



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 1, 2021 – 05:26 PM EDT

PDB ID : 4V88
Title : The structure of the eukaryotic ribosome at 3.0 Å resolution.
Authors : Ben-Shem, A.; Garreau de Loubresse, N.; Melnikov, S.; Jenner, L.; Yusupova, G.; Yusupov, M.
Deposited on : 2011-10-11
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

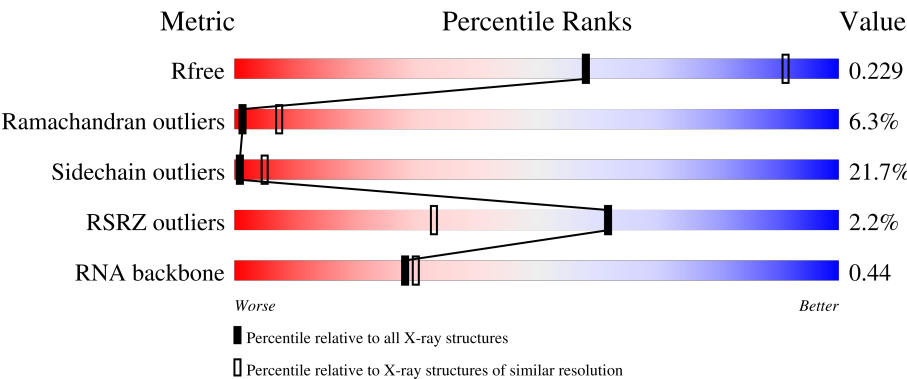
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



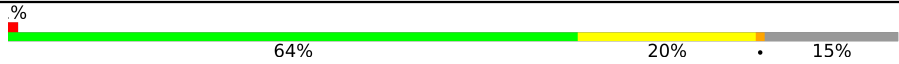

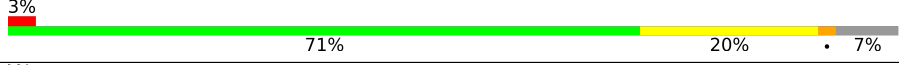

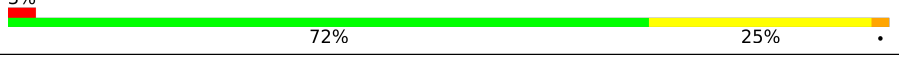
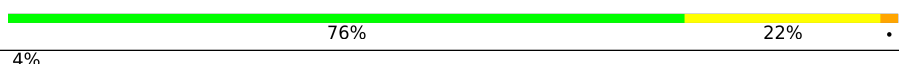
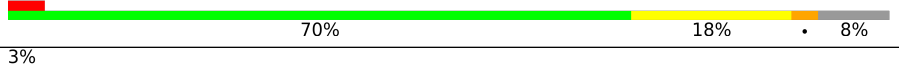

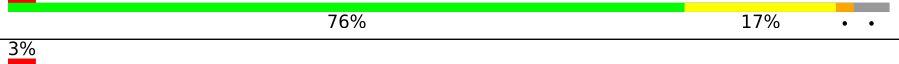


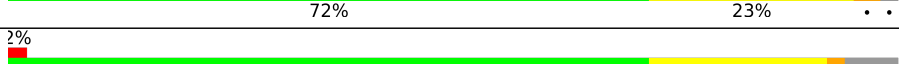
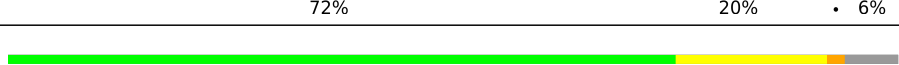
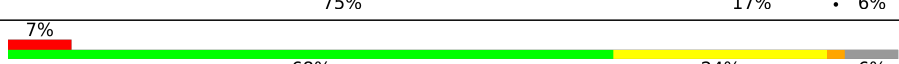

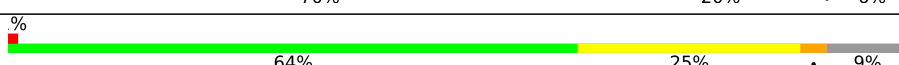
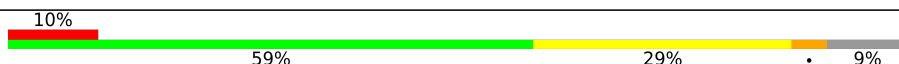
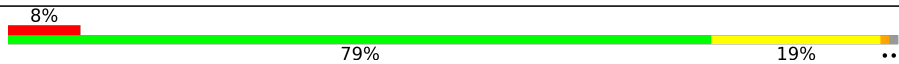
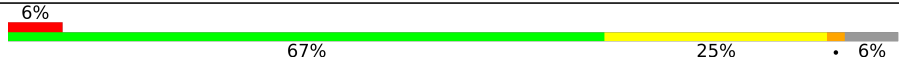



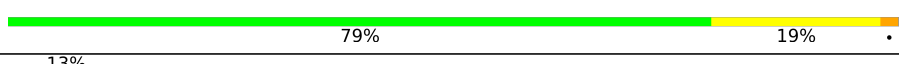


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	A2	1800	<div> <div>2%</div> <div>54% 36% 9%</div> </div>
2	AA	252	<div> <div>2%</div> <div>58% 21% 18%</div> </div>
2	CA	252	<div> <div>0%</div> <div>60% 19% 18%</div> </div>
3	AB	255	<div> <div>11%</div> <div>54% 24% 6% 16%</div> </div>
3	CB	255	<div> <div>0%</div> <div>63% 20% 15%</div> </div>

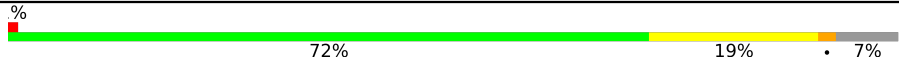

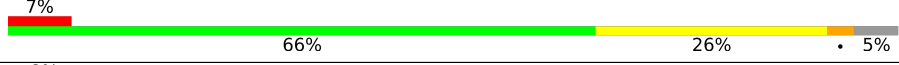

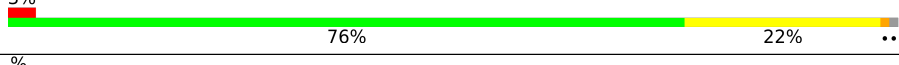
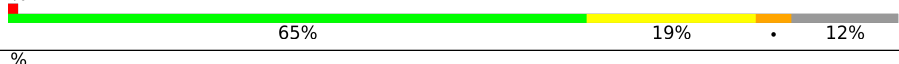
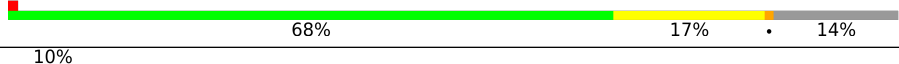

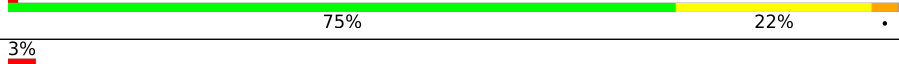


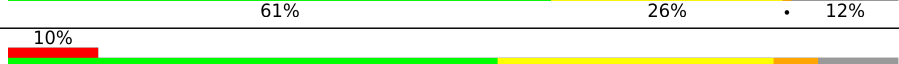
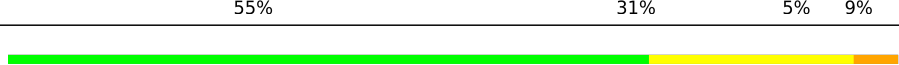
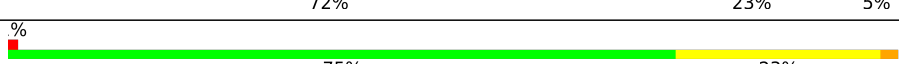

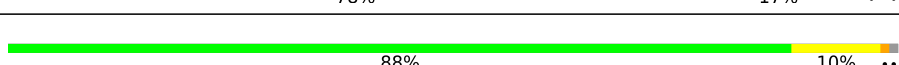
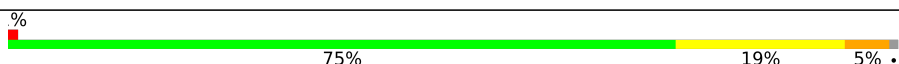
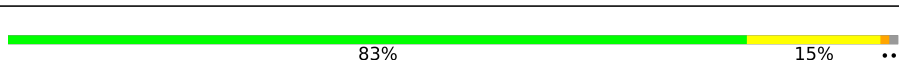
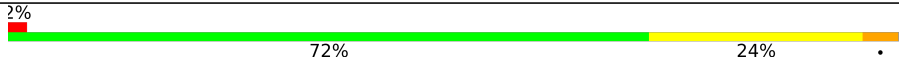

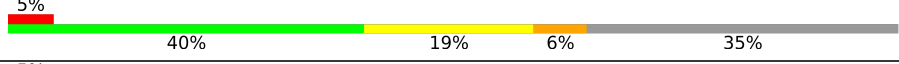
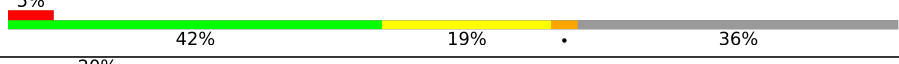
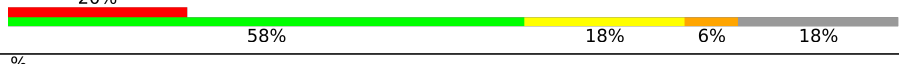


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Mol	Chain	Length	Quality of chain
4	AC	254	
4	CC	254	
5	AD	240	
5	CD	240	
6	AE	261	
6	CE	261	
7	AF	225	
7	CF	225	
8	AG	236	
8	CG	236	
9	AH	190	
9	CH	190	
10	AI	200	
10	CI	200	
11	AJ	197	
11	CJ	197	
12	AK	105	
12	CK	105	
13	AL	156	
13	CL	156	
14	AM	143	
14	CM	143	
15	AN	151	
15	CN	151	
16	AO	137	

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Mol	Chain	Length	Quality of chain
16	CO	137	
17	AP	142	
17	CP	142	
18	AQ	143	
18	CQ	143	
19	AR	136	
19	CR	136	
20	AS	146	
20	CS	146	
21	AT	144	
21	CT	144	
22	AU	121	
22	CU	121	
23	AV	87	
23	CV	87	
24	AW	130	
24	CW	130	
25	AX	145	
25	CX	145	
26	AY	135	
26	CY	135	
27	AZ	108	
27	CZ	108	
28	Aa	119	
28	Ca	119	

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Mol	Chain	Length	Quality of chain
29	Ab	82	
29	Cb	82	
30	Ac	67	
30	Cc	67	
31	Ad	56	
31	Cd	56	
32	Ae	63	
32	Ce	63	
33	Af	152	
33	Cf	152	
34	Ag	319	
34	Cg	319	
35	Ah	273	
36	A1	3396	
36	A5	3396	
37	A3	121	
37	A7	121	
38	A4	158	
38	A8	158	
39	BA	254	
39	DA	254	
40	BB	387	
40	DB	387	
41	BC	362	
41	DC	362	




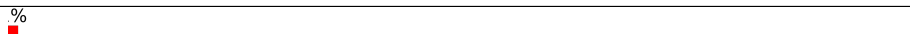
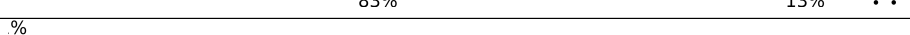
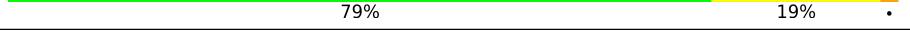



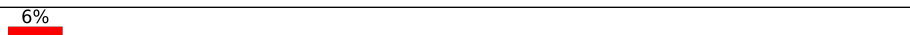
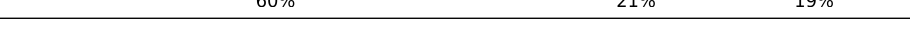




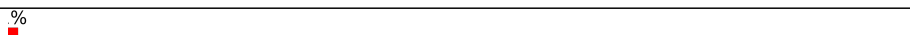






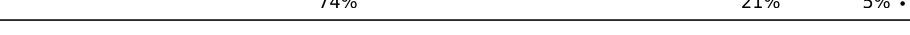


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Mol	Chain	Length	Quality of chain
42	BD	297	% 75% 23% .
42	DD	297	% 80% 18% ..
43	BE	176	74% 13% . 11%
43	DE	176	% 73% 15% . 11%
44	BF	244	77% 11% . 9%
44	DF	244	76% 14% . 9%
45	BG	256	71% 18% . 9%
45	DG	256	% 68% 21% . 10%
46	BH	191	% 75% 24% .
46	DH	191	% 78% 20% .
47	BI	221	76% 18% . 5%
47	DI	221	2% 71% 23% . .
48	BJ	174	% 68% 25% 5% .
48	DJ	174	72% 21% . . .
49	BL	199	75% 19% . .
49	DL	199	76% 19% . .
50	BM	138	77% 20% ..
50	DM	138	80% 17% ..
51	BN	204	81% 17% .
51	DN	204	79% 18% .
52	BO	219	75% 21% . . .
52	DO	219	% 71% 20% 9% .
53	BP	184	4% 76% 23% ..
53	DP	184	70% 12% . 16%
54	BQ	186	82% 15% ..

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Mol	Chain	Length	Quality of chain
54	DQ	186	
55	BR	189	
55	DR	189	
56	BS	172	
56	DS	172	
57	BT	160	
57	DT	160	
58	BU	121	
58	DU	121	
59	BV	137	
59	DV	137	
60	BW	155	
60	DW	155	
61	BX	142	
61	DX	142	
62	BY	127	
62	DY	127	
63	BZ	136	
63	DZ	136	
64	Ba	149	
64	Da	149	
65	Bb	59	
65	Db	59	
66	Bc	105	
66	Dc	105	



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Mol	Chain	Length	Quality of chain
67	Bd	113	<div> <div>3%</div> <div>75%</div> <div>19%</div> <div>• •</div> </div>
67	Dd	113	<div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
68	Be	130	<div> <div>2%</div> <div>75%</div> <div>21%</div> <div>• • •</div> </div>
68	De	130	<div> <div>2%</div> <div>76%</div> <div>19%</div> <div>• • •</div> </div>
69	Bf	107	<div> <div>•</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
69	Df	107	<div> <div>85%</div> <div>12%</div> <div>• •</div> </div>
70	Bg	121	<div> <div>2%</div> <div>69%</div> <div>20%</div> <div>• 7%</div> </div>
70	Dg	121	<div> <div>2%</div> <div>70%</div> <div>21%</div> <div>• 7%</div> </div>
71	Bh	120	<div> <div>•</div> <div>72%</div> <div>26%</div> <div>• •</div> </div>
71	Dh	120	<div> <div>•</div> <div>76%</div> <div>22%</div> <div>• •</div> </div>
72	Bi	100	<div> <div>66%</div> <div>31%</div> <div>• •</div> </div>
72	Di	100	<div> <div>•</div> <div>67%</div> <div>28%</div> <div>• •</div> </div>
73	Bj	88	<div> <div>•</div> <div>74%</div> <div>23%</div> <div>• •</div> </div>
73	Dj	88	<div> <div>2%</div> <div>74%</div> <div>25%</div> <div>•</div> </div>
74	Bk	78	<div> <div>72%</div> <div>27%</div> <div>•</div> </div>
74	Dk	78	<div> <div>•</div> <div>76%</div> <div>23%</div> <div>•</div> </div>
75	Bl	51	<div> <div>78%</div> <div>18%</div> <div>• •</div> </div>
75	Dl	51	<div> <div>2%</div> <div>75%</div> <div>22%</div> <div>• •</div> </div>
76	Bm	128	<div> <div>2%</div> <div>31%</div> <div>8%</div> <div>•</div> <div>59%</div> </div>
76	Dm	128	<div> <div>•</div> <div>30%</div> <div>9%</div> <div>•</div> <div>59%</div> </div>
77	Bn	25	<div> <div>4%</div> <div>68%</div> <div>24%</div> <div>8%</div> </div>
77	Dn	25	<div> <div>72%</div> <div>20%</div> <div>8%</div> </div>
78	Bo	106	<div> <div>•</div> <div>74%</div> <div>23%</div> <div>• •</div> </div>
78	Do	106	<div> <div>2%</div> <div>82%</div> <div>16%</div> <div>• •</div> </div>
79	Bp	92	<div> <div>79%</div> <div>18%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
79	Dp	92	
80	A6	1800	
81	Ch	273	
82	DK	155	
83	Dq	312	
84	Dr	47	
85	Ds	46	

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
86	OHX	A1	3753	-	-	-	X
86	OHX	A1	3779	-	-	-	X
86	OHX	A1	3805	-	-	-	X
86	OHX	A1	3814	-	-	-	X
86	OHX	A1	3815	-	-	-	X
86	OHX	A2	2051	-	-	-	X
86	OHX	A5	3768	-	-	-	X
86	OHX	A5	3780	-	-	-	X
86	OHX	A5	3792	-	-	-	X
86	OHX	A5	3810	-	-	-	X
86	OHX	A5	3819	-	-	-	X
86	OHX	A6	2083	-	-	-	X
86	OHX	A6	2086	-	-	-	X
86	OHX	A6	2090	-	-	-	X
86	OHX	A6	2095	-	-	-	X
86	OHX	A8	218	-	-	-	X
86	OHX	BI	303	-	-	-	X
86	OHX	CP	202	-	-	-	X
87	MG	A1	3848	-	-	-	X
87	MG	A1	3909	-	-	-	X
87	MG	A1	3912	-	-	-	X
87	MG	A1	3919	-	-	-	X
87	MG	A1	3922	-	-	-	X
87	MG	A1	3928	-	-	-	X
87	MG	A1	3978	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	A1	3990	-	-	-	X
87	MG	A1	4014	-	-	-	X
87	MG	A1	4059	-	-	-	X
87	MG	A1	4086	-	-	-	X
87	MG	A1	4135	-	-	-	X
87	MG	A1	4144	-	-	-	X
87	MG	A1	4150	-	-	-	X
87	MG	A1	4155	-	-	-	X
87	MG	A1	4187	-	-	-	X
87	MG	A1	4201	-	-	-	X
87	MG	A1	4226	-	-	-	X
87	MG	A1	4232	-	-	-	X
87	MG	A1	4248	-	-	-	X
87	MG	A1	4263	-	-	-	X
87	MG	A1	4269	-	-	-	X
87	MG	A1	4273	-	-	-	X
87	MG	A1	4277	-	-	-	X
87	MG	A1	4282	-	-	-	X
87	MG	A1	4298	-	-	-	X
87	MG	A1	4299	-	-	-	X
87	MG	A1	4302	-	-	-	X
87	MG	A1	4310	-	-	-	X
87	MG	A1	4316	-	-	-	X
87	MG	A1	4326	-	-	-	X
87	MG	A1	4329	-	-	-	X
87	MG	A1	4333	-	-	-	X
87	MG	A1	4337	-	-	-	X
87	MG	A1	4339	-	-	-	X
87	MG	A1	4360	-	-	-	X
87	MG	A1	4368	-	-	-	X
87	MG	A1	4374	-	-	-	X
87	MG	A1	4376	-	-	-	X
87	MG	A1	4385	-	-	-	X
87	MG	A1	4387	-	-	-	X
87	MG	A1	4407	-	-	-	X
87	MG	A1	4408	-	-	-	X
87	MG	A1	4419	-	-	-	X
87	MG	A1	4420	-	-	-	X
87	MG	A1	4432	-	-	-	X
87	MG	A1	4440	-	-	-	X
87	MG	A1	4444	-	-	-	X
87	MG	A1	4447	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	A1	4451	-	-	-	X
87	MG	A1	4453	-	-	-	X
87	MG	A1	4462	-	-	-	X
87	MG	A1	4480	-	-	-	X
87	MG	A1	4495	-	-	-	X
87	MG	A1	4501	-	-	-	X
87	MG	A1	4503	-	-	-	X
87	MG	A1	4504	-	-	-	X
87	MG	A2	2170	-	-	-	X
87	MG	A2	2194	-	-	-	X
87	MG	A2	2196	-	-	-	X
87	MG	A2	2209	-	-	-	X
87	MG	A2	2210	-	-	-	X
87	MG	A2	2211	-	-	-	X
87	MG	A2	2222	-	-	-	X
87	MG	A2	2225	-	-	-	X
87	MG	A2	2241	-	-	-	X
87	MG	A2	2256	-	-	-	X
87	MG	A3	220	-	-	-	X
87	MG	A3	230	-	-	-	X
87	MG	A4	220	-	-	-	X
87	MG	A4	245	-	-	-	X
87	MG	A5	3408	-	-	-	X
87	MG	A5	3826	-	-	-	X
87	MG	A5	3862	-	-	-	X
87	MG	A5	3887	-	-	-	X
87	MG	A5	3989	-	-	-	X
87	MG	A5	4022	-	-	-	X
87	MG	A5	4081	-	-	-	X
87	MG	A5	4084	-	-	-	X
87	MG	A5	4135	-	-	-	X
87	MG	A5	4155	-	-	-	X
87	MG	A5	4177	-	-	-	X
87	MG	A5	4202	-	-	-	X
87	MG	A5	4217	-	-	-	X
87	MG	A5	4250	-	-	-	X
87	MG	A5	4254	-	-	-	X
87	MG	A5	4256	-	-	-	X
87	MG	A5	4264	-	-	-	X
87	MG	A5	4265	-	-	-	X
87	MG	A5	4273	-	-	-	X
87	MG	A5	4279	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	A5	4283	-	-	-	X
87	MG	A5	4285	-	-	-	X
87	MG	A5	4309	-	-	-	X
87	MG	A5	4317	-	-	-	X
87	MG	A5	4337	-	-	-	X
87	MG	A5	4345	-	-	-	X
87	MG	A5	4349	-	-	-	X
87	MG	A5	4353	-	-	-	X
87	MG	A5	4372	-	-	-	X
87	MG	A5	4374	-	-	-	X
87	MG	A5	4375	-	-	-	X
87	MG	A5	4379	-	-	-	X
87	MG	A5	4382	-	-	-	X
87	MG	A5	4402	-	-	-	X
87	MG	A5	4409	-	-	-	X
87	MG	A5	4410	-	-	-	X
87	MG	A5	4414	-	-	-	X
87	MG	A5	4424	-	-	-	X
87	MG	A5	4432	-	-	-	X
87	MG	A5	4440	-	-	-	X
87	MG	A5	4464	-	-	-	X
87	MG	A5	4476	-	-	-	X
87	MG	A5	4477	-	-	-	X
87	MG	A5	4482	-	-	-	X
87	MG	A5	4485	-	-	-	X
87	MG	A5	4486	-	-	-	X
87	MG	A5	4488	-	-	-	X
87	MG	A5	4491	-	-	-	X
87	MG	A5	4492	-	-	-	X
87	MG	A5	4510	-	-	-	X
87	MG	A5	4511	-	-	-	X
87	MG	A5	4514	-	-	-	X
87	MG	A5	4515	-	-	-	X
87	MG	A5	4518	-	-	-	X
87	MG	A5	4529	-	-	-	X
87	MG	A5	4541	-	-	-	X
87	MG	A5	4549	-	-	-	X
87	MG	A5	4554	-	-	-	X
87	MG	A5	4561	-	-	-	X
87	MG	A5	4569	-	-	-	X
87	MG	A5	4575	-	-	-	X
87	MG	A5	4579	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	A6	2157	-	-	-	X
87	MG	A6	2158	-	-	-	X
87	MG	A6	2196	-	-	-	X
87	MG	A6	2244	-	-	-	X
87	MG	A6	2246	-	-	-	X
87	MG	A6	2250	-	-	-	X
87	MG	A6	2259	-	-	-	X
87	MG	A6	2262	-	-	-	X
87	MG	A6	2278	-	-	-	X
87	MG	A6	2281	-	-	-	X
87	MG	A6	2284	-	-	-	X
87	MG	A6	2287	-	-	-	X
87	MG	A6	2288	-	-	-	X
87	MG	A6	2296	-	-	-	X
87	MG	A6	2299	-	-	-	X
87	MG	A6	2316	-	-	-	X
87	MG	A6	2317	-	-	-	X
87	MG	A6	2320	-	-	-	X
87	MG	A6	2321	-	-	-	X
87	MG	A6	2322	-	-	-	X
87	MG	A6	2329	-	-	-	X
87	MG	A6	2332	-	-	-	X
87	MG	A6	2333	-	-	-	X
87	MG	A6	2335	-	-	-	X
87	MG	A6	2336	-	-	-	X
87	MG	A6	2338	-	-	-	X
87	MG	A7	227	-	-	-	X
87	MG	A7	228	-	-	-	X
87	MG	A7	229	-	-	-	X
87	MG	A8	235	-	-	-	X
87	MG	BA	306	-	-	-	X
87	MG	BI	307	-	-	-	X
87	MG	BO	205	-	-	-	X
87	MG	BP	211	-	-	-	X
87	MG	BQ	202	-	-	-	X
87	MG	BV	205	-	-	-	X
87	MG	Ba	207	-	-	-	X
87	MG	Ba	208	-	-	-	X
87	MG	Be	201	-	-	-	X
87	MG	Bj	107	-	-	-	X
87	MG	Bl	4500	-	-	-	X
87	MG	CL	204	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	CP	203	-	-	-	X
87	MG	DB	414	-	-	-	X
87	MG	DC	405	-	-	-	X
87	MG	DH	202	-	-	-	X
87	MG	DH	203	-	-	-	X
87	MG	DO	207	-	-	-	X
87	MG	Db	102	-	-	-	X
87	MG	De	203	-	-	-	X

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 416785 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 18S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A2	1781	Total	C	N	O	P	0	1	0
			37835	16910	6661	12482	1782			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AA	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	CA	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AB	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	CB	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AC	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	CC	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AD	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	CD	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AE	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	CE	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AF	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	CF	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AG	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	CG	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AH	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	CH	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AI	188	Total	C	N	O	0	0	0
			1489	925	298	264			
10	CI	188	Total	C	N	O	0	0	0
			1489	925	298	264			

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AJ	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	CJ	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AK	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
12	CK	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AL	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	CL	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AM	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
14	CM	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AN	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	CN	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AO	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	CO	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AP	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	CP	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AQ	141	Total	C	N	O		0	0	0
			1105	708	203	194				
18	CQ	142	Total	C	N	O		0	0	0
			1111	711	204	196				

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AR	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	CR	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AS	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	CS	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AT	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	CT	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AU	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	CU	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AV	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	CV	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	CW	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AX	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	CX	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AY	134	Total	C	N	O	0	0	0
			1073	676	208	189			
26	CY	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	AZ	70	Total	C	N	O	0	0	0
			563	360	104	99			
27	CZ	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 28 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Aa	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	Ca	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	Ab	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	Cb	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Ac	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	Cc	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Ad	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	Cd	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	Ae	60	Total 475	C 299	N 98	O 77	S 1	0	0	0
32	Ce	62	Total 491	C 309	N 101	O 80	S 1	0	0	0

- Molecule 33 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	Af	71	Total 516	C 328	N 93	O 91	S 4	0	0	0
33	Cf	76	Total 544	C 346	N 98	O 96	S 4	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Af	82	UNK	LYS	SEE REMARK 999	UNP P05759
Af	83	UNK	LYS	SEE REMARK 999	UNP P05759
Af	84	UNK	VAL	SEE REMARK 999	UNP P05759
Af	85	UNK	TYR	SEE REMARK 999	UNP P05759
Af	86	UNK	THR	SEE REMARK 999	UNP P05759
Af	87	UNK	THR	SEE REMARK 999	UNP P05759
Af	88	UNK	PRO	SEE REMARK 999	UNP P05759
Af	89	UNK	LYS	SEE REMARK 999	UNP P05759
Af	90	UNK	LYS	SEE REMARK 999	UNP P05759
Af	91	UNK	ILE	SEE REMARK 999	UNP P05759
Af	92	UNK	LYS	SEE REMARK 999	UNP P05759
Af	93	UNK	HIS	SEE REMARK 999	UNP P05759
Af	94	UNK	LYS	SEE REMARK 999	UNP P05759
Af	95	UNK	HIS	SEE REMARK 999	UNP P05759
Af	96	UNK	LYS	SEE REMARK 999	UNP P05759
Af	97	UNK	LYS	SEE REMARK 999	UNP P05759
Af	98	UNK	VAL	SEE REMARK 999	UNP P05759
Af	99	UNK	LYS	SEE REMARK 999	UNP P05759
Af	100	UNK	LEU	SEE REMARK 999	UNP P05759
Af	101	UNK	ALA	SEE REMARK 999	UNP P05759
Cf	77	UNK	GLY	SEE REMARK 999	UNP P05759
Cf	78	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	79	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	80	UNK	ARG	SEE REMARK 999	UNP P05759
Cf	81	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	82	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	83	UNK	LYS	SEE REMARK 999	UNP P05759

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Chain	Residue	Modelled	Actual	Comment	Reference
Cf	84	UNK	VAL	SEE REMARK 999	UNP P05759
Cf	85	UNK	TYR	SEE REMARK 999	UNP P05759
Cf	86	UNK	THR	SEE REMARK 999	UNP P05759
Cf	87	UNK	THR	SEE REMARK 999	UNP P05759
Cf	88	UNK	PRO	SEE REMARK 999	UNP P05759
Cf	89	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	90	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	91	UNK	ILE	SEE REMARK 999	UNP P05759
Cf	92	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	93	UNK	HIS	SEE REMARK 999	UNP P05759
Cf	94	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	95	UNK	HIS	SEE REMARK 999	UNP P05759
Cf	96	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	97	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	98	UNK	VAL	SEE REMARK 999	UNP P05759
Cf	99	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	100	UNK	LEU	SEE REMARK 999	UNP P05759
Cf	101	UNK	ALA	SEE REMARK 999	UNP P05759

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	Ag	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
34	Cg	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	Ah	159	Total	C	N	O	0	0	0
			1105	653	221	231			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	9	UNK	GLY	SEE REMARK 999	UNP P39015
Ah	10	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	11	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	12	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	13	UNK	GLU	SEE REMARK 999	UNP P39015

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Chain	Residue	Modelled	Actual	Comment	Reference
Ah	14	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	15	UNK	ALA	SEE REMARK 999	UNP P39015
Ah	16	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	17	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	18	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	19	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	20	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	151	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	152	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	153	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	154	UNK	TYR	SEE REMARK 999	UNP P39015
Ah	155	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	156	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	157	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	158	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	159	UNK	ALA	SEE REMARK 999	UNP P39015
Ah	160	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	161	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	162	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	163	UNK	PHE	SEE REMARK 999	UNP P39015
Ah	164	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	165	UNK	LYS	SEE REMARK 999	UNP P39015
Ah	166	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	167	UNK	PRO	SEE REMARK 999	UNP P39015
Ah	168	UNK	GLU	SEE REMARK 999	UNP P39015
Ah	169	UNK	ALA	SEE REMARK 999	UNP P39015
Ah	170	UNK	LYS	SEE REMARK 999	UNP P39015
Ah	171	UNK	LYS	SEE REMARK 999	UNP P39015
Ah	172	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	173	UNK	GLU	SEE REMARK 999	UNP P39015
Ah	174	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	175	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	176	UNK	ALA	SEE REMARK 999	UNP P39015

- Molecule 36 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	A1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	A5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	A3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	A7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 38 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	A4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	A8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BA	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	DA	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BB	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	DB	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BC	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	DC	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BD	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DD	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BE	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	DE	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BF	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	DF	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BG	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	DG	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BH	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	DH	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BI	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
47	DI	213	Total	C	N	O	S	0	0	0
			1722	1094	325	297	6			

- Molecule 48 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BJ	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
48	DJ	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BL	193	Total	C	N	O		0	0	0
			1543	962	315	266				
49	DL	194	Total	C	N	O		0	0	0
			1548	965	316	267				

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BM	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	DM	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BN	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	DN	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 52 is a protein called 60S ribosomal protein L16-A, 60S ribosomal protein L16-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BO	197	Total	C	N	O	S	0	197	0
			3119	2008	581	528	2			
52	DO	197	Total	C	N	O	S	0	197	0
			3119	2008	581	528	2			

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	BP	183	Total	C	N	O	0	0	0
			1420	882	281	257			
53	DP	155	Total	C	N	O	0	0	0
			1227	764	238	225			

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BQ	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	DQ	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BR	188	Total	C	N	O	0	0	0
			1521	935	326	260			
55	DR	188	Total	C	N	O	0	0	0
			1521	935	326	260			

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BS	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	DS	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BT	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
57	DT	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	BU	100	Total	C	N	O	0	0	0
			796	516	131	149			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	DU	98	Total	C	N	O	0	0	0
			778	505	127	146			

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BV	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
59	DV	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BW	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
60	DW	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	BX	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	DX	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	BY	126	Total	C	N	O	0	0	0
			993	625	192	176			
62	DY	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	BZ	135	Total	C	N	O	0	0	0
			1092	710	202	180			
63	DZ	135	Total	C	N	O	0	0	0
			1092	710	202	180			

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	Ba	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	Da	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	Bb	58	Total	C	N	O	S	0	0	0
			462	289	100	73				
65	Db	58	Total	C	N	O	S	0	0	0
			462	289	100	73				

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	Bc	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	Dc	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	Bd	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
67	Dd	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	Be	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	De	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	Bf	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	Df	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	Bg	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	Dg	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	Bh	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	Dh	119	Total	C	N	O	S	0	0	0
			965	612	185	167	1			

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	Bi	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	Di	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	Bj	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
73	Dj	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	Bk	77	Total	C	N	O	0	0	0
			612	391	115	106			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	Dk	77	Total	C	N	O	0	0	0
			608	388	114	106			

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	Bl	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
75	Dl	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 76 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Bm	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	Dm	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Bn	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	Dn	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Bo	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
78	Do	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	Bp	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	Dp	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 80 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	A6	1795	Total	C	N	O	P	0	1	0
			38021	16989	6669	12567	1796			

- Molecule 81 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
81	Ch	104	Total	C	N	O	0	0	0
			680	403	140	137			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	119	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	120	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	121	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	122	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	123	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	124	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	125	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	126	UNK	ASP	SEE REMARK 999	UNP P39015
Ch	127	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	128	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	129	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	130	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	131	UNK	ILE	SEE REMARK 999	UNP P39015
Ch	132	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	133	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	134	UNK	ASP	SEE REMARK 999	UNP P39015
Ch	135	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	136	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	137	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	138	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	139	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	155	UNK	LEU	SEE REMARK 999	UNP P39015
Ch	156	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	157	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	158	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	159	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	160	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	161	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	162	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	163	UNK	PHE	SEE REMARK 999	UNP P39015

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Chain	Residue	Modelled	Actual	Comment	Reference
Ch	164	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	165	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	166	UNK	VAL	SEE REMARK 999	UNP P39015
Ch	167	UNK	PRO	SEE REMARK 999	UNP P39015
Ch	168	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	169	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	170	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	171	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	172	UNK	VAL	SEE REMARK 999	UNP P39015
Ch	173	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	174	UNK	LEU	SEE REMARK 999	UNP P39015

- Molecule 82 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
82	DK	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	Dq	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Dq	199	UNK	SER	SEE REMARK 999	UNP P05317
Dq	200	UNK	SER	SEE REMARK 999	UNP P05317
Dq	201	UNK	ILE	SEE REMARK 999	UNP P05317
Dq	202	UNK	LEU	SEE REMARK 999	UNP P05317
Dq	203	UNK	ASP	SEE REMARK 999	UNP P05317
Dq	204	UNK	ILE	SEE REMARK 999	UNP P05317
Dq	205	UNK	THR	SEE REMARK 999	UNP P05317
Dq	206	UNK	ASP	SEE REMARK 999	UNP P05317
Dq	207	UNK	GLU	SEE REMARK 999	UNP P05317
Dq	208	UNK	GLU	SEE REMARK 999	UNP P05317
Dq	209	UNK	LEU	SEE REMARK 999	UNP P05317
Dq	210	UNK	VAL	SEE REMARK 999	UNP P05317
Dq	211	UNK	SER	SEE REMARK 999	UNP P05317
Dq	212	UNK	HIS	SEE REMARK 999	UNP P05317
Dq	213	UNK	PHE	SEE REMARK 999	UNP P05317

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Chain	Residue	Modelled	Actual	Comment	Reference
Dq	214	UNK	VAL	SEE REMARK 999	UNP P05317
Dq	215	UNK	SER	SEE REMARK 999	UNP P05317
Dq	216	UNK	ALA	SEE REMARK 999	UNP P05317
Dq	217	UNK	VAL	SEE REMARK 999	UNP P05317
Dq	218	UNK	SER	SEE REMARK 999	UNP P05317
Dq	219	UNK	THR	SEE REMARK 999	UNP P05317
Dq	220	UNK	ILE	SEE REMARK 999	UNP P05317
Dq	221	UNK	ALA	SEE REMARK 999	UNP P05317

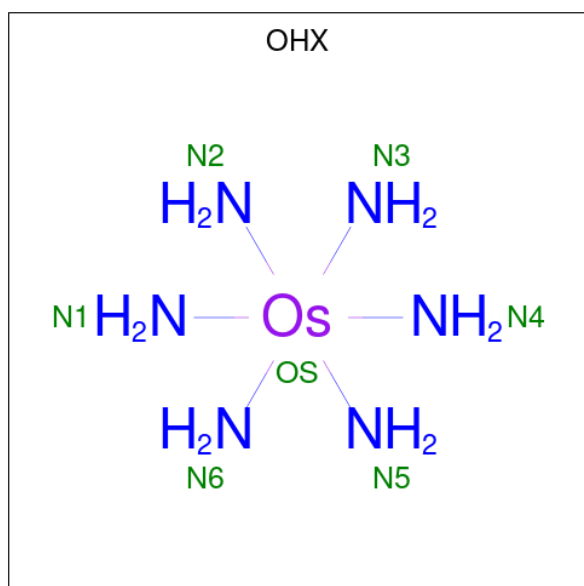
- Molecule 84 is a protein called Ribosomal protein P1 alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
84	Dr	47	Total	C	N	O	0	0	0
			235	141	47	47			

- Molecule 85 is a protein called Ribosomal protein P2 beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
85	Ds	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
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86	A2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
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86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
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86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
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86	A2	1	Total	N	Os	0	0
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86	A2	1	Total	N	Os	0	0
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86	A2	1	Total	N	Os	0	0
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86	A2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A2	1	Total	N	Os	0	0
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86	AC	1	Total	N	Os	0	0
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86	AI	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	AN	1	Total	N	Os	0	0
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86	AP	1	Total	N	Os	0	0
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86	Ad	1	Total	N	Os	0	0
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86	Ag	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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			7	6	1		
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A3	1	Total	N	Os	0	0
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86	A4	1	Total	N	Os	0	0
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86	A4	1	Total	N	Os	0	0
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86	A4	1	Total	N	Os	0	0
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86	A4	1	Total	N	Os	0	0
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			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A4	1	Total	N	Os	0	0
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86	A4	1	Total	N	Os	0	0
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86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
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86	BA	1	Total	N	Os	0	0
			7	6	1		
86	BB	1	Total	N	Os	0	0
			7	6	1		
86	BB	1	Total	N	Os	0	0
			7	6	1		
86	BC	1	Total	N	Os	0	0
			7	6	1		
86	BD	1	Total	N	Os	0	0
			7	6	1		
86	BI	1	Total	N	Os	0	0
			7	6	1		
86	BI	1	Total	N	Os	0	0
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86	BI	1	Total	N	Os	0	0
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86	BI	1	Total	N	Os	0	0
			7	6	1		
86	BN	1	Total	N	Os	0	0
			7	6	1		
86	BO	1	Total	N	Os	0	0
			7	6	1		
86	BP	1	Total	N	Os	0	0
			7	6	1		
86	BP	1	Total	N	Os	0	0
			7	6	1		
86	BR	1	Total	N	Os	0	0
			7	6	1		
86	BT	1	Total	N	Os	0	0
			7	6	1		
86	Bb	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	Bj	1	Total	N	Os	0	0
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86	Bj	1	Total	N	Os	0	0
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86	Bj	1	Total	N	Os	0	0
			7	6	1		
86	Bo	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A6	1	Total	N	Os	0	0
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86	A6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	CB	1	Total	N	Os	0	0
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86	CG	1	Total	N	Os	0	0
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86	CG	1	Total	N	Os	0	0
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86	CI	1	Total	N	Os	0	0
			7	6	1		
86	CJ	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	CP	1	Total	N	Os	0	0
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86	CS	1	Total	N	Os	0	0
			7	6	1		
86	CY	1	Total	N	Os	0	0
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86	CY	1	Total	N	Os	0	0
			7	6	1		
86	Cd	1	Total	N	Os	0	0
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86	Cg	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
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86	A5	1	Total	N	Os	0	0
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86	A5	1	Total	N	Os	0	0
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86	A5	1	Total	N	Os	0	0
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86	A5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A5	1	Total	N	Os	0	0
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86	A5	1	Total	N	Os	0	0
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86	A5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A5	1	Total	N	Os	0	0
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86	A5	1	Total	N	Os	0	0
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86	A5	1	Total	N	Os	0	0
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86	A5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		
86	DA	1	Total	N	Os	0	0
			7	6	1		
86	DB	1	Total	N	Os	0	0
			7	6	1		
86	DB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	DC	1	Total	N	Os	0	0
			7	6	1		
86	DC	1	Total	N	Os	0	0
			7	6	1		
86	DD	1	Total	N	Os	0	0
			7	6	1		
86	DG	1	Total	N	Os	0	0
			7	6	1		
86	DH	1	Total	N	Os	0	0
			7	6	1		
86	DI	1	Total	N	Os	0	0
			7	6	1		
86	DI	1	Total	N	Os	0	0
			7	6	1		
86	DJ	1	Total	N	Os	0	0
			7	6	1		
86	DM	1	Total	N	Os	0	0
			7	6	1		
86	DO	1	Total	N	Os	0	0
			7	6	1		
86	DP	1	Total	N	Os	0	0
			7	6	1		
86	DQ	1	Total	N	Os	0	0
			7	6	1		
86	DR	1	Total	N	Os	0	0
			7	6	1		
86	DV	1	Total	N	Os	0	0
			7	6	1		
86	Db	1	Total	N	Os	0	0
			7	6	1		
86	De	1	Total	N	Os	0	0
			7	6	1		
86	Df	1	Total	N	Os	0	0
			7	6	1		
86	Dg	1	Total	N	Os	0	0
			7	6	1		
86	Dh	1	Total	N	Os	0	0
			7	6	1		
86	Dj	1	Total	N	Os	0	0
			7	6	1		
86	Do	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	A2	171	Total 171	Mg 171	0	0
87	AB	2	Total 2	Mg 2	0	0
87	AC	1	Total 1	Mg 1	0	0
87	AE	1	Total 1	Mg 1	0	0
87	AI	2	Total 2	Mg 2	0	0
87	AJ	1	Total 1	Mg 1	0	0
87	AL	2	Total 2	Mg 2	0	0
87	AN	1	Total 1	Mg 1	0	0
87	AP	1	Total 1	Mg 1	0	0
87	AS	2	Total 2	Mg 2	0	0
87	AX	1	Total 1	Mg 1	0	0
87	Aa	1	Total 1	Mg 1	0	0
87	Ad	3	Total 3	Mg 3	0	0
87	Af	1	Total 1	Mg 1	0	0
87	A1	695	Total 695	Mg 695	0	0
87	A3	19	Total 19	Mg 19	0	0
87	A4	34	Total 34	Mg 34	0	0
87	BA	5	Total 5	Mg 5	0	0
87	BB	4	Total 4	Mg 4	0	0
87	BC	6	Total 6	Mg 6	0	0
87	BD	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	BE	1	Total 1	Mg 1	0	0
87	BF	2	Total 2	Mg 2	0	0
87	BG	1	Total 1	Mg 1	0	0
87	BI	4	Total 4	Mg 4	0	0
87	BJ	1	Total 1	Mg 1	0	0
87	BL	5	Total 5	Mg 5	0	0
87	BN	6	Total 6	Mg 6	0	0
87	BO	8	Total 8	Mg 8	0	0
87	BP	10	Total 10	Mg 10	0	0
87	BQ	4	Total 4	Mg 4	0	0
87	BR	4	Total 4	Mg 4	0	0
87	BS	2	Total 2	Mg 2	0	0
87	BT	1	Total 1	Mg 1	0	0
87	BV	5	Total 5	Mg 5	0	0
87	BY	2	Total 2	Mg 2	0	0
87	Ba	8	Total 8	Mg 8	0	0
87	Bd	1	Total 1	Mg 1	0	0
87	Be	2	Total 2	Mg 2	0	0
87	Bf	1	Total 1	Mg 1	0	0
87	Bg	1	Total 1	Mg 1	0	0
87	Bj	7	Total 7	Mg 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	Bl	1	Total 1	Mg 1	0	0
87	Bm	1	Total 1	Mg 1	0	0
87	Bo	3	Total 3	Mg 3	0	0
87	A6	239	Total 239	Mg 239	0	0
87	CB	1	Total 1	Mg 1	0	0
87	CE	1	Total 1	Mg 1	0	0
87	CF	2	Total 2	Mg 2	0	0
87	CG	2	Total 2	Mg 2	0	0
87	CI	2	Total 2	Mg 2	0	0
87	CL	3	Total 3	Mg 3	0	0
87	CP	1	Total 1	Mg 1	0	0
87	CQ	2	Total 2	Mg 2	0	0
87	CS	2	Total 2	Mg 2	0	0
87	CX	2	Total 2	Mg 2	0	0
87	CY	2	Total 2	Mg 2	0	0
87	CZ	1	Total 1	Mg 1	0	0
87	Ca	1	Total 1	Mg 1	0	0
87	Cd	1	Total 1	Mg 1	0	0
87	Ch	2	Total 2	Mg 2	0	0
87	A5	763	Total 763	Mg 763	0	0
87	A7	26	Total 26	Mg 26	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	A8	20	Total 20	Mg 20	0	0
87	DA	4	Total 4	Mg 4	0	0
87	DB	13	Total 13	Mg 13	0	0
87	DC	5	Total 5	Mg 5	0	0
87	DD	7	Total 7	Mg 7	0	0
87	DF	4	Total 4	Mg 4	0	0
87	DG	1	Total 1	Mg 1	0	0
87	DH	2	Total 2	Mg 2	0	0
87	DJ	2	Total 2	Mg 2	0	0
87	DL	1	Total 1	Mg 1	0	0
87	DM	2	Total 2	Mg 2	0	0
87	DN	1	Total 1	Mg 1	0	0
87	DO	8	Total 8	Mg 8	0	0
87	DP	7	Total 7	Mg 7	0	0
87	DQ	1	Total 1	Mg 1	0	0
87	DR	1	Total 1	Mg 1	0	0
87	DS	4	Total 4	Mg 4	0	0
87	DT	3	Total 3	Mg 3	0	0
87	DV	3	Total 3	Mg 3	0	0
87	DW	1	Total 1	Mg 1	0	0
87	DY	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	Da	4	Total 4	Mg 4	0	0
87	Db	1	Total 1	Mg 1	0	0
87	Dd	1	Total 1	Mg 1	0	0
87	De	2	Total 2	Mg 2	0	0
87	Df	4	Total 4	Mg 4	0	0
87	Dg	2	Total 2	Mg 2	0	0
87	Dj	3	Total 3	Mg 3	0	0
87	Dl	1	Total 1	Mg 1	0	0
87	Dm	1	Total 1	Mg 1	0	0
87	Dn	1	Total 1	Mg 1	0	0
87	Do	1	Total 1	Mg 1	0	0
87	Dp	3	Total 3	Mg 3	0	0
87	Dq	1	Total 1	Mg 1	0	0

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	Aa	1	Total 1	Zn 1	0	0
88	Ab	1	Total 1	Zn 1	0	0
88	Ad	1	Total 1	Zn 1	0	0
88	Af	1	Total 1	Zn 1	0	0
88	Bj	1	Total 1	Zn 1	0	0
88	Bm	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	Bo	1	Total 1	Zn 1	0	0
88	Bp	1	Total 1	Zn 1	0	0
88	Ca	1	Total 1	Zn 1	0	0
88	Cb	1	Total 1	Zn 1	0	0
88	Cd	1	Total 1	Zn 1	0	0
88	Cf	1	Total 1	Zn 1	0	0
88	Dj	1	Total 1	Zn 1	0	0
88	Dm	1	Total 1	Zn 1	0	0
88	Do	1	Total 1	Zn 1	0	0
88	Dp	1	Total 1	Zn 1	0	0

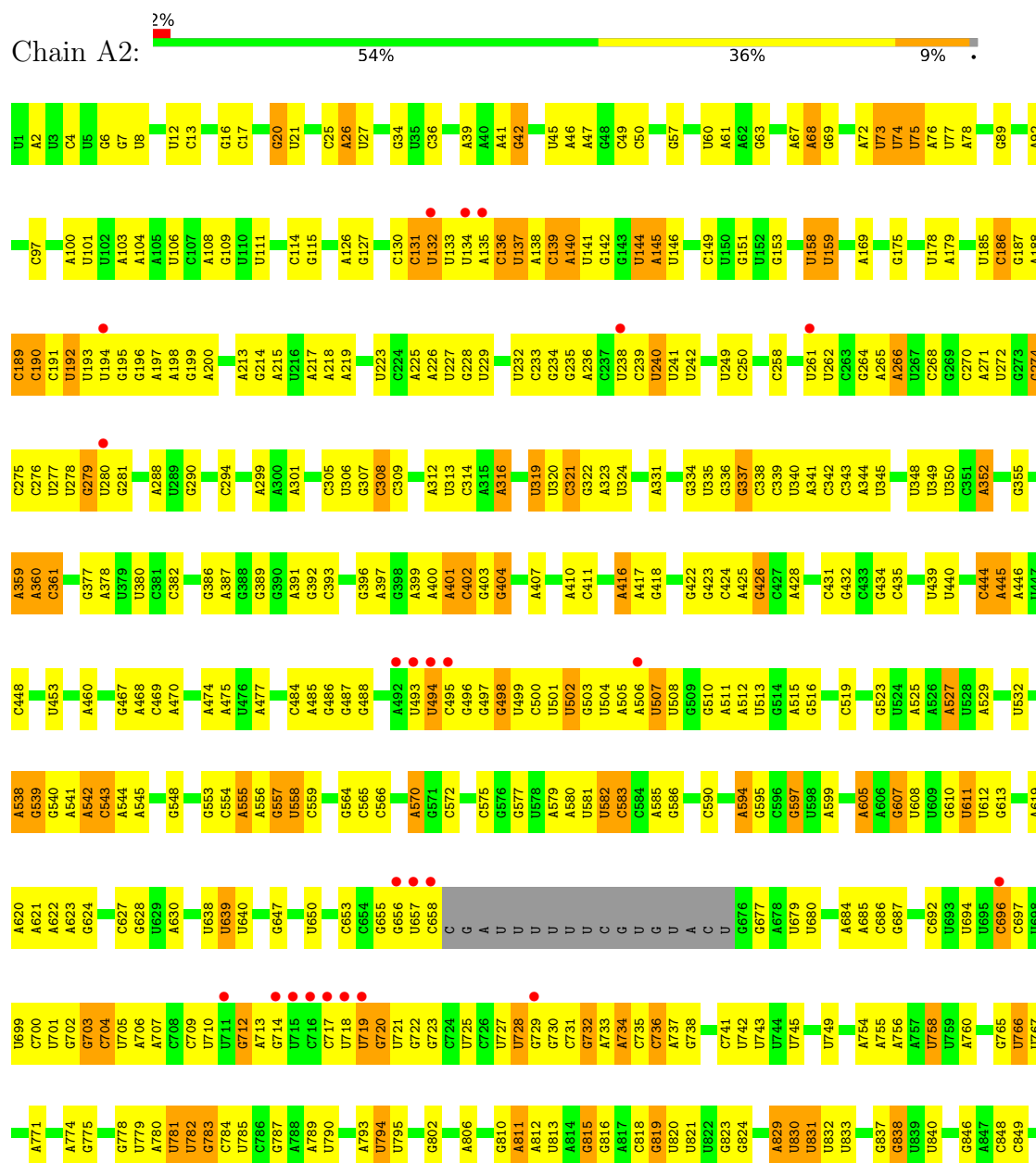
- Molecule 89 is water.

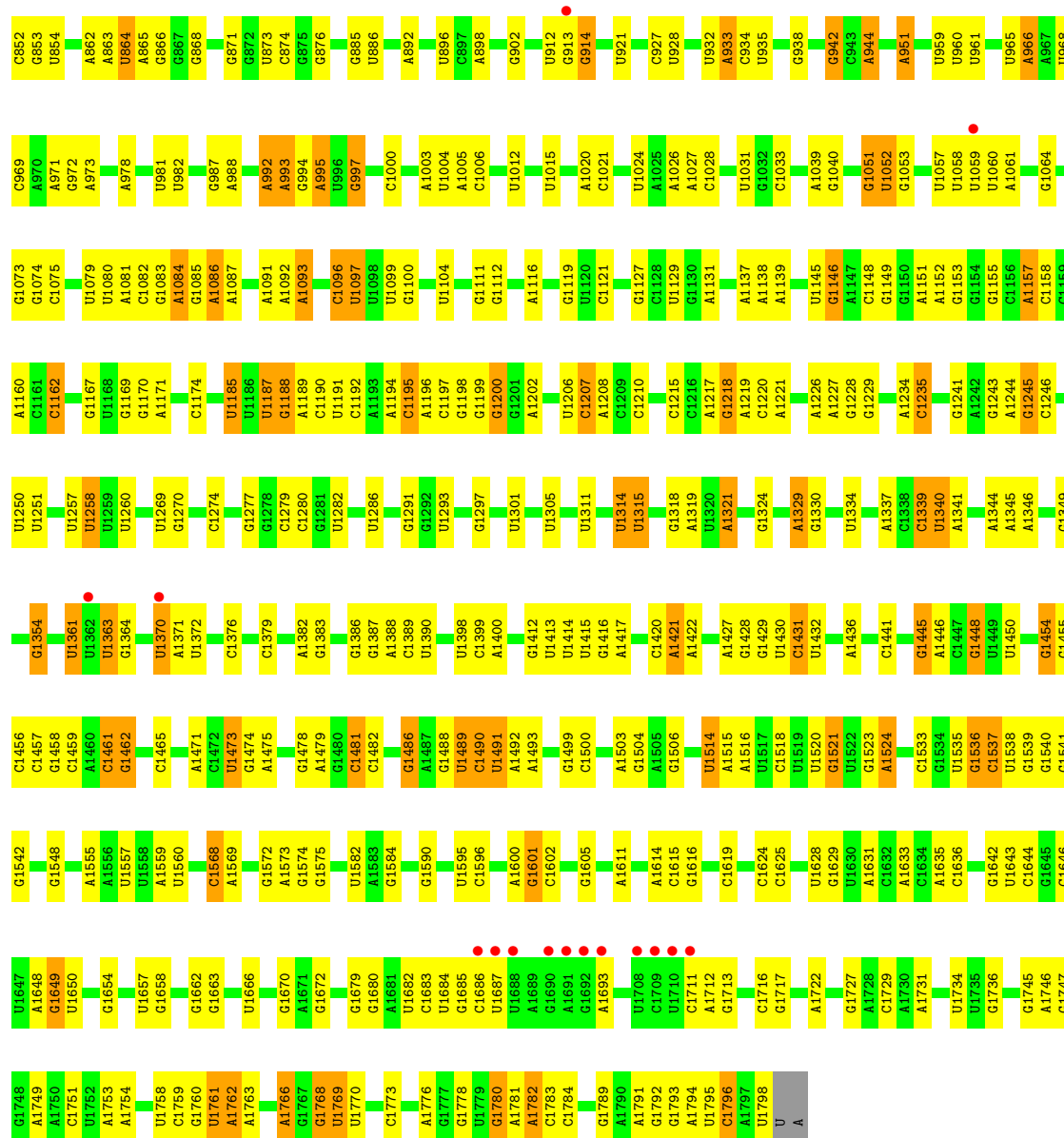
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	CI	1	Total 1	O 1	0	0
89	DB	1	Total 1	O 1	0	0

3 Residue-property plots

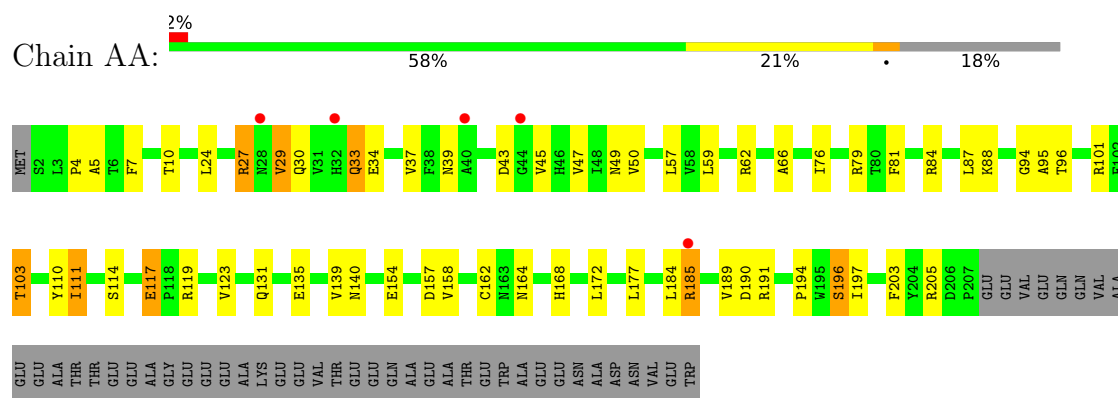
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

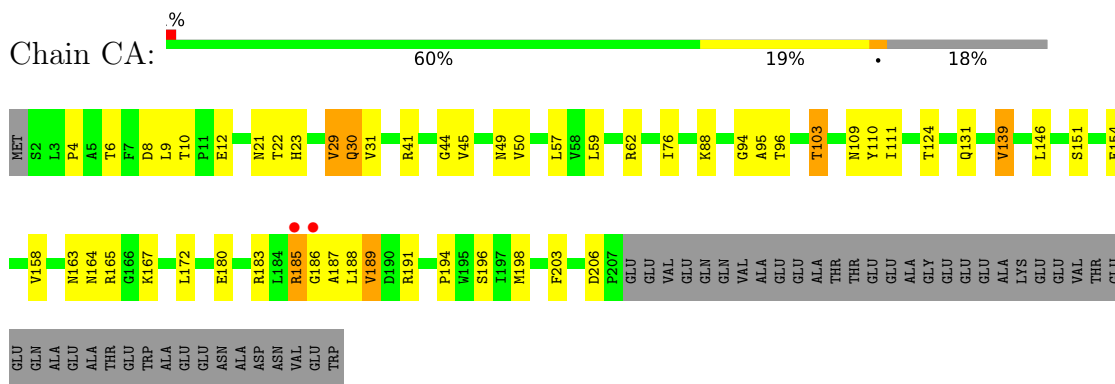
• Molecule 1: 18S RIBOSOMAL RNA



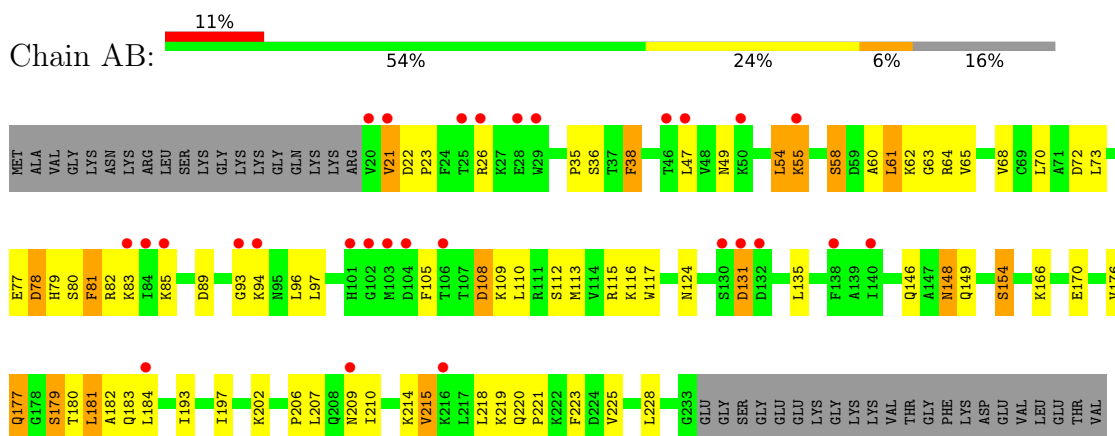


• Molecule 2: 40S ribosomal protein S0-A

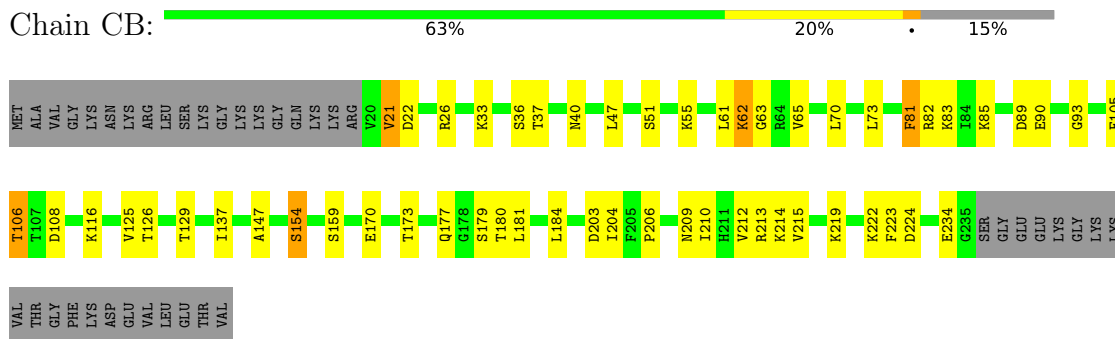




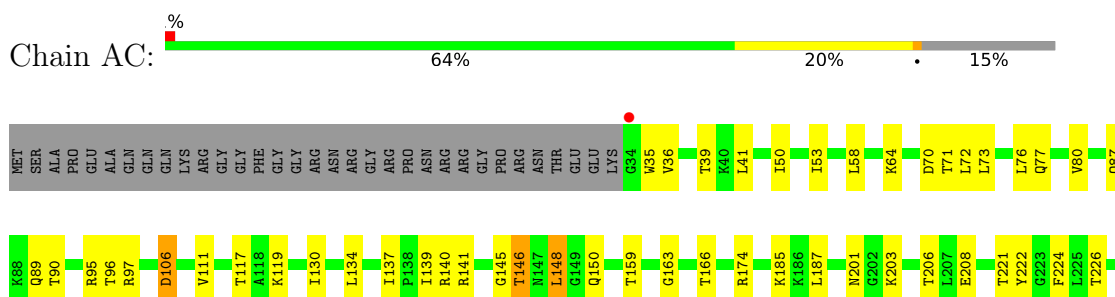
- Molecule 3: 40S ribosomal protein S1-A



- Molecule 3: 40S ribosomal protein S1-A

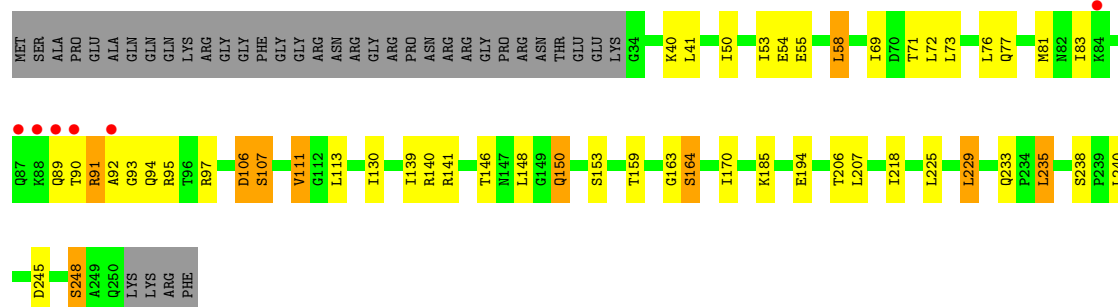


- Molecule 4: 40S ribosomal protein S2

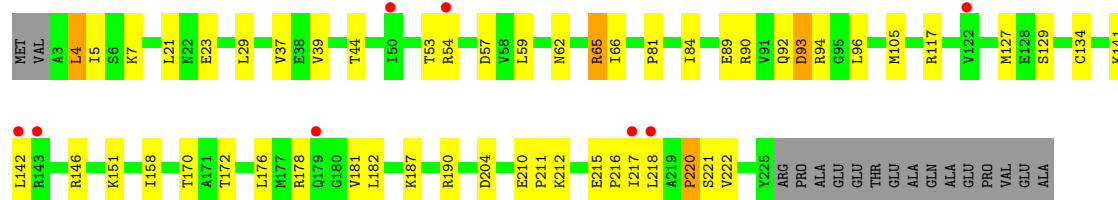
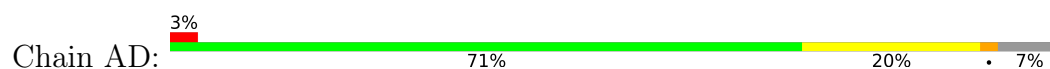




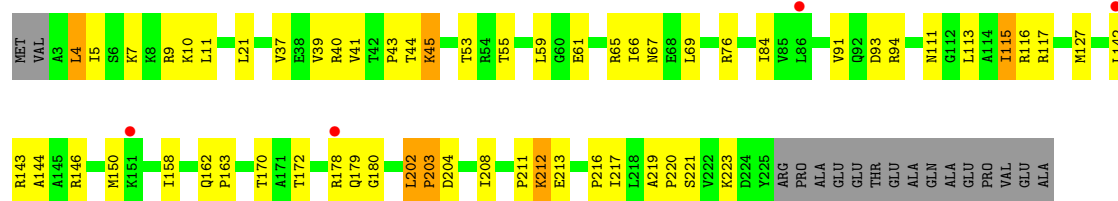
• Molecule 4: 40S ribosomal protein S2



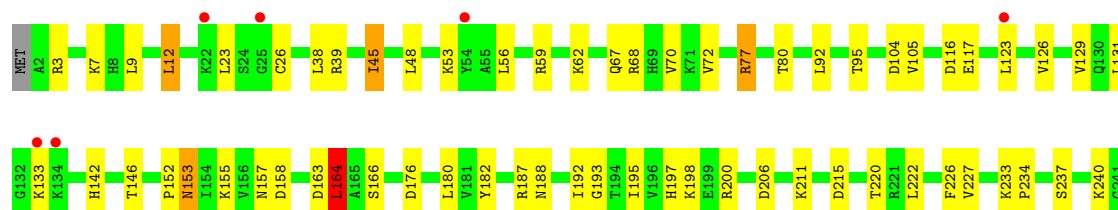
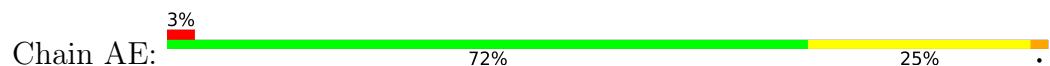
• Molecule 5: 40S ribosomal protein S3



• Molecule 5: 40S ribosomal protein S3



• Molecule 6: 40S ribosomal protein S4-A





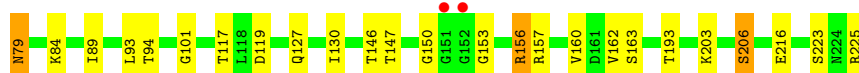
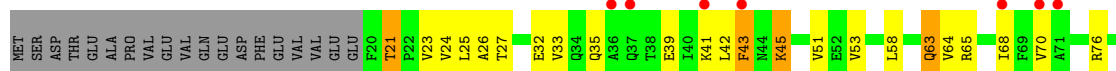
- Molecule 6: 40S ribosomal protein S4-A

Chain CE: 76% 22%



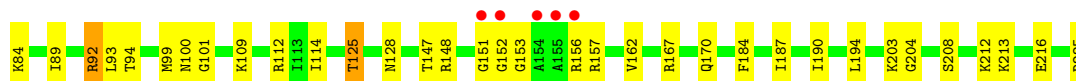
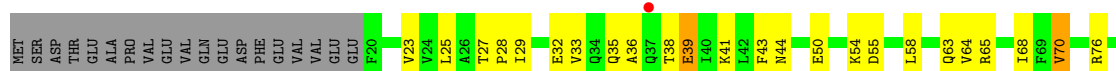
- Molecule 7: 40S ribosomal protein S5

Chain AF: 4% 70% 18% 8%



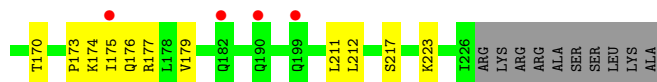
- Molecule 7: 40S ribosomal protein S5

Chain CF: 3% 66% 24% 8%



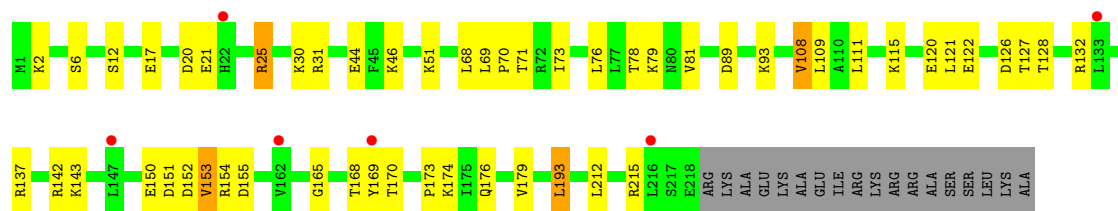
- Molecule 8: 40S ribosomal protein S6-A

Chain AG: 3% 76% 17% 2%

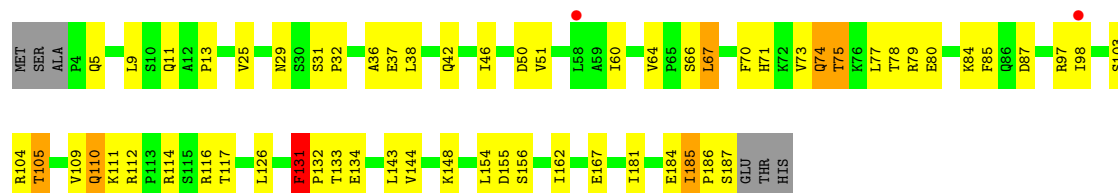


- Molecule 8: 40S ribosomal protein S6-A

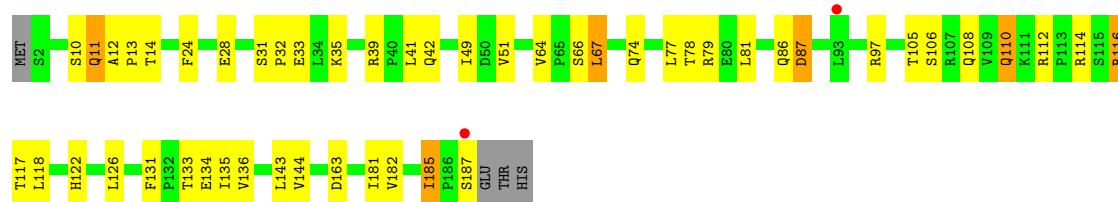
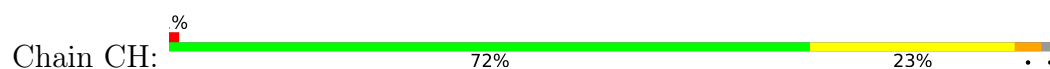
Chain CG: 3% 69% 21% 8%



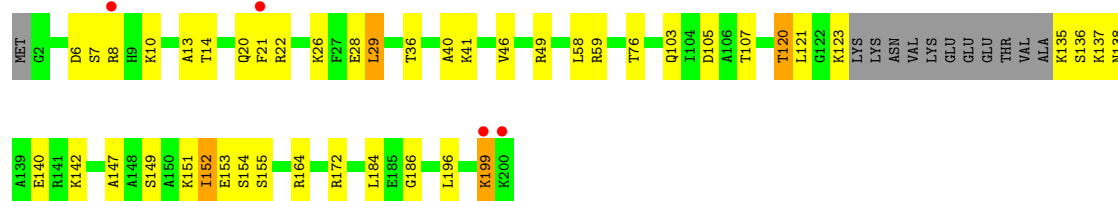
• Molecule 9: 40S ribosomal protein S7-A



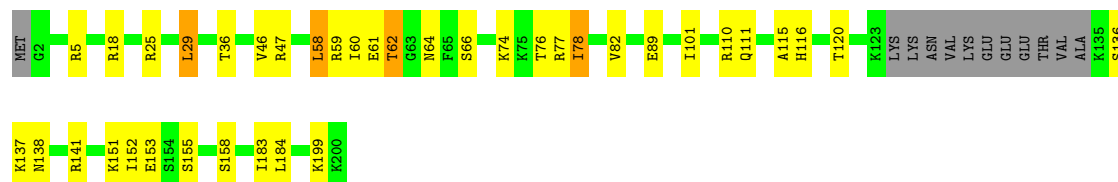
• Molecule 9: 40S ribosomal protein S7-A



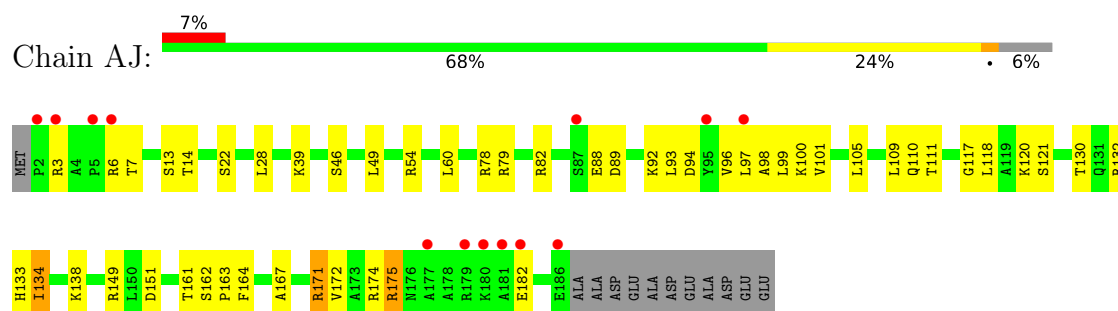
• Molecule 10: 40S ribosomal protein S8-A



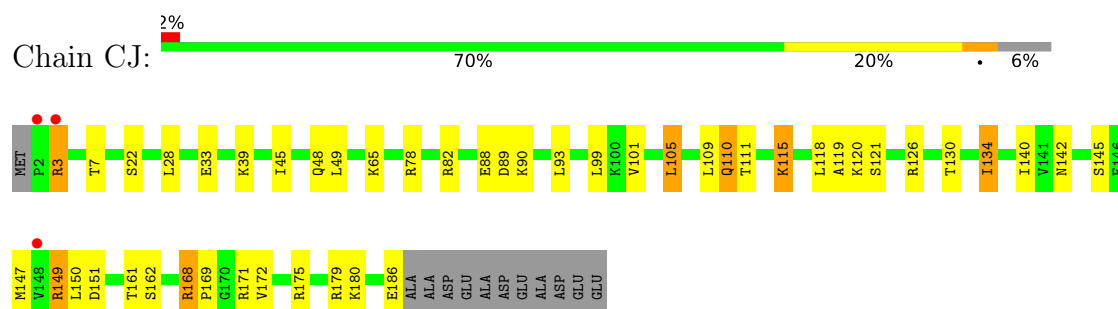
• Molecule 10: 40S ribosomal protein S8-A



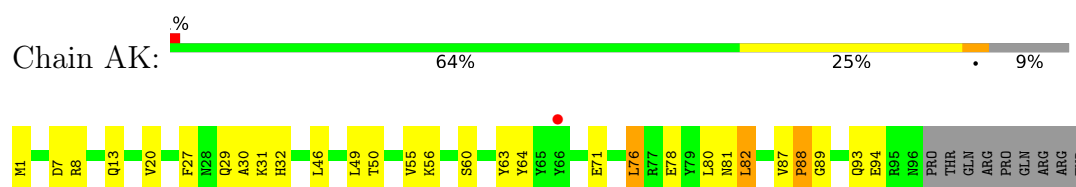
- Molecule 11: 40S ribosomal protein S9-A



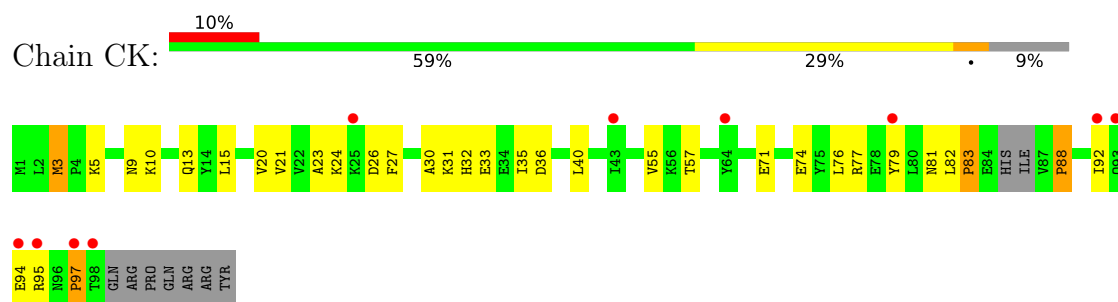
- Molecule 11: 40S ribosomal protein S9-A



