5MC	1A	1962	21/22	0.95	0.22	72,83,91,94	0
32	5MC	2a	1407	21/22	0.95	0.16	93,98,101,106	0
32	2MG	1a	1207	24/25	0.95	0.17	77,95,102,105	0
1	PSU	2A	2605	20/21	0.95	0.25	79,88,93,96	0
1	OMG	2A	2251	24/25	0.95	0.33	74,88,94,96	0
32	5MC	1a	1404	21/22	0.95	0.28	74,83,96,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MC	2A	1942	21/22	0.95	0.17	88,94,99,106	0
55	5MU	1x	54	21/22	0.95	0.14	86,97,101,105	0
55	PSU	1x	55	20/21	0.95	0.12	94,100,107,116	0
1	2MA	2A	2503	23/24	0.95	0.27	70,81,88,92	0
55	5MC	1x	32	21/22	0.95	0.23	84,95,100,102	0
1	2MU	1A	2552	21/23	0.96	0.31	58,78,84,92	0
32	5MC	1a	1400	21/22	0.96	0.26	81,91,96,104	0
1	4OC	1A	1920	21/23	0.96	0.21	76,89,95,96	0
32	5MC	1a	967	21/22	0.96	0.23	77,88,95,101	0
1	5MC	1A	1942	21/22	0.96	0.20	65,81,86,88	0
32	7MG	1a	527	24/25	0.96	0.20	78,89,96,98	0
32	MA6	2a	1518	24/25	0.96	0.22	90,97,101,102	0
1	5MU	1A	1939	21/22	0.96	0.26	66,78,86,90	0
1	5MU	2A	1939	21/22	0.96	0.23	75,86,91,95	0
32	M2G	1a	966	25/26	0.96	0.26	81,87,96,98	0
32	MA6	1a	1518	24/25	0.97	0.24	58,85,89,93	0
32	UR3	1a	1498	21/22	0.97	0.28	78,85,89,93	0
1	2MU	2A	2552	21/23	0.97	0.17	74,84,89,91	0
32	MA6	1a	1519	24/25	0.97	0.34	82,87,92,99	0
1	OMG	1A	2251	24/25	0.97	0.25	66,80,85,86	0
1	2MA	1A	2503	23/24	0.97	0.32	58,74,81,83	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	3317	1/1	0.32	0.65	92,92,92,92	0
56	MG	2A	3201	1/1	0.34	0.22	102,102,102,102	0
56	MG	1A	3190	1/1	0.34	0.48	118,118,118,118	0
56	MG	1A	3242	1/1	0.37	0.33	78,78,78,78	0
56	MG	2a	3060	1/1	0.37	0.43	101,101,101,101	0
56	MG	2a	3082	1/1	0.37	0.31	109,109,109,109	0
56	MG	2a	3154	1/1	0.38	0.16	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3315	1/1	0.40	0.84	103,103,103,103	0
56	MG	1A	3557	1/1	0.40	0.36	89,89,89,89	0
56	MG	1a	3094	1/1	0.44	1.77	96,96,96,96	0
56	MG	2A	3031	1/1	0.45	0.20	100,100,100,100	0
56	MG	1a	3214	1/1	0.45	0.26	103,103,103,103	0
56	MG	1A	3497	1/1	0.46	0.22	96,96,96,96	0
56	MG	1A	3104	1/1	0.46	0.98	90,90,90,90	0
56	MG	2A	3017	1/1	0.48	0.30	98,98,98,98	0
56	MG	1A	3377	1/1	0.48	0.45	102,102,102,102	0
56	MG	1A	3429	1/1	0.50	0.25	87,87,87,87	0
56	MG	1a	3111	1/1	0.51	0.42	103,103,103,103	0
56	MG	1A	3240	1/1	0.53	0.37	101,101,101,101	0
56	MG	1A	3194	1/1	0.53	0.26	72,72,72,72	0
56	MG	1A	3157	1/1	0.54	0.13	92,92,92,92	0
56	MG	1A	3036	1/1	0.54	0.80	99,99,99,99	0
56	MG	1A	3099	1/1	0.55	0.40	77,77,77,77	0
56	MG	1A	3133	1/1	0.55	0.36	76,76,76,76	0
56	MG	2a	3080	1/1	0.56	0.28	85,85,85,85	0
56	MG	1A	3433	1/1	0.56	1.77	97,97,97,97	0
56	MG	1A	3359	1/1	0.56	0.77	89,89,89,89	0
56	MG	1A	3041	1/1	0.56	0.23	105,105,105,105	0
56	MG	1A	3534	1/1	0.56	0.30	86,86,86,86	0
56	MG	2A	3205	1/1	0.57	0.32	111,111,111,111	0
56	MG	1A	3441	1/1	0.57	0.38	103,103,103,103	0
56	MG	2a	3059	1/1	0.57	0.46	79,79,79,79	0
56	MG	1a	3077	1/1	0.58	0.22	84,84,84,84	0
56	MG	1A	3367	1/1	0.58	0.25	104,104,104,104	0
56	MG	1A	3148	1/1	0.58	0.42	79,79,79,79	0
56	MG	2a	3034	1/1	0.59	0.23	79,79,79,79	0
56	MG	1a	3005	1/1	0.60	0.21	80,80,80,80	0
56	MG	2a	3107	1/1	0.60	0.10	106,106,106,106	0
56	MG	2A	3146	1/1	0.60	0.23	79,79,79,79	0
56	MG	1A	3615	1/1	0.60	0.22	95,95,95,95	0
56	MG	2A	3057	1/1	0.61	0.71	89,89,89,89	0
56	MG	2A	3074	1/1	0.61	0.30	102,102,102,102	0
56	MG	1A	3651	1/1	0.61	0.19	90,90,90,90	0
56	MG	2A	3034	1/1	0.61	0.17	71,71,71,71	0
56	MG	2a	3102	1/1	0.61	0.23	90,90,90,90	0
56	MG	1A	3527	1/1	0.61	0.24	74,74,74,74	0
56	MG	1a	3211	1/1	0.61	0.30	77,77,77,77	0
56	MG	2A	3111	1/1	0.61	0.67	81,81,81,81	0
56	MG	2A	3316	1/1	0.62	0.48	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3302	1/1	0.63	0.14	82,82,82,82	0
56	MG	2a	3007	1/1	0.64	0.54	99,99,99,99	0
56	MG	1a	3043	1/1	0.64	0.41	95,95,95,95	0
56	MG	1A	3142	1/1	0.64	0.53	73,73,73,73	0
56	MG	2a	3087	1/1	0.64	0.46	94,94,94,94	0
56	MG	1A	3105	1/1	0.64	0.25	74,74,74,74	0
56	MG	2a	3058	1/1	0.65	0.61	93,93,93,93	0
56	MG	1A	3569	1/1	0.65	0.11	95,95,95,95	0
56	MG	1a	3167	1/1	0.65	0.48	109,109,109,109	0
56	MG	2a	3015	1/1	0.65	0.15	98,98,98,98	0
56	MG	2A	3158	1/1	0.65	0.67	78,78,78,78	0
56	MG	1a	3122	1/1	0.65	1.05	93,93,93,93	0
56	MG	2a	3017	1/1	0.66	2.14	89,89,89,89	0
56	MG	2A	3323	1/1	0.66	0.15	104,104,104,104	0
56	MG	2a	3051	1/1	0.66	0.31	79,79,79,79	0
56	MG	1A	3364	1/1	0.66	0.30	96,96,96,96	0
56	MG	2A	3160	1/1	0.67	0.13	88,88,88,88	0
56	MG	1A	3145	1/1	0.67	0.27	93,93,93,93	0
56	MG	2a	3106	1/1	0.67	0.22	124,124,124,124	0
56	MG	1a	3008	1/1	0.67	0.15	66,66,66,66	0
56	MG	1a	3116	1/1	0.67	0.47	90,90,90,90	0
56	MG	1a	3149	1/1	0.67	0.21	110,110,110,110	0
57	ZN	14	501	1/1	0.67	0.04	162,162,162,162	0
56	MG	1A	3123	1/1	0.67	0.47	93,93,93,93	0
56	MG	2A	3184	1/1	0.67	0.28	82,82,82,82	0
56	MG	1A	3191	1/1	0.67	0.26	90,90,90,90	0
56	MG	1A	3098	1/1	0.67	1.35	80,80,80,80	0
56	MG	1A	3524	1/1	0.68	0.36	84,84,84,84	0
56	MG	2a	3138	1/1	0.68	0.28	95,95,95,95	0
56	MG	2A	3287	1/1	0.68	0.16	83,83,83,83	0
56	MG	2a	3049	1/1	0.68	0.18	79,79,79,79	0
56	MG	1a	3085	1/1	0.68	0.34	89,89,89,89	0
56	MG	1A	3408	1/1	0.68	0.20	96,96,96,96	0
56	MG	1A	3034	1/1	0.69	0.10	79,79,79,79	0
56	MG	1A	3573	1/1	0.69	0.21	88,88,88,88	0
56	MG	1A	3565	1/1	0.69	0.28	83,83,83,83	0
56	MG	2a	3158	1/1	0.69	0.22	116,116,116,116	0
56	MG	2A	3162	1/1	0.69	0.23	77,77,77,77	0
56	MG	1A	3128	1/1	0.70	0.22	75,75,75,75	0
56	MG	2a	3100	1/1	0.71	0.26	94,94,94,94	0
56	MG	1A	3506	1/1	0.71	0.52	118,118,118,118	0
56	MG	2a	3070	1/1	0.71	0.21	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3277	1/1	0.71	0.21	73,73,73,73	0
56	MG	2a	3053	1/1	0.71	0.82	90,90,90,90	0
56	MG	1a	3173	1/1	0.71	0.25	75,75,75,75	0
56	MG	1A	3303	1/1	0.71	0.27	78,78,78,78	0
56	MG	1A	3151	1/1	0.71	0.27	64,64,64,64	0
56	MG	1A	3585	1/1	0.71	0.19	76,76,76,76	0
56	MG	2A	3094	1/1	0.71	0.22	85,85,85,85	0
56	MG	2A	3196	1/1	0.71	0.33	81,81,81,81	0
56	MG	2A	3278	1/1	0.71	0.16	89,89,89,89	0
56	MG	1A	3160	1/1	0.71	0.26	76,76,76,76	0
56	MG	1A	3572	1/1	0.71	0.18	85,85,85,85	0
56	MG	2A	3166	1/1	0.71	0.27	79,79,79,79	0
56	MG	2A	3290	1/1	0.72	0.14	94,94,94,94	0
56	MG	1A	3533	1/1	0.72	0.37	114,114,114,114	0
56	MG	1a	3028	1/1	0.72	0.20	76,76,76,76	0
56	MG	2A	3099	1/1	0.72	0.62	89,89,89,89	0
56	MG	1a	3082	1/1	0.72	0.80	75,75,75,75	0
56	MG	2a	3077	1/1	0.72	0.17	95,95,95,95	0
56	MG	2a	3006	1/1	0.72	0.31	104,104,104,104	0
56	MG	2A	3022	1/1	0.72	0.16	96,96,96,96	0
56	MG	1a	3162	1/1	0.72	0.31	93,93,93,93	0
56	MG	2A	3119	1/1	0.72	0.15	90,90,90,90	0
56	MG	1A	3239	1/1	0.72	0.25	93,93,93,93	0
56	MG	1A	3636	1/1	0.73	0.34	73,73,73,73	0
56	MG	2A	3019	1/1	0.73	0.21	101,101,101,101	0
56	MG	2a	3054	1/1	0.73	0.18	90,90,90,90	0
56	MG	2A	3245	1/1	0.73	0.41	94,94,94,94	0
56	MG	2a	3130	1/1	0.73	0.09	74,74,74,74	0
56	MG	1A	3612	1/1	0.73	0.24	95,95,95,95	0
56	MG	2a	3179	1/1	0.73	0.12	106,106,106,106	0
56	MG	2a	3037	1/1	0.73	0.21	106,106,106,106	0
56	MG	1A	3505	1/1	0.73	0.15	70,70,70,70	0
56	MG	2A	3092	1/1	0.73	0.48	99,99,99,99	0
56	MG	1A	3513	1/1	0.73	0.63	88,88,88,88	0
56	MG	2A	3193	1/1	0.74	0.35	86,86,86,86	0
56	MG	2a	3088	1/1	0.74	0.32	97,97,97,97	0
56	MG	1A	3390	1/1	0.74	0.27	87,87,87,87	0
56	MG	2A	3192	1/1	0.74	0.12	77,77,77,77	0
56	MG	2a	3031	1/1	0.74	0.88	109,109,109,109	0
56	MG	1a	3105	1/1	0.74	0.25	86,86,86,86	0
56	MG	2A	3244	1/1	0.74	0.11	90,90,90,90	0
56	MG	1A	3583	1/1	0.74	0.15	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3070	1/1	0.74	0.35	74,74,74,74	0
56	MG	1A	3352	1/1	0.75	0.26	95,95,95,95	0
56	MG	2A	3087	1/1	0.75	0.28	88,88,88,88	0
56	MG	2A	3197	1/1	0.75	0.20	78,78,78,78	0
56	MG	1a	3163	1/1	0.75	0.41	66,66,66,66	0
56	MG	1A	3368	1/1	0.75	0.78	99,99,99,99	0
56	MG	1a	3092	1/1	0.75	0.71	85,85,85,85	0
56	MG	2a	3097	1/1	0.75	0.31	89,89,89,89	0
56	MG	1A	3268	1/1	0.75	0.21	68,68,68,68	0
56	MG	1A	3423	1/1	0.76	0.38	78,78,78,78	0
56	MG	1a	3016	1/1	0.76	0.92	87,87,87,87	0
56	MG	2A	3156	1/1	0.76	0.17	69,69,69,69	0
56	MG	1A	3014	1/1	0.76	0.39	93,93,93,93	0
56	MG	1a	3182	1/1	0.76	0.21	102,102,102,102	0
56	MG	2a	3166	1/1	0.76	0.14	115,115,115,115	0
56	MG	2A	3123	1/1	0.76	0.18	81,81,81,81	0
56	MG	1A	3555	1/1	0.76	0.23	80,80,80,80	0
56	MG	2A	3058	1/1	0.76	0.32	78,78,78,78	0
56	MG	1A	3257	1/1	0.76	0.27	80,80,80,80	0
56	MG	1A	3149	1/1	0.76	0.53	76,76,76,76	0
56	MG	1A	3244	1/1	0.77	0.23	81,81,81,81	0
56	MG	1A	3629	1/1	0.77	0.28	106,106,106,106	0
56	MG	2A	3243	1/1	0.77	0.13	88,88,88,88	0