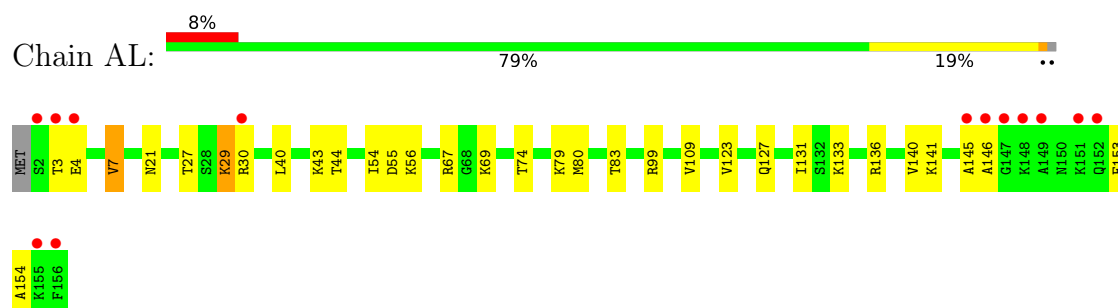
- Molecule 12: 40S ribosomal protein S10-A



- Molecule 12: 40S ribosomal protein S10-A

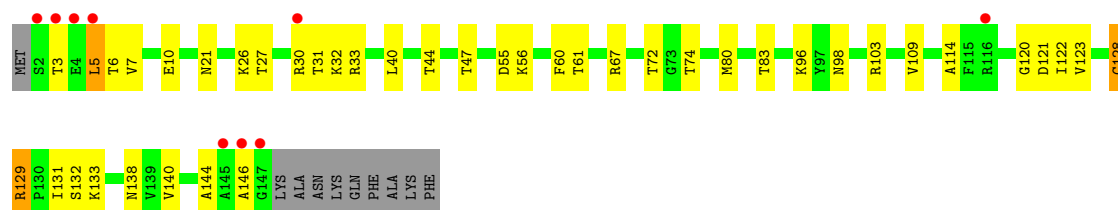


- Molecule 13: 40S ribosomal protein S11-A



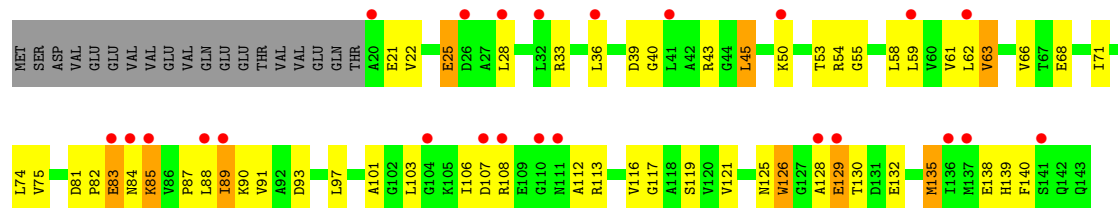
- Molecule 13: 40S ribosomal protein S11-A

Chain CL: 



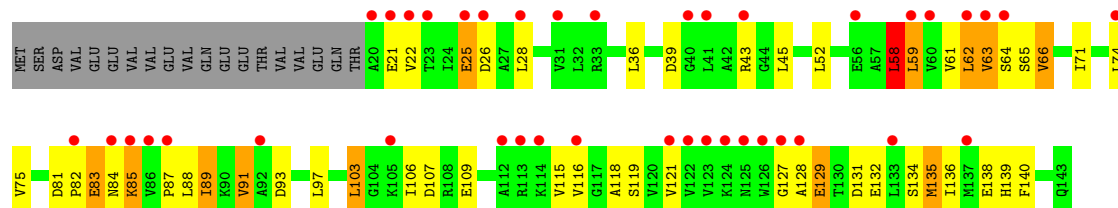
- Molecule 14: 40S ribosomal protein S12

Chain AM: 




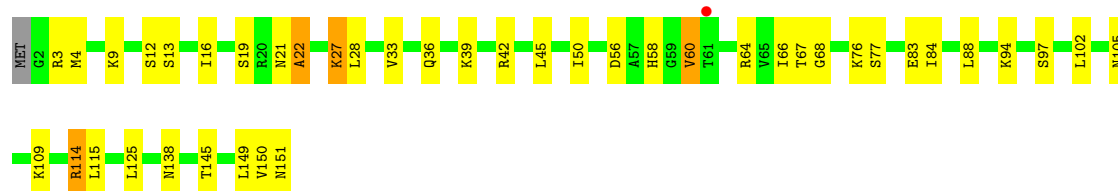
- Molecule 14: 40S ribosomal protein S12

Chain CM: 




- Molecule 15: 40S ribosomal protein S13

Chain AN: 

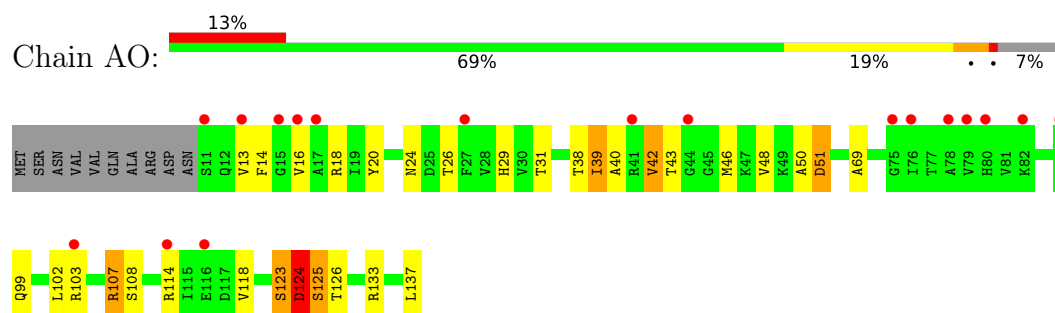


- Molecule 15: 40S ribosomal protein S13

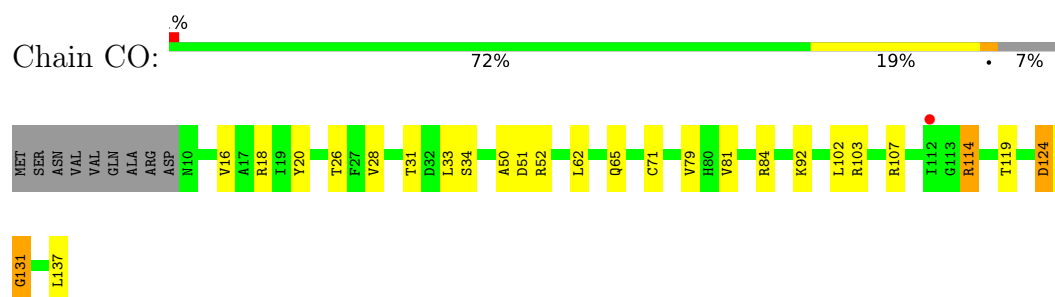
Chain CN: 



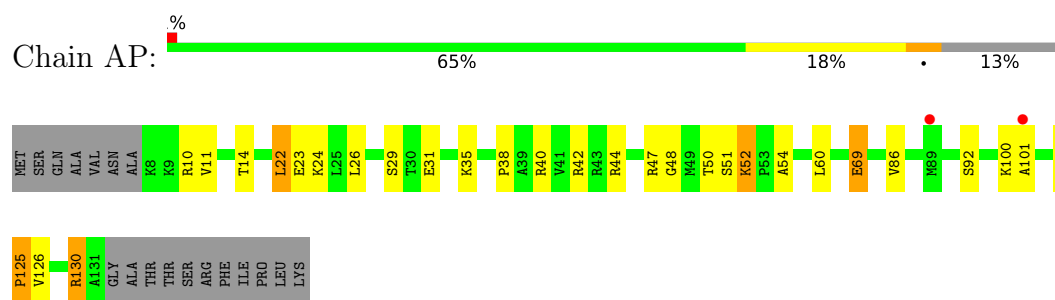
- Molecule 16: 40S ribosomal protein S14-A



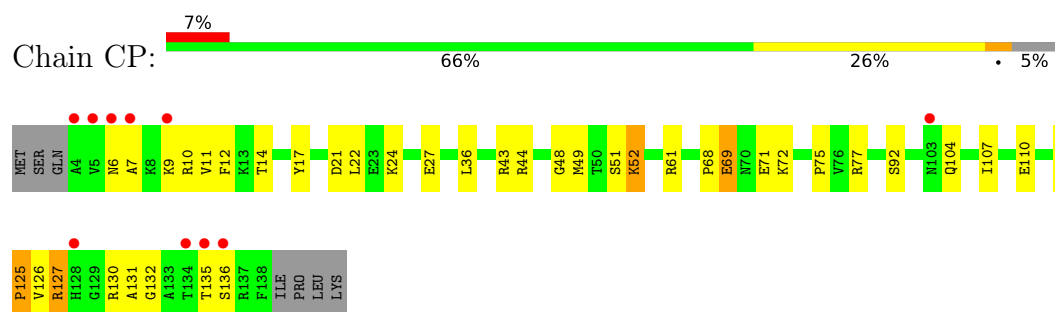
- Molecule 16: 40S ribosomal protein S14-A



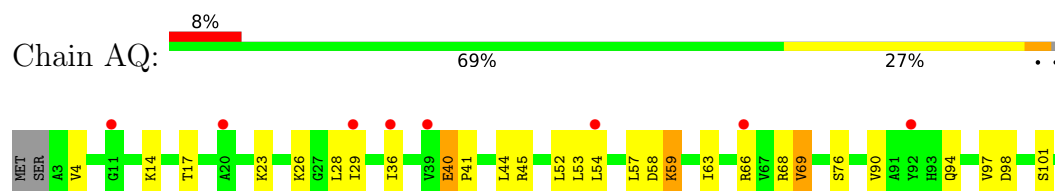
- Molecule 17: 40S ribosomal protein S15

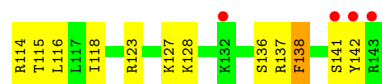


- Molecule 17: 40S ribosomal protein S15

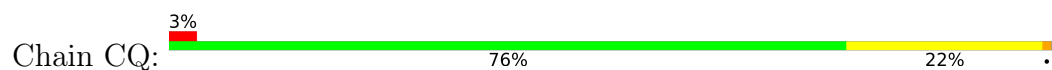


- Molecule 18: 40S ribosomal protein S16-A

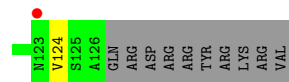




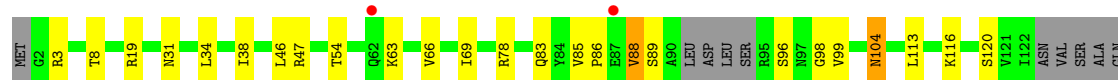
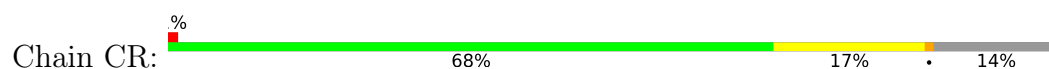
- Molecule 18: 40S ribosomal protein S16-A



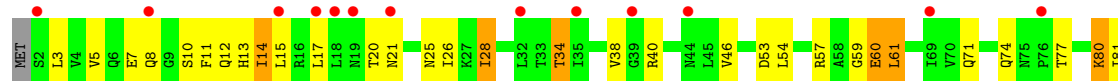
- Molecule 19: 40S ribosomal protein S17-A



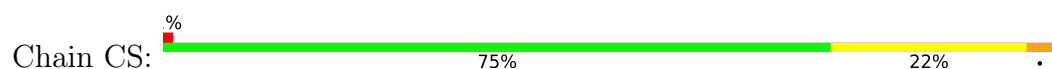
- Molecule 19: 40S ribosomal protein S17-A



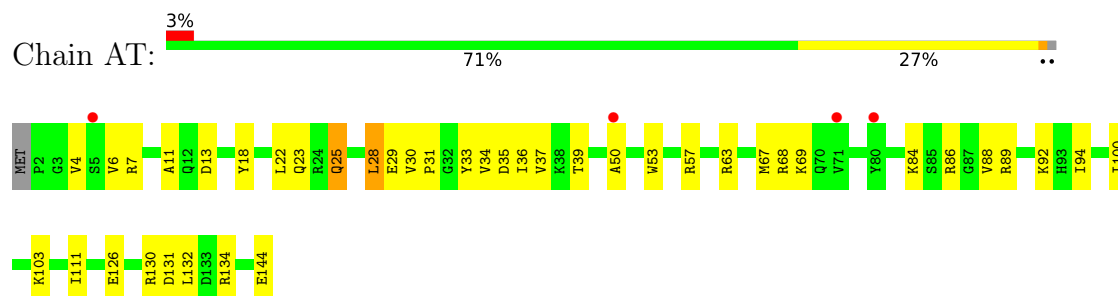
- Molecule 20: 40S ribosomal protein S18-A



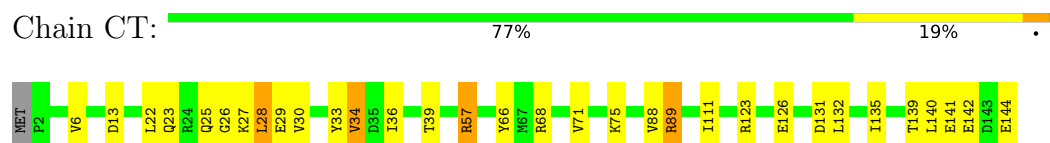
- Molecule 20: 40S ribosomal protein S18-A



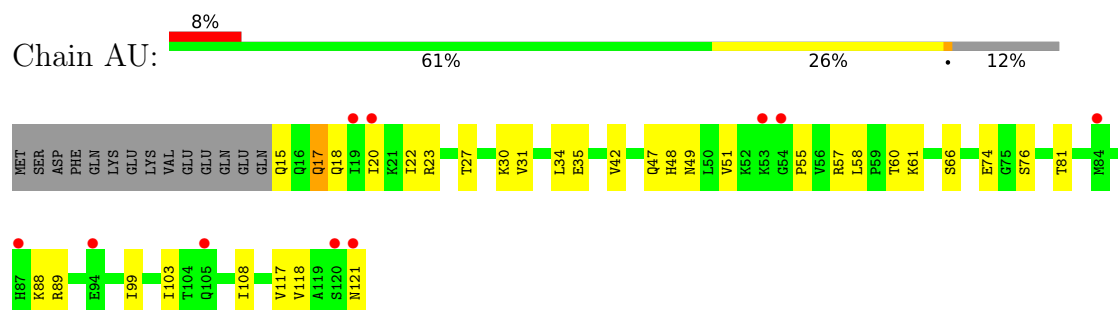
- Molecule 21: 40S ribosomal protein S19-A



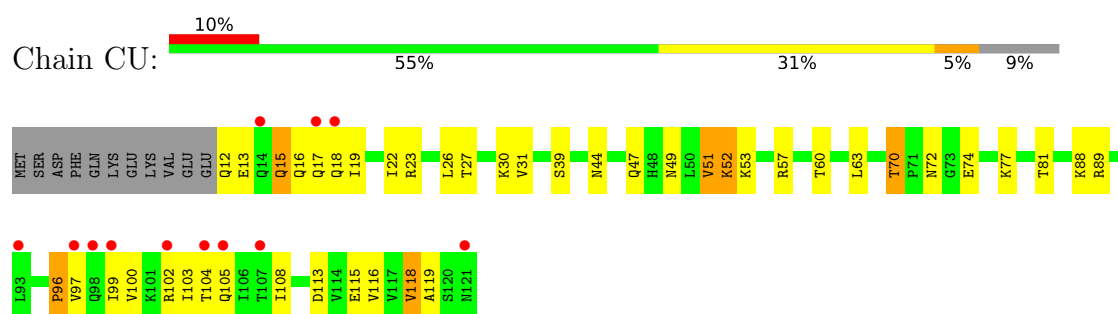
- Molecule 21: 40S ribosomal protein S19-A



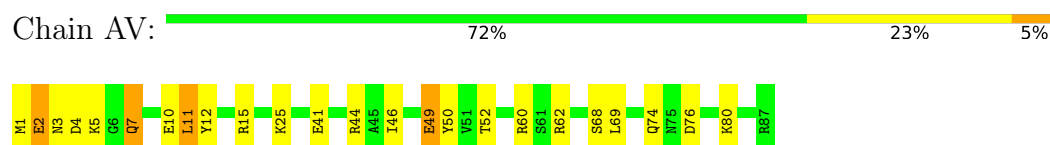
- Molecule 22: 40S ribosomal protein S20



- Molecule 22: 40S ribosomal protein S20



- Molecule 23: 40S ribosomal protein S21-A



- Molecule 23: 40S ribosomal protein S21-A





- Molecule 24: 40S ribosomal protein S22-A

Chain AW: 78% 17% ..



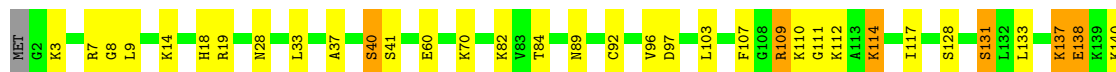
- Molecule 24: 40S ribosomal protein S22-A

Chain CW: 88% 10% ..



- Molecule 25: 40S ribosomal protein S23-A

Chain AX: 75% 19% 5% ..



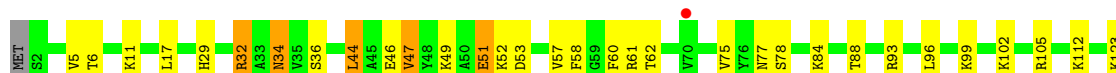
- Molecule 25: 40S ribosomal protein S23-A

Chain CX: 83% 15% ..



- Molecule 26: 40S ribosomal protein S24-A

Chain AY: 72% 24% ..

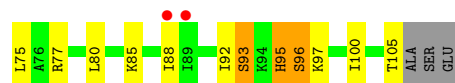
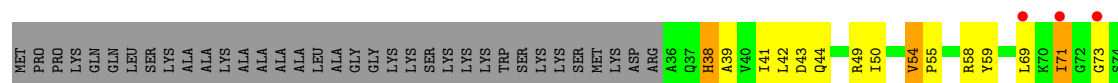


- Molecule 26: 40S ribosomal protein S24-A

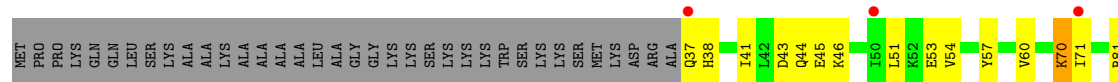
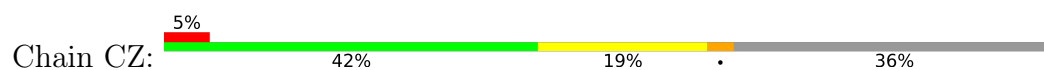
Chain CY: 73% 24% ..



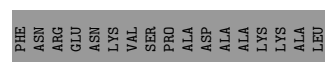
- Molecule 27: 40S ribosomal protein S25-A



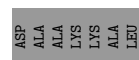
- Molecule 27: 40S ribosomal protein S25-A



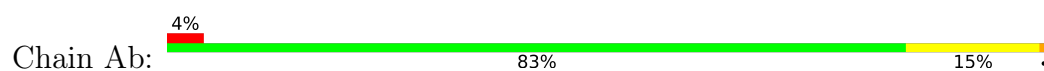
- Molecule 28: 40S ribosomal protein S26-A

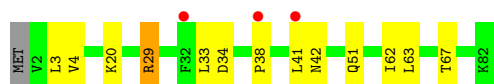


- Molecule 28: 40S ribosomal protein S26-A



- Molecule 29: 40S ribosomal protein S27-A





- Molecule 29: 40S ribosomal protein S27-A

Chain Cb: 73% 26% .



- Molecule 30: 40S ribosomal protein S28-A

Chain Ac: 4% 60% 34% 6%



- Molecule 30: 40S ribosomal protein S28-A

Chain Cc: 9% 64% 28% 6%



- Molecule 31: 40S ribosomal protein S29-A

Chain Ad: 4% 75% 16% 5%



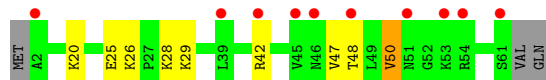
- Molecule 31: 40S ribosomal protein S29-A

Chain Cd: 5% 68% 23% 5%

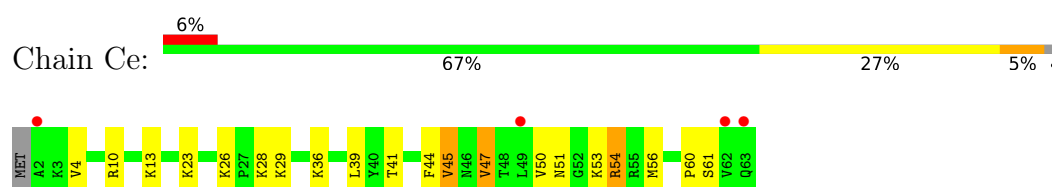


- Molecule 32: 40S ribosomal protein S30-A

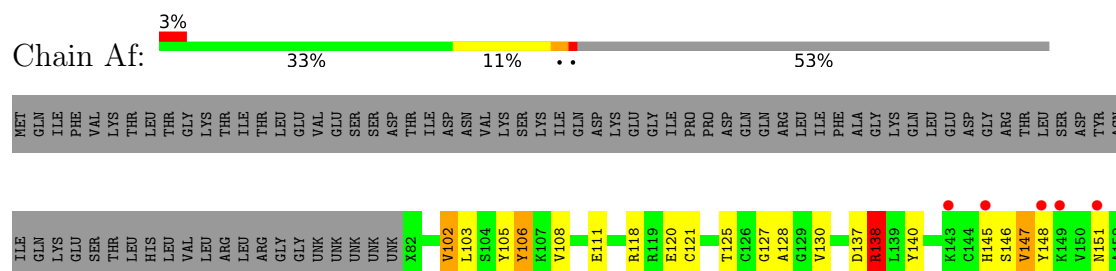
Chain Ae: 16% 81% 13% 5%



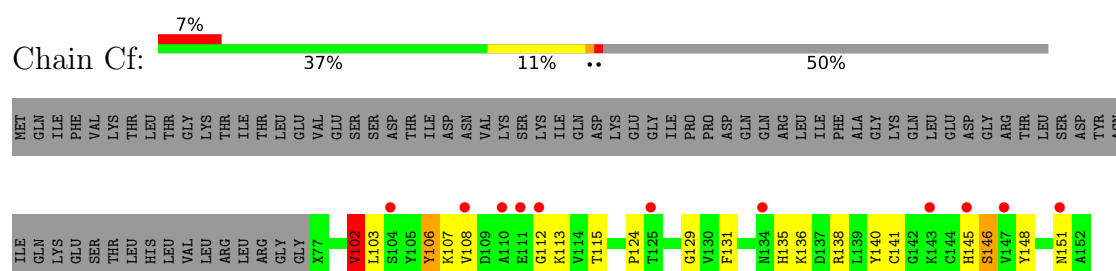
- Molecule 32: 40S ribosomal protein S30-A



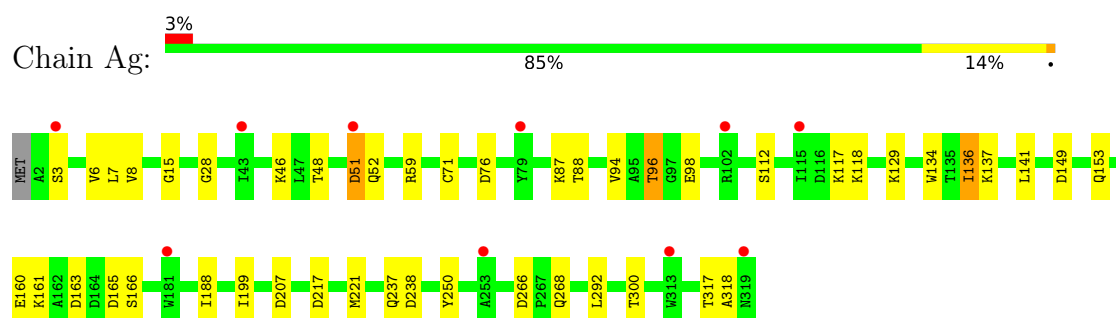
- Molecule 33: 40S ribosomal protein S31



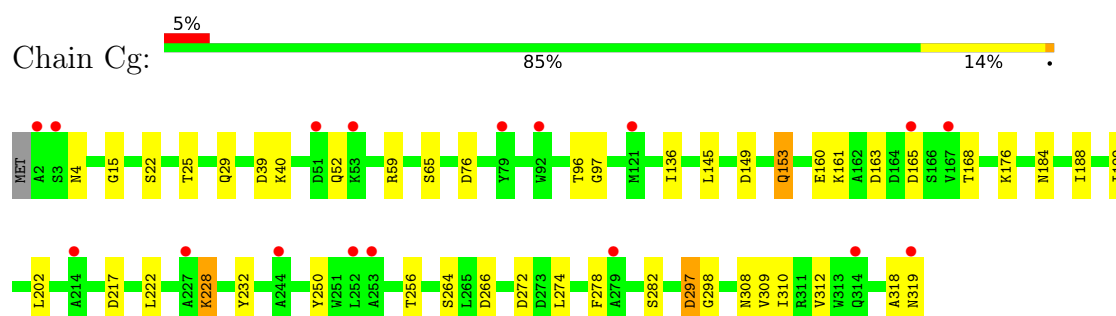
- Molecule 33: 40S ribosomal protein S31



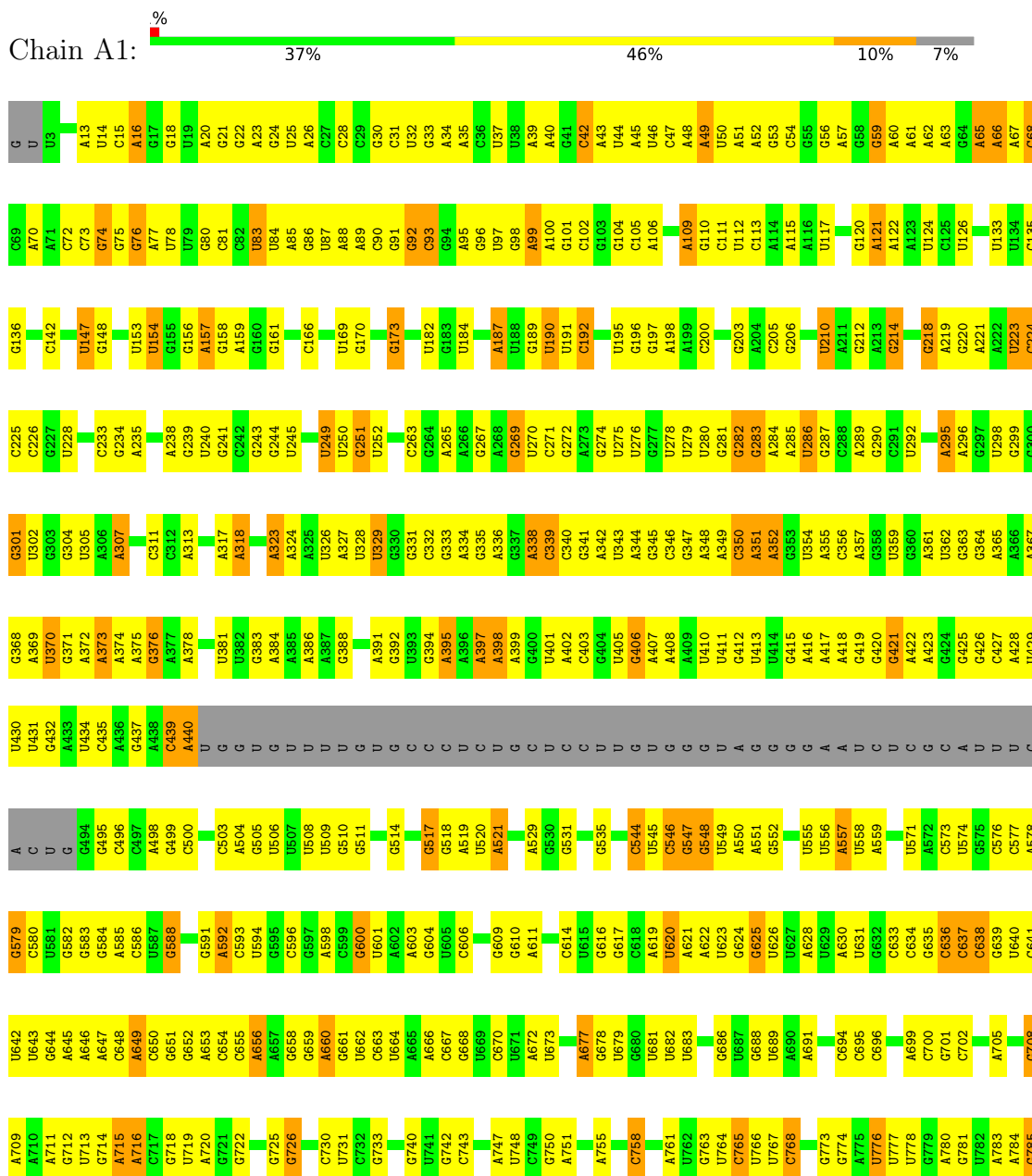
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1)



- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1)



- Molecule 35: Suppressor protein STM1



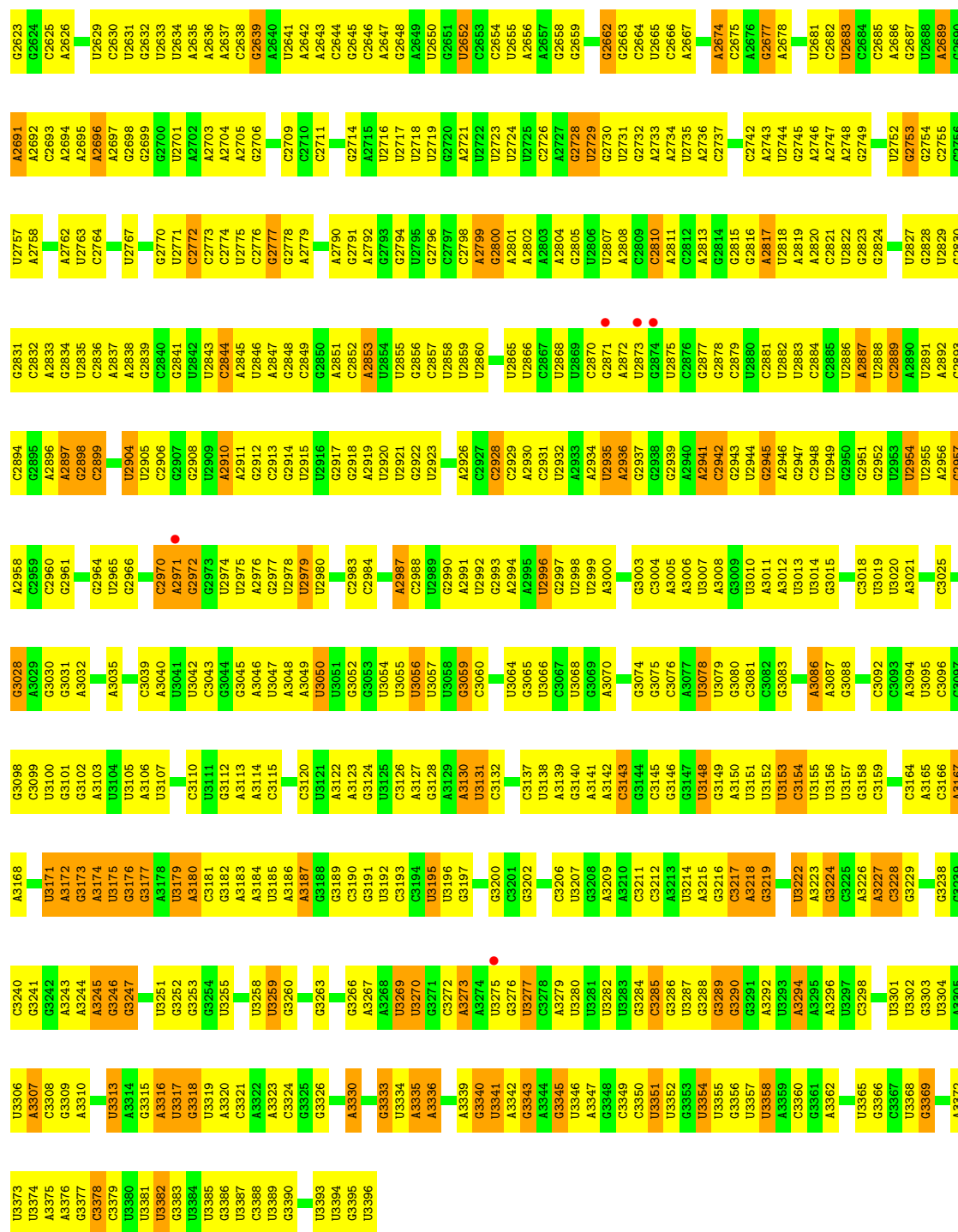
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U1765	U1554	U1555	G1643	A1482	U1556	G1414	U1351	C1280	A1204	G1140	U1071	U988	C923	G859	G787
G1766	U1556	U1557	A1643	U1483	U1558	G1415	A1352	G1281	G1209	G1141	U1072	A989	A924	G860	C788
G1767	U1558	U1559	U1644	G1484	U1559	G1416	U1353	U1285	U1210	A1142	U1073	G994	A925	G861	A789
G1770	A1559	G1560	U1645	G1488	A1560	G1417	U1354	A1286	U1211	A1143	U1074	G993	A926	G862	U790
G1773	G1561	G1562	U1646	A1489	U1561	A1418	U1355	A1287	A1212	G1144	U1075	U995	C928	G863	A791
G1778	A1490	C1563	A1654	A1490	G1564	A1419	G1357	U1292	U1214	G1147	A1079	A998	U930	G867	C793
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G1780	G1492	C1565	U1658	G1492	U1566	G1422	C1360	U1294	C1216	G1149	U1081	G999	U932	G868	U796
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	U1576	U1577		U1551	U1621			U1358							
	U1578	U1579		U1552	U1622			U1359							
	U1580	U1581		U1553	U1623			U1360							
	U1582	U1583		U1554	U1624			U1361							
	U1584	U1585		U1555	U1625			U1362							
	U1586	U1587		U1556	U1626			U1363							
	U1588	U1589		U1557	U1627			U1364							
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	U1598	U1599		U1562	U1632			U1369							
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A2635	U2550	A2635	U2550	G2415	G2355	G2206	U2141	C1869
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A2638	U2553	G2638	U2553	G2418	A2358	U2209	A2144	G1875
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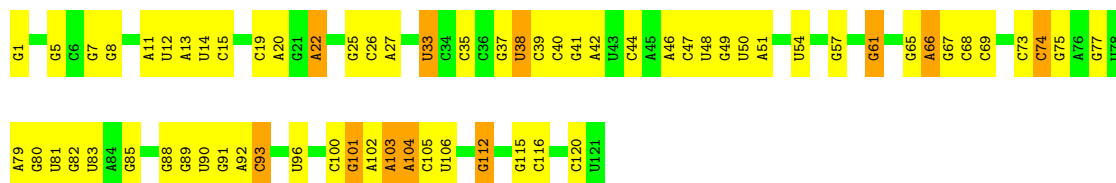
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A2357	A2358	C2359	C2360	A2361	C2362	A2363	G2364	C2365	C2366	A2367	A2368	G2369	G2370	G2371	A2372	C2373	G2374	G2375	G2376	G2377	C2378	U2379	G2380	G2381	G2382	C2383	A2384	C2385	A2386	A2387	U2388	C2389	G2390	G2391	G2392	G2393	G2394	G2395	G2396	A2397	A2398	A2399	G2400	A2401	A2402	G2403	A2404	A2405	C2406	C2407	U2408	G2409	U2410	U2411	U2412	A2413	G2414	G2415	U2416	G2417	U2418	G2419	U2420	G2421	U2422	G2423	A2424	G2425	U2426	G2427	U2428	G2429	U2430	G2431	A2432	U2433	U2434	G2435	U2436	G2437	A2438	A2439	G2440	A2441	G2442	A2443	G2444	U2445	U2446	G2447	U2448	G2449	U2450	G2451	U2452	G2453	U2454	G2455	U2456	G2457	U2458	G2459	U2460	G2461	U2462	G2463	U2464	G2465	U2466	G2467	U2468	G2469	U2470	G2471	U2472	G2473	U2474	G2475	U2476	G2477	U2478	G2479	U2480	G2481	U2482	G2483	U2484	G2485	U2486	G2487	U2488	G2489	U2490	G2491	U2492	G2493	U2494	G2495	U2496	G2497	U2498	G2499	U2500	G2501	U2502	G2503	U2504	G2505	U2506	G2507	U2508	U2509	U2510	A2511	G2512	U2513	U2514	A2515	U2516	G2517	G2518	G2522	U2604	G2605	G2606	G2607	G2608	A2609	G2610	U2611	U2612	U2613	G2614	G2615	G2616	U2617	G2618	G2619	G2620	G2621	G2622																																																																																																																																																																																																																																																																																																																																																											
A2143	A2144	A2145	C2146	A2147	U2148	A2149	A2158	U2162	C2163	A2164	G2165	A2166	A2167	G2168	U2170	G2171	A2172	U2173	G2174	U2175	U2176	G2177	A2178	C2179	G2180	C2181	G2182	A2183	U2184	A2188	U2189	U2190	U2191	C2192	U2193	G2194	C2197	A2198	G2201	C2202	U2203	C2204	U2205	G2206	A2207	U2208	U2209	G2210	U2211	G2212	A2213	U2214	A2215	G2216	U2217	A2222	A2223	U2228	G2229	C2230	C2231	G2234	C2237	G2238	G2239	A2242	A2243	A2244	C2245	G2246	G2247	C2248	G2249	G2250	G2253	U2254	A2255	A2256	C2257	U2258	G2261	A2262	C2263	U2264	A2270	G2271	G2272	G2273	G2276	C2277	C2278	A2279	A2280	A2281	U2282	A2283	A2284	C2285	U2286	G2287	U2288	C2289	A2290	G2291	U2292	G2293	U2294	U2298	G2299	U2300	G2301	A2302	G2303	G2305	C2306	C2307	C2308	A2309	U2310	G2311	A2312	U2313	U2314	G2315	C2316	A2317	U2318	U2319	A2320	C2321	G2322	U2323	A2324	G2325	U2326	C2327	U2328	C2329	C2330	U2334	G2335	U2336	C2337	C2338	G2339	U2340	A2341	U2342	C2343	U2344	A2345	U2346	U2347	A2348	U2349	C2350	U2351	A2352	G2353	C2354	U2355	A2356	G2357	U2358	C2359	A2360	U2361	G2362	U2363	A2364	C2365	U2366	G2367	A2368	U2369	G2370	G2371	A2372	C2373	G2374	G2375	G2376	G2377	C2378	U2379	G2380	G2381	G2382	C2383	A2384	C2385	A2386	A2387	U2388	C2389	G2390	G2391	G2392	G2393	G2394	G2395	G2396	A2397	A2398	A2399	G2400	A2401	A2402	G2403	A2404	A2405	C2406	C2407	U2408	G2409	U2410	U2411	U2412	A2413	G2414	G2415	U2416	G2417	U2418	G2419	U2420	G2421	U2422	G2423	A2424	G2425	U2426	G2427	U2428	G2429	U2430	G2431	A2432	U2433	U2434	G2435	U2436	G2437	A2438	A2439	G2440	A2441	G2442	A2443	G2444	U2445	U2446	G2447	U2448	G2449	U2450	G2451	U2452	G2453	U2454	G2455	U2456	G2457	U2458	G2459	U2460	G2461	U2462	G2463	U2464	G2465	U2466	G2467	U2468	G2469	U2470	G2471	U2472	G2473	U2474	G2475	U2476	G2477	U2478	G2479	U2480	G2481	U2482	G2483	U2484	G2485	U2486	G2487	U2488	G2489	U2490	G2491	U2492	G2493	U2494	G2495	U2496	G2497	U2498	G2499	U2500	G2501	U2502	G2503	U2504	G2505	U2506	G2507	U2508	U2509	U2510	A2511	G2512	U2513	U2514	A2515	U2516	G2517	G2518	G2522	U2604	G2605	G2606	G2607	G2608	A2609	G2610	U2611	U2612	U2613	G2614	G2615	G2616	U2617	G2618	G2619	G2620	G2621	G2622																																																																																																																																																																																								
U1876	U1877	G1878	A1879	U1880	A1881	G1882	A1883	U1885	A1886	G1887	U1888	C1889	U1890	A1891	G1892	A1893	U1894	A1895	G1896	G1897	G1898	A1901	G1902	U1903	U1904	G1905	G1906	C1907	U1908	A1909	U1910	A1911	U1912	A1913	G1914	C1917	U1918	U1919	A1921	U1925	C1926	G1927	U1928	G1929	A1930	U1931	U1932	U1937	U1938	C1939	G1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	U2000	U2001	U2002	U2003	U2004	U2005	U2006	U2007	U2008	U2009	U2010	U2011	U2012	U2013	U2014	U2015	U2016	U2017	U2018	U2019	U2020	U2021	U2022	U2023	U2024	U2025	U2026	U2027	U2028	U2029	U2030	U2031	U2032	U2033	U2034	U2035	U2036	U2037	U2038	U2039	U2040	U2041	U2042	U2043	U2044	U2045	U2046	U2047	U2048	U2049	U2050	U2051	U2052	U2053	U2054	U2055	U2056	U2057	U2058	U2059	U2060	U2061	U2062	U2063	U2064	U2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073	U2074	U2075	U2076	U2077	U2078	U2079	U2080	U2081	U2082	U2083	U2084	U2085	U2086	U2087	U2088	U2089	U2090	U2091	U2092	U2093	U2094	U2095	U2096	U2097	U2098	U2099	U2100	U2101	U2102	U2103	U2104	U2105	U2106	U2107	U2108	U2109	U2110	U2111	U2112	U2113	U2114	U2115	U2116	U2117	U2118	U2119	U2120	U2121	U2122	U2123	U2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	U2133	U2134	U2135	U2136	U2137	U2138	U2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	U2161	U2162	U2163	U2164	U2165	U2166	U2167	U2168	U2169	U2170	U2171	U2172	U2173	U2174	U2175	U2176	U2177	U2178	U2179	U2180	U2181	U2182	U2183	U2184	U2185	U2186	U2187	U2188	U2189	U2190	U2191	U2192	U2193	U2194	U2195	U2196	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230	U2231	U2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240	U2241	U2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2251	U2252	U2253	U2254	U2255	U2256	U2257	U2258	U2259	U2260	U2261	U2262	U2263	U2264	U2265	U2266	U2267	U2268	U2269	U2270	U2271	U2272	U2273	U2274	U2275	U2276	U2277	U2278	U2279	U2280	U2281	U2282	U2283	U2284	U2285	U2286	U2287	U2288	U2289	U2290	U2291	U2292	U2293	U2294	U2295	U2296	U2297	U2298	U2299	U2300	U2301	U2302	U2303	U2304	U2305	U2306	U2307	U2308	U2309	U2310	U2311	U2312	U2313	U2314	U2315	U2316	U2317	U2318	U2319	U2320	U2321	U2322	U2323	U2324	U2325	U2326	U2327	U2328	U2329	U2330	U2331	U2332	U2333	U2334	U2335	U2336	U2337	U2338	U2339	U2340	U2341	U2342	U2343	U2344	U2345	U2346	U2347	U2348	U2349	U2350	U2351	U2352	U2353	U2354	U2355	U2356	U2357	U2358	U2359	U2360	U2361	U2362	U2363	U2364	U2365	U2366	U2367	U2368	U2369	U2370	U2371	U2372	U2373	U2374	U2375	U2376	U2377	U2378	U2379	U2380	U2381	U2382	U2383	U2384	U2385	U2386	U2387	U2388	U2389	U2390	U2391	U2392	U2393	U2394	U2395	U2396	U2397	U2398	U2399	U2400	U2401	U2402	U2403	U2404	U2405	U2406	U2407	U2408	U2409	U2410	U2411	U2412	U2413	U2414	U2415	U2416	U2417





• Molecule 37: 5S rRNA

Chain A7: 45% 45% 9%



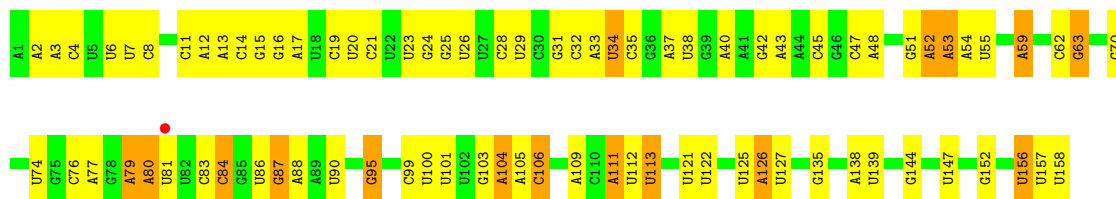
• Molecule 38: 5.8S rRNA

Chain A4: 39% 52% 9%



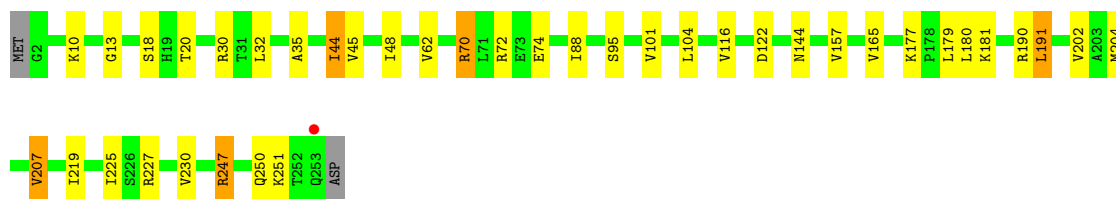
• Molecule 38: 5.8S rRNA

Chain A8: 48% 42% 10%




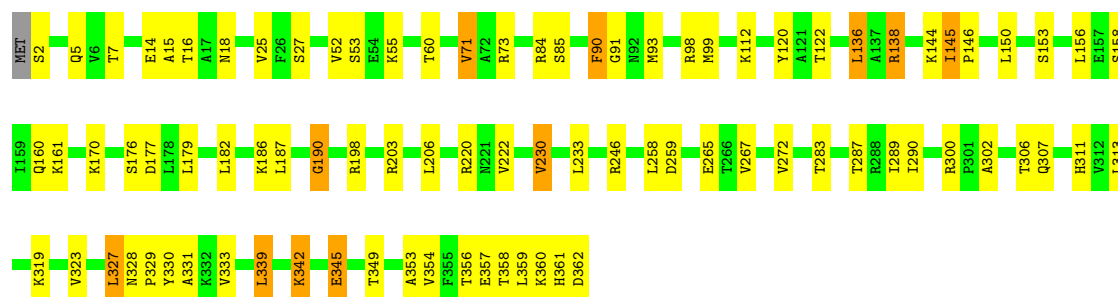
• Molecule 39: 60S ribosomal protein L2-A

Chain BA: 84% 13% 3%




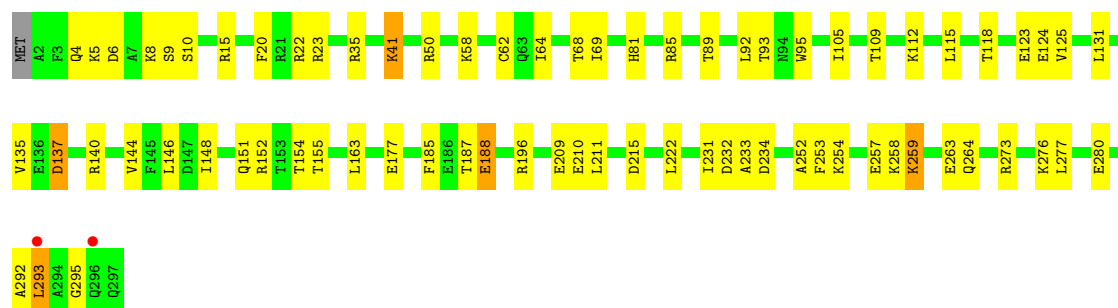
• Molecule 39: 60S ribosomal protein L2-A

Chain DC:  75% 21% .




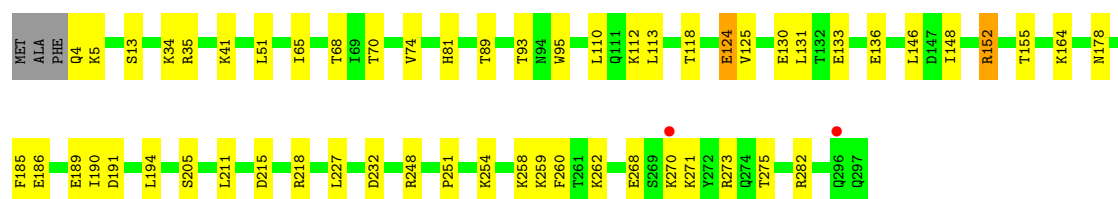
• Molecule 42: 60S ribosomal protein L5

Chain BD:  75% 23% .




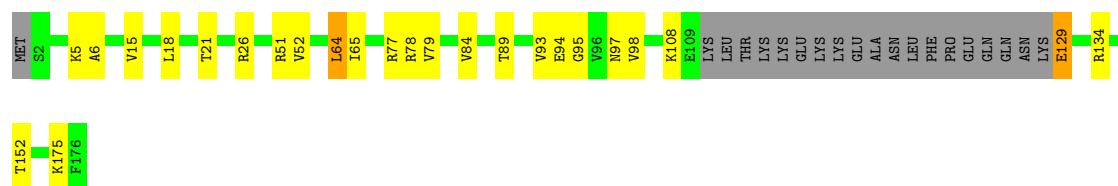
• Molecule 42: 60S ribosomal protein L5

Chain DD:  80% 18% ..




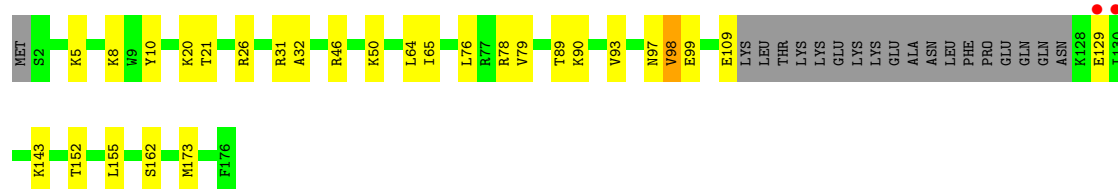
• Molecule 43: 60S ribosomal protein L6-A

Chain BE:  74% 13% 11% .



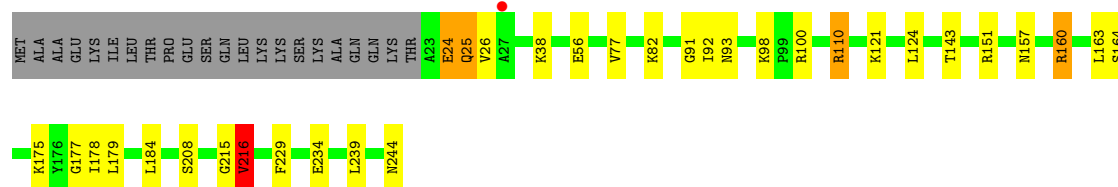
• Molecule 43: 60S ribosomal protein L6-A

Chain DE:  73% 15% 11% .



- Molecule 44: 60S ribosomal protein L7-A

Chain BF: 77% 11% 9%



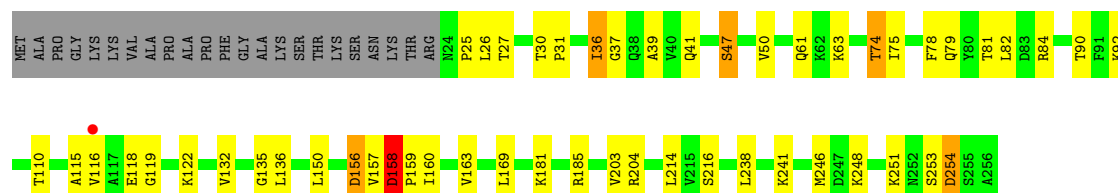
- Molecule 44: 60S ribosomal protein L7-A

Chain DF: 76% 14% 9%



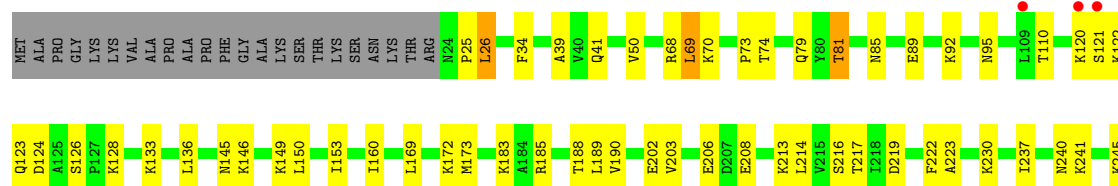
- Molecule 45: 60S ribosomal protein L8-A

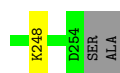
Chain BG: 71% 18% 9%



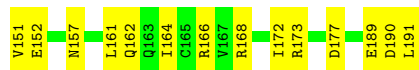
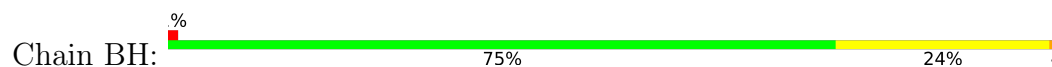
- Molecule 45: 60S ribosomal protein L8-A

Chain DG: 68% 21% 10%

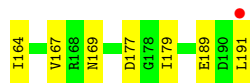
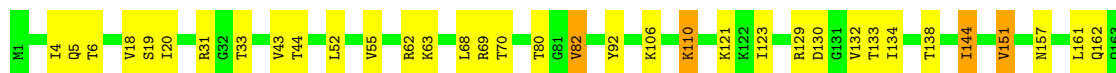
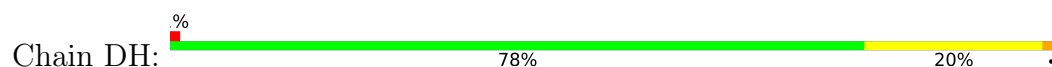




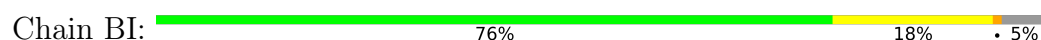
• Molecule 46: 60S ribosomal protein L9-A



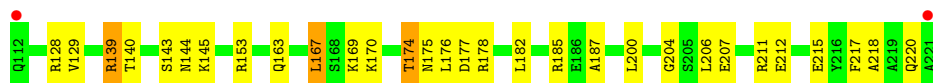
• Molecule 46: 60S ribosomal protein L9-A



• Molecule 47: 60S ribosomal protein L10

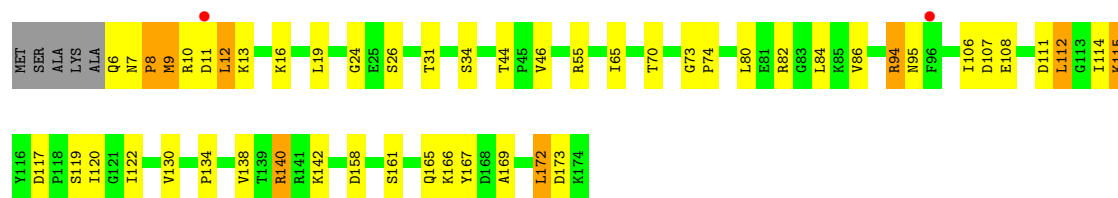


• Molecule 47: 60S ribosomal protein L10



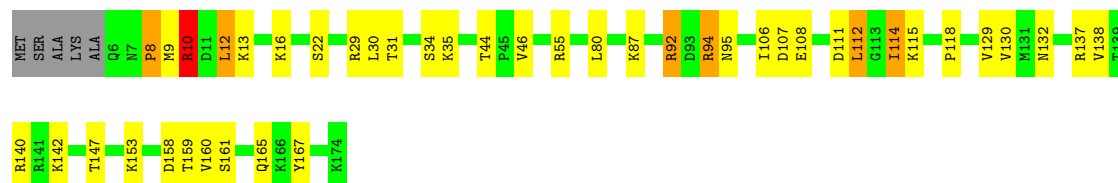
• Molecule 48: 60S ribosomal protein L11-A





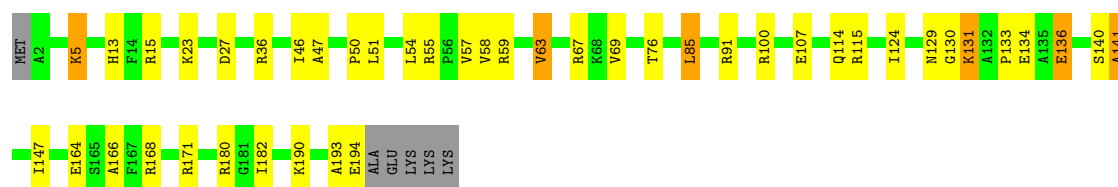
- Molecule 48: 60S ribosomal protein L11-A

Chain DJ: 72% 21% ..



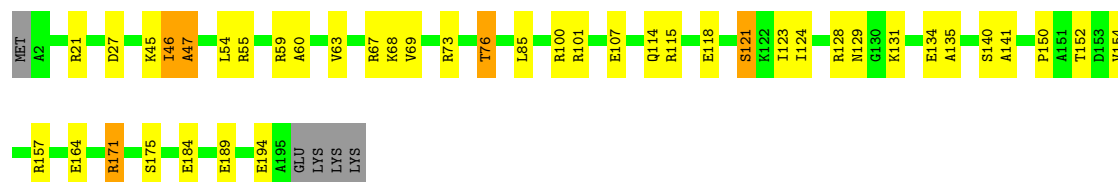
- Molecule 49: 60S ribosomal protein L13-A

Chain BL: 75% 19% ..



- Molecule 49: 60S ribosomal protein L13-A

Chain DL: 76% 19% ..



- Molecule 50: 60S ribosomal protein L14-A

Chain BM: 77% 20% ..



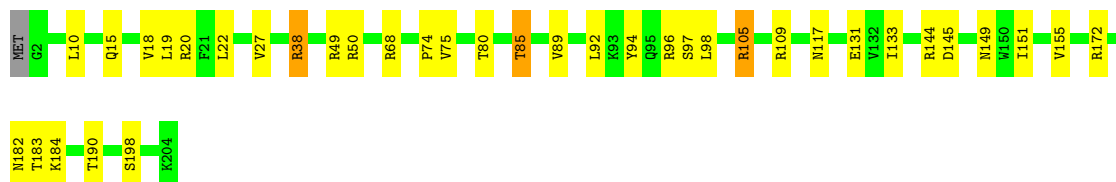
- Molecule 50: 60S ribosomal protein L14-A

Chain DM: 80% 17% ..



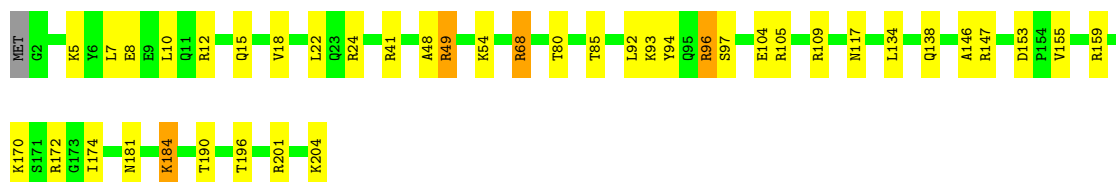
- Molecule 51: 60S ribosomal protein L15-A

Chain BN: 81% 17% .



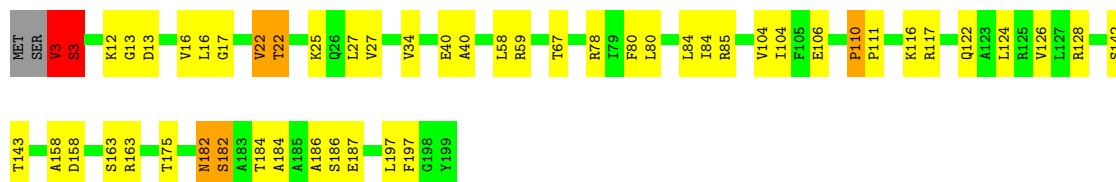
- Molecule 51: 60S ribosomal protein L15-A

Chain DN: 79% 18% .



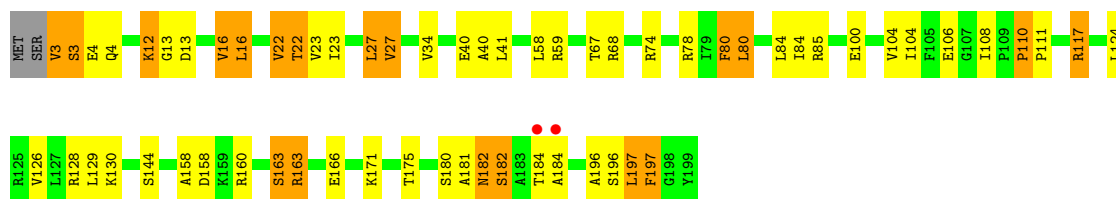
- Molecule 52: 60S ribosomal protein L16-A, 60S ribosomal protein L16-B

Chain BO: 75% 21% ...



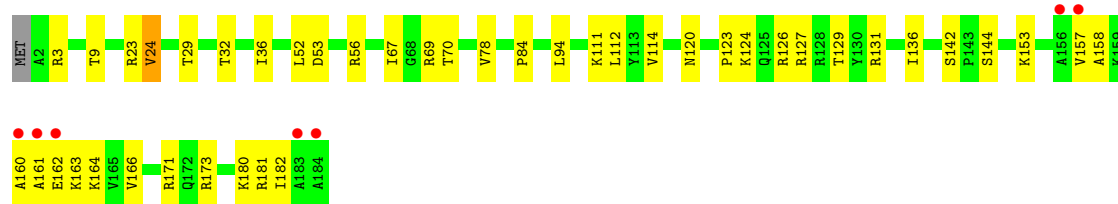
- Molecule 52: 60S ribosomal protein L16-A, 60S ribosomal protein L16-B

Chain DO: 71% 20% 9% .



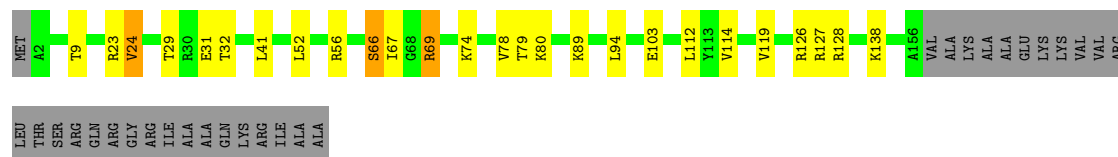
- Molecule 53: 60S ribosomal protein L17-A

Chain BP: 4% 76% 23% ..



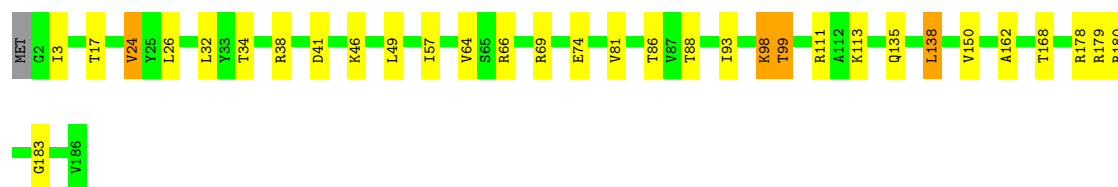
• Molecule 53: 60S ribosomal protein L17-A

Chain DP: 70% 12% 16%



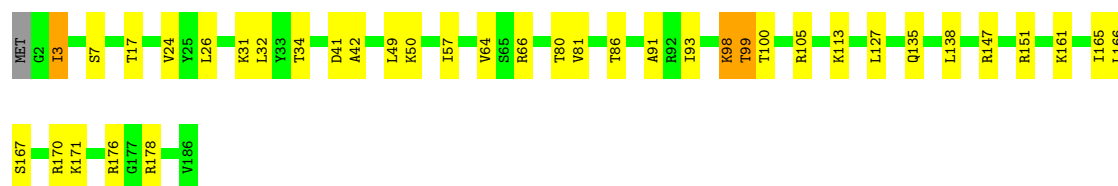
• Molecule 54: 60S ribosomal protein L18-A

Chain BQ: 82% 15% ..



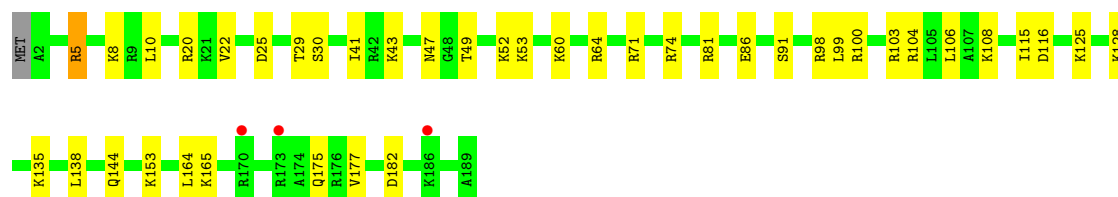
• Molecule 54: 60S ribosomal protein L18-A

Chain DQ: 79% 19% ..

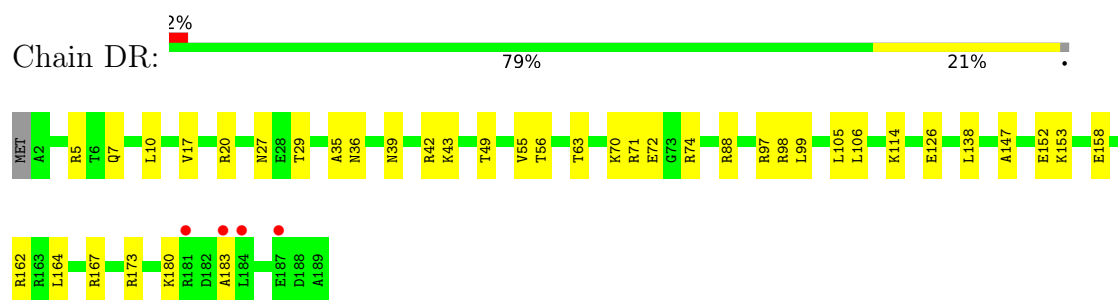


• Molecule 55: 60S ribosomal protein L19-A

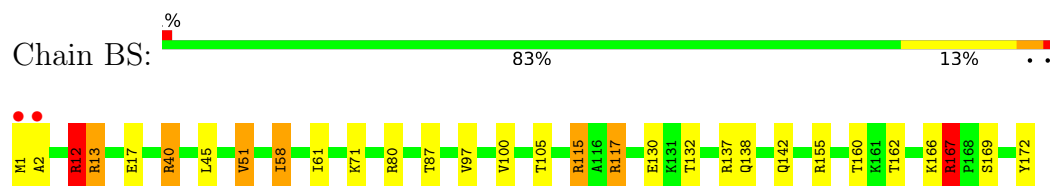
Chain BR: 78% 21% ..



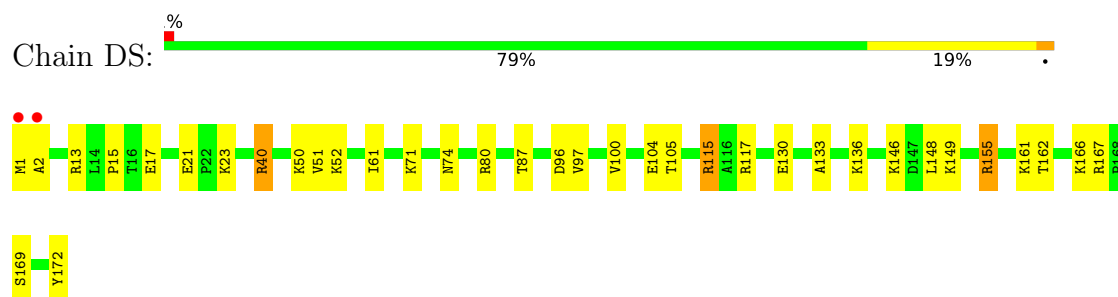
• Molecule 55: 60S ribosomal protein L19-A



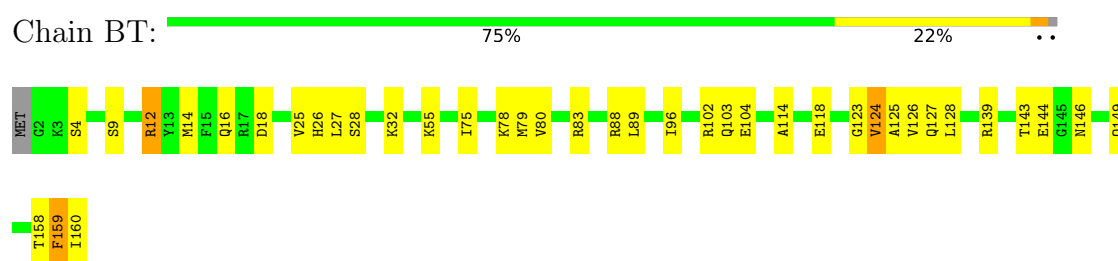
- Molecule 56: 60S ribosomal protein L20-A



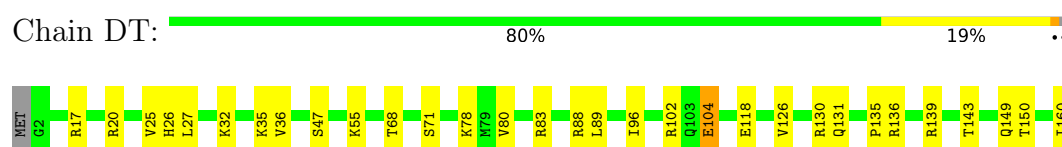
- Molecule 56: 60S ribosomal protein L20-A



- Molecule 57: 60S ribosomal protein L21-A



- Molecule 57: 60S ribosomal protein L21-A

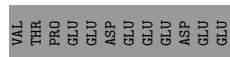


- Molecule 58: 60S ribosomal protein L22-A





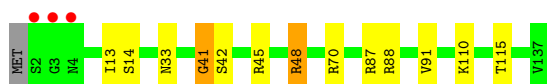
- Molecule 58: 60S ribosomal protein L22-A



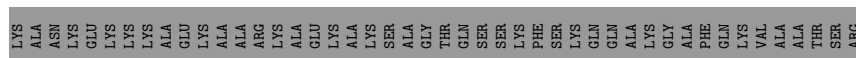
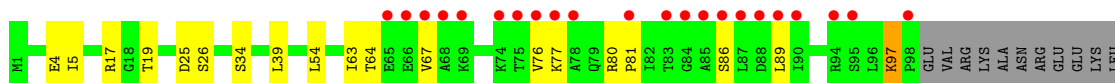
- Molecule 59: 60S ribosomal protein L23-A



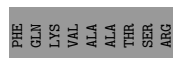
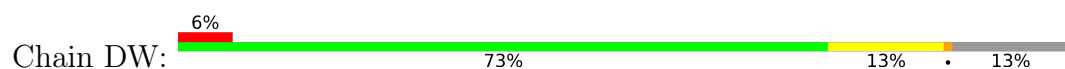
- Molecule 59: 60S ribosomal protein L23-A



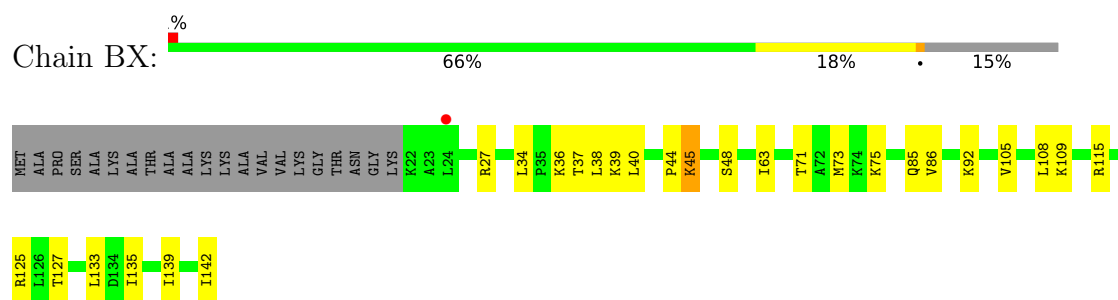
- Molecule 60: 60S ribosomal protein L24-A



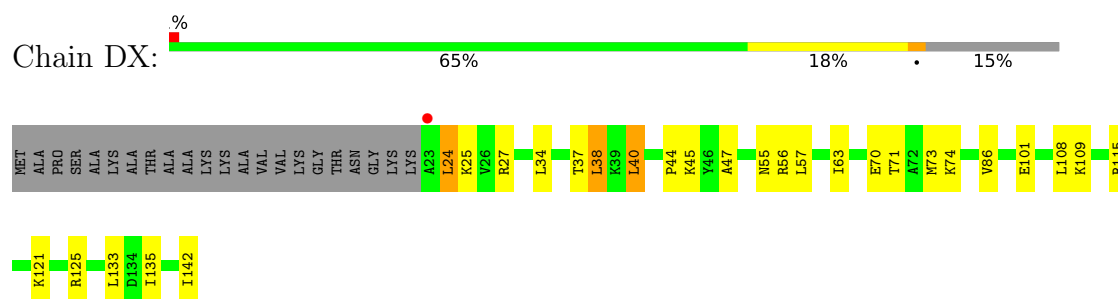
- Molecule 60: 60S ribosomal protein L24-A



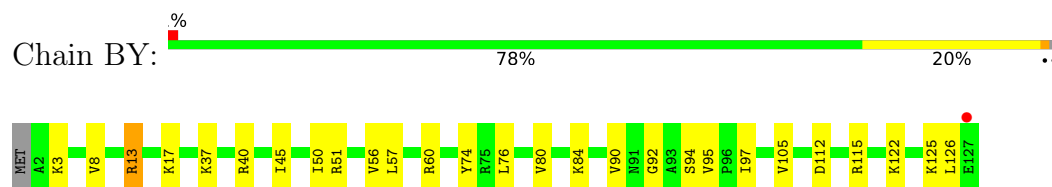
- Molecule 61: 60S ribosomal protein L25



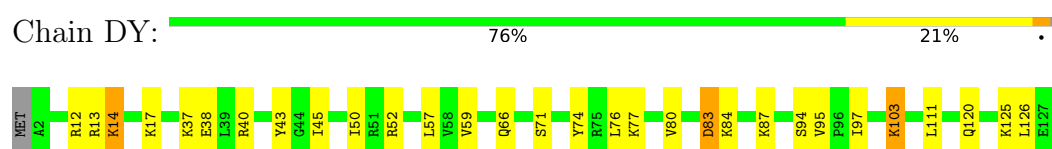
- Molecule 61: 60S ribosomal protein L25



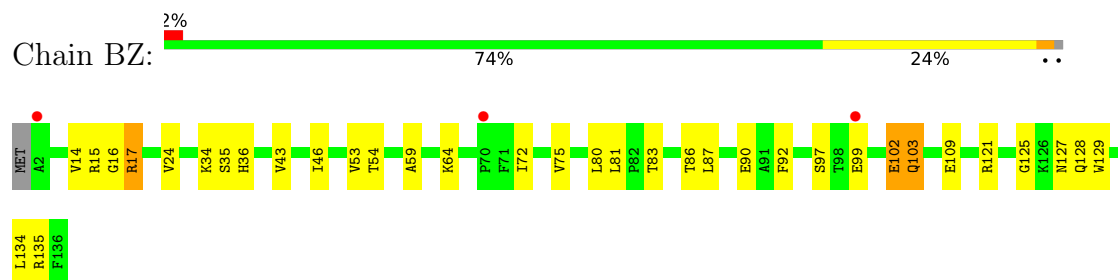
- Molecule 62: 60S ribosomal protein L26-A



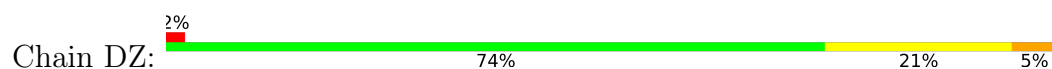
- Molecule 62: 60S ribosomal protein L26-A



- Molecule 63: 60S ribosomal protein L27-A



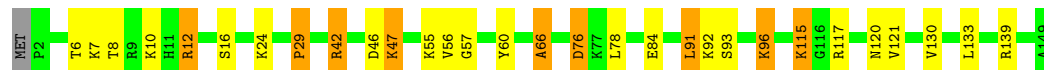
- Molecule 63: 60S ribosomal protein L27-A





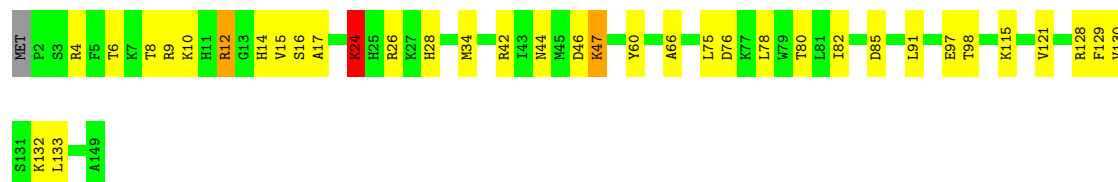
- Molecule 64: 60S ribosomal protein L28

Chain Ba: 79% 14% 6% .



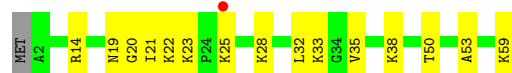
- Molecule 64: 60S ribosomal protein L28

Chain Da: 75% 22% ...



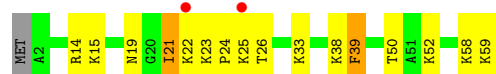
- Molecule 65: 60S ribosomal protein L29

Chain Bb: 2% 73% 25% .



- Molecule 65: 60S ribosomal protein L29

Chain Db: 3% 71% 24% ..



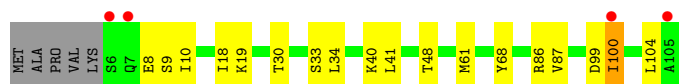
- Molecule 66: 60S ribosomal protein L30

Chain Bc: 75% 16% 8% .

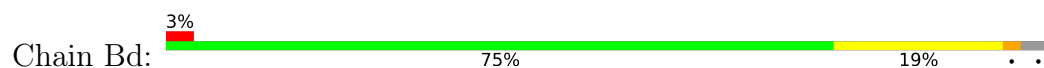


- Molecule 66: 60S ribosomal protein L30

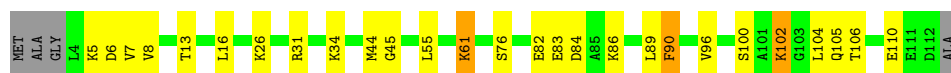
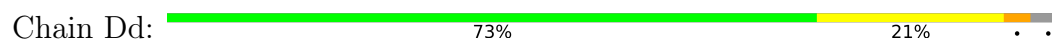
Chain Dc: 4% 78% 16% 5%



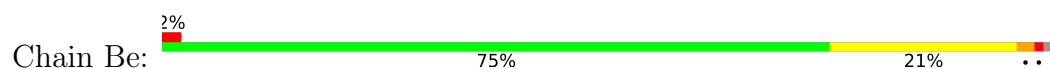
- Molecule 67: 60S ribosomal protein L31-A



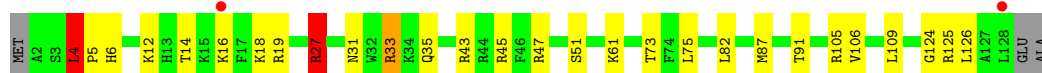
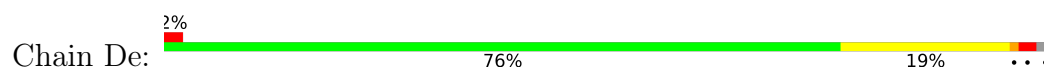
- Molecule 67: 60S ribosomal protein L31-A



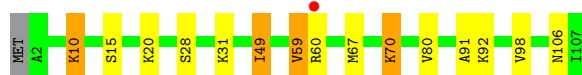
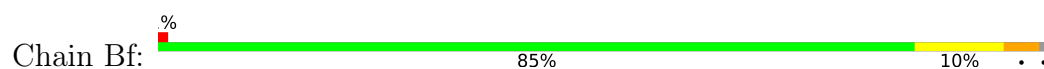
- Molecule 68: 60S ribosomal protein L32



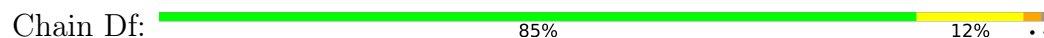
- Molecule 68: 60S ribosomal protein L32



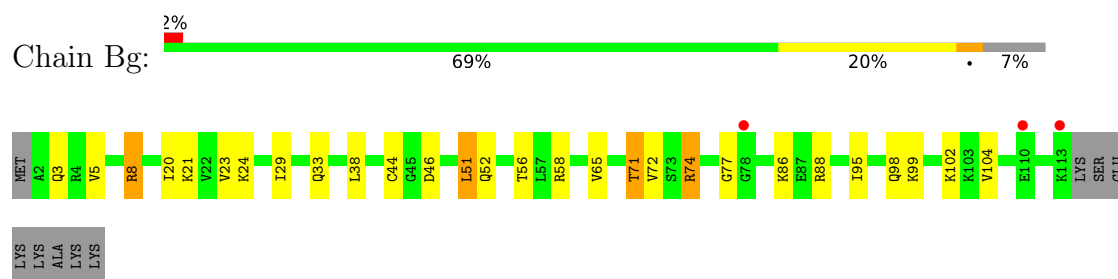
- Molecule 69: 60S ribosomal protein L33-A



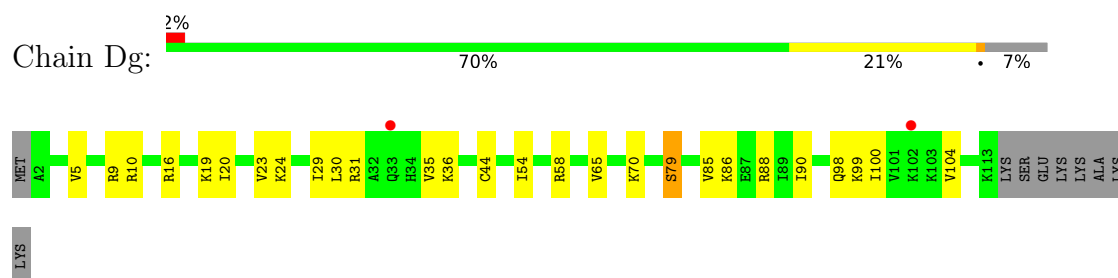
- Molecule 69: 60S ribosomal protein L33-A



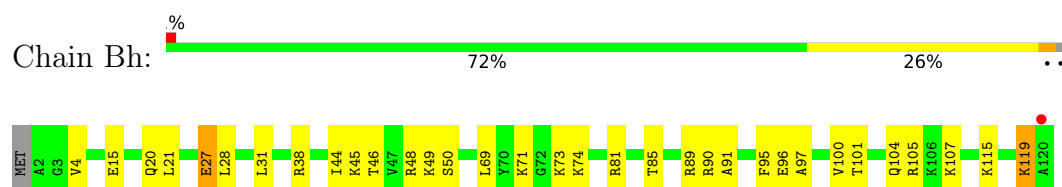
- Molecule 70: 60S ribosomal protein L34-A



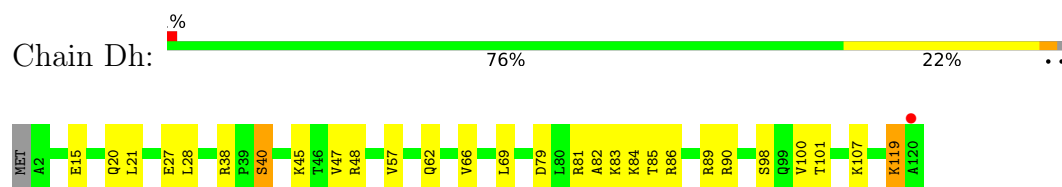
- Molecule 70: 60S ribosomal protein L34-A



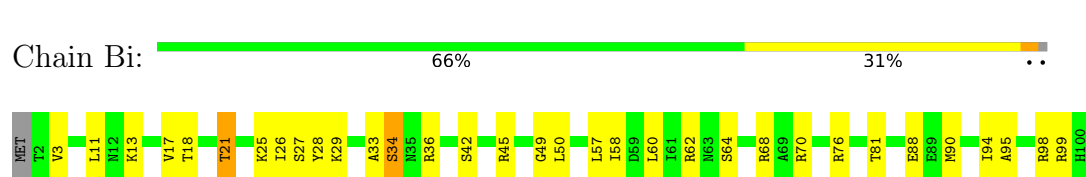
- Molecule 71: 60S ribosomal protein L35-A



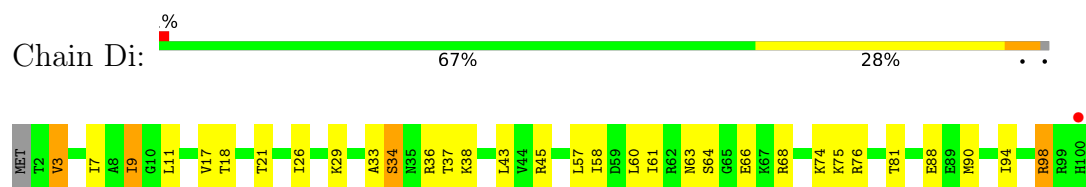
- Molecule 71: 60S ribosomal protein L35-A



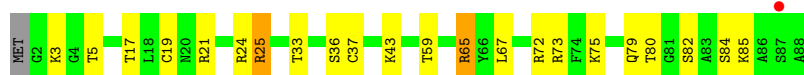
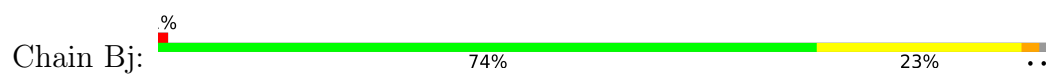
- Molecule 72: 60S ribosomal protein L36-A



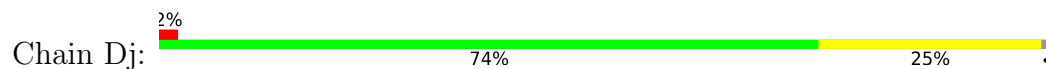
- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A



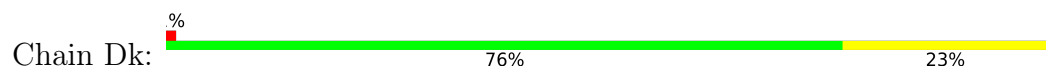
- Molecule 73: 60S ribosomal protein L37-A



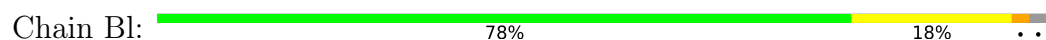
- Molecule 74: 60S ribosomal protein L38



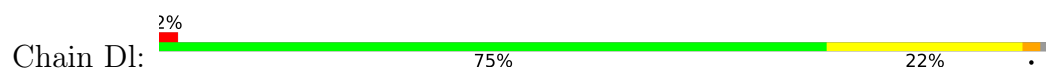
- Molecule 74: 60S ribosomal protein L38



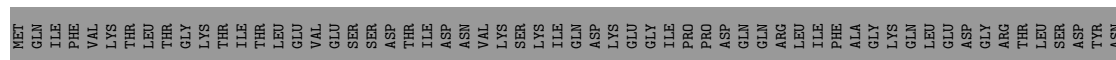
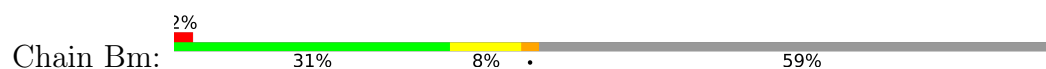
- Molecule 75: 60S ribosomal protein L39

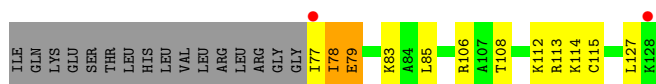


- Molecule 75: 60S ribosomal protein L39

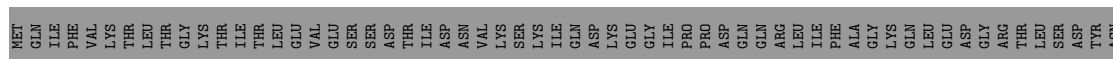
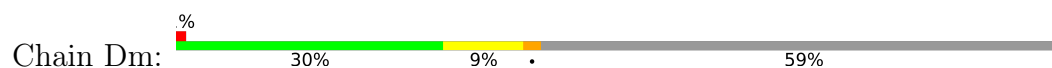


- Molecule 76: 60S ribosomal protein L40





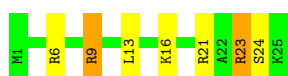
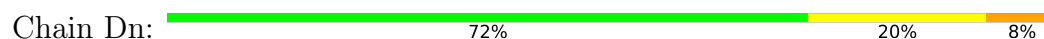
- Molecule 76: 60S ribosomal protein L40



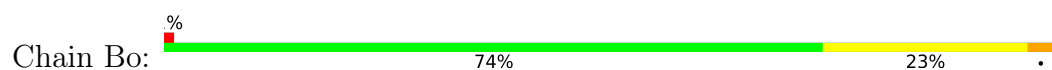
- Molecule 77: 60S ribosomal protein L41-A



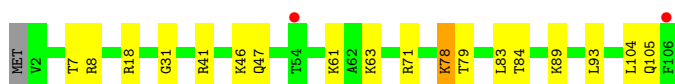
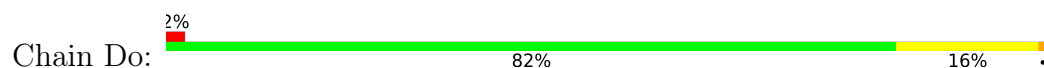
- Molecule 77: 60S ribosomal protein L41-A



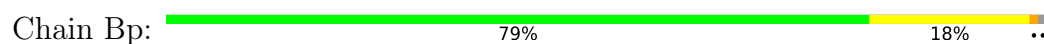
- Molecule 78: 60S ribosomal protein L42-A



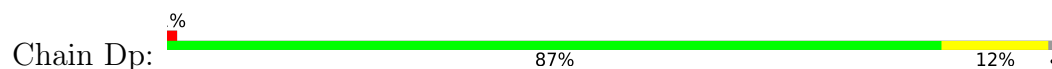
- Molecule 78: 60S ribosomal protein L42-A



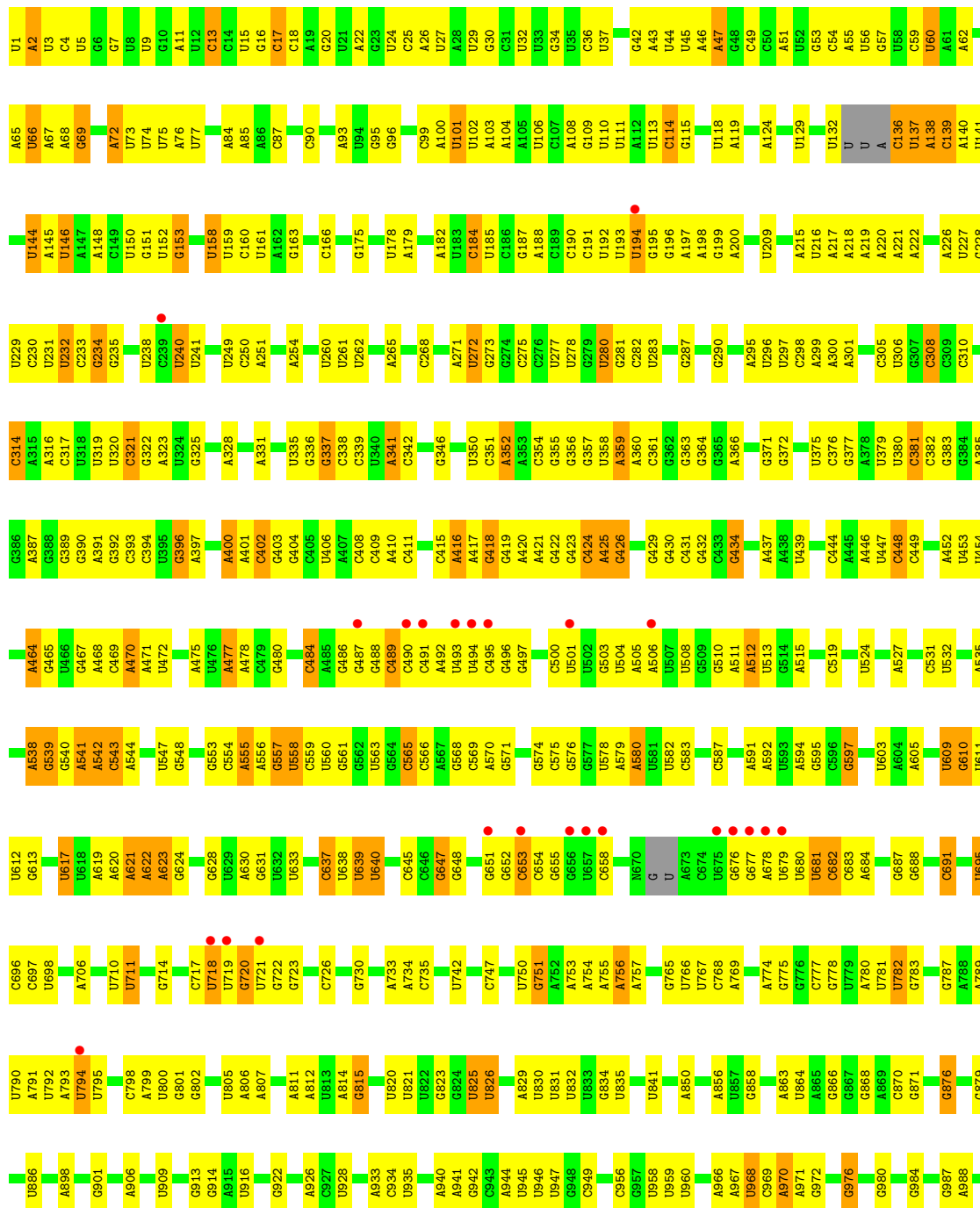
- Molecule 79: 60S ribosomal protein L43-A

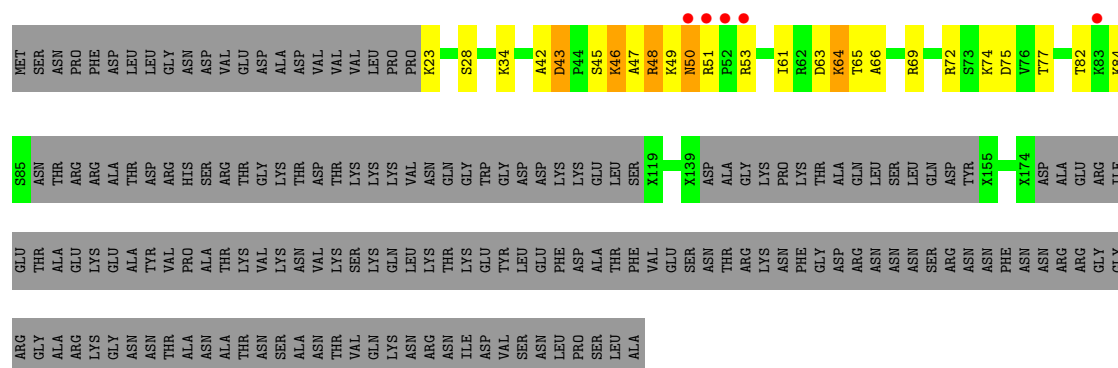


• Molecule 79: 60S ribosomal protein L43-A



• Molecule 80: 18S rRNA






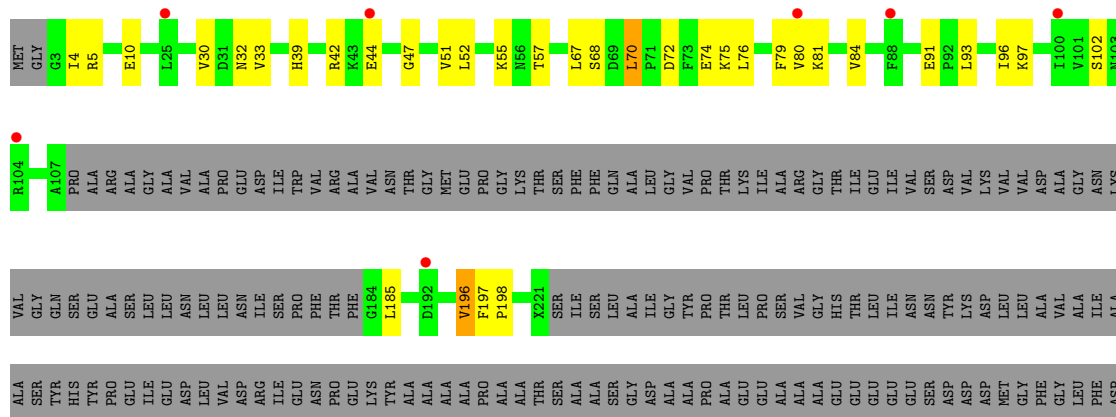
- Molecule 82: Ribosomal protein L12

Chain DK:  97%



- Molecule 83: 60S acidic ribosomal protein P0

Chain Dq:  2% 35% 10% 54%



- Molecule 84: Ribosomal protein P1 alpha

Chain Dr:  100%

There are no outlier residues recorded for this chain.

- Molecule 85: Ribosomal protein P2 beta

Chain Ds:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.43Å 288.22Å 305.08Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	300.00 – 3.00 301.33 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (300.00-3.00) 99.9 (301.33-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.229 0.189 , 0.229	Depositor DCC
R_{free} test set	32787 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	416785	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OHX, MG, ZN

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	A2	0.92	36/42128 (0.1%)	1.49	822/65642 (1.3%)
2	AA	0.54	0/1617	0.80	0/2215
2	CA	0.64	0/1623	0.88	0/2222
3	AB	0.45	0/1735	0.81	0/2335
3	CB	0.61	0/1748	0.80	1/2352 (0.0%)
4	AC	0.60	0/1665	0.77	0/2263
4	CC	0.70	0/1665	0.93	6/2263 (0.3%)
5	AD	0.59	0/1759	0.74	0/2368
5	CD	0.54	0/1759	0.76	1/2368 (0.0%)
6	AE	0.57	0/2109	0.86	1/2839 (0.0%)
6	CE	0.70	0/2109	0.94	2/2839 (0.1%)
7	AF	0.49	0/1629	0.72	0/2202
7	CF	0.62	0/1629	0.86	2/2202 (0.1%)
8	AG	0.55	0/1823	0.75	0/2439
8	CG	0.68	0/1779	0.87	2/2379 (0.1%)
9	AH	0.52	0/1506	0.77	0/2028
9	CH	0.59	0/1516	0.85	0/2043
10	AI	0.68	0/1514	0.89	3/2021 (0.1%)
10	CI	0.75	0/1514	0.99	2/2021 (0.1%)
11	AJ	0.59	0/1519	0.81	1/2035 (0.0%)
11	CJ	0.70	0/1519	0.91	3/2035 (0.1%)
12	AK	0.55	0/789	0.83	3/1067 (0.3%)
12	CK	0.51	0/776	0.83	3/1047 (0.3%)
13	AL	0.70	0/1239	0.81	0/1673
13	CL	0.76	0/1194	0.98	5/1610 (0.3%)
14	AM	0.49	0/898	0.76	0/1220
14	CM	0.44	0/898	0.77	2/1220 (0.2%)
15	AN	0.61	0/1215	0.83	3/1638 (0.2%)
15	CN	0.67	0/1215	0.89	1/1638 (0.1%)
16	AO	0.48	0/901	0.82	1/1217 (0.1%)
16	CO	0.70	0/960	0.92	0/1290
17	AP	0.60	0/998	0.86	2/1341 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CP	0.57	0/1060	0.83	0/1426
18	AQ	0.56	0/1125	0.85	3/1510 (0.2%)
18	CQ	0.66	0/1131	0.85	1/1518 (0.1%)
19	AR	0.54	0/935	0.82	0/1254
19	CR	0.60	0/914	0.86	0/1224
20	AS	0.59	0/1211	0.80	0/1628
20	CS	0.63	0/1211	0.92	3/1628 (0.2%)
21	AT	0.57	0/1130	0.81	0/1517
21	CT	0.66	0/1130	0.86	3/1517 (0.2%)
22	AU	0.55	0/865	0.76	0/1169
22	CU	0.62	0/892	0.86	0/1205
23	AV	0.52	0/693	0.75	0/935
23	CV	0.65	0/693	0.86	0/935
24	AW	0.65	0/1038	0.86	3/1395 (0.2%)
24	CW	0.81	0/1038	0.89	1/1395 (0.1%)
25	AX	0.72	0/1139	0.91	2/1518 (0.1%)
25	CX	0.86	0/1139	0.99	3/1518 (0.2%)
26	AY	0.56	0/1087	0.77	1/1449 (0.1%)
26	CY	0.65	0/1087	0.84	0/1449
27	AZ	0.49	0/571	0.85	1/768 (0.1%)
27	CZ	0.51	0/566	0.80	1/761 (0.1%)
28	Aa	0.54	0/782	0.77	0/1047
28	Ca	0.63	0/782	0.84	0/1047
29	Ab	0.53	0/620	0.82	1/838 (0.1%)
29	Cb	0.55	0/620	0.87	0/838
30	Ac	0.43	0/499	0.72	0/670
30	Cc	0.53	0/499	0.84	0/670
31	Ad	0.71	1/452 (0.2%)	0.94	1/600 (0.2%)
31	Cd	0.77	1/452 (0.2%)	0.94	1/600 (0.2%)
32	Ae	0.50	0/483	0.71	0/643
32	Ce	0.62	0/499	0.89	1/665 (0.2%)
33	Af	0.53	0/404	0.99	2/542 (0.4%)
33	Cf	0.46	0/404	0.84	0/542
34	Ag	0.49	0/2490	0.70	0/3389
34	Cg	0.51	0/2495	0.69	0/3395
35	Ah	0.86	2/925 (0.2%)	0.87	2/1240 (0.2%)
36	A1	1.42	515/75394 (0.7%)	1.91	3591/117545 (3.1%)
36	A5	1.46	607/75414 (0.8%)	1.88	3500/117575 (3.0%)
37	A3	1.15	5/2883 (0.2%)	1.59	68/4491 (1.5%)
37	A7	1.38	13/2883 (0.5%)	1.80	121/4491 (2.7%)
38	A4	1.31	18/3746 (0.5%)	1.79	159/5832 (2.7%)
38	A8	1.16	4/3746 (0.1%)	1.70	130/5832 (2.2%)
39	BA	0.84	0/1948	1.01	5/2617 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DA	0.87	1/1946 (0.1%)	1.05	4/2614 (0.2%)
40	BB	0.92	3/3146 (0.1%)	1.05	11/4228 (0.3%)
40	DB	1.02	4/3146 (0.1%)	1.11	13/4228 (0.3%)
41	BC	0.96	3/2800 (0.1%)	1.14	17/3790 (0.4%)
41	DC	0.87	0/2800	1.07	11/3790 (0.3%)
42	BD	0.71	2/2425 (0.1%)	0.87	1/3271 (0.0%)
42	DD	0.89	1/2408 (0.0%)	0.96	3/3248 (0.1%)
43	BE	0.88	0/1260	1.02	3/1694 (0.2%)
43	DE	0.90	1/1269 (0.1%)	1.00	3/1705 (0.2%)
44	BF	0.96	1/1821 (0.1%)	1.06	7/2451 (0.3%)
44	DF	0.99	1/1828 (0.1%)	1.04	6/2461 (0.2%)
45	BG	0.64	0/1836	0.82	1/2481 (0.0%)
45	DG	0.64	0/1795	0.81	1/2429 (0.0%)
46	BH	0.80	0/1539	0.97	5/2073 (0.2%)
46	DH	0.97	2/1539 (0.1%)	1.01	1/2073 (0.0%)
47	BI	0.90	2/1741 (0.1%)	0.97	5/2335 (0.2%)
47	DI	0.92	1/1758 (0.1%)	1.08	12/2358 (0.5%)
48	BJ	0.65	0/1374	0.85	1/1842 (0.1%)
48	DJ	0.81	1/1374 (0.1%)	0.99	4/1842 (0.2%)
49	BL	0.89	0/1568	1.02	8/2106 (0.4%)
49	DL	0.82	0/1573	1.04	6/2113 (0.3%)
50	BM	0.88	0/1068	0.91	0/1438
50	DM	0.95	0/1074	1.01	4/1446 (0.3%)
51	BN	0.88	0/1757	1.05	5/2354 (0.2%)
51	DN	0.83	1/1757 (0.1%)	1.00	6/2354 (0.3%)
52	BO	0.92	10/3160 (0.3%)	1.16	10/4208 (0.2%)
52	DO	0.98	11/3159 (0.3%)	1.02	25/4205 (0.6%)
53	BP	0.97	2/1443 (0.1%)	1.02	3/1944 (0.2%)
53	DP	1.05	1/1250 (0.1%)	1.09	5/1683 (0.3%)
54	BQ	0.98	0/1465	1.13	8/1965 (0.4%)
54	DQ	0.89	1/1465 (0.1%)	1.12	8/1965 (0.4%)
55	BR	0.71	1/1538 (0.1%)	0.87	1/2050 (0.0%)
55	DR	0.78	1/1538 (0.1%)	0.87	3/2050 (0.1%)
56	BS	0.89	0/1481	1.06	9/1990 (0.5%)
56	DS	1.02	0/1481	1.09	7/1990 (0.4%)
57	BT	0.93	0/1300	0.98	1/1743 (0.1%)
57	DT	1.01	2/1300 (0.2%)	1.01	1/1743 (0.1%)
58	BU	0.52	0/812	0.70	0/1099
58	DU	0.56	0/794	0.77	0/1076
59	BV	0.86	0/1018	1.03	3/1369 (0.2%)
59	DV	0.98	0/1018	1.09	4/1369 (0.3%)
60	BW	0.68	0/712	0.86	1/958 (0.1%)
60	DW	0.80	0/1052	0.90	1/1398 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	BX	0.73	0/979	0.87	0/1321
61	DX	0.72	0/974	0.86	0/1314
62	BY	0.78	0/1004	1.10	5/1341 (0.4%)
62	DY	0.79	1/1004 (0.1%)	0.98	2/1341 (0.1%)
63	BZ	0.59	0/1118	0.81	1/1497 (0.1%)
63	DZ	0.55	0/1118	0.83	2/1497 (0.1%)
64	Ba	0.97	2/1204 (0.2%)	1.16	7/1612 (0.4%)
64	Da	0.94	2/1204 (0.2%)	1.14	9/1612 (0.6%)
65	Bb	0.83	0/473	0.85	0/629
65	Db	0.91	0/473	1.14	1/629 (0.2%)
66	Bc	0.59	0/751	0.73	0/1008
66	Dc	0.61	0/775	0.77	0/1040
67	Bd	0.73	0/890	0.89	1/1196 (0.1%)
67	Dd	0.94	2/897 (0.2%)	0.95	1/1205 (0.1%)
68	Be	1.02	2/1041 (0.2%)	1.19	9/1394 (0.6%)
68	De	1.03	0/1041	1.27	11/1394 (0.8%)
69	Bf	1.19	4/868 (0.5%)	1.08	2/1168 (0.2%)
69	Df	1.12	1/868 (0.1%)	1.09	3/1168 (0.3%)
70	Bg	0.70	0/890	0.98	4/1189 (0.3%)
70	Dg	0.72	0/890	0.92	0/1189
71	Bh	0.83	0/978	0.94	2/1301 (0.2%)
71	Dh	0.67	0/974	0.80	0/1297
72	Bi	0.77	0/778	0.98	1/1034 (0.1%)
72	Di	0.67	0/777	0.85	0/1033
73	Bj	0.98	2/696 (0.3%)	1.19	6/923 (0.7%)
73	Dj	0.87	0/696	1.04	3/923 (0.3%)
74	Bk	0.59	0/618	0.75	0/826
74	Dk	0.50	0/614	0.70	0/822
75	Bl	0.90	1/443 (0.2%)	1.07	1/588 (0.2%)
75	Dl	0.90	0/443	1.02	1/588 (0.2%)
76	Bm	0.89	1/423 (0.2%)	0.97	1/562 (0.2%)
76	Dm	1.08	2/423 (0.5%)	1.13	1/562 (0.2%)
77	Bn	0.78	0/234	1.18	2/300 (0.7%)
77	Dn	0.90	0/234	1.15	1/300 (0.3%)
78	Bo	0.87	1/860 (0.1%)	0.97	2/1136 (0.2%)
78	Do	0.83	0/860	0.88	1/1136 (0.1%)
79	Bp	0.80	0/701	0.96	1/934 (0.1%)
79	Dp	0.86	0/701	0.98	1/934 (0.1%)
80	A6	1.13	97/42174 (0.2%)	1.61	1103/65711 (1.7%)
81	Ch	0.64	0/480	0.85	0/642
83	Dq	0.54	0/977	0.75	1/1313 (0.1%)
All	All	1.11	1373/432157 (0.3%)	1.51	9884/634038 (1.6%)

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
2	CA	0	1
3	AB	0	1
5	CD	0	1
7	CF	0	2
9	AH	0	1
11	CJ	0	3
13	AL	0	1
16	AO	0	1
16	CO	0	1
17	CP	0	1
18	CQ	0	1
19	AR	0	2
22	CU	0	1
25	CX	0	1
27	AZ	0	3
27	CZ	0	2
29	Ab	0	1
33	Af	0	2
33	Cf	0	2
35	Ah	0	1
36	A1	0	3
36	A5	0	1
39	DA	0	2
40	BB	0	1
41	BC	0	1
41	DC	0	1
42	DD	0	1
43	BE	0	2
43	DE	0	1
44	BF	0	1
44	DF	0	2
45	BG	0	3
46	BH	0	1
48	BJ	0	1
52	BO	0	2
52	DO	0	2
56	DS	0	1
57	BT	0	1
59	DV	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
62	DY	0	1
63	DZ	0	1
64	Da	0	3
65	Bb	0	2
65	Db	0	1
67	Bd	0	1
78	Bo	0	1
All	All	0	67