56	MG	1A	3280	1/1	0.77	0.20	77,77,77,77	0
56	MG	2A	3003	1/1	0.77	0.23	84,84,84,84	0
56	MG	1A	3304	1/1	0.77	0.21	76,76,76,76	0
56	MG	1A	3045	1/1	0.77	0.23	94,94,94,94	0
56	MG	1A	3518	1/1	0.77	0.27	97,97,97,97	0
56	MG	2A	3198	1/1	0.77	0.17	83,83,83,83	0
56	MG	1a	3027	1/1	0.77	0.18	76,76,76,76	0
56	MG	1a	3067	1/1	0.77	0.18	80,80,80,80	0
56	MG	1A	3415	1/1	0.77	0.21	78,78,78,78	0
56	MG	1A	3394	1/1	0.77	0.46	91,91,91,91	0
56	MG	2A	3138	1/1	0.77	0.20	102,102,102,102	0
56	MG	2A	3148	1/1	0.77	0.16	96,96,96,96	0
56	MG	1A	3442	1/1	0.77	0.15	77,77,77,77	0
56	MG	2A	3142	1/1	0.78	0.61	81,81,81,81	0
56	MG	2A	3297	1/1	0.78	0.19	93,93,93,93	0
56	MG	2A	3206	1/1	0.78	0.35	73,73,73,73	0
56	MG	1a	3051	1/1	0.78	0.33	99,99,99,99	0
56	MG	1A	3121	1/1	0.78	0.42	76,76,76,76	0
56	MG	1A	3318	1/1	0.78	0.46	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3331	1/1	0.78	0.28	67,67,67,67	0
56	MG	1A	3428	1/1	0.78	0.26	79,79,79,79	0
56	MG	1A	3125	1/1	0.78	0.30	77,77,77,77	0
56	MG	2A	3249	1/1	0.78	0.11	81,81,81,81	0
56	MG	1A	3176	1/1	0.78	0.23	95,95,95,95	0
56	MG	1A	3320	1/1	0.78	0.23	65,65,65,65	0
56	MG	1A	3252	1/1	0.78	0.20	73,73,73,73	0
56	MG	1A	3198	1/1	0.78	0.11	83,83,83,83	0
56	MG	2A	3110	1/1	0.78	0.15	79,79,79,79	0
56	MG	1A	3376	1/1	0.78	0.19	92,92,92,92	0
56	MG	1A	3549	1/1	0.78	0.26	83,83,83,83	0
56	MG	2a	3090	1/1	0.78	0.22	91,91,91,91	0
56	MG	2A	3318	1/1	0.78	0.21	87,87,87,87	0
56	MG	2A	3294	1/1	0.78	0.38	104,104,104,104	0
56	MG	2A	3078	1/1	0.79	0.23	75,75,75,75	0
56	MG	1a	3238	1/1	0.79	0.15	99,99,99,99	0
56	MG	1A	3479	1/1	0.79	0.14	86,86,86,86	0
56	MG	1A	3571	1/1	0.79	0.05	98,98,98,98	0
56	MG	1A	3554	1/1	0.79	0.14	109,109,109,109	0
56	MG	1A	3199	1/1	0.79	0.23	70,70,70,70	0
56	MG	2a	3169	1/1	0.79	0.25	78,78,78,78	0
56	MG	1a	3189	1/1	0.79	0.23	85,85,85,85	0
56	MG	2A	3101	1/1	0.79	0.46	83,83,83,83	0
56	MG	1a	3037	1/1	0.79	0.42	82,82,82,82	0
56	MG	1a	3134	1/1	0.79	0.39	77,77,77,77	0
56	MG	1a	3106	1/1	0.79	0.07	98,98,98,98	0
56	MG	1a	3152	1/1	0.79	0.18	102,102,102,102	0
56	MG	2a	3092	1/1	0.79	0.19	88,88,88,88	0
56	MG	2A	3143	1/1	0.79	0.24	93,93,93,93	0
56	MG	1A	3114	1/1	0.79	0.42	93,93,93,93	0
56	MG	2a	3141	1/1	0.79	0.10	82,82,82,82	0
56	MG	1A	3486	1/1	0.79	0.23	68,68,68,68	0
56	MG	1A	3161	1/1	0.79	0.17	90,90,90,90	0
56	MG	2a	3028	1/1	0.79	0.14	85,85,85,85	0
56	MG	2A	3310	1/1	0.79	0.06	91,91,91,91	0
56	MG	2A	3071	1/1	0.79	0.20	75,75,75,75	0
56	MG	2a	3036	1/1	0.80	0.10	95,95,95,95	0
56	MG	1a	3179	1/1	0.80	0.13	90,90,90,90	0
56	MG	1A	3056	1/1	0.80	0.27	80,80,80,80	0
56	MG	2A	3051	1/1	0.80	0.29	80,80,80,80	0
56	MG	1A	3579	1/1	0.80	0.51	118,118,118,118	0
56	MG	1A	3258	1/1	0.80	0.29	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3053	1/1	0.80	1.62	79,79,79,79	0
56	MG	1A	3511	1/1	0.80	0.17	62,62,62,62	0
56	MG	1a	3230	1/1	0.80	0.23	84,84,84,84	0
56	MG	2A	3234	1/1	0.80	0.72	84,84,84,84	0
56	MG	1a	3222	1/1	0.80	0.11	91,91,91,91	0
56	MG	2a	3048	1/1	0.80	0.33	94,94,94,94	0
56	MG	1A	3420	1/1	0.80	0.36	76,76,76,76	0
56	MG	2a	3063	1/1	0.80	0.25	83,83,83,83	0
56	MG	1A	3181	1/1	0.80	1.48	78,78,78,78	0
56	MG	2A	3112	1/1	0.80	0.31	89,89,89,89	0
56	MG	1a	3068	1/1	0.80	0.15	95,95,95,95	0
56	MG	1a	3072	1/1	0.80	0.20	94,94,94,94	0
56	MG	2A	3114	1/1	0.80	0.37	79,79,79,79	0
56	MG	2A	3237	1/1	0.80	0.18	92,92,92,92	0
56	MG	1A	3058	1/1	0.80	0.15	80,80,80,80	0
56	MG	1A	3661	1/1	0.80	0.35	87,87,87,87	0
56	MG	1a	3117	1/1	0.80	0.14	83,83,83,83	0
56	MG	2a	3050	1/1	0.80	0.29	105,105,105,105	0
56	MG	2A	3227	1/1	0.80	0.11	81,81,81,81	0
56	MG	2a	3144	1/1	0.80	0.24	101,101,101,101	0
56	MG	1A	3159	1/1	0.80	0.11	69,69,69,69	0
56	MG	1A	3002	1/1	0.81	0.17	72,72,72,72	0
56	MG	2A	3337	1/1	0.81	0.14	78,78,78,78	0
56	MG	1A	3015	1/1	0.81	0.13	86,86,86,86	0
56	MG	1A	3016	1/1	0.81	0.28	66,66,66,66	0
56	MG	2A	3258	1/1	0.81	0.34	103,103,103,103	0
56	MG	1a	3039	1/1	0.81	0.21	80,80,80,80	0
56	MG	1a	3033	1/1	0.81	0.28	87,87,87,87	0
56	MG	2A	3134	1/1	0.81	0.42	91,91,91,91	0
56	MG	1A	3174	1/1	0.81	0.39	77,77,77,77	0
56	MG	1A	3168	1/1	0.81	0.19	78,78,78,78	0
56	MG	1A	3580	1/1	0.81	0.15	74,74,74,74	0
56	MG	1a	3136	1/1	0.81	0.23	84,84,84,84	0
56	MG	1a	3203	1/1	0.81	0.34	105,105,105,105	0
56	MG	2A	3332	1/1	0.81	0.48	116,116,116,116	0
56	MG	1A	3291	1/1	0.81	0.18	79,79,79,79	0
56	MG	1A	3295	1/1	0.81	0.34	66,66,66,66	0
56	MG	2A	3055	1/1	0.81	0.13	92,92,92,92	0
56	MG	2A	3336	1/1	0.81	0.21	77,77,77,77	0
56	MG	1a	3004	1/1	0.81	0.19	101,101,101,101	0
56	MG	1a	3201	1/1	0.81	0.50	93,93,93,93	0
56	MG	2a	3167	1/1	0.81	0.30	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3116	1/1	0.81	0.20	82,82,82,82	0
56	MG	1a	3069	1/1	0.81	0.18	81,81,81,81	0
56	MG	2a	3004	1/1	0.81	0.29	98,98,98,98	0
56	MG	1a	3019	1/1	0.81	0.53	96,96,96,96	0
56	MG	1a	3110	1/1	0.81	0.10	90,90,90,90	0
56	MG	2a	3099	1/1	0.81	0.20	93,93,93,93	0
56	MG	1A	3053	1/1	0.81	0.38	95,95,95,95	0
56	MG	1A	3447	1/1	0.81	0.30	91,91,91,91	0
56	MG	2A	3216	1/1	0.81	0.75	87,87,87,87	0
56	MG	1A	3400	1/1	0.81	0.25	90,90,90,90	0
56	MG	1a	3030	1/1	0.81	0.47	105,105,105,105	0
56	MG	2A	3351	1/1	0.81	0.15	84,84,84,84	0
56	MG	2A	3298	1/1	0.82	0.56	76,76,76,76	0
56	MG	1A	3192	1/1	0.82	0.14	74,74,74,74	0
56	MG	1A	3196	1/1	0.82	0.23	81,81,81,81	0
56	MG	2A	3097	1/1	0.82	0.41	91,91,91,91	0
56	MG	2a	3177	1/1	0.82	0.16	86,86,86,86	0
56	MG	2A	3247	1/1	0.82	0.16	101,101,101,101	0
56	MG	1a	3133	1/1	0.82	0.15	90,90,90,90	0
56	MG	2a	3085	1/1	0.82	0.16	83,83,83,83	0
56	MG	1A	3249	1/1	0.82	0.34	77,77,77,77	0
56	MG	1A	3647	1/1	0.82	0.15	93,93,93,93	0
56	MG	2A	3217	1/1	0.82	0.52	82,82,82,82	0
56	MG	1A	3385	1/1	0.82	0.30	74,74,74,74	0
56	MG	1a	3090	1/1	0.82	0.53	87,87,87,87	0
56	MG	1A	3657	1/1	0.82	0.43	79,79,79,79	0
56	MG	1a	3220	1/1	0.82	0.35	80,80,80,80	0
56	MG	1A	3180	1/1	0.82	0.77	93,93,93,93	0
56	MG	2A	3344	1/1	0.82	0.10	106,106,106,106	0
56	MG	2A	3222	1/1	0.82	0.23	89,89,89,89	0
56	MG	2A	3165	1/1	0.82	0.14	77,77,77,77	0
56	MG	2A	3090	1/1	0.82	0.22	98,98,98,98	0
56	MG	2A	3098	1/1	0.82	0.57	79,79,79,79	0
56	MG	2a	3061	1/1	0.82	0.07	92,92,92,92	0
56	MG	1A	3567	1/1	0.82	0.13	87,87,87,87	0
56	MG	1A	3293	1/1	0.82	0.13	78,78,78,78	0
56	MG	1a	3233	1/1	0.82	0.19	76,76,76,76	0
56	MG	1a	3143	1/1	0.83	0.27	91,91,91,91	0
56	MG	1A	3147	1/1	0.83	0.15	86,86,86,86	0
56	MG	1A	3208	1/1	0.83	0.22	74,74,74,74	0
56	MG	2A	3186	1/1	0.83	0.20	79,79,79,79	0
56	MG	1A	3234	1/1	0.83	0.36	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3010	1/1	0.83	0.08	86,86,86,86	0
56	MG	1a	3169	1/1	0.83	0.16	80,80,80,80	0
56	MG	1A	3144	1/1	0.83	0.18	85,85,85,85	0
56	MG	2a	3009	1/1	0.83	0.32	84,84,84,84	0
56	MG	1a	3063	1/1	0.83	0.27	89,89,89,89	0
56	MG	1a	3062	1/1	0.83	0.27	71,71,71,71	0
56	MG	1a	3187	1/1	0.83	0.27	78,78,78,78	0
56	MG	2a	3161	1/1	0.83	0.14	104,104,104,104	0
56	MG	1A	3203	1/1	0.83	0.29	74,74,74,74	0
56	MG	2A	3011	1/1	0.83	0.21	87,87,87,87	0
56	MG	1A	3419	1/1	0.83	0.16	87,87,87,87	0
56	MG	1A	3319	1/1	0.83	0.54	100,100,100,100	0
56	MG	1A	3113	1/1	0.83	0.14	75,75,75,75	0
56	MG	1A	3620	1/1	0.83	0.51	91,91,91,91	0
56	MG	1a	3126	1/1	0.83	0.15	100,100,100,100	0
56	MG	2a	3047	1/1	0.83	0.14	83,83,83,83	0
56	MG	1A	3444	1/1	0.83	0.23	83,83,83,83	0
56	MG	1A	3459	1/1	0.83	0.11	62,62,62,62	0
56	MG	1A	3087	1/1	0.83	0.14	79,79,79,79	0
56	MG	2A	3060	1/1	0.83	0.17	79,79,79,79	0
56	MG	1a	3097	1/1	0.83	0.88	95,95,95,95	0
56	MG	1A	3197	1/1	0.83	0.25	72,72,72,72	0
56	MG	2A	3131	1/1	0.83	0.41	95,95,95,95	0
56	MG	2A	3277	1/1	0.83	0.40	93,93,93,93	0
56	MG	2A	3151	1/1	0.83	0.13	78,78,78,78	0
56	MG	2A	3104	1/1	0.83	0.16	98,98,98,98	0
56	MG	1A	3391	1/1	0.83	0.27	80,80,80,80	0
56	MG	2A	3283	1/1	0.83	0.20	84,84,84,84	0
56	MG	2A	3033	1/1	0.83	0.33	81,81,81,81	0
56	MG	2A	3313	1/1	0.83	0.15	96,96,96,96	0
57	ZN	24	501	1/1	0.83	0.06	168,168,168,168	0
56	MG	1a	3089	1/1	0.83	0.16	78,78,78,78	0
56	MG	1a	3165	1/1	0.83	0.49	87,87,87,87	0
56	MG	1A	3265	1/1	0.83	0.26	65,65,65,65	0
56	MG	2A	3153	1/1	0.83	0.35	81,81,81,81	0
56	MG	1a	3049	1/1	0.83	0.21	87,87,87,87	0
56	MG	2a	3089	1/1	0.83	0.14	86,86,86,86	0
56	MG	1a	3083	1/1	0.83	0.30	93,93,93,93	0
56	MG	2A	3127	1/1	0.84	0.10	78,78,78,78	0
56	MG	1A	3457	1/1	0.84	0.18	77,77,77,77	0
56	MG	2A	3100	1/1	0.84	0.21	86,86,86,86	0
56	MG	1a	3115	1/1	0.84	0.12	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3343	1/1	0.84	0.20	72,72,72,72	0