All (1373) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	BO	3[A]	VAL	C-N	26.80	1.95	1.34
36	A1	2777	G	C5-C6	-23.22	1.19	1.42
52	DO	197[B]	PHE	C-N	-21.96	0.93	1.33
52	DO	182[B]	SER	C-N	18.04	1.75	1.34
36	A5	1152	G	N9-C8	15.01	1.48	1.37
36	A5	1152	G	N9-C4	-14.78	1.26	1.38
52	BO	197[B]	PHE	C-N	-14.63	1.06	1.33
35	Ah	134	ASP	CG-OD1	13.92	1.57	1.25
36	A5	1152	G	C2-N3	-13.38	1.22	1.32
36	A1	3242	G	N9-C4	-13.12	1.27	1.38
36	A1	2777	G	C8-N7	-13.09	1.23	1.30
35	Ah	134	ASP	CG-OD2	12.58	1.54	1.25
36	A1	3242	G	C2-N3	-11.79	1.23	1.32
52	DO	23[B]	ILE	C-N	-11.03	1.08	1.34
80	A6	337	G	C2-N2	10.65	1.45	1.34
36	A1	2993	G	N9-C4	-10.48	1.29	1.38
52	BO	13[B]	ASP	C-N	10.23	1.57	1.34
40	BB	7	GLU	CG-CD	9.97	1.67	1.51
52	DO	3[B]	SER	C-N	9.61	1.56	1.34
52	BO	40[B]	ALA	C-N	-9.49	1.12	1.34
36	A5	3216	G	N7-C5	-9.44	1.33	1.39
36	A1	2714	G	N9-C4	-9.34	1.30	1.38
36	A1	942	U	C2-N3	-9.30	1.31	1.37
36	A1	39	A	N7-C5	-9.25	1.33	1.39
40	BB	7	GLU	CB-CG	9.23	1.69	1.52
36	A1	2777	G	C5-C4	-9.20	1.31	1.38
36	A1	2278	C	C2-O2	-9.19	1.16	1.24
36	A5	2941	A	N9-C4	-9.16	1.32	1.37
80	A6	163	G	N9-C4	-9.06	1.30	1.38
36	A5	2914	G	P-OP2	-9.06	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	1434	G	N7-C5	-9.05	1.33	1.39
36	A5	1449	A	N9-C4	-9.03	1.32	1.37
36	A1	1377	G	N1-C2	-8.96	1.30	1.37
36	A5	652	G	N1-C2	-8.88	1.30	1.37
80	A6	337	G	C8-N7	-8.88	1.25	1.30
36	A1	2714	G	N9-C8	8.83	1.44	1.37
36	A5	1450	G	C8-N7	-8.74	1.25	1.30
36	A1	3181	C	N3-C4	-8.72	1.27	1.33
36	A5	953	G	C5-C4	-8.71	1.32	1.38
36	A1	2419	A	N9-C4	-8.68	1.32	1.37
36	A5	367	A	N9-C4	-8.65	1.32	1.37
36	A1	1592	G	C6-O6	-8.58	1.16	1.24
52	DO	80[B]	LEU	C-N	8.57	1.53	1.34
36	A1	2867	C	N3-C4	-8.51	1.27	1.33
52	BO	22[B]	THR	C-N	8.49	1.53	1.34
36	A1	2777	G	N1-C2	-8.48	1.30	1.37
36	A5	3088	G	C6-O6	-8.43	1.16	1.24
36	A5	2278	C	C2-O2	-8.32	1.17	1.24
36	A1	49	A	N9-C4	-8.26	1.32	1.37
36	A5	2899	C	N3-C4	-8.26	1.28	1.33
80	A6	1652	C	N3-C4	-8.23	1.28	1.33
36	A1	2800	G	P-OP1	-8.20	1.35	1.49
36	A5	2191	U	C4-C5	-8.19	1.36	1.43
36	A5	1178	G	P-OP2	-8.17	1.35	1.49
80	A6	65	A	N9-C4	-8.17	1.32	1.37
1	A2	553	G	C6-N1	8.12	1.45	1.39
36	A5	1887	A	N9-C4	-8.12	1.32	1.37
36	A1	2356	A	N9-C4	-8.11	1.32	1.37
80	A6	337	G	N1-C2	8.08	1.44	1.37
36	A5	2393	G	C8-N7	-8.08	1.26	1.30
36	A5	2726	C	N3-C4	-8.06	1.28	1.33
80	A6	337	G	C2-N3	8.06	1.39	1.32
36	A5	2817	A	P-OP1	-8.02	1.35	1.49
36	A5	1152	G	C5-C6	-7.99	1.34	1.42
36	A5	2830	G	C6-N1	-7.98	1.33	1.39
36	A5	2280	A	N9-C4	-7.97	1.33	1.37
36	A5	3216	G	N9-C8	-7.97	1.32	1.37
36	A5	1849	C	N3-C4	-7.97	1.28	1.33
39	DA	211	HIS	C-O	7.97	1.38	1.23
36	A5	2314	U	N3-C4	7.95	1.45	1.38
36	A1	2777	G	N7-C5	-7.94	1.34	1.39
36	A5	1152	G	N3-C4	-7.91	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	3114	A	N9-C4	-7.89	1.33	1.37
36	A1	3242	G	N3-C4	-7.88	1.29	1.35
36	A5	3245	A	N9-C4	-7.88	1.33	1.37
36	A5	1311	G	C5-C4	-7.86	1.32	1.38
36	A5	953	G	N7-C5	-7.84	1.34	1.39
36	A1	652	G	N1-C2	-7.83	1.31	1.37
36	A5	917	A	N7-C5	-7.80	1.34	1.39
38	A4	12	A	N3-C4	-7.80	1.30	1.34
36	A1	2836	C	N3-C4	-7.79	1.28	1.33
80	A6	163	G	N3-C4	-7.77	1.30	1.35
75	B1	2	ALA	CA-CB	-7.77	1.36	1.52
36	A5	519	A	N7-C5	-7.75	1.34	1.39
36	A5	2703	A	N7-C5	-7.74	1.34	1.39
36	A5	631	U	C2-N3	-7.71	1.32	1.37
36	A5	2945	G	P-O5'	-7.71	1.52	1.59
80	A6	1595	U	C2-N3	-7.70	1.32	1.37
36	A5	1902	G	C5-C4	-7.69	1.32	1.38
36	A1	816	A	N3-C4	7.67	1.39	1.34
36	A1	317	A	N7-C5	-7.66	1.34	1.39
36	A1	1164	G	C6-N1	-7.66	1.34	1.39
36	A5	41	G	P-OP1	-7.66	1.35	1.49
57	DT	104	GLU	CB-CG	7.65	1.66	1.52
36	A1	966	U	C4-O4	-7.65	1.17	1.23
36	A5	345	G	N1-C2	-7.64	1.31	1.37
36	A5	1434	G	N9-C8	-7.63	1.32	1.37
36	A5	2804	A	N9-C4	-7.62	1.33	1.37
36	A1	1492	G	N9-C4	7.62	1.44	1.38
36	A5	2314	U	C2-N3	7.60	1.43	1.37
36	A5	1301	A	N7-C5	-7.59	1.34	1.39
36	A5	970	A	N9-C4	-7.58	1.33	1.37
36	A1	963	G	N7-C5	-7.56	1.34	1.39
80	A6	542	A	N7-C5	-7.55	1.34	1.39
36	A5	3006	A	N3-C4	-7.55	1.30	1.34
36	A5	2335	G	N3-C4	-7.54	1.30	1.35
36	A5	2272	G	C5-C4	-7.54	1.33	1.38
52	DO	84[B]	ILE	C-N	7.54	1.51	1.34
80	A6	1773	C	C4-N4	7.53	1.40	1.33
52	BO	182[B]	SER	C-N	-7.53	1.16	1.34
36	A1	895	A	N9-C8	7.53	1.43	1.37
36	A1	1507	G	N9-C8	-7.52	1.32	1.37
36	A1	970	A	N9-C4	-7.51	1.33	1.37
36	A1	2952	G	N9-C4	-7.51	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	282	G	N7-C5	-7.50	1.34	1.39
36	A5	1307	G	P-O5'	-7.48	1.52	1.59
54	DQ	171	LYS	CE-NZ	7.47	1.67	1.49
36	A1	659	G	N1-C2	-7.43	1.31	1.37
36	A5	960	U	N1-C2	7.43	1.45	1.38
36	A5	2191	U	C4-O4	-7.43	1.17	1.23
36	A1	2919	A	N9-C4	-7.41	1.33	1.37
36	A5	934	G	P-OP1	-7.40	1.36	1.49
36	A1	1886	A	N9-C4	-7.40	1.33	1.37
41	BC	94	CYS	CB-SG	-7.40	1.69	1.82
80	A6	1535	U	C2-N3	-7.39	1.32	1.37
36	A5	1303	A	C5-C4	-7.39	1.33	1.38
36	A1	35	A	N9-C4	-7.39	1.33	1.37
36	A5	2134	G	N1-C2	-7.39	1.31	1.37
36	A1	2777	G	N9-C4	-7.38	1.32	1.38
36	A5	1902	G	P-OP1	-7.36	1.36	1.49
36	A5	953	G	N9-C8	-7.36	1.32	1.37
36	A5	2948	C	N3-C4	-7.35	1.28	1.33
36	A1	2697	A	C6-N6	-7.34	1.28	1.33
36	A5	2385	G	N9-C4	-7.32	1.32	1.38
36	A5	3245	A	C5-C6	-7.32	1.34	1.41
36	A5	1443	G	C2-N3	-7.31	1.26	1.32
69	Bf	70	LYS	CE-NZ	7.29	1.67	1.49
36	A1	929	A	N3-C4	-7.29	1.30	1.34
36	A5	1374	G	N1-C2	-7.29	1.31	1.37
36	A1	644	G	N7-C5	-7.28	1.34	1.39
36	A1	2611	U	C4-O4	-7.28	1.17	1.23
78	Bo	77	CYS	CB-SG	-7.28	1.69	1.82
36	A1	799	G	N3-C4	-7.27	1.30	1.35
36	A5	345	G	C6-N1	-7.27	1.34	1.39
36	A5	2919	A	C6-N1	-7.26	1.30	1.35
36	A5	1515	A	C5-C6	-7.24	1.34	1.41
52	BO	27[B]	VAL	C-N	7.24	1.50	1.34
36	A1	637	C	N1-C6	-7.23	1.32	1.37
36	A1	644	G	C6-O6	7.23	1.30	1.24
36	A1	1308	A	P-OP2	-7.22	1.36	1.49
36	A1	660	A	C6-N6	-7.21	1.28	1.33
36	A5	3122	A	N3-C4	-7.21	1.30	1.34
36	A5	2141	U	P-OP2	-7.20	1.36	1.49
36	A5	2943	G	N7-C5	-7.18	1.34	1.39
36	A1	816	A	N9-C4	7.17	1.42	1.37
36	A1	1430	U	P-OP1	-7.17	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	339	C	N3-C4	-7.17	1.28	1.33
36	A1	2679	A	N9-C4	-7.16	1.33	1.37
36	A5	2949	U	P-OP1	-7.16	1.36	1.49
36	A5	1849	C	C2-N3	-7.15	1.30	1.35
37	A7	85	G	N1-C2	-7.15	1.32	1.37
36	A5	2364	G	C6-N1	-7.14	1.34	1.39
1	A2	377	G	N9-C4	-7.14	1.32	1.38
36	A5	644	G	N7-C5	-7.13	1.34	1.39
36	A5	1430	U	P-OP1	-7.12	1.36	1.49
80	A6	609	U	N3-C4	-7.09	1.32	1.38
36	A5	1112	A	N7-C5	-7.08	1.35	1.39
36	A5	2837	A	C5-C4	-7.07	1.33	1.38
36	A1	661	G	N7-C5	-7.07	1.35	1.39
36	A5	2689	A	N3-C4	-7.07	1.30	1.34
36	A1	1304	A	N9-C4	-7.07	1.33	1.37
36	A1	1099	A	N9-C4	-7.06	1.33	1.37
36	A5	1159	A	N9-C4	-7.05	1.33	1.37
37	A7	96	U	C2-O2	-7.05	1.16	1.22
38	A8	20	U	C4-O4	-7.05	1.18	1.23
80	A6	100	A	P-OP2	-7.04	1.36	1.49
36	A1	631	U	C2-O2	-7.03	1.16	1.22
36	A5	1110	U	C4-O4	-7.03	1.18	1.23
36	A5	420	G	N7-C5	-7.03	1.35	1.39
36	A5	2364	G	N3-C4	-7.02	1.30	1.35
36	A1	2640	A	C6-N1	-7.01	1.30	1.35
37	A3	89	G	N7-C5	-7.01	1.35	1.39
36	A1	889	U	C2-N3	-7.00	1.32	1.37
36	A5	1887	A	N7-C5	-7.00	1.35	1.39
36	A5	726	G	C5-C6	-7.00	1.35	1.42
64	Ba	24	LYS	CE-NZ	6.99	1.66	1.49
36	A1	1301	A	N7-C5	-6.98	1.35	1.39
80	A6	397	A	N9-C4	-6.97	1.33	1.37
36	A5	3180	A	N3-C4	-6.97	1.30	1.34
80	A6	1744	A	N9-C4	-6.95	1.33	1.37
36	A5	1200	A	N3-C4	-6.95	1.30	1.34
36	A5	2361	A	N9-C4	6.95	1.42	1.37
80	A6	1105	C	N1-C6	-6.95	1.32	1.37
36	A5	2887	A	P-OP2	-6.95	1.37	1.49
36	A1	148	G	N7-C5	-6.94	1.35	1.39
36	A5	2434	U	N3-C4	-6.94	1.32	1.38
38	A4	28	C	N3-C4	-6.93	1.29	1.33
36	A1	2279	A	C5-C6	-6.93	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	971	G	C5-C4	-6.93	1.33	1.38
36	A1	3227	A	N9-C4	-6.92	1.33	1.37
36	A5	2335	G	C6-N1	-6.91	1.34	1.39
36	A5	2399	A	N9-C4	-6.91	1.33	1.37
36	A5	1901	A	N7-C5	-6.89	1.35	1.39
36	A5	2138	A	N7-C5	-6.89	1.35	1.39
36	A1	658	G	C8-N7	-6.88	1.26	1.30
36	A5	1184	A	N9-C4	-6.88	1.33	1.37
36	A1	2394	G	C5-C4	-6.88	1.33	1.38
36	A1	3130	A	N7-C5	-6.88	1.35	1.39
36	A1	1153	A	N7-C5	-6.88	1.35	1.39
36	A5	2336	U	C2-N3	-6.87	1.32	1.37
36	A1	970	A	N3-C4	-6.86	1.30	1.34
36	A5	2836	C	C4-C5	6.86	1.48	1.43
1	A2	1456	C	N3-C4	-6.85	1.29	1.33
36	A1	66	A	N9-C4	-6.84	1.33	1.37
36	A5	334	A	C5-C4	-6.84	1.33	1.38
36	A5	340	C	P-OP1	-6.83	1.37	1.49
36	A1	2376	G	N9-C8	-6.83	1.33	1.37
80	A6	1503	A	N9-C8	6.82	1.43	1.37
36	A1	1117	G	C5-C4	-6.82	1.33	1.38
36	A1	2692	A	N9-C4	6.82	1.42	1.37
36	A5	1592	G	N1-C2	-6.82	1.32	1.37
36	A1	345	G	N9-C8	-6.82	1.33	1.37
36	A5	1042	U	C2-N3	-6.82	1.32	1.37
36	A1	1928	G	C2-N3	-6.80	1.27	1.32
36	A5	429	U	C2-N3	-6.79	1.32	1.37
36	A1	1114	U	C2-N3	-6.79	1.33	1.37
36	A5	986	U	C4-C5	-6.78	1.37	1.43
47	BI	14	ASN	CG-ND2	6.75	1.49	1.32
36	A5	2636	A	C6-N1	-6.75	1.30	1.35
36	A5	1449	A	P-OP2	-6.75	1.37	1.49
52	BO	184[B]	ALA	C-N	6.75	1.49	1.34
36	A5	3316	A	N9-C4	-6.74	1.33	1.37
36	A5	930	U	C4-O4	-6.74	1.18	1.23
80	A6	1600	A	N9-C4	-6.73	1.33	1.37
36	A5	1178	G	C2-N3	-6.73	1.27	1.32
37	A7	81	U	C4-O4	-6.72	1.18	1.23
36	A1	2816	G	C5-C4	-6.72	1.33	1.38
80	A6	1119	G	C6-N1	-6.71	1.34	1.39
36	A5	1592	G	C6-N1	-6.71	1.34	1.39
1	A2	1455	G	C6-O6	6.71	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	922	U	P-OP2	-6.71	1.37	1.49
1	A2	992	A	C2-N3	-6.70	1.27	1.33
36	A1	2188	A	N9-C4	-6.69	1.33	1.37
36	A5	2395	G	C5-C4	-6.69	1.33	1.38
36	A5	847	A	N9-C4	-6.69	1.33	1.37
36	A1	874	U	C2-N3	-6.68	1.33	1.37
36	A1	912	G	C5-C4	-6.68	1.33	1.38
36	A5	3137	C	N1-C6	6.68	1.41	1.37
1	A2	553	G	C6-O6	6.67	1.30	1.24
36	A5	2912	G	N7-C5	-6.67	1.35	1.39
36	A1	1887	A	N9-C4	-6.67	1.33	1.37
36	A1	2409	G	N3-C4	-6.66	1.30	1.35
80	A6	163	G	C5-C6	-6.66	1.35	1.42
36	A5	1371	G	C6-N1	-6.66	1.34	1.39
36	A1	910	G	N7-C5	-6.66	1.35	1.39
36	A1	1326	A	N9-C4	-6.66	1.33	1.37
36	A1	2657	A	N7-C5	-6.65	1.35	1.39
36	A5	1319	G	N7-C5	-6.65	1.35	1.39
36	A1	3216	G	N7-C5	-6.65	1.35	1.39
37	A7	85	G	C6-N1	-6.65	1.34	1.39
36	A1	654	C	N1-C6	-6.64	1.33	1.37
36	A5	2911	A	N7-C5	-6.64	1.35	1.39
36	A5	3006	A	N9-C4	-6.63	1.33	1.37
36	A5	1301	A	C5-C6	-6.63	1.35	1.41
36	A1	653	A	C6-N6	-6.63	1.28	1.33
36	A1	30	G	C6-N1	-6.63	1.34	1.39
36	A1	195	U	C2-O2	-6.63	1.16	1.22
36	A1	2601	A	N9-C4	-6.62	1.33	1.37
36	A1	85	A	N9-C4	-6.62	1.33	1.37
36	A1	2617	U	N3-C4	-6.62	1.32	1.38
80	A6	1773	C	N3-C4	6.61	1.38	1.33
36	A5	3209	A	C5-C4	6.61	1.43	1.38
80	A6	1773	C	C2-N3	6.61	1.41	1.35
80	A6	1119	G	N7-C5	-6.60	1.35	1.39
36	A1	1307	G	N1-C2	-6.60	1.32	1.37
36	A1	45	A	N7-C5	-6.60	1.35	1.39
36	A5	2693	C	C2-N3	-6.59	1.30	1.35
52	DO	158[B]	ASP	C-N	6.59	1.49	1.34
36	A1	643	U	N1-C2	-6.59	1.32	1.38
36	A1	1481	A	N7-C5	-6.59	1.35	1.39
36	A1	3222	U	C2-N3	-6.59	1.33	1.37
36	A5	3362	A	N3-C4	-6.59	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	942	U	N3-C4	-6.58	1.32	1.38
80	A6	351	C	N1-C6	-6.58	1.33	1.37
36	A5	2853	A	N9-C4	-6.58	1.33	1.37
36	A1	1154	A	N7-C5	-6.58	1.35	1.39
80	A6	337	G	N7-C5	-6.58	1.35	1.39
36	A5	2918	G	N7-C5	-6.58	1.35	1.39
36	A5	267	G	C8-N7	-6.56	1.27	1.30
36	A5	859	G	N1-C2	-6.56	1.32	1.37
52	DO	22[B]	THR	C-N	6.56	1.49	1.34
36	A5	1429	G	C6-N1	-6.56	1.34	1.39
80	A6	53	G	C6-N1	-6.54	1.34	1.39
36	A5	1515	A	C6-N1	-6.54	1.30	1.35
36	A5	91	G	N3-C4	-6.53	1.30	1.35
36	A1	931	C	N3-C4	-6.53	1.29	1.33
36	A5	642	U	N3-C4	-6.53	1.32	1.38
36	A5	1142	G	N7-C5	-6.53	1.35	1.39
36	A1	2899	C	N1-C6	-6.52	1.33	1.37
36	A1	965	A	N3-C4	-6.52	1.30	1.34
36	A5	942	U	P-OP1	-6.51	1.37	1.49
36	A5	1849	C	N1-C6	-6.51	1.33	1.37
36	A5	1307	G	C3'-O3'	6.50	1.51	1.42
36	A5	1833	G	N1-C2	-6.50	1.32	1.37
36	A5	3106	A	N7-C5	-6.49	1.35	1.39
36	A5	1490	A	N7-C5	-6.49	1.35	1.39
36	A1	3306	U	C4-C5	6.49	1.49	1.43
36	A1	884	A	N9-C4	-6.48	1.33	1.37
1	A2	1200	G	C6-N1	6.48	1.44	1.39
36	A1	1394	A	N7-C5	-6.47	1.35	1.39
36	A1	3129	A	N9-C4	-6.47	1.33	1.37
36	A5	637	C	C2-O2	-6.45	1.18	1.24
36	A1	417	A	N9-C4	-6.45	1.33	1.37
36	A5	1487	G	N1-C2	-6.45	1.32	1.37
36	A1	2606	G	N9-C8	-6.44	1.33	1.37
36	A5	1841	A	N7-C5	-6.44	1.35	1.39
36	A5	1370	G	N1-C2	-6.43	1.32	1.37
36	A1	2679	A	N3-C4	-6.43	1.30	1.34
36	A5	813	G	N7-C5	-6.42	1.35	1.39
36	A1	2355	G	N7-C5	-6.42	1.35	1.39
36	A1	2376	G	N7-C5	-6.42	1.35	1.39
36	A1	511	G	C6-N1	-6.41	1.35	1.39
36	A5	420	G	C5-C4	-6.41	1.33	1.38
36	A5	2123	G	C5-C4	-6.41	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	A6	101	U	P-OP2	-6.40	1.38	1.49
36	A5	2323	G	C6-N1	-6.40	1.35	1.39
36	A5	2987	A	N7-C5	-6.40	1.35	1.39
36	A1	1152	G	P-O5'	-6.40	1.53	1.59
36	A1	812	G	N7-C5	-6.40	1.35	1.39
36	A5	2147	A	C5-C6	-6.39	1.35	1.41
36	A5	1143	A	N9-C4	-6.39	1.34	1.37
36	A5	1117	G	C5-C4	-6.39	1.33	1.38
36	A1	895	A	C5-C4	6.39	1.43	1.38
36	A1	878	G	P-OP2	-6.39	1.38	1.49
36	A1	2364	G	N9-C4	-6.39	1.32	1.38
36	A5	802	C	N1-C6	-6.39	1.33	1.37
1	A2	992	A	N9-C4	-6.38	1.34	1.37
68	Be	41	VAL	CB-CG1	-6.37	1.39	1.52
80	A6	366	A	N9-C4	-6.37	1.34	1.37
36	A1	1606	U	C2-N3	-6.37	1.33	1.37
36	A1	2726	C	N3-C4	-6.37	1.29	1.33
36	A5	2816	G	C5-C4	-6.36	1.33	1.38
36	A1	364	G	N9-C4	-6.36	1.32	1.38
1	A2	1754	A	N9-C4	-6.35	1.34	1.37
36	A1	701	G	C6-O6	-6.35	1.18	1.24
36	A5	3102	G	C6-N1	-6.34	1.35	1.39
36	A1	628	A	N9-C4	-6.34	1.34	1.37
36	A5	342	A	N9-C4	-6.33	1.34	1.37
36	A1	2368	A	C6-N1	-6.33	1.31	1.35
36	A1	1130	A	N7-C5	-6.33	1.35	1.39
36	A5	2937	G	N9-C8	-6.32	1.33	1.37
36	A1	2952	G	C5-C6	-6.32	1.36	1.42
36	A1	940	G	C6-N1	-6.31	1.35	1.39
36	A5	1406	A	N3-C4	-6.31	1.31	1.34
36	A1	2983	C	N3-C4	-6.31	1.29	1.33
36	A1	3362	A	N7-C5	-6.30	1.35	1.39
38	A4	10	A	C6-N6	-6.29	1.28	1.33
36	A1	2958	A	C6-N6	-6.29	1.28	1.33
36	A1	3130	A	C6-N1	-6.28	1.31	1.35
36	A1	646	A	N7-C5	-6.28	1.35	1.39
36	A1	1180	A	C6-N1	-6.28	1.31	1.35
38	A4	13	A	C6-N6	-6.27	1.28	1.33
36	A5	2905	U	C2-N3	-6.26	1.33	1.37
36	A5	2128	C	N1-C6	-6.26	1.33	1.37
57	DT	32	LYS	CD-CE	6.26	1.66	1.51
80	A6	400	A	N9-C4	6.26	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	1913	A	C5-C6	-6.26	1.35	1.41
36	A1	1434	G	N9-C8	-6.25	1.33	1.37
80	A6	1503	A	C5-C4	6.25	1.43	1.38
36	A1	2800	G	N9-C4	-6.24	1.32	1.38
36	A5	1902	G	N9-C8	-6.24	1.33	1.37
36	A5	2291	A	N3-C4	-6.24	1.31	1.34
36	A5	2856	G	N9-C8	-6.24	1.33	1.37
36	A5	1449	A	C5-C6	-6.23	1.35	1.41
36	A1	2977	G	C5-C4	-6.23	1.33	1.38
36	A1	1150	A	N3-C4	-6.23	1.31	1.34
36	A1	1372	C	N3-C4	-6.23	1.29	1.33
69	Bf	10	LYS	CD-CE	6.22	1.66	1.51
36	A5	876	A	N3-C4	-6.22	1.31	1.34
36	A5	953	G	N9-C4	-6.22	1.32	1.38
52	BO	3[B]	SER	C-N	6.22	1.48	1.34
36	A5	2194	G	C5-C4	-6.21	1.33	1.38
36	A5	2754	G	P-OP1	-6.21	1.38	1.49
36	A5	3182	G	C6-N1	-6.21	1.35	1.39
36	A5	1487	G	C6-N1	-6.21	1.35	1.39
36	A1	2421	U	C4-O4	-6.21	1.18	1.23
36	A1	2800	G	N3-C4	-6.21	1.31	1.35
53	DP	66	SER	C-O	6.21	1.35	1.23
69	Bf	70	LYS	CD-CE	6.21	1.66	1.51
36	A5	795	G	C5-C4	-6.20	1.34	1.38
36	A5	884	A	C8-N7	6.20	1.35	1.31
36	A5	2737	C	N1-C6	-6.20	1.33	1.37
1	A2	49	C	P-OP2	-6.20	1.38	1.49
36	A1	2383	C	N3-C4	6.20	1.38	1.33
36	A1	2993	G	N3-C4	-6.20	1.31	1.35
36	A5	2314	U	C4-O4	6.19	1.28	1.23
36	A5	3172	A	C8-N7	-6.19	1.27	1.31
37	A7	91	G	N9-C8	-6.19	1.33	1.37
36	A1	1846	C	P-O5'	-6.19	1.53	1.59
36	A5	2823	G	N7-C5	-6.19	1.35	1.39
36	A5	1835	A	P-OP1	-6.18	1.38	1.49
36	A5	2858	U	N3-C4	-6.18	1.32	1.38
36	A5	872	U	C4-O4	-6.18	1.18	1.23
1	A2	1241	G	N9-C8	6.17	1.42	1.37
36	A5	1369	A	P-OP2	-6.17	1.38	1.49
36	A5	1847	A	N9-C4	-6.17	1.34	1.37
36	A1	347	G	C5-C4	-6.17	1.34	1.38
36	A1	1055	A	N9-C4	-6.17	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	1307	G	C3'-O3'	6.17	1.50	1.42
36	A1	584	G	C5-C4	-6.17	1.34	1.38
40	DB	367	LYS	CE-NZ	6.16	1.64	1.49
36	A5	421	G	C6-N1	-6.16	1.35	1.39
36	A1	2800	G	C5-C4	-6.16	1.34	1.38
36	A5	1152	G	C8-N7	6.15	1.34	1.30
80	A6	1097	U	C3'-O3'	6.15	1.50	1.42
36	A1	857	G	N1-C2	-6.14	1.32	1.37
36	A5	218	G	P-O5'	-6.14	1.53	1.59
36	A1	668	G	N3-C4	-6.14	1.31	1.35
36	A5	2881	C	C2-O2	-6.14	1.19	1.24
36	A1	1434	G	N7-C5	-6.14	1.35	1.39
36	A5	1851	G	N9-C8	-6.13	1.33	1.37
36	A5	3006	A	N7-C5	-6.13	1.35	1.39
36	A1	2169	G	C5-C6	6.13	1.48	1.42
36	A5	649	A	C5-C6	-6.13	1.35	1.41
36	A5	363	G	C5-C4	-6.13	1.34	1.38
43	DE	90	LYS	CD-CE	6.13	1.66	1.51
64	Da	24	LYS	CE-NZ	6.13	1.64	1.49
36	A5	1169	A	N9-C4	-6.13	1.34	1.37
36	A1	279	U	C4-O4	-6.12	1.18	1.23
36	A1	1164	G	N3-C4	-6.12	1.31	1.35
38	A4	82	U	P-O5'	6.12	1.65	1.59
36	A5	434	U	C2-N3	-6.12	1.33	1.37
36	A1	2853	A	N7-C5	-6.11	1.35	1.39
36	A5	2848	G	N7-C5	-6.11	1.35	1.39
37	A7	96	U	C4-O4	-6.11	1.18	1.23
36	A5	659	G	N7-C5	-6.10	1.35	1.39
36	A5	1797	A	N7-C5	-6.10	1.35	1.39
36	A1	1336	U	C2-N3	-6.10	1.33	1.37
36	A1	1902	G	C8-N7	-6.10	1.27	1.30
36	A5	2830	G	N3-C4	-6.10	1.31	1.35
36	A1	670	C	N3-C4	-6.09	1.29	1.33
36	A1	1433	A	N7-C5	-6.09	1.35	1.39
36	A1	1103	A	N9-C4	6.08	1.41	1.37
36	A1	921	A	N7-C5	-6.08	1.35	1.39
36	A5	2372	A	N3-C4	-6.08	1.31	1.34
36	A1	426	G	N1-C2	-6.08	1.32	1.37
36	A1	3006	A	N9-C4	-6.07	1.34	1.37
36	A1	34	A	N9-C4	-6.07	1.34	1.37
36	A5	2975	U	C4-O4	-6.07	1.18	1.23
36	A5	3308	C	N3-C4	-6.07	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	359	U	C4-O4	-6.07	1.18	1.23
36	A1	2138	A	N7-C5	-6.07	1.35	1.39
36	A1	3209	A	C6-N1	6.07	1.39	1.35
36	A5	2377	G	N9-C8	-6.07	1.33	1.37
36	A1	1467	A	C6-N1	-6.07	1.31	1.35
38	A4	12	A	N9-C4	-6.06	1.34	1.37
36	A5	3102	G	N1-C2	-6.06	1.32	1.37
36	A5	859	G	C6-N1	-6.06	1.35	1.39
36	A5	2733	A	N9-C4	-6.05	1.34	1.37
36	A5	1174	G	C5-C4	-6.05	1.34	1.38
36	A1	2827	U	C2-N3	-6.05	1.33	1.37
36	A5	2915	U	C2-O2	-6.05	1.17	1.22
36	A5	1490	A	C5-C6	-6.04	1.35	1.41
36	A1	800	G	C2-N3	-6.04	1.27	1.32
36	A5	1454	A	C6-N6	-6.03	1.29	1.33
40	DB	262	TRP	CB-CG	-6.03	1.39	1.50
36	A1	857	G	C6-O6	-6.03	1.18	1.24
36	A5	2948	C	C4-N4	-6.02	1.28	1.33
36	A1	348	A	P-OP1	-6.02	1.38	1.49
36	A5	2341	A	N3-C4	6.02	1.38	1.34
36	A1	1149	G	N3-C4	-6.01	1.31	1.35
36	A1	2147	A	N7-C5	-6.01	1.35	1.39
36	A5	1504	A	C6-N1	-6.01	1.31	1.35
36	A5	2980	U	C2-O2	-6.01	1.17	1.22
36	A1	347	G	N9-C4	-6.00	1.33	1.38
36	A1	576	C	N1-C6	-6.00	1.33	1.37
36	A5	744	A	N9-C4	-6.00	1.34	1.37
36	A5	2214	A	P-OP2	-6.00	1.38	1.49
36	A5	2704	A	N7-C5	-6.00	1.35	1.39
36	A5	2857	C	C4-N4	-6.00	1.28	1.33
36	A5	3008	A	N9-C4	-5.99	1.34	1.37
36	A5	1149	G	C5-C4	-5.99	1.34	1.38
36	A5	3005	A	C6-N1	-5.98	1.31	1.35
36	A5	1332	A	C5-C4	-5.98	1.34	1.38
36	A5	2730	G	N9-C4	-5.98	1.33	1.38
36	A1	189	G	N7-C5	-5.97	1.35	1.39
36	A5	2188	A	N3-C4	-5.97	1.31	1.34
36	A5	647	A	N3-C4	-5.97	1.31	1.34
36	A5	1152	G	N1-C2	5.96	1.42	1.37
36	A5	2706	G	C5-C4	-5.96	1.34	1.38
36	A1	1796	G	C6-N1	-5.96	1.35	1.39
36	A1	3054	U	C2-N3	-5.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2244	A	N3-C4	-5.95	1.31	1.34
80	A6	538	A	N9-C4	5.95	1.41	1.37
37	A7	89	G	C5-C4	-5.95	1.34	1.38
36	A1	3344	A	N7-C5	-5.95	1.35	1.39
1	A2	1782	A	C6-N1	-5.94	1.31	1.35
42	BD	41	LYS	CE-NZ	5.94	1.64	1.49
36	A5	416	A	N7-C5	-5.94	1.35	1.39
36	A1	2278	C	N1-C6	5.94	1.40	1.37
36	A1	826	G	C6-N1	-5.93	1.35	1.39
36	A5	1837	U	P-OP2	-5.93	1.38	1.49
36	A1	1507	G	C8-N7	-5.93	1.27	1.30
36	A5	3335	A	N9-C4	-5.93	1.34	1.37
73	Bj	19	CYS	CB-SG	-5.92	1.72	1.81
36	A5	348	A	P-OP1	-5.92	1.38	1.49
36	A5	1449	A	N7-C5	-5.92	1.35	1.39
36	A1	2983	C	C4-C5	5.92	1.47	1.43
36	A1	378	A	N7-C5	-5.92	1.35	1.39
38	A8	111	A	N9-C4	-5.92	1.34	1.37
37	A3	101	G	N3-C4	-5.92	1.31	1.35
36	A5	1138	U	C4-O4	-5.91	1.19	1.23
36	A1	2642	A	N9-C4	-5.91	1.34	1.37
69	Bf	10	LYS	CE-NZ	5.91	1.63	1.49
36	A1	1515	A	N7-C5	-5.91	1.35	1.39
36	A5	345	G	C5-C4	-5.91	1.34	1.38
36	A1	635	G	P-OP2	-5.90	1.39	1.49
41	BC	194	TYR	CD1-CE1	-5.90	1.30	1.39
36	A5	2524	A	C5-C4	5.90	1.42	1.38
36	A5	784	A	C5-C6	-5.89	1.35	1.41
36	A5	857	G	C6-O6	-5.89	1.18	1.24
36	A5	2335	G	C5-C4	-5.89	1.34	1.38
36	A1	2811	A	N3-C4	-5.89	1.31	1.34
80	A6	392	G	N1-C2	-5.89	1.33	1.37
36	A1	584	G	N7-C5	-5.89	1.35	1.39
36	A1	3057	U	N3-C4	-5.89	1.33	1.38
36	A5	868	C	N1-C6	-5.88	1.33	1.37
36	A5	3227	A	N3-C4	-5.88	1.31	1.34
38	A4	96	A	N9-C4	-5.88	1.34	1.37
80	A6	1723	U	C2-O2	-5.88	1.17	1.22
36	A5	922	U	P-OP2	-5.88	1.39	1.49
36	A5	2278	C	N1-C6	5.87	1.40	1.37
36	A1	1127	G	N7-C5	-5.87	1.35	1.39
36	A5	577	C	N1-C6	-5.87	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	3000	A	N9-C4	-5.86	1.34	1.37
36	A1	2798	C	P-OP1	-5.86	1.39	1.49
36	A1	2640	A	C5-C4	-5.86	1.34	1.38
36	A5	1203	A	C5-C6	-5.86	1.35	1.41
36	A5	1149	G	N9-C8	-5.85	1.33	1.37
36	A5	3010	U	C2-N3	-5.85	1.33	1.37
36	A5	931	C	C4-N4	-5.85	1.28	1.33
36	A1	367	A	N9-C4	-5.85	1.34	1.37
36	A1	1375	G	C5-C4	-5.85	1.34	1.38
36	A1	2409	G	N7-C5	-5.84	1.35	1.39
36	A5	2946	A	C6-N1	-5.84	1.31	1.35
36	A5	3047	U	C2-N3	-5.84	1.33	1.37
36	A1	1902	G	N1-C2	5.83	1.42	1.37
36	A5	2884	C	C2-O2	-5.83	1.19	1.24
80	A6	553	G	N7-C5	-5.83	1.35	1.39
80	A6	17	C	C4-N4	-5.83	1.28	1.33
36	A5	1429	G	N9-C8	-5.83	1.33	1.37
36	A5	1332	A	C6-N1	-5.82	1.31	1.35
36	A5	2971	A	N9-C4	5.82	1.41	1.37
36	A5	1172	G	N1-C2	-5.82	1.33	1.37
36	A1	2413	A	C5-C6	-5.81	1.35	1.41
80	A6	1765	A	N9-C4	-5.81	1.34	1.37
1	A2	1291	G	N3-C4	-5.81	1.31	1.35
36	A1	747	A	N3-C4	-5.81	1.31	1.34
36	A5	1156	C	C4-N4	-5.81	1.28	1.33
36	A1	909	G	C5-C4	-5.81	1.34	1.38
36	A5	2977	G	C6-N1	-5.80	1.35	1.39
36	A1	3114	A	N3-C4	-5.80	1.31	1.34
80	A6	1655	A	N3-C4	-5.80	1.31	1.34
36	A1	338	A	N7-C5	-5.80	1.35	1.39
80	A6	1322	A	N3-C4	-5.79	1.31	1.34
36	A1	1145	G	C5-C4	-5.79	1.34	1.38
37	A3	95	A	C6-N1	-5.79	1.31	1.35
36	A5	1903	U	C4-O4	5.79	1.28	1.23
36	A5	1308	A	N9-C8	-5.79	1.33	1.37
36	A1	345	G	C5-C4	-5.79	1.34	1.38
36	A5	2915	U	C2-N3	-5.78	1.33	1.37
36	A5	3095	U	C4-O4	-5.78	1.19	1.23
36	A1	99	A	N7-C5	-5.78	1.35	1.39
36	A1	1429	G	N9-C8	-5.78	1.33	1.37
36	A1	799	G	N9-C4	-5.78	1.33	1.38
36	A5	2732	G	C6-N1	-5.78	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2827	U	N3-C4	-5.77	1.33	1.38
36	A5	805	G	N7-C5	5.77	1.42	1.39
36	A5	2612	U	C2-N3	-5.77	1.33	1.37
36	A5	2960	C	C4-N4	-5.77	1.28	1.33
36	A5	1305	U	N1-C6	-5.77	1.32	1.38
36	A5	369	A	C6-N6	-5.77	1.29	1.33
36	A5	518	G	C5-C4	-5.77	1.34	1.38
36	A5	3245	A	N7-C5	-5.77	1.35	1.39
36	A1	2341	A	N9-C4	-5.76	1.34	1.37
36	A5	1127	G	C5-C4	-5.76	1.34	1.38
36	A1	624	G	N7-C5	-5.76	1.35	1.39
1	A2	992	A	N9-C8	5.76	1.42	1.37
36	A5	3005	A	N7-C5	-5.76	1.35	1.39
36	A1	1592	G	N7-C5	-5.76	1.35	1.39
36	A5	1208	U	N3-C4	-5.76	1.33	1.38
36	A5	2401	A	N9-C4	5.76	1.41	1.37
36	A5	2412	G	N1-C2	-5.76	1.33	1.37
36	A1	2621	G	N3-C4	-5.75	1.31	1.35
80	A6	1388	A	N3-C4	-5.75	1.31	1.34
36	A5	2367	A	N9-C4	5.75	1.41	1.37
36	A1	1156	C	N3-C4	-5.75	1.29	1.33
36	A5	1112	A	C6-N1	-5.75	1.31	1.35
36	A1	1197	A	C6-N1	-5.75	1.31	1.35
36	A5	100	A	N9-C4	-5.75	1.34	1.37
36	A1	421	G	N1-C2	-5.74	1.33	1.37
36	A1	1171	G	N7-C5	-5.74	1.35	1.39
36	A1	1592	G	C5-C6	-5.74	1.36	1.42
80	A6	331	A	N9-C4	-5.74	1.34	1.37
36	A5	1213	G	N1-C2	-5.74	1.33	1.37
36	A5	2858	U	C2-N3	-5.74	1.33	1.37
36	A1	851	C	C4-C5	-5.74	1.38	1.43
36	A5	1365	G	C6-N1	-5.74	1.35	1.39
36	A1	50	U	C4-O4	-5.74	1.19	1.23
36	A5	1462	A	N9-C4	-5.74	1.34	1.37
36	A5	2957	G	C8-N7	-5.74	1.27	1.30
36	A1	2415	C	C4-N4	-5.73	1.28	1.33
36	A1	3273	A	N7-C5	-5.73	1.35	1.39
36	A5	1898	G	C5-C4	-5.73	1.34	1.38
36	A1	909	G	N9-C8	-5.73	1.33	1.37
36	A5	1450	G	C5-C4	-5.73	1.34	1.38
36	A5	2921	U	C4-O4	-5.73	1.19	1.23
36	A5	2860	U	C4-O4	5.72	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	DO	40[B]	ALA	C-N	-5.72	1.20	1.34
36	A5	883	A	P-OP1	5.72	1.58	1.49
36	A5	953	G	N3-C4	-5.72	1.31	1.35
36	A5	1477	A	N3-C4	-5.72	1.31	1.34
42	BD	62	CYS	CB-SG	-5.71	1.72	1.81
36	A5	339	C	N3-C4	-5.71	1.29	1.33
36	A5	2375	G	C6-N1	-5.71	1.35	1.39
36	A1	3174	A	C8-N7	5.71	1.35	1.31
36	A5	428	A	N7-C5	-5.71	1.35	1.39
1	A2	1560	U	N3-C4	-5.71	1.33	1.38
36	A5	2888	U	C2-N3	-5.71	1.33	1.37
36	A1	636	C	C4-N4	-5.71	1.28	1.33
1	A2	993	A	N7-C5	-5.71	1.35	1.39
36	A1	421	G	C6-O6	-5.71	1.19	1.24
36	A1	3114	A	N9-C4	-5.71	1.34	1.37
36	A5	1910	A	C5-C4	-5.70	1.34	1.38
36	A5	326	U	C4-O4	-5.70	1.19	1.23
36	A5	1189	C	N1-C6	-5.70	1.33	1.37
36	A1	803	C	C4-N4	-5.70	1.28	1.33
36	A1	867	G	C5-C4	-5.70	1.34	1.38
36	A1	1874	A	N7-C5	-5.70	1.35	1.39
80	A6	357	G	N9-C8	-5.70	1.33	1.37
36	A5	1338	C	N1-C6	-5.69	1.33	1.37
36	A5	1849	C	C4-C5	-5.69	1.38	1.43
36	A1	635	G	C5-C4	-5.69	1.34	1.38
36	A5	2888	U	C4-C5	-5.69	1.38	1.43
36	A5	2350	C	N1-C6	-5.69	1.33	1.37
36	A1	1330	A	C5-C6	-5.69	1.35	1.41
36	A1	701	G	C6-N1	-5.68	1.35	1.39
36	A5	2646	C	N1-C6	-5.68	1.33	1.37
36	A1	1910	A	N9-C4	-5.68	1.34	1.37
36	A5	652	G	C5-C4	-5.68	1.34	1.38
36	A5	876	A	N1-C2	-5.68	1.29	1.34
1	A2	1555	A	N3-C4	-5.68	1.31	1.34
36	A1	2944	U	C4-O4	-5.68	1.19	1.23
36	A1	963	G	C5-C6	-5.67	1.36	1.42
36	A1	1911	A	C5-C6	-5.67	1.35	1.41
36	A5	924	G	C2-N3	-5.67	1.28	1.32
36	A5	2134	G	C6-N1	-5.67	1.35	1.39
38	A8	54	A	N9-C4	-5.67	1.34	1.37
36	A1	187	A	N9-C4	5.67	1.41	1.37
37	A7	39	C	N3-C4	-5.67	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2418	G	O3'-P	5.67	1.68	1.61
80	A6	1537	C	N3-C4	5.67	1.38	1.33
36	A5	984	G	N7-C5	-5.67	1.35	1.39
36	A5	2361	A	N7-C5	-5.67	1.35	1.39
36	A5	200	C	N3-C4	-5.66	1.29	1.33
36	A1	2213	A	N7-C5	-5.66	1.35	1.39
36	A1	2946	A	N9-C4	-5.66	1.34	1.37
36	A5	1145	G	N3-C4	-5.66	1.31	1.35
36	A1	1664	G	C6-N1	-5.66	1.35	1.39
36	A5	2892	A	C6-N1	-5.65	1.31	1.35
31	Cd	7	TRP	CB-CG	5.65	1.60	1.50
38	A4	103	G	N9-C4	5.65	1.42	1.38
80	A6	423	G	C6-N1	-5.64	1.35	1.39
36	A5	39	A	N3-C4	-5.64	1.31	1.34
36	A5	1370	G	C6-N1	-5.64	1.35	1.39
36	A5	2340	U	C4-O4	-5.63	1.19	1.23
36	A1	780	A	N3-C4	-5.63	1.31	1.34
36	A1	1180	A	N3-C4	-5.63	1.31	1.34
36	A1	2794	G	C6-N1	-5.63	1.35	1.39
36	A5	3039	C	N1-C6	-5.63	1.33	1.37
1	A2	865	A	C6-N1	-5.63	1.31	1.35
36	A1	44	U	C4-O4	-5.63	1.19	1.23
36	A1	822	G	C2-N3	-5.63	1.28	1.32
36	A1	2130	G	C6-N1	-5.63	1.35	1.39
36	A5	900	G	C6-N1	-5.63	1.35	1.39
36	A5	2147	A	N7-C5	-5.63	1.35	1.39
1	A2	1746	A	N9-C4	-5.63	1.34	1.37
36	A1	2315	G	C6-N1	-5.63	1.35	1.39
36	A1	2393	G	C8-N7	-5.63	1.27	1.30
36	A5	1043	C	N3-C4	-5.62	1.30	1.33
62	DY	38	GLU	CG-CD	5.62	1.60	1.51
36	A1	1150	A	N9-C4	-5.62	1.34	1.37
36	A5	657	A	N3-C4	-5.62	1.31	1.34
36	A1	92	G	C6-O6	-5.62	1.19	1.24
36	A1	2326	A	N9-C4	-5.62	1.34	1.37
36	A5	1370	G	N9-C8	-5.62	1.33	1.37
36	A5	2419	A	C6-N1	-5.61	1.31	1.35
36	A5	2647	A	N3-C4	-5.61	1.31	1.34
76	Bm	115	CYS	CB-SG	-5.61	1.72	1.81
36	A5	2810	C	N1-C6	-5.61	1.33	1.37
36	A5	1099	A	C6-N1	-5.61	1.31	1.35
36	A1	1173	U	C4-O4	-5.60	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2846	U	N3-C4	-5.60	1.33	1.38
36	A5	1320	C	C4-C5	-5.60	1.38	1.43
52	DO	4[B]	GLN	C-N	-5.60	1.23	1.34
80	A6	542	A	C5-C6	-5.60	1.36	1.41
36	A5	2148	U	C4-O4	-5.60	1.19	1.23
36	A1	649	A	C6-N1	-5.60	1.31	1.35
36	A1	365	A	N7-C5	-5.59	1.35	1.39
36	A5	1414	G	C6-N1	-5.59	1.35	1.39
36	A5	1434	G	C5-C4	-5.59	1.34	1.38
36	A1	1396	C	C4-N4	-5.59	1.28	1.33
47	BI	8	CYS	CB-SG	-5.59	1.72	1.81
36	A1	2946	A	C5-C6	-5.58	1.36	1.41
36	A5	3218	A	N9-C4	-5.58	1.34	1.37
36	A5	2382	G	N7-C5	-5.58	1.35	1.39
36	A5	817	A	C4'-C3'	-5.58	1.47	1.52
36	A5	1309	U	N1-C2	-5.58	1.33	1.38
36	A5	2626	A	N9-C8	-5.58	1.33	1.37
36	A5	3088	G	C5-C6	-5.58	1.36	1.42
36	A1	307	A	N7-C5	-5.57	1.35	1.39
36	A5	559	A	N7-C5	-5.57	1.35	1.39
36	A5	3374	U	C4-O4	-5.57	1.19	1.23
36	A5	3013	U	C2-N3	-5.57	1.33	1.37
36	A5	2302	G	N1-C2	-5.57	1.33	1.37
36	A1	1305	U	C4-O4	-5.57	1.19	1.23
36	A1	3226	A	N9-C4	-5.57	1.34	1.37
36	A1	1459	C	N3-C4	-5.56	1.30	1.33
36	A1	2957	G	N9-C8	-5.56	1.33	1.37
36	A5	2301	U	C2-O2	-5.56	1.17	1.22
36	A1	2647	A	N3-C4	-5.56	1.31	1.34
36	A1	2728	G	C5-C4	-5.56	1.34	1.38
36	A5	640	U	C2-N3	-5.56	1.33	1.37
36	A5	2323	G	N1-C2	-5.56	1.33	1.37
36	A5	657	A	N9-C4	-5.56	1.34	1.37
36	A5	2860	U	P-OP2	-5.56	1.39	1.49
36	A1	1510	G	C6-N1	-5.56	1.35	1.39
36	A1	2605	G	C5-C4	-5.55	1.34	1.38
36	A1	2909	U	C2-N3	5.55	1.41	1.37
80	A6	1118	G	N3-C4	-5.55	1.31	1.35
36	A5	1433	A	N7-C5	-5.55	1.35	1.39
36	A1	1668	G	C6-N1	-5.55	1.35	1.39
36	A1	2880	U	C2-N3	5.55	1.41	1.37
36	A5	49	A	C5-C4	-5.55	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2640	A	N3-C4	-5.55	1.31	1.34
36	A5	949	C	N3-C4	-5.55	1.30	1.33
36	A5	2823	G	C5-C4	-5.55	1.34	1.38
36	A1	659	G	N7-C5	-5.54	1.35	1.39
36	A1	1432	C	C2-O2	-5.54	1.19	1.24
36	A5	1413	G	C6-N1	-5.54	1.35	1.39
1	A2	577	G	C5-C6	-5.54	1.36	1.42
36	A5	2609	A	C5-C4	-5.54	1.34	1.38
80	A6	1478	G	N7-C5	-5.54	1.35	1.39
36	A5	824	C	N3-C4	-5.54	1.30	1.33
36	A5	987	U	C2-O2	-5.54	1.17	1.22
36	A1	1446	A	N9-C8	-5.53	1.33	1.37
36	A5	2932	U	C2-N3	-5.52	1.33	1.37
36	A5	3052	G	N1-C2	-5.52	1.33	1.37
36	A1	953	G	C2-N3	-5.52	1.28	1.32
36	A1	2750	U	C2-N3	-5.52	1.33	1.37
80	A6	1749	A	N3-C4	5.52	1.38	1.34
36	A5	891	G	N9-C4	-5.52	1.33	1.38
36	A1	86	G	C6-N1	-5.52	1.35	1.39
36	A5	1875	G	C6-N1	-5.52	1.35	1.39
36	A5	2164	A	N7-C5	-5.52	1.35	1.39
36	A5	420	G	N9-C8	-5.52	1.33	1.37
36	A5	1432	C	N1-C6	-5.52	1.33	1.37
36	A5	899	U	C4-O4	-5.52	1.19	1.23
36	A5	1174	G	C8-N7	-5.52	1.27	1.30
36	A5	1901	A	N9-C8	-5.52	1.33	1.37
36	A5	2908	G	C2-N3	-5.52	1.28	1.32
36	A1	1592	G	N3-C4	5.51	1.39	1.35
36	A1	1369	A	N7-C5	-5.51	1.35	1.39
36	A5	2391	G	C6-O6	-5.51	1.19	1.24
36	A1	2169	G	N7-C5	5.51	1.42	1.39
36	A1	1153	A	N3-C4	-5.50	1.31	1.34
36	A1	2971	A	N9-C4	5.50	1.41	1.37
41	BC	106	TRP	CB-CG	-5.50	1.40	1.50
36	A5	421	G	N1-C2	-5.50	1.33	1.37
36	A5	1177	G	N7-C5	-5.50	1.35	1.39
36	A5	1330	A	N3-C4	-5.50	1.31	1.34
36	A5	1443	G	N3-C4	-5.50	1.31	1.35
36	A5	2419	A	P-O5'	5.50	1.65	1.59
36	A5	2920	U	P-OP1	-5.50	1.39	1.49
36	A5	2904	U	C2-N3	-5.50	1.33	1.37
36	A1	1379	G	C6-N1	-5.50	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A4	73	U	C4-O4	-5.50	1.19	1.23
36	A5	2417	U	C4-O4	5.50	1.28	1.23
36	A5	3184	A	N9-C4	-5.50	1.34	1.37
36	A1	670	C	N1-C6	-5.50	1.33	1.37
36	A5	344	A	N9-C8	-5.50	1.33	1.37
36	A5	706	A	C5-C4	-5.49	1.34	1.38
36	A5	1195	A	N1-C2	-5.49	1.29	1.34
36	A1	2385	G	N9-C4	-5.49	1.33	1.38
40	DB	349	LYS	CD-CE	5.49	1.65	1.51
36	A1	3344	A	C5-C6	-5.49	1.36	1.41
36	A5	2987	A	C6-N1	-5.49	1.31	1.35
36	A1	1126	G	C5-C4	-5.49	1.34	1.38
37	A7	5	G	N9-C8	-5.49	1.34	1.37
36	A1	2434	U	N3-C4	-5.49	1.33	1.38
36	A5	360	G	N9-C8	-5.48	1.34	1.37
36	A5	1911	A	C5-C6	-5.48	1.36	1.41
1	A2	1084	A	N3-C4	-5.48	1.31	1.34
36	A1	1395	G	C5-C4	-5.48	1.34	1.38
38	A4	25	G	C6-N1	-5.48	1.35	1.39
36	A5	2122	G	C5-C4	-5.48	1.34	1.38
36	A1	867	G	N3-C4	-5.48	1.31	1.35
1	A2	542	A	N9-C4	-5.48	1.34	1.37
36	A1	48	A	C5-C4	-5.48	1.34	1.38
36	A1	1394	A	N9-C8	-5.48	1.33	1.37
36	A5	1319	G	N9-C8	-5.48	1.34	1.37
36	A1	789	A	N3-C4	-5.48	1.31	1.34
38	A4	10	A	N7-C5	-5.48	1.35	1.39
36	A1	282	G	C5-C4	-5.47	1.34	1.38
80	A6	1118	G	C5-C4	-5.47	1.34	1.38
36	A5	2744	U	C2-N3	-5.47	1.33	1.37
36	A5	889	U	C4-O4	-5.47	1.19	1.23
36	A1	2367	A	C8-N7	-5.47	1.27	1.31
36	A1	3042	U	N3-C4	-5.47	1.33	1.38
36	A5	3088	G	N7-C5	-5.47	1.35	1.39
36	A1	339	C	N1-C6	-5.46	1.33	1.37
36	A5	635	G	P-OP2	-5.46	1.39	1.49
36	A1	369	A	C6-N6	-5.46	1.29	1.33
36	A1	1369	A	N9-C4	-5.46	1.34	1.37
36	A1	2817	A	C6-N1	-5.46	1.31	1.35
36	A1	2611	U	N3-C4	-5.46	1.33	1.38
80	A6	341	A	N3-C4	-5.46	1.31	1.34
36	A5	834	U	C4-O4	-5.46	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	2941	A	N9-C8	-5.46	1.33	1.37
36	A1	1197	A	C5-C6	-5.46	1.36	1.41
36	A5	1147	G	N9-C8	-5.46	1.34	1.37
36	A1	885	U	C2-N3	-5.45	1.33	1.37
80	A6	418	G	N7-C5	-5.45	1.35	1.39
80	A6	1670	G	C5-C4	-5.45	1.34	1.38
36	A5	1324	U	C2-N3	-5.45	1.33	1.37
80	A6	314	C	C2-O2	-5.45	1.19	1.24
36	A5	1301	A	N9-C8	-5.45	1.33	1.37
36	A5	2824	G	N7-C5	-5.45	1.35	1.39
36	A1	672	A	C6-N1	5.45	1.39	1.35
36	A1	1122	U	N3-C4	-5.45	1.33	1.38
36	A5	354	U	C2-N3	-5.45	1.33	1.37
36	A5	3107	U	C2-N3	-5.45	1.33	1.37
80	A6	1109	G	C6-N1	-5.45	1.35	1.39
36	A5	1130	A	N1-C2	-5.45	1.29	1.34
1	A2	553	G	N1-C2	5.44	1.42	1.37
36	A5	522	A	P-O5'	-5.44	1.54	1.59
36	A5	1492	G	C2-N3	5.44	1.37	1.32
80	A6	553	G	C6-O6	5.44	1.29	1.24
36	A1	1858	A	N7-C5	-5.44	1.35	1.39
36	A5	3096	C	N1-C6	-5.44	1.33	1.37
36	A1	2286	U	N3-C4	-5.44	1.33	1.38
36	A1	2867	C	C2-N3	-5.44	1.31	1.35
36	A5	2336	U	C2-O2	-5.44	1.17	1.22
36	A1	1147	G	N1-C2	-5.44	1.33	1.37
36	A1	2737	C	N1-C2	-5.44	1.34	1.40
36	A5	2198	A	N9-C4	-5.44	1.34	1.37
36	A1	656	A	N7-C5	-5.43	1.35	1.39
36	A5	2717	U	C2-N3	-5.43	1.33	1.37
36	A1	899	U	C2-N3	-5.43	1.33	1.37
36	A1	2147	A	N9-C4	-5.43	1.34	1.37
36	A5	2342	U	C2-N3	-5.43	1.33	1.37
1	A2	331	A	N9-C4	-5.43	1.34	1.37
36	A1	1169	A	P-O5'	-5.43	1.54	1.59
36	A5	2397	A	C5-C6	5.43	1.46	1.41
36	A5	2912	G	N9-C8	-5.43	1.34	1.37
36	A5	3273	A	N9-C4	-5.43	1.34	1.37
36	A5	1845	G	C5-C4	-5.42	1.34	1.38
36	A5	36	C	N1-C2	-5.42	1.34	1.40
68	Be	8	LYS	CD-CE	5.42	1.64	1.51
36	A5	1320	C	C4-N4	-5.42	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	2611	U	P-OP1	-5.42	1.39	1.49
36	A1	867	G	N7-C5	-5.42	1.35	1.39
36	A1	2372	A	N3-C4	-5.41	1.31	1.34
36	A5	2128	C	C4-N4	-5.41	1.29	1.33
36	A5	2336	U	N3-C4	-5.41	1.33	1.38
36	A5	2775	U	C2-N3	-5.41	1.33	1.37
36	A1	1122	U	C4-O4	-5.41	1.19	1.23
36	A1	2177	G	N7-C5	-5.41	1.36	1.39
36	A1	1307	G	C5-C4	-5.40	1.34	1.38
36	A5	1908	A	C6-N1	-5.40	1.31	1.35
36	A1	912	G	C8-N7	-5.40	1.27	1.30
36	A1	984	G	N7-C5	-5.40	1.36	1.39
36	A1	2345	A	C6-N1	-5.40	1.31	1.35
36	A1	1446	A	N7-C5	-5.40	1.36	1.39
36	A1	1151	U	C4-O4	5.40	1.27	1.23
36	A5	39	A	C5-C4	-5.39	1.34	1.38
36	A5	365	A	N7-C5	-5.39	1.36	1.39
36	A1	1124	U	C5-C6	-5.39	1.29	1.34
36	A1	426	G	C8-N7	-5.39	1.27	1.30
36	A1	2400	G	N9-C4	-5.39	1.33	1.38
37	A3	88	G	C6-N1	-5.39	1.35	1.39
80	A6	1670	G	N7-C5	-5.39	1.36	1.39
36	A5	3307	A	C2-N3	-5.39	1.28	1.33
37	A7	88	G	N1-C2	-5.39	1.33	1.37
36	A1	2699	G	N1-C2	-5.39	1.33	1.37
36	A1	3296	A	C6-N1	-5.39	1.31	1.35
36	A5	2834	G	C2-N3	-5.39	1.28	1.32
36	A1	1117	G	P-OP1	-5.39	1.39	1.49
1	A2	377	G	C6-N1	5.38	1.43	1.39
36	A1	647	A	C6-N6	-5.38	1.29	1.33
36	A1	2309	A	N9-C4	-5.38	1.34	1.37
36	A5	2365	C	N3-C4	-5.38	1.30	1.33
36	A5	831	G	N7-C5	-5.38	1.36	1.39
36	A1	1164	G	N1-C2	-5.38	1.33	1.37
36	A5	631	U	N3-C4	-5.38	1.33	1.38
36	A5	1086	C	C4-C5	-5.38	1.38	1.43
36	A5	41	G	N9-C4	-5.38	1.33	1.38
36	A5	417	A	N7-C5	-5.38	1.36	1.39
36	A5	1327	C	N3-C4	-5.38	1.30	1.33
36	A1	3136	G	C6-N1	-5.37	1.35	1.39
36	A5	895	A	N3-C4	-5.37	1.31	1.34
1	A2	538	A	N3-C4	5.37	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	46	U	C2-N3	-5.37	1.33	1.37
36	A1	423	A	N3-C4	-5.37	1.31	1.34
36	A1	2737	C	N1-C6	-5.37	1.33	1.37
36	A5	1895	A	N3-C4	-5.37	1.31	1.34
37	A7	66	A	P-OP2	-5.37	1.39	1.49
1	A2	555	A	N9-C4	5.37	1.41	1.37
36	A1	2357	A	N7-C5	-5.37	1.36	1.39
36	A1	2919	A	N7-C5	-5.37	1.36	1.39
36	A1	1337	A	N9-C4	5.37	1.41	1.37
38	A8	25	G	N1-C2	-5.37	1.33	1.37
36	A5	755	A	C6-N1	-5.36	1.31	1.35
36	A1	1145	G	C6-N1	-5.36	1.35	1.39
36	A1	626	U	C2-N3	-5.36	1.33	1.37
36	A1	718	G	N9-C8	5.36	1.41	1.37
36	A5	508	U	C5-C6	-5.36	1.29	1.34
36	A5	3112	G	C5-C4	-5.36	1.34	1.38
36	A1	1170	A	N3-C4	5.36	1.38	1.34
36	A1	2828	G	C6-N1	-5.36	1.35	1.39
36	A1	2920	U	C2-N3	-5.36	1.34	1.37
44	BF	234	GLU	CD-OE2	5.36	1.31	1.25
80	A6	1600	A	C5-C4	5.36	1.42	1.38
36	A5	864	G	C5-C4	-5.36	1.34	1.38
36	A5	1296	C	N3-C4	-5.35	1.30	1.33
53	BP	124	LYS	CE-NZ	5.35	1.62	1.49
36	A5	363	G	N3-C4	-5.35	1.31	1.35
36	A5	2974	U	C2-N3	-5.35	1.34	1.37
40	DB	287	LYS	CD-CE	5.35	1.64	1.51
36	A5	1833	G	C6-N1	-5.35	1.35	1.39
36	A1	37	U	N1-C2	-5.35	1.33	1.38
36	A1	938	C	C4-N4	-5.35	1.29	1.33
36	A1	2281	A	N9-C4	-5.35	1.34	1.37
36	A1	2800	G	N9-C8	-5.35	1.34	1.37
36	A5	95	A	C5-C4	-5.35	1.35	1.38
36	A5	666	A	N3-C4	-5.34	1.31	1.34
36	A5	1338	C	C4-C5	-5.34	1.38	1.43
36	A5	990	U	C2-N3	-5.34	1.34	1.37
36	A1	317	A	C5-C6	-5.34	1.36	1.41
36	A5	2697	A	N9-C4	5.34	1.41	1.37
36	A5	3039	C	C4-C5	-5.34	1.38	1.43
36	A1	658	G	P-OP2	-5.34	1.39	1.49
36	A1	791	A	P-O5'	-5.34	1.54	1.59
36	A1	3301	U	C2-N3	-5.34	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	A6	317	C	N1-C6	-5.34	1.33	1.37
80	A6	1596	C	N3-C4	-5.34	1.30	1.33
36	A5	784	A	N7-C5	-5.34	1.36	1.39
36	A1	1537	A	N7-C5	-5.34	1.36	1.39
36	A1	2397	A	N3-C4	5.34	1.38	1.34
36	A5	1415	U	C2-O2	-5.33	1.17	1.22
36	A1	1893	A	C6-N1	-5.33	1.31	1.35
36	A5	2395	G	C6-N1	-5.33	1.35	1.39
36	A1	939	U	N1-C2	-5.33	1.33	1.38
80	A6	1087	A	C6-N1	-5.33	1.31	1.35
36	A1	883	A	P-OP1	-5.33	1.39	1.49
80	A6	314	C	N3-C4	-5.33	1.30	1.33
80	A6	1119	G	N3-C4	-5.33	1.31	1.35
36	A5	1902	G	C6-N1	-5.33	1.35	1.39
36	A1	637	C	C3'-C2'	-5.32	1.46	1.52
36	A5	806	A	P-OP2	-5.32	1.40	1.49
36	A5	2619	G	C6-O6	-5.32	1.19	1.24
36	A5	903	U	C2-N3	-5.32	1.34	1.37
36	A5	1190	A	C6-N1	-5.32	1.31	1.35
36	A5	2643	A	C6-N1	5.32	1.39	1.35
36	A5	3216	G	C5-C4	-5.32	1.34	1.38
47	DI	96	VAL	CB-CG2	-5.32	1.41	1.52
36	A5	1404	G	N9-C8	-5.32	1.34	1.37
1	A2	973	A	N7-C5	-5.32	1.36	1.39
36	A5	2693	C	N1-C6	-5.32	1.33	1.37
36	A5	2937	G	C5-C4	-5.32	1.34	1.38
36	A1	592	A	N3-C4	5.32	1.38	1.34
36	A1	3180	A	N3-C4	-5.32	1.31	1.34
36	A1	2958	A	N9-C8	-5.31	1.33	1.37
36	A5	1840	U	C2-N3	-5.31	1.34	1.37
36	A5	1851	G	C8-N7	-5.31	1.27	1.30
36	A5	1425	U	C2-N3	-5.31	1.34	1.37
36	A5	1468	A	N7-C5	-5.31	1.36	1.39
36	A1	95	A	N3-C4	-5.31	1.31	1.34
36	A1	937	G	C5-C4	-5.31	1.34	1.38
36	A5	290	G	C6-N1	-5.31	1.35	1.39
36	A5	2204	C	N3-C4	-5.31	1.30	1.33
36	A1	3209	A	C5-C4	5.30	1.42	1.38
36	A5	52	A	N7-C5	-5.30	1.36	1.39
36	A5	1443	G	N1-C2	-5.30	1.33	1.37
36	A5	3114	A	N3-C4	-5.30	1.31	1.34
36	A1	933	A	C6-N1	-5.30	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	2632	G	C8-N7	5.30	1.34	1.30
36	A1	45	A	C6-N6	-5.30	1.29	1.33
36	A5	3065	G	C6-N1	-5.30	1.35	1.39
36	A1	2093	A	N9-C4	5.30	1.41	1.37
36	A1	1902	G	N7-C5	-5.30	1.36	1.39
38	A4	16	G	C5-C4	-5.30	1.34	1.38
36	A5	2730	G	N7-C5	-5.30	1.36	1.39
1	A2	582	U	P-O5'	-5.29	1.54	1.59
36	A1	963	G	C5-C4	-5.29	1.34	1.38
36	A5	2272	G	C6-N1	-5.29	1.35	1.39
36	A5	3032	A	N7-C5	-5.29	1.36	1.39
36	A1	815	G	C6-N1	-5.29	1.35	1.39
36	A1	279	U	C2-O2	-5.29	1.17	1.22
36	A5	925	A	N7-C5	-5.29	1.36	1.39
40	BB	200	GLU	CG-CD	5.29	1.59	1.51
36	A5	2434	U	C2-N3	-5.29	1.34	1.37
36	A5	2734	A	N9-C4	-5.29	1.34	1.37
36	A5	2376	G	C6-O6	-5.29	1.19	1.24
36	A1	318	A	N7-C5	-5.28	1.36	1.39
36	A1	591	G	C8-N7	-5.28	1.27	1.30
36	A5	1151	U	C4-O4	-5.28	1.19	1.23
36	A1	2988	C	C2-O2	-5.28	1.19	1.24
36	A5	818	C	P-OP1	-5.28	1.40	1.49
36	A5	1115	G	N7-C5	-5.28	1.36	1.39
36	A5	1888	U	N1-C6	-5.28	1.33	1.38
36	A5	1362	G	C6-N1	-5.28	1.35	1.39
36	A1	2821	C	N3-C4	5.28	1.37	1.33
36	A1	2939	G	N7-C5	-5.28	1.36	1.39
36	A5	956	U	N3-C4	-5.28	1.33	1.38
36	A5	3115	C	N3-C4	-5.28	1.30	1.33
52	DO	196[B]	SER	C-N	-5.28	1.22	1.34
64	Da	15	VAL	C-O	5.28	1.33	1.23
80	A6	119	A	N9-C4	-5.28	1.34	1.37
80	A6	623	A	N9-C4	-5.28	1.34	1.37
80	A6	377	G	N1-C2	-5.27	1.33	1.37
36	A5	1409	G	C6-N1	-5.27	1.35	1.39
36	A1	2816	G	C6-N1	-5.27	1.35	1.39
36	A5	505	G	N3-C4	-5.27	1.31	1.35
36	A5	1131	G	N7-C5	-5.27	1.36	1.39
36	A5	1209	G	C2-N3	-5.27	1.28	1.32
36	A5	658	G	N3-C4	-5.27	1.31	1.35
36	A5	994	G	C5-C4	-5.27	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	1117	G	N7-C5	-5.27	1.36	1.39
36	A1	91	G	C8-N7	5.27	1.34	1.30
36	A5	2191	U	N3-C4	-5.26	1.33	1.38
36	A1	323	A	N9-C4	-5.26	1.34	1.37
80	A6	478	A	N9-C4	-5.26	1.34	1.37
80	A6	1780	G	N1-C2	-5.26	1.33	1.37
36	A5	798	G	C6-O6	-5.26	1.19	1.24
36	A5	2341	A	N9-C8	-5.26	1.33	1.37
36	A5	3070	A	C6-N1	-5.26	1.31	1.35
36	A1	2983	C	P-O5'	-5.26	1.54	1.59
36	A5	1135	A	N9-C8	-5.26	1.33	1.37
36	A1	641	C	N3-C4	-5.25	1.30	1.33
36	A1	2649	A	C5-C4	-5.25	1.35	1.38
36	A5	2318	U	N3-C4	-5.25	1.33	1.38
80	A6	1654	G	N3-C4	-5.25	1.31	1.35
36	A1	289	A	N7-C5	-5.25	1.36	1.39
36	A1	1492	G	C6-N1	-5.25	1.35	1.39
36	A5	1838	G	C5-C4	-5.25	1.34	1.38
36	A5	2706	G	C8-N7	-5.25	1.27	1.30
80	A6	337	G	C5-C6	-5.25	1.37	1.42
36	A5	1171	G	N7-C5	-5.25	1.36	1.39
36	A1	361	A	C6-N6	-5.24	1.29	1.33
36	A1	653	A	C5-C6	-5.24	1.36	1.41
36	A1	45	A	C5-C6	-5.24	1.36	1.41
36	A1	2662	G	N7-C5	-5.24	1.36	1.39
80	A6	1781	A	N9-C4	5.24	1.41	1.37
36	A5	912	G	N3-C4	5.24	1.39	1.35
36	A5	1326	A	C5-C4	-5.24	1.35	1.38
36	A5	2734	A	N3-C4	-5.24	1.31	1.34
36	A1	2426	U	C2-O2	-5.24	1.17	1.22
53	BP	129	THR	CB-CG2	-5.24	1.35	1.52
36	A1	805	G	N7-C5	5.24	1.42	1.39
36	A5	1515	A	N7-C5	-5.24	1.36	1.39
44	DF	131	GLU	CD-OE2	5.24	1.31	1.25
36	A1	2317	A	C6-N1	-5.24	1.31	1.35
36	A5	2617	U	C4-O4	-5.23	1.19	1.23
36	A5	433	A	N9-C4	-5.23	1.34	1.37
36	A1	420	G	C6-N1	-5.23	1.35	1.39
36	A5	2163	C	N3-C4	-5.23	1.30	1.33
36	A5	3372	A	N9-C4	5.23	1.41	1.37
36	A1	430	U	N1-C6	-5.23	1.33	1.38
36	A1	2938	G	C2-N3	-5.23	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	A6	352	A	N9-C4	-5.23	1.34	1.37
37	A3	95	A	C5-C6	-5.23	1.36	1.41
36	A5	2214	A	N9-C4	-5.22	1.34	1.37
76	Dm	79	GLU	CD-OE1	5.22	1.31	1.25
80	A6	647	G	N3-C4	-5.22	1.31	1.35
36	A5	934	G	C5-C4	-5.22	1.34	1.38
36	A5	2620	G	N1-C2	-5.22	1.33	1.37
36	A1	673	U	C4-O4	-5.22	1.19	1.23
36	A1	1124	U	C4-O4	-5.22	1.19	1.23
36	A5	917	A	N3-C4	-5.22	1.31	1.34
36	A1	942	U	N1-C2	-5.22	1.33	1.38
36	A1	1422	G	C6-N1	-5.22	1.35	1.39
36	A5	658	G	N9-C4	-5.22	1.33	1.38
36	A1	286	U	C2-N3	-5.21	1.34	1.37
36	A5	3000	A	C5-C4	-5.21	1.35	1.38
36	A1	1507	G	C5-C4	-5.21	1.34	1.38
36	A5	3179	U	C4-O4	-5.21	1.19	1.23
36	A1	49	A	N3-C4	-5.21	1.31	1.34
36	A1	278	U	C2-O2	-5.21	1.17	1.22
36	A1	2626	A	N9-C4	5.21	1.41	1.37
80	A6	597	G	C6-N1	-5.21	1.35	1.39
36	A1	795	G	C5-C4	-5.21	1.34	1.38
36	A5	1477	A	C6-N1	-5.21	1.31	1.35
36	A5	645	A	C8-N7	-5.21	1.27	1.31
80	A6	992	A	N9-C4	-5.20	1.34	1.37
36	A5	693	A	N9-C4	-5.20	1.34	1.37
36	A1	1845	G	C5-C4	-5.20	1.34	1.38
80	A6	1655	A	C5-C4	-5.20	1.35	1.38
36	A1	106	A	N9-C4	-5.20	1.34	1.37
36	A1	1304	A	N9-C8	-5.20	1.33	1.37
36	A1	584	G	N3-C4	-5.20	1.31	1.35
36	A5	1311	G	N7-C5	-5.20	1.36	1.39
80	A6	392	G	C5-C4	-5.20	1.34	1.38
80	A6	592	A	N3-C4	-5.20	1.31	1.34
36	A1	359	U	C2-N3	-5.19	1.34	1.37
36	A5	2922	G	C6-O6	-5.19	1.19	1.24
36	A1	28	C	C2-N3	-5.19	1.31	1.35
36	A1	345	G	P-OP2	-5.19	1.40	1.49
36	A5	282	G	C2-N3	-5.19	1.28	1.32
36	A5	1114	U	C2-N3	-5.19	1.34	1.37
36	A1	640	U	N1-C6	-5.19	1.33	1.38
36	A1	1117	G	N9-C8	-5.19	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2377	G	C6-N1	-5.19	1.35	1.39
36	A5	1170	A	C8-N7	-5.19	1.27	1.31
36	A5	2327	U	N3-C4	-5.19	1.33	1.38
36	A5	2692	A	N7-C5	-5.19	1.36	1.39
36	A5	2912	G	C5-C4	-5.19	1.34	1.38
80	A6	375	U	C4-O4	-5.19	1.19	1.23
36	A1	3215	A	N9-C4	-5.18	1.34	1.37
80	A6	434	G	C6-N1	-5.18	1.35	1.39
80	A6	980	G	N9-C8	-5.18	1.34	1.37
36	A5	1056	U	C2-N3	5.18	1.41	1.37
36	A5	2375	G	P-OP2	-5.18	1.40	1.49
1	A2	352	A	N9-C8	-5.18	1.33	1.37
36	A5	835	G	C5-C4	-5.18	1.34	1.38
36	A5	1116	G	N9-C8	-5.18	1.34	1.37
36	A1	1170	A	N9-C4	5.18	1.41	1.37
36	A1	2277	C	C4-N4	-5.18	1.29	1.33
36	A5	345	G	C6-O6	-5.18	1.19	1.24
36	A5	627	U	C2-N3	-5.18	1.34	1.37
36	A5	1832	C	N1-C6	-5.18	1.34	1.37
36	A1	826	G	C5-C4	-5.18	1.34	1.38
38	A4	10	A	C6-N1	-5.18	1.31	1.35
36	A5	49	A	N3-C4	-5.18	1.31	1.34
36	A5	884	A	C5-C6	-5.18	1.36	1.41
36	A1	642	U	P-O5'	-5.17	1.54	1.59
36	A1	2877	G	N7-C5	-5.17	1.36	1.39
36	A5	2372	A	C6-N1	-5.17	1.31	1.35
36	A1	1178	G	N3-C4	-5.17	1.31	1.35
36	A5	649	A	N7-C5	-5.17	1.36	1.39
36	A5	1607	U	C3'-O3'	5.17	1.49	1.42
80	A6	1644	C	N3-C4	-5.17	1.30	1.33
36	A5	284	A	N9-C4	5.17	1.41	1.37
36	A1	42	C	N1-C6	5.17	1.40	1.37
36	A5	859	G	C2-N3	-5.17	1.28	1.32
1	A2	474	A	N9-C4	-5.17	1.34	1.37
36	A1	1497	C	P-OP2	5.17	1.57	1.49
36	A5	70	A	N7-C5	-5.17	1.36	1.39
36	A5	2634	U	N3-C4	5.17	1.43	1.38
36	A1	987	U	C2-O2	-5.16	1.17	1.22
36	A1	2426	U	C4-O4	-5.16	1.19	1.23
36	A5	2837	A	N3-C4	-5.16	1.31	1.34
36	A5	2859	U	C2-N3	-5.16	1.34	1.37
42	DD	95	TRP	CG-CD1	5.16	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2278	C	N3-C4	-5.16	1.30	1.33
36	A1	583	G	C6-N1	-5.16	1.35	1.39
36	A5	436	A	C5-C4	5.16	1.42	1.38
36	A5	1157	G	N9-C8	-5.16	1.34	1.37
48	DJ	8	PRO	CB-CG	5.16	1.75	1.50
36	A1	1409	G	C6-N1	-5.16	1.35	1.39
36	A1	1908	A	P-OP2	-5.16	1.40	1.49
36	A1	3216	G	N9-C8	-5.16	1.34	1.37
36	A1	795	G	N1-C2	-5.16	1.33	1.37
36	A5	2414	G	C5-C4	-5.16	1.34	1.38
36	A5	2858	U	C2-O2	-5.16	1.17	1.22
36	A1	1202	A	C6-N1	-5.15	1.31	1.35
36	A1	1741	A	C5-C6	-5.15	1.36	1.41
36	A1	2595	A	N9-C8	5.15	1.41	1.37
36	A1	1450	G	C2-N3	-5.15	1.28	1.32
38	A4	21	C	P-O5'	-5.15	1.54	1.59
36	A5	984	G	C6-N1	-5.15	1.35	1.39
36	A5	1151	U	C2-N3	-5.15	1.34	1.37
36	A1	2364	G	N3-C4	-5.15	1.31	1.35
36	A5	1208	U	C2-N3	-5.14	1.34	1.37
36	A5	2172	A	N9-C4	-5.14	1.34	1.37
36	A5	404	G	N9-C8	-5.14	1.34	1.37
36	A1	638	C	C2-O2	-5.14	1.19	1.24
36	A1	2394	G	C8-N7	-5.14	1.27	1.30
36	A1	2920	U	C2-O2	-5.14	1.17	1.22
38	A4	48	A	N7-C5	-5.14	1.36	1.39
36	A1	892	U	C4-O4	-5.14	1.19	1.23
36	A1	1133	A	N9-C4	-5.14	1.34	1.37
80	A6	1	U	N1-C2	5.13	1.43	1.38
36	A5	3316	A	N3-C4	-5.13	1.31	1.34
36	A1	832	G	C6-N1	-5.13	1.35	1.39
36	A1	1480	G	C8-N7	-5.13	1.27	1.30
46	DH	82	VAL	CB-CG2	-5.13	1.42	1.52
36	A1	1131	G	C6-N1	-5.13	1.35	1.39
36	A1	1837	U	P-OP2	-5.13	1.40	1.49
36	A1	1328	C	N1-C6	-5.13	1.34	1.37
36	A5	609	G	N3-C4	-5.13	1.31	1.35
36	A1	1841	A	N9-C4	5.13	1.41	1.37
80	A6	687	G	N9-C4	-5.12	1.33	1.38
36	A5	1338	C	C4-N4	-5.12	1.29	1.33
36	A1	221	A	N9-C8	-5.12	1.33	1.37
36	A1	951	A	N9-C4	-5.12	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2149	A	C6-N1	-5.12	1.31	1.35
36	A5	1797	A	C5-C4	-5.12	1.35	1.38
36	A5	2666	C	N1-C6	-5.12	1.34	1.37
36	A5	2859	U	N3-C4	-5.12	1.33	1.38
36	A1	73	C	N1-C6	-5.12	1.34	1.37
36	A1	2642	A	N3-C4	-5.12	1.31	1.34
36	A1	2877	G	C6-N1	-5.12	1.35	1.39
36	A5	2865	U	N1-C2	5.12	1.43	1.38
36	A1	3319	U	N1-C2	5.11	1.43	1.38
36	A5	2928	C	C4'-C3'	-5.11	1.47	1.52
36	A5	2936	A	C4'-C3'	-5.11	1.47	1.52
1	A2	387	A	N7-C5	5.11	1.42	1.39
36	A1	159	A	N9-C4	-5.11	1.34	1.37
36	A1	338	A	C5-C4	-5.11	1.35	1.38
36	A5	1117	G	C6-O6	-5.11	1.19	1.24
38	A4	13	A	C5-C6	-5.11	1.36	1.41
36	A1	835	G	C5-C4	-5.11	1.34	1.38
36	A5	891	G	N3-C4	-5.11	1.31	1.35
36	A5	984	G	N9-C8	-5.11	1.34	1.37
36	A1	1481	A	P-O5'	-5.10	1.54	1.59
36	A5	1179	A	P-OP2	-5.10	1.40	1.49
36	A5	1886	A	N3-C4	-5.10	1.31	1.34
36	A1	1431	G	C6-N1	-5.10	1.35	1.39
36	A1	287	G	N3-C4	-5.10	1.31	1.35
80	A6	55	A	C5-C4	-5.10	1.35	1.38
36	A5	1143	A	N3-C4	-5.10	1.31	1.34
36	A5	1902	G	C8-N7	-5.10	1.27	1.30
67	Dd	61	LYS	CD-CE	5.10	1.64	1.51
36	A1	1060	U	C2-N3	-5.10	1.34	1.37
36	A5	38	U	O3'-P	-5.10	1.55	1.61
36	A1	907	G	N7-C5	-5.10	1.36	1.39
36	A1	952	A	C5-C6	-5.10	1.36	1.41
36	A1	1845	G	N7-C5	-5.10	1.36	1.39
36	A5	1898	G	N9-C8	-5.10	1.34	1.37
36	A5	2243	A	N3-C4	-5.09	1.31	1.34
36	A1	1305	U	C2-N3	-5.09	1.34	1.37
36	A1	2160	G	N7-C5	-5.09	1.36	1.39
36	A5	2934	A	C6-N1	-5.09	1.31	1.35
36	A1	2888	U	C4-O4	-5.09	1.19	1.23
36	A5	2371	G	N1-C2	-5.09	1.33	1.37
64	Ba	42	ARG	CZ-NH2	5.09	1.39	1.33
52	BO	158[B]	ASP	C-N	-5.09	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	397	A	N3-C4	-5.09	1.31	1.34
36	A5	2659	G	N1-C2	-5.09	1.33	1.37
80	A6	49	C	P-OP2	-5.08	1.40	1.49
36	A5	2147	A	C5-C4	-5.08	1.35	1.38
36	A5	2620	G	C5-C4	-5.08	1.34	1.38
36	A5	2693	C	N3-C4	-5.08	1.30	1.33
36	A5	999	G	C5-C4	-5.08	1.34	1.38
36	A1	2987	A	C6-N1	-5.08	1.31	1.35
1	A2	142	G	N9-C4	-5.08	1.33	1.38
36	A1	1164	G	N9-C4	-5.08	1.33	1.38
36	A5	2141	U	P-OP1	-5.08	1.40	1.49
36	A1	2132	C	P-OP1	-5.08	1.40	1.49
36	A1	2147	A	C5-C4	-5.08	1.35	1.38
36	A5	652	G	N7-C5	-5.08	1.36	1.39
36	A5	1910	A	C6-N6	-5.08	1.29	1.33
36	A1	679	U	C2-N3	-5.07	1.34	1.37
80	A6	420	A	N9-C4	-5.07	1.34	1.37
36	A5	1145	G	C2-N3	-5.07	1.28	1.32
36	A1	1124	U	C4-C5	-5.07	1.39	1.43
38	A4	23	U	C2-N3	5.07	1.41	1.37
36	A5	656	A	O3'-P	-5.07	1.55	1.61
36	A5	1117	G	C8-N7	-5.07	1.27	1.30
36	A1	50	U	N3-C4	-5.07	1.33	1.38
36	A5	987	U	C4-C5	5.07	1.48	1.43
36	A5	2302	G	C6-N1	-5.07	1.36	1.39
36	A5	2922	G	C5-C6	-5.07	1.37	1.42
36	A1	2370	G	N7-C5	-5.06	1.36	1.39
36	A1	923	C	N1-C2	-5.06	1.35	1.40
36	A5	34	A	N3-C4	-5.06	1.31	1.34
36	A5	3122	A	N7-C5	-5.06	1.36	1.39
36	A1	1454	A	N9-C4	-5.06	1.34	1.37
36	A5	1188	U	C2-N3	-5.06	1.34	1.37
36	A1	1299	U	C4-O4	-5.06	1.19	1.23
36	A1	1310	G	N1-C2	-5.06	1.33	1.37
36	A1	1417	G	C5-C4	-5.05	1.34	1.38
36	A1	3063	C	N3-C4	-5.05	1.30	1.33
80	A6	539	G	C5-C4	5.05	1.41	1.38
36	A5	2372	A	C3'-O3'	5.05	1.49	1.42
36	A1	2412	G	N7-C5	-5.05	1.36	1.39
36	A1	2860	U	P-O5'	-5.05	1.54	1.59
36	A5	1188	U	C5-C6	-5.05	1.29	1.34
36	A5	2717	U	C2-O2	-5.05	1.17	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A5	2855	U	C4-O4	-5.05	1.19	1.23
36	A1	960	U	C2-O2	5.05	1.26	1.22
36	A1	1165	A	C6-N6	-5.05	1.29	1.33
36	A5	585	A	N3-C4	-5.05	1.31	1.34
51	DN	94	TYR	CE1-CZ	5.05	1.45	1.38
76	Dm	79	GLU	CD-OE2	5.05	1.31	1.25
36	A1	936	A	C6-N6	-5.05	1.29	1.33
36	A5	2993	G	N1-C2	-5.05	1.33	1.37
36	A1	3307	A	C6-N1	-5.04	1.32	1.35
36	A5	2882	U	C2-O2	-5.04	1.17	1.22
55	BR	125	LYS	CD-CE	5.04	1.63	1.51
36	A5	1295	G	C6-N1	-5.04	1.36	1.39
46	DH	110	LYS	CD-CE	5.04	1.63	1.51
36	A1	574	U	C4-O4	-5.04	1.19	1.23
80	A6	335	U	N1-C2	-5.04	1.34	1.38
36	A1	1852	G	C6-O6	5.04	1.28	1.24
80	A6	158	U	C3'-O3'	5.04	1.49	1.42
36	A5	877	C	C4-N4	-5.04	1.29	1.33
36	A5	1123	U	N3-C4	-5.04	1.33	1.38
36	A5	1435	A	C6-N6	-5.04	1.29	1.33
55	DR	72	GLU	CG-CD	5.04	1.59	1.51
36	A1	345	G	N7-C5	-5.04	1.36	1.39
36	A1	893	C	P-OP2	-5.04	1.40	1.49
36	A1	2833	A	N9-C4	-5.04	1.34	1.37
36	A5	2958	A	N9-C4	-5.04	1.34	1.37
1	A2	1773	C	C4-N4	5.03	1.38	1.33
36	A5	652	G	N9-C8	-5.03	1.34	1.37
36	A1	198	A	C6-N1	-5.03	1.32	1.35
36	A5	726	G	N7-C5	-5.03	1.36	1.39
36	A5	1427	U	C2-N3	-5.03	1.34	1.37
36	A1	2393	G	N9-C8	-5.03	1.34	1.37
36	A1	919	U	C4-O4	-5.03	1.19	1.23
36	A1	1145	G	C8-N7	-5.03	1.27	1.30
36	A1	3375	A	N7-C5	-5.03	1.36	1.39
80	A6	1723	U	C2-N3	-5.03	1.34	1.37
36	A5	1049	C	C4-N4	-5.03	1.29	1.33
37	A7	88	G	C2-N3	-5.03	1.28	1.32
36	A1	2302	G	N1-C2	-5.02	1.33	1.37
36	A5	1299	U	C4-O4	-5.02	1.19	1.23
36	A5	333	G	C6-N1	-5.02	1.36	1.39
36	A5	2743	A	C6-N6	-5.02	1.29	1.33
1	A2	1782	A	N3-C4	-5.02	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Ad	7	TRP	CB-CG	5.02	1.59	1.50
36	A1	2919	A	C6-N1	-5.02	1.32	1.35
80	A6	609	U	C2-N3	-5.02	1.34	1.37
36	A5	2366	C	C2-N3	5.02	1.39	1.35
36	A1	952	A	N7-C5	-5.01	1.36	1.39
80	A6	47	A	C5'-C4'	-5.01	1.45	1.51
36	A5	106	A	N9-C4	-5.01	1.34	1.37
67	Dd	102	LYS	CD-CE	5.01	1.63	1.51
36	A1	952	A	C6-N6	-5.01	1.29	1.33
36	A1	2350	C	N1-C6	-5.01	1.34	1.37
36	A1	3139	A	C6-N6	-5.01	1.29	1.33
38	A4	36	G	N9-C4	-5.01	1.33	1.38
80	A6	1595	U	N3-C4	-5.01	1.33	1.38
36	A5	282	G	N3-C4	-5.01	1.31	1.35
36	A5	867	G	C2-N3	-5.01	1.28	1.32
36	A5	3187	A	C6-N1	-5.01	1.32	1.35
1	A2	1758	U	N1-C2	5.01	1.43	1.38
36	A1	357	A	N3-C4	-5.01	1.31	1.34
36	A1	413	U	C4-O4	-5.01	1.19	1.23
36	A1	1056	U	C4-O4	-5.01	1.19	1.23
80	A6	1602	C	N3-C4	-5.01	1.30	1.33
36	A5	2190	U	C2-O2	-5.01	1.17	1.22
80	A6	437	A	N9-C4	-5.01	1.34	1.37
36	A1	372	A	N3-C4	5.01	1.37	1.34
80	A6	163	G	N9-C8	5.01	1.41	1.37
36	A5	2375	G	C6-O6	-5.01	1.19	1.24
36	A5	3245	A	N1-C2	5.01	1.38	1.34
73	Bj	43	LYS	CD-CE	5.00	1.63	1.51
36	A5	2930	A	N3-C4	5.00	1.37	1.34
36	A1	406	G	C6-N1	-5.00	1.36	1.39
36	A1	2369	G	N9-C8	-5.00	1.34	1.37
36	A5	2291	A	N9-C4	-5.00	1.34	1.37
36	A5	2652	U	N1-C2	-5.00	1.34	1.38
36	A5	2944	U	C4-O4	-5.00	1.19	1.23
69	Df	91	ALA	N-CA	5.00	1.56	1.46
36	A1	668	G	C5-C4	-5.00	1.34	1.38
36	A1	2697	A	C6-N1	-5.00	1.32	1.35
36	A5	1184	A	N3-C4	-5.00	1.31	1.34
36	A5	1388	U	C2-O2	-5.00	1.17	1.22
36	A5	2315	G	N9-C4	-5.00	1.33	1.38
37	A7	12	U	C4-O4	-5.00	1.19	1.23

All (9884) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2777	G	C4-C5-N7	50.47	130.99	110.80
36	A1	2777	G	N9-C4-C5	-40.53	89.19	105.40
36	A1	2777	G	C5-C6-O6	-39.10	105.14	128.60
52	BO	3[A]	VAL	CA-C-N	-39.08	31.23	117.20
36	A5	1152	G	N3-C4-C5	33.63	145.41	128.60
36	A1	2777	G	N1-C6-O6	32.55	139.43	119.90
36	A1	2777	G	C6-C5-N7	-32.03	111.18	130.40
36	A5	1152	G	N3-C4-N9	-31.59	107.05	126.00
52	BO	3[A]	VAL	C-N-CA	-31.16	43.80	121.70
36	A5	1152	G	N3-C2-N2	-26.99	101.01	119.90
36	A1	2777	G	C5-N7-C8	-26.62	90.99	104.30
36	A1	3242	G	N3-C4-N9	-25.00	111.00	126.00
36	A5	1152	G	C2-N3-C4	-24.03	99.89	111.90
36	A1	2714	G	N3-C4-C5	22.55	139.87	128.60
36	A5	922	U	C5-C6-N1	-22.08	111.66	122.70
36	A5	922	U	C2-N3-C4	-21.60	114.04	127.00
80	A6	1773	C	N3-C4-C5	-21.52	113.29	121.90
36	A1	2777	G	N3-C4-N9	20.18	138.11	126.00
36	A5	1152	G	C5-N7-C8	-20.02	94.29	104.30
36	A1	1495	U	C5-C6-N1	-19.83	112.79	122.70
36	A1	2714	G	N3-C4-N9	-19.57	114.26	126.00
36	A5	922	U	N1-C2-N3	19.47	126.58	114.90
36	A5	1152	G	C8-N9-C1'	18.98	151.68	127.00
36	A5	3245	A	C2-N3-C4	-18.87	101.16	110.60
36	A1	2714	G	C2-N3-C4	-18.73	102.53	111.90
1	A2	553	G	N1-C6-O6	18.62	131.07	119.90
36	A5	3245	A	C5-N7-C8	-18.61	94.59	103.90
36	A1	3242	G	N3-C4-C5	18.44	137.82	128.60
1	A2	1200	G	N1-C6-O6	17.86	130.61	119.90
36	A1	1492	G	N3-C4-C5	-17.61	119.79	128.60
80	A6	609	U	C5-C6-N1	-17.30	114.05	122.70
36	A5	1152	G	N1-C6-O6	17.20	130.22	119.90
36	A1	2617	U	C5-C6-N1	-16.99	114.21	122.70
36	A5	1152	G	C4-N9-C1'	-16.85	104.59	126.50
36	A5	1152	G	C4-C5-N7	16.78	117.51	110.80
36	A1	2777	G	C8-N9-C4	16.56	113.03	106.40
80	A6	609	U	C5-C4-O4	16.48	135.79	125.90
36	A1	2952	G	C5-C6-O6	-16.45	118.73	128.60
36	A5	1152	G	N1-C2-N2	16.25	130.82	116.20
36	A1	1495	U	C4-C5-C6	16.12	129.37	119.70
36	A5	922	U	N1-C2-O2	-16.09	111.53	122.80
36	A5	3245	A	N7-C8-N9	15.82	121.71	113.80
80	A6	553	G	N1-C6-O6	15.73	129.34	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	337	G	C6-C5-N7	-15.69	120.99	130.40
36	A5	776	U	C5-C6-N1	-15.52	114.94	122.70
36	A5	2726	C	C6-N1-C2	-15.44	114.12	120.30
36	A1	1308	A	N7-C8-N9	15.43	121.51	113.80
36	A1	517	G	C8-N9-C4	-15.42	100.23	106.40
36	A1	1495	U	N1-C2-N3	15.31	124.09	114.90
36	A1	3242	G	N3-C2-N2	-15.29	109.20	119.90
36	A1	2846	U	C5-C4-O4	15.27	135.06	125.90
36	A5	1450	G	C5-N7-C8	15.24	111.92	104.30
36	A1	644	G	C5-C6-O6	15.20	137.72	128.60
36	A1	1409	G	N1-C6-O6	-15.20	110.78	119.90
36	A1	3242	G	C8-N9-C1'	15.18	146.74	127.00
36	A1	804	C	N1-C2-O2	-15.14	109.82	118.90
1	A2	577	G	C4-C5-N7	15.02	116.81	110.80
36	A5	3245	A	C4-C5-N7	14.99	118.19	110.70
80	A6	163	G	C5-N7-C8	-14.81	96.89	104.30
36	A5	3245	A	N1-C6-N6	14.78	127.47	118.60
36	A1	1308	A	C8-N9-C4	-14.71	99.92	105.80
36	A1	3306	U	N1-C2-N3	14.70	123.72	114.90
36	A1	1492	G	C5-N7-C8	14.61	111.61	104.30
36	A5	3245	A	C6-C5-N7	-14.56	122.11	132.30
36	A1	1902	G	N1-C6-O6	14.47	128.58	119.90
36	A1	3242	G	N9-C4-C5	14.45	111.18	105.40
80	A6	337	G	C8-N9-C1'	-14.40	108.28	127.00
36	A5	1152	G	C5-C6-O6	-14.38	119.97	128.60
36	A1	2827	U	C5-C6-N1	-14.27	115.57	122.70
36	A1	1592	G	C5-C6-N1	14.27	118.63	111.50
1	A2	1200	G	C5-C6-O6	-14.23	120.06	128.60
36	A1	2278	C	N1-C2-O2	-14.20	110.38	118.90
80	A6	163	G	N3-C4-C5	14.20	135.70	128.60
80	A6	163	G	N3-C4-N9	-14.19	117.48	126.00
36	A1	3306	U	N3-C2-O2	-14.18	112.27	122.20
1	A2	1773	C	N3-C4-C5	-14.15	116.24	121.90
36	A5	2353	G	C5-C6-O6	-14.14	120.12	128.60
36	A1	2434	U	C5-C4-O4	14.07	134.34	125.90
36	A1	1492	G	C2-N3-C4	14.07	118.93	111.90
36	A5	2726	C	C5-C4-N4	14.02	130.02	120.20
36	A5	2634	U	C2-N3-C4	-13.99	118.61	127.00
36	A1	885	U	C5-C6-N1	-13.96	115.72	122.70
36	A5	2634	U	C5-C4-O4	-13.96	117.53	125.90
36	A5	776	U	N1-C2-N3	13.95	123.27	114.90
36	A1	2298	U	C5-C6-N1	-13.92	115.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1592	G	N1-C6-O6	-13.92	111.55	119.90
36	A1	2679	A	C2-N3-C4	-13.84	103.68	110.60
36	A1	709	A	C8-N9-C4	13.83	111.33	105.80
36	A1	776	U	C4-C5-C6	13.82	128.00	119.70
80	A6	163	G	C2-N3-C4	-13.82	104.99	111.90
80	A6	609	U	N3-C4-O4	-13.74	109.78	119.40
36	A1	2278	C	N1-C2-N3	13.64	128.75	119.20
36	A1	2617	U	C5-C4-O4	13.48	133.99	125.90
36	A5	2245	C	C6-N1-C2	-13.44	114.93	120.30
36	A5	776	U	C4-C5-C6	13.41	127.75	119.70
1	A2	1560	U	C5-C4-O4	13.36	133.91	125.90
36	A5	2372	A	C8-N9-C4	-13.34	100.47	105.80
80	A6	308	C	C5-C6-N1	-13.32	114.34	121.00
80	A6	337	G	C4-N9-C1'	13.31	143.80	126.50
36	A5	1450	G	N7-C8-N9	-13.30	106.45	113.10
36	A1	1216	C	C6-N1-C2	-13.27	114.99	120.30
1	A2	1773	C	C6-N1-C2	-13.23	115.01	120.30
36	A5	922	U	C4-C5-C6	13.22	127.63	119.70
36	A1	3242	G	C4-N9-C1'	-13.22	109.31	126.50
36	A1	1592	G	C4-C5-N7	13.19	116.08	110.80
36	A1	2836	C	C5-C4-N4	13.19	129.43	120.20
80	A6	1280	C	N3-C4-C5	-13.12	116.65	121.90
36	A5	631	U	N3-C2-O2	-13.11	113.02	122.20
36	A1	2278	C	C6-N1-C2	-13.07	115.07	120.30
80	A6	1773	C	N3-C4-N4	13.03	127.12	118.00
36	A1	2983	C	C5-C6-N1	-13.02	114.49	121.00
36	A5	2278	C	N1-C2-O2	-12.99	111.11	118.90
36	A5	2303	A	C2-N3-C4	12.97	117.08	110.60
36	A5	2361	A	C2-N3-C4	12.96	117.08	110.60
36	A5	3214	U	C5-C4-O4	12.88	133.63	125.90
36	A1	1846	C	N1-C2-O2	-12.87	111.18	118.90
36	A1	1342	C	N3-C4-C5	12.86	127.04	121.90
36	A5	2726	C	N1-C2-N3	12.84	128.19	119.20
36	A1	2983	C	C5-C4-N4	12.79	129.15	120.20
36	A1	3242	G	N1-C2-N2	12.77	127.69	116.20
36	A5	1208	U	N3-C4-O4	-12.77	110.46	119.40
36	A1	1592	G	N3-C2-N2	12.74	128.82	119.90
36	A1	2617	U	N3-C4-O4	-12.71	110.51	119.40
80	A6	453	U	N3-C2-O2	-12.70	113.31	122.20
1	A2	577	G	C5-N7-C8	-12.68	97.96	104.30
36	A5	1208	U	C5-C4-O4	12.68	133.51	125.90
36	A5	2308	C	N1-C2-O2	-12.67	111.30	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2617	U	C2-N3-C4	-12.66	119.40	127.00
36	A5	2327	U	C5-C6-N1	-12.66	116.37	122.70
36	A5	3214	U	N3-C2-O2	-12.64	113.35	122.20
36	A5	1152	G	C4-C5-C6	-12.63	111.22	118.80
36	A1	3269	U	N3-C2-O2	-12.62	113.37	122.20
68	De	43	ARG	NE-CZ-NH1	12.58	126.59	120.30
36	A1	3306	U	C5-C4-O4	12.57	133.44	125.90
36	A1	1492	G	C4-C5-N7	-12.56	105.78	110.80
36	A1	2314	U	N1-C2-N3	-12.56	107.36	114.90
36	A5	2758	A	C2-N3-C4	12.56	116.88	110.60
1	A2	1541	G	N1-C6-O6	-12.55	112.37	119.90
36	A1	709	A	N7-C8-N9	-12.51	107.54	113.80
36	A1	1911	A	N1-C6-N6	12.50	126.10	118.60
80	A6	308	C	C2-N3-C4	-12.46	113.67	119.90
36	A1	2726	C	C6-N1-C2	-12.44	115.33	120.30
36	A5	1371	G	N1-C6-O6	-12.43	112.44	119.90
36	A1	2983	C	N3-C4-N4	-12.43	109.30	118.00
36	A1	2899	C	C4-C5-C6	12.41	123.61	117.40
36	A5	776	U	N3-C2-O2	-12.40	113.52	122.20
36	A5	1846	C	C5-C6-N1	-12.38	114.81	121.00
80	A6	1773	C	C6-N1-C2	-12.38	115.35	120.30
80	A6	337	G	N9-C4-C5	-12.38	100.45	105.40
36	A1	1904	C	N1-C2-O2	-12.36	111.48	118.90
36	A1	2836	C	C4-C5-C6	12.35	123.58	117.40
36	A1	1495	U	N1-C2-O2	-12.35	114.16	122.80
36	A1	1902	G	C5-C6-O6	-12.34	121.19	128.60
36	A1	2952	G	N1-C6-O6	12.32	127.29	119.90
36	A5	1434	G	C5-N7-C8	12.31	110.46	104.30
36	A5	1450	G	C4-C5-N7	-12.30	105.88	110.80
36	A1	54	C	N3-C4-N4	-12.30	109.39	118.00
80	A6	65	A	C2-N3-C4	-12.30	104.45	110.60
36	A1	3344	A	N7-C8-N9	12.29	119.94	113.80
36	A1	1858	A	C2-N3-C4	12.29	116.74	110.60
36	A1	672	A	N1-C6-N6	12.28	125.97	118.60
37	A7	120	C	C6-N1-C2	12.26	125.20	120.30
36	A5	591	G	C5-C6-O6	-12.24	121.25	128.60
36	A1	295	A	C8-N9-C4	-12.24	100.90	105.80
36	A1	3362	A	N1-C6-N6	12.21	125.93	118.60
36	A1	3362	A	C6-C5-N7	-12.16	123.79	132.30
36	A1	1902	G	C6-C5-N7	-12.14	123.12	130.40
62	BY	13	ARG	NE-CZ-NH2	-12.11	114.25	120.30
36	A1	2726	C	N3-C2-O2	-12.08	113.44	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2340	U	N3-C4-O4	-12.06	110.96	119.40
36	A1	2846	U	N3-C2-O2	-12.02	113.79	122.20
36	A1	2952	G	C4-C5-N7	12.01	115.60	110.80
80	A6	144	U	N3-C2-O2	-12.00	113.80	122.20
36	A5	3245	A	N1-C2-N3	12.00	135.30	129.30
36	A1	517	G	N7-C8-N9	11.93	119.07	113.10
36	A1	1336	U	N3-C2-O2	-11.93	113.85	122.20
36	A5	1308	A	N7-C8-N9	11.93	119.76	113.80
36	A5	2726	C	C4-C5-C6	11.93	123.36	117.40
80	A6	553	G	C6-C5-N7	-11.92	123.25	130.40
36	A1	1495	U	C2-N3-C4	-11.91	119.85	127.00
36	A5	1056	U	C4-C5-C6	11.91	126.85	119.70
1	A2	1200	G	N3-C2-N2	-11.91	111.56	119.90
36	A1	2617	U	C4-C5-C6	11.89	126.83	119.70
36	A1	435	C	C6-N1-C2	11.84	125.04	120.30
36	A1	2130	G	N1-C6-O6	-11.83	112.80	119.90
36	A5	290	G	N1-C6-O6	-11.82	112.81	119.90
36	A5	966	U	N3-C2-O2	-11.77	113.96	122.20
36	A1	3306	U	N3-C4-O4	-11.76	111.17	119.40
36	A1	2617	U	N1-C2-N3	11.75	121.95	114.90
80	A6	553	G	C5-C6-O6	-11.75	121.55	128.60
36	A1	895	A	C5-N7-C8	-11.75	98.03	103.90
36	A5	667	C	C6-N1-C2	11.72	124.99	120.30
36	A1	2777	G	N3-C2-N2	11.72	128.10	119.90
36	A5	2278	C	N1-C2-N3	11.71	127.40	119.20
1	A2	577	G	C5-C6-O6	-11.69	121.58	128.60
36	A5	2726	C	N3-C4-C5	-11.67	117.23	121.90
36	A1	2633	U	N3-C2-O2	-11.64	114.05	122.20
36	A5	2808	A	N9-C4-C5	-11.64	101.14	105.80
36	A1	979	U	C6-N1-C2	-11.64	114.02	121.00
36	A1	942	U	N3-C4-O4	-11.61	111.27	119.40
36	A1	1156	C	N3-C4-C5	11.59	126.54	121.90
36	A1	3344	A	C6-C5-N7	-11.58	124.19	132.30
36	A1	2679	A	N1-C2-N3	11.57	135.09	129.30
80	A6	1773	C	N1-C2-O2	-11.56	111.96	118.90
80	A6	163	G	C4-C5-N7	11.55	115.42	110.80
80	A6	687	G	N3-C2-N2	-11.55	111.81	119.90
36	A5	1389	G	C4-C5-N7	11.53	115.41	110.80
36	A1	2278	C	C2-N3-C4	-11.52	114.14	119.90
36	A1	2817	A	C6-N1-C2	-11.51	111.69	118.60
1	A2	1782	A	N9-C4-C5	11.51	110.40	105.80
36	A1	2827	U	N3-C2-O2	-11.47	114.17	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1027	A	C8-N9-C4	-11.47	101.21	105.80
36	A1	3362	A	C5-N7-C8	-11.46	98.17	103.90
36	A1	645	A	C6-N1-C2	-11.46	111.72	118.60
36	A1	591	G	C5-C6-O6	-11.45	121.73	128.60
36	A1	2983	C	C4-C5-C6	11.44	123.12	117.40
36	A5	1130	A	C2-N3-C4	11.44	116.32	110.60
36	A1	1202	A	C2-N3-C4	-11.43	104.89	110.60
36	A1	3214	U	N3-C2-O2	-11.42	114.21	122.20
36	A5	1592	G	N3-C2-N2	11.41	127.89	119.90
80	A6	609	U	N3-C2-O2	-11.40	114.22	122.20
36	A1	2413	A	N1-C2-N3	-11.36	123.62	129.30
36	A5	2899	C	N3-C2-O2	-11.35	113.96	121.90
36	A5	1797	A	C5-N7-C8	11.34	109.57	103.90
1	A2	553	G	N3-C2-N2	-11.34	111.96	119.90
36	A1	664	U	C5-C6-N1	-11.33	117.04	122.70
36	A1	2726	C	N1-C2-N3	11.32	127.12	119.20
36	A1	1307	G	N1-C6-O6	-11.31	113.11	119.90
36	A1	963	G	C5-C6-O6	-11.31	121.81	128.60
80	A6	609	U	N1-C2-N3	11.31	121.68	114.90
36	A1	776	U	C5-C6-N1	-11.27	117.07	122.70
36	A5	2142	A	C5-C6-N1	11.26	123.33	117.70
1	A2	393	C	C6-N1-C2	11.25	124.80	120.30
36	A1	2353	G	C5-C6-O6	-11.24	121.86	128.60
36	A5	414	U	C4-C5-C6	11.24	126.44	119.70
36	A1	776	U	N1-C2-N3	11.24	121.64	114.90
37	A3	81	U	C5-C4-O4	-11.23	119.16	125.90
80	A6	1600	A	C2-N3-C4	-11.23	104.99	110.60
1	A2	639	U	N3-C2-O2	-11.22	114.35	122.20
36	A1	645	A	C5-C6-N1	11.21	123.31	117.70
80	A6	1596	C	N3-C2-O2	-11.20	114.06	121.90
1	A2	1280	C	N3-C4-C5	-11.19	117.42	121.90
36	A5	3377	G	C5-C6-O6	-11.18	121.89	128.60
36	A1	2772	C	C2-N1-C1'	11.18	131.09	118.80
1	A2	1600	A	C2-N3-C4	-11.17	105.02	110.60
36	A5	2744	U	N3-C2-O2	-11.17	114.38	122.20
36	A5	1004	U	N1-C2-O2	11.16	130.61	122.80
36	A1	1838	G	N1-C6-O6	11.16	126.59	119.90
36	A1	3362	A	N1-C2-N3	11.16	134.88	129.30
36	A1	895	A	C8-N9-C4	-11.15	101.34	105.80
1	A2	577	G	N1-C6-O6	11.13	126.58	119.90
36	A5	15	C	C6-N1-C2	-11.12	115.85	120.30
36	A1	895	A	N7-C8-N9	11.12	119.36	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1858	A	N3-C4-C5	-11.12	119.02	126.80
36	A1	3362	A	C2-N3-C4	-11.11	105.04	110.60
80	A6	639	U	N3-C2-O2	-11.11	114.42	122.20
36	A1	1741	A	C2-N3-C4	-11.11	105.04	110.60
36	A5	2278	C	N3-C4-N4	-11.08	110.25	118.00
38	A4	113	U	N1-C2-N3	11.06	121.53	114.90
80	A6	337	G	N1-C6-O6	11.05	126.53	119.90
80	A6	1560	U	N3-C2-O2	-11.05	114.47	122.20
36	A1	2634	U	C2-N3-C4	-11.02	120.39	127.00
36	A5	2836	C	C2-N3-C4	-11.02	114.39	119.90
36	A1	2993	G	N3-C4-N9	-11.01	119.40	126.00
36	A5	3060	C	N1-C2-O2	-11.00	112.30	118.90
36	A1	2169	G	N1-C6-O6	-10.98	113.31	119.90
36	A5	3138	U	N1-C2-O2	-10.98	115.12	122.80
36	A1	3362	A	N7-C8-N9	10.96	119.28	113.80
80	A6	1514	U	C5-C4-O4	10.96	132.47	125.90
80	A6	1773	C	C4-C5-C6	10.96	122.88	117.40
80	A6	453	U	C5-C4-O4	10.93	132.46	125.90
80	A6	1745	G	C5-C6-N1	10.93	116.97	111.50
1	A2	1782	A	C8-N9-C4	-10.91	101.43	105.80
36	A5	947	G	N3-C4-C5	-10.90	123.15	128.60
36	A5	776	U	C5-C4-O4	10.88	132.43	125.90
36	A5	931	C	C2-N3-C4	-10.88	114.46	119.90
36	A5	1119	C	N3-C4-C5	10.88	126.25	121.90
36	A1	2198	A	C8-N9-C4	10.88	110.15	105.80
36	A1	645	A	C2-N3-C4	10.87	116.04	110.60
36	A5	1403	C	C6-N1-C2	10.87	124.65	120.30
36	A5	420	G	C6-N1-C2	-10.87	118.58	125.10
36	A1	3375	A	C8-N9-C4	-10.86	101.45	105.80
36	A5	41	G	N1-C6-O6	10.86	126.42	119.90
36	A5	41	G	C5-C6-O6	-10.86	122.09	128.60
36	A1	2827	U	C5-C4-O4	10.85	132.41	125.90
36	A1	1929	G	C8-N9-C4	10.85	110.74	106.40
36	A5	2341	A	C8-N9-C4	10.84	110.14	105.80
36	A1	1409	G	C5-C6-O6	10.81	135.09	128.60
36	A1	644	G	C8-N9-C4	-10.81	102.08	106.40
36	A5	2343	C	N3-C4-C5	10.81	126.22	121.90
36	A1	3092	C	C6-N1-C2	10.80	124.62	120.30
36	A1	1048	A	N1-C2-N3	-10.79	123.90	129.30
36	A5	2726	C	N3-C2-O2	-10.79	114.35	121.90
1	A2	144	U	N3-C2-O2	-10.79	114.65	122.20
36	A5	2634	U	C5-C6-N1	-10.78	117.31	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	922	U	C2-N1-C1'	-10.76	104.79	117.70
36	A1	105	C	C2-N3-C4	-10.76	114.52	119.90
36	A1	1403	C	C2-N3-C4	-10.75	114.52	119.90
36	A5	2632	G	N1-C6-O6	-10.75	113.45	119.90
36	A1	2726	C	C5-C4-N4	10.74	127.72	120.20
36	A1	2179	C	N3-C4-C5	10.73	126.19	121.90
1	A2	1560	U	N3-C2-O2	-10.71	114.70	122.20
1	A2	1455	G	C5-C6-N1	-10.71	106.15	111.50
80	A6	1595	U	N3-C4-O4	-10.70	111.91	119.40
36	A5	1147	G	C4-C5-N7	-10.70	106.52	110.80
36	A1	2142	A	C6-N1-C2	-10.69	112.19	118.60
36	A5	2234	G	C5-C6-O6	-10.69	122.19	128.60
80	A6	1634	C	N1-C2-O2	10.69	125.31	118.90
36	A1	929	A	N1-C2-N3	10.69	134.64	129.30
36	A5	2288	G	C5-C6-N1	10.68	116.84	111.50
36	A1	340	C	N3-C4-N4	-10.68	110.53	118.00
36	A1	963	G	N1-C6-O6	10.67	126.30	119.90
36	A5	2899	C	N1-C2-N3	10.66	126.66	119.20
36	A5	2353	G	N1-C6-O6	10.66	126.30	119.90
36	A5	1434	G	N7-C8-N9	-10.66	107.77	113.10
36	A1	1305	U	N1-C2-O2	10.65	130.25	122.80
36	A5	2290	C	C5-C6-N1	-10.64	115.68	121.00
36	A1	2242	A	N1-C2-N3	10.63	134.61	129.30
36	A1	2298	U	C2-N3-C4	-10.61	120.64	127.00
36	A5	2631	U	C2-N3-C4	-10.61	120.64	127.00
36	A5	2905	U	C5-C6-N1	-10.60	117.40	122.70
38	A4	113	U	C5-C4-O4	10.59	132.26	125.90
1	A2	553	G	C5-C6-N1	-10.57	106.21	111.50
38	A4	113	U	C5-C6-N1	-10.57	117.42	122.70
36	A5	957	C	N3-C4-C5	10.57	126.13	121.90
36	A5	2512	C	C6-N1-C2	-10.57	116.07	120.30
36	A5	1592	G	N1-C2-N2	-10.54	106.71	116.20
36	A1	1589	A	C5-C6-N6	-10.53	115.27	123.70
1	A2	577	G	C6-C5-N7	-10.53	124.08	130.40
36	A5	3122	A	C8-N9-C4	-10.53	101.59	105.80
36	A1	821	U	N3-C4-O4	-10.53	112.03	119.40
36	A1	2434	U	N3-C4-O4	-10.52	112.03	119.40
36	A1	3046	A	C8-N9-C4	-10.52	101.59	105.80
36	A5	546	C	C2-N1-C1'	10.50	130.35	118.80
36	A5	2314	U	C5-C4-O4	-10.50	119.60	125.90
36	A1	3181	C	C6-N1-C2	-10.50	116.10	120.30
36	A5	1911	A	C8-N9-C4	10.49	110.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1389	G	C5-C6-O6	-10.49	122.31	128.60
36	A1	340	C	N3-C2-O2	-10.48	114.56	121.90
36	A5	1907	C	C6-N1-C2	-10.48	116.11	120.30
80	A6	1539	G	N3-C4-C5	10.48	133.84	128.60
36	A5	2211	U	C4-C5-C6	10.48	125.99	119.70
36	A1	30	G	N1-C6-O6	-10.47	113.62	119.90
36	A1	1492	G	N3-C4-N9	10.47	132.28	126.00
36	A1	2868	U	C5-C6-N1	-10.47	117.47	122.70
36	A1	3344	A	C5-N7-C8	-10.46	98.67	103.90
36	A1	1119	C	C2-N3-C4	-10.44	114.68	119.90
36	A5	2314	U	N3-C4-O4	10.44	126.71	119.40
36	A1	2846	U	N1-C2-N3	10.44	121.16	114.90
80	A6	163	G	N7-C8-N9	10.43	118.32	113.10
36	A5	1848	G	C5-C6-O6	-10.43	122.34	128.60
36	A1	3217	C	N1-C2-O2	10.43	125.16	118.90
36	A1	2392	C	N3-C4-C5	10.42	126.07	121.90
80	A6	337	G	C4-C5-N7	10.42	114.97	110.80
36	A1	1367	G	N3-C2-N2	10.42	127.19	119.90
36	A1	2279	A	N9-C4-C5	-10.41	101.64	105.80
36	A5	3172	A	C8-N9-C4	10.41	109.97	105.80
1	A2	639	U	N1-C2-O2	10.40	130.08	122.80
36	A1	785	G	C2-N3-C4	10.40	117.10	111.90
36	A5	1301	A	N1-C6-N6	10.40	124.84	118.60
1	A2	1782	A	C5-C6-N6	10.40	132.02	123.70
36	A1	785	G	N3-C4-C5	-10.39	123.40	128.60
36	A1	931	C	C5-C6-N1	-10.39	115.80	121.00
68	De	27	ARG	NE-CZ-NH2	-10.39	115.10	120.30
80	A6	308	C	C2-N1-C1'	-10.39	107.37	118.80
36	A1	2983	C	N3-C2-O2	-10.38	114.64	121.90
80	A6	1329	A	N1-C6-N6	10.37	124.82	118.60
36	A1	2392	C	C2-N3-C4	-10.36	114.72	119.90
36	A5	965	A	C2-N3-C4	10.36	115.78	110.60
36	A5	2836	C	C5-C6-N1	-10.36	115.82	121.00
36	A1	2899	C	C2-N1-C1'	10.35	130.18	118.80
36	A5	930	U	N3-C4-C5	10.33	120.80	114.60
36	A5	2364	G	N1-C6-O6	-10.32	113.71	119.90
36	A1	1433	A	C5-C6-N1	10.32	122.86	117.70
36	A5	2211	U	C5-C4-O4	10.31	132.09	125.90
36	A1	847	A	N1-C6-N6	10.30	124.78	118.60
36	A5	1797	A	N7-C8-N9	-10.30	108.65	113.80
36	A1	2879	C	N3-C4-C5	-10.29	117.78	121.90
36	A1	2361	A	C8-N9-C4	-10.29	101.68	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1341	U	C5-C4-O4	10.29	132.07	125.90
80	A6	543	C	N3-C2-O2	-10.29	114.70	121.90
36	A5	1303	A	N1-C2-N3	-10.29	124.16	129.30
36	A1	2156	C	C6-N1-C2	10.28	124.41	120.30
36	A5	819	U	C5-C6-N1	-10.28	117.56	122.70
36	A1	3242	G	C5-C6-N1	-10.28	106.36	111.50
36	A5	1391	C	N1-C2-O2	-10.28	112.73	118.90
36	A1	2836	C	N1-C2-N3	10.27	126.39	119.20
36	A5	1004	U	N3-C4-O4	-10.26	112.22	119.40
36	A5	1429	G	N3-C2-N2	10.26	127.08	119.90
36	A5	1903	U	N3-C4-O4	10.26	126.58	119.40
36	A1	1164	G	C5-C6-O6	10.24	134.74	128.60
36	A5	2148	U	N1-C2-O2	-10.23	115.64	122.80
36	A1	1164	G	N1-C6-O6	-10.23	113.76	119.90
38	A8	8	C	C6-N1-C2	-10.22	116.21	120.30
36	A1	2289	U	N3-C2-O2	-10.21	115.05	122.20
36	A5	1513	G	C8-N9-C4	-10.21	102.32	106.40
36	A1	979	U	N1-C2-N3	10.20	121.02	114.90
36	A1	2314	U	C5-C4-O4	-10.20	119.78	125.90
36	A1	645	A	C5-C6-N6	-10.19	115.55	123.70
36	A5	1297	C	C2-N3-C4	-10.19	114.80	119.90
36	A5	847	A	C8-N9-C4	10.19	109.88	105.80
36	A1	2983	C	C2-N3-C4	-10.18	114.81	119.90
36	A1	979	U	N3-C2-O2	-10.18	115.08	122.20
36	A5	2257	C	C6-N1-C2	-10.18	116.23	120.30
36	A1	1119	C	N3-C4-C5	10.16	125.96	121.90
36	A5	1056	U	C6-N1-C2	-10.14	114.91	121.00
36	A1	2278	C	N3-C4-N4	-10.14	110.90	118.00
36	A5	414	U	C5-C6-N1	-10.13	117.63	122.70
36	A1	968	G	C8-N9-C4	-10.13	102.35	106.40
36	A1	369	A	C2-N3-C4	10.12	115.66	110.60
36	A1	2369	G	N3-C4-C5	-10.12	123.54	128.60
36	A5	2343	C	C2-N3-C4	-10.12	114.84	119.90
36	A5	1481	A	C8-N9-C4	-10.12	101.75	105.80
36	A5	3096	C	C4-C5-C6	10.11	122.46	117.40
36	A1	3143	C	C6-N1-C2	10.10	124.34	120.30
36	A1	3306	U	C2-N3-C4	-10.10	120.94	127.00
36	A1	644	G	C5-C6-N1	-10.10	106.45	111.50
36	A1	2279	A	N1-C6-N6	10.10	124.66	118.60
36	A5	652	G	N1-C2-N2	-10.09	107.12	116.20
36	A1	2942	C	N1-C2-O2	-10.09	112.85	118.90
36	A1	639	G	N1-C6-O6	10.09	125.95	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2632	G	C5-C6-O6	10.06	134.64	128.60
68	Be	33	ARG	NE-CZ-NH1	10.06	125.33	120.30
36	A5	1124	U	C4-C5-C6	-10.06	113.66	119.70
36	A1	1480	G	C5-C6-O6	-10.05	122.57	128.60
36	A5	1208	U	N3-C2-O2	-10.05	115.16	122.20
80	A6	1572	G	C5-C6-O6	-10.05	122.57	128.60
36	A1	3344	A	C8-N9-C4	-10.04	101.78	105.80
80	A6	314	C	C6-N1-C2	-10.04	116.28	120.30
36	A5	877	C	N3-C4-C5	10.04	125.92	121.90
36	A5	1389	G	N9-C4-C5	-10.03	101.39	105.40
36	A5	1440	G	N1-C6-O6	-10.03	113.88	119.90
1	A2	1486	G	C5-N7-C8	-10.03	99.29	104.30
36	A1	2719	U	C5-C6-N1	-10.02	117.69	122.70
36	A5	3006	A	C2-N3-C4	-10.02	105.59	110.60
36	A1	1902	G	N9-C4-C5	-10.02	101.39	105.40
36	A1	2870	C	C6-N1-C1'	10.01	132.81	120.80
36	A1	1119	C	C5-C6-N1	-10.00	116.00	121.00
38	A8	25	G	N1-C6-O6	-10.00	113.90	119.90
36	A1	966	U	N3-C2-O2	-9.99	115.21	122.20
36	A5	340	C	C2-N3-C4	-9.98	114.91	119.90
36	A5	1308	A	C8-N9-C4	-9.98	101.81	105.80
1	A2	507	U	N3-C2-O2	-9.97	115.22	122.20
36	A1	2292	U	C2-N3-C4	-9.97	121.02	127.00
38	A8	32	C	N1-C2-O2	-9.97	112.92	118.90
36	A1	2292	U	C5-C4-O4	-9.96	119.93	125.90
36	A1	2827	U	C4-C5-C6	9.96	125.67	119.70
36	A1	1137	C	C2-N3-C4	-9.94	114.93	119.90
36	A1	2572	C	N1-C2-O2	9.94	124.87	118.90
36	A5	339	C	N3-C4-N4	-9.94	111.04	118.00
36	A5	3362	A	C2-N3-C4	-9.94	105.63	110.60
36	A5	2905	U	C2-N3-C4	-9.94	121.03	127.00
36	A1	958	C	N3-C4-N4	-9.93	111.05	118.00
80	A6	553	G	C4-C5-C6	9.93	124.76	118.80
36	A1	2138	A	C8-N9-C4	-9.92	101.83	105.80
36	A1	2356	A	C5-N7-C8	-9.92	98.94	103.90
36	A1	808	A	N1-C6-N6	-9.91	112.65	118.60
36	A5	2824	G	N3-C2-N2	-9.91	112.96	119.90
36	A5	2366	C	C5-C6-N1	9.91	125.95	121.00
36	A1	743	C	C6-N1-C2	9.91	124.26	120.30
36	A5	2952	G	C5-C6-O6	-9.91	122.66	128.60
36	A5	420	G	C5-C6-O6	-9.90	122.66	128.60
1	A2	542	A	N7-C8-N9	9.90	118.75	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2617	U	N3-C2-O2	-9.90	115.27	122.20
1	A2	1096	C	C2-N1-C1'	9.89	129.68	118.80
36	A1	2306	C	N1-C2-O2	9.89	124.83	118.90
36	A1	498	A	N1-C6-N6	-9.89	112.67	118.60
36	A1	2611	U	C5-C6-N1	-9.89	117.76	122.70
36	A5	1484	U	C5-C6-N1	-9.89	117.75	122.70
36	A1	1489	A	N1-C6-N6	9.88	124.53	118.60
1	A2	1745	G	C5-C6-O6	-9.88	122.67	128.60
36	A1	960	U	C6-N1-C2	9.87	126.92	121.00
80	A6	1634	C	C2-N1-C1'	9.87	129.66	118.80
36	A5	2808	A	C8-N9-C4	9.86	109.75	105.80
80	A6	448	C	C6-N1-C2	-9.86	116.36	120.30
36	A5	2118	C	N3-C2-O2	-9.86	115.00	121.90
36	A1	1492	G	N1-C6-O6	-9.84	113.99	119.90
1	A2	1456	C	N3-C4-N4	-9.84	111.11	118.00
36	A1	2353	G	N1-C6-O6	9.83	125.80	119.90
1	A2	553	G	C5-C6-O6	-9.82	122.71	128.60
1	A2	1198	G	C8-N9-C4	-9.82	102.47	106.40
36	A1	2176	U	N3-C2-O2	-9.82	115.33	122.20
36	A5	1152	G	N7-C8-N9	9.82	118.01	113.10
36	A5	1392	G	C8-N9-C4	9.81	110.33	106.40
36	A1	2846	U	N3-C4-O4	-9.81	112.53	119.40
52	DO	182[B]	SER	O-C-N	-9.81	107.01	122.70
36	A5	1655	G	N7-C8-N9	9.80	118.00	113.10
36	A5	1655	G	C8-N9-C4	-9.80	102.48	106.40
36	A1	1475	A	C2-N3-C4	9.79	115.50	110.60
36	A1	940	G	N1-C6-O6	-9.79	114.03	119.90
36	A1	406	G	O4'-C1'-N9	9.78	116.02	108.20
36	A1	50	U	N1-C2-N3	9.78	120.77	114.90
36	A5	835	G	C5-C6-O6	-9.78	122.73	128.60
36	A1	938	C	C2-N3-C4	-9.77	115.01	119.90
36	A1	2609	A	N1-C6-N6	-9.76	112.74	118.60
36	A5	2917	G	C5-C6-O6	-9.76	122.75	128.60
36	A1	2165	G	C5-C6-O6	-9.75	122.75	128.60
36	A5	947	G	C5-C6-N1	9.75	116.38	111.50
36	A5	2134	G	N1-C6-O6	-9.75	114.05	119.90
36	A5	1064	A	N1-C6-N6	9.75	124.45	118.60
36	A1	867	G	N3-C2-N2	-9.75	113.08	119.90
36	A5	2246	G	N9-C4-C5	9.75	109.30	105.40
36	A1	1216	C	C5-C6-N1	9.75	125.87	121.00
36	A5	815	G	N1-C6-O6	-9.75	114.05	119.90
36	A1	3362	A	C4-C5-N7	9.75	115.57	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A4	113	U	N3-C2-O2	-9.74	115.38	122.20
36	A5	1147	G	C5-N7-C8	9.74	109.17	104.30
36	A5	3096	C	C2-N3-C4	-9.73	115.03	119.90
36	A5	1448	U	C5-C6-N1	-9.73	117.83	122.70
36	A5	2361	A	N3-C4-C5	-9.73	119.99	126.80
36	A1	350	C	C6-N1-C2	-9.73	116.41	120.30
80	A6	609	U	C4-C5-C6	9.73	125.54	119.70
36	A5	2948	C	N3-C4-N4	-9.73	111.19	118.00
36	A5	1057	A	N1-C6-N6	9.72	124.43	118.60
36	A1	645	A	N3-C4-C5	-9.71	120.00	126.80
36	A5	645	A	C6-N1-C2	-9.71	112.77	118.60
36	A1	2679	A	N1-C6-N6	9.71	124.43	118.60
36	A1	716	A	N1-C6-N6	9.70	124.42	118.60
36	A1	2993	G	N3-C4-C5	9.70	133.45	128.60
36	A1	635	G	C5-C6-O6	-9.69	122.78	128.60
36	A5	2278	C	C6-N1-C2	-9.69	116.42	120.30
1	A2	553	G	C6-C5-N7	-9.69	124.59	130.40
36	A1	2350	C	C2-N3-C4	-9.68	115.06	119.90
36	A1	30	G	C5-C6-O6	9.68	134.41	128.60
80	A6	163	G	C8-N9-C4	-9.68	102.53	106.40
38	A4	81	U	N3-C2-O2	-9.67	115.43	122.20
36	A5	591	G	N1-C6-O6	9.67	125.70	119.90
36	A5	2211	U	N1-C2-N3	9.67	120.70	114.90
80	A6	1749	A	N1-C6-N6	9.67	124.40	118.60
36	A1	2283	G	N1-C6-O6	9.67	125.70	119.90
80	A6	1027	A	N7-C8-N9	9.67	118.63	113.80
36	A5	2391	G	C8-N9-C4	-9.66	102.54	106.40
36	A5	1888	U	C5-C6-N1	-9.65	117.88	122.70
36	A5	1327	C	N3-C4-N4	-9.64	111.25	118.00
36	A1	2142	A	N3-C4-C5	-9.64	120.05	126.80
36	A1	331	G	N1-C6-O6	-9.64	114.12	119.90
36	A1	2343	C	N3-C4-C5	9.63	125.75	121.90
36	A1	2817	A	C5-C6-N1	9.63	122.52	117.70
80	A6	99	C	C2-N3-C4	-9.63	115.08	119.90
36	A5	2757	U	N1-C2-N3	9.63	120.68	114.90
36	A5	3060	C	N3-C4-N4	9.63	124.74	118.00
36	A5	776	U	C2-N3-C4	-9.63	121.22	127.00
1	A2	1782	A	N1-C6-N6	-9.63	112.83	118.60
36	A5	1152	G	C8-N9-C4	-9.63	102.55	106.40
1	A2	1280	C	N3-C4-N4	9.62	124.73	118.00
36	A5	1042	U	N3-C4-O4	-9.62	112.67	119.40
37	A7	49	G	N1-C6-O6	9.62	125.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	3181	C	N1-C2-N3	9.61	125.93	119.20
36	A5	518	G	C5-C6-O6	-9.61	122.83	128.60
36	A1	2572	C	N3-C2-O2	-9.61	115.17	121.90
36	A1	1114	U	C6-N1-C2	9.60	126.76	121.00
40	DB	10	ARG	NE-CZ-NH2	-9.60	115.50	120.30
36	A1	1122	U	C2-N3-C4	-9.59	121.24	127.00
36	A1	1480	G	N1-C6-O6	9.58	125.65	119.90
36	A1	3242	G	C6-C5-N7	9.58	136.15	130.40
36	A1	1405	U	N3-C4-C5	9.58	120.35	114.60
36	A1	952	A	C5-C6-N6	-9.58	116.04	123.70
38	A4	140	G	C8-N9-C4	-9.58	102.57	106.40
36	A5	2424	A	N1-C6-N6	9.58	124.35	118.60
36	A5	340	C	C5-C6-N1	-9.57	116.21	121.00
46	BH	91	ARG	NE-CZ-NH2	9.57	125.09	120.30
36	A5	1127	G	C5-C6-O6	-9.57	122.86	128.60
36	A1	2356	A	C4-C5-N7	9.57	115.48	110.70
36	A1	2944	U	N3-C4-C5	9.57	120.34	114.60
37	A3	81	U	N3-C4-C5	9.57	120.34	114.60
36	A1	2633	U	N1-C2-O2	9.56	129.49	122.80
36	A5	2899	C	C5-C4-N4	9.56	126.89	120.20
80	A6	1514	U	N3-C4-O4	-9.55	112.72	119.40
36	A5	2572	C	N1-C2-O2	9.55	124.63	118.90
1	A2	1486	G	N7-C8-N9	9.54	117.87	113.10
36	A1	2550	U	C5-C4-O4	9.54	131.62	125.90
36	A1	631	U	N1-C2-N3	9.54	120.62	114.90
36	A5	1056	U	N1-C2-N3	9.53	120.62	114.90
36	A1	2595	A	C5-N7-C8	-9.53	99.14	103.90
36	A5	905	U	C5-C4-O4	-9.53	120.18	125.90
36	A1	1339	C	C2-N3-C4	-9.52	115.14	119.90
36	A1	895	A	C2-N3-C4	-9.52	105.84	110.60
80	A6	1614	A	C5-N7-C8	-9.52	99.14	103.90
36	A5	1403	C	C5-C4-N4	-9.52	113.54	120.20
36	A5	1848	G	N1-C6-O6	9.51	125.61	119.90
36	A1	3083	G	N3-C4-C5	-9.51	123.85	128.60
80	A6	1537	C	C5-C6-N1	9.50	125.75	121.00
36	A1	2860	U	N3-C2-O2	9.49	128.84	122.20
80	A6	639	U	N1-C2-O2	9.49	129.45	122.80
36	A1	3214	U	C5-C4-O4	9.49	131.59	125.90
36	A5	1902	G	C5-C6-O6	-9.49	122.91	128.60
36	A1	637	C	C2-N1-C1'	-9.48	108.37	118.80
36	A1	637	C	C6-N1-C1'	9.48	132.18	120.80
1	A2	1456	C	C5-C4-N4	9.48	126.83	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2156	C	N3-C4-C5	9.48	125.69	121.90
36	A5	546	C	N1-C2-O2	9.47	124.58	118.90
36	A5	1239	C	C5-C6-N1	9.47	125.73	121.00
80	A6	553	G	N3-C2-N2	-9.46	113.28	119.90
36	A5	947	G	C2-N3-C4	9.46	116.63	111.90
36	A1	3217	C	N3-C2-O2	-9.46	115.28	121.90
38	A4	73	U	N3-C4-C5	9.46	120.27	114.60
36	A5	1888	U	C4-C5-C6	9.45	125.37	119.70
38	A8	113	U	C5-C6-N1	9.45	127.42	122.70
36	A5	2705	A	C5-C6-N1	9.45	122.42	117.70
80	A6	1481	C	C6-N1-C2	-9.45	116.52	120.30
80	A6	1560	U	C5-C4-O4	9.44	131.57	125.90
36	A1	1117	G	C8-N9-C4	9.44	110.18	106.40
36	A5	2202	C	C5-C4-N4	-9.44	113.59	120.20
36	A1	3344	A	N1-C6-N6	9.44	124.26	118.60
1	A2	139	C	C6-N1-C2	-9.44	116.53	120.30
36	A1	3344	A	C2-N3-C4	-9.43	105.88	110.60
36	A5	282	G	C8-N9-C4	-9.43	102.63	106.40
36	A5	3362	A	N7-C8-N9	9.43	118.51	113.80
36	A1	80	G	C6-N1-C2	-9.42	119.45	125.10
36	A5	644	G	C2-N3-C4	9.42	116.61	111.90
36	A5	386	A	N1-C6-N6	9.42	124.25	118.60
36	A5	708	G	C4-C5-N7	9.42	114.57	110.80
36	A5	40	A	N1-C2-N3	9.42	134.01	129.30
36	A5	1210	U	C5-C4-O4	9.42	131.55	125.90
36	A5	966	U	N1-C2-O2	9.42	129.39	122.80
36	A5	2899	C	C6-N1-C2	-9.41	116.54	120.30
1	A2	453	U	N3-C2-O2	-9.40	115.62	122.20
36	A1	2726	C	N3-C4-N4	-9.40	111.42	118.00
36	A5	2364	G	N9-C4-C5	9.40	109.16	105.40
36	A5	3376	A	C8-N9-C4	-9.39	102.04	105.80
1	A2	1282	U	N3-C2-O2	-9.39	115.63	122.20
36	A1	1169	A	C4-C5-C6	9.38	121.69	117.00
36	A5	1449	A	C2-N3-C4	-9.38	105.91	110.60
36	A5	1858	A	C8-N9-C4	-9.38	102.05	105.80
36	A1	1173	U	C5-C6-N1	-9.37	118.01	122.70
80	A6	1280	C	C6-N1-C2	-9.38	116.55	120.30
1	A2	1654	G	C5-C6-N1	9.37	116.19	111.50
36	A1	112	U	C2-N1-C1'	9.37	128.94	117.70
36	A1	970	A	C5-N7-C8	-9.37	99.22	103.90
36	A5	811	U	C5-C6-N1	-9.37	118.02	122.70
36	A1	295	A	N7-C8-N9	9.36	118.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1480	G	N9-C4-C5	-9.36	101.66	105.40
36	A5	2978	U	N3-C2-O2	-9.36	115.65	122.20
1	A2	1258	U	N3-C2-O2	-9.35	115.66	122.20
36	A1	1857	C	N1-C2-O2	-9.34	113.29	118.90
36	A5	3218	A	C5-N7-C8	-9.34	99.23	103.90
36	A1	2389	C	C5-C6-N1	-9.34	116.33	121.00
1	A2	1169	G	C8-N9-C4	-9.33	102.67	106.40
36	A1	24	G	C5-C6-O6	-9.33	123.00	128.60
36	A1	2827	U	N3-C4-O4	-9.33	112.87	119.40
68	Be	33	ARG	NE-CZ-NH2	-9.33	115.64	120.30
36	A5	1437	C	C6-N1-C2	-9.33	116.57	120.30
36	A5	21	G	C2-N3-C4	-9.33	107.24	111.90
36	A1	2621	G	N3-C2-N2	-9.32	113.37	119.90
80	A6	415	C	C6-N1-C2	9.32	124.03	120.30
36	A5	2340	U	N3-C4-C5	9.32	120.19	114.60
36	A5	2830	G	N9-C4-C5	9.31	109.12	105.40
36	A1	2719	U	N1-C2-O2	-9.31	116.28	122.80
36	A1	641	C	N3-C4-C5	9.30	125.62	121.90
80	A6	1596	C	C5-C4-N4	9.30	126.71	120.20
36	A5	721	G	N1-C6-O6	-9.30	114.32	119.90
36	A1	2823	G	C5-C6-O6	9.29	134.18	128.60
36	A1	3057	U	C5-C4-O4	9.29	131.47	125.90
36	A5	1447	G	C8-N9-C4	-9.29	102.68	106.40
36	A1	1295	G	N1-C6-O6	-9.29	114.33	119.90
36	A1	718	G	N3-C4-C5	9.28	133.24	128.60
80	A6	687	G	N3-C4-N9	-9.28	120.43	126.00
36	A5	1151	U	N3-C4-O4	-9.29	112.90	119.40
36	A1	2772	C	C6-N1-C1'	-9.28	109.67	120.80
36	A1	2174	G	C8-N9-C4	-9.28	102.69	106.40
36	A5	1879	A	N1-C6-N6	9.27	124.16	118.60
36	A5	3050	U	N3-C2-O2	-9.27	115.71	122.20
36	A1	2634	U	N1-C2-N3	9.27	120.46	114.90
36	A5	3186	A	C8-N9-C4	-9.26	102.10	105.80
36	A5	994	G	C5-C6-N1	9.26	116.13	111.50
36	A5	1064	A	N9-C4-C5	-9.26	102.10	105.80
36	A1	410	U	N1-C2-O2	-9.25	116.32	122.80
36	A1	2320	A	C2-N3-C4	-9.25	105.97	110.60
36	A5	1849	C	N1-C2-O2	9.25	124.45	118.90
36	A1	2302	G	C5-C6-O6	9.24	134.15	128.60
36	A1	2763	U	N1-C2-O2	-9.24	116.33	122.80
36	A1	2302	G	N1-C6-O6	-9.23	114.36	119.90
36	A1	3057	U	N3-C2-O2	-9.23	115.74	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1600	A	C5-N7-C8	-9.23	99.28	103.90
36	A1	2222	A	C8-N9-C4	-9.23	102.11	105.80
36	A5	3060	C	C5-C4-N4	-9.23	113.74	120.20
38	A8	80	A	C8-N9-C4	-9.23	102.11	105.80
36	A1	645	A	N3-C4-N9	9.23	134.78	127.40
36	A1	2393	G	C8-N9-C4	9.23	110.09	106.40
36	A5	1449	A	N1-C6-N6	9.23	124.14	118.60
36	A5	3309	G	N3-C4-C5	-9.23	123.99	128.60
36	A5	1371	G	C5-C6-N1	9.22	116.11	111.50
36	A5	3214	U	N3-C4-O4	-9.22	112.95	119.40
36	A5	2246	G	C4-C5-N7	-9.22	107.11	110.80
36	A5	1156	C	N3-C4-C5	9.22	125.59	121.90
36	A1	2378	C	N3-C4-C5	-9.20	118.22	121.90
36	A1	3242	G	C2-N3-C4	-9.20	107.30	111.90
36	A5	968	G	N3-C2-N2	9.20	126.34	119.90
36	A5	3377	G	C4-C5-N7	9.20	114.48	110.80
36	A1	931	C	N3-C4-N4	-9.20	111.56	118.00
36	A1	2283	G	N3-C2-N2	-9.20	113.46	119.90
36	A5	3245	A	C8-N9-C4	-9.20	102.12	105.80
36	A1	3181	C	N3-C2-O2	-9.19	115.46	121.90
36	A1	154	U	C5-C6-N1	-9.19	118.10	122.70
36	A1	1480	G	C8-N9-C4	9.19	110.08	106.40
36	A5	2550	U	C5-C4-O4	9.19	131.41	125.90
36	A1	3181	C	C5-C4-N4	9.18	126.63	120.20
36	A5	1101	G	N3-C2-N2	9.17	126.32	119.90
40	DB	2	SER	N-CA-C	-9.17	86.24	111.00
36	A1	2247	G	N1-C6-O6	9.17	125.40	119.90
36	A5	1050	U	N3-C2-O2	-9.17	115.78	122.20
36	A5	3266	G	C5-C6-O6	9.17	134.10	128.60
36	A5	2693	C	N3-C2-O2	-9.17	115.48	121.90
36	A1	857	G	C5-C6-N1	9.17	116.08	111.50
36	A1	3377	G	C5-C6-N1	9.16	116.08	111.50
80	A6	1105	C	N3-C2-O2	-9.15	115.49	121.90
36	A1	2280	A	C8-N9-C4	9.15	109.46	105.80
80	A6	163	G	N1-C6-O6	9.15	125.39	119.90
36	A1	2356	A	N9-C4-C5	-9.14	102.14	105.80
36	A1	3057	U	N3-C4-O4	-9.14	113.00	119.40
36	A1	3278	C	N1-C2-O2	9.14	124.39	118.90
36	A1	1514	G	N1-C6-O6	-9.14	114.42	119.90
36	A5	2142	A	C6-N1-C2	-9.14	113.12	118.60
36	A5	2354	C	N1-C2-O2	-9.14	113.42	118.90
36	A1	939	U	N1-C2-O2	-9.14	116.41	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	558	U	N3-C2-O2	-9.13	115.81	122.20
36	A5	1911	A	N9-C4-C5	-9.13	102.15	105.80
36	A5	2365	C	N3-C4-N4	-9.12	111.61	118.00
36	A5	3308	C	C4-C5-C6	9.12	121.96	117.40
36	A5	834	U	N3-C4-C5	9.12	120.07	114.60
36	A5	3362	A	C5-N7-C8	-9.11	99.34	103.90
36	A5	2942	C	N3-C4-N4	9.11	124.38	118.00
40	DB	4	ARG	NE-CZ-NH1	9.11	124.85	120.30
36	A1	959	C	C6-N1-C2	9.10	123.94	120.30
36	A5	2176	U	N3-C2-O2	-9.10	115.83	122.20
1	A2	142	G	N3-C2-N2	-9.09	113.53	119.90
1	A2	402	C	C6-N1-C2	9.09	123.94	120.30
36	A1	907	G	N3-C4-C5	-9.09	124.05	128.60
36	A1	88	A	N1-C6-N6	9.09	124.06	118.60
36	A1	3181	C	N3-C4-N4	-9.09	111.64	118.00
80	A6	1456	C	C5-C4-N4	9.09	126.56	120.20
36	A1	591	G	N1-C6-O6	9.08	125.35	119.90
36	A5	1843	C	C6-N1-C2	-9.08	116.67	120.30
52	BO	158[B]	ASP	O-C-N	9.08	137.22	122.70
1	A2	1596	C	N3-C2-O2	-9.07	115.55	121.90
36	A1	1902	G	N3-C4-N9	9.07	131.44	126.00
36	A5	1133	A	C2-N3-C4	9.07	115.14	110.60
36	A1	641	C	C2-N1-C1'	-9.07	108.82	118.80
36	A1	818	C	C6-N1-C2	-9.06	116.67	120.30
36	A1	644	G	N1-C2-N2	-9.06	108.05	116.20
36	A5	2744	U	N1-C2-O2	9.05	129.14	122.80
36	A1	1341	U	N3-C2-O2	-9.05	115.86	122.20
36	A1	1405	U	C2-N3-C4	-9.05	121.57	127.00
36	A5	1911	A	N1-C6-N6	9.05	124.03	118.60
36	A1	2851	A	C8-N9-C4	9.05	109.42	105.80
54	DQ	66	ARG	NE-CZ-NH2	-9.04	115.78	120.30
36	A5	1450	G	C8-N9-C4	9.03	110.01	106.40
37	A3	81	U	C6-N1-C2	9.03	126.42	121.00
36	A1	2814	G	C8-N9-C4	9.03	110.01	106.40
36	A5	1181	U	C5-C6-N1	-9.02	118.19	122.70
36	A1	2884	C	N3-C4-C5	9.01	125.50	121.90
36	A1	2299	A	C4-C5-C6	9.01	121.50	117.00
36	A1	655	C	C5-C6-N1	-9.00	116.50	121.00
36	A5	369	A	C8-N9-C4	-9.00	102.20	105.80
80	A6	352	A	C8-N9-C4	9.00	109.40	105.80
36	A5	1317	A	C5-C6-N6	-9.00	116.50	123.70
36	A1	1592	G	N9-C4-C5	-9.00	101.80	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A4	20	U	N3-C4-O4	-8.99	113.10	119.40
36	A1	2434	U	C5-C6-N1	-8.99	118.20	122.70
36	A5	2830	G	N1-C2-N3	8.99	129.30	123.90
36	A1	1510	G	N3-C2-N2	8.99	126.19	119.90
36	A5	1487	G	N1-C6-O6	-8.99	114.51	119.90
1	A2	794	U	N1-C2-O2	8.99	129.09	122.80
36	A5	2836	C	C4-C5-C6	8.99	121.89	117.40
36	A5	631	U	N1-C2-N3	8.98	120.29	114.90
36	A5	2320	A	C5-C6-N6	8.98	130.88	123.70
38	A4	140	G	N9-C4-C5	8.98	108.99	105.40
80	A6	321	C	N3-C2-O2	-8.98	115.62	121.90
36	A5	2857	C	N3-C4-C5	8.97	125.49	121.90
36	A1	112	U	C5-C6-N1	8.97	127.19	122.70
36	A1	365	A	N1-C6-N6	8.97	123.98	118.60
1	A2	969	C	C6-N1-C2	8.97	123.89	120.30
36	A5	3212	C	C2-N3-C4	-8.97	115.42	119.90
37	A7	101	G	N1-C6-O6	8.97	125.28	119.90
37	A3	86	U	C5-C4-O4	-8.96	120.52	125.90
1	A2	542	A	C5-N7-C8	-8.95	99.42	103.90
36	A5	2202	C	N1-C2-O2	-8.95	113.53	118.90
38	A8	113	U	C2-N1-C1'	8.95	128.44	117.70
36	A5	2327	U	N3-C4-O4	-8.95	113.13	119.40
36	A5	2372	A	N7-C8-N9	8.95	118.28	113.80
36	A5	1116	G	C4-C5-N7	-8.95	107.22	110.80
36	A5	726	G	C4-C5-N7	8.95	114.38	110.80
36	A5	802	C	C4-C5-C6	8.95	121.87	117.40
36	A5	2824	G	C6-N1-C2	-8.95	119.73	125.10
36	A1	2899	C	N3-C2-O2	-8.94	115.64	121.90
36	A5	2905	U	N3-C4-O4	-8.94	113.14	119.40
36	A5	2327	U	C2-N3-C4	-8.94	121.64	127.00
36	A1	2899	C	C2-N3-C4	-8.94	115.43	119.90
36	A5	2728	G	N9-C4-C5	8.94	108.97	105.40
80	A6	1105	C	N1-C2-O2	8.94	124.26	118.90
36	A5	802	C	C5-C6-N1	-8.94	116.53	121.00
36	A5	2833	A	N1-C6-N6	-8.94	113.24	118.60
1	A2	1596	C	C6-N1-C2	-8.93	116.73	120.30
4	CC	58	LEU	CA-CB-CG	8.93	135.85	115.30
36	A5	2808	A	C2-N3-C4	-8.92	106.14	110.60
36	A5	887	G	C5-C6-N1	-8.92	107.04	111.50
36	A5	1450	G	C6-C5-N7	8.92	135.75	130.40
36	A5	2382	G	C5-C6-O6	8.92	133.95	128.60
36	A1	2376	G	C8-N9-C4	-8.92	102.83	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A3	86	U	C2-N3-C4	-8.92	121.65	127.00
36	A1	1377	G	C5-C6-N1	8.91	115.96	111.50
36	A5	1044	U	N3-C4-O4	-8.91	113.16	119.40
1	A2	1745	G	N3-C4-N9	8.91	131.35	126.00
37	A3	101	G	C8-N9-C4	8.91	109.96	106.40
80	A6	1503	A	C5-N7-C8	-8.91	99.45	103.90
80	A6	1745	G	C6-N1-C2	-8.91	119.76	125.10
36	A5	3382	U	C2-N1-C1'	8.91	128.39	117.70
36	A5	881	C	N1-C2-O2	8.90	124.24	118.90
12	AK	88	PRO	N-CA-CB	8.90	113.98	103.30
36	A1	2983	C	N1-C2-N3	8.89	125.43	119.20
36	A1	1404	G	C8-N9-C4	8.89	109.96	106.40
80	A6	1572	G	N1-C6-O6	8.89	125.23	119.90
36	A1	2808	A	N1-C6-N6	8.88	123.93	118.60
36	A5	2719	U	C2-N1-C1'	-8.88	107.04	117.70
80	A6	163	G	N3-C2-N2	-8.88	113.68	119.90
36	A5	1429	G	N1-C2-N2	-8.87	108.21	116.20
36	A5	1314	C	C2-N3-C4	-8.87	115.46	119.90
36	A5	3049	A	C5-C6-N1	-8.86	113.27	117.70
36	A5	1158	A	N1-C6-N6	8.86	123.92	118.60
1	A2	1455	G	N3-C2-N2	-8.86	113.70	119.90
36	A1	2298	U	N3-C4-O4	-8.86	113.20	119.40
80	A6	29	U	C5-C4-O4	8.86	131.21	125.90
80	A6	1539	G	N3-C4-N9	-8.86	120.69	126.00
80	A6	1596	C	N3-C4-N4	-8.85	111.81	118.00
36	A5	420	G	C5-C6-N1	8.85	115.92	111.50
36	A5	631	U	N3-C4-O4	-8.85	113.21	119.40
36	A5	3040	A	C8-N9-C4	8.85	109.34	105.80
36	A5	433	A	C2-N3-C4	-8.84	106.18	110.60
36	A5	3047	U	C5-C6-N1	-8.84	118.28	122.70
36	A1	1495	U	C2-N1-C1'	-8.84	107.10	117.70
80	A6	1537	C	C5-C4-N4	-8.84	114.02	120.20
36	A5	2881	C	C2-N3-C4	-8.83	115.48	119.90
36	A1	3000	A	C8-N9-C4	8.83	109.33	105.80
36	A5	1931	U	C2-N1-C1'	-8.83	107.10	117.70
36	A1	644	G	N9-C4-C5	8.83	108.93	105.40
36	A1	2280	A	N9-C4-C5	-8.82	102.27	105.80
36	A1	2142	A	C2-N3-C4	8.81	115.01	110.60
36	A5	2647	A	N9-C4-C5	8.81	109.33	105.80
37	A3	82	G	N1-C2-N2	-8.81	108.27	116.20
36	A5	819	U	C4-C5-C6	8.81	124.99	119.70
36	A1	2821	C	C5-C6-N1	8.81	125.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2393	G	C8-N9-C4	8.81	109.92	106.40
36	A1	1832	C	N3-C2-O2	-8.81	115.73	121.90
38	A4	57	C	C6-N1-C2	8.81	123.82	120.30
80	A6	539	G	N7-C8-N9	8.81	117.50	113.10
38	A4	39	G	N3-C2-N2	8.80	126.06	119.90
36	A5	1113	G	C2-N3-C4	-8.80	107.50	111.90
36	A5	2757	U	C4-C5-C6	8.80	124.98	119.70
36	A5	947	G	C6-N1-C2	-8.80	119.82	125.10
1	A2	1761	U	C5-C4-O4	8.80	131.18	125.90
36	A1	1049	C	N3-C4-C5	8.80	125.42	121.90
37	A3	103	A	C8-N9-C4	8.80	109.32	105.80
36	A1	1279	C	C6-N1-C2	-8.80	116.78	120.30
80	A6	1	U	C2-N1-C1'	8.80	128.26	117.70
36	A1	1911	A	C5-C6-N6	-8.79	116.67	123.70
36	A1	2870	C	N3-C4-N4	-8.79	111.84	118.00
36	A1	3143	C	N1-C2-O2	-8.79	113.62	118.90
80	A6	1456	C	N3-C2-O2	-8.79	115.74	121.90
36	A5	437	G	C8-N9-C4	-8.79	102.88	106.40
80	A6	687	G	N1-C2-N2	8.79	124.11	116.20
59	DV	48	ARG	NE-CZ-NH1	8.79	124.69	120.30
36	A5	1311	G	C2-N3-C4	8.78	116.29	111.90
1	A2	1749	A	N1-C6-N6	8.78	123.87	118.60
36	A1	730	C	N3-C4-C5	8.78	125.41	121.90
36	A5	3127	A	N1-C6-N6	-8.78	113.33	118.60
1	A2	1654	G	C6-N1-C2	-8.78	119.83	125.10
36	A1	2314	U	C5-C6-N1	8.78	127.09	122.70
36	A5	1907	C	N3-C4-C5	-8.78	118.39	121.90
1	A2	507	U	N1-C2-O2	8.77	128.94	122.80
38	A4	25	G	C4-C5-N7	-8.77	107.29	110.80
80	A6	1600	A	N1-C2-N3	8.77	133.69	129.30
80	A6	371	G	N1-C6-O6	8.77	125.16	119.90
36	A1	1115	G	N3-C2-N2	8.76	126.03	119.90
36	A1	3344	A	N1-C2-N3	8.76	133.68	129.30
36	A5	2434	U	C5-C6-N1	-8.76	118.32	122.70
1	A2	992	A	N3-C4-C5	8.75	132.93	126.80
36	A1	2828	G	N1-C6-O6	-8.75	114.65	119.90
36	A1	1329	U	N1-C2-N3	8.74	120.14	114.90
36	A1	2865	U	N3-C4-C5	8.74	119.84	114.60
36	A5	1149	G	C2-N3-C4	8.73	116.27	111.90
1	A2	1503	A	C2-N3-C4	-8.73	106.23	110.60
36	A1	1589	A	N1-C6-N6	8.73	123.84	118.60
36	A1	159	A	C8-N9-C4	8.73	109.29	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1161	G	C5-C6-N1	8.73	115.86	111.50
36	A5	1903	U	C4-C5-C6	8.73	124.94	119.70
36	A5	1846	C	C2-N3-C4	-8.72	115.54	119.90
36	A5	2416	U	C6-N1-C2	-8.72	115.77	121.00
36	A1	439	C	N1-C2-O2	8.71	124.13	118.90
36	A5	3123	A	C8-N9-C4	8.71	109.29	105.80
1	A2	453	U	C2-N1-C1'	8.71	128.16	117.70
36	A1	1007	U	C6-N1-C2	8.71	126.23	121.00
36	A1	1138	U	N3-C2-O2	-8.71	116.10	122.20
1	A2	558	U	N1-C2-O2	8.71	128.90	122.80
36	A1	369	A	C8-N9-C4	-8.71	102.32	105.80
36	A1	2714	G	C5-N7-C8	-8.70	99.95	104.30
36	A1	1120	A	N1-C2-N3	8.70	133.65	129.30
36	A5	834	U	C4-C5-C6	-8.70	114.48	119.70
80	A6	337	G	C4-C5-C6	8.70	124.02	118.80
36	A5	1840	U	N3-C2-O2	-8.70	116.11	122.20
36	A1	2413	A	C4-C5-C6	-8.70	112.65	117.00
36	A5	726	G	C6-C5-N7	-8.70	125.18	130.40
36	A5	1412	G	C8-N9-C4	-8.70	102.92	106.40
36	A5	2271	A	N7-C8-N9	-8.70	109.45	113.80
36	A5	2730	G	N1-C6-O6	8.69	125.11	119.90
36	A1	49	A	C5-C6-N1	-8.69	113.36	117.70
36	A1	2977	G	C5-C6-N1	8.69	115.84	111.50
38	A4	15	G	C5-C6-O6	-8.68	123.39	128.60
80	A6	1537	C	N3-C4-N4	8.68	124.08	118.00
36	A5	2858	U	N3-C2-O2	-8.68	116.12	122.20
36	A5	2409	G	C8-N9-C4	-8.68	102.93	106.40
36	A5	2865	U	C5-C6-N1	8.68	127.04	122.70
36	A1	718	G	C5-N7-C8	-8.68	99.96	104.30
36	A1	960	U	N3-C4-C5	8.67	119.80	114.60
36	A5	1134	G	C5-C6-O6	-8.67	123.40	128.60
36	A5	2292	U	N3-C2-O2	-8.67	116.13	122.20
36	A5	2832	C	C5-C6-N1	-8.67	116.66	121.00
36	A1	2653	C	N3-C4-N4	-8.67	111.93	118.00
36	A1	2679	A	C6-C5-N7	-8.67	126.23	132.30
40	BB	21	ARG	NE-CZ-NH2	8.67	124.63	120.30
36	A5	2434	U	N3-C4-O4	-8.67	113.33	119.40
36	A5	1119	C	C2-N3-C4	-8.66	115.57	119.90
36	A5	2290	C	C2-N3-C4	-8.66	115.57	119.90
37	A7	48	U	C2-N3-C4	-8.66	121.80	127.00
36	A1	2368	A	N1-C6-N6	-8.66	113.41	118.60
36	A1	3259	U	N1-C2-O2	-8.66	116.74	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2198	A	N1-C6-N6	8.65	123.79	118.60
36	A1	2406	C	C6-N1-C2	8.65	123.76	120.30
36	A5	2190	U	C5-C4-O4	8.65	131.09	125.90
36	A1	959	C	C5-C6-N1	-8.65	116.68	121.00
38	A8	17	A	N1-C6-N6	8.65	123.79	118.60
36	A5	2961	G	C8-N9-C4	-8.64	102.94	106.40
1	A2	92	A	C8-N9-C4	-8.64	102.34	105.80
1	A2	1291	G	N7-C8-N9	8.64	117.42	113.10
36	A5	3040	A	N7-C8-N9	-8.64	109.48	113.80
36	A5	796	U	N3-C2-O2	-8.64	116.15	122.20
36	A1	2728	G	C5-C6-O6	-8.63	123.42	128.60
36	A5	3143	C	N1-C2-O2	-8.64	113.72	118.90
54	DQ	151	ARG	NE-CZ-NH1	-8.64	115.98	120.30
36	A1	2777	G	C2-N3-C4	-8.63	107.58	111.90
36	A1	864	G	N3-C4-C5	-8.63	124.28	128.60
36	A1	1110	U	C5-C4-O4	-8.63	120.72	125.90
36	A5	66	A	C8-N9-C4	8.63	109.25	105.80
80	A6	558	U	C2-N1-C1'	8.62	128.05	117.70
36	A5	339	C	C5-C4-N4	8.62	126.24	120.20
36	A1	2168	A	C8-N9-C4	8.62	109.25	105.80
36	A1	2836	C	C5-C6-N1	-8.62	116.69	121.00
36	A5	938	C	C2-N3-C4	-8.62	115.59	119.90
36	A1	2836	C	N3-C4-N4	-8.62	111.97	118.00
1	A2	17	C	C6-N1-C2	-8.62	116.85	120.30
36	A5	821	U	C5-C6-N1	-8.62	118.39	122.70
80	A6	858	G	C4-C5-N7	8.61	114.25	110.80
36	A5	2385	G	N3-C4-C5	8.61	132.91	128.60
36	A5	3374	U	N3-C4-C5	8.61	119.77	114.60
36	A1	1929	G	N9-C4-C5	-8.61	101.96	105.40
36	A1	2314	U	C6-N1-C1'	-8.61	109.15	121.20
36	A1	2376	G	N3-C4-C5	-8.61	124.30	128.60
36	A1	3242	G	C6-N1-C2	8.61	130.26	125.10
36	A5	1327	C	N1-C2-O2	8.61	124.06	118.90
38	A4	53	A	C2-N3-C4	8.61	114.90	110.60
36	A1	197	G	N1-C6-O6	8.60	125.06	119.90
36	A5	644	G	C5-C6-N1	8.60	115.80	111.50
36	A1	407	A	C8-N9-C4	-8.60	102.36	105.80
36	A5	2728	G	N3-C2-N2	-8.60	113.88	119.90
37	A7	92	A	N1-C6-N6	8.60	123.76	118.60
1	A2	794	U	N3-C2-O2	-8.60	116.18	122.20
36	A5	2687	G	N1-C6-O6	-8.60	114.74	119.90
36	A1	2621	G	N9-C4-C5	8.59	108.84	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2638	C	N1-C2-O2	-8.59	113.75	118.90
36	A5	2913	C	C4-C5-C6	8.59	121.70	117.40
1	A2	7	G	N1-C6-O6	-8.59	114.75	119.90
36	A5	2391	G	N1-C6-O6	-8.59	114.75	119.90
36	A1	1911	A	C4-C5-N7	8.59	114.99	110.70
36	A1	44	U	C5-C6-N1	-8.59	118.41	122.70
36	A5	2988	C	N3-C2-O2	-8.59	115.89	121.90
36	A1	53	G	C8-N9-C4	8.58	109.83	106.40
36	A1	2867	C	N3-C4-N4	-8.58	111.99	118.00
36	A1	2393	G	N3-C4-N9	8.58	131.15	126.00
38	A4	96	A	C2-N3-C4	-8.58	106.31	110.60
36	A1	804	C	N3-C2-O2	8.58	127.91	121.90
36	A1	3001	C	C6-N1-C2	8.58	123.73	120.30
80	A6	512	A	N1-C6-N6	8.58	123.75	118.60
36	A5	2392	C	C2-N3-C4	-8.58	115.61	119.90
36	A5	2699	G	C5-C6-O6	-8.58	123.45	128.60
1	A2	1189	A	C8-N9-C4	8.57	109.23	105.80
36	A1	2151	C	N1-C2-O2	-8.57	113.76	118.90
1	A2	992	A	C5-C6-N1	-8.57	113.42	117.70
36	A5	2758	A	N1-C2-N3	-8.57	125.02	129.30
36	A1	1060	U	C5-C6-N1	-8.56	118.42	122.70
36	A1	37	U	N1-C2-O2	-8.56	116.81	122.80
80	A6	1085	G	N1-C6-O6	-8.56	114.76	119.90
36	A5	341	G	C5-C6-O6	-8.56	123.47	128.60
36	A5	345	G	C5-C6-N1	8.55	115.78	111.50
36	A1	785	G	N1-C6-O6	-8.55	114.77	119.90
36	A1	922	U	N3-C2-O2	-8.55	116.22	122.20
36	A1	3208	G	N3-C4-N9	-8.55	120.87	126.00
36	A1	709	A	C5-N7-C8	8.54	108.17	103.90
36	A1	3217	C	C2-N1-C1'	8.54	128.20	118.80
36	A1	1904	C	C6-N1-C2	-8.54	116.88	120.30
36	A1	2823	G	C4-C5-N7	-8.54	107.38	110.80
36	A1	2899	C	C6-N1-C1'	-8.54	110.55	120.80
36	A5	2634	U	N1-C2-O2	-8.54	116.82	122.80
36	A1	907	G	C8-N9-C4	-8.54	102.98	106.40
36	A1	2395	G	C6-N1-C2	-8.54	119.98	125.10
80	A6	1037	C	C6-N1-C2	8.54	123.72	120.30
1	A2	1745	G	C5-C6-N1	8.53	115.77	111.50
36	A1	1339	C	N1-C2-O2	-8.53	113.78	118.90
80	A6	453	U	C2-N1-C1'	8.53	127.94	117.70
36	A5	726	G	C5-C6-O6	-8.53	123.48	128.60
36	A5	2988	C	C4-C5-C6	8.53	121.67	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1749	A	N9-C4-C5	-8.53	102.39	105.80
36	A5	1050	U	N1-C2-O2	8.53	128.77	122.80
36	A5	946	U	N3-C2-O2	-8.53	116.23	122.20
36	A1	2823	G	N1-C6-O6	-8.53	114.78	119.90
36	A5	3010	U	N3-C2-O2	-8.53	116.23	122.20
36	A1	883	A	N1-C2-N3	-8.52	125.04	129.30
80	A6	858	G	C5-N7-C8	-8.52	100.04	104.30
1	A2	719	U	C2-N1-C1'	8.52	127.92	117.70
1	A2	1773	C	N3-C4-N4	8.52	123.96	118.00
36	A1	2165	G	C4-C5-N7	8.52	114.21	110.80
36	A5	326	U	C5-C4-O4	-8.52	120.79	125.90
36	A1	2282	U	C2-N3-C4	-8.51	121.89	127.00
36	A5	1409	G	N1-C6-O6	-8.51	114.79	119.90
36	A5	2301	U	C2-N3-C4	-8.51	121.89	127.00
38	A8	14	C	C5-C6-N1	-8.51	116.74	121.00
36	A1	2868	U	C2-N3-C4	-8.51	121.89	127.00
36	A1	588	G	N3-C4-C5	-8.51	124.35	128.60
80	A6	1269	U	N1-C2-N3	8.51	120.00	114.90
80	A6	314	C	N3-C2-O2	-8.50	115.95	121.90
36	A5	1143	A	C5-C6-N1	-8.50	113.45	117.70
1	A2	647	G	N3-C4-N9	-8.50	120.90	126.00
36	A1	2289	U	N1-C2-O2	8.50	128.75	122.80
36	A5	2524	A	C5-N7-C8	-8.50	99.65	103.90
36	A5	2952	G	N3-C2-N2	-8.50	113.95	119.90
80	A6	144	U	C2-N1-C1'	8.50	127.89	117.70
36	A1	931	C	C2-N3-C4	-8.49	115.66	119.90
1	A2	992	A	N3-C4-N9	-8.48	120.61	127.40
36	A5	2978	U	C5-C6-N1	-8.48	118.46	122.70
36	A1	1142	G	N3-C4-C5	-8.48	124.36	128.60
36	A1	1295	G	C5-C6-O6	8.48	133.69	128.60
36	A1	1142	G	C5-C6-O6	-8.48	123.51	128.60
36	A5	1085	A	N7-C8-N9	8.48	118.04	113.80
36	A5	1342	C	C5-C6-N1	-8.48	116.76	121.00
36	A1	2631	U	C5-C6-N1	-8.48	118.46	122.70
36	A5	887	G	C5-C6-O6	8.48	133.69	128.60
36	A5	2732	G	N1-C6-O6	-8.48	114.81	119.90
36	A1	2349	U	C2-N3-C4	-8.47	121.92	127.00
36	A1	592	A	N9-C4-C5	-8.47	102.41	105.80
36	A5	3377	G	C5-C6-N1	8.47	115.74	111.50
36	A1	95	A	C8-N9-C4	8.47	109.19	105.80
36	A1	633	C	C5-C6-N1	-8.47	116.77	121.00
36	A1	2870	C	C6-N1-C2	-8.47	116.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	3321	C	C5-C6-N1	-8.46	116.77	121.00
1	A2	1486	G	C4-C5-N7	8.46	114.19	110.80
36	A5	1942	U	N1-C2-O2	-8.46	116.88	122.80
36	A1	895	A	C4-C5-N7	8.46	114.93	110.70
36	A5	343	U	N3-C2-O2	-8.46	116.28	122.20
36	A5	1047	A	C2-N3-C4	8.46	114.83	110.60
36	A1	2892	A	N1-C6-N6	-8.46	113.53	118.60
36	A5	224	C	N1-C2-O2	8.45	123.97	118.90
36	A1	3344	A	C4-C5-N7	8.45	114.93	110.70
36	A5	652	G	N3-C4-C5	-8.45	124.37	128.60
36	A5	2913	C	C2-N3-C4	-8.45	115.67	119.90
36	A1	1481	A	C8-N9-C4	-8.45	102.42	105.80
36	A5	2870	C	C6-N1-C2	-8.44	116.92	120.30
36	A1	3077	A	C8-N9-C4	-8.44	102.42	105.80
1	A2	1200	G	C6-C5-N7	-8.44	125.34	130.40
80	A6	1298	U	C5-C6-N1	-8.44	118.48	122.70
36	A5	2980	U	N1-C2-N3	8.44	119.96	114.90
36	A1	3306	U	C5-C6-N1	-8.43	118.48	122.70
36	A1	106	A	C8-N9-C4	8.43	109.17	105.80
37	A7	96	U	C2-N3-C4	-8.43	121.94	127.00
36	A5	945	C	N3-C4-C5	8.43	125.27	121.90
36	A1	1481	A	N7-C8-N9	8.43	118.01	113.80
80	A6	1596	C	C6-N1-C2	-8.43	116.93	120.30
36	A1	2277	C	N3-C4-C5	8.42	125.27	121.90
36	A5	3137	C	N3-C4-C5	8.42	125.27	121.90
36	A1	1592	G	N1-C2-N2	-8.42	108.62	116.20
36	A5	1402	C	N3-C2-O2	-8.42	116.00	121.90
36	A1	63	A	N1-C2-N3	-8.42	125.09	129.30
1	A2	1387	G	N1-C6-O6	8.42	124.95	119.90
36	A5	999	G	N1-C6-O6	-8.42	114.85	119.90
36	A5	1156	C	C2-N3-C4	-8.42	115.69	119.90
36	A5	2683	U	N1-C2-O2	8.42	128.69	122.80
36	A1	2418	G	C2-N3-C4	8.41	116.11	111.90
36	A5	1064	A	C5-C6-N6	-8.41	116.97	123.70
1	A2	577	G	N7-C8-N9	8.41	117.31	113.10
36	A5	2928	C	C4-C5-C6	8.41	121.61	117.40
36	A1	2334	U	C5-C6-N1	-8.41	118.50	122.70
36	A5	2345	A	N1-C6-N6	8.41	123.65	118.60
36	A1	2642	A	C8-N9-C4	8.41	109.16	105.80
36	A1	2752	U	N3-C4-O4	-8.40	113.52	119.40
36	A1	3083	G	C2-N3-C4	8.40	116.10	111.90
36	A5	1469	C	N3-C4-C5	-8.40	118.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1336	U	N1-C2-N3	8.40	119.94	114.90
36	A1	1403	C	N3-C4-C5	8.40	125.26	121.90
80	A6	1535	U	N1-C2-O2	8.40	128.68	122.80
36	A1	24	G	N3-C2-N2	-8.39	114.02	119.90
36	A1	2595	A	N7-C8-N9	8.39	118.00	113.80
1	A2	966	A	C8-N9-C4	8.39	109.16	105.80
36	A1	2909	U	N1-C2-O2	-8.39	116.92	122.80
80	A6	17	C	N3-C2-O2	-8.39	116.02	121.90
36	A5	580	C	C6-N1-C2	-8.39	116.94	120.30
36	A5	811	U	C2-N3-C4	-8.39	121.97	127.00
36	A1	2719	U	C2-N3-C4	-8.39	121.97	127.00
38	A8	55	U	N1-C2-N3	8.39	119.93	114.90
36	A1	3222	U	N3-C2-O2	-8.39	116.33	122.20
36	A1	573	C	N3-C4-C5	8.38	125.25	121.90
36	A1	938	C	N3-C4-C5	8.38	125.25	121.90
37	A7	48	U	C5-C4-O4	-8.38	120.87	125.90
36	A1	1119	C	C6-N1-C2	8.38	123.65	120.30
80	A6	1614	A	N1-C6-N6	8.38	123.63	118.60
36	A1	1382	G	C8-N9-C4	8.38	109.75	106.40
80	A6	1	U	N3-C2-O2	-8.38	116.33	122.20
80	A6	114	C	N1-C2-O2	8.38	123.93	118.90
1	A2	1541	G	C5-C6-O6	8.38	133.62	128.60
1	A2	1387	G	C6-C5-N7	-8.37	125.38	130.40
36	A1	2314	U	C4-C5-C6	-8.38	114.67	119.70
36	A5	2307	G	N3-C4-C5	-8.38	124.41	128.60
80	A6	1745	G	C5-C6-O6	-8.37	123.58	128.60
80	A6	102	U	N1-C2-O2	-8.36	116.94	122.80
36	A1	104	G	C5-C6-O6	-8.36	123.58	128.60
36	A5	3102	G	N3-C2-N2	8.36	125.75	119.90
36	A1	368	G	N1-C2-N3	8.36	128.92	123.90
36	A1	2944	U	N1-C2-O2	8.36	128.65	122.80
36	A1	2279	A	C5-C6-N6	-8.36	117.02	123.70
36	A5	817	A	C8-N9-C4	-8.36	102.46	105.80