56	MG	1A	3453	1/1	0.84	0.19	84,84,84,84	0
56	MG	1A	3674	1/1	0.84	0.33	81,81,81,81	0
56	MG	1a	3107	1/1	0.84	0.17	84,84,84,84	0
56	MG	1a	3174	1/1	0.84	0.15	87,87,87,87	0
56	MG	2A	3328	1/1	0.84	0.12	90,90,90,90	0
56	MG	2a	3121	1/1	0.84	0.26	114,114,114,114	0
56	MG	1A	3617	1/1	0.84	0.14	69,69,69,69	0
56	MG	2A	3194	1/1	0.84	0.16	85,85,85,85	0
56	MG	1a	3205	1/1	0.84	0.11	102,102,102,102	0
56	MG	1A	3299	1/1	0.84	0.20	90,90,90,90	0
56	MG	2A	3018	1/1	0.84	0.20	85,85,85,85	0
56	MG	1a	3007	1/1	0.84	0.19	67,67,67,67	0
56	MG	1a	3191	1/1	0.84	0.12	93,93,93,93	0
56	MG	2A	3266	1/1	0.84	0.10	88,88,88,88	0
56	MG	2a	3159	1/1	0.84	0.33	92,92,92,92	0
56	MG	2A	3013	1/1	0.84	0.36	79,79,79,79	0
56	MG	1a	3052	1/1	0.84	0.15	84,84,84,84	0
56	MG	1A	3371	1/1	0.84	0.29	52,52,52,52	0
56	MG	1A	3633	1/1	0.84	0.22	75,75,75,75	0
56	MG	2A	3061	1/1	0.84	0.18	76,76,76,76	0
56	MG	1A	3658	1/1	0.84	0.23	98,98,98,98	0
56	MG	2A	3026	1/1	0.84	0.19	92,92,92,92	0
56	MG	1A	3287	1/1	0.84	0.13	80,80,80,80	0
56	MG	1A	3253	1/1	0.84	0.28	71,71,71,71	0
56	MG	1A	3601	1/1	0.84	0.91	102,102,102,102	0
56	MG	1A	3339	1/1	0.84	1.46	112,112,112,112	0
56	MG	1A	3622	1/1	0.84	0.19	91,91,91,91	0
56	MG	1A	3026	1/1	0.84	0.27	77,77,77,77	0
56	MG	1A	3001	1/1	0.84	0.10	70,70,70,70	0
56	MG	1a	3070	1/1	0.84	0.20	85,85,85,85	0
56	MG	1A	3137	1/1	0.84	0.20	82,82,82,82	0
56	MG	1A	3030	1/1	0.84	0.50	69,69,69,69	0
56	MG	2A	3204	1/1	0.84	0.53	90,90,90,90	0
56	MG	2a	3160	1/1	0.84	0.11	104,104,104,104	0
56	MG	2A	3215	1/1	0.84	0.18	86,86,86,86	0
56	MG	2a	3012	1/1	0.84	0.14	79,79,79,79	0
56	MG	2a	3078	1/1	0.84	0.15	85,85,85,85	0
56	MG	1A	3012	1/1	0.84	0.13	78,78,78,78	0
56	MG	1A	3548	1/1	0.84	0.62	91,91,91,91	0
56	MG	2A	3152	1/1	0.85	0.68	85,85,85,85	0
56	MG	1A	3521	1/1	0.85	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3372	1/1	0.85	0.17	63,63,63,63	0
56	MG	1a	3099	1/1	0.85	0.10	90,90,90,90	0
56	MG	1A	3019	1/1	0.85	0.19	81,81,81,81	0
56	MG	2A	3253	1/1	0.85	0.17	74,74,74,74	0
56	MG	1A	3063	1/1	0.85	0.16	80,80,80,80	0
56	MG	1A	3519	1/1	0.85	0.17	88,88,88,88	0
56	MG	2a	3062	1/1	0.85	0.32	94,94,94,94	0
56	MG	2A	3181	1/1	0.85	0.69	90,90,90,90	0
56	MG	1A	3417	1/1	0.85	0.19	79,79,79,79	0
56	MG	1A	3219	1/1	0.85	0.13	84,84,84,84	0
56	MG	1A	3205	1/1	0.85	0.15	78,78,78,78	0
56	MG	2A	3024	1/1	0.85	0.22	95,95,95,95	0
56	MG	1A	3246	1/1	0.85	0.14	78,78,78,78	0
56	MG	2A	3207	1/1	0.85	0.46	68,68,68,68	0
56	MG	2A	3190	1/1	0.85	0.11	98,98,98,98	0
56	MG	1a	3127	1/1	0.85	0.21	82,82,82,82	0
56	MG	2a	3076	1/1	0.85	0.17	99,99,99,99	0
56	MG	1A	3543	1/1	0.85	0.28	86,86,86,86	0
56	MG	2A	3203	1/1	0.85	0.43	87,87,87,87	0
56	MG	2A	3080	1/1	0.85	0.08	80,80,80,80	0
56	MG	1A	3608	1/1	0.85	0.12	87,87,87,87	0
56	MG	1A	3007	1/1	0.85	0.12	91,91,91,91	0
56	MG	1a	3166	1/1	0.85	0.15	100,100,100,100	0
56	MG	1a	3108	1/1	0.85	0.24	93,93,93,93	0
56	MG	2A	3263	1/1	0.85	0.52	86,86,86,86	0
56	MG	2A	3028	1/1	0.85	0.40	68,68,68,68	0
56	MG	1A	3354	1/1	0.85	0.21	83,83,83,83	0
56	MG	2A	3041	1/1	0.85	0.23	69,69,69,69	0
56	MG	2a	3162	1/1	0.85	0.15	126,126,126,126	0
56	MG	1a	3224	1/1	0.85	0.21	77,77,77,77	0
56	MG	1A	3552	1/1	0.85	0.14	100,100,100,100	0
56	MG	1A	3455	1/1	0.85	0.15	63,63,63,63	0
56	MG	2A	3209	1/1	0.85	0.38	83,83,83,83	0
56	MG	1a	3036	1/1	0.85	0.14	90,90,90,90	0
56	MG	1a	3060	1/1	0.85	0.17	83,83,83,83	0
56	MG	2A	3295	1/1	0.85	0.31	91,91,91,91	0
56	MG	2A	3195	1/1	0.85	0.31	84,84,84,84	0
56	MG	1A	3153	1/1	0.85	0.37	72,72,72,72	0
56	MG	2a	3118	1/1	0.85	0.04	115,115,115,115	0
56	MG	2a	3120	1/1	0.85	0.67	103,103,103,103	0
56	MG	1a	3180	1/1	0.85	0.19	90,90,90,90	0
56	MG	1a	3213	1/1	0.86	1.10	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3053	1/1	0.86	0.10	77,77,77,77	0
56	MG	1A	3621	1/1	0.86	0.13	69,69,69,69	0
56	MG	1a	3058	1/1	0.86	0.30	75,75,75,75	0
56	MG	2A	3154	1/1	0.86	0.70	74,74,74,74	0
56	MG	2A	3072	1/1	0.86	0.18	74,74,74,74	0
56	MG	1A	3237	1/1	0.86	0.33	74,74,74,74	0
56	MG	1A	3122	1/1	0.86	0.24	77,77,77,77	0
56	MG	2A	3025	1/1	0.86	0.21	88,88,88,88	0
56	MG	1A	3075	1/1	0.86	0.15	78,78,78,78	0
56	MG	1A	3443	1/1	0.86	0.09	82,82,82,82	0
56	MG	1A	3154	1/1	0.86	0.18	59,59,59,59	0
56	MG	1A	3330	1/1	0.86	0.26	96,96,96,96	0
56	MG	2A	3084	1/1	0.86	0.26	90,90,90,90	0
56	MG	1A	3529	1/1	0.86	0.16	71,71,71,71	0
56	MG	2A	3048	1/1	0.86	0.23	83,83,83,83	0
56	MG	1A	3103	1/1	0.86	0.86	68,68,68,68	0
56	MG	2a	3066	1/1	0.86	0.22	106,106,106,106	0
56	MG	1A	3150	1/1	0.86	0.20	91,91,91,91	0
56	MG	1A	3425	1/1	0.86	0.31	62,62,62,62	0
56	MG	1A	3022	1/1	0.86	0.38	83,83,83,83	0
56	MG	1A	3609	1/1	0.86	0.67	74,74,74,74	0
56	MG	1A	3525	1/1	0.86	0.21	101,101,101,101	0
56	MG	2A	3144	1/1	0.86	0.42	75,75,75,75	0
56	MG	1A	3589	1/1	0.86	0.11	86,86,86,86	0
56	MG	2a	3043	1/1	0.86	0.66	70,70,70,70	0
56	MG	1A	3493	1/1	0.86	0.16	69,69,69,69	0
56	MG	1a	3140	1/1	0.86	0.33	84,84,84,84	0
56	MG	2A	3333	1/1	0.86	0.12	101,101,101,101	0
56	MG	1A	3566	1/1	0.86	0.10	93,93,93,93	0
56	MG	2a	3168	1/1	0.86	0.15	112,112,112,112	0
56	MG	1A	3065	1/1	0.86	0.43	71,71,71,71	0
56	MG	1A	3556	1/1	0.86	0.18	81,81,81,81	0
56	MG	1A	3251	1/1	0.86	0.43	69,69,69,69	0
56	MG	1A	3452	1/1	0.86	0.16	97,97,97,97	0
56	MG	1A	3139	1/1	0.86	0.21	79,79,79,79	0
56	MG	1A	3177	1/1	0.86	0.66	89,89,89,89	0
56	MG	1a	3103	1/1	0.86	0.19	79,79,79,79	0
56	MG	1a	3018	1/1	0.86	0.37	74,74,74,74	0
56	MG	2A	3286	1/1	0.86	0.15	93,93,93,93	0
56	MG	1A	3431	1/1	0.86	0.14	76,76,76,76	0
56	MG	2A	3188	1/1	0.86	0.12	92,92,92,92	0
56	MG	2a	3142	1/1	0.86	0.24	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3011	1/1	0.86	0.38	65,65,65,65	0
56	MG	1A	3100	1/1	0.87	0.60	61,61,61,61	0
56	MG	1A	3186	1/1	0.87	0.15	95,95,95,95	0
56	MG	2a	3064	1/1	0.87	0.14	99,99,99,99	0
56	MG	1a	3170	1/1	0.87	0.13	76,76,76,76	0
56	MG	1a	3120	1/1	0.87	0.57	87,87,87,87	0
56	MG	2A	3157	1/1	0.87	0.84	70,70,70,70	0
56	MG	1A	3023	1/1	0.87	1.07	88,88,88,88	0
56	MG	1A	3545	1/1	0.87	0.17	67,67,67,67	0
56	MG	2A	3140	1/1	0.87	0.45	81,81,81,81	0
56	MG	1a	3042	1/1	0.87	0.11	74,74,74,74	0
56	MG	1A	3167	1/1	0.87	0.20	90,90,90,90	0
56	MG	2a	3117	1/1	0.87	0.11	92,92,92,92	0
56	MG	2a	3024	1/1	0.87	0.10	90,90,90,90	0
56	MG	1A	3048	1/1	0.87	0.51	74,74,74,74	0
56	MG	2A	3038	1/1	0.87	0.39	65,65,65,65	0
56	MG	2A	3115	1/1	0.87	1.18	80,80,80,80	0
56	MG	2a	3183	1/1	0.87	0.07	98,98,98,98	0
56	MG	1A	3637	1/1	0.87	0.13	100,100,100,100	0
56	MG	2a	3042	1/1	0.87	0.19	82,82,82,82	0
56	MG	1A	3541	1/1	0.87	0.15	72,72,72,72	0
56	MG	2A	3106	1/1	0.87	0.25	73,73,73,73	0
56	MG	2A	3254	1/1	0.87	0.15	78,78,78,78	0
56	MG	1a	3071	1/1	0.87	0.84	75,75,75,75	0
56	MG	1A	3437	1/1	0.87	0.31	79,79,79,79	0
56	MG	1a	3139	1/1	0.87	0.41	81,81,81,81	0
56	MG	1a	3020	1/1	0.87	0.15	74,74,74,74	0
56	MG	2a	3176	1/1	0.87	0.14	83,83,83,83	0
56	MG	1A	3032	1/1	0.87	0.14	75,75,75,75	0
56	MG	1a	3184	1/1	0.87	0.27	71,71,71,71	0
56	MG	2A	3334	1/1	0.87	0.46	105,105,105,105	0
56	MG	1A	3613	1/1	0.87	0.15	64,64,64,64	0
56	MG	1A	3118	1/1	0.87	0.11	60,60,60,60	0
56	MG	2a	3055	1/1	0.87	0.23	95,95,95,95	0
56	MG	2a	3069	1/1	0.87	0.19	103,103,103,103	0
56	MG	1A	3183	1/1	0.87	0.42	74,74,74,74	0
56	MG	2A	3327	1/1	0.87	0.52	96,96,96,96	0
56	MG	1A	3288	1/1	0.87	0.12	70,70,70,70	0
56	MG	2a	3129	1/1	0.87	0.14	92,92,92,92	0
56	MG	1A	3600	1/1	0.87	0.10	77,77,77,77	0
56	MG	1a	3035	1/1	0.87	0.23	81,81,81,81	0
56	MG	1A	3358	1/1	0.87	0.19	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3138	1/1	0.87	0.48	82,82,82,82	0
56	MG	1A	3322	1/1	0.87	0.15	92,92,92,92	0
56	MG	1A	3494	1/1	0.88	0.11	75,75,75,75	0
56	MG	1a	3217	1/1	0.88	0.10	85,85,85,85	0
56	MG	2a	3105	1/1	0.88	0.26	95,95,95,95	0
56	MG	2A	3343	1/1	0.88	0.23	99,99,99,99	0
56	MG	1A	3614	1/1	0.88	0.15	89,89,89,89	0
56	MG	1A	3004	1/1	0.88	0.17	56,56,56,56	0
56	MG	1A	3263	1/1	0.88	0.20	78,78,78,78	0
56	MG	1a	3146	1/1	0.88	0.20	79,79,79,79	0
56	MG	1A	3301	1/1	0.88	0.24	85,85,85,85	0
56	MG	1a	3113	1/1	0.88	0.13	86,86,86,86	0
56	MG	2a	3164	1/1	0.88	0.10	114,114,114,114	0
56	MG	1A	3481	1/1	0.88	0.22	83,83,83,83	0
56	MG	1a	3175	1/1	0.88	0.07	87,87,87,87	0
56	MG	2a	3096	1/1	0.88	0.27	84,84,84,84	0
56	MG	2A	3147	1/1	0.88	0.13	84,84,84,84	0
56	MG	1A	3436	1/1	0.88	0.18	68,68,68,68	0
56	MG	1A	3185	1/1	0.88	1.14	80,80,80,80	0
56	MG	1A	3465	1/1	0.88	0.18	80,80,80,80	0