37	A7	96	U	N1-C2-N3	8.36	119.91	114.90
1	A2	736	C	C2-N1-C1'	8.35	127.99	118.80
36	A1	1838	G	C6-C5-N7	-8.35	125.39	130.40
36	A5	511	G	N1-C6-O6	-8.35	114.89	119.90
36	A5	916	G	C5-C6-O6	8.35	133.61	128.60
36	A1	1858	A	N3-C4-N9	8.35	134.08	127.40
36	A5	926	A	C5-C6-N1	8.35	121.88	117.70
36	A5	2234	G	N9-C4-C5	-8.35	102.06	105.40
36	A5	2820	A	C8-N9-C4	-8.35	102.46	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	136	C	C2-N1-C1'	8.35	127.98	118.80
80	A6	359	A	C4-C5-C6	-8.35	112.83	117.00
36	A5	616	G	C5-C6-N1	8.35	115.67	111.50
37	A7	93	C	C2-N3-C4	-8.35	115.73	119.90
36	A5	3173	G	C5-C6-O6	-8.34	123.59	128.60
36	A1	3143	C	C5-C6-N1	-8.34	116.83	121.00
36	A1	347	G	C5-C6-O6	-8.34	123.60	128.60
36	A1	2356	A	N1-C6-N6	8.33	123.60	118.60
36	A1	2763	U	C5-C6-N1	-8.33	118.53	122.70
36	A1	2393	G	N9-C4-C5	-8.33	102.07	105.40
36	A1	3180	A	C8-N9-C4	-8.33	102.47	105.80
36	A1	2237	C	C6-N1-C2	8.33	123.63	120.30
36	A1	2409	G	C5-C6-O6	8.33	133.60	128.60
36	A5	1487	G	C5-C6-O6	8.33	133.60	128.60
36	A5	2320	A	C2-N3-C4	-8.33	106.44	110.60
36	A1	47	C	C4-C5-C6	8.32	121.56	117.40
36	A1	2400	G	N3-C4-C5	8.32	132.76	128.60
80	A6	376	C	N3-C4-C5	8.32	125.23	121.90
37	A3	28	C	N3-C4-N4	8.32	123.82	118.00
36	A1	1191	U	C5-C6-N1	-8.32	118.54	122.70
36	A1	1507	G	N3-C2-N2	-8.31	114.08	119.90
36	A1	2283	G	C5-C6-O6	-8.31	123.61	128.60
36	A5	3050	U	C5-C4-O4	8.31	130.89	125.90
73	Bj	21	ARG	NE-CZ-NH2	-8.31	116.14	120.30
36	A1	702	C	C6-N1-C2	-8.31	116.98	120.30
36	A1	1918	C	C6-N1-C2	-8.31	116.98	120.30
36	A1	646	A	C8-N9-C4	-8.30	102.48	105.80
36	A1	1115	G	N1-C6-O6	-8.30	114.92	119.90
36	A1	2827	U	N1-C2-N3	8.30	119.88	114.90
38	A4	21	C	C6-N1-C2	8.30	123.62	120.30
36	A5	2683	U	N3-C2-O2	-8.30	116.39	122.20
36	A5	1898	G	C2-N3-C4	8.30	116.05	111.90
36	A1	2836	C	N3-C4-C5	-8.29	118.58	121.90
36	A1	2958	A	C5-C6-N1	8.29	121.85	117.70
36	A5	986	U	C5-C4-O4	-8.29	120.92	125.90
36	A5	1480	G	N7-C8-N9	-8.29	108.95	113.10
52	DO	197[B]	PHE	C-N-CA	-8.29	104.88	122.30
36	A5	715	A	N1-C6-N6	-8.29	113.62	118.60
38	A8	80	A	N7-C8-N9	8.29	117.94	113.80
1	A2	542	A	C4-N9-C1'	8.28	141.20	126.30
36	A1	106	A	C2-N3-C4	-8.28	106.46	110.60
36	A1	1890	U	C5-C6-N1	-8.28	118.56	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2977	G	N7-C8-N9	-8.27	108.96	113.10
1	A2	1280	C	N1-C2-O2	-8.27	113.94	118.90
36	A1	39	A	C4-C5-C6	8.27	121.14	117.00
36	A1	957	C	C6-N1-C2	8.27	123.61	120.30
36	A5	2360	C	C4-C5-C6	8.27	121.53	117.40
1	A2	1131	A	C8-N9-C4	8.27	109.11	105.80
36	A5	1392	G	N7-C8-N9	-8.27	108.97	113.10
36	A1	2814	G	C5-C6-O6	-8.26	123.64	128.60
37	A7	69	C	C6-N1-C2	8.26	123.61	120.30
38	A4	73	U	N3-C4-O4	-8.26	113.62	119.40
80	A6	272	U	N3-C2-O2	-8.26	116.42	122.20
36	A5	1604	G	C8-N9-C1'	-8.26	116.26	127.00
80	A6	1614	A	C4-C5-N7	8.26	114.83	110.70
36	A5	715	A	C2-N3-C4	8.26	114.73	110.60
36	A1	2130	G	C5-C6-O6	8.26	133.55	128.60
36	A1	2642	A	N7-C8-N9	-8.26	109.67	113.80
36	A5	2621	G	N1-C6-O6	8.26	124.85	119.90
37	A7	93	C	C5-C6-N1	-8.26	116.87	121.00
47	DI	128	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	A2	1782	A	N1-C2-N3	8.25	133.42	129.30
47	BI	24	ARG	NE-CZ-NH1	8.25	124.42	120.30
36	A1	2169	G	C4-C5-N7	-8.24	107.50	110.80
80	A6	1119	G	C5-C6-O6	8.24	133.55	128.60
36	A1	2714	G	C8-N9-C1'	8.24	137.72	127.00
36	A1	1122	U	N3-C4-C5	8.24	119.54	114.60
38	A8	55	U	C6-N1-C2	-8.24	116.06	121.00
36	A5	2695	A	C8-N9-C4	-8.23	102.51	105.80
36	A1	3143	C	N3-C2-O2	8.23	127.66	121.90
38	A4	125	U	N1-C2-O2	8.23	128.56	122.80
36	A5	1494	U	C6-N1-C2	8.23	125.94	121.00
36	A5	2371	G	N3-C2-N2	8.23	125.66	119.90
36	A1	2426	U	N3-C4-O4	-8.23	113.64	119.40
36	A1	2808	A	C6-C5-N7	-8.23	126.54	132.30
1	A2	1119	G	N1-C6-O6	-8.23	114.96	119.90
80	A6	342	C	C5-C6-N1	-8.23	116.89	121.00
36	A1	973	A	C8-N9-C4	-8.23	102.51	105.80
36	A1	3269	U	N1-C2-N3	8.23	119.84	114.90
36	A1	2123	G	C8-N9-C4	8.22	109.69	106.40
36	A5	2859	U	N3-C4-O4	-8.22	113.65	119.40
36	A1	369	A	N1-C6-N6	-8.22	113.67	118.60
1	A2	992	A	C5-N7-C8	-8.22	99.79	103.90
36	A5	818	C	N1-C2-O2	-8.22	113.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1178	G	C8-N9-C4	-8.22	103.11	106.40
1	A2	319	U	N3-C2-O2	8.22	127.95	122.20
1	A2	1096	C	N1-C2-O2	8.22	123.83	118.90
38	A4	79	A	C8-N9-C4	-8.21	102.51	105.80
36	A5	15	C	C5-C6-N1	8.21	125.11	121.00
36	A5	1586	G	C5-C6-O6	-8.21	123.67	128.60
36	A1	2293	C	C5-C4-N4	-8.21	114.45	120.20
36	A5	2735	U	C5-C6-N1	8.21	126.81	122.70
36	A5	435	C	N3-C4-C5	8.21	125.18	121.90
36	A1	1515	A	C4-C5-C6	8.21	121.11	117.00
80	A6	1595	U	C5-C4-O4	8.21	130.82	125.90
36	A5	1015	U	C5-C6-N1	8.21	126.80	122.70
36	A5	2211	U	N3-C2-O2	-8.21	116.45	122.20
36	A1	2909	U	N3-C4-O4	8.20	125.14	119.40
36	A5	591	G	N9-C4-C5	-8.21	102.12	105.40
36	A5	922	U	C6-N1-C1'	8.21	132.69	121.20
36	A5	1404	G	C8-N9-C4	8.20	109.68	106.40
36	A1	2169	G	C6-C5-N7	8.20	135.32	130.40
36	A1	2816	G	C5-C6-N1	8.20	115.60	111.50
36	A5	2202	C	N3-C2-O2	8.20	127.64	121.90
36	A1	345	G	N3-C4-C5	-8.20	124.50	128.60
36	A1	432	G	C2-N3-C4	-8.20	107.80	111.90
36	A1	2572	C	C6-N1-C2	-8.20	117.02	120.30
36	A5	1054	A	C8-N9-C4	8.20	109.08	105.80
36	A5	968	G	N9-C4-C5	-8.20	102.12	105.40
36	A1	3318	G	C4-N9-C1'	8.20	137.16	126.50
36	A1	2618	G	C5-C6-N1	8.20	115.60	111.50
36	A1	1133	A	C8-N9-C4	8.19	109.08	105.80
36	A5	514	G	C5-C6-O6	-8.19	123.68	128.60
36	A1	1142	G	N3-C4-N9	8.19	130.91	126.00
36	A1	2990	G	C4-C5-N7	-8.19	107.52	110.80
38	A4	58	G	N3-C4-N9	8.19	130.91	126.00
36	A1	2777	G	N3-C4-C5	8.19	132.69	128.60
36	A5	2190	U	N3-C4-O4	-8.19	113.67	119.40
36	A5	343	U	N1-C2-O2	8.19	128.53	122.80
36	A1	874	U	N3-C4-O4	-8.18	113.67	119.40
36	A5	949	C	C4-C5-C6	8.18	121.49	117.40
38	A4	103	G	N1-C6-O6	-8.18	114.99	119.90
56	DS	115	ARG	NE-CZ-NH1	8.18	124.39	120.30
36	A1	1180	A	N1-C2-N3	8.18	133.39	129.30
36	A1	544	C	C6-N1-C2	-8.17	117.03	120.30
36	A5	2913	C	N1-C2-N3	8.17	124.92	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A4	32	C	N1-C2-O2	-8.17	114.00	118.90
36	A5	2609	A	C5-N7-C8	8.17	107.99	103.90
36	A1	2595	A	C4-C5-N7	8.17	114.78	110.70
36	A5	805	G	C8-N9-C4	8.17	109.67	106.40
36	A5	280	U	C2-N3-C4	-8.17	122.10	127.00
36	A5	435	C	C5-C4-N4	-8.17	114.48	120.20
36	A5	1110	U	N3-C4-C5	8.17	119.50	114.60
36	A5	3317	U	C5-C4-O4	8.17	130.80	125.90
36	A1	631	U	C2-N3-C4	-8.16	122.10	127.00
36	A5	926	A	C5-C6-N6	-8.16	117.17	123.70
36	A5	726	G	N1-C6-O6	8.16	124.80	119.90
36	A5	1445	U	C5-C4-O4	-8.16	121.00	125.90
36	A5	2302	G	C5-C6-O6	8.15	133.49	128.60
36	A5	3122	A	N9-C4-C5	8.15	109.06	105.80
36	A5	708	G	C5-N7-C8	-8.15	100.22	104.30
36	A1	2176	U	N1-C2-O2	8.15	128.50	122.80
36	A5	2970	C	C4-C5-C6	8.15	121.47	117.40
36	A1	2572	C	C2-N1-C1'	8.15	127.76	118.80
36	A1	2409	G	N9-C4-C5	8.14	108.66	105.40
36	A1	2622	C	C6-N1-C2	-8.14	117.04	120.30
1	A2	1241	G	C5-N7-C8	-8.14	100.23	104.30
36	A1	883	A	C2-N3-C4	8.14	114.67	110.60
36	A1	2278	C	N3-C4-C5	8.14	125.16	121.90
80	A6	17	C	N1-C2-O2	8.14	123.78	118.90
36	A5	987	U	N1-C2-N3	8.14	119.78	114.90
36	A1	2356	A	N1-C2-N3	-8.13	125.23	129.30
36	A5	1176	C	C5-C6-N1	-8.13	116.93	121.00
36	A5	2412	G	C8-N9-C4	-8.13	103.15	106.40
1	A2	308	C	C5-C6-N1	-8.13	116.94	121.00
36	A1	1434	G	C4-C5-C6	8.13	123.68	118.80
36	A5	1085	A	C5-N7-C8	-8.13	99.83	103.90
36	A1	1617	G	C8-N9-C4	8.13	109.65	106.40
1	A2	1129	U	N3-C4-C5	8.13	119.48	114.60
36	A5	2838	A	C5-C6-N6	-8.13	117.20	123.70
36	A1	405	U	C5-C4-O4	-8.12	121.03	125.90
36	A1	1049	C	C5-C4-N4	-8.12	114.52	120.20
36	A1	1362	G	C8-N9-C4	8.12	109.65	106.40
38	A4	113	U	C4-C5-C6	8.12	124.57	119.70
36	A5	2665	U	N1-C2-N3	-8.12	110.03	114.90
36	A5	2859	U	C5-C4-O4	8.12	130.77	125.90
1	A2	1291	G	N1-C2-N3	8.11	128.77	123.90
36	A1	3049	A	C5-C6-N1	-8.12	113.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	769	G	C8-N9-C4	8.12	109.65	106.40
36	A5	842	G	C5-C6-O6	-8.11	123.73	128.60
36	A1	651	G	N3-C4-C5	-8.11	124.54	128.60
36	A1	653	A	C5-C6-N1	8.11	121.76	117.70
36	A5	2634	U	N3-C4-C5	8.11	119.47	114.60
36	A1	847	A	N9-C4-C5	-8.11	102.56	105.80
36	A1	1132	C	N3-C4-N4	-8.11	112.33	118.00
36	A1	1947	G	N3-C2-N2	-8.11	114.23	119.90
36	A5	637	C	N1-C2-O2	-8.10	114.04	118.90
36	A1	1523	U	N1-C2-O2	-8.10	117.13	122.80
36	A5	2246	G	N1-C6-O6	-8.10	115.04	119.90
36	A5	290	G	C5-C6-O6	8.10	133.46	128.60
36	A5	817	A	C2-N3-C4	8.10	114.65	110.60
36	A1	1123	U	C5-C6-N1	-8.10	118.65	122.70
36	A1	2165	G	N1-C6-O6	8.09	124.76	119.90
36	A1	2288	G	C8-N9-C4	-8.09	103.16	106.40
36	A5	2175	U	C5-C6-N1	-8.09	118.65	122.70
36	A5	916	G	N1-C6-O6	-8.09	115.05	119.90
36	A1	2200	U	C6-N1-C2	-8.09	116.15	121.00
36	A5	2278	C	C5-C4-N4	8.09	125.86	120.20
36	A5	2440	G	C8-N9-C4	-8.09	103.17	106.40
36	A5	3362	A	N1-C2-N3	8.09	133.34	129.30
36	A1	2550	U	N1-C2-N3	8.08	119.75	114.90
36	A1	3207	U	C5-C4-O4	8.08	130.75	125.90
36	A5	329	U	C5-C6-N1	-8.08	118.66	122.70
36	A5	1512	U	N1-C2-N3	8.08	119.75	114.90
36	A5	2182	A	N1-C6-N6	-8.08	113.75	118.60
36	A5	3215	A	N1-C6-N6	8.08	123.45	118.60
38	A8	38	U	C5-C6-N1	-8.08	118.66	122.70
36	A5	2290	C	C4-C5-C6	8.08	121.44	117.40
1	A2	1773	C	C5-C6-N1	8.08	125.04	121.00
36	A5	1390	A	N9-C4-C5	8.07	109.03	105.80
36	A5	1516	C	C2-N3-C4	-8.07	115.86	119.90
36	A5	945	C	C2-N3-C4	-8.07	115.86	119.90
38	A8	2	A	C8-N9-C4	-8.07	102.57	105.80
80	A6	418	G	C6-C5-N7	-8.07	125.56	130.40
36	A5	41	G	C5-N7-C8	-8.07	100.27	104.30
37	A7	112	G	N1-C6-O6	-8.07	115.06	119.90
36	A5	1879	A	C8-N9-C4	-8.07	102.57	105.80
1	A2	1436	A	N1-C6-N6	8.07	123.44	118.60
38	A8	113	U	N3-C4-O4	8.06	125.04	119.40
36	A1	2735	U	N3-C4-C5	8.05	119.43	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A4	32	C	C2-N1-C1'	-8.05	109.94	118.80
36	A5	1449	A	C5-N7-C8	-8.05	99.88	103.90
80	A6	1000	C	C2-N1-C1'	8.05	127.65	118.80
36	A5	359	U	C2-N3-C4	-8.05	122.17	127.00
36	A5	1193	A	N1-C2-N3	8.05	133.32	129.30
36	A5	1858	A	N3-C4-C5	-8.05	121.17	126.80
1	A2	1200	G	N1-C2-N2	8.04	123.44	116.20
36	A1	2318	U	C2-N3-C4	-8.04	122.17	127.00
36	A5	413	U	C2-N3-C4	-8.04	122.17	127.00
36	A5	631	U	C2-N3-C4	-8.04	122.17	127.00
1	A2	1324	G	N3-C4-N9	-8.04	121.17	126.00
36	A1	2382	G	N1-C6-O6	-8.04	115.08	119.90
36	A1	2893	C	N3-C4-C5	8.04	125.12	121.90
36	A1	2952	G	C5-N7-C8	-8.04	100.28	104.30
36	A5	3110	C	C4-C5-C6	8.04	121.42	117.40
36	A1	2284	C	C2-N3-C4	-8.04	115.88	119.90
54	BQ	178	ARG	NE-CZ-NH1	-8.04	116.28	120.30
52	DO	3[B]	SER	O-C-N	8.04	135.56	122.70
80	A6	100	A	C8-N9-C4	8.04	109.02	105.80
36	A5	1879	A	C6-C5-N7	-8.04	126.67	132.30
44	DF	88	ARG	NE-CZ-NH2	-8.04	116.28	120.30
36	A1	2595	A	C2-N3-C4	-8.04	106.58	110.60
36	A1	2821	C	C6-N1-C2	-8.04	117.08	120.30
36	A1	2836	C	C6-N1-C2	-8.04	117.09	120.30
36	A1	3180	A	N9-C4-C5	8.04	109.01	105.80
36	A5	278	U	C5-C6-N1	8.03	126.72	122.70
80	A6	1389	C	C2-N1-C1'	8.03	127.64	118.80
36	A5	945	C	C6-N1-C2	8.03	123.51	120.30
36	A5	2278	C	C2-N3-C4	-8.03	115.89	119.90
36	A1	3119	U	N3-C4-O4	-8.03	113.78	119.40
36	A5	824	C	C6-N1-C2	-8.03	117.09	120.30
36	A1	2860	U	C5-C4-O4	-8.03	121.08	125.90
36	A5	2189	U	N1-C2-N3	8.03	119.72	114.90
80	A6	1782	A	C8-N9-C4	-8.03	102.59	105.80
38	A8	74	U	C5-C4-O4	-8.02	121.09	125.90
36	A1	1848	G	C5-C6-O6	-8.02	123.79	128.60
36	A1	2328	U	N3-C4-O4	-8.02	113.79	119.40
1	A2	1662	G	N1-C6-O6	-8.02	115.09	119.90
36	A1	817	A	C6-N1-C2	-8.02	113.79	118.60
36	A1	2329	C	N1-C2-O2	-8.02	114.09	118.90
80	A6	1735	U	N3-C4-C5	8.02	119.41	114.60
36	A5	2572	C	C2-N1-C1'	8.02	127.62	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1395	G	N3-C2-N2	8.02	125.51	119.90
36	A5	2630	C	N3-C4-C5	8.02	125.11	121.90
1	A2	1490	C	C6-N1-C2	-8.01	117.09	120.30
36	A1	1397	C	N1-C2-O2	-8.01	114.09	118.90
36	A5	2281	A	C8-N9-C4	8.01	109.00	105.80
36	A1	1483	G	N1-C6-O6	-8.01	115.09	119.90
80	A6	418	G	C8-N9-C4	-8.01	103.20	106.40
80	A6	1644	C	C2-N3-C4	-8.01	115.90	119.90
36	A5	1592	G	C5-C6-N1	8.01	115.50	111.50
1	A2	316	A	C8-N9-C4	8.00	109.00	105.80
36	A5	857	G	C5-C6-N1	8.00	115.50	111.50
36	A5	3309	G	N3-C4-N9	8.00	130.80	126.00
37	A3	81	U	C6-N1-C1'	-8.00	110.00	121.20
65	Db	39	PHE	N-CA-CB	8.00	125.00	110.60
1	A2	349	U	N3-C2-O2	-8.00	116.60	122.20
36	A1	1881	A	C8-N9-C4	8.00	109.00	105.80
36	A1	2360	C	C4-C5-C6	8.00	121.40	117.40
80	A6	65	A	N1-C6-N6	8.00	123.40	118.60
36	A5	3362	A	C8-N9-C4	-8.00	102.60	105.80
80	A6	858	G	N7-C8-N9	7.99	117.10	113.10
36	A5	1481	A	N7-C8-N9	7.99	117.80	113.80
36	A5	1441	G	N1-C6-O6	-7.99	115.11	119.90
36	A1	620	U	C6-N1-C2	-7.99	116.21	121.00
36	A1	891	G	C5-C6-O6	7.99	133.39	128.60
36	A5	1113	G	C8-N9-C4	7.99	109.60	106.40
36	A5	2777	G	C5-C6-O6	7.99	133.39	128.60
36	A1	3214	U	N1-C2-N3	7.99	119.69	114.90
37	A3	82	G	N1-C2-N3	7.99	128.69	123.90
36	A1	56	G	C5-C6-O6	-7.98	123.81	128.60
36	A5	2350	C	C5-C6-N1	-7.98	117.01	121.00
36	A1	695	C	N3-C4-N4	-7.98	112.41	118.00
37	A7	81	U	N3-C4-C5	7.98	119.39	114.60
36	A1	2395	G	N3-C4-C5	-7.98	124.61	128.60
36	A5	3215	A	C2-N3-C4	-7.98	106.61	110.60
36	A1	966	U	N3-C4-C5	7.98	119.39	114.60
36	A5	2317	A	C8-N9-C4	-7.97	102.61	105.80
36	A5	2512	C	C5-C6-N1	7.97	124.99	121.00
36	A5	3343	G	N9-C4-C5	-7.97	102.21	105.40
37	A7	85	G	N1-C6-O6	-7.97	115.12	119.90
36	A1	281	G	C8-N9-C4	-7.97	103.21	106.40
36	A1	960	U	C2-N3-C4	-7.97	122.22	127.00
80	A6	826	U	C5-C6-N1	7.97	126.68	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1100	G	C6-N1-C2	-7.97	120.32	125.10
36	A5	345	G	N1-C6-O6	-7.97	115.12	119.90
36	A5	1148	G	C2-N3-C4	7.97	115.88	111.90
36	A1	24	G	N1-C6-O6	7.97	124.68	119.90
36	A5	1297	C	C5-C6-N1	-7.97	117.02	121.00
36	A5	2366	C	N3-C4-N4	7.96	123.58	118.00
36	A5	3343	G	N3-C4-N9	7.96	130.78	126.00
36	A5	2288	G	C2-N3-C4	7.96	115.88	111.90
36	A1	54	C	N3-C4-C5	7.96	125.08	121.90
36	A1	1309	U	C5-C4-O4	-7.96	121.12	125.90
36	A1	2369	G	N3-C4-N9	7.96	130.78	126.00
36	A5	2870	C	C6-N1-C1'	7.96	130.35	120.80
80	A6	400	A	N1-C6-N6	7.95	123.37	118.60
36	A5	784	A	N1-C6-N6	7.95	123.37	118.60
36	A1	1003	A	N1-C6-N6	7.95	123.37	118.60
36	A1	2138	A	N9-C4-C5	7.95	108.98	105.80
80	A6	1749	A	C4-C5-N7	7.95	114.67	110.70
36	A1	121	A	C8-N9-C4	7.95	108.98	105.80
36	A1	962	A	N1-C2-N3	7.95	133.27	129.30
36	A1	2751	G	C5-C6-O6	-7.95	123.83	128.60
52	BO	158[B]	ASP	C-N-CA	-7.95	101.84	121.70
36	A5	3377	G	N9-C4-C5	-7.94	102.22	105.40
36	A1	1556	C	C6-N1-C2	-7.94	117.12	120.30
36	A1	2885	C	N3-C4-C5	7.94	125.08	121.90
36	A1	2952	G	N9-C4-C5	-7.94	102.22	105.40
36	A5	3151	U	C6-N1-C2	7.94	125.76	121.00
1	A2	1611	A	N7-C8-N9	7.94	117.77	113.80
36	A1	3278	C	N3-C2-O2	-7.94	116.34	121.90
36	A5	1317	A	N1-C6-N6	7.94	123.36	118.60
36	A5	2757	U	N3-C4-O4	7.94	124.96	119.40
36	A1	1907	C	C2-N3-C4	7.94	123.87	119.90
36	A1	2356	A	C5-C6-N6	-7.94	117.35	123.70
36	A1	3277	U	N3-C2-O2	-7.94	116.64	122.20
36	A5	355	A	C2-N3-C4	-7.94	106.63	110.60
36	A5	629	U	N3-C4-C5	7.94	119.36	114.60
36	A1	2829	U	N3-C2-O2	-7.93	116.65	122.20
36	A5	3102	G	N1-C6-O6	-7.93	115.14	119.90
36	A5	1484	U	C6-N1-C2	7.93	125.76	121.00
1	A2	145	A	C8-N9-C4	-7.93	102.63	105.80
36	A1	3375	A	N7-C8-N9	7.93	117.76	113.80
36	A1	909	G	C8-N9-C4	7.92	109.57	106.40
36	A1	1741	A	N1-C2-N3	7.92	133.26	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1432	U	C6-N1-C2	7.92	125.75	121.00
1	A2	189	C	C2-N1-C1'	7.92	127.51	118.80
38	A4	58	G	C5-C6-O6	-7.92	123.85	128.60
36	A5	277	G	N1-C6-O6	-7.92	115.15	119.90
80	A6	453	U	N3-C4-O4	-7.92	113.86	119.40
36	A5	2550	U	N1-C2-N3	7.91	119.65	114.90
1	A2	1481	C	C6-N1-C2	-7.91	117.14	120.30
36	A1	1307	G	N3-C2-N2	7.91	125.44	119.90
36	A1	963	G	C6-C5-N7	-7.91	125.65	130.40
36	A1	2117	A	N1-C6-N6	-7.91	113.86	118.60
68	De	43	ARG	NE-CZ-NH2	-7.91	116.35	120.30
36	A5	2836	C	N1-C2-N3	7.91	124.73	119.20
36	A5	934	G	C5-C6-O6	-7.91	123.86	128.60
36	A5	2531	C	C2-N1-C1'	7.91	127.50	118.80
52	DO	27[B]	VAL	O-C-N	-7.90	110.05	122.70
36	A1	2776	C	C2-N3-C4	-7.90	115.95	119.90
80	A6	864	U	N3-C2-O2	-7.90	116.67	122.20
36	A5	960	U	C5-C6-N1	-7.90	118.75	122.70
36	A5	1940	G	N3-C2-N2	7.90	125.43	119.90
36	A1	47	C	C5-C6-N1	-7.90	117.05	121.00
36	A5	2381	G	C8-N9-C4	-7.90	103.24	106.40
36	A5	851	C	C6-N1-C2	-7.90	117.14	120.30
36	A1	2714	G	C4-C5-C6	-7.89	114.06	118.80
80	A6	1	U	C6-N1-C2	-7.89	116.26	121.00
36	A1	1919	G	N1-C6-O6	-7.89	115.16	119.90
36	A1	2380	U	C2-N3-C4	-7.89	122.26	127.00
36	A5	2618	G	C5-C6-O6	-7.89	123.86	128.60
36	A1	3302	U	C6-N1-C2	7.89	125.73	121.00
80	A6	1535	U	N3-C2-O2	-7.89	116.68	122.20
36	A5	2913	C	C5-C6-N1	-7.89	117.06	121.00
36	A5	1939	G	C5-C6-O6	7.89	133.33	128.60
36	A1	2281	A	C8-N9-C4	7.88	108.95	105.80
36	A5	2919	A	N1-C6-N6	-7.88	113.87	118.60
36	A5	2993	G	C5-C6-O6	-7.88	123.87	128.60
1	A2	864	U	N3-C2-O2	-7.88	116.68	122.20
36	A1	508	U	C5-C4-O4	-7.88	121.17	125.90
37	A7	26	C	C4-C5-C6	7.88	121.34	117.40
36	A5	2130	G	N3-C2-N2	7.88	125.41	119.90
36	A1	1048	A	C6-N1-C2	7.87	123.32	118.60
36	A5	2865	U	C5-C4-O4	-7.87	121.18	125.90
36	A1	1138	U	N1-C2-N3	7.87	119.62	114.90
80	A6	1489	U	N3-C2-O2	-7.87	116.69	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	3146	G	C5-C6-O6	7.87	133.32	128.60
36	A5	630	A	N1-C2-N3	7.87	133.23	129.30
36	A5	2366	C	C2-N1-C1'	7.87	127.46	118.80
36	A1	660	A	N1-C6-N6	-7.87	113.88	118.60
36	A1	718	G	C4-C5-N7	7.87	113.95	110.80
36	A1	62	A	C2-N3-C4	7.87	114.53	110.60
36	A1	3034	C	N1-C2-O2	7.87	123.62	118.90
36	A5	1480	G	C5-N7-C8	7.87	108.23	104.30
44	DF	88	ARG	NE-CZ-NH1	7.87	124.23	120.30
36	A1	344	A	N1-C6-N6	-7.86	113.88	118.60
36	A1	2870	C	C2-N1-C1'	-7.86	110.15	118.80
80	A6	542	A	C8-N9-C4	-7.86	102.66	105.80
36	A1	301	G	N1-C6-O6	-7.86	115.19	119.90
36	A1	1858	A	C8-N9-C4	-7.86	102.66	105.80
36	A1	2996	U	N1-C2-O2	7.86	128.30	122.80
80	A6	337	G	N3-C4-N9	7.86	130.71	126.00
36	A1	340	C	N3-C4-C5	7.85	125.04	121.90
36	A1	1403	C	C5-C6-N1	-7.85	117.07	121.00
36	A1	3275	U	C5-C6-N1	7.85	126.62	122.70
36	A5	813	G	C8-N9-C4	-7.85	103.26	106.40
41	DC	339	LEU	CA-CB-CG	7.85	133.35	115.30
80	A6	1456	C	N3-C4-N4	-7.85	112.51	118.00
36	A5	1140	G	N1-C6-O6	-7.85	115.19	119.90
36	A5	1793	C	N3-C4-C5	-7.85	118.76	121.90
36	A5	1834	U	C2-N1-C1'	-7.85	108.28	117.70
36	A5	1845	G	C5-C6-N1	7.85	115.42	111.50
36	A1	1796	G	C8-N9-C4	-7.85	103.26	106.40
1	A2	581	U	C2-N1-C1'	7.84	127.11	117.70
36	A1	2777	G	C5-C6-N1	7.84	115.42	111.50
36	A5	343	U	N3-C4-O4	-7.84	113.91	119.40
36	A5	2400	G	C2-N3-C4	-7.84	107.98	111.90
80	A6	1745	G	N3-C4-N9	7.84	130.70	126.00
36	A5	2303	A	N9-C4-C5	7.84	108.93	105.80
36	A5	3130	A	N1-C2-N3	7.84	133.22	129.30
36	A1	434	U	C4-C5-C6	-7.83	115.00	119.70
36	A1	1341	U	N1-C2-O2	7.83	128.28	122.80
36	A1	2814	G	N7-C8-N9	-7.83	109.18	113.10
36	A1	655	C	C4-C5-C6	7.83	121.31	117.40
36	A5	530	G	N1-C6-O6	-7.83	115.20	119.90
36	A1	1392	G	N3-C4-N9	7.83	130.70	126.00
36	A1	1494	U	C5-C6-N1	-7.83	118.79	122.70
36	A1	2214	A	N1-C6-N6	7.83	123.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	397	A	C2-N3-C4	-7.82	106.69	110.60
36	A1	545	U	C2-N1-C1'	7.82	127.09	117.70
80	A6	1185	U	N1-C2-O2	7.82	128.28	122.80
36	A5	2288	G	C6-N1-C2	-7.82	120.41	125.10
36	A1	2719	U	N1-C2-N3	7.82	119.59	114.90
36	A1	2400	G	N3-C4-N9	-7.81	121.31	126.00
1	A2	555	A	C8-N9-C4	-7.81	102.67	105.80
36	A1	2156	C	C5-C6-N1	-7.81	117.09	121.00
36	A5	1392	G	N3-C4-N9	7.81	130.69	126.00
36	A5	3096	C	N1-C2-N3	7.81	124.67	119.20
36	A1	1152	G	N1-C2-N3	7.81	128.59	123.90
36	A1	3209	A	N1-C6-N6	7.81	123.29	118.60
36	A5	226	C	C6-N1-C2	7.81	123.42	120.30
36	A5	2395	G	C5-N7-C8	7.81	108.20	104.30
36	A5	2705	A	C5-C6-N6	-7.81	117.45	123.70
36	A1	644	G	C4-C5-N7	-7.80	107.68	110.80
36	A1	644	G	N3-C2-N2	7.80	125.36	119.90
36	A5	1295	G	N1-C6-O6	-7.80	115.22	119.90
36	A5	1390	A	C8-N9-C4	-7.80	102.68	105.80
1	A2	1751	C	N3-C4-C5	7.80	125.02	121.90
36	A1	50	U	C2-N3-C4	-7.80	122.32	127.00
36	A1	659	G	N3-C2-N2	7.80	125.36	119.90
36	A5	276	U	C5-C6-N1	-7.80	118.80	122.70
36	A5	2882	U	N1-C2-N3	7.80	119.58	114.90
36	A5	1364	C	N1-C2-O2	-7.80	114.22	118.90
36	A5	2807	U	C5-C4-O4	-7.80	121.22	125.90
36	A5	641	C	N1-C2-O2	-7.80	114.22	118.90
36	A5	708	G	C5-C6-O6	-7.79	123.92	128.60
1	A2	1560	U	N3-C4-O4	-7.79	113.94	119.40
36	A5	3206	C	N3-C2-O2	-7.79	116.44	121.90
36	A1	50	U	N3-C4-O4	-7.79	113.95	119.40
36	A1	634	C	N3-C2-O2	-7.79	116.45	121.90
36	A1	635	G	C5-C6-N1	7.79	115.39	111.50
80	A6	421	A	C8-N9-C4	7.79	108.92	105.80
36	A1	2787	G	C5-C6-O6	-7.79	123.93	128.60
36	A5	216	G	N1-C6-O6	7.79	124.57	119.90
36	A5	2905	U	N3-C4-C5	7.79	119.27	114.60
36	A1	2203	U	N1-C2-N3	7.79	119.57	114.90
36	A1	1164	G	N9-C4-C5	7.79	108.52	105.40
36	A5	1311	G	C5-C6-N1	7.79	115.39	111.50
36	A5	1440	G	C5-C6-O6	7.79	133.27	128.60
36	A1	53	G	N9-C4-C5	-7.79	102.29	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1291	G	C8-N9-C4	-7.78	103.29	106.40
36	A5	2303	A	C8-N9-C4	-7.78	102.69	105.80
36	A5	3050	U	N1-C2-O2	7.78	128.25	122.80
36	A5	3187	A	C5-N7-C8	7.78	107.79	103.90
36	A5	1150	A	C2-N3-C4	-7.78	106.71	110.60
36	A5	2975	U	N3-C4-C5	7.78	119.27	114.60
36	A1	1733	G	N3-C4-C5	-7.78	124.71	128.60
36	A1	2363	A	N1-C6-N6	-7.78	113.93	118.60
80	A6	306	U	C5-C6-N1	-7.78	118.81	122.70
36	A1	282	G	C8-N9-C4	-7.78	103.29	106.40
36	A1	1520	G	C5-N7-C8	7.78	108.19	104.30
36	A1	290	G	C5-C6-N1	7.78	115.39	111.50
36	A1	2311	G	C5-C6-O6	-7.78	123.93	128.60
80	A6	364	G	C5-C6-O6	-7.78	123.93	128.60
80	A6	1514	U	C5-C6-N1	-7.78	118.81	122.70
36	A5	2134	G	C5-C6-N1	7.78	115.39	111.50
36	A1	2130	G	N3-C4-C5	-7.78	124.71	128.60
80	A6	194	U	C2-N1-C1'	7.78	127.03	117.70
36	A5	2891	U	C2-N3-C4	-7.78	122.33	127.00
36	A1	1400	G	C8-N9-C4	7.77	109.51	106.40
36	A5	3187	A	N1-C6-N6	-7.77	113.94	118.60
36	A1	573	C	C2-N3-C4	-7.77	116.01	119.90
36	A5	1792	C	N1-C2-O2	-7.77	114.24	118.90
36	A1	651	G	N3-C4-N9	7.77	130.66	126.00
36	A5	2550	U	N3-C4-O4	-7.77	113.96	119.40
80	A6	539	G	C8-N9-C4	-7.76	103.29	106.40
36	A5	1391	C	N3-C2-O2	7.76	127.33	121.90
36	A1	3344	A	C4-C5-C6	7.76	120.88	117.00
36	A1	1150	A	C5-C6-N6	7.76	129.91	123.70
36	A5	3266	G	N9-C4-C5	7.76	108.50	105.40
1	A2	992	A	C6-N1-C2	7.76	123.26	118.60
36	A1	368	G	N1-C2-N2	-7.76	109.22	116.20
36	A1	2714	G	C4-N9-C1'	-7.76	116.41	126.50
36	A5	1480	G	C8-N9-C4	7.76	109.50	106.40
36	A5	2246	G	C5-C6-O6	7.76	133.26	128.60
36	A5	3185	U	C2-N3-C4	-7.76	122.34	127.00
36	A5	2899	C	N3-C4-N4	-7.76	112.57	118.00
36	A1	2632	G	N3-C2-N2	7.76	125.33	119.90
36	A1	519	A	N1-C6-N6	7.75	123.25	118.60
36	A5	859	G	C8-N9-C4	-7.75	103.30	106.40
36	A5	990	U	N1-C2-O2	7.75	128.23	122.80
36	A5	3377	G	N3-C4-N9	7.75	130.65	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1143	A	C5-N7-C8	-7.75	100.02	103.90
36	A5	2393	G	N1-C6-O6	7.75	124.55	119.90
36	A1	664	U	C2-N3-C4	-7.75	122.35	127.00
38	A4	85	G	C8-N9-C4	-7.75	103.30	106.40
36	A1	2827	U	C2-N3-C4	-7.75	122.35	127.00
80	A6	1620	C	C6-N1-C2	-7.75	117.20	120.30
36	A1	1126	G	N7-C8-N9	-7.74	109.23	113.10
36	A1	2719	U	C2-N1-C1'	-7.74	108.41	117.70
36	A5	2202	C	N3-C4-N4	7.74	123.42	118.00
80	A6	769	A	C8-N9-C4	-7.74	102.70	105.80
36	A5	1370	G	N1-C6-O6	-7.74	115.25	119.90
36	A1	2306	C	N3-C2-O2	-7.74	116.48	121.90
64	Ba	42	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A2	142	G	N3-C4-N9	-7.74	121.36	126.00
36	A5	904	A	N1-C6-N6	-7.74	113.96	118.60
36	A5	2278	C	C6-N1-C1'	7.74	130.08	120.80
80	A6	36	C	C5-C4-N4	-7.74	114.78	120.20
80	A6	1568	C	C6-N1-C2	-7.74	117.21	120.30
1	A2	704	C	N1-C2-O2	7.73	123.54	118.90
36	A1	2653	C	N3-C2-O2	-7.73	116.49	121.90
80	A6	1634	C	C6-N1-C1'	-7.73	111.52	120.80
36	A5	2960	C	N3-C4-C5	7.73	124.99	121.90
36	A1	1492	G	C4-N9-C1'	7.73	136.55	126.50
47	DI	167	LEU	CA-CB-CG	7.73	133.08	115.30
1	A2	1486	G	C8-N9-C4	-7.73	103.31	106.40
36	A5	974	G	N3-C4-C5	-7.73	124.74	128.60
36	A1	1841	A	C2-N3-C4	7.73	114.46	110.60
36	A1	891	G	N1-C6-O6	-7.72	115.27	119.90
36	A1	3112	G	C5-C6-O6	-7.72	123.97	128.60
36	A5	3308	C	N1-C2-N3	7.72	124.60	119.20
80	A6	1549	C	N3-C4-C5	-7.72	118.81	121.90
36	A1	386	A	N1-C6-N6	7.71	123.23	118.60
36	A1	1448	U	C2-N3-C4	-7.71	122.37	127.00
36	A5	1833	G	N1-C6-O6	-7.71	115.27	119.90
36	A5	546	C	C6-N1-C1'	-7.71	111.55	120.80
36	A1	664	U	C4-C5-C6	7.71	124.32	119.70
36	A1	3208	G	C8-N9-C1'	7.71	137.02	127.00
36	A1	2249	G	C3'-C2'-C1'	-7.70	95.34	101.50
36	A5	1889	G	N1-C6-O6	-7.70	115.28	119.90
36	A5	2757	U	C2-N3-C4	-7.70	122.38	127.00
1	A2	1455	G	C4-C5-N7	-7.70	107.72	110.80
36	A1	1117	G	N7-C8-N9	-7.70	109.25	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	363	G	N1-C2-N3	7.70	128.52	123.90
36	A5	376	G	C5-C6-N1	7.70	115.35	111.50
36	A5	2315	G	C8-N9-C4	7.70	109.48	106.40
36	A5	2584	G	C4-N9-C1'	7.70	136.50	126.50
80	A6	1473	U	N3-C2-O2	-7.69	116.81	122.20
36	A5	753	C	C2-N3-C4	-7.69	116.05	119.90
36	A1	2339	C	N1-C2-O2	-7.69	114.29	118.90
36	A1	1143	A	N1-C6-N6	7.69	123.21	118.60
36	A1	218	G	C2-N3-C4	7.68	115.74	111.90
36	A1	2376	G	C5-C6-N1	7.68	115.34	111.50
68	De	45	ARG	NE-CZ-NH2	-7.68	116.46	120.30
36	A1	384	A	C8-N9-C4	7.68	108.87	105.80
70	Bg	51	LEU	CA-CB-CG	7.68	132.96	115.30
1	A2	334	G	C2-N3-C4	-7.68	108.06	111.90
36	A1	1156	C	N3-C4-N4	-7.68	112.63	118.00
36	A1	1846	C	C5-C6-N1	-7.68	117.16	121.00
36	A1	2811	A	N1-C6-N6	-7.68	113.99	118.60
49	DL	21	ARG	NE-CZ-NH1	-7.68	116.46	120.30
36	A1	2777	G	N1-C2-N3	-7.67	119.30	123.90
36	A5	2346	C	C2-N3-C4	-7.67	116.06	119.90
36	A5	3065	G	N1-C6-O6	-7.67	115.30	119.90
36	A5	1604	G	C4-N9-C1'	7.67	136.47	126.50
38	A8	11	C	N3-C2-O2	-7.67	116.53	121.90
37	A3	96	U	C5-C6-N1	-7.67	118.86	122.70
38	A4	35	C	C6-N1-C2	-7.67	117.23	120.30
36	A5	630	A	C2-N3-C4	-7.67	106.76	110.60
36	A5	519	A	N1-C6-N6	7.67	123.20	118.60
36	A5	2703	A	C8-N9-C4	-7.67	102.73	105.80
36	A5	2887	A	C5-C6-N1	-7.67	113.87	117.70
36	A1	1507	G	C6-N1-C2	-7.67	120.50	125.10
37	A7	39	C	C6-N1-C2	-7.67	117.23	120.30
36	A1	24	G	C8-N9-C4	7.66	109.47	106.40
36	A1	874	U	C4-C5-C6	-7.66	115.10	119.70
36	A1	1305	U	N3-C2-O2	-7.66	116.83	122.20
80	A6	46	A	C2-N3-C4	-7.66	106.77	110.60
36	A1	583	G	N1-C6-O6	-7.66	115.30	119.90
80	A6	1644	C	C5-C6-N1	-7.66	117.17	121.00
36	A1	1386	A	C6-N1-C2	-7.66	114.00	118.60
36	A1	1489	A	C2-N3-C4	-7.66	106.77	110.60
36	A5	594	U	C6-N1-C2	-7.66	116.40	121.00
1	A2	1305	U	C5-C4-O4	7.66	130.49	125.90
36	A1	643	U	N3-C2-O2	7.66	127.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2643	A	C2-N3-C4	7.66	114.43	110.60
36	A1	970	A	C8-N9-C4	-7.65	102.74	105.80
36	A1	1124	U	N3-C4-C5	7.65	119.19	114.60
36	A5	3245	A	C5-C6-N1	-7.65	113.87	117.70
37	A7	11	A	C8-N9-C4	7.65	108.86	105.80
36	A5	2634	U	C6-N1-C2	7.65	125.59	121.00
36	A5	3330	A	C5-C6-N1	7.65	121.52	117.70
1	A2	553	G	C4-C5-C6	7.65	123.39	118.80
36	A5	1124	U	N1-C2-N3	-7.65	110.31	114.90
36	A5	1381	A	C8-N9-C4	7.65	108.86	105.80
36	A1	1130	A	C8-N9-C4	-7.64	102.74	105.80
36	A1	832	G	N1-C6-O6	-7.64	115.31	119.90
36	A1	2776	C	N3-C4-C5	7.64	124.96	121.90
36	A1	39	A	C5-N7-C8	7.64	107.72	103.90
36	A1	3382	U	N3-C2-O2	-7.64	116.85	122.20
36	A1	810	A	N1-C6-N6	-7.64	114.02	118.60
36	A1	2541	U	C2-N1-C1'	7.64	126.86	117.70
36	A5	2237	C	N3-C4-N4	-7.64	112.65	118.00
36	A5	1402	C	C5-C6-N1	-7.63	117.18	121.00
36	A5	2611	U	C5-C6-N1	-7.63	118.88	122.70
36	A1	3318	G	N3-C4-C5	-7.63	124.78	128.60
36	A1	1335	C	N3-C4-C5	7.63	124.95	121.90
80	A6	1305	U	N1-C2-O2	-7.63	117.46	122.80
36	A5	2234	G	C8-N9-C4	7.63	109.45	106.40
36	A1	30	G	C8-N9-C4	-7.63	103.35	106.40
36	A1	1420	C	N3-C2-O2	-7.63	116.56	121.90
36	A1	2389	C	C2-N3-C4	-7.62	116.09	119.90
36	A1	678	G	N3-C2-N2	-7.62	114.56	119.90
36	A1	1110	U	N3-C4-C5	7.62	119.17	114.60
36	A1	2343	C	C2-N3-C4	-7.62	116.09	119.90
12	CK	97	PRO	N-CA-CB	7.62	112.45	103.30
36	A5	665	A	N1-C6-N6	7.62	123.17	118.60
36	A1	963	G	N9-C4-C5	-7.62	102.35	105.40
36	A1	1543	G	C2-N3-C4	7.62	115.71	111.90
1	A2	704	C	C2-N1-C1'	7.62	127.18	118.80
36	A1	417	A	N1-C6-N6	7.62	123.17	118.60
36	A5	3055	U	N3-C2-O2	-7.62	116.87	122.20
80	A6	1280	C	N1-C2-O2	-7.62	114.33	118.90
36	A1	2415	C	C6-N1-C2	7.61	123.34	120.30
36	A5	121	A	C8-N9-C4	7.61	108.85	105.80
36	A1	847	A	C5-C6-N6	-7.61	117.61	123.70
36	A5	877	C	C4-C5-C6	-7.61	113.59	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2433	U	C6-N1-C2	7.61	125.57	121.00
38	A8	144	G	N1-C6-O6	7.61	124.47	119.90
36	A1	2281	A	N9-C4-C5	-7.61	102.76	105.80
36	A5	1890	U	C4-C5-C6	7.61	124.27	119.70
36	A1	3159	C	N3-C2-O2	-7.61	116.58	121.90
36	A5	1163	A	N1-C6-N6	-7.61	114.04	118.60
36	A1	545	U	N1-C2-O2	7.61	128.12	122.80
36	A1	890	C	N3-C4-C5	7.60	124.94	121.90
36	A1	1313	G	C5-C6-O6	-7.60	124.04	128.60
80	A6	418	G	C4-N9-C1'	7.60	136.38	126.50
36	A5	1370	G	C5-C6-N1	7.60	115.30	111.50
36	A5	3088	G	C4-C5-N7	7.60	113.84	110.80
36	A1	2857	C	C5-C4-N4	-7.60	114.88	120.20
80	A6	1310	U	N3-C2-O2	-7.60	116.88	122.20
37	A7	67	G	N3-C2-N2	-7.60	114.58	119.90
36	A1	54	C	C5-C4-N4	7.59	125.52	120.20
80	A6	359	A	N1-C2-N3	-7.59	125.50	129.30
36	A5	1342	C	C2-N3-C4	-7.59	116.10	119.90
36	A1	1392	G	C2-N3-C4	7.59	115.69	111.90
80	A6	1572	G	C4-C5-N7	7.59	113.84	110.80
36	A1	1478	C	C5-C6-N1	-7.59	117.20	121.00
36	A5	2698	G	C8-N9-C4	7.59	109.44	106.40
38	A8	6	U	C2-N3-C4	-7.59	122.45	127.00
36	A1	1115	G	N1-C2-N2	-7.59	109.37	116.20
36	A5	419	G	C5-C6-O6	-7.59	124.05	128.60
36	A5	2289	U	N1-C2-O2	7.59	128.11	122.80
36	A5	2372	A	N9-C4-C5	7.59	108.83	105.80
36	A5	3006	A	C5-C6-N1	-7.59	113.91	117.70
36	A5	2138	A	C8-N9-C4	-7.59	102.77	105.80
36	A5	2693	C	N3-C4-C5	7.59	124.94	121.90
36	A1	218	G	N3-C4-C5	-7.58	124.81	128.60
36	A1	2278	C	C6-N1-C1'	7.58	129.90	120.80
80	A6	565	C	N1-C2-O2	7.58	123.45	118.90
36	A1	61	A	C8-N9-C4	7.58	108.83	105.80
36	A5	1014	U	C2-N1-C1'	7.58	126.79	117.70
36	A5	1390	A	N1-C6-N6	-7.58	114.05	118.60
36	A1	835	G	C8-N9-C4	7.58	109.43	106.40
36	A1	339	C	N3-C4-N4	-7.58	112.70	118.00
36	A1	2187	G	C4-C5-N7	7.57	113.83	110.80
36	A5	2271	A	C8-N9-C4	7.57	108.83	105.80
36	A1	83	U	C5-C4-O4	-7.57	121.36	125.90
36	A1	1467	A	N9-C4-C5	7.57	108.83	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2179	C	C5-C4-N4	-7.57	114.90	120.20
36	A1	2897	A	C8-N9-C4	7.57	108.83	105.80
36	A5	1305	U	C5-C4-O4	-7.57	121.36	125.90
80	A6	1016	C	N3-C4-C5	7.57	124.93	121.90
36	A1	2948	C	N3-C4-C5	7.56	124.92	121.90
36	A5	929	A	C8-N9-C4	7.56	108.83	105.80
36	A5	1163	A	C5-N7-C8	7.56	107.68	103.90
36	A5	3154	C	N1-C2-O2	7.56	123.44	118.90
36	A5	3172	A	N7-C8-N9	-7.56	110.02	113.80
36	A1	1055	A	C8-N9-C4	7.56	108.82	105.80
36	A1	106	A	N9-C4-C5	-7.56	102.78	105.80
80	A6	308	C	N3-C4-N4	-7.56	112.71	118.00
36	A5	81	C	N3-C4-C5	7.56	124.92	121.90
36	A5	2849	C	N3-C4-C5	-7.56	118.88	121.90
37	A7	49	G	C5-C6-O6	-7.56	124.06	128.60
36	A1	15	C	C6-N1-C2	-7.56	117.28	120.30
36	A1	54	C	C2-N1-C1'	-7.56	110.49	118.80
36	A5	1396	C	N3-C4-C5	7.55	124.92	121.90
36	A1	2409	G	C8-N9-C4	-7.55	103.38	106.40
36	A5	641	C	N3-C4-N4	-7.55	112.71	118.00
36	A1	2246	G	N9-C4-C5	7.55	108.42	105.40
36	A5	289	A	C6-N1-C2	-7.55	114.07	118.60
36	A5	1848	G	C4-C5-N7	7.55	113.82	110.80
36	A1	2777	G	C8-N9-C1'	-7.55	117.19	127.00
36	A5	633	C	N1-C2-O2	-7.55	114.37	118.90
36	A5	3096	C	C5-C6-N1	-7.55	117.23	121.00
1	A2	1291	G	C2-N3-C4	-7.54	108.13	111.90
36	A1	2846	U	C6-N1-C2	-7.54	116.47	121.00
36	A5	1130	A	C5-C6-N1	7.54	121.47	117.70
36	A5	3378	C	N3-C4-C5	7.54	124.92	121.90
36	A5	324	A	C8-N9-C4	-7.54	102.78	105.80
36	A5	1176	C	C2-N3-C4	-7.54	116.13	119.90
36	A5	2838	A	N1-C6-N6	7.54	123.13	118.60
36	A1	2714	G	C4-C5-N7	7.54	113.82	110.80
36	A5	851	C	C5-C6-N1	7.54	124.77	121.00
36	A5	2234	G	C4-C5-N7	7.54	113.82	110.80
36	A1	1403	C	C5-C4-N4	-7.54	114.92	120.20
36	A5	928	C	C4-C5-C6	7.54	121.17	117.40
36	A1	88	A	C8-N9-C4	7.54	108.82	105.80
80	A6	308	C	C6-N1-C1'	7.54	129.85	120.80
1	A2	647	G	N9-C4-C5	7.54	108.42	105.40
36	A1	3218	A	C8-N9-C4	-7.54	102.78	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	163	G	C5-C6-O6	-7.54	124.08	128.60
36	A5	400	G	C5-C6-O6	-7.54	124.08	128.60
59	DV	45	ARG	NE-CZ-NH1	-7.54	116.53	120.30
36	A1	270	U	N3-C2-O2	-7.54	116.93	122.20
36	A1	1476	G	C5-C6-O6	7.54	133.12	128.60
36	A5	1216	C	N1-C2-O2	-7.54	114.38	118.90
36	A1	582	G	N9-C4-C5	7.53	108.41	105.40
36	A5	42	C	C4-C5-C6	-7.53	113.63	117.40
38	A8	144	G	N3-C2-N2	-7.53	114.63	119.90
36	A5	2625	C	C2-N3-C4	-7.53	116.13	119.90
80	A6	65	A	N3-C4-C5	7.53	132.07	126.80
36	A5	1910	A	C8-N9-C4	7.53	108.81	105.80
1	A2	1280	C	C6-N1-C2	-7.53	117.29	120.30
36	A5	2381	G	N9-C4-C5	7.53	108.41	105.40
80	A6	555	A	C8-N9-C4	-7.53	102.79	105.80
38	A8	2	A	N9-C4-C5	7.53	108.81	105.80
36	A1	1467	A	N1-C6-N6	-7.53	114.08	118.60
36	A1	1494	U	C6-N1-C2	7.53	125.52	121.00
1	A2	1758	U	N3-C2-O2	-7.52	116.94	122.20
36	A1	1157	G	N1-C6-O6	-7.52	115.39	119.90
1	A2	323	A	C8-N9-C4	-7.52	102.79	105.80
1	A2	871	G	N3-C4-C5	-7.52	124.84	128.60
36	A1	2142	A	C5-C6-N1	7.52	121.46	117.70
36	A1	2932	U	C5-C4-O4	7.52	130.41	125.90
36	A5	1515	A	C2-N3-C4	-7.52	106.84	110.60
36	A5	2342	U	N3-C4-O4	-7.52	114.14	119.40
36	A5	2524	A	N7-C8-N9	7.52	117.56	113.80
36	A1	1308	A	C5-N7-C8	-7.52	100.14	103.90
36	A1	2826	U	C5-C4-O4	-7.52	121.39	125.90
80	A6	1280	C	N3-C4-N4	7.52	123.26	118.00
36	A1	1142	G	C2-N3-C4	7.52	115.66	111.90
80	A6	542	A	C6-C5-N7	-7.52	127.04	132.30
36	A5	1057	A	C5-C6-N6	-7.51	117.69	123.70
36	A1	2152	A	N1-C6-N6	-7.51	114.09	118.60
36	A1	662	U	N3-C4-O4	-7.51	114.14	119.40
36	A1	2756	C	N1-C2-O2	-7.51	114.39	118.90
36	A1	3058	U	C2-N1-C1'	7.51	126.71	117.70
80	A6	768	C	C6-N1-C2	7.51	123.30	120.30
36	A5	3140	G	C4-C5-N7	7.51	113.80	110.80
1	A2	758	U	N3-C2-O2	-7.51	116.94	122.20
36	A1	2856	G	C8-N9-C4	7.51	109.40	106.40
36	A1	2369	G	C2-N3-C4	7.51	115.65	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2948	C	N3-C4-N4	-7.51	112.75	118.00
36	A1	880	G	C5-C6-N1	7.50	115.25	111.50
38	A8	12	A	C5-N7-C8	-7.50	100.15	103.90
1	A2	978	A	C8-N9-C4	7.50	108.80	105.80
36	A5	2791	G	C5-C6-O6	-7.50	124.10	128.60
36	A5	426	G	C8-N9-C4	7.50	109.40	106.40
36	A5	971	G	C2-N3-C4	7.50	115.65	111.90
36	A5	2726	C	N3-C4-N4	-7.50	112.75	118.00
36	A1	228	U	N3-C2-O2	-7.50	116.95	122.20
38	A4	20	U	C5-C4-O4	7.50	130.40	125.90
80	A6	603	U	N1-C2-N3	7.50	119.40	114.90
36	A5	622	A	N1-C6-N6	7.50	123.10	118.60
36	A5	971	G	N7-C8-N9	-7.50	109.35	113.10
36	A5	2718	U	N1-C2-N3	7.50	119.40	114.90
36	A1	1052	U	N3-C4-C5	7.50	119.10	114.60
36	A5	971	G	C5-N7-C8	7.50	108.05	104.30
36	A5	1516	C	N1-C2-O2	-7.50	114.40	118.90
36	A1	88	A	N9-C4-C5	-7.50	102.80	105.80
80	A6	1478	G	C4-N9-C1'	7.50	136.24	126.50
36	A5	1389	G	N3-C2-N2	7.49	125.14	119.90
36	A5	1887	A	N1-C6-N6	7.49	123.09	118.60
36	A5	2630	C	C2-N3-C4	-7.49	116.16	119.90
1	A2	594	A	C2-N3-C4	7.49	114.34	110.60
38	A8	14	C	C4-C5-C6	7.49	121.14	117.40
36	A1	678	G	N1-C2-N2	7.49	122.94	116.20
36	A1	2653	C	C5-C4-N4	7.49	125.44	120.20
80	A6	144	U	C6-N1-C2	-7.49	116.51	121.00
36	A5	924	G	N1-C2-N2	7.49	122.94	116.20
36	A5	1407	A	C6-N1-C2	7.49	123.09	118.60
36	A5	3138	U	C2-N3-C4	-7.49	122.51	127.00
36	A5	3308	C	N1-C2-O2	-7.49	114.41	118.90
1	A2	1291	G	C5-N7-C8	-7.48	100.56	104.30
36	A1	1370	G	C5-C6-O6	7.48	133.09	128.60
36	A5	1459	C	N3-C4-C5	7.48	124.89	121.90
36	A5	3007	U	C2-N3-C4	-7.48	122.51	127.00
80	A6	308	C	N1-C2-N3	7.48	124.44	119.20
36	A5	150	A	N1-C6-N6	7.48	123.09	118.60
1	A2	507	U	C2-N1-C1'	7.48	126.67	117.70
36	A1	730	C	C2-N3-C4	-7.48	116.16	119.90
36	A1	2093	A	C2-N3-C4	7.48	114.34	110.60
36	A1	1592	G	N3-C4-N9	7.48	130.49	126.00
36	A1	1848	G	N1-C6-O6	7.47	124.38	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	307	A	N1-C6-N6	-7.47	114.12	118.60
36	A1	1503	A	C2-N3-C4	-7.47	106.86	110.60
80	A6	308	C	C4-C5-C6	7.47	121.14	117.40
36	A1	686	G	C4-C5-N7	-7.47	107.81	110.80
36	A1	2276	G	C2-N3-C4	7.47	115.63	111.90
36	A1	3279	A	C8-N9-C4	-7.47	102.81	105.80
36	A1	3312	U	C2-N3-C4	-7.47	122.52	127.00
36	A5	2366	C	C5-C4-N4	-7.47	114.97	120.20
36	A5	74	G	N1-C6-O6	-7.47	115.42	119.90
36	A5	2341	A	N7-C8-N9	-7.47	110.07	113.80
36	A1	426	G	C8-N9-C4	7.46	109.39	106.40
36	A1	2969	A	C8-N9-C4	-7.46	102.81	105.80
36	A5	1879	A	N7-C8-N9	7.46	117.53	113.80
36	A5	3025	C	N3-C4-N4	-7.46	112.78	118.00
36	A1	2323	G	C5-C6-O6	7.46	133.08	128.60
1	A2	1761	U	C6-N1-C2	-7.46	116.52	121.00
36	A1	93	C	C6-N1-C2	-7.46	117.31	120.30
36	A1	1279	C	C5-C6-N1	7.46	124.73	121.00
80	A6	453	U	N1-C2-O2	7.46	128.02	122.80
36	A1	2376	G	N7-C8-N9	7.46	116.83	113.10
36	A5	931	C	N3-C4-C5	7.46	124.88	121.90
36	A5	1205	A	C8-N9-C4	-7.46	102.82	105.80
36	A5	3192	U	C5-C6-N1	-7.46	118.97	122.70
37	A7	41	G	C8-N9-C4	7.46	109.38	106.40
36	A1	3209	A	N9-C4-C5	-7.46	102.82	105.80
36	A1	686	G	N9-C4-C5	7.45	108.38	105.40
36	A1	1351	U	N3-C2-O2	-7.45	116.98	122.20
80	A6	901	G	C4-C5-N7	7.45	113.78	110.80
36	A5	3167	A	C8-N9-C4	-7.45	102.82	105.80
38	A8	2	A	N1-C6-N6	-7.45	114.13	118.60
36	A1	963	G	C8-N9-C4	7.45	109.38	106.40
36	A1	80	G	N1-C2-N3	7.45	128.37	123.90
80	A6	610	G	C8-N9-C1'	-7.45	117.32	127.00
36	A5	1586	G	N3-C4-N9	7.45	130.47	126.00
36	A5	2621	G	N3-C2-N2	-7.45	114.69	119.90
1	A2	608	U	C2-N3-C4	-7.45	122.53	127.00
36	A1	2647	A	N9-C4-C5	7.45	108.78	105.80
36	A5	1124	U	C5-C6-N1	7.45	126.42	122.70
36	A5	1317	A	C2-N3-C4	7.45	114.32	110.60
36	A5	3381	U	N3-C4-O4	-7.45	114.19	119.40
80	A6	359	A	C6-N1-C2	7.44	123.07	118.60
36	A5	645	A	C5-C6-N6	-7.44	117.75	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2395	G	N7-C8-N9	-7.44	109.38	113.10
1	A2	1432	U	C5-C6-N1	-7.44	118.98	122.70
36	A1	1351	U	N1-C2-O2	7.44	128.01	122.80
36	A1	1145	G	N7-C8-N9	-7.44	109.38	113.10
36	A5	2743	A	C8-N9-C4	7.44	108.78	105.80
36	A5	1014	U	C5-C4-O4	-7.44	121.44	125.90
36	A5	436	A	N1-C6-N6	7.44	123.06	118.60
36	A5	2311	G	C8-N9-C4	7.44	109.37	106.40
1	A2	1075	C	N1-C2-O2	-7.43	114.44	118.90
36	A1	46	U	N3-C4-O4	-7.43	114.20	119.40
36	A1	1396	C	N3-C4-C5	7.43	124.87	121.90
36	A5	2179	C	C6-N1-C2	7.43	123.27	120.30
36	A5	3081	C	N3-C4-C5	7.43	124.87	121.90
36	A1	576	C	C2-N3-C4	-7.43	116.18	119.90
36	A1	646	A	N1-C2-N3	7.43	133.02	129.30
36	A5	1144	U	N1-C2-N3	7.43	119.36	114.90
36	A5	1372	C	N1-C2-O2	-7.43	114.44	118.90
36	A1	1130	A	C2-N3-C4	7.43	114.31	110.60
36	A5	2908	G	C8-N9-C4	-7.43	103.43	106.40
36	A5	2991	A	N1-C6-N6	-7.43	114.14	118.60
36	A1	2600	C	N1-C2-O2	7.42	123.35	118.90
36	A5	1506	A	C8-N9-C4	-7.42	102.83	105.80
36	A1	857	G	N3-C2-N2	7.42	125.09	119.90
36	A1	1145	G	C8-N9-C4	7.42	109.37	106.40
36	A5	2245	C	C5-C6-N1	7.42	124.71	121.00
1	A2	1012	U	C2-N3-C4	7.42	131.45	127.00
80	A6	1423	U	C5-C6-N1	-7.42	118.99	122.70
36	A5	2996	U	N1-C2-O2	7.42	127.99	122.80
80	A6	392	G	N1-C6-O6	-7.42	115.45	119.90
36	A5	1327	C	N3-C4-C5	7.42	124.87	121.90
36	A5	1340	G	C8-N9-C4	7.42	109.37	106.40
36	A5	2308	C	N3-C2-O2	7.41	127.09	121.90
18	AQ	40	GLU	C-N-CD	-7.41	104.29	120.60
36	A1	2985	C	N1-C2-O2	-7.41	114.45	118.90
36	A5	2350	C	C4-C5-C6	7.41	121.11	117.40
1	A2	831	U	C5-C6-N1	7.41	126.41	122.70
36	A1	1100	U	C2-N3-C4	-7.41	122.55	127.00
36	A1	2631	U	C2-N3-C4	-7.41	122.55	127.00
36	A1	1476	G	N1-C6-O6	-7.41	115.45	119.90
80	A6	60	U	N1-C2-O2	7.41	127.99	122.80
80	A6	807	A	C8-N9-C4	-7.41	102.84	105.80
36	A5	2572	C	N3-C2-O2	-7.41	116.71	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	3207	U	N1-C2-N3	7.41	119.34	114.90
36	A5	1085	A	C2-N3-C4	-7.41	106.90	110.60
36	A5	1484	U	C2-N3-C4	-7.41	122.56	127.00
36	A5	3151	U	N1-C2-N3	-7.41	110.46	114.90
37	A7	96	U	N3-C2-O2	-7.41	117.02	122.20
1	A2	1762	A	N1-C6-N6	7.40	123.04	118.60
36	A5	2851	A	N1-C2-N3	7.40	133.00	129.30
36	A1	988	U	C5-C6-N1	-7.40	119.00	122.70
36	A1	2139	A	C5-N7-C8	7.40	107.60	103.90
36	A5	2943	G	N3-C2-N2	7.40	125.08	119.90
36	A1	942	U	N3-C4-C5	7.40	119.04	114.60
36	A1	1180	A	C2-N3-C4	-7.40	106.90	110.60
80	A6	609	U	C2-N3-C4	-7.40	122.56	127.00
80	A6	1644	C	N3-C4-C5	7.40	124.86	121.90
36	A5	280	U	C5-C6-N1	-7.40	119.00	122.70
36	A5	2717	U	C5-C6-N1	-7.40	119.00	122.70
38	A8	144	G	C5-C6-O6	-7.40	124.16	128.60
80	A6	1643	U	C5-C6-N1	-7.40	119.00	122.70
36	A1	3208	G	N9-C4-C5	7.40	108.36	105.40
36	A5	1117	G	C5-C6-N1	7.40	115.20	111.50
36	A5	3102	G	N1-C2-N2	-7.40	109.54	116.20
38	A8	2	A	C5-C6-N6	7.40	129.62	123.70
36	A1	1165	A	C8-N9-C4	7.39	108.76	105.80
36	A5	1192	C	C4-C5-C6	7.39	121.10	117.40
38	A8	99	C	C6-N1-C2	7.39	123.26	120.30
36	A1	1911	A	C6-C5-N7	-7.39	127.12	132.30
80	A6	622	A	N9-C4-C5	7.39	108.76	105.80
36	A5	1604	G	N3-C4-N9	7.39	130.44	126.00
36	A5	2370	G	C6-N1-C2	-7.39	120.67	125.10
36	A1	909	G	N7-C8-N9	-7.39	109.41	113.10
36	A1	994	G	N1-C6-O6	-7.39	115.47	119.90
36	A1	3373	U	C5-C6-N1	-7.39	119.00	122.70
80	A6	1304	G	C5-C6-O6	-7.39	124.17	128.60
36	A5	2245	C	N3-C2-O2	-7.39	116.73	121.90
80	A6	815	G	C4-C5-N7	7.39	113.75	110.80
36	A1	374	A	N1-C6-N6	-7.39	114.17	118.60
36	A1	124	U	N3-C2-O2	-7.38	117.03	122.20
36	A1	966	U	N1-C2-O2	7.38	127.97	122.80
36	A1	1118	C	C4-C5-C6	7.38	121.09	117.40
36	A5	2142	A	C2-N3-C4	7.38	114.29	110.60
36	A5	2639	G	C5-C6-O6	-7.38	124.17	128.60
1	A2	355	G	C5-C6-N1	7.38	115.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	583	C	C6-N1-C2	-7.38	117.35	120.30
36	A1	333	G	C5-C6-O6	7.38	133.03	128.60
36	A1	1082	U	C2-N1-C1'	7.38	126.55	117.70
36	A5	1437	C	C5-C6-N1	7.38	124.69	121.00
38	A4	39	G	N1-C2-N2	-7.38	109.56	116.20
36	A5	957	C	C2-N3-C4	-7.38	116.21	119.90
36	A1	1464	G	C8-N9-C4	7.38	109.35	106.40
1	A2	1389	C	N1-C2-O2	7.37	123.32	118.90
36	A1	1634	G	C8-N9-C4	-7.37	103.45	106.40
36	A1	2756	C	C5-C4-N4	-7.37	115.04	120.20
36	A1	2867	C	N3-C4-C5	7.37	124.85	121.90
80	A6	1269	U	N3-C2-O2	-7.37	117.04	122.20
80	A6	1503	A	N7-C8-N9	7.37	117.49	113.80
36	A5	2531	C	N1-C2-O2	7.37	123.32	118.90
36	A5	2621	G	C5-C6-N1	-7.37	107.81	111.50
36	A1	98	G	C8-N9-C4	7.37	109.35	106.40
36	A1	666	A	N7-C8-N9	-7.37	110.11	113.80
36	A1	768	C	C6-N1-C2	-7.37	117.35	120.30
36	A1	1359	C	C5-C4-N4	-7.37	115.04	120.20
36	A1	2891	U	C5-C4-O4	-7.37	121.48	125.90
36	A5	65	A	C8-N9-C4	-7.37	102.85	105.80
36	A1	210	U	N3-C2-O2	-7.37	117.04	122.20
36	A5	2541	U	C2-N1-C1'	7.37	126.54	117.70
36	A5	2810	C	N3-C2-O2	-7.37	116.74	121.90
56	DS	40	ARG	NE-CZ-NH1	7.37	123.98	120.30
36	A1	3047	U	C2-N3-C4	-7.37	122.58	127.00
37	A3	53	U	N1-C2-O2	-7.37	117.64	122.80
36	A5	3369	G	C5-C6-O6	-7.37	124.18	128.60
36	A1	327	A	C8-N9-C4	7.37	108.75	105.80
36	A1	952	A	N1-C6-N6	7.37	123.02	118.60
36	A1	2242	A	C2-N3-C4	-7.37	106.92	110.60
36	A1	2958	A	N1-C6-N6	-7.37	114.18	118.60
38	A4	38	U	N3-C2-O2	-7.37	117.04	122.20
36	A5	1855	U	C2-N3-C4	-7.37	122.58	127.00
36	A1	2772	C	C3'-C2'-C1'	-7.36	95.61	101.50
36	A5	795	G	N7-C8-N9	-7.36	109.42	113.10
36	A5	2307	G	N3-C4-N9	7.36	130.42	126.00
36	A5	2385	G	C4-N9-C1'	-7.36	116.93	126.50
36	A1	644	G	C2-N3-C4	-7.36	108.22	111.90
36	A1	776	U	C5-C4-O4	7.36	130.32	125.90
36	A1	816	A	N1-C2-N3	-7.36	125.62	129.30
36	A5	98	G	C5-C6-N1	7.36	115.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2743	A	N7-C8-N9	-7.36	110.12	113.80
36	A1	1422	G	N1-C6-O6	-7.36	115.48	119.90
36	A1	3190	C	N3-C4-C5	7.36	124.84	121.90
36	A1	416	A	N1-C6-N6	-7.36	114.19	118.60
36	A1	643	U	C4-C5-C6	-7.36	115.29	119.70
36	A1	1492	G	C5-C6-O6	7.36	133.01	128.60
80	A6	815	G	N1-C6-O6	7.36	124.31	119.90
36	A1	650	C	C5-C6-N1	-7.35	117.32	121.00
1	A2	1241	G	N7-C8-N9	7.35	116.78	113.10
36	A1	1510	G	N3-C4-N9	7.35	130.41	126.00
36	A1	3217	C	C6-N1-C1'	-7.35	111.98	120.80
36	A5	2802	A	C2-N3-C4	7.35	114.28	110.60
1	A2	142	G	N3-C4-C5	7.35	132.28	128.60
36	A1	689	U	N1-C2-O2	7.35	127.95	122.80
36	A1	1081	U	C5-C6-N1	7.35	126.38	122.70
36	A1	1480	G	N7-C8-N9	-7.35	109.42	113.10
36	A5	2954	U	C6-N1-C1'	-7.35	110.91	121.20
36	A1	899	U	N3-C4-O4	-7.35	114.26	119.40
36	A1	2395	G	C5-C6-N1	7.35	115.17	111.50
36	A1	1378	U	C2-N3-C4	-7.35	122.59	127.00
36	A1	2123	G	N7-C8-N9	-7.35	109.43	113.10
36	A1	1137	C	C5-C4-N4	-7.34	115.06	120.20
36	A1	3294	A	C8-N9-C4	-7.34	102.86	105.80
38	A4	125	U	C2-N1-C1'	7.34	126.51	117.70
36	A5	3290	G	C8-N9-C4	-7.34	103.46	106.40
36	A1	517	G	N3-C4-C5	-7.34	124.93	128.60
36	A1	821	U	C5-C6-N1	-7.34	119.03	122.70
36	A1	1041	U	C5-C6-N1	-7.34	119.03	122.70
36	A1	716	A	N9-C4-C5	-7.34	102.86	105.80
36	A1	1665	C	N3-C4-C5	7.34	124.84	121.90
36	A1	1848	G	C6-C5-N7	-7.34	126.00	130.40
36	A1	2124	G	N1-C6-O6	7.34	124.30	119.90
36	A5	2288	G	N3-C4-N9	7.34	130.41	126.00
1	A2	377	G	N3-C2-N2	-7.34	114.76	119.90
36	A5	3218	A	C4-C5-N7	7.34	114.37	110.70
57	DT	130	ARG	NE-CZ-NH2	-7.34	116.63	120.30
36	A1	652	G	N1-C2-N2	-7.34	109.60	116.20
36	A1	1496	C	C5-C6-N1	7.34	124.67	121.00
36	A1	510	G	C5-C6-O6	-7.34	124.20	128.60
36	A5	3289	G	C8-N9-C4	-7.34	103.47	106.40
36	A1	35	A	C5-N7-C8	-7.33	100.23	103.90
36	A1	874	U	N3-C4-C5	7.33	119.00	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	962	A	C6-N1-C2	-7.33	114.20	118.60
37	A7	41	G	N9-C4-C5	-7.33	102.47	105.40
36	A5	2234	G	N1-C6-O6	7.33	124.30	119.90
80	A6	240	U	C2-N1-C1'	7.33	126.50	117.70
36	A5	804	C	C4-C5-C6	7.33	121.06	117.40
36	A5	1449	A	C4-C5-N7	7.33	114.36	110.70
36	A1	689	U	N3-C2-O2	-7.33	117.07	122.20
36	A5	931	C	C5-C6-N1	-7.33	117.34	121.00
36	A5	2410	U	C4-C5-C6	-7.33	115.30	119.70
36	A5	2701	U	C5-C4-O4	-7.33	121.50	125.90
36	A1	649	A	C5-N7-C8	7.32	107.56	103.90
36	A1	1902	G	C4-C5-N7	7.32	113.73	110.80
36	A1	2963	C	C4-C5-C6	7.32	121.06	117.40
1	A2	89	G	C8-N9-C4	7.32	109.33	106.40
36	A5	2884	C	C2-N3-C4	-7.32	116.24	119.90
36	A1	959	C	N1-C2-O2	-7.32	114.51	118.90
36	A1	2247	G	C5-C6-O6	-7.32	124.21	128.60
38	A4	32	C	N3-C2-O2	7.32	127.02	121.90
38	A4	85	G	N7-C8-N9	7.32	116.76	113.10
80	A6	421	A	N1-C6-N6	7.32	122.99	118.60
36	A5	2320	A	C5-C6-N1	-7.32	114.04	117.70
36	A5	2736	A	N1-C6-N6	-7.32	114.21	118.60
36	A1	957	C	C5-C6-N1	-7.32	117.34	121.00
36	A1	3382	U	N1-C2-O2	7.32	127.92	122.80
80	A6	800	U	C6-N1-C2	-7.32	116.61	121.00
36	A5	834	U	C6-N1-C2	7.31	125.39	121.00
36	A5	924	G	N1-C6-O6	7.31	124.29	119.90
36	A1	1717	U	C6-N1-C2	-7.31	116.61	121.00
36	A1	83	U	N3-C4-C5	7.31	118.98	114.60
36	A1	1201	C	C6-N1-C2	-7.31	117.38	120.30
80	A6	794	U	C2-N1-C1'	7.31	126.47	117.70
36	A5	578	A	N1-C6-N6	7.31	122.99	118.60
36	A5	971	G	C4-C5-N7	-7.31	107.88	110.80
36	A5	1921	A	N1-C6-N6	7.31	122.98	118.60
36	A1	2163	C	N3-C4-N4	-7.31	112.89	118.00
80	A6	542	A	N7-C8-N9	7.31	117.45	113.80
80	A6	1542	G	N9-C4-C5	7.31	108.32	105.40
36	A1	2130	G	C4-C5-N7	-7.31	107.88	110.80
36	A1	2632	G	N1-C6-O6	-7.30	115.52	119.90
36	A1	2967	A	C8-N9-C4	7.30	108.72	105.80
36	A5	1133	A	C5-C6-N1	7.30	121.35	117.70
36	A1	2977	G	C8-N9-C4	7.30	109.32	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A4	28	C	C5-C6-N1	-7.30	117.35	121.00
80	A6	56	U	C5-C6-N1	-7.30	119.05	122.70
36	A5	3382	U	N1-C2-O2	7.30	127.91	122.80
69	Df	18	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A2	1096	C	C6-N1-C1'	-7.30	112.04	120.80
36	A5	1014	U	C6-N1-C1'	-7.30	110.98	121.20
36	A5	1506	A	N7-C8-N9	7.30	117.45	113.80
36	A5	2892	A	C5-C6-N6	7.30	129.54	123.70
37	A7	104	A	N1-C6-N6	7.30	122.98	118.60
36	A1	2798	C	C4-C5-C6	7.29	121.05	117.40
36	A5	2620	G	C5-C6-N1	7.29	115.15	111.50
36	A1	954	U	C6-N1-C2	-7.29	116.62	121.00
80	A6	160	C	N1-C2-O2	7.29	123.28	118.90
80	A6	1796	C	C5-C6-N1	-7.29	117.35	121.00
36	A5	800	G	C8-N9-C4	7.29	109.32	106.40
36	A1	2857	C	N3-C4-C5	7.29	124.82	121.90
36	A5	3122	A	N7-C8-N9	7.29	117.44	113.80
36	A5	2611	U	N3-C2-O2	-7.29	117.10	122.20
36	A1	944	C	N3-C4-C5	-7.29	118.99	121.90
36	A5	3131	U	N3-C4-C5	7.29	118.97	114.60
80	A6	1560	U	N3-C4-O4	-7.28	114.30	119.40
36	A1	821	U	C5-C4-O4	7.28	130.27	125.90
36	A1	2357	A	N1-C6-N6	7.28	122.97	118.60
36	A5	2758	A	C8-N9-C4	-7.28	102.89	105.80
36	A1	1656	A	C8-N9-C4	7.28	108.71	105.80
68	Be	45	ARG	NE-CZ-NH1	7.28	123.94	120.30
36	A5	1189	C	N1-C2-O2	-7.28	114.53	118.90
36	A5	2836	C	N3-C4-N4	-7.28	112.90	118.00
36	A1	3046	A	N7-C8-N9	7.28	117.44	113.80
37	A3	83	U	C2-N3-C4	-7.28	122.63	127.00
36	A5	669	U	N1-C2-N3	7.28	119.27	114.90
36	A5	2942	C	C4-C5-C6	7.28	121.04	117.40
36	A1	28	C	C6-N1-C2	7.28	123.21	120.30
36	A1	2376	G	C6-N1-C2	-7.28	120.73	125.10
36	A5	1426	C	N3-C4-C5	7.28	124.81	121.90
36	A1	960	U	C2-N1-C1'	-7.27	108.97	117.70
36	A1	3362	A	C4-C5-C6	7.27	120.64	117.00
36	A1	1858	A	C5-C6-N1	7.27	121.34	117.70
36	A1	2615	G	C5-C6-O6	-7.27	124.24	128.60
36	A5	1049	C	N3-C4-C5	7.27	124.81	121.90
80	A6	1781	A	C5-N7-C8	7.27	107.53	103.90
80	A6	410	A	N1-C6-N6	-7.27	114.24	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1781	A	C5-C6-N1	-7.27	114.07	117.70
36	A5	267	G	C8-N9-C4	7.27	109.31	106.40
36	A1	345	G	N3-C4-N9	7.26	130.36	126.00
80	A6	1542	G	C8-N9-C4	-7.26	103.49	106.40
36	A5	2815	G	C8-N9-C4	7.26	109.31	106.40
36	A1	2902	A	C8-N9-C4	7.26	108.70	105.80
36	A5	652	G	N3-C2-N2	7.26	124.98	119.90
36	A5	1430	U	C5-C6-N1	-7.26	119.07	122.70
36	A1	272	G	N7-C8-N9	-7.26	109.47	113.10
36	A1	885	U	N3-C4-O4	-7.26	114.32	119.40
80	A6	1600	A	N7-C8-N9	7.26	117.43	113.80
80	A6	800	U	N3-C4-C5	-7.26	110.24	114.60
36	A5	1364	C	C2-N3-C4	-7.26	116.27	119.90
80	A6	1304	G	N9-C4-C5	-7.26	102.50	105.40
36	A1	1902	G	C4-C5-C6	7.26	123.15	118.80
1	A2	728	U	C2-N1-C1'	7.25	126.41	117.70
36	A1	786	A	C2-N3-C4	7.25	114.23	110.60
36	A5	2848	G	N3-C2-N2	-7.25	114.82	119.90
36	A5	3255	U	C5-C4-O4	-7.25	121.55	125.90
36	A1	666	A	C8-N9-C4	7.25	108.70	105.80
36	A5	1538	G	C8-N9-C4	7.25	109.30	106.40
36	A5	1846	C	C4-C5-C6	7.25	121.03	117.40
36	A5	283	G	C6-C5-N7	-7.25	126.05	130.40
36	A5	580	C	C4-C5-C6	7.25	121.03	117.40
80	A6	1073	G	N1-C6-O6	-7.25	115.55	119.90
36	A5	2699	G	C2-N3-C4	7.25	115.52	111.90
36	A1	508	U	C5-C6-N1	-7.25	119.08	122.70
36	A5	514	G	C4-C5-N7	7.25	113.70	110.80
80	A6	1596	C	N1-C2-N3	7.24	124.27	119.20
36	A1	521	A	N1-C6-N6	7.24	122.94	118.60
36	A1	696	C	N3-C4-C5	7.24	124.80	121.90
36	A1	919	U	N3-C4-C5	7.24	118.94	114.60
36	A5	2372	A	P-O3'-C3'	7.24	128.39	119.70
80	A6	1145	U	N1-C2-O2	-7.24	117.73	122.80
36	A1	1122	U	C5-C6-N1	-7.24	119.08	122.70
47	BI	57	LEU	CA-CB-CG	7.24	131.94	115.30