56	MG	2a	3124	1/1	0.88	0.18	83,83,83,83	0
56	MG	1A	3066	1/1	0.88	0.37	78,78,78,78	0
56	MG	1a	3073	1/1	0.88	0.16	78,78,78,78	0
56	MG	1A	3286	1/1	0.88	0.12	96,96,96,96	0
56	MG	1a	3147	1/1	0.88	0.27	71,71,71,71	0
56	MG	1a	3153	1/1	0.88	0.15	84,84,84,84	0
56	MG	1A	3175	1/1	0.88	0.24	75,75,75,75	0
56	MG	1A	3279	1/1	0.88	0.15	82,82,82,82	0
56	MG	2A	3121	1/1	0.88	0.34	79,79,79,79	0
56	MG	2A	3296	1/1	0.88	0.21	102,102,102,102	0
56	MG	1A	3396	1/1	0.88	0.28	99,99,99,99	0
56	MG	1A	3645	1/1	0.88	0.24	82,82,82,82	0
56	MG	2A	3301	1/1	0.88	0.22	83,83,83,83	0
56	MG	1A	3184	1/1	0.88	1.24	73,73,73,73	0
56	MG	1A	3021	1/1	0.88	1.00	55,55,55,55	0
56	MG	1A	3267	1/1	0.88	0.22	76,76,76,76	0
56	MG	1A	3173	1/1	0.88	0.16	74,74,74,74	0
56	MG	1a	3064	1/1	0.88	0.32	87,87,87,87	0
56	MG	1A	3544	1/1	0.88	0.18	71,71,71,71	0
56	MG	2A	3136	1/1	0.88	0.23	71,71,71,71	0
56	MG	1A	3052	1/1	0.88	0.21	77,77,77,77	0
56	MG	1A	3261	1/1	0.88	0.22	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3150	1/1	0.88	0.43	88,88,88,88	0
56	MG	1A	3214	1/1	0.88	0.27	96,96,96,96	0
56	MG	1A	3347	1/1	0.88	0.23	70,70,70,70	0
56	MG	1a	3190	1/1	0.88	1.15	95,95,95,95	0
56	MG	1A	3210	1/1	0.88	0.15	71,71,71,71	0
56	MG	2A	3035	1/1	0.88	0.16	92,92,92,92	0
56	MG	2a	3101	1/1	0.88	0.80	101,101,101,101	0
56	MG	2a	3143	1/1	0.88	0.10	107,107,107,107	0
56	MG	2A	3265	1/1	0.88	0.34	93,93,93,93	0
56	MG	2a	3074	1/1	0.88	0.14	98,98,98,98	0
56	MG	1a	3024	1/1	0.88	0.41	83,83,83,83	0
56	MG	1a	3032	1/1	0.88	0.07	76,76,76,76	0
56	MG	1A	3042	1/1	0.88	0.17	64,64,64,64	0
56	MG	2a	3180	1/1	0.88	0.26	102,102,102,102	0
56	MG	1A	3127	1/1	0.88	0.16	72,72,72,72	0
56	MG	2A	3223	1/1	0.88	0.21	72,72,72,72	0
56	MG	2a	3178	1/1	0.88	0.26	96,96,96,96	0
56	MG	1A	3639	1/1	0.89	0.20	67,67,67,67	0
56	MG	1A	3136	1/1	0.89	0.69	78,78,78,78	0
56	MG	1a	3192	1/1	0.89	0.19	85,85,85,85	0
56	MG	1A	3662	1/1	0.89	0.16	90,90,90,90	0
56	MG	2A	3047	1/1	0.89	0.26	89,89,89,89	0
56	MG	1A	3648	1/1	0.89	0.32	127,127,127,127	0
56	MG	2a	3005	1/1	0.89	0.43	96,96,96,96	0
56	MG	1A	3092	1/1	0.89	0.09	70,70,70,70	0
56	MG	1A	3308	1/1	0.89	0.13	80,80,80,80	0
56	MG	2A	3118	1/1	0.89	0.62	72,72,72,72	0
56	MG	1A	3575	1/1	0.89	0.25	83,83,83,83	0
56	MG	1a	3101	1/1	0.89	0.39	88,88,88,88	0
56	MG	2a	3003	1/1	0.89	0.48	69,69,69,69	0
56	MG	2a	3115	1/1	0.89	0.24	103,103,103,103	0
56	MG	2A	3042	1/1	0.89	0.12	89,89,89,89	0
56	MG	1A	3363	1/1	0.89	0.18	79,79,79,79	0
56	MG	2A	3105	1/1	0.89	0.18	71,71,71,71	0
56	MG	2A	3008	1/1	0.89	0.11	79,79,79,79	0
56	MG	1A	3560	1/1	0.89	0.27	88,88,88,88	0
56	MG	2A	3141	1/1	0.89	0.72	81,81,81,81	0
56	MG	1A	3353	1/1	0.89	0.13	66,66,66,66	0
56	MG	1A	3346	1/1	0.89	0.41	92,92,92,92	0
56	MG	1A	3323	1/1	0.89	0.20	81,81,81,81	0
56	MG	1A	3062	1/1	0.89	0.84	92,92,92,92	0
56	MG	1a	3121	1/1	0.89	0.41	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3039	1/1	0.89	0.32	88,88,88,88	0
56	MG	1A	3515	1/1	0.89	0.30	63,63,63,63	0
56	MG	1a	3048	1/1	0.89	0.20	73,73,73,73	0
56	MG	1A	3306	1/1	0.89	0.28	82,82,82,82	0
56	MG	2a	3175	1/1	0.89	0.20	76,76,76,76	0
56	MG	1A	3078	1/1	0.89	0.91	79,79,79,79	0
56	MG	1A	3407	1/1	0.89	0.14	91,91,91,91	0
56	MG	2a	3079	1/1	0.89	0.37	90,90,90,90	0
56	MG	2A	3079	1/1	0.89	0.25	89,89,89,89	0
56	MG	2a	3163	1/1	0.89	0.19	103,103,103,103	0
56	MG	1A	3416	1/1	0.89	0.34	82,82,82,82	0
56	MG	1a	3124	1/1	0.89	0.22	70,70,70,70	0
56	MG	1A	3169	1/1	0.89	0.25	84,84,84,84	0
56	MG	1A	3164	1/1	0.89	0.14	72,72,72,72	0
56	MG	1A	3503	1/1	0.89	0.27	90,90,90,90	0
56	MG	2A	3282	1/1	0.89	0.12	87,87,87,87	0
56	MG	1A	3588	1/1	0.89	0.23	82,82,82,82	0
56	MG	2a	3170	1/1	0.89	0.13	80,80,80,80	0
56	MG	1A	3676	1/1	0.89	0.15	84,84,84,84	0
56	MG	1a	3158	1/1	0.89	0.15	81,81,81,81	0
56	MG	1A	3434	1/1	0.89	0.10	81,81,81,81	0
56	MG	1A	3112	1/1	0.89	0.29	66,66,66,66	0
56	MG	2A	3126	1/1	0.89	0.21	80,80,80,80	0
56	MG	1a	3045	1/1	0.89	0.12	85,85,85,85	0
56	MG	1a	3236	1/1	0.89	0.15	85,85,85,85	0
56	MG	2A	3293	1/1	0.89	0.13	95,95,95,95	0
56	MG	1A	3165	1/1	0.89	0.41	86,86,86,86	0
56	MG	1a	3050	1/1	0.89	0.11	80,80,80,80	0
56	MG	2a	3014	1/1	0.90	0.30	89,89,89,89	0
56	MG	2A	3077	1/1	0.90	0.42	77,77,77,77	0
56	MG	2a	3029	1/1	0.90	0.20	87,87,87,87	0
56	MG	1a	3209	1/1	0.90	0.33	90,90,90,90	0
56	MG	1a	3065	1/1	0.90	0.19	87,87,87,87	0
56	MG	1A	3327	1/1	0.90	0.18	78,78,78,78	0
56	MG	2A	3040	1/1	0.90	0.14	82,82,82,82	0
56	MG	2A	3130	1/1	0.90	0.24	90,90,90,90	0
56	MG	1A	3577	1/1	0.90	0.12	94,94,94,94	0
56	MG	2a	3040	1/1	0.90	0.14	78,78,78,78	0
56	MG	1a	3215	1/1	0.90	0.15	84,84,84,84	0
56	MG	1A	3472	1/1	0.90	0.14	72,72,72,72	0
56	MG	1A	3547	1/1	0.90	0.18	71,71,71,71	0
56	MG	1A	3374	1/1	0.90	0.20	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3568	1/1	0.90	0.09	79,79,79,79	0
57	ZN	2Y	501	1/1	0.90	0.13	138,138,138,138	0
56	MG	2A	3089	1/1	0.90	0.15	82,82,82,82	0
56	MG	1A	3489	1/1	0.90	0.34	78,78,78,78	0
56	MG	1A	3188	1/1	0.90	0.27	91,91,91,91	0
56	MG	1A	3520	1/1	0.90	0.10	88,88,88,88	0
56	MG	1A	3679	1/1	0.90	0.59	83,83,83,83	0
56	MG	1A	3156	1/1	0.90	0.14	66,66,66,66	0
56	MG	1A	3049	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3324	1/1	0.90	0.36	67,67,67,67	0
56	MG	1A	3044	1/1	0.90	0.16	89,89,89,89	0
56	MG	1a	3009	1/1	0.90	0.36	91,91,91,91	0
56	MG	1A	3250	1/1	0.90	0.30	94,94,94,94	0
56	MG	1A	3009	1/1	0.90	0.28	75,75,75,75	0
56	MG	1A	3468	1/1	0.90	0.73	83,83,83,83	0
56	MG	1A	3531	1/1	0.90	0.20	92,92,92,92	0
56	MG	2A	3173	1/1	0.90	0.11	70,70,70,70	0
56	MG	2a	3139	1/1	0.90	0.15	81,81,81,81	0
56	MG	1a	3066	1/1	0.90	0.11	101,101,101,101	0
56	MG	1A	3218	1/1	0.90	0.21	96,96,96,96	0
56	MG	1a	3012	1/1	0.90	0.49	93,93,93,93	0
56	MG	2a	3151	1/1	0.90	0.20	111,111,111,111	0
56	MG	2A	3330	1/1	0.90	0.16	101,101,101,101	0
56	MG	2A	3213	1/1	0.90	0.14	90,90,90,90	0
56	MG	1a	3109	1/1	0.90	0.61	103,103,103,103	0
56	MG	1a	3093	1/1	0.90	0.39	88,88,88,88	0
56	MG	1A	3439	1/1	0.90	0.30	84,84,84,84	0
56	MG	2A	3004	1/1	0.90	0.16	91,91,91,91	0
56	MG	1A	3067	1/1	0.90	0.08	65,65,65,65	0
56	MG	2a	3157	1/1	0.90	0.29	114,114,114,114	0
56	MG	2A	3273	1/1	0.90	0.20	86,86,86,86	0
56	MG	1A	3405	1/1	0.90	0.18	78,78,78,78	0
56	MG	2A	3256	1/1	0.90	0.08	98,98,98,98	0
56	MG	1a	3014	1/1	0.90	0.10	78,78,78,78	0
56	MG	2A	3076	1/1	0.90	0.47	77,77,77,77	0
56	MG	2a	3011	1/1	0.90	0.10	101,101,101,101	0
56	MG	1A	3584	1/1	0.90	0.16	92,92,92,92	0
56	MG	1a	3118	1/1	0.90	0.75	101,101,101,101	0
56	MG	1A	3094	1/1	0.90	0.10	63,63,63,63	0
56	MG	1A	3665	1/1	0.90	0.21	74,74,74,74	0
56	MG	2a	3155	1/1	0.90	0.11	84,84,84,84	0
56	MG	2A	3139	1/1	0.90	0.25	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3096	1/1	0.90	0.09	90,90,90,90	0
56	MG	2A	3159	1/1	0.90	0.14	91,91,91,91	0
56	MG	1A	3231	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3070	1/1	0.90	0.23	52,52,52,52	0
56	MG	1a	3046	1/1	0.90	0.24	73,73,73,73	0
56	MG	1A	3270	1/1	0.90	0.41	75,75,75,75	0
56	MG	1A	3607	1/1	0.90	0.12	58,58,58,58	0
56	MG	2a	3072	1/1	0.90	0.12	107,107,107,107	0
56	MG	2A	3086	1/1	0.91	0.92	78,78,78,78	0
56	MG	1A	3024	1/1	0.91	0.82	83,83,83,83	0
56	MG	1A	3300	1/1	0.91	0.19	77,77,77,77	0
56	MG	1A	3140	1/1	0.91	0.20	89,89,89,89	0
56	MG	1a	3154	1/1	0.91	0.32	78,78,78,78	0
56	MG	1a	3226	1/1	0.91	0.27	89,89,89,89	0
56	MG	1A	3006	1/1	0.91	0.45	69,69,69,69	0
56	MG	1A	3095	1/1	0.91	0.17	81,81,81,81	0
56	MG	1a	3095	1/1	0.91	0.26	62,62,62,62	0
56	MG	1A	3050	1/1	0.91	0.16	76,76,76,76	0
56	MG	2A	3124	1/1	0.91	0.20	86,86,86,86	0
56	MG	2a	3126	1/1	0.91	0.31	86,86,86,86	0
56	MG	2A	3246	1/1	0.91	0.88	105,105,105,105	0
56	MG	1A	3232	1/1	0.91	0.24	52,52,52,52	0
56	MG	2a	3001	1/1	0.91	0.12	74,74,74,74	0
56	MG	1A	3333	1/1	0.91	0.30	73,73,73,73	0
56	MG	1A	3285	1/1	0.91	0.26	56,56,56,56	0
56	MG	1A	3328	1/1	0.91	0.34	94,94,94,94	0
56	MG	1a	3185	1/1	0.91	0.11	90,90,90,90	0
56	MG	1a	3021	1/1	0.91	0.24	102,102,102,102	0
56	MG	1A	3652	1/1	0.91	0.13	86,86,86,86	0
56	MG	1A	3010	1/1	0.91	0.64	65,65,65,65	0
56	MG	1a	3216	1/1	0.91	0.14	81,81,81,81	0
56	MG	2A	3268	1/1	0.91	0.06	82,82,82,82	0
56	MG	1A	3553	1/1	0.91	0.22	89,89,89,89	0
56	MG	2A	3168	1/1	0.91	0.30	98,98,98,98	0
56	MG	1A	3380	1/1	0.91	0.14	67,67,67,67	0
56	MG	1A	3256	1/1	0.91	0.42	84,84,84,84	0
56	MG	1A	3119	1/1	0.91	0.23	107,107,107,107	0
56	MG	2A	3314	1/1	0.91	0.13	94,94,94,94	0
56	MG	1A	3294	1/1	0.91	0.38	87,87,87,87	0
56	MG	2a	3091	1/1	0.91	0.24	92,92,92,92	0
56	MG	2A	3284	1/1	0.91	0.09	79,79,79,79	0
56	MG	1a	3061	1/1	0.91	0.35	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3033	1/1	0.91	0.31	86,86,86,86	0
56	MG	1A	3335	1/1	0.91	0.14	66,66,66,66	0
56	MG	1A	3426	1/1	0.91	0.25	72,72,72,72	0
56	MG	2A	3321	1/1	0.91	0.10	101,101,101,101	0
56	MG	1A	3478	1/1	0.91	0.30	83,83,83,83	0
56	MG	2A	3149	1/1	0.91	0.27	84,84,84,84	0
56	MG	2a	3145	1/1	0.91	0.20	90,90,90,90	0
56	MG	1A	3178	1/1	0.91	0.43	82,82,82,82	0
56	MG	2A	3320	1/1	0.91	0.10	79,79,79,79	0
56	MG	2A	3036	1/1	0.91	0.94	87,87,87,87	0
56	MG	1A	3035	1/1	0.91	0.15	70,70,70,70	0
56	MG	2A	3169	1/1	0.91	0.26	79,79,79,79	0
56	MG	1a	3232	1/1	0.91	0.19	76,76,76,76	0
56	MG	1A	3357	1/1	0.91	0.32	76,76,76,76	0
56	MG	1A	3361	1/1	0.91	0.27	71,71,71,71	0
56	MG	2a	3095	1/1	0.91	0.27	75,75,75,75	0
56	MG	1A	3388	1/1	0.91	0.34	69,69,69,69	0
56	MG	1A	3141	1/1	0.91	0.21	70,70,70,70	0
56	MG	1A	3243	1/1	0.91	0.12	81,81,81,81	0
56	MG	1A	3504	1/1	0.91	0.19	77,77,77,77	0
56	MG	2A	3091	1/1	0.91	0.28	74,74,74,74	0
56	MG	1A	3460	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3559	1/1	0.91	0.10	115,115,115,115	0
56	MG	2a	3127	1/1	0.91	0.10	100,100,100,100	0
56	MG	2A	3170	1/1	0.91	0.20	95,95,95,95	0
56	MG	2A	3054	1/1	0.91	0.17	89,89,89,89	0
56	MG	2A	3257	1/1	0.91	0.26	76,76,76,76	0
56	MG	1A	3616	1/1	0.91	0.27	84,84,84,84	0
56	MG	1a	3025	1/1	0.91	0.09	85,85,85,85	0
56	MG	1a	3112	1/1	0.91	0.25	70,70,70,70	0
56	MG	1A	3454	1/1	0.91	0.20	66,66,66,66	0
56	MG	2A	3348	1/1	0.91	0.25	79,79,79,79	0
56	MG	1A	3350	1/1	0.91	0.13	76,76,76,76	0
56	MG	2A	3009	1/1	0.91	0.90	89,89,89,89	0
56	MG	2A	3210	1/1	0.91	0.12	75,75,75,75	0
56	MG	1A	3201	1/1	0.91	0.29	68,68,68,68	0
56	MG	1A	3470	1/1	0.91	0.31	100,100,100,100	0
56	MG	1A	3427	1/1	0.91	0.20	78,78,78,78	0
56	MG	1a	3098	1/1	0.91	0.35	87,87,87,87	0
56	MG	1A	3060	1/1	0.91	0.17	75,75,75,75	0
56	MG	2a	3023	1/1	0.91	0.47	80,80,80,80	0
56	MG	2A	3303	1/1	0.91	0.65	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3202	1/1	0.91	0.22	89,89,89,89	0
56	MG	1A	3310	1/1	0.91	0.14	76,76,76,76	0
56	MG	1a	3015	1/1	0.91	0.39	90,90,90,90	0
56	MG	1a	3031	1/1	0.91	0.49	103,103,103,103	0
56	MG	1a	3186	1/1	0.91	0.19	85,85,85,85	0
56	MG	2a	3071	1/1	0.91	0.41	88,88,88,88	0
56	MG	1A	3290	1/1	0.92	0.35	90,90,90,90	0
56	MG	2A	3187	1/1	0.92	0.14	81,81,81,81	0
56	MG	1a	3079	1/1	0.92	0.19	73,73,73,73	0
56	MG	2A	3164	1/1	0.92	0.16	82,82,82,82	0
56	MG	2a	3123	1/1	0.92	0.16	79,79,79,79	0
56	MG	1A	3275	1/1	0.92	0.19	61,61,61,61	0
56	MG	1A	3551	1/1	0.92	0.24	97,97,97,97	0
56	MG	1A	3126	1/1	0.92	0.64	76,76,76,76	0
56	MG	2a	3086	1/1	0.92	0.14	87,87,87,87	0
56	MG	2a	3152	1/1	0.92	0.19	111,111,111,111	0
56	MG	1A	3642	1/1	0.92	0.29	74,74,74,74	0
56	MG	1A	3491	1/1	0.92	0.23	84,84,84,84	0
56	MG	1A	3313	1/1	0.92	0.29	72,72,72,72	0
56	MG	1A	3340	1/1	0.92	0.32	78,78,78,78	0
56	MG	1A	3171	1/1	0.92	0.14	77,77,77,77	0
56	MG	1A	3449	1/1	0.92	0.27	76,76,76,76	0
56	MG	2A	3242	1/1	0.92	0.18	70,70,70,70	0
56	MG	2A	3180	1/1	0.92	0.15	74,74,74,74	0
56	MG	2A	3231	1/1	0.92	0.17	74,74,74,74	0
56	MG	1a	3059	1/1	0.92	0.68	82,82,82,82	0
56	MG	1a	3091	1/1	0.92	0.57	83,83,83,83	0
56	MG	1A	3563	1/1	0.92	0.17	97,97,97,97	0
56	MG	2A	3020	1/1	0.92	0.29	69,69,69,69	0
56	MG	1A	3204	1/1	0.92	0.19	60,60,60,60	0
56	MG	1A	3211	1/1	0.92	0.30	88,88,88,88	0
56	MG	2a	3046	1/1	0.92	0.10	85,85,85,85	0
56	MG	1A	3110	1/1	0.92	0.67	82,82,82,82	0
56	MG	1A	3207	1/1	0.92	0.11	74,74,74,74	0
56	MG	1A	3618	1/1	0.92	0.19	98,98,98,98	0
56	MG	1a	3178	1/1	0.92	0.32	81,81,81,81	0
56	MG	1A	3409	1/1	0.92	0.33	70,70,70,70	0
56	MG	1a	3229	1/1	0.92	0.24	85,85,85,85	0
56	MG	2A	3044	1/1	0.92	0.22	78,78,78,78	0
56	MG	1a	3207	1/1	0.92	0.20	96,96,96,96	0
56	MG	1A	3055	1/1	0.92	0.22	79,79,79,79	0
56	MG	2A	3211	1/1	0.92	0.29	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3033	1/1	0.92	0.13	86,86,86,86	0
56	MG	1A	3672	1/1	0.92	0.28	68,68,68,68	0
56	MG	1a	3034	1/1	0.92	0.12	73,73,73,73	0
56	MG	1A	3495	1/1	0.92	0.23	66,66,66,66	0
56	MG	1A	3581	1/1	0.92	0.13	84,84,84,84	0
56	MG	2A	3116	1/1	0.92	0.35	91,91,91,91	0
56	MG	2A	3068	1/1	0.92	0.18	106,106,106,106	0
56	MG	1A	3411	1/1	0.92	0.17	66,66,66,66	0
56	MG	2a	3156	1/1	0.92	0.08	104,104,104,104	0
56	MG	1A	3461	1/1	0.92	0.15	59,59,59,59	0
56	MG	1A	3582	1/1	0.92	0.20	73,73,73,73	0
56	MG	2A	3182	1/1	0.92	0.23	81,81,81,81	0
56	MG	1A	3356	1/1	0.92	0.67	61,61,61,61	0
56	MG	1A	3274	1/1	0.92	0.24	78,78,78,78	0
56	MG	2A	3335	1/1	0.92	0.09	100,100,100,100	0
56	MG	1A	3550	1/1	0.92	0.31	101,101,101,101	0
56	MG	2A	3252	1/1	0.92	0.13	73,73,73,73	0
56	MG	1A	3599	1/1	0.92	0.30	100,100,100,100	0
56	MG	2A	3007	1/1	0.92	0.14	80,80,80,80	0
56	MG	2A	3229	1/1	0.92	0.18	90,90,90,90	0
56	MG	2a	3073	1/1	0.92	0.19	113,113,113,113	0
56	MG	1A	3488	1/1	0.92	0.16	80,80,80,80	0
56	MG	1a	3010	1/1	0.92	0.26	85,85,85,85	0
56	MG	1A	3466	1/1	0.92	0.16	92,92,92,92	0
56	MG	1A	3596	1/1	0.92	0.16	81,81,81,81	0
56	MG	1A	3329	1/1	0.92	0.20	77,77,77,77	0
56	MG	2A	3135	1/1	0.92	0.25	78,78,78,78	0
56	MG	1A	3389	1/1	0.92	0.49	75,75,75,75	0
56	MG	2A	3145	1/1	0.92	0.11	77,77,77,77	0
56	MG	2A	3043	1/1	0.92	0.21	82,82,82,82	0
56	MG	1A	3500	1/1	0.92	0.17	86,86,86,86	0
56	MG	1A	3283	1/1	0.92	0.25	58,58,58,58	0
56	MG	2A	3238	1/1	0.92	0.17	93,93,93,93	0
56	MG	2a	3039	1/1	0.92	0.13	89,89,89,89	0
56	MG	1a	3197	1/1	0.92	0.12	102,102,102,102	0
56	MG	1a	3022	1/1	0.92	0.21	89,89,89,89	0
56	MG	2A	3066	1/1	0.92	0.13	92,92,92,92	0
56	MG	2a	3113	1/1	0.92	0.08	111,111,111,111	0
56	MG	1a	3123	1/1	0.92	0.16	72,72,72,72	0
56	MG	1A	3187	1/1	0.92	0.14	75,75,75,75	0
56	MG	1A	3325	1/1	0.92	0.19	69,69,69,69	0
56	MG	2A	3050	1/1	0.92	0.36	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3081	1/1	0.92	0.10	79,79,79,79	0
56	MG	1a	3026	1/1	0.92	0.22	80,80,80,80	0
56	MG	1A	3124	1/1	0.92	0.79	86,86,86,86	0
56	MG	2A	3326	1/1	0.92	0.16	91,91,91,91	0
56	MG	1A	3384	1/1	0.92	0.46	75,75,75,75	0
56	MG	2A	3312	1/1	0.92	0.10	74,74,74,74	0
56	MG	2a	3119	1/1	0.92	0.12	107,107,107,107	0
56	MG	2a	3026	1/1	0.92	0.15	90,90,90,90	0
56	MG	1A	3115	1/1	0.92	0.23	87,87,87,87	0
56	MG	1A	3638	1/1	0.92	0.13	80,80,80,80	0
56	MG	1a	3084	1/1	0.92	0.20	94,94,94,94	0
56	MG	1A	3143	1/1	0.92	0.32	84,84,84,84	0
56	MG	2A	3305	1/1	0.92	0.11	85,85,85,85	0
56	MG	2a	3075	1/1	0.92	0.30	98,98,98,98	0
56	MG	1A	3365	1/1	0.92	0.31	75,75,75,75	0
56	MG	2A	3046	1/1	0.92	0.13	68,68,68,68	0
56	MG	1a	3160	1/1	0.93	0.23	76,76,76,76	0
56	MG	1A	3038	1/1	0.93	0.16	74,74,74,74	0
56	MG	1a	3003	1/1	0.93	0.11	92,92,92,92	0
56	MG	1A	3233	1/1	0.93	0.09	58,58,58,58	0
56	MG	2a	3104	1/1	0.93	0.11	100,100,100,100	0
56	MG	2A	3202	1/1	0.93	0.32	88,88,88,88	0
56	MG	1A	3542	1/1	0.93	0.42	77,77,77,77	0
56	MG	1A	3158	1/1	0.93	0.19	67,67,67,67	0
56	MG	1A	3334	1/1	0.93	0.18	64,64,64,64	0
56	MG	1A	3223	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3271	1/1	0.93	0.18	83,83,83,83	0
56	MG	1A	3469	1/1	0.93	0.37	84,84,84,84	0
56	MG	1A	3235	1/1	0.93	0.13	73,73,73,73	0
56	MG	1a	3125	1/1	0.93	0.21	106,106,106,106	0
56	MG	1A	3047	1/1	0.93	0.99	68,68,68,68	0
56	MG	1a	3198	1/1	0.93	0.28	89,89,89,89	0
56	MG	2a	3025	1/1	0.93	0.08	86,86,86,86	0
56	MG	2A	3107	1/1	0.93	0.27	92,92,92,92	0
56	MG	1A	3640	1/1	0.93	0.26	81,81,81,81	0
56	MG	1A	3025	1/1	0.93	0.29	87,87,87,87	0
56	MG	1A	3537	1/1	0.93	1.62	113,113,113,113	0
56	MG	2A	3311	1/1	0.93	0.22	106,106,106,106	0
56	MG	1A	3438	1/1	0.93	0.10	71,71,71,71	0
56	MG	2A	3137	1/1	0.93	0.28	91,91,91,91	0
56	MG	2A	3177	1/1	0.93	0.22	74,74,74,74	0
56	MG	2A	3341	1/1	0.93	0.15	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3476	1/1	0.93	0.11	89,89,89,89	0
56	MG	1A	3029	1/1	0.93	0.21	65,65,65,65	0
56	MG	2A	3309	1/1	0.93	0.12	85,85,85,85	0
56	MG	1A	3355	1/1	0.93	0.23	68,68,68,68	0
56	MG	1A	3081	1/1	0.93	0.17	60,60,60,60	0
56	MG	1A	3273	1/1	0.93	0.23	62,62,62,62	0
56	MG	2a	3114	1/1	0.93	0.34	92,92,92,92	0
56	MG	2A	3001	1/1	0.93	0.14	75,75,75,75	0
56	MG	1a	3159	1/1	0.93	0.28	72,72,72,72	0
56	MG	1A	3530	1/1	0.93	0.79	79,79,79,79	0
56	MG	1a	3132	1/1	0.93	0.12	101,101,101,101	0
56	MG	2A	3280	1/1	0.93	0.83	94,94,94,94	0
56	MG	1A	3523	1/1	0.93	0.11	96,96,96,96	0
56	MG	2A	3230	1/1	0.93	0.35	82,82,82,82	0
56	MG	1A	3413	1/1	0.93	0.24	71,71,71,71	0
56	MG	2A	3322	1/1	0.93	0.15	86,86,86,86	0