10	CI	29	LEU	CA-CB-CG	7.24	131.94	115.30
36	A5	643	U	N3-C4-C5	7.24	118.94	114.60
36	A5	1144	U	C5-C6-N1	-7.24	119.08	122.70
36	A5	2758	A	N9-C4-C5	7.24	108.69	105.80
37	A7	11	A	N7-C8-N9	-7.24	110.18	113.80
36	A1	1741	A	C6-C5-N7	-7.23	127.24	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A4	21	C	N1-C2-O2	-7.23	114.56	118.90
36	A5	1660	C	C6-N1-C2	-7.23	117.41	120.30
36	A5	1887	A	C2-N3-C4	-7.23	106.98	110.60
36	A1	112	U	C6-N1-C1'	-7.23	111.08	121.20
36	A1	1327	C	C4-C5-C6	-7.23	113.78	117.40
36	A1	2857	C	C2-N3-C4	-7.23	116.28	119.90
80	A6	999	U	N3-C4-O4	-7.23	114.34	119.40
36	A5	1336	U	C5-C4-O4	-7.23	121.56	125.90
36	A5	2370	G	C5-C6-O6	-7.23	124.26	128.60
36	A5	1724	U	C6-N1-C2	-7.23	116.66	121.00
36	A1	3302	U	N3-C4-O4	-7.23	114.34	119.40
36	A1	3318	G	C6-C5-N7	-7.23	126.06	130.40
80	A6	815	G	C6-C5-N7	-7.23	126.06	130.40
36	A5	1833	G	N3-C2-N2	7.23	124.96	119.90
36	A1	2161	G	C8-N9-C4	-7.23	103.51	106.40
36	A5	1518	U	N3-C4-O4	-7.23	114.34	119.40
36	A1	1387	G	C4-C5-N7	-7.22	107.91	110.80
80	A6	1000	C	C6-N1-C2	-7.22	117.41	120.30
1	A2	1329	A	N1-C6-N6	7.22	122.93	118.60
1	A2	1611	A	C5-N7-C8	-7.22	100.29	103.90
80	A6	1091	A	N1-C6-N6	7.22	122.93	118.60
1	A2	1654	G	C5-C6-O6	-7.22	124.27	128.60
36	A1	695	C	C5-C6-N1	-7.22	117.39	121.00
36	A1	2169	G	C5-C6-O6	7.22	132.93	128.60
80	A6	1787	C	N1-C2-O2	-7.22	114.57	118.90
36	A5	2662	G	C8-N9-C4	-7.22	103.51	106.40
36	A1	1496	C	C2-N1-C1'	7.22	126.74	118.80
36	A5	2383	C	N1-C2-O2	-7.22	114.57	118.90
80	A6	18	C	C6-N1-C2	-7.22	117.41	120.30
36	A1	636	C	C5-C6-N1	-7.22	117.39	121.00
80	A6	1649	G	C5-C6-O6	7.22	132.93	128.60
36	A5	2754	G	N1-C2-N2	-7.22	109.70	116.20
1	A2	1745	G	C4-C5-N7	7.21	113.69	110.80
36	A5	810	A	N1-C6-N6	-7.21	114.27	118.60
36	A5	2964	G	C8-N9-C4	7.21	109.28	106.40
37	A7	49	G	N3-C2-N2	-7.21	114.85	119.90
36	A1	816	A	C2-N3-C4	7.21	114.20	110.60
36	A5	594	U	N3-C2-O2	-7.21	117.15	122.20
36	A5	643	U	C2-N3-C4	-7.21	122.67	127.00
36	A5	1407	A	C5-C6-N1	-7.21	114.09	117.70
1	A2	1000	C	N3-C4-N4	-7.21	112.95	118.00
36	A1	1372	C	C2-N3-C4	-7.21	116.30	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1116	G	C8-N9-C4	-7.21	103.52	106.40
36	A1	1376	C	C4-C5-C6	7.21	121.00	117.40
36	A1	1442	U	C5-C4-O4	-7.21	121.58	125.90
36	A1	1510	G	N1-C2-N2	-7.21	109.71	116.20
36	A5	46	U	N1-C2-O2	7.21	127.85	122.80
36	A5	2911	A	C2-N3-C4	7.21	114.20	110.60
80	A6	53	G	N1-C6-O6	-7.21	115.58	119.90
36	A5	2584	G	C6-C5-N7	-7.21	126.08	130.40
36	A5	639	G	N1-C6-O6	7.21	124.22	119.90
36	A1	1304	A	N9-C4-C5	7.20	108.68	105.80
36	A1	2179	C	C6-N1-C2	7.20	123.18	120.30
80	A6	1793	G	C4-C5-N7	-7.20	107.92	110.80
36	A5	39	A	C4-C5-C6	7.20	120.60	117.00
36	A5	2148	U	C2-N3-C4	-7.20	122.68	127.00
36	A5	3060	C	N3-C2-O2	7.20	126.94	121.90
38	A4	103	G	N3-C4-C5	-7.20	125.00	128.60
36	A1	1657	C	N3-C2-O2	7.20	126.94	121.90
36	A1	153	U	N3-C4-C5	-7.20	110.28	114.60
36	A1	2768	U	N1-C2-O2	7.20	127.84	122.80
80	A6	1634	C	C5-C6-N1	7.20	124.60	121.00
36	A5	1858	A	C2-N3-C4	7.20	114.20	110.60
36	A1	281	G	N9-C4-C5	7.20	108.28	105.40
1	A2	1642	G	C2-N3-C4	7.19	115.50	111.90
40	DB	266	ARG	NE-CZ-NH2	-7.19	116.70	120.30
36	A1	2318	U	N1-C2-N3	7.19	119.22	114.90
36	A1	2550	U	N3-C2-O2	-7.19	117.17	122.20
38	A4	16	G	N7-C8-N9	-7.19	109.50	113.10
80	A6	1190	C	C6-N1-C2	7.19	123.18	120.30
36	A5	37	U	C2-N3-C4	-7.19	122.68	127.00
36	A5	1172	G	N1-C6-O6	-7.19	115.58	119.90
36	A5	272	G	C8-N9-C4	7.19	109.28	106.40
36	A5	1169	A	C5-C6-N1	-7.19	114.11	117.70
36	A5	1434	G	C4-C5-C6	7.19	123.11	118.80
36	A1	340	C	C2-N3-C4	-7.19	116.31	119.90
36	A1	1017	C	C6-N1-C2	-7.19	117.42	120.30
80	A6	1031	U	C6-N1-C2	7.19	125.31	121.00
52	DO	16[B]	LEU	C-N-CA	7.19	137.40	122.30
1	A2	1174	C	N1-C2-O2	7.19	123.21	118.90
80	A6	321	C	N1-C2-O2	7.19	123.21	118.90
36	A5	2337	C	C6-N1-C2	7.19	123.17	120.30
36	A1	1411	C	N3-C4-N4	-7.18	112.97	118.00
36	A1	2339	C	N3-C2-O2	7.18	126.93	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	960	U	N1-C2-O2	7.18	127.83	122.80
36	A5	1406	A	C6-N1-C2	-7.18	114.29	118.60
36	A5	2824	G	N9-C4-C5	7.18	108.27	105.40
36	A1	279	U	N3-C2-O2	-7.18	117.17	122.20
80	A6	29	U	N3-C4-O4	-7.18	114.37	119.40
36	A5	1140	G	N3-C2-N2	7.18	124.93	119.90
36	A1	878	G	C2-N3-C4	-7.18	108.31	111.90
80	A6	542	A	C4-N9-C1'	7.18	139.22	126.30
36	A5	2244	A	N1-C6-N6	-7.18	114.29	118.60
36	A5	2870	C	N3-C4-N4	-7.18	112.97	118.00
36	A5	838	G	N1-C6-O6	-7.18	115.59	119.90
36	A5	2732	G	C5-C6-O6	7.18	132.91	128.60
36	A1	641	C	N3-C4-N4	-7.17	112.98	118.00
52	BO	158[B]	ASP	CA-C-N	-7.17	101.42	117.20
80	A6	1106	U	N1-C2-N3	7.17	119.20	114.90
36	A5	39	A	N1-C6-N6	7.17	122.90	118.60
36	A1	813	G	C5-C6-N1	7.17	115.09	111.50
36	A1	672	A	C5-C6-N6	-7.17	117.96	123.70
36	A1	2389	C	N3-C4-C5	7.17	124.77	121.90
38	A8	54	A	C2-N3-C4	-7.17	107.02	110.60
1	A2	1241	G	C4-C5-N7	7.17	113.67	110.80
36	A1	351	A	C8-N9-C4	7.17	108.67	105.80
36	A1	2302	G	N1-C2-N2	-7.17	109.75	116.20
57	BT	14	MET	CG-SD-CE	-7.17	88.73	100.20
36	A5	1403	C	C5-C6-N1	-7.17	117.42	121.00
36	A5	2320	A	C4-C5-N7	-7.17	107.12	110.70
36	A1	285	A	N1-C6-N6	7.17	122.90	118.60
80	A6	376	C	C6-N1-C2	7.17	123.17	120.30
36	A5	419	G	N9-C4-C5	-7.17	102.53	105.40
36	A5	1167	U	C5-C4-O4	-7.17	121.60	125.90
36	A5	2908	G	N9-C4-C5	7.17	108.27	105.40
36	A5	3040	A	C5-N7-C8	7.17	107.48	103.90
36	A1	640	U	N3-C2-O2	-7.16	117.19	122.20
36	A1	2763	U	C2-N3-C4	-7.16	122.70	127.00
36	A1	3317	U	N3-C2-O2	-7.16	117.19	122.20
36	A5	969	C	C2-N3-C4	-7.16	116.32	119.90
36	A5	974	G	C4-N9-C1'	7.16	135.81	126.50
36	A1	2679	A	C5-N7-C8	-7.16	100.32	103.90
36	A1	2960	C	C2-N3-C4	-7.16	116.32	119.90
37	A3	48	U	C5-C4-O4	-7.16	121.60	125.90
36	A5	2965	U	C4-C5-C6	7.16	124.00	119.70
36	A5	3052	G	N1-C6-O6	-7.16	115.60	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A7	44	C	N1-C2-O2	-7.16	114.60	118.90
68	Be	45	ARG	NE-CZ-NH2	-7.16	116.72	120.30
36	A5	2305	G	N9-C4-C5	-7.16	102.54	105.40
36	A1	1405	U	C6-N1-C2	7.16	125.29	121.00
80	A6	337	G	N3-C2-N2	7.16	124.91	119.90
36	A1	969	C	C2-N3-C4	-7.16	116.32	119.90
36	A5	629	U	C2-N3-C4	-7.16	122.71	127.00
36	A5	1206	G	N9-C4-C5	7.16	108.26	105.40
36	A5	2979	U	C6-N1-C2	7.16	125.29	121.00
36	A1	2726	C	C2-N3-C4	-7.15	116.32	119.90
36	A5	518	G	N9-C4-C5	-7.15	102.54	105.40
36	A1	907	G	N3-C4-N9	7.15	130.29	126.00
36	A1	1472	U	C6-N1-C2	7.15	125.29	121.00
36	A5	1591	G	N1-C6-O6	-7.15	115.61	119.90
36	A1	50	U	C5-C4-O4	7.15	130.19	125.90
36	A5	801	A	C5-C6-N1	-7.15	114.12	117.70
36	A5	1209	G	N3-C2-N2	-7.15	114.89	119.90
36	A5	2396	G	N9-C4-C5	7.15	108.26	105.40
36	A5	2917	G	C6-C5-N7	-7.15	126.11	130.40
1	A2	1611	A	C2-N3-C4	-7.15	107.03	110.60
80	A6	387	A	N1-C6-N6	-7.15	114.31	118.60
36	A5	563	U	N1-C2-O2	7.15	127.80	122.80
36	A5	2942	C	N3-C4-C5	-7.15	119.04	121.90
36	A1	2952	G	C6-C5-N7	-7.15	126.11	130.40
36	A5	1158	A	C5-C6-N6	-7.15	117.98	123.70
36	A1	1507	G	C5-C6-O6	-7.15	124.31	128.60
36	A5	922	U	N3-C4-O4	-7.14	114.40	119.40
1	A2	628	G	C2-N3-C4	-7.14	108.33	111.90
36	A1	921	A	N1-C6-N6	7.14	122.89	118.60
36	A1	2647	A	C6-N1-C2	-7.14	114.31	118.60
36	A5	3379	C	C5-C6-N1	-7.14	117.43	121.00
36	A5	1458	U	C2-N3-C4	-7.14	122.72	127.00
36	A1	1164	G	N1-C2-N3	7.14	128.18	123.90
36	A5	46	U	C5-C4-O4	7.14	130.18	125.90
36	A5	2363	A	C8-N9-C4	-7.14	102.94	105.80
36	A1	548	G	N3-C4-N9	-7.14	121.72	126.00
36	A5	3005	A	N9-C4-C5	7.14	108.66	105.80
36	A1	2289	U	C5-C4-O4	7.14	130.18	125.90
36	A5	1292	C	C6-N1-C2	7.14	123.15	120.30
1	A2	992	A	C2-N3-C4	-7.13	107.03	110.60
36	A1	2899	C	N3-C4-N4	7.13	122.99	118.00
80	A6	93	A	N1-C6-N6	7.13	122.88	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2305	G	N3-C2-N2	7.13	124.89	119.90
36	A1	2372	A	C8-N9-C4	-7.13	102.95	105.80
36	A1	2945	G	C8-N9-C4	7.13	109.25	106.40
1	A2	783	G	C4-C5-N7	7.13	113.65	110.80
80	A6	22	A	C8-N9-C4	7.13	108.65	105.80
36	A1	104	G	C4-C5-N7	7.13	113.65	110.80
36	A1	2620	G	C5-C6-N1	7.13	115.06	111.50
37	A3	81	U	C2-N3-C4	-7.13	122.72	127.00
80	A6	653	C	C2-N1-C1'	7.13	126.64	118.80
36	A5	577	C	C2-N3-C4	-7.13	116.34	119.90
80	A6	371	G	C6-C5-N7	-7.13	126.12	130.40
36	A5	928	C	N1-C2-N3	7.13	124.19	119.20
36	A5	1548	C	C2-N3-C4	-7.13	116.34	119.90
36	A5	2344	U	C5-C6-N1	-7.13	119.14	122.70
36	A1	1335	C	N3-C4-N4	-7.12	113.01	118.00
36	A1	1414	G	C8-N9-C4	-7.12	103.55	106.40
36	A5	384	A	C8-N9-C4	7.12	108.65	105.80
36	A5	2242	A	N1-C6-N6	-7.12	114.33	118.60
36	A1	2817	A	N1-C2-N3	7.12	132.86	129.30
53	DP	69	ARG	NE-CZ-NH2	-7.12	116.74	120.30
36	A1	650	C	C2-N3-C4	-7.12	116.34	119.90
36	A1	2808	A	C5-C6-N1	-7.12	114.14	117.70
36	A5	1939	G	N3-C2-N2	7.12	124.88	119.90
36	A1	1142	G	C5-C6-N1	7.12	115.06	111.50
36	A5	3245	A	N3-C4-C5	7.12	131.78	126.80
36	A1	851	C	C5-C6-N1	7.12	124.56	121.00
36	A1	2747	A	N1-C6-N6	-7.12	114.33	118.60
36	A1	2762	A	C8-N9-C4	7.12	108.65	105.80
36	A5	3086	A	N7-C8-N9	-7.12	110.24	113.80
1	A2	1274	C	C5-C6-N1	-7.11	117.44	121.00
36	A5	1004	U	N3-C4-C5	7.11	118.87	114.60
36	A1	1719	G	N1-C6-O6	7.11	124.17	119.90
36	A1	369	A	N9-C4-C5	7.11	108.64	105.80
36	A1	1719	G	C6-C5-N7	-7.11	126.13	130.40
36	A5	434	U	N3-C4-C5	7.11	118.87	114.60
36	A5	1902	G	C8-N9-C4	7.11	109.24	106.40
36	A5	3076	C	N3-C4-C5	7.11	124.74	121.90
36	A1	415	G	C5-C6-O6	7.11	132.87	128.60
36	A1	821	U	N3-C2-O2	-7.11	117.22	122.20
36	A5	327	A	N7-C8-N9	-7.11	110.25	113.80
1	A2	1456	C	N3-C2-O2	-7.11	116.92	121.90
36	A5	24	G	N1-C6-O6	7.11	124.17	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	511	G	C5-C6-O6	7.11	132.86	128.60
38	A8	42	G	C8-N9-C4	7.11	109.24	106.40
36	A1	2323	G	N1-C6-O6	-7.11	115.64	119.90
36	A1	3269	U	C5-C4-O4	7.11	130.16	125.90
38	A4	113	U	N3-C4-O4	-7.11	114.43	119.40
36	A1	973	A	N9-C4-C5	7.10	108.64	105.80
36	A1	1520	G	N7-C8-N9	-7.10	109.55	113.10
36	A1	718	G	N3-C4-N9	-7.10	121.74	126.00
36	A1	2710	C	N3-C4-C5	7.10	124.74	121.90
48	DJ	112	LEU	CA-CB-CG	7.10	131.64	115.30
36	A1	1342	C	C2-N3-C4	-7.10	116.35	119.90
36	A1	2177	G	C5-C6-O6	-7.10	124.34	128.60
1	A2	1121	C	C4-C5-C6	7.10	120.95	117.40
1	A2	1324	G	N3-C2-N2	-7.10	114.93	119.90
36	A1	1741	A	N1-C6-N6	7.10	122.86	118.60
36	A5	3086	A	C5-N7-C8	7.10	107.45	103.90
36	A5	3110	C	N1-C2-N3	7.10	124.17	119.20
1	A2	1749	A	C2-N3-C4	-7.10	107.05	110.60
37	A7	101	G	C5-C6-O6	-7.10	124.34	128.60
36	A1	2957	G	C4-C5-N7	-7.10	107.96	110.80
36	A1	1395	G	C5-C6-N1	7.09	115.05	111.50
80	A6	876	G	C5-N7-C8	7.09	107.85	104.30
80	A6	1000	C	N3-C2-O2	-7.09	116.93	121.90
36	A5	2993	G	C4-C5-N7	7.09	113.64	110.80
38	A8	139	U	N3-C4-O4	-7.09	114.43	119.40
36	A1	1878	G	C5-C6-O6	-7.09	124.34	128.60
36	A1	652	G	N3-C2-N2	7.09	124.86	119.90
36	A1	1888	U	C5-C6-N1	-7.09	119.15	122.70
36	A5	436	A	C6-C5-N7	-7.09	127.33	132.30
36	A5	2616	C	C6-N1-C2	7.09	123.14	120.30
1	A2	1654	G	N3-C4-C5	-7.09	125.06	128.60
36	A1	302	U	C2-N3-C4	-7.09	122.75	127.00
36	A1	1125	U	C2-N3-C4	-7.09	122.75	127.00
36	A1	1507	G	C5-N7-C8	7.09	107.84	104.30
36	A5	1328	C	C4-C5-C6	7.09	120.94	117.40
36	A5	3006	A	N1-C2-N3	7.09	132.84	129.30
36	A1	1175	C	C2-N3-C4	-7.09	116.36	119.90
80	A6	421	A	N9-C4-C5	-7.09	102.97	105.80
36	A5	2169	G	C5-C6-N1	7.09	115.04	111.50
36	A5	2584	G	N3-C4-N9	7.09	130.25	126.00
36	A1	31	C	N3-C4-C5	7.08	124.73	121.90
36	A1	920	A	N1-C2-N3	7.08	132.84	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1042	U	N1-C2-O2	7.08	127.76	122.80
36	A1	2413	A	C5-C6-N1	7.08	121.24	117.70
37	A3	36	C	N3-C2-O2	-7.08	116.94	121.90
80	A6	1269	U	C4-C5-C6	7.08	123.95	119.70
80	A6	1503	A	C2-N3-C4	-7.08	107.06	110.60
36	A5	622	A	N9-C4-C5	-7.08	102.97	105.80
36	A5	1340	G	N1-C2-N2	-7.08	109.82	116.20
36	A5	2881	C	C5-C6-N1	-7.08	117.46	121.00
36	A1	2389	C	C6-N1-C2	7.08	123.13	120.30
36	A1	3092	C	N3-C4-C5	7.08	124.73	121.90
36	A5	1085	A	C8-N9-C4	-7.08	102.97	105.80
36	A5	2127	U	N1-C2-N3	7.08	119.15	114.90
36	A5	2631	U	N3-C4-C5	7.08	118.85	114.60
56	DS	115	ARG	NE-CZ-NH2	-7.08	116.76	120.30
36	A1	994	G	C5-C6-N1	7.08	115.04	111.50
36	A1	2696	A	N1-C6-N6	-7.08	114.35	118.60
36	A5	1917	C	N1-C2-O2	-7.08	114.65	118.90
36	A5	2327	U	C6-N1-C2	7.08	125.25	121.00
1	A2	577	G	N9-C4-C5	-7.08	102.57	105.40
36	A1	1166	G	C5-C6-O6	-7.08	124.35	128.60
36	A1	1307	G	C5-C6-O6	7.08	132.85	128.60
36	A1	2198	A	N9-C4-C5	-7.08	102.97	105.80
36	A1	2373	A	N1-C6-N6	7.08	122.85	118.60
80	A6	1796	C	C5-C4-N4	7.08	125.15	120.20
1	A2	108	A	N1-C2-N3	7.08	132.84	129.30
36	A1	1592	G	N1-C6-O6	-7.08	115.65	119.90
36	A1	1150	A	C2-N3-C4	-7.07	107.06	110.60
36	A1	1339	C	C4-C5-C6	7.07	120.94	117.40
36	A5	3052	G	C5-C6-O6	7.07	132.84	128.60
36	A5	872	U	N3-C4-C5	7.07	118.84	114.60
36	A1	711	A	N1-C6-N6	-7.07	114.36	118.60
36	A1	2727	A	C2-N3-C4	7.07	114.14	110.60
36	A5	546	C	C5-C6-N1	7.07	124.53	121.00
36	A5	2149	A	C8-N9-C4	-7.07	102.97	105.80
36	A1	876	A	N1-C6-N6	-7.07	114.36	118.60
36	A1	1118	C	C2-N3-C4	-7.07	116.37	119.90
36	A1	742	G	C8-N9-C4	7.07	109.23	106.40
36	A1	3362	A	C5-C6-N6	-7.07	118.05	123.70
36	A5	2988	C	C5-C6-N1	-7.07	117.47	121.00
36	A1	2145	A	C2-N3-C4	7.06	114.13	110.60
36	A1	2595	A	N1-C6-N6	7.06	122.84	118.60
80	A6	3	U	C5-C6-N1	-7.06	119.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1879	A	C5-N7-C8	-7.06	100.37	103.90
36	A5	3107	U	N3-C2-O2	-7.06	117.26	122.20
36	A5	3192	U	N3-C4-O4	-7.06	114.46	119.40
38	A8	101	U	C6-N1-C2	-7.06	116.76	121.00
36	A1	1589	A	C6-N1-C2	-7.06	114.37	118.60
36	A1	1447	G	N9-C4-C5	7.06	108.22	105.40
36	A1	1528	G	C8-N9-C4	-7.06	103.58	106.40
36	A1	1870	C	N3-C4-C5	7.06	124.72	121.90
36	A1	3052	G	C5-C6-O6	7.06	132.83	128.60
41	BC	313	LEU	CA-CB-CG	7.06	131.53	115.30
38	A8	126	A	C8-N9-C4	-7.05	102.98	105.80
80	A6	1789	G	C5-N7-C8	7.05	107.83	104.30
36	A5	641	C	C6-N1-C1'	7.05	129.26	120.80
36	A5	1592	G	C5-C6-O6	7.05	132.83	128.60
36	A1	95	A	N7-C8-N9	-7.05	110.27	113.80
80	A6	310	C	N1-C2-O2	-7.05	114.67	118.90
36	A5	437	G	N7-C8-N9	7.05	116.63	113.10
36	A1	2139	A	N1-C6-N6	-7.05	114.37	118.60
36	A1	3208	G	C4-N9-C1'	-7.05	117.33	126.50
37	A3	28	C	N1-C2-O2	-7.05	114.67	118.90
80	A6	512	A	C5-C6-N6	-7.05	118.06	123.70
80	A6	1188	G	C5-C6-O6	-7.05	124.37	128.60
36	A5	834	U	N3-C4-O4	-7.05	114.47	119.40
1	A2	610	G	C8-N9-C1'	-7.05	117.84	127.00
36	A5	2832	C	C2-N3-C4	-7.05	116.38	119.90
52	DO	4[B]	GLN	O-C-N	7.05	134.49	121.10
36	A5	929	A	N7-C8-N9	-7.04	110.28	113.80
1	A2	1057	U	C5-C6-N1	7.04	126.22	122.70
1	A2	1462	G	C8-N9-C4	7.04	109.22	106.40
36	A1	2406	C	C5-C6-N1	-7.04	117.48	121.00
36	A1	2799	A	C6-N1-C2	-7.04	114.37	118.60
80	A6	371	G	C5-C6-O6	-7.04	124.37	128.60
36	A5	1370	G	N3-C2-N2	7.04	124.83	119.90
36	A5	2618	G	C6-N1-C2	-7.04	120.87	125.10
36	A1	700	C	C6-N1-C2	7.04	123.12	120.30
80	A6	1606	C	C6-N1-C2	7.04	123.12	120.30
80	A6	543	C	N1-C2-O2	7.04	123.12	118.90
80	A6	756	A	N7-C8-N9	7.04	117.32	113.80
36	A5	1417	G	N1-C6-O6	-7.04	115.68	119.90
36	A5	2300	G	N3-C2-N2	7.04	124.83	119.90
36	A1	1145	G	N1-C6-O6	-7.04	115.68	119.90
36	A1	1200	A	N9-C4-C5	7.04	108.61	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1389	G	C5-C6-O6	-7.04	124.38	128.60
36	A1	788	C	C6-N1-C2	7.04	123.11	120.30
36	A1	1480	G	N3-C4-N9	7.04	130.22	126.00
36	A1	2325	G	C5-C6-N1	7.04	115.02	111.50
36	A5	708	G	N7-C8-N9	7.04	116.62	113.10
36	A5	2618	G	N3-C4-N9	7.04	130.22	126.00
36	A5	2189	U	C2-N3-C4	-7.03	122.78	127.00
36	A5	2350	C	C2-N3-C4	-7.03	116.38	119.90
36	A5	2426	U	N1-C2-O2	7.03	127.72	122.80
36	A5	3154	C	N3-C2-O2	-7.03	116.98	121.90
36	A5	2190	U	N1-C2-N3	7.03	119.12	114.90
1	A2	1773	C	C2-N3-C4	7.03	123.42	119.90
36	A1	22	G	N9-C4-C5	7.03	108.21	105.40
36	A1	28	C	N3-C4-C5	7.03	124.71	121.90
36	A1	895	A	N3-C4-C5	7.03	131.72	126.80
36	A5	1314	C	C2-N1-C1'	7.03	126.53	118.80
36	A5	1434	G	C4-C5-N7	-7.03	107.99	110.80
36	A5	2280	A	C2-N3-C4	-7.03	107.08	110.60
36	A5	3317	U	C6-N1-C2	-7.03	116.78	121.00
36	A1	357	A	C6-N1-C2	-7.03	114.38	118.60
80	A6	114	C	N3-C2-O2	-7.03	116.98	121.90
36	A1	153	U	C5-C4-O4	7.03	130.12	125.90
36	A1	1495	U	C5-C4-O4	7.03	130.12	125.90
36	A5	2167	A	C6-N1-C2	-7.03	114.38	118.60
1	A2	1747	G	C2-N3-C4	-7.03	108.39	111.90
36	A1	2369	G	C8-N9-C4	-7.03	103.59	106.40
36	A1	3111	U	N3-C4-O4	-7.03	114.48	119.40
36	A5	1152	G	N1-C2-N3	7.03	128.12	123.90
36	A5	2293	C	N3-C4-C5	7.03	124.71	121.90
36	A1	1838	G	C5-C6-O6	-7.02	124.39	128.60
36	A1	3126	C	C5-C6-N1	-7.02	117.49	121.00
80	A6	1560	U	N1-C2-N3	7.02	119.11	114.90
36	A5	1441	G	N7-C8-N9	-7.02	109.59	113.10
36	A5	2302	G	N1-C6-O6	-7.02	115.69	119.90
36	A1	2595	A	C8-N9-C4	-7.02	102.99	105.80
36	A5	2917	G	C6-N1-C2	-7.02	120.89	125.10
1	A2	159	U	C6-N1-C2	7.02	125.21	121.00
36	A1	95	A	C5-C6-N1	-7.02	114.19	117.70
36	A1	2130	G	C5-N7-C8	7.02	107.81	104.30
64	Da	12	ARG	NE-CZ-NH2	-7.02	116.79	120.30
36	A1	81	C	C2-N3-C4	-7.02	116.39	119.90
36	A1	3129	A	C8-N9-C4	7.02	108.61	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	11	A	C2-N3-C4	7.02	114.11	110.60
36	A5	2693	C	C2-N3-C4	-7.02	116.39	119.90
36	A1	709	A	N9-C4-C5	-7.02	102.99	105.80
36	A1	1127	G	N1-C6-O6	7.02	124.11	119.90
36	A1	2146	C	C6-N1-C2	-7.02	117.49	120.30
36	A5	3098	G	C5-C6-O6	7.02	132.81	128.60
36	A1	84	U	C5-C4-O4	-7.01	121.69	125.90
36	A1	889	U	N3-C2-O2	-7.01	117.29	122.20
36	A1	1893	A	N1-C2-N3	7.01	132.81	129.30
36	A5	81	C	N3-C4-N4	-7.01	113.09	118.00
36	A5	706	A	C8-N9-C4	7.01	108.61	105.80
36	A1	814	U	C5-C6-N1	-7.01	119.19	122.70
36	A1	908	G	C8-N9-C1'	-7.01	117.89	127.00
36	A5	859	G	N1-C6-O6	-7.01	115.69	119.90
1	A2	321	C	C6-N1-C2	-7.01	117.50	120.30
36	A1	2274	U	N1-C2-O2	7.01	127.70	122.80
36	A5	804	C	N3-C4-C5	-7.00	119.10	121.90
36	A5	945	C	C5-C6-N1	-7.00	117.50	121.00
36	A1	1389	G	C4-C5-N7	7.00	113.60	110.80
36	A1	1947	G	N1-C2-N2	7.00	122.50	116.20
36	A5	591	G	C4-C5-N7	7.00	113.60	110.80
36	A5	1110	U	C4-C5-C6	-7.00	115.50	119.70
1	A2	74	U	O4'-C1'-N1	7.00	113.80	108.20
36	A1	895	A	C5-C6-N1	-7.00	114.20	117.70
36	A1	2814	G	N1-C6-O6	7.00	124.10	119.90
80	A6	610	G	C4-N9-C1'	7.00	135.60	126.50
36	A5	3214	U	N1-C2-N3	7.00	119.10	114.90
37	A3	28	C	C5-C4-N4	-7.00	115.30	120.20
36	A5	418	A	N1-C6-N6	7.00	122.80	118.60
36	A1	662	U	N3-C2-O2	-7.00	117.30	122.20
36	A1	926	A	C2-N3-C4	7.00	114.10	110.60
80	A6	297	U	C2-N1-C1'	7.00	126.10	117.70
36	A5	3182	G	N1-C6-O6	-7.00	115.70	119.90
36	A1	987	U	N1-C2-N3	7.00	119.10	114.90
36	A1	950	G	C6-N1-C2	6.99	129.30	125.10
36	A1	2139	A	C4-C5-N7	-6.99	107.20	110.70
80	A6	424	C	C6-N1-C2	6.99	123.10	120.30
36	A5	32	U	N3-C4-C5	-6.99	110.40	114.60
36	A5	802	C	C2-N3-C4	-6.99	116.40	119.90
36	A5	1925	U	C2-N3-C4	-6.99	122.80	127.00
36	A1	361	A	C2-N3-C4	6.99	114.09	110.60
36	A5	2943	G	N1-C6-O6	-6.99	115.70	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	930	U	N3-C4-O4	-6.99	114.51	119.40
36	A5	2169	G	C6-C5-N7	6.99	134.59	130.40
36	A5	2932	U	N1-C2-O2	6.99	127.69	122.80
36	A1	78	U	C2-N3-C4	-6.99	122.81	127.00
52	DO	104[B]	ILE	O-C-N	6.99	133.88	122.70
36	A1	636	C	C2-N3-C4	-6.98	116.41	119.90
1	A2	1600	A	C5-C6-N1	-6.98	114.21	117.70
80	A6	408	C	C6-N1-C2	-6.98	117.51	120.30
36	A1	363	G	N3-C2-N2	-6.98	115.01	119.90
36	A1	791	A	C8-N9-C4	6.98	108.59	105.80
36	A1	1156	C	C2-N3-C4	-6.98	116.41	119.90
36	A5	2882	U	C2-N3-C4	-6.98	122.81	127.00
36	A1	33	G	N3-C2-N2	-6.98	115.02	119.90
36	A1	54	C	C6-N1-C2	6.98	123.09	120.30
36	A1	2364	G	C5-C6-O6	-6.98	124.41	128.60
80	A6	9	U	C5-C6-N1	-6.98	119.21	122.70
36	A1	3304	U	C2-N1-C1'	-6.98	109.33	117.70
36	A5	1118	C	N3-C4-C5	6.98	124.69	121.90
36	A5	2290	C	C6-N1-C2	6.98	123.09	120.30
36	A5	3218	A	C2-N3-C4	-6.98	107.11	110.60
36	A5	1149	G	N9-C4-C5	6.97	108.19	105.40
36	A1	359	U	C2-N3-C4	-6.97	122.82	127.00
36	A1	958	C	C5-C4-N4	6.97	125.08	120.20
36	A5	933	A	N1-C2-N3	6.97	132.79	129.30
36	A5	2917	G	N3-C4-N9	6.97	130.18	126.00
36	A5	1673	G	N1-C6-O6	-6.97	115.72	119.90
1	A2	1533	C	C4-C5-C6	6.97	120.88	117.40
36	A1	427	C	C2-N3-C4	-6.97	116.42	119.90
36	A1	2678	A	N1-C6-N6	-6.97	114.42	118.60
80	A6	605	A	C8-N9-C4	6.97	108.59	105.80
38	A8	70	G	C8-N9-C4	6.97	109.19	106.40
1	A2	1162	C	C6-N1-C2	-6.96	117.51	120.30
38	A4	6	U	C5-C4-O4	-6.96	121.72	125.90
36	A5	2314	U	C5-C6-N1	6.96	126.18	122.70
36	A5	369	A	N7-C8-N9	6.96	117.28	113.80
36	A1	650	C	N1-C2-O2	-6.96	114.72	118.90
36	A1	1132	C	C5-C4-N4	6.96	125.07	120.20
36	A1	1741	A	C4-C5-N7	6.96	114.18	110.70
36	A1	2169	G	C2-N3-C4	6.96	115.38	111.90
38	A8	112	U	C2-N1-C1'	-6.96	109.35	117.70
80	A6	1455	G	N9-C4-C5	6.96	108.18	105.40
36	A5	3172	A	C5-N7-C8	6.96	107.38	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	61	A	N7-C8-N9	6.96	117.28	113.80
36	A1	2757	U	N1-C2-N3	6.96	119.08	114.90
80	A6	411	C	C4-C5-C6	6.96	120.88	117.40
36	A5	2631	U	C5-C6-N1	-6.96	119.22	122.70
36	A5	3070	A	C2-N3-C4	-6.96	107.12	110.60
36	A5	3099	C	C5-C6-N1	-6.96	117.52	121.00
80	A6	144	U	N1-C2-O2	6.96	127.67	122.80
38	A8	139	U	C5-C6-N1	-6.96	119.22	122.70
36	A1	352	A	C5-C6-N1	-6.95	114.22	117.70
36	A1	376	G	C4-C5-N7	-6.95	108.02	110.80
36	A1	1491	A	N7-C8-N9	-6.95	110.32	113.80
80	A6	647	G	N3-C4-N9	-6.95	121.83	126.00
36	A5	2644	C	N1-C2-O2	-6.95	114.73	118.90
36	A5	2689	A	C6-N1-C2	-6.95	114.43	118.60
36	A1	885	U	C2-N3-C4	-6.95	122.83	127.00
36	A1	2958	A	N7-C8-N9	-6.95	110.33	113.80
36	A5	751	A	C2-N3-C4	-6.95	107.12	110.60
36	A5	2249	G	C3'-C2'-C1'	-6.95	95.94	101.50
36	A1	963	G	N7-C8-N9	-6.95	109.62	113.10
36	A1	1371	G	N1-C6-O6	-6.95	115.73	119.90
36	A5	1199	C	C4-C5-C6	6.95	120.87	117.40
36	A1	653	A	C6-N1-C2	-6.95	114.43	118.60
36	A5	2626	A	C5-C6-N6	6.95	129.26	123.70
36	A5	3333	G	C5-C6-O6	-6.95	124.43	128.60
1	A2	981	U	N3-C2-O2	-6.95	117.34	122.20
1	A2	1782	A	N7-C8-N9	6.95	117.27	113.80
36	A1	1429	G	N1-C2-N2	-6.95	109.95	116.20
1	A2	542	A	C8-N9-C1'	-6.94	115.20	127.70
36	A1	1926	C	N3-C4-C5	6.94	124.68	121.90
36	A5	2184	U	C2-N3-C4	-6.94	122.83	127.00
80	A6	351	C	C2-N1-C1'	6.94	126.44	118.80
36	A1	2600	C	N3-C2-O2	-6.94	117.04	121.90
36	A1	3372	A	C5-C6-N1	6.94	121.17	117.70
36	A1	407	A	N7-C8-N9	6.94	117.27	113.80
36	A5	835	G	C5-C6-N1	6.94	114.97	111.50
36	A5	1834	U	N3-C4-O4	-6.94	114.54	119.40
1	A2	360	A	N9-C4-C5	-6.94	103.03	105.80
39	BA	207	VAL	CB-CA-C	-6.94	98.22	111.40
80	A6	1681	A	C2-N3-C4	-6.94	107.13	110.60
15	AN	22	ALA	C-N-CD	-6.93	105.34	120.60
36	A1	1182	A	C8-N9-C4	6.93	108.57	105.80
36	A1	2899	C	C5-C6-N1	-6.93	117.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1793	G	N1-C6-O6	-6.93	115.74	119.90
1	A2	1548	G	C2-N3-C4	6.93	115.36	111.90
36	A1	1858	A	C6-N1-C2	-6.93	114.44	118.60
36	A1	2977	G	C6-N1-C2	-6.93	120.94	125.10
80	A6	310	C	C4-C5-C6	6.93	120.86	117.40
36	A5	1285	G	C8-N9-C4	6.93	109.17	106.40
36	A5	1589	A	C2-N3-C4	6.93	114.06	110.60
36	A5	1833	G	C8-N9-C4	6.93	109.17	106.40
1	A2	1749	A	N9-C4-C5	-6.93	103.03	105.80
36	A5	857	G	N9-C4-C5	-6.93	102.63	105.40
36	A1	371	G	N9-C4-C5	-6.93	102.63	105.40
36	A1	987	U	C2-N3-C4	-6.93	122.84	127.00
36	A1	873	C	C6-N1-C2	-6.92	117.53	120.30
36	A1	1839	A	C8-N9-C4	-6.92	103.03	105.80
46	BH	62	ARG	NE-CZ-NH1	6.92	123.76	120.30
80	A6	385	A	C5-N7-C8	6.92	107.36	103.90
13	CL	103	ARG	NE-CZ-NH1	6.92	123.76	120.30
80	A6	65	A	N9-C4-C5	-6.92	103.03	105.80
36	A5	96	G	C5-C6-O6	6.92	132.75	128.60
36	A1	1851	G	N3-C4-N9	6.92	130.15	126.00
36	A1	2184	U	C2-N1-C1'	6.92	126.01	117.70
36	A5	343	U	C5-C4-O4	6.92	130.05	125.90
80	A6	339	C	N1-C2-O2	-6.92	114.75	118.90
80	A6	687	G	N9-C4-C5	6.92	108.17	105.40
1	A2	313	U	N3-C4-O4	-6.91	114.56	119.40
36	A1	903	U	C2-N3-C4	-6.91	122.85	127.00
36	A1	2393	G	C5-C6-O6	-6.91	124.45	128.60
36	A1	2631	U	N3-C4-O4	-6.91	114.56	119.40
37	A3	67	G	N1-C6-O6	6.91	124.05	119.90
36	A5	784	A	C5-C6-N6	-6.91	118.17	123.70
36	A5	2412	G	N3-C4-C5	-6.91	125.14	128.60
37	A7	74	C	N1-C2-O2	-6.91	114.75	118.90
52	DO	3[B]	SER	CA-C-N	-6.91	101.99	117.20
68	De	33	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A2	736	C	C6-N1-C1'	-6.91	112.51	120.80
36	A1	2941	A	C5-C6-N1	6.91	121.16	117.70
36	A5	3020	U	N1-C2-O2	-6.91	117.96	122.80
36	A1	57	A	C2-N3-C4	-6.91	107.14	110.60
36	A1	83	U	C2-N3-C4	-6.91	122.85	127.00
36	A1	644	G	N1-C6-O6	-6.91	115.75	119.90
36	A1	2836	C	N3-C2-O2	-6.91	117.06	121.90
36	A1	3057	U	N1-C2-N3	6.91	119.05	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	24	G	C6-N1-C2	-6.91	120.95	125.10
36	A1	1460	A	C5-C6-N1	6.91	121.15	117.70
36	A1	1515	A	C6-C5-N7	-6.91	127.46	132.30
38	A4	13	A	C5-C6-N6	-6.91	118.17	123.70
36	A5	942	U	C5-C4-O4	-6.91	121.75	125.90
36	A5	1210	U	N3-C2-O2	-6.91	117.36	122.20
36	A5	3362	A	C5-C6-N1	-6.91	114.25	117.70
36	A5	3362	A	C6-C5-N7	-6.91	127.46	132.30
36	A1	967	A	N7-C8-N9	-6.91	110.35	113.80
36	A1	2252	A	C8-N9-C4	-6.91	103.04	105.80
37	A3	88	G	N1-C6-O6	-6.91	115.76	119.90
36	A1	1646	G	C5-C6-O6	-6.91	124.46	128.60
36	A1	302	U	N3-C4-C5	6.90	118.74	114.60
36	A1	917	A	N1-C6-N6	-6.90	114.46	118.60
36	A5	1609	C	N3-C4-N4	6.90	122.83	118.00
73	Dj	73	ARG	NE-CZ-NH2	-6.90	116.85	120.30
36	A1	1130	A	C5-C6-N6	-6.90	118.18	123.70
36	A1	3179	U	N3-C2-O2	-6.90	117.37	122.20
36	A5	2732	G	N3-C2-N2	6.90	124.73	119.90
36	A1	339	C	C5-C4-N4	6.90	125.03	120.20
80	A6	868	G	C5-C6-O6	-6.90	124.46	128.60
36	A5	3019	U	C2-N3-C4	-6.90	122.86	127.00
80	A6	29	U	N3-C2-O2	-6.90	117.37	122.20
36	A5	1883	A	N1-C6-N6	-6.90	114.46	118.60
36	A1	1741	A	C5-N7-C8	-6.89	100.45	103.90
36	A5	221	A	C8-N9-C4	6.89	108.56	105.80
36	A1	980	A	C8-N9-C4	-6.89	103.04	105.80
80	A6	987	G	C5-C6-O6	-6.89	124.46	128.60
48	DJ	9	MET	N-CA-C	-6.89	92.39	111.00
80	A6	354	C	N3-C4-C5	6.89	124.66	121.90
36	A5	419	G	N3-C4-N9	6.89	130.13	126.00
36	A1	1150	A	C5-C6-N1	-6.89	114.25	117.70
46	BH	91	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	A2	1206	U	N3-C4-O4	6.89	124.22	119.40
38	A4	142	C	N1-C2-O2	-6.89	114.77	118.90
80	A6	638	U	N1-C2-O2	6.89	127.62	122.80
36	A5	1603	A	C8-N9-C4	-6.89	103.05	105.80
36	A1	1932	A	C2-N3-C4	6.88	114.04	110.60
36	A1	2288	G	N7-C8-N9	6.88	116.54	113.10
36	A5	1370	G	N1-C2-N2	-6.88	110.00	116.20
36	A5	2246	G	C8-N9-C4	-6.88	103.65	106.40
1	A2	305	C	C6-N1-C2	-6.88	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1361	U	N1-C2-O2	6.88	127.62	122.80
80	A6	1124	A	C8-N9-C4	6.88	108.55	105.80
80	A6	1631	A	C2-N3-C4	-6.88	107.16	110.60
36	A5	833	G	C6-N1-C2	-6.88	120.97	125.10
36	A5	1875	G	N1-C6-O6	-6.88	115.77	119.90
36	A1	356	C	C2-N3-C4	-6.88	116.46	119.90
80	A6	1592	A	N1-C2-N3	6.88	132.74	129.30
36	A1	317	A	N1-C2-N3	-6.88	125.86	129.30
36	A1	2641	U	C5-C6-N1	-6.88	119.26	122.70
36	A1	2669	G	C2-N3-C4	-6.88	108.46	111.90
80	A6	418	G	N7-C8-N9	6.88	116.54	113.10
36	A5	2978	U	N3-C4-O4	-6.88	114.58	119.40
36	A1	2980	U	N3-C2-O2	-6.88	117.39	122.20
36	A5	1406	A	N1-C2-N3	6.88	132.74	129.30
36	A1	2306	C	C6-N1-C2	-6.88	117.55	120.30
36	A1	2952	G	N3-C4-C5	6.88	132.04	128.60
1	A2	92	A	N9-C4-C5	6.87	108.55	105.80
36	A5	864	G	C6-N1-C2	-6.87	120.98	125.10
36	A5	2207	A	N1-C6-N6	6.87	122.72	118.60
36	A5	2695	A	N7-C8-N9	6.87	117.24	113.80
36	A5	3308	C	C6-N1-C2	-6.87	117.55	120.30
36	A1	369	A	N1-C2-N3	-6.87	125.86	129.30
36	A1	3343	G	N1-C2-N2	-6.87	110.02	116.20
36	A5	3376	A	N7-C8-N9	6.87	117.24	113.80
36	A1	1374	G	N3-C2-N2	6.87	124.71	119.90
36	A5	857	G	C8-N9-C4	6.87	109.15	106.40
36	A5	1513	G	N7-C8-N9	6.87	116.53	113.10
36	A5	1903	U	N3-C4-C5	-6.87	110.48	114.60
36	A1	1346	G	C2-N3-C4	-6.87	108.47	111.90
56	BS	167	ARG	NE-CZ-NH1	6.87	123.73	120.30
36	A5	2705	A	C2-N3-C4	6.87	114.03	110.60
36	A1	1409	G	N9-C4-C5	6.87	108.15	105.40
36	A1	2921	U	N3-C4-C5	6.87	118.72	114.60
36	A1	3268	A	C2-N3-C4	-6.87	107.17	110.60
38	A4	67	U	C5-C6-N1	-6.87	119.27	122.70
36	A5	1417	G	C5-C6-N1	6.86	114.93	111.50
36	A5	2382	G	N1-C6-O6	-6.86	115.78	119.90
36	A1	580	C	C6-N1-C2	-6.86	117.56	120.30
36	A1	2279	A	C4-C5-N7	6.86	114.13	110.70
80	A6	18	C	N1-C2-O2	-6.86	114.78	118.90
80	A6	467	G	N1-C6-O6	-6.86	115.78	119.90
36	A5	2884	C	N1-C2-O2	-6.86	114.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2306	C	C5-C4-N4	6.86	125.00	120.20
80	A6	87	C	C4-C5-C6	6.86	120.83	117.40
51	BN	105	ARG	NE-CZ-NH1	6.86	123.73	120.30
80	A6	638	U	N3-C2-O2	-6.86	117.40	122.20
1	A2	453	U	N1-C2-O2	6.86	127.60	122.80
36	A5	189	G	N1-C6-O6	-6.86	115.78	119.90
36	A5	3105	U	N3-C2-O2	6.86	127.00	122.20
36	A1	281	G	N7-C8-N9	6.86	116.53	113.10
80	A6	1782	A	N7-C8-N9	6.86	117.23	113.80
36	A1	3230	G	C6-N1-C2	-6.85	120.99	125.10
36	A5	2729	U	C5-C6-N1	6.85	126.13	122.70
36	A1	187	A	N3-C4-C5	-6.85	122.00	126.80
36	A1	988	U	N3-C4-O4	-6.85	114.60	119.40
36	A5	2524	A	C3'-C2'-C1'	-6.85	96.02	101.50
36	A5	2987	A	C5-N7-C8	6.85	107.33	103.90
36	A1	1191	U	N1-C2-N3	6.85	119.01	114.90
36	A1	715	A	N7-C8-N9	6.85	117.22	113.80
36	A1	2982	A	C8-N9-C4	6.85	108.54	105.80
36	A5	693	A	N1-C6-N6	-6.85	114.49	118.60
36	A5	2385	G	C2-N3-C4	-6.85	108.47	111.90
36	A5	3176	G	N1-C2-N3	6.85	128.01	123.90
80	A6	9	U	C2-N3-C4	-6.85	122.89	127.00
36	A5	881	C	C2-N3-C4	6.85	123.32	119.90
37	A7	112	G	C5-C6-O6	6.85	132.71	128.60
36	A1	517	G	N9-C4-C5	6.85	108.14	105.40
36	A1	1515	A	N1-C6-N6	6.84	122.71	118.60
36	A5	3149	G	C2-N3-C4	-6.84	108.48	111.90
36	A1	2823	G	C5-N7-C8	6.84	107.72	104.30
1	A2	934	C	C2-N1-C1'	6.84	126.33	118.80
80	A6	337	G	N1-C2-N3	-6.84	119.80	123.90
80	A6	351	C	N3-C4-C5	-6.84	119.16	121.90
36	A1	1076	C	C6-N1-C2	6.84	123.04	120.30
36	A5	2237	C	N1-C2-O2	6.84	123.00	118.90
36	A5	2359	C	C6-N1-C2	6.84	123.04	120.30
36	A1	1136	A	C5-C6-N1	6.84	121.12	117.70
80	A6	372	G	C8-N9-C4	6.84	109.14	106.40
80	A6	617	U	C6-N1-C2	-6.84	116.90	121.00
36	A5	815	G	C4-C5-N7	-6.84	108.06	110.80
36	A5	1297	C	N1-C2-O2	-6.84	114.80	118.90
36	A5	2362	C	N3-C4-C5	6.84	124.64	121.90
36	A5	2401	A	C2-N3-C4	6.84	114.02	110.60
36	A1	584	G	N9-C4-C5	6.83	108.13	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A3	22	A	N1-C6-N6	6.83	122.70	118.60
80	A6	1030	A	N9-C4-C5	6.83	108.53	105.80
80	A6	1796	C	N3-C4-N4	-6.83	113.22	118.00
36	A5	3056	U	N1-C2-N3	6.83	119.00	114.90
1	A2	73	U	O4'-C1'-N1	6.83	113.67	108.20
36	A1	2816	G	C5-C6-O6	-6.83	124.50	128.60
36	A1	3015	G	C5-C6-N1	6.83	114.92	111.50
38	A4	25	G	C5-N7-C8	6.83	107.72	104.30
80	A6	342	C	C4-C5-C6	6.83	120.81	117.40
36	A1	1592	G	C5-N7-C8	-6.83	100.89	104.30
40	BB	7	GLU	OE1-CD-OE2	-6.83	115.10	123.30
36	A5	2664	C	N3-C4-C5	6.83	124.63	121.90
36	A5	3081	C	C4-C5-C6	-6.83	113.98	117.40
36	A1	750	G	C5-C6-O6	6.83	132.70	128.60
36	A1	2280	A	N1-C6-N6	6.83	122.70	118.60
80	A6	1246	C	N3-C2-O2	-6.83	117.12	121.90
36	A5	1868	G	C8-N9-C4	6.83	109.13	106.40
1	A2	1146	G	C8-N9-C4	-6.83	103.67	106.40
36	A1	1169	A	C6-C5-N7	-6.83	127.52	132.30
36	A1	1695	U	C5-C6-N1	-6.83	119.29	122.70
36	A5	622	A	C5-C6-N6	-6.83	118.24	123.70
36	A5	1902	G	C6-N1-C2	-6.83	121.00	125.10
36	A5	1941	C	C2-N3-C4	-6.83	116.49	119.90
1	A2	607	G	N1-C6-O6	6.82	123.99	119.90
36	A1	3172	A	C8-N9-C4	6.82	108.53	105.80
80	A6	453	U	C6-N1-C2	-6.82	116.91	121.00
80	A6	1472	C	N3-C4-N4	-6.82	113.22	118.00
1	A2	1319	A	N1-C6-N6	6.82	122.69	118.60
36	A1	331	G	C4-C5-N7	-6.82	108.07	110.80
36	A1	1858	A	C4-N9-C1'	6.82	138.58	126.30
36	A5	2400	G	N3-C4-C5	6.82	132.01	128.60
36	A5	3321	C	C4-C5-C6	6.82	120.81	117.40
36	A5	1481	A	P-O3'-C3'	6.82	127.88	119.70
38	A8	23	U	N1-C2-N3	6.82	118.99	114.90
36	A1	639	G	C6-C5-N7	-6.82	126.31	130.40
36	A5	578	A	C5-C6-N6	-6.82	118.25	123.70
41	DC	90	PHE	C-N-CA	-6.82	107.98	122.30
38	A4	7	U	C5-C6-N1	-6.82	119.29	122.70
36	A5	1124	U	N1-C2-O2	6.81	127.57	122.80
36	A5	1941	C	N3-C4-C5	6.81	124.62	121.90
36	A1	851	C	C2-N1-C1'	6.81	126.30	118.80
36	A5	1138	U	N3-C4-C5	6.81	118.69	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1940	G	N1-C6-O6	-6.81	115.81	119.90
36	A5	2389	C	C2-N3-C4	-6.81	116.49	119.90
36	A5	2821	C	C6-N1-C2	-6.81	117.58	120.30
1	A2	240	U	C2-N1-C1'	6.81	125.87	117.70
36	A1	1489	A	C6-C5-N7	-6.81	127.53	132.30
1	A2	1611	A	N1-C2-N3	6.81	132.71	129.30
36	A1	545	U	N3-C2-O2	-6.81	117.43	122.20
36	A5	327	A	C8-N9-C4	6.81	108.52	105.80
36	A5	1369	A	C8-N9-C4	6.81	108.52	105.80
36	A5	3101	G	C5-C6-O6	6.81	132.69	128.60
36	A1	2678	A	N9-C4-C5	6.81	108.52	105.80
36	A1	2865	U	C5-C4-O4	-6.81	121.82	125.90
36	A5	41	G	C4-C5-N7	6.81	113.52	110.80
36	A5	1448	U	C2-N3-C4	-6.81	122.92	127.00
1	A2	410	A	C8-N9-C4	6.81	108.52	105.80
40	BB	19	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A2	1195	C	C6-N1-C2	-6.80	117.58	120.30
38	A4	63	G	N1-C6-O6	-6.80	115.82	119.90
36	A5	1652	G	N7-C8-N9	-6.80	109.70	113.10
36	A5	2524	A	C4-C5-N7	6.80	114.10	110.70
36	A1	637	C	N1-C2-N3	6.80	123.96	119.20
36	A1	864	G	N1-C6-O6	-6.80	115.82	119.90
36	A1	2111	G	C5-C6-O6	6.80	132.68	128.60
36	A5	1556	C	C6-N1-C2	-6.80	117.58	120.30
36	A5	2341	A	N9-C4-C5	-6.80	103.08	105.80
1	A2	360	A	C8-N9-C4	6.80	108.52	105.80
36	A5	564	G	C4-C5-N7	-6.80	108.08	110.80
36	A1	1411	C	N3-C2-O2	-6.80	117.14	121.90
36	A1	2222	A	N9-C4-C5	6.80	108.52	105.80
36	A5	3374	U	N3-C4-O4	-6.80	114.64	119.40
36	A1	347	G	C8-N9-C4	6.80	109.12	106.40
36	A5	669	U	C2-N3-C4	-6.80	122.92	127.00
36	A1	1906	G	C5-C6-O6	-6.80	124.52	128.60
36	A1	2237	C	N3-C4-C5	6.80	124.62	121.90
36	A5	1205	A	N7-C8-N9	6.80	117.20	113.80
36	A5	2434	U	C5-C4-O4	6.80	129.98	125.90
36	A1	948	C	C4-C5-C6	6.79	120.80	117.40
36	A1	1173	U	C2-N3-C4	-6.79	122.92	127.00
80	A6	1085	G	C5-C6-O6	6.79	132.68	128.60
37	A7	11	A	C5-N7-C8	6.79	107.30	103.90
1	A2	1006	C	C6-N1-C2	-6.79	117.58	120.30
36	A5	2619	G	C5-C6-O6	-6.79	124.52	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2639	G	C8-N9-C4	6.79	109.12	106.40
36	A5	63	A	N1-C6-N6	6.79	122.67	118.60
36	A1	394	G	N3-C2-N2	6.79	124.65	119.90
36	A1	521	A	N9-C4-C5	-6.79	103.08	105.80
36	A1	548	G	N3-C4-C5	6.79	132.00	128.60
36	A1	2362	C	N1-C2-O2	6.79	122.97	118.90
36	A1	2826	U	C5-C6-N1	-6.79	119.31	122.70
36	A1	2830	G	N3-C2-N2	-6.79	115.15	119.90
36	A5	2692	A	N1-C6-N6	-6.79	114.53	118.60
1	A2	1318	G	N1-C6-O6	6.79	123.97	119.90
36	A1	1060	U	C2-N3-C4	-6.79	122.93	127.00
36	A1	1200	A	N1-C6-N6	-6.79	114.53	118.60
36	A1	1329	U	N3-C2-O2	-6.79	117.45	122.20
36	A1	2351	U	N3-C2-O2	-6.79	117.45	122.20
79	Dp	17	ARG	NE-CZ-NH1	-6.79	116.91	120.30
80	A6	622	A	C4-C5-N7	-6.79	107.31	110.70
1	A2	142	G	N1-C2-N2	6.79	122.31	116.20
36	A1	383	G	C8-N9-C4	6.79	109.11	106.40
36	A1	1137	C	N1-C2-N3	6.79	123.95	119.20
47	DI	48	LEU	CA-CB-CG	6.79	130.91	115.30
38	A8	38	U	C4-C5-C6	6.78	123.77	119.70
1	A2	1762	A	C8-N9-C4	6.78	108.51	105.80
36	A1	895	A	N3-C4-N9	-6.78	121.97	127.40
36	A1	2650	U	C5-C4-O4	6.78	129.97	125.90
36	A5	1327	C	N3-C2-O2	-6.78	117.15	121.90
36	A1	304	G	N1-C2-N2	6.78	122.30	116.20
36	A1	1300	G	C8-N9-C4	6.78	109.11	106.40
36	A1	1432	C	C6-N1-C2	-6.78	117.59	120.30
80	A6	622	A	C8-N9-C4	-6.78	103.09	105.80
36	A5	838	G	C5-C6-O6	6.78	132.67	128.60
36	A5	1449	A	C6-C5-N7	-6.78	127.55	132.30
36	A5	2824	G	C4-C5-N7	-6.78	108.09	110.80
37	A7	49	G	C8-N9-C4	6.78	109.11	106.40
36	A1	3137	C	N1-C2-O2	-6.78	114.83	118.90
36	A1	30	G	N1-C2-N2	-6.78	110.10	116.20
80	A6	430	G	C5-C6-O6	-6.78	124.53	128.60
36	A5	2730	G	C2-N3-C4	-6.78	108.51	111.90
36	A5	2810	C	C4-C5-C6	6.78	120.79	117.40
36	A5	3076	C	C2-N3-C4	-6.78	116.51	119.90
36	A5	48	A	C8-N9-C4	-6.78	103.09	105.80
36	A5	413	U	C4-C5-C6	6.78	123.77	119.70
36	A5	1130	A	N1-C2-N3	-6.77	125.91	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1469	C	C6-N1-C2	-6.77	117.59	120.30
36	A1	2231	C	C6-N1-C2	6.77	123.01	120.30
36	A5	652	G	C6-N1-C2	-6.77	121.04	125.10
36	A5	1685	C	N3-C2-O2	-6.77	117.16	121.90
36	A1	2831	G	N3-C2-N2	-6.77	115.16	119.90
36	A5	146	U	C5-C4-O4	6.77	129.96	125.90
36	A5	2693	C	N1-C2-O2	6.77	122.96	118.90
1	A2	553	G	N1-C2-N2	6.77	122.29	116.20
31	Ad	36	LEU	CA-CB-CG	6.77	130.87	115.30
36	A1	2357	A	C4-C5-C6	6.77	120.39	117.00
80	A6	297	U	N3-C4-O4	6.77	124.14	119.40
80	A6	777	C	C5-C6-N1	6.77	124.38	121.00
80	A6	1614	A	N7-C8-N9	6.77	117.19	113.80
36	A5	2899	C	C4-C5-C6	6.77	120.78	117.40
37	A7	22	A	N1-C6-N6	6.77	122.66	118.60
36	A1	2350	C	N3-C4-C5	6.77	124.61	121.90
36	A1	2392	C	C5-C4-N4	-6.77	115.46	120.20
36	A5	2932	U	N3-C2-O2	-6.77	117.46	122.20
1	A2	1190	C	C6-N1-C2	6.77	123.01	120.30
36	A1	1495	U	C6-N1-C1'	6.77	130.67	121.20
36	A1	2378	C	N3-C4-N4	6.77	122.74	118.00
80	A6	163	G	C8-N9-C1'	6.77	135.80	127.00
36	A1	593	C	N1-C2-O2	-6.76	114.84	118.90
36	A1	2808	A	C4-C5-C6	6.76	120.38	117.00
36	A1	3083	G	N3-C4-N9	6.76	130.06	126.00
4	CC	235	LEU	CA-CB-CG	6.76	130.86	115.30
36	A5	644	G	N3-C4-C5	-6.76	125.22	128.60
36	A5	960	U	N3-C2-O2	-6.76	117.46	122.20
36	A5	1843	C	N3-C2-O2	-6.76	117.17	121.90
36	A1	1007	U	C5-C6-N1	-6.76	119.32	122.70
36	A1	1417	G	C8-N9-C4	6.76	109.11	106.40
36	A1	1615	C	C2-N3-C4	-6.76	116.52	119.90
36	A1	2984	C	N3-C4-N4	-6.76	113.27	118.00
36	A1	3034	C	N3-C2-O2	-6.76	117.17	121.90
38	A4	58	G	N9-C4-C5	-6.76	102.70	105.40
80	A6	677	G	N3-C4-C5	6.76	131.98	128.60
80	A6	1008	G	C5-C6-O6	-6.76	124.54	128.60
36	A5	749	C	C6-N1-C2	-6.76	117.59	120.30
36	A5	888	A	C5-C6-N1	-6.76	114.32	117.70
36	A5	2820	A	C6-N1-C2	-6.76	114.54	118.60
36	A5	3088	G	N3-C2-N2	6.76	124.63	119.90
36	A5	3313	U	C5-C4-O4	6.76	129.96	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1665	C	C2-N3-C4	-6.76	116.52	119.90
36	A5	205	C	N3-C2-O2	-6.76	117.17	121.90
36	A5	1116	G	N9-C4-C5	6.76	108.10	105.40
36	A5	1421	G	C2-N3-C4	-6.76	108.52	111.90
36	A5	3375	A	C2-N3-C4	6.76	113.98	110.60
36	A1	1405	U	C5-C6-N1	-6.76	119.32	122.70
36	A1	2611	U	C2-N3-C4	-6.76	122.94	127.00
80	A6	617	U	C2-N1-C1'	6.76	125.81	117.70
36	A1	1492	G	C4-C5-C6	6.76	122.85	118.80
36	A1	2274	U	N3-C2-O2	-6.76	117.47	122.20
80	A6	354	C	C4-C5-C6	-6.76	114.02	117.40
36	A5	2391	G	N7-C8-N9	6.76	116.48	113.10
36	A5	2647	A	N1-C6-N6	-6.76	114.55	118.60
1	A2	539	G	N7-C8-N9	6.75	116.48	113.10
36	A1	2415	C	C5-C6-N1	-6.75	117.62	121.00
36	A5	345	G	N1-C2-N2	-6.75	110.12	116.20
36	A5	890	C	N3-C4-C5	6.75	124.60	121.90
36	A1	3279	A	N7-C8-N9	6.75	117.17	113.80
80	A6	95	G	C8-N9-C4	-6.75	103.70	106.40
80	A6	426	G	N3-C4-C5	-6.75	125.22	128.60
36	A5	1910	A	N7-C8-N9	-6.75	110.42	113.80
37	A7	50	U	C5-C6-N1	6.75	126.08	122.70
1	A2	1210	C	N3-C4-C5	-6.75	119.20	121.90
36	A5	908	G	C4-N9-C1'	6.75	135.27	126.50
36	A5	2908	G	C5-C6-O6	6.75	132.65	128.60
36	A1	2286	U	N1-C2-N3	6.75	118.95	114.90
80	A6	44	U	N1-C2-N3	6.75	118.95	114.90
80	A6	543	C	C5-C4-N4	6.75	124.92	120.20
80	A6	624	G	C8-N9-C4	6.75	109.10	106.40
80	A6	1280	C	C4-C5-C6	6.75	120.77	117.40
36	A5	776	U	N3-C4-O4	-6.75	114.68	119.40
36	A5	1197	A	N1-C2-N3	6.75	132.67	129.30
36	A5	2584	G	C8-N9-C1'	-6.75	118.23	127.00
36	A1	2174	G	N7-C8-N9	6.75	116.47	113.10
36	A5	95	A	C5-C6-N6	-6.75	118.30	123.70
36	A1	96	G	C2-N3-C4	-6.74	108.53	111.90
36	A1	397	A	N1-C6-N6	-6.74	114.55	118.60
36	A1	1181	U	C5-C6-N1	-6.74	119.33	122.70
36	A1	2702	A	C8-N9-C4	-6.74	103.10	105.80
36	A5	3324	C	C6-N1-C2	6.74	123.00	120.30
36	A5	2685	C	C2-N3-C4	-6.74	116.53	119.90
36	A1	2153	U	N1-C2-N3	6.74	118.94	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	3319	U	N3-C2-O2	-6.74	117.48	122.20
36	A5	887	G	C2-N3-C4	-6.74	108.53	111.90
36	A5	2830	G	C4-C5-N7	-6.74	108.10	110.80
36	A1	1138	U	C2-N3-C4	-6.74	122.96	127.00
80	A6	382	C	N3-C4-C5	6.74	124.59	121.90
36	A5	322	U	C5-C4-O4	-6.74	121.86	125.90
36	A5	644	G	C8-N9-C4	-6.74	103.70	106.40
36	A1	1517	G	C5-N7-C8	6.74	107.67	104.30
36	A5	1134	G	C5-C6-N1	6.74	114.87	111.50
36	A1	374	A	C5-C6-N6	6.74	129.09	123.70
36	A1	649	A	C5-C6-N6	6.74	129.09	123.70
36	A1	1911	A	N9-C4-C5	-6.74	103.11	105.80
36	A5	1375	G	C2-N3-C4	6.74	115.27	111.90
36	A5	2317	A	N7-C8-N9	6.74	117.17	113.80
36	A5	3336	A	N1-C2-N3	6.74	132.67	129.30
36	A5	1911	A	C5-C6-N6	-6.73	118.31	123.70
36	A1	197	G	C5-C6-O6	-6.73	124.56	128.60
36	A1	1339	C	C5-C6-N1	-6.73	117.63	121.00
80	A6	1329	A	N9-C4-C5	-6.73	103.11	105.80
36	A5	2145	A	N1-C6-N6	-6.73	114.56	118.60
36	A1	1491	A	C8-N9-C4	6.73	108.49	105.80
36	A1	1507	G	C4-C5-C6	6.73	122.84	118.80
36	A5	1686	U	C5-C4-O4	-6.73	121.86	125.90
36	A5	2231	C	C4-C5-C6	6.73	120.77	117.40
56	DS	40	ARG	CG-CD-NE	6.73	125.94	111.80
1	A2	89	G	N7-C8-N9	-6.73	109.74	113.10
36	A1	928	C	C6-N1-C2	-6.73	117.61	120.30
36	A5	1056	U	N3-C4-O4	6.73	124.11	119.40
36	A5	1652	G	C5-N7-C8	6.73	107.66	104.30
36	A1	1309	U	N1-C2-O2	-6.73	118.09	122.80
80	A6	1095	U	C5-C6-N1	-6.73	119.34	122.70
36	A5	587	U	N3-C4-C5	6.73	118.64	114.60
36	A5	1044	U	C5-C6-N1	-6.73	119.34	122.70
36	A5	2920	U	C2-N3-C4	-6.73	122.96	127.00
36	A1	758	C	C6-N1-C2	-6.72	117.61	120.30
36	A1	1164	G	C8-N9-C4	-6.72	103.71	106.40
80	A6	1478	G	C6-C5-N7	-6.72	126.37	130.40
36	A5	1496	C	C2-N1-C1'	6.72	126.20	118.80
36	A1	410	U	N1-C2-N3	6.72	118.93	114.90
53	BP	131	ARG	NE-CZ-NH1	-6.72	116.94	120.30
36	A5	518	G	C4-C5-N7	6.72	113.49	110.80
36	A5	1392	G	C5-N7-C8	6.72	107.66	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1113	G	N3-C4-C5	6.72	131.96	128.60
36	A5	3309	G	C5-C6-O6	-6.72	124.57	128.60
36	A5	3140	G	C5-C6-O6	-6.72	124.57	128.60
36	A5	3050	U	N3-C4-O4	-6.72	114.70	119.40
36	A1	251	G	C4-N9-C1'	6.71	135.23	126.50
36	A1	1169	A	C5-C6-N1	-6.71	114.34	117.70
44	BF	160	ARG	NE-CZ-NH1	6.71	123.66	120.30
36	A5	215	G	C8-N9-C4	-6.71	103.71	106.40
1	A2	838	G	C8-N9-C4	6.71	109.08	106.40
36	A5	413	U	C5-C6-N1	-6.71	119.34	122.70
36	A5	1206	G	C8-N9-C4	-6.71	103.72	106.40
36	A5	2868	U	N3-C4-C5	6.71	118.63	114.60
1	A2	1246	C	N3-C2-O2	-6.71	117.20	121.90
1	A2	1521	G	N3-C4-C5	-6.71	125.24	128.60
36	A1	1339	C	N1-C2-N3	6.71	123.90	119.20
36	A1	2187	G	C6-C5-N7	-6.71	126.37	130.40
36	A1	2735	U	C4-C5-C6	-6.71	115.67	119.70
80	A6	119	A	C2-N3-C4	-6.71	107.24	110.60
36	A5	2892	A	N9-C4-C5	6.71	108.48	105.80
36	A5	3140	G	N1-C6-O6	6.71	123.93	119.90
36	A1	196	G	N9-C4-C5	-6.71	102.72	105.40
36	A5	2767	U	C5-C4-O4	6.71	129.93	125.90
36	A5	1042	U	C5-C4-O4	6.71	129.93	125.90
36	A5	2407	C	C5-C4-N4	-6.71	115.50	120.20
36	A5	3266	G	N1-C6-O6	-6.71	115.87	119.90
36	A1	943	U	C2-N3-C4	-6.71	122.98	127.00
40	BB	323	MET	CG-SD-CE	-6.71	89.47	100.20
36	A1	2909	U	C5-C4-O4	-6.71	121.88	125.90
36	A5	2422	C	N1-C2-O2	6.71	122.92	118.90
36	A1	637	C	O4'-C1'-N1	6.70	113.56	108.20
36	A1	1478	C	C6-N1-C2	6.70	122.98	120.30
36	A5	2135	U	C6-N1-C2	6.70	125.02	121.00
37	A7	25	G	N1-C6-O6	6.70	123.92	119.90
1	A2	192	U	C2-N1-C1'	6.70	125.74	117.70
36	A1	2649	A	N7-C8-N9	-6.70	110.45	113.80
36	A5	1882	G	C4-C5-N7	-6.70	108.12	110.80
38	A8	42	G	C4-N9-C1'	-6.70	117.79	126.50
36	A5	3214	U	N1-C2-O2	6.70	127.49	122.80
36	A5	614	C	C6-N1-C2	6.70	122.98	120.30
36	A5	2929	C	N1-C2-O2	-6.70	114.88	118.90
36	A1	1452	A	C8-N9-C4	6.70	108.48	105.80
36	A5	835	G	C6-N1-C2	-6.70	121.08	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1042	U	N1-C2-O2	6.70	127.49	122.80
36	A1	2860	U	N1-C2-N3	-6.69	110.88	114.90
1	A2	266	A	N9-C4-C5	-6.69	103.12	105.80
1	A2	340	U	N1-C2-O2	6.69	127.48	122.80
36	A1	426	G	N9-C4-C5	-6.69	102.72	105.40
80	A6	110	U	N3-C4-C5	6.69	118.61	114.60
36	A5	1057	A	N9-C4-C5	-6.69	103.12	105.80
38	A8	25	G	C5-C6-O6	6.69	132.62	128.60
36	A1	660	A	C8-N9-C4	6.69	108.48	105.80
36	A1	1305	U	N3-C4-O4	-6.69	114.72	119.40
36	A5	376	G	C2-N3-C4	6.69	115.25	111.90
50	DM	72	LEU	CA-CB-CG	6.69	130.69	115.30
36	A5	649	A	C8-N9-C4	-6.69	103.12	105.80
1	A2	736	C	C5-C6-N1	6.69	124.34	121.00
36	A1	361	A	N1-C6-N6	-6.69	114.59	118.60
36	A1	1387	G	C5-N7-C8	6.69	107.64	104.30
36	A1	2390	A	C6-N1-C2	-6.69	114.59	118.60
36	A1	2809	C	N1-C2-O2	6.69	122.91	118.90
80	A6	1783	C	C4-C5-C6	6.69	120.74	117.40
4	CC	111	VAL	CB-CA-C	-6.69	98.69	111.40
36	A5	400	G	C4-C5-N7	6.69	113.47	110.80
36	A1	339	C	N3-C2-O2	-6.69	117.22	121.90
36	A1	2175	U	C5-C6-N1	-6.68	119.36	122.70
36	A1	3110	C	C6-N1-C2	-6.68	117.63	120.30
36	A5	620	U	C5-C6-N1	6.68	126.04	122.70
36	A5	2411	U	N3-C4-O4	-6.68	114.72	119.40
36	A5	3138	U	N1-C2-N3	6.68	118.91	114.90
39	DA	246	LEU	CA-CB-CG	6.68	130.68	115.30
36	A1	1325	U	N1-C2-O2	-6.68	118.12	122.80
36	A1	1451	C	C6-N1-C2	6.68	122.97	120.30
36	A1	1513	G	C8-N9-C4	-6.68	103.73	106.40
36	A1	1537	A	N1-C6-N6	6.68	122.61	118.60
36	A1	2808	A	N9-C4-C5	-6.68	103.13	105.80
36	A5	436	A	N7-C8-N9	6.68	117.14	113.80
36	A5	1392	G	N9-C4-C5	-6.68	102.73	105.40
36	A5	1848	G	C6-C5-N7	-6.68	126.39	130.40
36	A5	3185	U	C5-C6-N1	-6.68	119.36	122.70
36	A1	2870	C	C4-C5-C6	-6.68	114.06	117.40
80	A6	232	U	C2-N1-C1'	6.68	125.72	117.70
36	A5	2279	A	N1-C2-N3	6.68	132.64	129.30
1	A2	1679	G	N3-C4-C5	-6.68	125.26	128.60
52	BO	104[B]	ILE	O-C-N	6.68	133.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1206	U	N3-C4-O4	6.68	124.07	119.40
1	A2	1258	U	C5-C4-O4	6.68	129.91	125.90
36	A5	3128	G	C5-C6-O6	-6.68	124.59	128.60
36	A1	546	C	C6-N1-C2	-6.67	117.63	120.30
36	A5	1359	C	C5-C4-N4	-6.67	115.53	120.20
36	A1	421	G	C5-C6-N1	6.67	114.83	111.50
36	A1	1382	G	C5-C6-O6	-6.67	124.60	128.60
36	A1	1402	C	C2-N3-C4	-6.67	116.56	119.90
36	A5	1389	G	C6-C5-N7	-6.67	126.40	130.40
36	A1	32	U	C5-C6-N1	-6.67	119.36	122.70
36	A1	2314	U	C2-N1-C1'	6.67	125.70	117.70
80	A6	1767	G	C8-N9-C4	6.67	109.07	106.40
36	A1	2808	A	C2-N3-C4	-6.67	107.27	110.60
36	A5	1307	G	C2-N3-C4	6.67	115.23	111.90
36	A1	791	A	C2-N3-C4	-6.67	107.27	110.60
36	A1	1112	A	N1-C6-N6	6.67	122.60	118.60
80	A6	1235	C	C5-C6-N1	6.67	124.33	121.00
80	A6	1609	U	N3-C2-O2	6.67	126.87	122.20
36	A1	664	U	C5-C4-O4	-6.67	121.90	125.90
36	A5	2403	G	C5-N7-C8	6.67	107.63	104.30
80	A6	1778	G	N1-C6-O6	-6.66	115.90	119.90
36	A5	332	C	C4-C5-C6	6.66	120.73	117.40
36	A5	930	U	C4-C5-C6	-6.66	115.70	119.70
36	A5	1159	A	C4-C5-N7	6.66	114.03	110.70
1	A2	131	C	C6-N1-C2	-6.66	117.64	120.30
36	A1	922	U	N1-C2-O2	6.66	127.46	122.80
36	A5	615	U	C5-C4-O4	-6.66	121.90	125.90
36	A5	3376	A	N9-C4-C5	6.66	108.46	105.80
36	A1	935	U	C5-C6-N1	-6.66	119.37	122.70
36	A1	2977	G	N1-C6-O6	-6.66	115.91	119.90
36	A1	3362	A	C4-N9-C1'	6.66	138.28	126.30
80	A6	65	A	C4-C5-N7	6.66	114.03	110.70
36	A5	652	G	N1-C2-N3	6.66	127.89	123.90
36	A5	2717	U	N1-C2-N3	6.66	118.89	114.90
1	A2	566	C	N1-C2-O2	6.66	122.89	118.90
36	A1	1807	G	C8-N9-C4	-6.66	103.74	106.40
36	A5	267	G	N9-C4-C5	-6.66	102.74	105.40
36	A1	633	C	C4-C5-C6	6.65	120.73	117.40
36	A1	2325	G	C2-N3-C4	6.65	115.23	111.90
36	A1	2111	G	N1-C6-O6	-6.65	115.91	119.90
36	A1	2187	G	C5-C6-O6	-6.65	124.61	128.60
80	A6	355	G	N1-C6-O6	-6.65	115.91	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	934	G	C2-N3-C4	6.65	115.22	111.90
36	A5	1439	U	C2-N3-C4	-6.65	123.01	127.00
36	A5	1890	U	C5-C6-N1	-6.65	119.38	122.70
36	A5	2292	U	C2-N1-C1'	6.65	125.68	117.70
36	A5	2743	A	C5-N7-C8	6.65	107.22	103.90
36	A5	3049	A	C6-N1-C2	6.65	122.59	118.60
36	A5	355	A	N1-C2-N3	6.65	132.62	129.30
36	A1	1056	U	C6-N1-C2	-6.65	117.01	121.00
36	A1	2550	U	N3-C4-O4	-6.65	114.75	119.40
36	A1	2799	A	N1-C2-N3	6.65	132.62	129.30
36	A1	2993	G	C5-C6-O6	6.65	132.59	128.60
36	A5	669	U	C4-C5-C6	6.65	123.69	119.70
36	A5	1146	C	N3-C2-O2	-6.65	117.25	121.90
36	A5	1208	U	C5-C6-N1	-6.65	119.38	122.70
36	A5	1844	C	N1-C2-O2	-6.65	114.91	118.90
36	A5	1931	U	N3-C4-O4	-6.65	114.75	119.40
36	A5	3007	U	N3-C4-C5	6.65	118.59	114.60
36	A1	1429	G	N3-C2-N2	6.65	124.55	119.90
36	A1	508	U	C6-N1-C2	6.64	124.99	121.00
36	A1	2899	C	N1-C2-N3	6.64	123.85	119.20
36	A5	361	A	N1-C6-N6	-6.64	114.61	118.60
36	A5	1409	G	C5-C6-O6	6.64	132.59	128.60
36	A5	3216	G	C6-C5-N7	-6.64	126.41	130.40
10	AI	172	ARG	NE-CZ-NH1	6.64	123.62	120.30
36	A1	432	G	C5-C6-N1	-6.64	108.18	111.50
36	A1	546	C	C2-N1-C1'	6.64	126.11	118.80
36	A1	903	U	N3-C2-O2	-6.64	117.55	122.20
36	A1	2286	U	N3-C2-O2	-6.64	117.55	122.20
80	A6	364	G	C5-C6-N1	6.64	114.82	111.50
36	A1	2952	G	C2-N3-C4	-6.64	108.58	111.90
80	A6	825	U	C6-N1-C2	6.64	124.98	121.00
36	A1	1050	U	N1-C2-O2	6.64	127.45	122.80
38	A4	13	A	C5-C6-N1	6.64	121.02	117.70
36	A1	1799	A	C8-N9-C4	6.64	108.45	105.80
36	A1	2172	A	N1-C6-N6	6.64	122.58	118.60
36	A5	2961	G	C5-C6-O6	6.64	132.58	128.60
36	A1	2184	U	C5-C6-N1	6.64	126.02	122.70
36	A1	3174	A	C5-N7-C8	-6.64	100.58	103.90
36	A5	625	G	N9-C4-C5	6.64	108.05	105.40
36	A5	3244	A	C2-N3-C4	-6.64	107.28	110.60
1	A2	1462	G	N9-C4-C5	-6.63	102.75	105.40
36	A5	2889	C	N3-C2-O2	-6.63	117.26	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1455	G	C5-C6-N1	-6.63	108.18	111.50
36	A5	3333	G	N1-C6-O6	6.63	123.88	119.90
36	A1	44	U	N3-C4-C5	6.63	118.58	114.60
38	A4	96	A	C8-N9-C4	6.63	108.45	105.80
1	A2	608	U	N1-C2-N3	6.63	118.88	114.90
36	A1	2657	A	C8-N9-C4	-6.63	103.15	105.80
36	A1	2884	C	C6-N1-C2	6.63	122.95	120.30
36	A5	1312	C	C6-N1-C2	-6.63	117.65	120.30
36	A5	226	C	N3-C4-C5	6.62	124.55	121.90
36	A1	112	U	N1-C2-O2	6.62	127.44	122.80
80	A6	36	C	N3-C4-N4	6.62	122.64	118.00
36	A5	2719	U	C6-N1-C1'	6.62	130.47	121.20
36	A5	3025	C	C5-C4-N4	6.62	124.84	120.20
36	A5	3039	C	C6-N1-C2	-6.62	117.65	120.30
1	A2	1297	G	C8-N9-C4	6.62	109.05	106.40
36	A1	2113	A	C8-N9-C4	6.62	108.45	105.80
36	A1	2638	C	C6-N1-C2	6.62	122.95	120.30
36	A5	1007	U	C5-C6-N1	-6.62	119.39	122.70
36	A5	2392	C	N1-C2-O2	-6.62	114.93	118.90
36	A1	923	C	N3-C2-O2	6.62	126.53	121.90
80	A6	380	U	N3-C2-O2	-6.62	117.57	122.20
80	A6	538	A	N1-C6-N6	-6.62	114.63	118.60
36	A1	1408	G	C5-C6-O6	6.62	132.57	128.60
36	A1	3295	A	C8-N9-C4	-6.62	103.15	105.80
80	A6	484	C	C5-C6-N1	6.62	124.31	121.00
36	A5	600	G	N7-C8-N9	6.62	116.41	113.10
36	A5	640	U	N3-C2-O2	-6.62	117.57	122.20
36	A5	966	U	C2-N3-C4	-6.62	123.03	127.00
36	A5	1876	U	C5-C6-N1	6.62	126.01	122.70
36	A5	925	A	C4-C5-C6	6.62	120.31	117.00
36	A1	326	U	C5-C4-O4	-6.62	121.93	125.90
36	A1	1297	C	C5-C6-N1	-6.62	117.69	121.00
44	BF	216	VAL	N-CA-C	6.62	128.86	111.00
36	A5	2201	G	N1-C6-O6	-6.62	115.93	119.90
36	A1	3349	C	C6-N1-C2	-6.61	117.66	120.30
36	A5	145	G	N3-C4-N9	-6.61	122.03	126.00
38	A8	24	G	N1-C6-O6	-6.61	115.93	119.90
36	A1	2198	A	N7-C8-N9	-6.61	110.50	113.80
80	A6	346	G	N1-C6-O6	-6.61	115.93	119.90
80	A6	1273	G	C5-C6-N1	6.61	114.81	111.50