56	MG	2A	3133	1/1	0.93	0.19	65,65,65,65	0
56	MG	2A	3037	1/1	0.93	0.26	75,75,75,75	0
56	MG	2A	3260	1/1	0.93	0.24	87,87,87,87	0
56	MG	2a	3084	1/1	0.93	0.14	78,78,78,78	0
56	MG	1A	3289	1/1	0.93	0.71	92,92,92,92	0
56	MG	1A	3331	1/1	0.93	0.12	75,75,75,75	0
56	MG	2a	3173	1/1	0.93	0.35	115,115,115,115	0
56	MG	1A	3512	1/1	0.93	0.29	82,82,82,82	0
56	MG	1a	3151	1/1	0.93	0.21	80,80,80,80	0
56	MG	1a	3206	1/1	0.93	0.10	89,89,89,89	0
56	MG	2A	3075	1/1	0.93	0.34	83,83,83,83	0
56	MG	1A	3255	1/1	0.93	0.26	59,59,59,59	0
56	MG	1A	3278	1/1	0.93	0.28	59,59,59,59	0
56	MG	1A	3414	1/1	0.93	0.36	82,82,82,82	0
56	MG	2A	3308	1/1	0.93	0.13	103,103,103,103	0
56	MG	1A	3074	1/1	0.93	0.14	81,81,81,81	0
56	MG	1A	3670	1/1	0.93	0.13	76,76,76,76	0
56	MG	1A	3221	1/1	0.93	0.31	79,79,79,79	0
56	MG	1A	3120	1/1	0.93	0.23	111,111,111,111	0
56	MG	1A	3202	1/1	0.93	0.28	73,73,73,73	0
56	MG	1A	3189	1/1	0.93	0.49	78,78,78,78	0
56	MG	1A	3592	1/1	0.93	0.25	84,84,84,84	0
56	MG	1A	3624	1/1	0.93	0.29	64,64,64,64	0
56	MG	1A	3229	1/1	0.93	0.21	74,74,74,74	0
56	MG	1a	3102	1/1	0.93	0.13	72,72,72,72	0
56	MG	1A	3312	1/1	0.93	0.30	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	3204	1/1	0.93	0.17	80,80,80,80	0
56	MG	2A	3219	1/1	0.93	0.13	80,80,80,80	0
56	MG	2a	3020	1/1	0.93	0.08	98,98,98,98	0
56	MG	2a	3008	1/1	0.93	0.10	85,85,85,85	0
56	MG	2a	3027	1/1	0.93	0.12	83,83,83,83	0
56	MG	1a	3141	1/1	0.93	0.20	59,59,59,59	0
56	MG	2A	3285	1/1	0.93	0.11	82,82,82,82	0
56	MG	1A	3166	1/1	0.93	0.33	77,77,77,77	0
56	MG	2A	3129	1/1	0.93	0.32	73,73,73,73	0
56	MG	1A	3241	1/1	0.93	0.32	68,68,68,68	0
56	MG	1a	3041	1/1	0.93	0.14	81,81,81,81	0
56	MG	2A	3208	1/1	0.93	0.12	71,71,71,71	0
56	MG	2a	3148	1/1	0.93	0.13	92,92,92,92	0
56	MG	1a	3196	1/1	0.93	0.15	85,85,85,85	0
56	MG	1a	3235	1/1	0.93	0.32	93,93,93,93	0
56	MG	1A	3496	1/1	0.93	0.24	72,72,72,72	0
56	MG	1A	3132	1/1	0.93	0.22	82,82,82,82	0
56	MG	2a	3137	1/1	0.94	0.09	81,81,81,81	0
56	MG	1A	3623	1/1	0.94	0.15	87,87,87,87	0
56	MG	1A	3305	1/1	0.94	0.20	65,65,65,65	0
56	MG	2A	3056	1/1	0.94	0.67	73,73,73,73	0
56	MG	1A	3264	1/1	0.94	0.43	67,67,67,67	0
56	MG	1A	3227	1/1	0.94	0.18	72,72,72,72	0
56	MG	1A	3603	1/1	0.94	0.21	67,67,67,67	0
56	MG	1a	3078	1/1	0.94	0.18	65,65,65,65	0
56	MG	1A	3134	1/1	0.94	0.30	63,63,63,63	0
56	MG	2a	3056	1/1	0.94	0.11	97,97,97,97	0
56	MG	2A	3251	1/1	0.94	0.13	73,73,73,73	0
56	MG	1A	3663	1/1	0.94	0.23	89,89,89,89	0
56	MG	1A	3668	1/1	0.94	0.11	82,82,82,82	0
56	MG	2a	3128	1/1	0.94	0.17	74,74,74,74	0
56	MG	1A	3224	1/1	0.94	0.22	65,65,65,65	0
56	MG	2A	3218	1/1	0.94	0.23	83,83,83,83	0
56	MG	2a	3136	1/1	0.94	0.27	85,85,85,85	0
56	MG	2A	3128	1/1	0.94	0.16	54,54,54,54	0
56	MG	2A	3045	1/1	0.94	0.21	76,76,76,76	0
56	MG	2a	3081	1/1	0.94	0.10	61,61,61,61	0
56	MG	2a	3153	1/1	0.94	0.13	106,106,106,106	0
56	MG	1A	3605	1/1	0.94	0.20	93,93,93,93	0
56	MG	2a	3013	1/1	0.94	0.28	85,85,85,85	0
56	MG	2A	3082	1/1	0.94	0.05	85,85,85,85	0
56	MG	1A	3650	1/1	0.94	1.24	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3112	1/1	0.94	0.14	87,87,87,87	0
56	MG	1a	3006	1/1	0.94	0.21	90,90,90,90	0
56	MG	1A	3116	1/1	0.94	0.41	113,113,113,113	0
56	MG	2a	3132	1/1	0.94	0.20	83,83,83,83	0
56	MG	1A	3595	1/1	0.94	0.32	69,69,69,69	0
56	MG	1A	3039	1/1	0.94	0.12	70,70,70,70	0
56	MG	1A	3370	1/1	0.94	0.17	82,82,82,82	0
56	MG	1a	3234	1/1	0.94	0.18	85,85,85,85	0
56	MG	2A	3212	1/1	0.94	0.52	83,83,83,83	0
56	MG	1a	3218	1/1	0.94	0.21	80,80,80,80	0
56	MG	1A	3366	1/1	0.94	0.14	72,72,72,72	0
56	MG	2A	3108	1/1	0.94	0.25	72,72,72,72	0
56	MG	2a	3174	1/1	0.94	0.12	101,101,101,101	0
56	MG	1A	3017	1/1	0.94	0.27	64,64,64,64	0
56	MG	1A	3574	1/1	0.94	0.23	77,77,77,77	0
56	MG	2A	3109	1/1	0.94	0.14	93,93,93,93	0
56	MG	1a	3193	1/1	0.94	0.24	88,88,88,88	0
56	MG	1A	3473	1/1	0.94	0.12	86,86,86,86	0
56	MG	1A	3422	1/1	0.94	0.32	67,67,67,67	0
56	MG	2a	3067	1/1	0.94	0.09	112,112,112,112	0
56	MG	2A	3185	1/1	0.94	0.32	76,76,76,76	0
56	MG	1A	3209	1/1	0.94	0.19	56,56,56,56	0
56	MG	2a	3182	1/1	0.94	0.17	106,106,106,106	0
56	MG	2A	3226	1/1	0.94	0.11	73,73,73,73	0
56	MG	1A	3578	1/1	0.94	0.12	86,86,86,86	0
56	MG	1A	3254	1/1	0.94	0.14	78,78,78,78	0
56	MG	1A	3659	1/1	0.94	0.18	80,80,80,80	0
56	MG	1A	3412	1/1	0.94	0.45	79,79,79,79	0
56	MG	1A	3088	1/1	0.94	0.18	71,71,71,71	0
56	MG	2A	3261	1/1	0.94	0.40	98,98,98,98	0
56	MG	2A	3095	1/1	0.94	0.43	89,89,89,89	0
56	MG	1a	3017	1/1	0.94	0.12	81,81,81,81	0
56	MG	1A	3316	1/1	0.94	0.29	83,83,83,83	0
56	MG	2A	3171	1/1	0.94	0.19	86,86,86,86	0
56	MG	1A	3351	1/1	0.94	0.24	58,58,58,58	0
56	MG	1A	3220	1/1	0.94	0.18	71,71,71,71	0
56	MG	2A	3103	1/1	0.94	0.24	83,83,83,83	0
56	MG	1A	3332	1/1	0.94	0.24	77,77,77,77	0
56	MG	1A	3558	1/1	0.94	0.14	97,97,97,97	0
56	MG	2A	3346	1/1	0.94	0.27	78,78,78,78	0
56	MG	1A	3383	1/1	0.94	0.24	69,69,69,69	0
56	MG	1A	3576	1/1	0.94	0.14	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3012	1/1	0.94	0.30	92,92,92,92	0
56	MG	2A	3304	1/1	0.94	0.46	92,92,92,92	0
56	MG	2a	3083	1/1	0.94	0.52	76,76,76,76	0
56	MG	1A	3387	1/1	0.94	0.17	80,80,80,80	0
56	MG	1a	3055	1/1	0.94	0.18	83,83,83,83	0
56	MG	2A	3220	1/1	0.94	0.33	74,74,74,74	0
56	MG	1A	3077	1/1	0.94	0.30	93,93,93,93	0
56	MG	2a	3110	1/1	0.94	0.13	80,80,80,80	0
56	MG	2a	3109	1/1	0.94	0.11	82,82,82,82	0
56	MG	1A	3130	1/1	0.94	0.36	81,81,81,81	0
56	MG	1A	3561	1/1	0.94	0.17	64,64,64,64	0
56	MG	2A	3174	1/1	0.94	0.13	79,79,79,79	0
56	MG	1a	3137	1/1	0.94	0.10	79,79,79,79	0
56	MG	1a	3155	1/1	0.94	0.08	74,74,74,74	0
56	MG	1a	3199	1/1	0.94	0.31	93,93,93,93	0
56	MG	2A	3235	1/1	0.94	0.19	69,69,69,69	0
56	MG	1A	3266	1/1	0.94	0.30	65,65,65,65	0
56	MG	1A	3337	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3644	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3586	1/1	0.94	0.32	71,71,71,71	0
56	MG	1A	3080	1/1	0.94	0.19	66,66,66,66	0
56	MG	1A	3649	1/1	0.94	0.05	86,86,86,86	0
56	MG	2A	3233	1/1	0.94	0.25	71,71,71,71	0
56	MG	1A	3666	1/1	0.94	0.17	92,92,92,92	0
56	MG	2A	3113	1/1	0.94	0.20	73,73,73,73	0
56	MG	1A	3381	1/1	0.94	0.27	68,68,68,68	0
56	MG	1A	3051	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3564	1/1	0.94	0.10	97,97,97,97	0
56	MG	2a	3131	1/1	0.94	0.13	84,84,84,84	0
56	MG	2A	3214	1/1	0.94	0.49	92,92,92,92	0
56	MG	1A	3152	1/1	0.94	0.67	84,84,84,84	0
56	MG	2a	3032	1/1	0.94	0.17	79,79,79,79	0
56	MG	1A	3677	1/1	0.94	0.23	55,55,55,55	0
56	MG	1A	3245	1/1	0.94	0.31	56,56,56,56	0
56	MG	2A	3088	1/1	0.94	0.17	77,77,77,77	0
56	MG	1A	3321	1/1	0.94	0.21	62,62,62,62	0
56	MG	2A	3289	1/1	0.94	0.07	102,102,102,102	0
56	MG	1A	3418	1/1	0.94	0.35	75,75,75,75	0
56	MG	1A	3593	1/1	0.94	0.17	65,65,65,65	0
56	MG	2A	3032	1/1	0.94	0.25	78,78,78,78	0
56	MG	1A	3326	1/1	0.94	0.20	83,83,83,83	0
56	MG	2a	3018	1/1	0.94	0.13	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3610	1/1	0.94	0.21	79,79,79,79	0
56	MG	1a	3056	1/1	0.94	0.11	83,83,83,83	0
56	MG	1A	3079	1/1	0.94	0.12	96,96,96,96	0
56	MG	2A	3228	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3272	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3206	1/1	0.94	0.07	76,76,76,76	0
56	MG	2a	3111	1/1	0.94	0.13	86,86,86,86	0
56	MG	1A	3656	1/1	0.94	0.20	70,70,70,70	0
56	MG	2A	3342	1/1	0.94	0.26	78,78,78,78	0
56	MG	1A	3404	1/1	0.95	0.16	62,62,62,62	0
56	MG	1a	3104	1/1	0.95	0.15	74,74,74,74	0
56	MG	1A	3669	1/1	0.95	0.19	79,79,79,79	0
56	MG	1A	3484	1/1	0.95	0.25	80,80,80,80	0
56	MG	1A	3342	1/1	0.95	0.20	64,64,64,64	0
56	MG	2A	3255	1/1	0.95	0.60	91,91,91,91	0
56	MG	1A	3230	1/1	0.95	0.20	72,72,72,72	0
56	MG	2A	3010	1/1	0.95	0.14	85,85,85,85	0
56	MG	1A	3386	1/1	0.95	0.49	68,68,68,68	0
56	MG	1A	3360	1/1	0.95	0.14	68,68,68,68	0
56	MG	2a	3019	1/1	0.95	0.13	95,95,95,95	0
56	MG	1A	3528	1/1	0.95	0.28	78,78,78,78	0
56	MG	1A	3675	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3382	1/1	0.95	0.23	60,60,60,60	0
56	MG	2A	3338	1/1	0.95	0.64	97,97,97,97	0
56	MG	1A	3182	1/1	0.95	0.69	72,72,72,72	0
56	MG	2A	3274	1/1	0.95	0.23	92,92,92,92	0
56	MG	1A	3083	1/1	0.95	0.21	71,71,71,71	0
56	MG	1A	3540	1/1	0.95	0.10	94,94,94,94	0
56	MG	1a	3181	1/1	0.95	0.28	66,66,66,66	0
56	MG	2A	3125	1/1	0.95	0.28	88,88,88,88	0
56	MG	2A	3281	1/1	0.95	0.10	88,88,88,88	0
56	MG	1a	3157	1/1	0.95	0.45	89,89,89,89	0
56	MG	1A	3054	1/1	0.95	0.24	86,86,86,86	0
56	MG	2A	3049	1/1	0.95	0.15	81,81,81,81	0
56	MG	1A	3522	1/1	0.95	0.10	69,69,69,69	0
56	MG	1A	3664	1/1	0.95	0.21	82,82,82,82	0
56	MG	2a	3147	1/1	0.95	0.36	89,89,89,89	0
56	MG	1a	3145	1/1	0.95	0.48	97,97,97,97	0
56	MG	1A	3373	1/1	0.95	0.35	54,54,54,54	0
56	MG	1a	3040	1/1	0.95	0.08	89,89,89,89	0
56	MG	2A	3016	1/1	0.95	0.14	82,82,82,82	0
56	MG	1A	3501	1/1	0.95	0.28	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3134	1/1	0.95	0.19	100,100,100,100	0
56	MG	1A	3402	1/1	0.95	0.21	51,51,51,51	0
56	MG	1A	3236	1/1	0.95	0.29	60,60,60,60	0
56	MG	1a	3081	1/1	0.95	0.16	81,81,81,81	0
56	MG	1a	3164	1/1	0.95	0.73	81,81,81,81	0
56	MG	1a	3172	1/1	0.95	0.14	90,90,90,90	0
56	MG	2a	3135	1/1	0.95	0.14	108,108,108,108	0
56	MG	2a	3122	1/1	0.95	0.09	114,114,114,114	0
56	MG	1A	3446	1/1	0.95	0.16	65,65,65,65	0
56	MG	2A	3262	1/1	0.95	0.66	84,84,84,84	0
56	MG	1A	3076	1/1	0.95	0.60	54,54,54,54	0
56	MG	1A	3403	1/1	0.95	0.36	59,59,59,59	0
56	MG	1A	3458	1/1	0.95	0.14	82,82,82,82	0
56	MG	1A	3626	1/1	0.95	0.16	86,86,86,86	0
56	MG	1A	3393	1/1	0.95	0.18	82,82,82,82	0
56	MG	1A	3487	1/1	0.95	0.11	81,81,81,81	0
56	MG	2a	3057	1/1	0.95	0.13	74,74,74,74	0
56	MG	1A	3432	1/1	0.95	0.32	57,57,57,57	0
56	MG	1A	3570	1/1	0.95	0.32	99,99,99,99	0
56	MG	1a	3195	1/1	0.95	0.22	80,80,80,80	0
56	MG	1A	3031	1/1	0.95	0.10	62,62,62,62	0
56	MG	2A	3349	1/1	0.95	0.26	81,81,81,81	0
56	MG	2A	3248	1/1	0.95	0.11	85,85,85,85	0
56	MG	1A	3536	1/1	0.95	0.22	74,74,74,74	0
56	MG	2A	3005	1/1	0.95	0.09	84,84,84,84	0
56	MG	1A	3462	1/1	0.95	0.11	64,64,64,64	0
56	MG	1A	3018	1/1	0.95	0.56	84,84,84,84	0
56	MG	2A	3324	1/1	0.95	0.27	83,83,83,83	0
56	MG	1A	3309	1/1	0.95	0.10	67,67,67,67	0
56	MG	1A	3631	1/1	0.95	0.08	82,82,82,82	0
56	MG	1A	3162	1/1	0.95	0.09	83,83,83,83	0
56	MG	1A	3602	1/1	0.95	0.22	67,67,67,67	0
56	MG	2a	3021	1/1	0.95	0.09	101,101,101,101	0
56	MG	2A	3347	1/1	0.95	0.16	86,86,86,86	0
56	MG	1A	3108	1/1	0.95	0.43	84,84,84,84	0
56	MG	1A	3008	1/1	0.95	0.13	74,74,74,74	0
56	MG	1A	3238	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3020	1/1	0.95	0.36	89,89,89,89	0
56	MG	2A	3183	1/1	0.95	0.15	80,80,80,80	0
56	MG	2a	3002	1/1	0.95	0.13	98,98,98,98	0
56	MG	2a	3030	1/1	0.95	0.12	77,77,77,77	0
56	MG	1a	3128	1/1	0.95	0.22	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3114	1/1	0.95	0.09	86,86,86,86	0
56	MG	1A	3397	1/1	0.95	0.09	83,83,83,83	0
56	MG	2a	3068	1/1	0.95	0.16	83,83,83,83	0
56	MG	1A	3587	1/1	0.95	0.18	80,80,80,80	0
56	MG	2A	3015	1/1	0.95	0.53	84,84,84,84	0
56	MG	2A	3200	1/1	0.95	0.26	86,86,86,86	0
56	MG	2a	3172	1/1	0.95	0.38	89,89,89,89	0
56	MG	1a	3228	1/1	0.95	0.19	72,72,72,72	0
56	MG	1A	3260	1/1	0.95	0.26	62,62,62,62	0
56	MG	2A	3062	1/1	0.95	0.12	84,84,84,84	0
56	MG	1a	3212	1/1	0.95	0.10	71,71,71,71	0
56	MG	1A	3341	1/1	0.95	0.21	70,70,70,70	0
56	MG	2A	3052	1/1	0.95	0.15	72,72,72,72	0
56	MG	1A	3302	1/1	0.95	0.26	59,59,59,59	0
56	MG	1A	3109	1/1	0.95	0.16	78,78,78,78	0
56	MG	2A	3027	1/1	0.95	0.16	87,87,87,87	0
56	MG	1A	3349	1/1	0.95	0.25	72,72,72,72	0
56	MG	1A	3082	1/1	0.95	0.15	69,69,69,69	0
56	MG	1A	3225	1/1	0.95	0.38	65,65,65,65	0
56	MG	1A	3131	1/1	0.95	0.18	84,84,84,84	0
56	MG	1A	3395	1/1	0.95	0.14	72,72,72,72	0
56	MG	1A	3003	1/1	0.95	0.39	60,60,60,60	0
56	MG	1A	3546	1/1	0.95	0.21	69,69,69,69	0
56	MG	1A	3091	1/1	0.95	0.29	75,75,75,75	0
56	MG	1A	3336	1/1	0.95	0.41	81,81,81,81	0
56	MG	1A	3369	1/1	0.95	0.31	86,86,86,86	0
56	MG	1A	3281	1/1	0.96	0.17	64,64,64,64	0
56	MG	1A	3392	1/1	0.96	0.36	80,80,80,80	0
56	MG	1A	3514	1/1	0.96	0.12	94,94,94,94	0
56	MG	2A	3221	1/1	0.96	0.14	107,107,107,107	0
57	ZN	29	501	1/1	0.96	0.19	105,105,105,105	0
56	MG	1a	3096	1/1	0.96	0.10	95,95,95,95	0
56	MG	1a	3237	1/1	0.96	0.06	106,106,106,106	0
56	MG	1A	3430	1/1	0.96	0.24	61,61,61,61	0
56	MG	1A	3627	1/1	0.96	0.20	60,60,60,60	0
56	MG	2A	3096	1/1	0.96	0.17	90,90,90,90	0
56	MG	2a	3038	1/1	0.96	0.20	101,101,101,101	0
56	MG	2A	3029	1/1	0.96	0.21	94,94,94,94	0
56	MG	1A	3193	1/1	0.96	0.17	62,62,62,62	0
56	MG	2a	3016	1/1	0.96	0.29	91,91,91,91	0
56	MG	1A	3634	1/1	0.96	0.19	83,83,83,83	0
56	MG	1A	3641	1/1	0.96	0.17	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	3146	1/1	0.96	0.17	100,100,100,100	0
56	MG	1A	3172	1/1	0.96	0.26	94,94,94,94	0
56	MG	1A	3440	1/1	0.96	0.14	77,77,77,77	0
56	MG	1a	3100	1/1	0.96	0.13	78,78,78,78	0
56	MG	1A	3163	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3362	1/1	0.96	0.21	53,53,53,53	0
56	MG	2a	3171	1/1	0.96	0.07	115,115,115,115	0
56	MG	2A	3270	1/1	0.96	0.11	80,80,80,80	0
56	MG	1a	3210	1/1	0.96	0.23	91,91,91,91	0
56	MG	2A	3272	1/1	0.96	0.15	89,89,89,89	0
56	MG	1A	3344	1/1	0.96	0.19	79,79,79,79	0
56	MG	1A	3027	1/1	0.96	1.18	68,68,68,68	0
56	MG	1A	3399	1/1	0.96	0.28	68,68,68,68	0
56	MG	1a	3074	1/1	0.96	0.12	88,88,88,88	0
56	MG	1A	3591	1/1	0.96	0.34	83,83,83,83	0
56	MG	1A	3538	1/1	0.96	0.09	87,87,87,87	0
56	MG	1a	3011	1/1	0.96	0.20	94,94,94,94	0
56	MG	1a	3130	1/1	0.96	0.27	99,99,99,99	0
56	MG	1A	3590	1/1	0.96	0.21	68,68,68,68	0
56	MG	1A	3170	1/1	0.96	0.30	99,99,99,99	0
56	MG	1A	3222	1/1	0.96	0.22	64,64,64,64	0
56	MG	1A	3348	1/1	0.96	0.34	74,74,74,74	0
56	MG	1A	3406	1/1	0.96	0.22	59,59,59,59	0
56	MG	2a	3133	1/1	0.96	0.23	92,92,92,92	0
56	MG	2A	3083	1/1	0.96	0.10	80,80,80,80	0
56	MG	2A	3340	1/1	0.96	0.19	67,67,67,67	0
56	MG	1A	3654	1/1	0.96	0.16	89,89,89,89	0
56	MG	2A	3236	1/1	0.96	0.18	69,69,69,69	0
56	MG	2A	3264	1/1	0.96	0.10	91,91,91,91	0
56	MG	1A	3037	1/1	0.96	0.18	83,83,83,83	0
56	MG	2A	3199	1/1	0.96	0.37	74,74,74,74	0
56	MG	1A	3317	1/1	0.96	0.30	56,56,56,56	0
56	MG	1A	3059	1/1	0.96	0.13	81,81,81,81	0
56	MG	1a	3225	1/1	0.96	0.57	85,85,85,85	0
56	MG	2A	3240	1/1	0.96	0.12	84,84,84,84	0
56	MG	2a	3181	1/1	0.96	0.17	90,90,90,90	0
56	MG	1A	3678	1/1	0.96	0.23	75,75,75,75	0
56	MG	1a	3161	1/1	0.96	0.10	82,82,82,82	0
56	MG	1a	3057	1/1	0.96	0.24	92,92,92,92	0
56	MG	2A	3279	1/1	0.96	0.25	70,70,70,70	0
56	MG	1a	3176	1/1	0.96	0.10	84,84,84,84	0
56	MG	2A	3299	1/1	0.96	0.48	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3421	1/1	0.96	0.22	68,68,68,68	0
56	MG	1a	3168	1/1	0.96	0.14	111,111,111,111	0
56	MG	1A	3562	1/1	0.96	0.10	60,60,60,60	0
56	MG	2A	3269	1/1	0.96	0.75	74,74,74,74	0
56	MG	2a	3035	1/1	0.96	0.15	94,94,94,94	0
56	MG	1A	3195	1/1	0.96	0.33	78,78,78,78	0
56	MG	1A	3282	1/1	0.96	0.29	63,63,63,63	0
56	MG	1A	3117	1/1	0.96	0.10	98,98,98,98	0
56	MG	1a	3044	1/1	0.96	0.29	90,90,90,90	0
56	MG	2A	3014	1/1	0.96	0.38	72,72,72,72	0
56	MG	2a	3108	1/1	0.96	0.05	98,98,98,98	0
56	MG	1A	3467	1/1	0.96	0.11	73,73,73,73	0
56	MG	1a	3142	1/1	0.96	0.16	85,85,85,85	0
56	MG	1A	3539	1/1	0.96	0.33	85,85,85,85	0
56	MG	1A	3445	1/1	0.96	0.20	80,80,80,80	0
56	MG	1A	3226	1/1	0.96	0.22	62,62,62,62	0
56	MG	1A	3284	1/1	0.96	0.16	86,86,86,86	0
56	MG	1A	3597	1/1	0.96	0.16	87,87,87,87	0
56	MG	2A	3176	1/1	0.96	0.22	89,89,89,89	0
56	MG	2A	3161	1/1	0.96	0.11	69,69,69,69	0
56	MG	1A	3297	1/1	0.96	0.13	77,77,77,77	0
56	MG	2a	3052	1/1	0.96	0.09	95,95,95,95	0
56	MG	2A	3259	1/1	0.96	0.21	76,76,76,76	0
56	MG	1A	3480	1/1	0.96	0.27	104,104,104,104	0
56	MG	1A	3248	1/1	0.96	0.20	76,76,76,76	0
56	MG	1A	3450	1/1	0.96	0.38	76,76,76,76	0
56	MG	1A	3673	1/1	0.96	0.30	77,77,77,77	0
56	MG	1A	3398	1/1	0.96	0.14	67,67,67,67	0
56	MG	2A	3155	1/1	0.96	0.07	66,66,66,66	0
57	ZN	16	501	1/1	0.96	0.23	87,87,87,87	0
56	MG	1A	3653	1/1	0.96	0.17	95,95,95,95	0
56	MG	2A	3307	1/1	0.96	0.17	79,79,79,79	0
56	MG	1A	3516	1/1	0.96	0.07	81,81,81,81	0
56	MG	1a	3023	1/1	0.96	0.23	87,87,87,87	0
56	MG	2A	3132	1/1	0.96	0.19	97,97,97,97	0
56	MG	2A	3329	1/1	0.96	0.29	100,100,100,100	0
56	MG	1a	3001	1/1	0.96	0.25	90,90,90,90	0
56	MG	1a	3087	1/1	0.96	0.13	100,100,100,100	0
56	MG	1A	3471	1/1	0.96	0.19	88,88,88,88	0
56	MG	2A	3006	1/1	0.96	0.24	71,71,71,71	0
56	MG	1a	3223	1/1	0.96	0.24	84,84,84,84	0
56	MG	1A	3269	1/1	0.96	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3625	1/1	0.96	0.17	66,66,66,66	0
56	MG	1A	3598	1/1	0.96	0.27	74,74,74,74	0
56	MG	2A	3325	1/1	0.96	0.20	91,91,91,91	0
56	MG	1A	3410	1/1	0.96	0.17	77,77,77,77	0
56	MG	2a	3094	1/1	0.96	0.29	89,89,89,89	0
56	MG	1a	3171	1/1	0.96	0.23	86,86,86,86	0
56	MG	1A	3535	1/1	0.96	0.34	90,90,90,90	0
56	MG	1A	3630	1/1	0.96	0.17	77,77,77,77	0
56	MG	1a	3150	1/1	0.96	0.15	83,83,83,83	0
56	MG	2A	3189	1/1	0.96	0.23	89,89,89,89	0
56	MG	2a	3093	1/1	0.96	0.23	87,87,87,87	0
56	MG	1A	3671	1/1	0.96	0.16	79,79,79,79	0
56	MG	1A	3298	1/1	0.96	0.42	83,83,83,83	0
56	MG	1A	3216	1/1	0.96	0.32	50,50,50,50	0
56	MG	1A	3378	1/1	0.96	0.43	73,73,73,73	0
56	MG	1a	3013	1/1	0.96	0.09	77,77,77,77	0
56	MG	1A	3213	1/1	0.96	0.16	66,66,66,66	0
56	MG	1A	3315	1/1	0.96	0.12	57,57,57,57	0
56	MG	1a	3208	1/1	0.96	0.14	80,80,80,80	0
56	MG	1A	3228	1/1	0.96	0.17	59,59,59,59	0
56	MG	1A	3508	1/1	0.96	0.12	86,86,86,86	0
56	MG	1A	3090	1/1	0.96	0.50	84,84,84,84	0
56	MG	2A	3175	1/1	0.97	0.16	65,65,65,65	0
56	MG	1A	3215	1/1	0.97	0.15	49,49,49,49	0
56	MG	1a	3119	1/1	0.97	0.58	88,88,88,88	0
56	MG	1A	3071	1/1	0.97	0.21	74,74,74,74	0
56	MG	1A	3680	1/1	0.97	0.19	85,85,85,85	0
57	ZN	1n	501	1/1	0.97	0.20	105,105,105,105	0
56	MG	1A	3499	1/1	0.97	0.09	72,72,72,72	0
56	MG	2A	3021	1/1	0.97	0.43	98,98,98,98	0
56	MG	2A	3191	1/1	0.97	0.36	74,74,74,74	0
57	ZN	2n	501	1/1	0.97	0.10	117,117,117,117	0
56	MG	1A	3401	1/1	0.97	0.27	90,90,90,90	0
56	MG	2a	3149	1/1	0.97	0.09	74,74,74,74	0
56	MG	1A	3068	1/1	0.97	0.08	74,74,74,74	0
56	MG	2A	3002	1/1	0.97	0.22	81,81,81,81	0
56	MG	1a	3231	1/1	0.97	0.16	82,82,82,82	0
56	MG	1A	3606	1/1	0.97	0.47	71,71,71,71	0
56	MG	2A	3241	1/1	0.97	0.12	89,89,89,89	0
56	MG	1A	3619	1/1	0.97	0.15	86,86,86,86	0
56	MG	2A	3065	1/1	0.97	0.36	88,88,88,88	0
56	MG	1A	3643	1/1	0.97	0.13	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3474	1/1	0.97	0.24	74,74,74,74	0
56	MG	1a	3131	1/1	0.97	0.25	107,107,107,107	0
56	MG	2A	3102	1/1	0.97	0.55	72,72,72,72	0
56	MG	2A	3291	1/1	0.97	0.10	87,87,87,87	0
56	MG	2a	3098	1/1	0.97	0.37	101,101,101,101	0
56	MG	2A	3093	1/1	0.97	0.16	71,71,71,71	0
56	MG	2A	3345	1/1	0.97	0.60	77,77,77,77	0
56	MG	1A	3311	1/1	0.97	0.34	61,61,61,61	0
56	MG	1A	3628	1/1	0.97	0.16	56,56,56,56	0
56	MG	1A	3475	1/1	0.97	0.30	88,88,88,88	0
56	MG	2A	3063	1/1	0.97	0.07	67,67,67,67	0
56	MG	2a	3041	1/1	0.97	0.20	69,69,69,69	0
56	MG	1A	3296	1/1	0.97	0.12	76,76,76,76	0
56	MG	1A	3483	1/1	0.97	0.07	77,77,77,77	0
56	MG	1A	3061	1/1	0.97	0.21	77,77,77,77	0
56	MG	1A	3085	1/1	0.97	0.37	92,92,92,92	0
56	MG	1A	3611	1/1	0.97	0.30	75,75,75,75	0
56	MG	1a	3038	1/1	0.97	0.12	88,88,88,88	0
56	MG	1A	3292	1/1	0.97	0.13	50,50,50,50	0
56	MG	1A	3146	1/1	0.97	0.17	62,62,62,62	0
56	MG	1A	3526	1/1	0.97	0.12	76,76,76,76	0
56	MG	2A	3073	1/1	0.97	0.16	85,85,85,85	0
56	MG	2A	3172	1/1	0.97	0.23	80,80,80,80	0
56	MG	1a	3194	1/1	0.97	0.22	102,102,102,102	0
56	MG	2A	3350	1/1	0.97	0.33	70,70,70,70	0
56	MG	2A	3275	1/1	0.97	0.34	81,81,81,81	0
56	MG	1a	3054	1/1	0.97	0.21	85,85,85,85	0
56	MG	1a	3029	1/1	0.97	0.12	64,64,64,64	0
56	MG	2a	3022	1/1	0.97	0.15	83,83,83,83	0
56	MG	1A	3043	1/1	0.97	0.13	74,74,74,74	0
56	MG	2a	3044	1/1	0.97	0.29	86,86,86,86	0
56	MG	1A	3106	1/1	0.97	0.26	63,63,63,63	0
56	MG	1a	3183	1/1	0.97	0.34	78,78,78,78	0
56	MG	1A	3307	1/1	0.97	0.28	60,60,60,60	0
56	MG	1a	3138	1/1	0.97	0.20	91,91,91,91	0
56	MG	1A	3155	1/1	0.97	0.15	65,65,65,65	0
56	MG	1A	3464	1/1	0.97	0.15	73,73,73,73	0
56	MG	1A	3005	1/1	0.97	0.13	74,74,74,74	0
56	MG	1a	3148	1/1	0.97	0.21	112,112,112,112	0
56	MG	1A	3084	1/1	0.97	0.28	71,71,71,71	0
56	MG	1A	3093	1/1	0.97	0.15	73,73,73,73	0
56	MG	1A	3040	1/1	0.97	0.24	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3117	1/1	0.97	0.17	83,83,83,83	0
56	MG	1A	3338	1/1	0.97	0.21	45,45,45,45	0
56	MG	1A	3212	1/1	0.97	0.21	54,54,54,54	0
56	MG	1a	3135	1/1	0.97	0.10	82,82,82,82	0
56	MG	1a	3144	1/1	0.97	0.18	71,71,71,71	0
56	MG	1a	3002	1/1	0.97	0.12	83,83,83,83	0
56	MG	2A	3232	1/1	0.97	0.24	53,53,53,53	0
56	MG	1A	3271	1/1	0.97	0.17	49,49,49,49	0
56	MG	2A	3085	1/1	0.97	0.66	101,101,101,101	0
56	MG	1A	3448	1/1	0.97	0.15	78,78,78,78	0
56	MG	1A	3594	1/1	0.97	0.17	77,77,77,77	0
56	MG	1A	3510	1/1	0.97	0.17	64,64,64,64	0
56	MG	2A	3319	1/1	0.97	0.14	78,78,78,78	0
56	MG	2A	3239	1/1	0.97	0.08	77,77,77,77	0
56	MG	1A	3660	1/1	0.97	0.25	65,65,65,65	0
56	MG	1A	3424	1/1	0.97	1.40	81,81,81,81	0
56	MG	2a	3103	1/1	0.97	0.27	73,73,73,73	0
56	MG	1a	3156	1/1	0.97	0.19	73,73,73,73	0
56	MG	2A	3276	1/1	0.97	0.12	82,82,82,82	0
56	MG	1A	3490	1/1	0.97	0.19	79,79,79,79	0
56	MG	2A	3292	1/1	0.97	0.08	91,91,91,91	0
56	MG	1A	3086	1/1	0.97	0.17	70,70,70,70	0
56	MG	2A	3023	1/1	0.97	0.07	71,71,71,71	0
56	MG	1A	3635	1/1	0.97	0.20	78,78,78,78	0
56	MG	1A	3217	1/1	0.97	0.11	60,60,60,60	0
56	MG	1A	3492	1/1	0.97	0.12	77,77,77,77	0
56	MG	2A	3179	1/1	0.97	0.14	74,74,74,74	0
56	MG	1A	3463	1/1	0.97	0.29	75,75,75,75	0
56	MG	2a	3150	1/1	0.97	0.21	87,87,87,87	0
56	MG	1A	3276	1/1	0.98	0.24	64,64,64,64	0
56	MG	1a	3188	1/1	0.98	0.12	81,81,81,81	0
56	MG	1a	3088	1/1	0.98	0.18	96,96,96,96	0
56	MG	2A	3224	1/1	0.98	0.18	62,62,62,62	0
56	MG	1A	3345	1/1	0.98	0.15	66,66,66,66	0
56	MG	1A	3262	1/1	0.98	0.22	64,64,64,64	0
56	MG	2A	3069	1/1	0.98	0.15	82,82,82,82	0
56	MG	1A	3097	1/1	0.98	0.11	94,94,94,94	0
56	MG	1a	3075	1/1	0.98	0.24	72,72,72,72	0
56	MG	1A	3655	1/1	0.98	0.35	67,67,67,67	0
56	MG	1a	3076	1/1	0.98	0.21	58,58,58,58	0
56	MG	1A	3247	1/1	0.98	0.10	55,55,55,55	0
56	MG	2a	3065	1/1	0.98	0.17	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3030	1/1	0.98	0.11	81,81,81,81	0
56	MG	1A	3069	1/1	0.98	0.90	67,67,67,67	0
56	MG	1A	3632	1/1	0.98	0.16	63,63,63,63	0
56	MG	2A	3267	1/1	0.98	0.21	93,93,93,93	0
56	MG	2A	3300	1/1	0.98	0.35	79,79,79,79	0
56	MG	2a	3045	1/1	0.98	0.08	102,102,102,102	0
56	MG	1A	3451	1/1	0.98	0.11	85,85,85,85	0
56	MG	1A	3200	1/1	0.98	0.22	63,63,63,63	0
56	MG	1A	3046	1/1	0.98	0.09	54,54,54,54	0
56	MG	1A	3517	1/1	0.98	0.20	77,77,77,77	0
56	MG	1A	3435	1/1	0.98	0.17	59,59,59,59	0
56	MG	1A	3072	1/1	0.98	0.47	67,67,67,67	0
56	MG	1a	3200	1/1	0.98	0.17	83,83,83,83	0
56	MG	2a	3140	1/1	0.98	0.14	88,88,88,88	0
56	MG	1A	3667	1/1	0.98	0.45	68,68,68,68	0
56	MG	1A	3532	1/1	0.98	0.09	88,88,88,88	0
56	MG	1A	3456	1/1	0.98	0.25	96,96,96,96	0
56	MG	1A	3101	1/1	0.98	0.23	86,86,86,86	0
56	MG	2a	3165	1/1	0.98	0.08	116,116,116,116	0
56	MG	1a	3129	1/1	0.98	0.11	88,88,88,88	0
57	ZN	1Y	501	1/1	0.98	0.18	100,100,100,100	0
56	MG	2A	3339	1/1	0.98	0.14	92,92,92,92	0
56	MG	1A	3259	1/1	0.98	0.20	54,54,54,54	0
56	MG	1a	3080	1/1	0.98	0.17	88,88,88,88	0
56	MG	1A	3507	1/1	0.98	0.25	92,92,92,92	0
56	MG	1A	3477	1/1	0.98	0.15	56,56,56,56	0
56	MG	1a	3221	1/1	0.98	0.20	79,79,79,79	0
56	MG	1A	3509	1/1	0.98	0.28	75,75,75,75	0
56	MG	1A	3604	1/1	0.98	0.14	67,67,67,67	0
56	MG	2A	3120	1/1	0.98	0.13	94,94,94,94	0
56	MG	2A	3178	1/1	0.98	0.17	63,63,63,63	0
56	MG	2A	3059	1/1	0.98	0.12	93,93,93,93	0
56	MG	1A	3129	1/1	0.98	0.16	93,93,93,93	0
56	MG	1A	3502	1/1	0.98	0.27	61,61,61,61	0
56	MG	1A	3179	1/1	0.98	0.34	90,90,90,90	0
56	MG	2A	3306	1/1	0.98	0.19	74,74,74,74	0
56	MG	2A	3122	1/1	0.98	0.21	86,86,86,86	0
56	MG	1A	3646	1/1	0.98	0.31	92,92,92,92	0
56	MG	2A	3163	1/1	0.98	0.22	79,79,79,79	0
56	MG	1a	3219	1/1	0.98	0.20	74,74,74,74	0
56	MG	1a	3047	1/1	0.98	0.20	82,82,82,82	0
56	MG	1A	3482	1/1	0.98	0.22	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3064	1/1	0.98	0.34	82,82,82,82	0
56	MG	1A	3314	1/1	0.98	0.29	54,54,54,54	0
56	MG	2A	3067	1/1	0.98	0.14	82,82,82,82	0
56	MG	2a	3125	1/1	0.98	0.14	75,75,75,75	0
56	MG	1A	3089	1/1	0.98	0.66	59,59,59,59	0
56	MG	2A	3167	1/1	0.98	0.12	87,87,87,87	0
56	MG	1a	3177	1/1	0.99	0.14	73,73,73,73	0
56	MG	1A	3064	1/1	0.99	0.17	84,84,84,84	0
56	MG	1A	3107	1/1	0.99	0.27	81,81,81,81	0
56	MG	1A	3498	1/1	0.99	0.14	85,85,85,85	0
56	MG	2A	3288	1/1	0.99	0.19	71,71,71,71	0
57	ZN	19	501	1/1	0.99	0.25	77,77,77,77	0
56	MG	1A	3379	1/1	0.99	0.26	55,55,55,55	0
56	MG	1A	3102	1/1	0.99	0.12	78,78,78,78	0
56	MG	1A	3073	1/1	0.99	0.25	81,81,81,81	0
56	MG	1A	3111	1/1	0.99	0.10	83,83,83,83	0
56	MG	1A	3135	1/1	0.99	0.10	59,59,59,59	0
58	SF4	2d	501	8/8	0.99	0.18	95,106,118,119	0
56	MG	1A	3375	1/1	0.99	0.24	62,62,62,62	0
57	ZN	26	501	1/1	0.99	0.26	98,98,98,98	0
58	SF4	1d	501	8/8	0.99	0.23	76,91,99,101	0
56	MG	2A	3225	1/1	0.99	0.27	75,75,75,75	0
56	MG	1a	3086	1/1	0.99	0.33	76,76,76,76	0
56	MG	1A	3057	1/1	0.99	0.16	79,79,79,79	0
56	MG	2A	3250	1/1	0.99	0.24	65,65,65,65	0
57	ZN	25	501	1/1	0.99	0.23	97,97,97,97	0
57	ZN	15	501	1/1	0.99	0.21	87,87,87,87	0
56	MG	1A	3485	1/1	0.99	0.18	61,61,61,61	0
56	MG	1A	3013	1/1	0.99	0.25	69,69,69,69	0
56	MG	1a	3227	1/1	0.99	0.33	64,64,64,64	0
56	MG	1A	3028	1/1	0.99	0.23	68,68,68,68	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.