36	A1	1367	G	N1-C2-N2	-6.61	110.25	116.20
36	A5	1518	U	N3-C4-C5	6.61	118.57	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1008	G	N1-C6-O6	6.61	123.86	119.90
80	A6	1030	A	N1-C6-N6	-6.61	114.64	118.60
36	A5	986	U	N3-C4-O4	6.61	124.03	119.40
36	A5	1754	G	N1-C6-O6	-6.61	115.94	119.90
36	A5	3303	G	N3-C2-N2	6.61	124.53	119.90
47	DI	10	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	A2	687	G	N3-C2-N2	-6.61	115.28	119.90
36	A5	3335	A	C2-N3-C4	-6.60	107.30	110.60
36	A1	970	A	N7-C8-N9	6.60	117.10	113.80
36	A1	2752	U	C5-C4-O4	6.60	129.86	125.90
36	A1	3000	A	N7-C8-N9	-6.60	110.50	113.80
36	A5	1049	C	C4-C5-C6	-6.60	114.10	117.40
80	A6	240	U	N1-C2-O2	6.60	127.42	122.80
36	A5	990	U	N3-C2-O2	-6.60	117.58	122.20
36	A1	35	A	N7-C8-N9	6.60	117.10	113.80
36	A1	1152	G	C2-N3-C4	-6.60	108.60	111.90
36	A1	1507	G	N1-C6-O6	6.60	123.86	119.90
36	A1	2552	C	N3-C2-O2	-6.60	117.28	121.90
36	A5	2357	A	N1-C6-N6	6.60	122.56	118.60
36	A5	2954	U	C2-N1-C1'	6.60	125.62	117.70
36	A1	885	U	C6-N1-C2	6.60	124.96	121.00
36	A1	1717	U	C5-C4-O4	6.60	129.86	125.90
36	A5	2207	A	C6-C5-N7	-6.60	127.68	132.30
36	A5	784	A	C6-C5-N7	-6.60	127.68	132.30
36	A5	792	G	N1-C2-N3	6.60	127.86	123.90
36	A5	2851	A	C8-N9-C4	6.60	108.44	105.80
36	A5	3122	A	C4-C5-C6	6.60	120.30	117.00
36	A1	391	A	N1-C6-N6	-6.59	114.64	118.60
80	A6	565	C	C6-N1-C1'	-6.59	112.89	120.80
49	DL	171	ARG	NE-CZ-NH1	-6.59	117.00	120.30
36	A1	954	U	N1-C2-N3	6.59	118.86	114.90
36	A5	721	G	C5-C6-N1	6.59	114.80	111.50
36	A5	2114	C	C6-N1-C2	-6.59	117.66	120.30
1	A2	783	G	N9-C4-C5	-6.59	102.76	105.40
36	A1	1903	U	N1-C2-O2	6.59	127.42	122.80
36	A1	2400	G	C2-N3-C4	-6.59	108.60	111.90
80	A6	1200	G	C8-N9-C1'	6.59	135.57	127.00
36	A1	1846	C	C4-C5-C6	6.59	120.69	117.40
36	A1	2115	G	C5-C6-O6	-6.59	124.65	128.60
36	A1	2293	C	N3-C4-C5	6.59	124.54	121.90
36	A1	2958	A	C8-N9-C4	6.59	108.44	105.80
80	A6	1	U	N1-C2-O2	6.59	127.41	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	3204	C	N3-C4-C5	6.59	124.53	121.90
80	A6	1258	U	N3-C2-O2	-6.59	117.59	122.20
36	A5	1004	U	N3-C2-O2	-6.59	117.59	122.20
36	A5	2811	A	C6-N1-C2	-6.59	114.65	118.60
36	A5	3115	C	N1-C2-O2	-6.59	114.95	118.90
36	A5	3289	G	N7-C8-N9	6.58	116.39	113.10
36	A1	2916	U	N3-C4-O4	6.58	124.01	119.40
36	A5	1159	A	N1-C2-N3	-6.58	126.01	129.30
36	A5	2866	U	N1-C2-O2	-6.58	118.19	122.80
36	A1	817	A	C8-N9-C4	-6.58	103.17	105.80
36	A1	2349	U	C5-C6-N1	-6.58	119.41	122.70
36	A5	828	A	N3-C4-C5	-6.58	122.19	126.80
36	A5	880	G	C5-C6-O6	-6.58	124.65	128.60
36	A5	2169	G	C2-N3-C4	6.58	115.19	111.90
36	A5	2647	A	C8-N9-C4	-6.58	103.17	105.80
36	A1	798	G	N3-C2-N2	-6.58	115.29	119.90
36	A1	1513	G	C6-N1-C2	-6.58	121.15	125.10
36	A1	2616	C	C5-C4-N4	-6.58	115.59	120.20
36	A1	3318	G	C8-N9-C4	-6.58	103.77	106.40
80	A6	711	U	C5-C6-N1	6.58	125.99	122.70
80	A6	1389	C	C6-N1-C1'	-6.58	112.91	120.80
37	A7	92	A	C5-N7-C8	-6.58	100.61	103.90
36	A1	1148	G	C2-N3-C4	6.58	115.19	111.90
36	A1	2381	G	N7-C8-N9	-6.58	109.81	113.10
80	A6	539	G	C5-N7-C8	-6.58	101.01	104.30
80	A6	1514	U	N3-C2-O2	-6.58	117.60	122.20
36	A5	2309	A	N1-C2-N3	-6.58	126.01	129.30
1	A2	557	G	C4-N9-C1'	6.58	135.05	126.50
39	BA	191	LEU	CA-CB-CG	-6.58	100.17	115.30
80	A6	1299	G	N3-C4-C5	-6.58	125.31	128.60
41	DC	138	ARG	NE-CZ-NH2	-6.58	117.01	120.30
36	A1	2328	U	C5-C4-O4	6.57	129.84	125.90
38	A4	55	U	N3-C2-O2	-6.57	117.60	122.20
36	A5	518	G	N1-C6-O6	6.57	123.84	119.90
36	A5	1200	A	C4-C5-C6	6.57	120.29	117.00
36	A5	3270	U	N3-C4-O4	-6.57	114.80	119.40
36	A5	3310	A	N1-C6-N6	-6.57	114.66	118.60
36	A5	360	G	C8-N9-C4	6.57	109.03	106.40
36	A1	1556	C	N3-C2-O2	-6.57	117.30	121.90
36	A5	1906	G	N1-C2-N3	6.57	127.84	123.90
36	A5	3105	U	N1-C2-O2	-6.57	118.20	122.80
38	A8	59	A	C2-N3-C4	6.57	113.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	916	G	C8-N9-C4	-6.57	103.77	106.40
36	A5	1151	U	N3-C4-C5	6.57	118.54	114.60
36	A1	500	C	C4-C5-C6	6.57	120.68	117.40
36	A5	2675	C	N1-C2-O2	-6.57	114.96	118.90
36	A1	1472	U	N3-C2-O2	6.57	126.80	122.20
36	A1	2860	U	C4-C5-C6	-6.57	115.76	119.70
36	A5	2257	C	N3-C2-O2	-6.57	117.30	121.90
38	A8	11	C	C4-C5-C6	6.57	120.68	117.40
36	A1	3208	G	N1-C2-N2	6.56	122.11	116.20
36	A1	1174	G	C5-C6-O6	-6.56	124.66	128.60
36	A1	1947	G	N3-C4-N9	-6.56	122.06	126.00
36	A1	3142	A	N1-C2-N3	6.56	132.58	129.30
36	A5	1788	C	N3-C4-C5	-6.56	119.28	121.90
37	A7	57	G	C4-C5-N7	-6.56	108.17	110.80
36	A1	3094	A	C5-C6-N1	6.56	120.98	117.70
37	A3	36	C	N1-C2-O2	6.56	122.84	118.90
80	A6	1781	A	C4-C5-N7	-6.56	107.42	110.70
36	A5	2347	U	N3-C4-O4	-6.56	114.81	119.40
36	A1	2649	A	C5-N7-C8	6.56	107.18	103.90
36	A5	1151	U	C4-C5-C6	-6.56	115.77	119.70
36	A5	1342	C	C4-C5-C6	6.56	120.68	117.40
36	A5	2301	U	C5-C6-N1	-6.56	119.42	122.70
36	A5	3153	U	N1-C2-O2	6.56	127.39	122.80
36	A5	2385	G	C8-N9-C4	6.56	109.02	106.40
36	A1	519	A	C5-C6-N6	-6.55	118.46	123.70
80	A6	282	C	C6-N1-C2	6.55	122.92	120.30
80	A6	901	G	N1-C6-O6	6.55	123.83	119.90
36	A5	1138	U	C2-N3-C4	-6.55	123.07	127.00
36	A5	1365	G	C8-N9-C1'	-6.55	118.48	127.00
36	A1	765	C	N1-C2-O2	6.55	122.83	118.90
80	A6	1170	G	N3-C4-N9	6.55	129.93	126.00
36	A1	2369	G	C6-N1-C2	-6.55	121.17	125.10
38	A4	1	A	C4-C5-N7	6.55	113.98	110.70
36	A5	2884	C	N1-C2-N3	6.55	123.79	119.20
36	A5	3263	G	N3-C2-N2	6.55	124.49	119.90
36	A5	3341	U	C6-N1-C2	-6.55	117.07	121.00
1	A2	647	G	N3-C2-N2	-6.55	115.31	119.90
36	A1	2967	A	N7-C8-N9	-6.55	110.53	113.80
80	A6	1414	U	N1-C2-N3	6.55	118.83	114.90
36	A5	2957	G	C8-N9-C4	6.55	109.02	106.40
36	A5	435	C	C2-N3-C4	-6.55	116.63	119.90
36	A5	2377	G	C2-N3-C4	6.55	115.17	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	785	G	C5-C6-N1	6.55	114.77	111.50
80	A6	1310	U	N1-C2-O2	6.55	127.38	122.80
36	A5	648	C	C6-N1-C2	-6.55	117.68	120.30
36	A5	815	G	C5-C6-O6	6.55	132.53	128.60
36	A1	823	C	C2-N3-C4	-6.54	116.63	119.90
36	A1	1801	U	C4-C5-C6	6.54	123.63	119.70
36	A5	2336	U	N3-C4-O4	-6.54	114.82	119.40
36	A5	3126	C	N3-C4-C5	6.54	124.52	121.90
36	A1	628	A	C8-N9-C4	6.54	108.42	105.80
36	A1	2870	C	C5-C4-N4	6.54	124.78	120.20
80	A6	1106	U	C4-C5-C6	6.54	123.63	119.70
36	A5	3186	A	N9-C4-C5	6.54	108.42	105.80
36	A1	654	C	C4-C5-C6	6.54	120.67	117.40
36	A1	2697	A	C5-C6-N1	6.54	120.97	117.70
36	A1	3304	U	C6-N1-C1'	6.54	130.36	121.20
80	A6	1106	U	C6-N1-C2	-6.54	117.08	121.00
80	A6	1652	C	C6-N1-C2	-6.54	117.68	120.30
36	A1	1911	A	C5-N7-C8	-6.54	100.63	103.90
36	A5	299	G	C2-N3-C4	6.54	115.17	111.90
36	A5	424	G	N3-C2-N2	6.54	124.48	119.90
37	A7	68	C	C2-N3-C4	-6.54	116.63	119.90
1	A2	6	G	N1-C2-N3	6.54	127.82	123.90
36	A1	63	A	C2-N3-C4	6.54	113.87	110.60
36	A1	2198	A	N1-C2-N3	6.54	132.57	129.30
36	A1	2388	U	N1-C2-O2	-6.54	118.22	122.80
36	A1	2958	A	C5-N7-C8	6.54	107.17	103.90
36	A5	828	A	C2-N3-C4	6.54	113.87	110.60
36	A5	1722	U	N3-C2-O2	6.54	126.78	122.20
36	A5	3306	U	C5-C6-N1	-6.54	119.43	122.70
36	A1	153	U	C6-N1-C2	-6.54	117.08	121.00
36	A1	281	G	N3-C2-N2	-6.54	115.33	119.90
80	A6	280	U	N3-C2-O2	-6.54	117.62	122.20
80	A6	352	A	N7-C8-N9	-6.54	110.53	113.80
36	A5	386	A	C6-C5-N7	-6.54	127.73	132.30
36	A5	884	A	N3-C4-N9	-6.54	122.17	127.40
36	A5	1215	U	N3-C4-O4	6.54	123.97	119.40
1	A2	557	G	C8-N9-C1'	-6.53	118.51	127.00
36	A1	785	G	C4-C5-N7	-6.53	108.19	110.80
80	A6	113	U	N1-C2-O2	-6.53	118.23	122.80
36	A5	641	C	C2-N1-C1'	-6.53	111.61	118.80
36	A5	2549	G	C6-C5-N7	-6.53	126.48	130.40
36	A5	2617	U	N3-C4-O4	-6.53	114.83	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	DI	182	LEU	CA-CB-CG	-6.53	100.27	115.30
1	A2	558	U	C2-N1-C1'	6.53	125.54	117.70
36	A1	1351	U	C2-N1-C1'	6.53	125.54	117.70
36	A1	3317	U	C6-N1-C2	-6.53	117.08	121.00
36	A5	859	G	N9-C4-C5	6.53	108.01	105.40
36	A1	1114	U	N3-C4-C5	6.53	118.52	114.60
80	A6	432	G	N3-C2-N2	-6.53	115.33	119.90
36	A5	1516	C	C5-C6-N1	-6.53	117.73	121.00
38	A8	6	U	C5-C6-N1	-6.53	119.44	122.70
1	A2	355	G	C6-N1-C2	-6.53	121.18	125.10
36	A1	1433	A	C6-N1-C2	-6.53	114.68	118.60
80	A6	1110	G	C4-C5-N7	-6.53	108.19	110.80
36	A5	2211	U	C5-C6-N1	-6.53	119.44	122.70
1	A2	266	A	C8-N9-C4	6.53	108.41	105.80
1	A2	1274	C	N3-C4-N4	-6.53	113.43	118.00
80	A6	101	U	C6-N1-C2	-6.53	117.08	121.00
36	A5	675	C	N3-C4-N4	6.53	122.57	118.00
36	A5	2626	A	C4-C5-N7	-6.53	107.44	110.70
1	A2	1282	U	C5-C4-O4	6.53	129.82	125.90
36	A1	2787	G	C2-N3-C4	6.53	115.16	111.90
68	Be	19	ARG	NE-CZ-NH2	6.53	123.56	120.30
80	A6	1542	G	N1-C6-O6	-6.53	115.98	119.90
36	A5	1211	U	N3-C4-C5	6.53	118.52	114.60
36	A5	2626	A	C5-C6-N1	-6.53	114.44	117.70
36	A5	3148	U	C5-C4-O4	-6.53	121.98	125.90
36	A1	800	G	C5-C6-N1	-6.52	108.24	111.50
80	A6	999	U	N3-C2-O2	-6.52	117.63	122.20
36	A5	1901	A	C4-C5-C6	6.52	120.26	117.00
36	A5	2147	A	N1-C6-N6	6.52	122.51	118.60
36	A1	3268	A	N1-C6-N6	6.52	122.51	118.60
36	A5	1448	U	N1-C2-O2	-6.52	118.23	122.80
36	A5	2699	G	N1-C6-O6	6.52	123.81	119.90
36	A5	3306	U	C6-N1-C2	6.52	124.91	121.00
37	A7	20	A	C5-C6-N6	-6.52	118.48	123.70
69	Df	49	ILE	CB-CA-C	-6.52	98.56	111.60
36	A5	370	U	N3-C2-O2	-6.52	117.64	122.20
36	A1	279	U	N3-C4-O4	-6.52	114.84	119.40
36	A5	1131	G	C2-N3-C4	-6.52	108.64	111.90
36	A5	2833	A	C8-N9-C4	6.52	108.41	105.80
1	A2	1503	A	N1-C2-N3	6.52	132.56	129.30
36	A1	623	U	C2-N1-C1'	-6.52	109.88	117.70
36	A1	1515	A	C2-N3-C4	-6.52	107.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2198	A	C5-C6-N6	-6.52	118.49	123.70
37	A3	97	A	N1-C6-N6	-6.52	114.69	118.60
36	A5	1215	U	N1-C2-O2	-6.52	118.24	122.80
36	A5	2800	G	N9-C4-C5	6.52	108.01	105.40
38	A8	54	A	C5-N7-C8	-6.52	100.64	103.90
36	A1	1851	G	N3-C4-C5	-6.52	125.34	128.60
36	A1	2145	A	N1-C2-N3	-6.52	126.04	129.30
80	A6	1473	U	N1-C2-N3	6.52	118.81	114.90
36	A5	1408	G	N3-C4-N9	-6.52	122.09	126.00
36	A1	903	U	C5-C6-N1	-6.51	119.44	122.70
36	A1	1902	G	C8-N9-C1'	-6.51	118.53	127.00
36	A1	2177	G	C5-C6-N1	6.51	114.76	111.50
80	A6	1087	A	C2-N3-C4	-6.51	107.34	110.60
36	A5	290	G	N3-C2-N2	6.51	124.46	119.90
36	A5	2303	A	N3-C4-C5	-6.51	122.24	126.80
36	A5	3190	C	C6-N1-C2	-6.51	117.69	120.30
36	A1	371	G	C8-N9-C4	6.51	109.00	106.40
36	A5	1496	C	C6-N1-C2	-6.51	117.69	120.30
80	A6	801	G	N1-C6-O6	-6.51	115.99	119.90
1	A2	1422	A	C8-N9-C4	6.51	108.40	105.80
36	A1	573	C	C5-C6-N1	-6.51	117.75	121.00
80	A6	151	G	N9-C4-C5	6.51	108.00	105.40
80	A6	394	C	C4-C5-C6	6.51	120.66	117.40
80	A6	448	C	C6-N1-C1'	6.51	128.61	120.80
80	A6	1510	U	C5-C4-O4	6.51	129.81	125.90
36	A5	2984	C	C2-N3-C4	-6.51	116.64	119.90
36	A5	3174	A	C4-C5-N7	6.51	113.95	110.70
35	Ah	134	ASP	OD1-CG-OD2	-6.51	110.94	123.30
80	A6	3	U	C6-N1-C2	6.51	124.91	121.00
36	A1	102	C	C5-C4-N4	-6.51	115.65	120.20
36	A1	1819	U	C2-N1-C1'	6.51	125.51	117.70
36	A5	420	G	N3-C4-C5	-6.51	125.35	128.60
36	A5	692	A	N1-C2-N3	-6.51	126.05	129.30
36	A1	819	U	N1-C2-O2	-6.50	118.25	122.80
36	A1	2885	C	C2-N3-C4	-6.50	116.65	119.90
36	A5	2904	U	C5-C6-N1	-6.50	119.45	122.70
40	DB	21	ARG	NE-CZ-NH1	6.50	123.55	120.30
36	A5	2849	C	C5-C6-N1	6.50	124.25	121.00
36	A1	506	U	C5-C6-N1	-6.50	119.45	122.70
36	A1	2647	A	C8-N9-C4	-6.50	103.20	105.80
20	CS	18	LEU	CA-CB-CG	6.50	130.25	115.30
36	A1	1060	U	C6-N1-C2	6.50	124.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2948	C	C5-C6-N1	-6.50	117.75	121.00
37	A3	93	C	N3-C4-C5	6.50	124.50	121.90
80	A6	1650	U	C2-N3-C4	-6.50	123.10	127.00
36	A5	370	U	C6-N1-C2	-6.50	117.10	121.00
36	A5	2320	A	N1-C2-N3	6.50	132.55	129.30
36	A5	3330	A	N1-C6-N6	-6.50	114.70	118.60
1	A2	132	U	C2-N1-C1'	-6.50	109.91	117.70
36	A1	2679	A	C4-C5-N7	6.50	113.95	110.70
49	BL	57	VAL	CB-CA-C	-6.50	99.06	111.40
80	A6	1340	U	N3-C2-O2	-6.50	117.65	122.20
38	A4	81	U	N1-C2-N3	6.50	118.80	114.90
36	A5	519	A	C5-C6-N6	-6.50	118.50	123.70
36	A1	1905	G	C5-C6-N1	6.49	114.75	111.50
36	A1	2152	A	C5-C6-N6	6.49	128.89	123.70
38	A4	53	A	C5-C6-N1	6.49	120.95	117.70
36	A5	783	A	N1-C6-N6	6.49	122.50	118.60
36	A5	2314	U	C2-N1-C1'	6.49	125.49	117.70
36	A1	859	G	C6-C5-N7	-6.49	126.50	130.40
36	A1	1180	A	N9-C4-C5	6.49	108.40	105.80
36	A1	2852	C	C6-N1-C1'	-6.49	113.01	120.80
36	A5	2258	U	N3-C2-O2	-6.49	117.66	122.20
36	A1	2662	G	C6-C5-N7	-6.49	126.50	130.40
36	A1	2945	G	N3-C2-N2	6.49	124.44	119.90
36	A5	345	G	N3-C2-N2	6.49	124.44	119.90
36	A5	429	U	N3-C4-C5	6.49	118.49	114.60
36	A5	947	G	N1-C6-O6	-6.49	116.01	119.90
36	A5	1434	G	C8-N9-C4	6.49	109.00	106.40
35	Ah	134	ASP	CB-CG-OD2	-6.49	112.46	118.30
36	A1	3063	C	N3-C2-O2	-6.49	117.36	121.90
36	A5	1190	A	C5-C6-N6	6.49	128.89	123.70
36	A1	184	U	N3-C2-O2	-6.49	117.66	122.20
38	A4	91	C	N1-C2-O2	6.49	122.79	118.90
36	A5	1215	U	C5-C4-O4	-6.49	122.01	125.90
36	A5	2288	G	C5-C6-O6	-6.49	124.71	128.60
36	A5	2433	U	N3-C4-C5	6.49	118.49	114.60
1	A2	830	U	N3-C2-O2	-6.49	117.66	122.20
1	A2	1473	U	N3-C2-O2	-6.49	117.66	122.20
36	A1	1604	G	C4-N9-C1'	6.49	134.93	126.50
36	A5	3043	C	N3-C4-C5	6.49	124.49	121.90
36	A1	644	G	C4-C5-C6	6.48	122.69	118.80
80	A6	580	A	C8-N9-C4	-6.48	103.21	105.80
1	A2	404	G	C5-C6-O6	-6.48	124.71	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2909	U	N3-C2-O2	6.48	126.74	122.20
80	A6	695	U	N1-C2-N3	6.48	118.79	114.90
36	A5	2396	G	N3-C4-C5	-6.48	125.36	128.60
1	A2	1024	U	N3-C2-O2	-6.48	117.66	122.20
36	A1	80	G	C5-C6-N1	6.48	114.74	111.50
36	A1	1329	U	C4-C5-C6	6.48	123.59	119.70
80	A6	1634	C	C2-N3-C4	6.48	123.14	119.90
36	A5	963	G	C5-C6-O6	-6.48	124.71	128.60
1	A2	965	U	C5-C6-N1	6.48	125.94	122.70
36	A5	3004	C	C5-C4-N4	-6.48	115.67	120.20
36	A1	359	U	C5-C6-N1	-6.48	119.46	122.70
36	A1	715	A	N1-C6-N6	6.48	122.49	118.60
36	A1	953	G	C8-N9-C1'	6.48	135.42	127.00
36	A1	1141	C	C4-C5-C6	6.48	120.64	117.40
36	A1	1578	C	C2-N1-C1'	6.48	125.93	118.80
51	DN	68	ARG	NE-CZ-NH1	6.48	123.54	120.30
80	A6	1478	G	C4-C5-C6	6.48	122.69	118.80
80	A6	1721	A	C8-N9-C4	6.48	108.39	105.80
36	A5	1298	C	N1-C2-O2	-6.48	115.01	118.90
36	A5	1897	G	C5-C6-O6	-6.48	124.71	128.60
36	A5	2857	C	C6-N1-C2	6.48	122.89	120.30
1	A2	1455	G	N1-C6-O6	6.47	123.78	119.90
36	A1	1523	U	N3-C2-O2	6.47	126.73	122.20
36	A1	1608	C	N1-C2-O2	6.47	122.78	118.90
36	A5	1408	G	N3-C4-C5	6.47	131.84	128.60
36	A5	2431	C	N3-C4-C5	-6.47	119.31	121.90
80	A6	815	G	C5-N7-C8	-6.47	101.06	104.30
80	A6	1298	U	C2-N3-C4	-6.47	123.12	127.00
36	A5	1392	G	C8-N9-C1'	-6.47	118.59	127.00
36	A5	2320	A	C5-N7-C8	6.47	107.14	103.90
36	A5	2518	C	C5-C6-N1	-6.47	117.76	121.00
36	A5	2719	U	C5-C6-N1	-6.47	119.46	122.70
67	Dd	90	PHE	CB-CA-C	-6.47	97.45	110.40
36	A1	427	C	N1-C2-O2	-6.47	115.02	118.90
36	A5	1161	G	N7-C8-N9	-6.47	109.86	113.10
36	A5	1399	A	C8-N9-C4	6.47	108.39	105.80
36	A5	1879	A	C4-C5-N7	6.47	113.94	110.70
36	A5	2351	U	N3-C4-O4	-6.47	114.87	119.40
36	A5	2837	A	C2-N3-C4	6.47	113.83	110.60
36	A1	579	G	N3-C2-N2	6.47	124.43	119.90
36	A1	1717	U	N3-C4-C5	-6.47	110.72	114.60
36	A5	217	U	C5-C6-N1	-6.47	119.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1284	C	C6-N1-C2	-6.47	117.71	120.30
1	A2	1085	G	N3-C2-N2	6.47	124.43	119.90
36	A1	610	G	C5-C6-N1	6.47	114.73	111.50
80	A6	1503	A	C4-C5-N7	6.47	113.93	110.70
36	A5	2746	A	C8-N9-C4	6.47	108.39	105.80
52	DO	27[B]	VAL	C-N-CA	6.47	137.87	121.70
36	A1	686	G	N1-C6-O6	-6.46	116.02	119.90
36	A1	3060	C	C5-C4-N4	-6.46	115.68	120.20
36	A1	646	A	C4-C5-C6	6.46	120.23	117.00
36	A1	974	G	N3-C4-C5	-6.46	125.37	128.60
36	A1	1083	G	N3-C4-C5	-6.46	125.37	128.60
36	A1	1371	G	C5-C6-O6	6.46	132.48	128.60
36	A1	1202	A	N1-C2-N3	6.46	132.53	129.30
80	A6	941	A	N1-C6-N6	-6.46	114.72	118.60
36	A5	2998	U	C5-C6-N1	-6.46	119.47	122.70
37	A7	12	U	N3-C4-C5	6.46	118.48	114.60
1	A2	1536	G	N3-C4-N9	6.46	129.88	126.00
38	A4	32	C	C6-N1-C1'	6.46	128.55	120.80
36	A5	284	A	C2-N3-C4	6.46	113.83	110.60
36	A5	369	A	N9-C4-C5	6.46	108.38	105.80
36	A5	1929	G	C8-N9-C4	6.46	108.98	106.40
36	A5	2631	U	N1-C2-N3	6.46	118.78	114.90
36	A5	2930	A	N1-C6-N6	-6.46	114.72	118.60
1	A2	1235	C	N1-C2-O2	-6.46	115.03	118.90
36	A1	948	C	C5-C6-N1	-6.46	117.77	121.00
36	A1	1042	U	N3-C2-O2	-6.46	117.68	122.20
36	A1	1126	G	C5-N7-C8	6.46	107.53	104.30
36	A1	1450	G	N3-C2-N2	-6.46	115.38	119.90
36	A1	2763	U	N3-C2-O2	6.46	126.72	122.20
36	A5	2440	G	N7-C8-N9	6.46	116.33	113.10
36	A1	324	A	C4-C5-C6	6.46	120.23	117.00
36	A1	2276	G	N9-C4-C5	6.46	107.98	105.40
36	A1	327	A	C5-C6-N6	-6.45	118.54	123.70
36	A1	2376	G	C2-N3-C4	6.45	115.13	111.90
36	A1	3151	U	C5-C4-O4	-6.45	122.03	125.90
38	A4	25	G	C5-C6-O6	6.45	132.47	128.60
38	A4	96	A	N9-C4-C5	-6.45	103.22	105.80
36	A5	1749	A	C8-N9-C4	6.45	108.38	105.80
36	A5	1894	U	C2-N3-C4	-6.45	123.13	127.00
37	A7	93	C	C4-C5-C6	6.45	120.63	117.40
36	A1	3204	C	C2-N3-C4	-6.45	116.67	119.90
80	A6	1000	C	C4-C5-C6	6.45	120.63	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	588	G	C5-C6-N1	6.45	114.73	111.50
36	A1	944	C	C6-N1-C2	-6.45	117.72	120.30
36	A1	966	U	C2-N3-C4	-6.45	123.13	127.00
36	A1	2202	C	C4-C5-C6	6.45	120.63	117.40
80	A6	139	C	C6-N1-C2	-6.45	117.72	120.30
37	A7	38	U	C6-N1-C1'	-6.45	112.17	121.20
38	A4	17	A	C5-C6-N1	-6.45	114.48	117.70
80	A6	565	C	C2-N1-C1'	6.45	125.89	118.80
80	A6	1035	G	C8-N9-C4	6.45	108.98	106.40
36	A5	894	G	C5-C6-O6	-6.45	124.73	128.60
36	A5	2662	G	C3'-C2'-C1'	-6.45	96.34	101.50
80	A6	687	G	C8-N9-C1'	6.45	135.38	127.00
1	A2	136	C	N1-C2-O2	6.45	122.77	118.90
36	A1	660	A	C5-C6-N1	6.45	120.92	117.70
36	A1	1148	G	C5-C6-N1	6.45	114.72	111.50
36	A1	1389	G	N1-C6-O6	6.45	123.77	119.90
36	A1	2368	A	N9-C4-C5	6.45	108.38	105.80
36	A5	343	U	C5-C6-N1	-6.45	119.48	122.70
1	A2	407	A	C4-C5-C6	6.44	120.22	117.00
1	A2	732	G	N9-C4-C5	-6.44	102.82	105.40
36	A1	802	C	N3-C2-O2	-6.44	117.39	121.90
36	A1	1727	G	C8-N9-C4	-6.44	103.82	106.40
36	A1	1934	G	C8-N9-C4	-6.44	103.82	106.40
36	A5	2993	G	N9-C4-C5	-6.44	102.82	105.40
1	A2	554	C	C2-N1-C1'	6.44	125.89	118.80
36	A1	864	G	N1-C2-N2	-6.44	110.40	116.20
36	A1	1931	U	C2-N1-C1'	-6.44	109.97	117.70
36	A1	2369	G	N7-C8-N9	6.44	116.32	113.10
36	A1	3382	U	C2-N1-C1'	6.44	125.43	117.70
80	A6	1755	A	C5-N7-C8	-6.44	100.68	103.90
36	A5	971	G	N1-C2-N2	6.44	122.00	116.20
36	A5	1451	C	C5-C6-N1	-6.44	117.78	121.00
36	A5	1607	U	N1-C2-N3	6.44	118.77	114.90
36	A5	1843	C	C2-N1-C1'	6.44	125.89	118.80
36	A5	2124	G	C8-N9-C4	6.44	108.98	106.40
36	A5	3306	U	N3-C4-C5	6.44	118.47	114.60
1	A2	75	U	N1-C2-O2	6.44	127.31	122.80
36	A1	386	A	C6-C5-N7	-6.44	127.79	132.30
80	A6	805	U	C6-N1-C2	-6.44	117.14	121.00
36	A5	3175	U	N3-C4-C5	-6.44	110.74	114.60
36	A1	1107	C	N3-C4-C5	6.44	124.48	121.90
36	A1	952	A	C5-C6-N1	6.44	120.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1413	G	N1-C6-O6	-6.44	116.04	119.90
80	A6	1473	U	C2-N1-C1'	6.44	125.42	117.70
37	A7	1	G	C4-N9-C1'	6.44	134.87	126.50
36	A1	105	C	N3-C4-C5	6.43	124.47	121.90
36	A5	3006	A	N3-C4-N9	-6.43	122.25	127.40
1	A2	1200	G	C4-C5-C6	6.43	122.66	118.80
36	A1	2349	U	N1-C2-N3	6.43	118.76	114.90
36	A5	393	U	N3-C2-O2	-6.43	117.70	122.20
36	A5	1840	U	C5-C6-N1	-6.43	119.48	122.70
36	A5	2246	G	N3-C4-C5	-6.43	125.38	128.60
36	A5	2879	C	N1-C2-O2	6.43	122.76	118.90
36	A1	2257	C	N3-C2-O2	-6.43	117.40	121.90
36	A1	1834	U	C5-C6-N1	-6.43	119.49	122.70
36	A5	667	C	N3-C4-C5	6.43	124.47	121.90
36	A1	91	G	C5-N7-C8	-6.43	101.09	104.30
38	A4	51	G	N1-C6-O6	6.43	123.76	119.90
36	A1	922	U	C5-C6-N1	6.43	125.91	122.70
80	A6	612	U	N3-C4-O4	-6.43	114.90	119.40
80	A6	653	C	N3-C4-N4	6.43	122.50	118.00
36	A1	205	C	N3-C4-C5	6.42	124.47	121.90
36	A5	824	C	C4-C5-C6	6.42	120.61	117.40
36	A5	2754	G	N3-C2-N2	6.42	124.40	119.90
1	A2	1169	G	N7-C8-N9	6.42	116.31	113.10
36	A5	1402	C	C4-C5-C6	6.42	120.61	117.40
38	A4	25	G	N1-C2-N3	6.42	127.75	123.90
38	A4	38	U	N1-C2-O2	6.42	127.30	122.80
36	A5	436	A	C4-N9-C1'	6.42	137.86	126.30
36	A5	1403	C	N3-C4-N4	6.42	122.50	118.00
36	A1	3155	U	N1-C2-O2	6.42	127.29	122.80
36	A5	779	G	C8-N9-C4	-6.42	103.83	106.40
1	A2	610	G	C4-N9-C1'	6.42	134.84	126.50
80	A6	1571	C	C4-C5-C6	6.42	120.61	117.40
36	A5	651	G	C8-N9-C4	-6.42	103.83	106.40
36	A5	2891	U	C5-C6-N1	-6.42	119.49	122.70
36	A1	1481	A	C6-C5-N7	-6.42	127.81	132.30
36	A1	1948	G	N3-C4-N9	6.42	129.85	126.00
80	A6	1652	C	N1-C2-N3	6.42	123.69	119.20
36	A5	1907	C	N1-C2-O2	-6.42	115.05	118.90
36	A5	2340	U	C2-N3-C4	-6.42	123.15	127.00
42	DD	152	ARG	NE-CZ-NH1	6.42	123.51	120.30
38	A4	16	G	C8-N9-C4	6.42	108.97	106.40
36	A5	1064	A	C4-C5-N7	6.42	113.91	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	843	A	C2-N3-C4	-6.41	107.39	110.60
80	A6	317	C	C2-N3-C4	-6.41	116.69	119.90
13	CL	5	LEU	CA-CB-CG	6.41	130.05	115.30
36	A5	950	G	N3-C2-N2	6.41	124.39	119.90
36	A5	1321	G	C5-C6-N1	-6.41	108.29	111.50
1	A2	1185	U	C2-N1-C1'	6.41	125.39	117.70
36	A1	2639	G	N9-C4-C5	-6.41	102.84	105.40
36	A1	2987	A	N1-C2-N3	6.41	132.50	129.30
80	A6	1112	G	C6-N1-C2	-6.41	121.25	125.10
36	A5	2231	C	N3-C4-C5	-6.41	119.34	121.90
36	A1	2356	A	C8-N9-C4	6.41	108.36	105.80
36	A5	679	U	C5-C6-N1	-6.41	119.50	122.70
36	A5	2302	G	N1-C2-N2	-6.41	110.43	116.20
37	A7	40	C	N1-C2-O2	-6.41	115.05	118.90
36	A5	2611	U	C4-C5-C6	6.41	123.54	119.70
36	A1	641	C	C2-N3-C4	-6.41	116.70	119.90
80	A6	1649	G	N3-C2-N2	6.41	124.38	119.90
36	A5	2408	U	N1-C2-N3	6.41	118.74	114.90
36	A5	3354	U	N3-C2-O2	-6.41	117.72	122.20
36	A1	1042	U	N3-C4-C5	6.40	118.44	114.60
36	A5	584	G	C5-C6-O6	6.40	132.44	128.60
1	A2	1000	C	N1-C2-O2	6.40	122.74	118.90
36	A1	77	A	N1-C6-N6	-6.40	114.76	118.60
36	A1	2866	U	N3-C2-O2	-6.40	117.72	122.20
36	A5	2345	A	C5-C6-N6	-6.40	118.58	123.70
68	De	45	ARG	NE-CZ-NH1	6.40	123.50	120.30
80	A6	621	A	C8-N9-C4	6.40	108.36	105.80
36	A5	2817	A	N3-C4-C5	-6.40	122.32	126.80
36	A1	66	A	C2-N3-C4	-6.40	107.40	110.60
36	A1	408	A	N1-C6-N6	-6.40	114.76	118.60
36	A1	582	G	C6-C5-N7	6.40	134.24	130.40
36	A1	1891	A	C2-N3-C4	-6.40	107.40	110.60
36	A1	2987	A	C2-N3-C4	-6.40	107.40	110.60
37	A3	10	C	C6-N1-C2	-6.40	117.74	120.30
36	A5	1390	A	C5-C6-N6	6.40	128.82	123.70
36	A1	2653	C	N1-C2-N3	6.40	123.68	119.20
36	A1	2980	U	N1-C2-N3	6.40	118.74	114.90
36	A5	2134	G	N3-C4-C5	-6.40	125.40	128.60
36	A5	3003	G	C5-C6-N1	6.40	114.70	111.50
36	A1	87	U	N1-C2-N3	6.39	118.74	114.90
36	A1	1166	G	C4-C5-N7	6.39	113.36	110.80
80	A6	1484	G	N3-C4-N9	6.39	129.84	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1115	G	C4-N9-C1'	6.39	134.81	126.50
41	BC	95	ARG	NE-CZ-NH2	6.39	123.50	120.30
36	A5	1793	C	C2-N3-C4	6.39	123.10	119.90
36	A5	2130	G	N1-C6-O6	-6.39	116.06	119.90
36	A5	2365	C	C5-C4-N4	6.39	124.67	120.20
36	A5	3303	G	N1-C2-N2	-6.39	110.45	116.20
54	DQ	176	ARG	NE-CZ-NH1	-6.39	117.10	120.30
36	A1	641	C	C6-N1-C1'	6.39	128.47	120.80
37	A3	98	C	C5-C6-N1	-6.39	117.81	121.00
80	A6	603	U	N1-C2-O2	-6.39	118.33	122.80
36	A5	65	A	N7-C8-N9	6.39	117.00	113.80
36	A5	943	U	C5-C6-N1	-6.39	119.50	122.70
36	A5	3174	A	C5-N7-C8	-6.39	100.70	103.90
37	A7	48	U	N1-C2-O2	-6.39	118.33	122.80
1	A2	136	C	C6-N1-C1'	-6.39	113.13	120.80
36	A1	2193	U	N1-C2-N3	6.39	118.73	114.90
80	A6	1111	G	C5-C6-O6	-6.39	124.77	128.60
36	A5	2677	G	N3-C2-N2	-6.39	115.43	119.90
37	A7	15	C	N3-C4-C5	6.39	124.46	121.90
36	A1	582	G	N3-C4-N9	-6.39	122.17	126.00
36	A5	645	A	C5-C6-N1	6.39	120.89	117.70
36	A5	909	G	C4-C5-N7	-6.39	108.25	110.80
36	A1	630	A	N1-C6-N6	-6.39	114.77	118.60
36	A1	2973	G	C8-N9-C4	6.39	108.95	106.40
36	A1	3362	A	C8-N9-C4	-6.39	103.25	105.80
80	A6	541	A	C8-N9-C4	-6.39	103.25	105.80
36	A5	1211	U	C4-C5-C6	-6.39	115.87	119.70
36	A5	1518	U	N1-C2-O2	6.39	127.27	122.80
36	A5	2389	C	N3-C4-C5	6.39	124.45	121.90
36	A1	835	G	N9-C4-C5	-6.38	102.85	105.40
36	A1	973	A	N7-C8-N9	6.38	116.99	113.80
36	A1	1719	G	N9-C4-C5	-6.38	102.85	105.40
36	A5	2117	A	N1-C6-N6	-6.38	114.77	118.60
36	A5	2349	U	N3-C4-C5	6.38	118.43	114.60
36	A5	2753	G	N3-C2-N2	-6.38	115.43	119.90
25	AX	33	LEU	CA-CB-CG	-6.38	100.62	115.30
36	A1	3072	C	N1-C2-O2	6.38	122.73	118.90
36	A5	2416	U	C5-C6-N1	6.38	125.89	122.70
36	A1	1060	U	N3-C4-O4	-6.38	114.93	119.40
36	A1	2870	C	C5-C6-N1	6.38	124.19	121.00
36	A5	1851	G	C4-C5-C6	6.38	122.63	118.80
54	BQ	111	ARG	NE-CZ-NH1	-6.38	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	652	G	N3-C4-N9	6.38	129.83	126.00
36	A5	891	G	C5-C6-O6	6.38	132.43	128.60
38	A8	29	U	C2-N3-C4	-6.38	123.17	127.00
64	Da	28	HIS	N-CA-C	6.38	128.23	111.00
1	A2	1096	C	N3-C2-O2	-6.38	117.44	121.90
36	A1	102	C	N3-C4-N4	6.38	122.47	118.00
36	A1	2377	G	C5-C6-O6	6.38	132.43	128.60
36	A1	2661	G	C5-C6-O6	-6.38	124.77	128.60
38	A8	19	C	C4-C5-C6	6.38	120.59	117.40
36	A1	1589	A	C5-C6-N1	6.38	120.89	117.70
36	A1	1846	C	N1-C2-N3	6.38	123.66	119.20
36	A1	2921	U	C2-N3-C4	-6.38	123.17	127.00
80	A6	7	G	C5-C6-N1	6.38	114.69	111.50
36	A5	75	G	C5-C6-O6	-6.38	124.77	128.60
36	A5	2964	G	N7-C8-N9	-6.38	109.91	113.10
38	A8	28	C	N3-C4-C5	6.38	124.45	121.90
36	A5	2363	A	C2-N3-C4	6.38	113.79	110.60
1	A2	1758	U	C6-N1-C2	-6.37	117.17	121.00
36	A1	2187	G	N1-C6-O6	6.37	123.72	119.90
80	A6	470	A	N7-C8-N9	6.37	116.99	113.80
36	A5	2146	C	C6-N1-C2	-6.37	117.75	120.30
36	A5	2351	U	N3-C2-O2	-6.37	117.74	122.20
36	A5	2894	C	N3-C4-C5	6.37	124.45	121.90
36	A1	21	G	N1-C6-O6	-6.37	116.08	119.90
59	BV	48	ARG	NE-CZ-NH1	6.37	123.48	120.30
25	CX	79	ASN	CB-CA-C	-6.37	97.66	110.40
36	A5	2288	G	N3-C4-C5	-6.37	125.42	128.60
36	A5	2948	C	C5-C4-N4	6.37	124.66	120.20
1	A2	144	U	C6-N1-C2	-6.37	117.18	121.00
36	A1	72	C	C2-N3-C4	-6.37	116.72	119.90
36	A1	716	A	C4-C5-N7	6.37	113.88	110.70
36	A1	1520	G	C2-N3-C4	6.37	115.08	111.90
80	A6	101	U	N3-C2-O2	-6.37	117.74	122.20
80	A6	402	C	C6-N1-C2	6.37	122.85	120.30
36	A5	1832	C	C2-N3-C4	-6.37	116.72	119.90
36	A5	2261	G	C8-N9-C4	6.37	108.95	106.40
36	A1	1082	U	C5-C6-N1	6.37	125.88	122.70
36	A1	1801	U	C5-C6-N1	-6.37	119.52	122.70
36	A1	2353	G	C4-C5-N7	6.37	113.35	110.80
80	A6	1082	C	C2-N1-C1'	6.37	125.80	118.80
1	A2	628	G	N3-C2-N2	6.36	124.35	119.90
36	A1	702	C	C2-N3-C4	-6.36	116.72	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2533	G	N3-C4-N9	6.36	129.82	126.00
36	A1	2616	C	C2-N3-C4	-6.36	116.72	119.90
80	A6	1188	G	N1-C6-O6	6.36	123.72	119.90
36	A5	1042	U	C5-C6-N1	-6.36	119.52	122.70
36	A5	1416	C	N3-C2-O2	-6.36	117.45	121.90
52	DO	23[B]	ILE	O-C-N	6.36	132.88	122.70
36	A1	670	C	C4-C5-C6	6.36	120.58	117.40
36	A1	2198	A	C2-N3-C4	-6.36	107.42	110.60
80	A6	1099	U	C5-C4-O4	6.36	129.72	125.90
55	BR	125	LYS	CD-CE-NZ	6.36	126.33	111.70
80	A6	539	G	N3-C4-N9	-6.36	122.18	126.00
80	A6	639	U	C2-N1-C1'	6.36	125.33	117.70
36	A5	665	A	C2-N3-C4	-6.36	107.42	110.60
37	A7	92	A	C4-C5-N7	6.36	113.88	110.70
1	A2	1611	A	C8-N9-C4	-6.36	103.26	105.80
1	A2	1745	G	N9-C4-C5	-6.36	102.86	105.40
36	A1	196	G	C5-C6-N1	6.36	114.68	111.50
36	A1	875	G	N1-C6-O6	-6.36	116.08	119.90
36	A1	1177	G	N3-C2-N2	-6.36	115.45	119.90
36	A1	1379	G	C5-C6-O6	6.36	132.41	128.60
36	A1	2203	U	N1-C2-O2	-6.36	118.35	122.80
80	A6	795	U	N3-C2-O2	-6.36	117.75	122.20
80	A6	1113	A	N1-C2-N3	6.36	132.48	129.30
36	A5	903	U	N3-C2-O2	-6.36	117.75	122.20
36	A5	1172	G	N3-C2-N2	6.36	124.35	119.90
36	A1	2291	A	C2-N3-C4	6.36	113.78	110.60
80	A6	1091	A	C5-C6-N1	-6.36	114.52	117.70
36	A5	2817	A	C6-N1-C2	-6.36	114.79	118.60
38	A8	17	A	C4-C5-N7	6.36	113.88	110.70
55	DR	88	ARG	NE-CZ-NH1	-6.36	117.12	120.30
36	A5	3189	G	N1-C2-N3	6.35	127.71	123.90
36	A1	331	G	C5-C6-O6	6.35	132.41	128.60
36	A1	1919	G	C5-C6-O6	6.35	132.41	128.60
36	A1	2298	U	N3-C4-C5	6.35	118.41	114.60
36	A1	2703	A	N7-C8-N9	6.35	116.98	113.80
36	A5	833	G	N1-C2-N3	6.35	127.71	123.90
36	A5	940	G	C8-N9-C4	-6.35	103.86	106.40
36	A5	1147	G	N7-C8-N9	-6.35	109.92	113.10
36	A5	42	C	C5-C6-N1	6.35	124.17	121.00
36	A1	823	C	C5-C6-N1	-6.35	117.83	121.00
36	A5	1403	C	C6-N1-C1'	-6.35	113.18	120.80
36	A5	3167	A	N7-C8-N9	6.35	116.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	761	A	C2-N3-C4	-6.35	107.43	110.60
36	A1	1371	G	C4-C5-N7	-6.35	108.26	110.80
36	A1	3092	C	C2-N3-C4	-6.35	116.73	119.90
80	A6	364	G	C8-N9-C4	6.35	108.94	106.40
36	A5	787	G	C2-N3-C4	-6.35	108.73	111.90
36	A5	1200	A	N1-C2-N3	6.35	132.47	129.30
38	A8	111	A	C2-N3-C4	-6.35	107.43	110.60
36	A5	2802	A	N1-C2-N3	-6.35	126.13	129.30
38	A4	32	C	N3-C4-C5	6.34	124.44	121.90
80	A6	1030	A	C8-N9-C4	-6.34	103.26	105.80
36	A5	938	C	C6-N1-C2	6.34	122.84	120.30
36	A5	1690	C	N1-C2-O2	-6.34	115.09	118.90
36	A1	2409	G	N1-C6-O6	-6.34	116.09	119.90
41	DC	327	LEU	CA-CB-CG	6.34	129.89	115.30
36	A1	1411	C	N1-C2-O2	6.34	122.70	118.90
36	A5	1340	G	N3-C2-N2	6.34	124.34	119.90
36	A5	2361	A	C8-N9-C4	-6.34	103.26	105.80
36	A5	2625	C	N3-C2-O2	-6.34	117.46	121.90
36	A5	2633	U	C5-C6-N1	-6.34	119.53	122.70
36	A1	688	G	N1-C6-O6	-6.34	116.10	119.90
36	A1	295	A	N9-C4-C5	6.34	108.33	105.80
80	A6	1520	U	N1-C2-O2	-6.34	118.36	122.80
36	A5	2305	G	C4-C5-N7	6.34	113.33	110.80
36	A5	3309	G	C4-N9-C1'	6.34	134.74	126.50
36	A5	1149	G	N1-C2-N3	-6.33	120.10	123.90
36	A5	1496	C	C5-C6-N1	6.33	124.17	121.00
80	A6	392	G	C5-C6-N1	6.33	114.67	111.50
36	A1	1003	A	C6-C5-N7	-6.33	127.87	132.30
36	A1	2935	U	C2-N3-C4	6.33	130.80	127.00
36	A5	1041	U	C6-N1-C2	6.33	124.80	121.00
36	A5	2277	C	C6-N1-C2	6.33	122.83	120.30
77	Dn	9	ARG	NE-CZ-NH2	-6.33	117.14	120.30
36	A1	327	A	N9-C4-C5	-6.33	103.27	105.80
38	A8	29	U	N1-C2-N3	6.33	118.70	114.90
1	A2	557	G	C4-C5-C6	6.33	122.60	118.80
36	A1	1425	U	N3-C4-O4	-6.33	114.97	119.40
36	A1	2795	U	N3-C4-O4	-6.33	114.97	119.40
80	A6	351	C	C4-C5-C6	6.33	120.56	117.40
36	A5	1858	A	N7-C8-N9	6.33	116.97	113.80
36	A5	2123	G	C2-N3-C4	6.33	115.06	111.90
36	A1	953	G	N3-C4-N9	-6.33	122.20	126.00
80	A6	1627	U	C5-C4-O4	6.33	129.69	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1869	C	N3-C4-C5	6.32	124.43	121.90
36	A1	2608	G	N3-C2-N2	6.32	124.33	119.90
80	A6	756	A	C8-N9-C4	-6.32	103.27	105.80
80	A6	1619	C	C6-N1-C2	-6.32	117.77	120.30
32	Ce	10	ARG	NE-CZ-NH1	-6.32	117.14	120.30
36	A5	2393	G	N9-C4-C5	-6.32	102.87	105.40
36	A1	2973	G	N1-C6-O6	6.32	123.69	119.90
38	A4	81	U	C6-N1-C2	-6.32	117.21	121.00
80	A6	355	G	C5-C6-N1	6.32	114.66	111.50
36	A5	2375	G	C5-C6-N1	6.32	114.66	111.50
1	A2	1246	C	C5-C4-N4	6.32	124.62	120.20
36	A1	1474	A	C2-N3-C4	-6.32	107.44	110.60
36	A5	248	U	N1-C2-O2	6.32	127.22	122.80
36	A5	892	U	N3-C4-C5	6.32	118.39	114.60
36	A5	1733	G	N1-C6-O6	6.32	123.69	119.90
36	A5	1407	A	C8-N9-C4	6.32	108.33	105.80
36	A5	2996	U	C2-N1-C1'	6.32	125.28	117.70
36	A5	625	G	C5-C6-O6	6.32	132.39	128.60
36	A5	947	G	N3-C4-N9	6.32	129.79	126.00
36	A5	1833	G	N7-C8-N9	-6.32	109.94	113.10
36	A5	2614	G	C8-N9-C1'	-6.32	118.79	127.00
1	A2	377	G	C5-C6-O6	-6.32	124.81	128.60
36	A1	335	G	C8-N9-C4	-6.32	103.87	106.40
36	A1	1294	A	C8-N9-C4	-6.32	103.27	105.80
36	A1	1518	U	N1-C2-N3	6.32	118.69	114.90
36	A1	3001	C	N3-C4-C5	6.32	124.43	121.90
36	A5	436	A	C5-N7-C8	-6.32	100.74	103.90
36	A5	3011	A	N1-C2-N3	-6.32	126.14	129.30
36	A5	3309	G	C6-N1-C2	-6.32	121.31	125.10
36	A1	1472	U	N1-C2-O2	-6.31	118.38	122.80
36	A1	1492	G	N9-C4-C5	6.31	107.93	105.40
80	A6	350	U	N3-C2-O2	-6.31	117.78	122.20
36	A5	510	G	C5-C6-N1	6.31	114.66	111.50
36	A5	631	U	N3-C4-C5	6.31	118.39	114.60
36	A5	1130	A	N3-C4-C5	-6.31	122.38	126.80
1	A2	1430	U	C5-C4-O4	6.31	129.69	125.90
36	A1	1846	C	C2-N3-C4	-6.31	116.74	119.90
36	A1	2369	G	C5-C6-N1	6.31	114.66	111.50
36	A5	676	G	C8-N9-C4	-6.31	103.88	106.40
36	A5	1188	U	C5-C4-O4	-6.31	122.11	125.90
36	A5	1300	G	C5-C6-O6	-6.31	124.81	128.60
36	A5	1902	G	N3-C4-N9	6.31	129.79	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	3245	A	C5-C6-N6	-6.31	118.65	123.70
36	A1	434	U	N1-C2-O2	6.31	127.22	122.80
36	A5	904	A	C8-N9-C4	-6.31	103.28	105.80
36	A5	2420	C	C5-C4-N4	-6.31	115.78	120.20
36	A1	2906	C	N1-C2-N3	6.31	123.62	119.20
80	A6	65	A	C5-C6-N1	-6.31	114.55	117.70
36	A5	3187	A	C4-C5-N7	-6.31	107.55	110.70
36	A1	953	G	C4-N9-C1'	-6.31	118.30	126.50
36	A1	1136	A	C6-N1-C2	-6.31	114.82	118.60
36	A1	1646	G	C4-C5-N7	6.31	113.32	110.80
36	A5	600	G	C8-N9-C4	-6.31	103.88	106.40
36	A5	1123	U	C5-C6-N1	-6.31	119.55	122.70
36	A5	3270	U	C5-C6-N1	-6.31	119.55	122.70
39	DA	204	MET	CG-SD-CE	-6.31	90.11	100.20
36	A5	3258	U	C6-N1-C2	6.31	124.78	121.00
1	A2	1027	A	N7-C8-N9	6.30	116.95	113.80
36	A1	285	A	C5-C6-N6	-6.30	118.66	123.70
36	A1	658	G	C4-N9-C1'	6.30	134.69	126.50
36	A1	1153	A	N1-C6-N6	6.30	122.38	118.60
64	Ba	12	ARG	NE-CZ-NH2	-6.30	117.15	120.30
80	A6	653	C	C6-N1-C1'	-6.30	113.23	120.80
36	A5	1449	A	C5-C6-N1	-6.30	114.55	117.70
36	A5	1844	C	C2-N3-C4	-6.30	116.75	119.90
36	A5	2821	C	C5-C6-N1	6.30	124.15	121.00
1	A2	189	C	N1-C2-O2	6.30	122.68	118.90
68	De	47	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A2	973	A	C2-N3-C4	-6.30	107.45	110.60
36	A1	509	U	N1-C2-N3	6.30	118.68	114.90
36	A1	1000	C	C6-N1-C1'	-6.30	113.24	120.80
36	A1	2851	A	N7-C8-N9	-6.30	110.65	113.80
62	BY	13	ARG	NE-CZ-NH1	6.30	123.45	120.30
80	A6	87	C	N1-C2-O2	-6.30	115.12	118.90
36	A5	112	U	C5-C4-O4	-6.30	122.12	125.90
36	A5	1306	G	C6-N1-C2	-6.30	121.32	125.10
36	A5	2303	A	N1-C6-N6	-6.30	114.82	118.60
37	A7	48	U	N3-C4-C5	6.30	118.38	114.60
1	A2	159	U	C2-N1-C1'	-6.30	110.14	117.70
36	A1	228	U	N1-C2-O2	6.30	127.21	122.80
36	A1	954	U	N1-C2-O2	-6.30	118.39	122.80
36	A1	2806	U	C2-N3-C4	-6.30	123.22	127.00
36	A5	582	G	C5-C6-O6	6.30	132.38	128.60
36	A5	2389	C	C5-C6-N1	-6.30	117.85	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	90	C	C2-N3-C4	-6.30	116.75	119.90
49	DL	27	ASP	CB-CG-OD2	6.30	123.97	118.30
36	A1	3328	G	C8-N9-C4	-6.30	103.88	106.40
38	A4	2	A	N7-C8-N9	6.30	116.95	113.80
36	A5	2364	G	C5-C6-O6	6.30	132.38	128.60
36	A5	2777	G	C4-C5-N7	-6.30	108.28	110.80
36	A5	3317	U	N3-C4-O4	-6.30	114.99	119.40
1	A2	213	A	C8-N9-C4	6.29	108.32	105.80
36	A1	1082	U	C6-N1-C2	-6.29	117.22	121.00
36	A1	2390	A	N1-C2-N3	6.29	132.45	129.30
42	DD	248	ARG	NE-CZ-NH2	-6.29	117.15	120.30
36	A1	91	G	N3-C4-N9	-6.29	122.22	126.00
36	A1	405	U	C2-N3-C4	-6.29	123.22	127.00
36	A1	1433	A	C2-N3-C4	6.29	113.75	110.60
36	A1	1948	G	C5-C6-O6	-6.29	124.82	128.60
36	A5	276	U	C2-N3-C4	-6.29	123.22	127.00
36	A5	3360	C	C6-N1-C2	-6.29	117.78	120.30
36	A1	2805	G	N3-C2-N2	6.29	124.31	119.90
36	A5	1115	G	C8-N9-C4	-6.29	103.88	106.40
36	A5	1314	C	C6-N1-C1'	-6.29	113.25	120.80
36	A5	3330	A	C2-N3-C4	6.29	113.75	110.60
38	A4	21	C	N3-C2-O2	6.29	126.30	121.90
36	A5	793	C	N1-C2-O2	-6.29	115.13	118.90
36	A5	2211	U	N3-C4-C5	-6.29	110.83	114.60
36	A1	907	G	C2-N3-C4	6.29	115.04	111.90
80	A6	768	C	N3-C4-N4	6.29	122.40	118.00
36	A5	1940	G	N1-C2-N2	-6.29	110.54	116.20
36	A5	2833	A	N7-C8-N9	-6.29	110.66	113.80
36	A1	394	G	N1-C2-N3	-6.29	120.13	123.90
36	A1	1948	G	N9-C4-C5	-6.29	102.89	105.40
56	BS	40	ARG	CG-CD-NE	6.29	125.00	111.80
36	A5	1506	A	C5-N7-C8	-6.29	100.76	103.90
38	A8	52	A	C8-N9-C4	-6.29	103.29	105.80
1	A2	590	C	C2-N1-C1'	6.28	125.71	118.80
36	A1	1460	A	C6-N1-C2	-6.28	114.83	118.60
80	A6	687	G	C6-C5-N7	6.28	134.17	130.40
80	A6	1469	A	C8-N9-C4	6.28	108.31	105.80
80	A6	1793	G	C5-N7-C8	6.28	107.44	104.30
36	A5	2289	U	N3-C4-O4	-6.28	115.00	119.40
1	A2	68	A	C8-N9-C4	-6.28	103.29	105.80
1	A2	942	G	N1-C6-O6	-6.28	116.13	119.90
1	A2	627	C	N3-C4-N4	6.28	122.40	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	365	A	C5-C6-N1	-6.28	114.56	117.70
36	A1	938	C	N1-C2-O2	-6.28	115.13	118.90
36	A1	942	U	C5-C4-O4	6.28	129.67	125.90
36	A1	2930	A	N9-C4-C5	6.28	108.31	105.80
80	A6	453	U	N1-C2-N3	6.28	118.67	114.90
80	A6	565	C	N3-C2-O2	-6.28	117.50	121.90
80	A6	1438	G	C8-N9-C4	6.28	108.91	106.40
36	A5	2616	C	C5-C4-N4	-6.28	115.80	120.20
36	A5	1168	U	N3-C4-C5	6.28	118.37	114.60
36	A5	1408	G	C2-N3-C4	-6.28	108.76	111.90
36	A5	2952	G	N1-C6-O6	6.28	123.67	119.90
36	A1	398	A	C2-N3-C4	6.28	113.74	110.60
36	A1	1341	U	N3-C4-O4	-6.28	115.01	119.40
80	A6	1044	U	N3-C2-O2	-6.28	117.81	122.20
1	A2	1000	C	C5-C6-N1	-6.28	117.86	121.00
1	A2	1515	A	C8-N9-C4	-6.28	103.29	105.80
36	A1	2417	U	C2-N3-C4	-6.28	123.23	127.00
36	A5	1056	U	N3-C4-C5	-6.28	110.83	114.60
36	A1	832	G	C8-N9-C4	6.27	108.91	106.40
36	A1	2284	C	N1-C2-O2	-6.27	115.14	118.90
36	A1	2299	A	C6-N1-C2	-6.27	114.84	118.60
37	A3	86	U	N1-C2-O2	-6.27	118.41	122.80
80	A6	402	C	C5-C4-N4	-6.27	115.81	120.20
38	A8	84	C	C6-N1-C2	-6.27	117.79	120.30
36	A1	808	A	C5-C6-N6	6.27	128.72	123.70
36	A1	1007	U	C5-C4-O4	-6.27	122.14	125.90
36	A1	1393	A	C6-N1-C2	-6.27	114.84	118.60
38	A4	15	G	N7-C8-N9	-6.27	109.96	113.10
80	A6	449	C	N3-C4-N4	-6.27	113.61	118.00
36	A5	2352	A	N1-C2-N3	6.27	132.44	129.30
36	A5	3317	U	C5-C6-N1	6.27	125.84	122.70
1	A2	1363	U	N1-C2-O2	6.27	127.19	122.80
1	A2	1456	C	C6-N1-C2	-6.27	117.79	120.30
1	A2	1465	C	N3-C4-C5	-6.27	119.39	121.90
36	A5	586	C	N3-C4-C5	6.27	124.41	121.90
36	A5	1383	G	N1-C6-O6	-6.27	116.14	119.90
36	A5	1511	U	C5-C6-N1	-6.27	119.56	122.70
1	A2	75	U	N3-C2-O2	-6.27	117.81	122.20
1	A2	1198	G	N9-C4-C5	6.27	107.91	105.40
36	A1	1297	C	C6-N1-C2	6.27	122.81	120.30
80	A6	1073	G	C5-C6-N1	6.27	114.63	111.50
36	A5	2735	U	C6-N1-C2	-6.27	117.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	3218	A	N3-C4-C5	6.27	131.19	126.80
1	A2	340	U	N3-C2-O2	-6.27	117.81	122.20
1	A2	377	G	N3-C4-C5	6.27	131.73	128.60
36	A1	1144	U	N3-C4-C5	6.27	118.36	114.60
36	A1	1492	G	C8-N9-C1'	-6.27	118.85	127.00
38	A4	10	A	N9-C4-C5	6.27	108.31	105.80
64	Ba	46	ASP	N-CA-C	-6.27	94.08	111.00
36	A5	2139	A	C5-N7-C8	6.27	107.03	103.90
36	A1	1448	U	N1-C2-O2	-6.27	118.41	122.80
36	A1	1796	G	N3-C4-C5	-6.27	125.47	128.60
36	A5	1411	C	N1-C2-O2	-6.27	115.14	118.90
36	A1	124	U	N3-C4-O4	-6.26	115.02	119.40
36	A1	1336	U	C6-N1-C2	-6.26	117.24	121.00
36	A1	3260	G	C5-C6-O6	6.26	132.36	128.60
40	BB	21	ARG	NE-CZ-NH1	-6.26	117.17	120.30
80	A6	62	A	N1-C6-N6	6.26	122.36	118.60
80	A6	1550	A	C5-C6-N6	-6.26	118.69	123.70
36	A5	637	C	C2-N1-C1'	-6.26	111.91	118.80
36	A5	2164	A	C8-N9-C4	-6.26	103.29	105.80
38	A8	38	U	C5-C4-O4	6.26	129.66	125.90
1	A2	404	G	C8-N9-C4	6.26	108.91	106.40
1	A2	868	G	N1-C6-O6	6.26	123.66	119.90
1	A2	942	G	C8-N9-C4	-6.26	103.89	106.40
36	A1	1003	A	C5-C6-N6	-6.26	118.69	123.70
36	A1	2382	G	C5-C6-O6	6.26	132.36	128.60
80	A6	382	C	C2-N3-C4	-6.26	116.77	119.90
80	A6	769	A	N9-C4-C5	6.26	108.31	105.80
36	A1	847	A	C6-C5-N7	-6.26	127.92	132.30
36	A1	3143	C	C2-N1-C1'	-6.26	111.91	118.80
38	A4	12	A	N9-C4-C5	6.26	108.31	105.80
36	A5	950	G	C8-N9-C4	6.26	108.91	106.40
36	A5	1211	U	N3-C4-O4	-6.26	115.02	119.40
36	A1	2340	U	N3-C4-O4	-6.26	115.02	119.40
36	A1	2361	A	C6-N1-C2	-6.26	114.84	118.60
36	A5	314	U	C5-C4-O4	6.26	129.66	125.90
36	A5	674	G	C8-N9-C4	-6.26	103.90	106.40
1	A2	810	G	C6-C5-N7	-6.26	126.64	130.40
36	A1	281	G	C6-N1-C2	-6.26	121.34	125.10
36	A1	2308	C	N1-C2-O2	-6.26	115.14	118.90
36	A1	3219	G	N3-C4-N9	6.26	129.75	126.00
38	A4	135	G	N9-C4-C5	6.26	107.90	105.40
36	A1	304	G	C2-N3-C4	6.26	115.03	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	347	G	C4-C5-N7	6.26	113.30	110.80
36	A1	2249	G	C5-C6-N1	6.26	114.63	111.50
41	BC	283	THR	CB-CA-C	-6.26	94.70	111.60
36	A5	1297	C	C4-C5-C6	6.26	120.53	117.40
36	A5	2808	A	N1-C2-N3	6.26	132.43	129.30
37	A7	92	A	C6-C5-N7	-6.26	127.92	132.30
40	DB	10	ARG	NE-CZ-NH1	6.26	123.43	120.30
36	A1	498	A	C5-C6-N6	6.25	128.70	123.70
36	A1	80	G	N3-C4-C5	-6.25	125.47	128.60
36	A1	278	U	C6-N1-C2	-6.25	117.25	121.00
36	A1	421	G	C4-C5-N7	6.25	113.30	110.80
36	A1	1204	A	C5-C6-N1	-6.25	114.57	117.70
36	A5	2429	G	C8-N9-C4	-6.25	103.90	106.40
36	A1	365	A	C2-N3-C4	-6.25	107.47	110.60
36	A1	1052	U	N3-C4-O4	-6.25	115.02	119.40
80	A6	396	G	C4-C5-N7	6.25	113.30	110.80
80	A6	400	A	C5-C6-N6	-6.25	118.70	123.70
36	A5	2516	U	C2-N3-C4	-6.25	123.25	127.00
36	A5	2886	U	N3-C2-O2	-6.25	117.82	122.20
80	A6	767	U	C5-C4-O4	6.25	129.65	125.90
36	A5	2128	C	N3-C2-O2	-6.25	117.53	121.90
36	A1	656	A	C4-C5-C6	6.25	120.12	117.00
36	A1	808	A	C4-C5-N7	-6.25	107.58	110.70
36	A1	2877	G	C4-C5-N7	-6.25	108.30	110.80
36	A5	1389	G	C5-N7-C8	-6.25	101.18	104.30
36	A5	1688	U	N1-C2-O2	6.25	127.17	122.80
37	A7	44	C	N3-C4-C5	-6.25	119.40	121.90
1	A2	1654	G	C8-N9-C4	-6.25	103.90	106.40
36	A1	407	A	C5-N7-C8	-6.25	100.78	103.90
36	A1	979	U	C5-C4-O4	6.25	129.65	125.90
36	A1	1173	U	N3-C4-C5	6.25	118.35	114.60
36	A1	1337	A	C5-C6-N1	6.25	120.82	117.70
80	A6	391	A	C5-N7-C8	6.25	107.02	103.90
80	A6	1471	A	C8-N9-C4	-6.25	103.30	105.80
49	BL	85	LEU	CA-CB-CG	6.25	129.66	115.30
36	A5	644	G	N1-C6-O6	-6.25	116.15	119.90
36	A5	3052	G	N7-C8-N9	-6.25	109.98	113.10
1	A2	543	C	N3-C2-O2	-6.24	117.53	121.90
1	A2	1633	A	N9-C4-C5	6.24	108.30	105.80
7	CF	92	ARG	NE-CZ-NH1	6.24	123.42	120.30
36	A5	2777	G	N9-C4-C5	6.24	107.90	105.40
36	A1	417	A	C8-N9-C4	6.24	108.30	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1455	U	C5-C6-N1	-6.24	119.58	122.70
36	A1	2305	G	C8-N9-C1'	-6.24	118.89	127.00
36	A5	1449	A	N3-C4-C5	6.24	131.17	126.80
36	A1	1163	A	N7-C8-N9	6.24	116.92	113.80
36	A1	1464	G	N7-C8-N9	-6.24	109.98	113.10
36	A1	2867	C	N3-C2-O2	-6.24	117.53	121.90
80	A6	372	G	C6-C5-N7	6.24	134.14	130.40
36	A5	2930	A	C8-N9-C4	-6.24	103.30	105.80
1	A2	1670	G	C8-N9-C1'	-6.24	118.89	127.00
36	A1	1400	G	N7-C8-N9	-6.24	109.98	113.10
36	A1	2517	U	C5-C6-N1	-6.24	119.58	122.70
80	A6	1643	U	C5-C4-O4	6.24	129.64	125.90
36	A5	146	U	N3-C4-O4	-6.24	115.03	119.40
36	A5	2754	G	N1-C6-O6	-6.24	116.16	119.90
1	A2	1766	A	C8-N9-C4	6.24	108.30	105.80
36	A5	2728	G	C8-N9-C4	-6.24	103.91	106.40
1	A2	933	A	C8-N9-C4	-6.24	103.31	105.80
36	A1	784	A	N1-C6-N6	6.24	122.34	118.60
36	A1	797	U	N3-C4-C5	6.24	118.34	114.60
38	A4	88	A	C5-C6-N6	-6.24	118.71	123.70
36	A5	891	G	C8-N9-C4	6.24	108.89	106.40
36	A5	1425	U	N3-C4-O4	-6.24	115.03	119.40
36	A5	1500	G	C8-N9-C4	6.24	108.89	106.40
36	A1	331	G	C6-C5-N7	6.23	134.14	130.40
36	A1	416	A	C5-C6-N6	6.23	128.69	123.70
1	A2	494	U	N1-C2-O2	6.23	127.16	122.80
12	AK	76	LEU	CA-CB-CG	6.23	129.63	115.30
36	A1	328	U	N3-C2-O2	-6.23	117.84	122.20
36	A1	786	A	C5-N7-C8	6.23	107.02	103.90
36	A5	670	C	N3-C4-C5	6.23	124.39	121.90
36	A5	1009	A	C8-N9-C4	-6.23	103.31	105.80
1	A2	1595	U	C5-C4-O4	-6.23	122.16	125.90
36	A1	576	C	C5-C6-N1	-6.23	117.88	121.00
38	A4	30	C	N3-C4-N4	-6.23	113.64	118.00
44	BF	163	LEU	CA-CB-CG	-6.23	100.97	115.30
36	A5	1911	A	N7-C8-N9	-6.23	110.69	113.80
36	A5	2133	U	N3-C4-C5	6.23	118.34	114.60
36	A5	3216	G	C6-N1-C2	-6.23	121.36	125.10
36	A5	3298	C	N1-C2-O2	-6.23	115.16	118.90
36	A5	1115	G	N3-C4-C5	-6.23	125.49	128.60
36	A5	1753	G	N3-C4-C5	-6.23	125.49	128.60
1	A2	1329	A	C5-C6-N6	-6.23	118.72	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	940	G	C5-C6-O6	6.23	132.34	128.60
36	A1	1392	G	N1-C2-N3	-6.23	120.16	123.90
80	A6	1027	A	C5-N7-C8	-6.23	100.79	103.90
80	A6	1410	A	N1-C6-N6	6.23	122.34	118.60
36	A5	437	G	N3-C2-N2	-6.23	115.54	119.90
36	A5	2716	U	C6-N1-C2	-6.23	117.26	121.00
36	A1	1515	A	C5-C6-N1	-6.23	114.59	117.70
36	A5	974	G	N3-C4-N9	6.23	129.74	126.00
36	A1	677	A	N9-C4-C5	-6.22	103.31	105.80
36	A1	2197	C	C2-N3-C4	6.22	123.01	119.90
36	A1	2985	C	N3-C4-C5	-6.22	119.41	121.90
54	BQ	99	THR	N-CA-C	6.22	127.81	111.00
80	A6	66	U	C5-C6-N1	-6.22	119.59	122.70
36	A5	691	A	C2-N3-C4	-6.22	107.49	110.60
36	A5	2301	U	N3-C4-C5	6.22	118.33	114.60
38	A8	53	A	C2-N3-C4	6.22	113.71	110.60
1	A2	1297	G	N7-C8-N9	-6.22	109.99	113.10
1	A2	1454	G	C5-C6-O6	6.22	132.33	128.60
36	A1	935	U	C4-C5-C6	6.22	123.43	119.70
36	A1	1051	U	C5-C4-O4	6.22	129.63	125.90
36	A1	2762	A	N7-C8-N9	-6.22	110.69	113.80
36	A1	2960	C	N3-C4-C5	6.22	124.39	121.90
36	A1	3119	U	N3-C2-O2	-6.22	117.84	122.20
36	A1	3190	C	C2-N3-C4	-6.22	116.79	119.90
80	A6	1030	A	C5-C6-N6	6.22	128.68	123.70
80	A6	1257	U	N3-C2-O2	-6.22	117.84	122.20
36	A5	514	G	N1-C6-O6	6.22	123.63	119.90
36	A5	3308	C	C5-C6-N1	-6.22	117.89	121.00
1	A2	523	G	N3-C4-C5	-6.22	125.49	128.60
36	A1	702	C	N1-C2-O2	-6.22	115.17	118.90
36	A1	867	G	N1-C2-N2	6.22	121.80	116.20
36	A1	2828	G	N3-C2-N2	6.22	124.25	119.90
36	A5	32	U	N1-C2-O2	-6.22	118.44	122.80
36	A5	150	A	C5-C6-N6	-6.22	118.72	123.70
36	A1	439	C	C2-N1-C1'	6.22	125.64	118.80
36	A1	2246	G	C8-N9-C4	-6.22	103.91	106.40
36	A1	3344	A	C4-N9-C1'	6.22	137.50	126.30
80	A6	1478	G	C8-N9-C1'	-6.22	118.91	127.00
36	A5	2242	A	C5-C6-N6	6.22	128.68	123.70
1	A2	1747	G	C8-N9-C4	6.22	108.89	106.40
36	A1	909	G	C5-C6-N1	6.22	114.61	111.50
36	A1	1374	G	C4-C5-N7	6.22	113.29	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1148	G	C5-C6-O6	-6.22	124.87	128.60
36	A5	2572	C	C6-N1-C2	-6.22	117.81	120.30
36	A1	496	C	N1-C2-O2	-6.22	115.17	118.90
36	A1	3318	G	N3-C4-N9	6.22	129.73	126.00
12	CK	83	PRO	N-CA-CB	6.22	110.76	103.30
36	A1	576	C	C5-C4-N4	-6.21	115.85	120.20
36	A1	998	A	C2-N3-C4	6.21	113.71	110.60
36	A1	1889	G	C5-C6-N1	-6.21	108.39	111.50
80	A6	396	G	N3-C2-N2	6.21	124.25	119.90
36	A5	1300	G	C4-C5-N7	6.21	113.29	110.80
36	A5	2198	A	C2-N3-C4	-6.21	107.49	110.60
36	A5	3000	A	C8-N9-C4	6.21	108.29	105.80
36	A5	1468	A	C8-N9-C4	-6.21	103.31	105.80
36	A1	701	G	N1-C6-O6	-6.21	116.17	119.90
36	A5	624	G	C8-N9-C4	6.21	108.88	106.40
36	A5	656	A	C8-N9-C4	6.21	108.28	105.80
1	A2	1218	G	N1-C6-O6	6.21	123.63	119.90
36	A1	2246	G	N3-C2-N2	-6.21	115.55	119.90
80	A6	1396	U	C6-N1-C2	-6.21	117.27	121.00
36	A1	2276	G	C8-N9-C4	-6.21	103.92	106.40
36	A1	2361	A	N9-C4-C5	6.21	108.28	105.80
38	A4	74	U	C5-C6-N1	-6.21	119.60	122.70
56	BS	58	ILE	CG1-CB-CG2	-6.21	97.74	111.40
36	A5	359	U	C5-C4-O4	-6.21	122.17	125.90
36	A5	1161	G	C2-N3-C4	6.21	115.00	111.90
36	A5	1888	U	C2-N3-C4	-6.21	123.28	127.00
36	A5	2117	A	C6-N1-C2	-6.21	114.87	118.60
36	A5	2645	G	C6-N1-C2	-6.21	121.38	125.10
1	A2	736	C	N1-C2-O2	6.21	122.62	118.90
80	A6	290	G	C8-N9-C4	-6.21	103.92	106.40
37	A7	25	G	N3-C2-N2	-6.21	115.56	119.90
36	A5	994	G	N3-C2-N2	6.21	124.24	119.90
36	A5	2133	U	N3-C4-O4	-6.21	115.06	119.40
36	A1	2679	A	C5-C6-N1	-6.20	114.60	117.70
37	A3	103	A	N7-C8-N9	-6.20	110.70	113.80
80	A6	447	U	N1-C2-N3	6.20	118.62	114.90
36	A5	726	G	C5-N7-C8	-6.20	101.20	104.30
36	A1	1307	G	C2-N3-C4	6.20	115.00	111.90
36	A1	2957	G	N3-C2-N2	-6.20	115.56	119.90
80	A6	364	G	C6-N1-C2	-6.20	121.38	125.10
80	A6	987	G	N3-C2-N2	-6.20	115.56	119.90
36	A5	3014	U	C5-C4-O4	-6.20	122.18	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	3175	U	C6-N1-C2	-6.20	117.28	121.00
53	DP	127	ARG	NE-CZ-NH1	6.20	123.40	120.30
36	A1	751	A	N1-C2-N3	-6.20	126.20	129.30
36	A1	1369	A	N9-C4-C5	-6.20	103.32	105.80
41	BC	138	ARG	NE-CZ-NH2	-6.20	117.20	120.30
80	A6	1200	G	C4-N9-C1'	-6.20	118.44	126.50
80	A6	1600	A	C4-C5-N7	6.20	113.80	110.70
36	A5	425	G	N7-C8-N9	-6.20	110.00	113.10
36	A5	1307	G	C8-N9-C4	-6.20	103.92	106.40
36	A5	1810	A	C8-N9-C4	6.20	108.28	105.80
36	A5	2930	A	N9-C4-C5	6.20	108.28	105.80
36	A1	352	A	C2-N3-C4	-6.20	107.50	110.60
36	A1	3218	A	N9-C4-C5	6.20	108.28	105.80
80	A6	1354	G	C8-N9-C4	-6.20	103.92	106.40
80	A6	1666	U	C5-C4-O4	6.20	129.62	125.90
36	A5	326	U	N3-C4-C5	6.20	118.32	114.60
36	A5	911	C	N1-C2-O2	-6.20	115.18	118.90
36	A5	3334	U	N3-C2-O2	-6.20	117.86	122.20
36	A1	2856	G	N7-C8-N9	-6.20	110.00	113.10
36	A5	2169	G	N1-C6-O6	-6.20	116.18	119.90
36	A5	2524	A	C6-N1-C2	6.20	122.32	118.60
36	A5	2552	C	N3-C2-O2	-6.20	117.56	121.90
1	A2	186	C	C5-C6-N1	6.20	124.10	121.00
1	A2	189	C	C6-N1-C1'	-6.20	113.36	120.80
1	A2	1436	A	N9-C4-C5	-6.20	103.32	105.80
1	A2	1560	U	N1-C2-N3	6.20	118.62	114.90
36	A1	104	G	C5-C6-N1	6.20	114.60	111.50
36	A1	1326	A	C8-N9-C4	6.20	108.28	105.80
36	A1	2733	A	C8-N9-C4	6.20	108.28	105.80
80	A6	152	U	C5-C4-O4	6.20	129.62	125.90
36	A5	511	G	N3-C2-N2	6.20	124.24	119.90
36	A5	1389	G	N3-C4-N9	6.20	129.72	126.00
36	A1	420	G	C8-N9-C4	6.19	108.88	106.40
36	A1	2826	U	C4-C5-C6	6.19	123.42	119.70
36	A5	35	A	C2-N3-C4	-6.19	107.50	110.60
36	A5	494	G	N3-C4-C5	-6.19	125.50	128.60
36	A5	819	U	C6-N1-C2	6.19	124.72	121.00
36	A5	2615	G	C5-C6-O6	-6.19	124.88	128.60
36	A1	44	U	C6-N1-C2	6.19	124.72	121.00
36	A1	576	C	C6-N1-C2	6.19	122.78	120.30
36	A1	713	U	N3-C2-O2	-6.19	117.87	122.20
36	A1	2204	C	N1-C2-N3	6.19	123.53	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1749	A	C2-N3-C4	-6.19	107.50	110.60
36	A5	294	U	C5-C4-O4	-6.19	122.19	125.90
36	A5	823	C	N3-C4-C5	6.19	124.38	121.90
36	A5	2865	U	N1-C2-N3	-6.19	111.18	114.90
68	De	4	LEU	C-N-CD	6.19	141.40	128.40
36	A1	1114	U	N1-C2-O2	6.19	127.13	122.80
80	A6	1127	G	C8-N9-C4	-6.19	103.92	106.40
36	A5	1346	G	N3-C4-C5	6.19	131.70	128.60
36	A5	1883	A	N9-C4-C5	6.19	108.28	105.80
36	A5	3365	U	N1-C2-N3	6.19	118.61	114.90
36	A1	2314	U	N3-C2-O2	6.19	126.53	122.20
36	A5	83	U	C5-C4-O4	-6.19	122.19	125.90
36	A5	1035	G	N3-C4-N9	6.19	129.71	126.00
36	A5	2846	U	N1-C2-O2	-6.19	118.47	122.80
36	A1	1387	G	N7-C8-N9	-6.19	110.01	113.10
36	A1	2182	A	N1-C6-N6	-6.19	114.89	118.60
36	A1	2618	G	C6-N1-C2	-6.19	121.39	125.10
36	A1	3301	U	N3-C2-O2	-6.19	117.87	122.20
80	A6	359	A	C4-N9-C1'	-6.19	115.16	126.30
36	A5	818	C	N3-C4-C5	-6.19	119.42	121.90
36	A5	2808	A	N1-C6-N6	6.19	122.31	118.60
1	A2	874	C	C5-C6-N1	6.19	124.09	121.00
24	AW	65	LEU	CA-CB-CG	6.19	129.53	115.30
36	A1	592	A	C5-C6-N6	-6.19	118.75	123.70
36	A5	436	A	C8-N9-C1'	-6.19	116.56	127.70
36	A5	1430	U	C6-N1-C2	6.19	124.71	121.00
36	A1	1415	U	C5-C4-O4	6.18	129.61	125.90
41	BC	309	ARG	NE-CZ-NH1	6.18	123.39	120.30
36	A5	904	A	N9-C4-C5	6.18	108.27	105.80
36	A5	1143	A	C6-N1-C2	6.18	122.31	118.60
36	A5	1161	G	C8-N9-C4	6.18	108.87	106.40
1	A2	767	U	N3-C4-O4	-6.18	115.07	119.40
1	A2	1628	U	N3-C2-O2	-6.18	117.87	122.20
36	A1	2422	C	N1-C2-O2	6.18	122.61	118.90
36	A1	2786	G	N3-C4-C5	-6.18	125.51	128.60
36	A5	1119	C	C5-C4-N4	-6.18	115.87	120.20
52	DO	3[B]	SER	C-N-CA	-6.18	106.24	121.70
1	A2	1305	U	N1-C2-N3	6.18	118.61	114.90
36	A5	3065	G	C5-C6-O6	6.18	132.31	128.60
1	A2	1670	G	C4-N9-C1'	6.18	134.53	126.50
36	A1	857	G	N1-C6-O6	-6.18	116.19	119.90
36	A1	1382	G	N9-C4-C5	-6.18	102.93	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2197	C	N1-C2-O2	6.18	122.61	118.90
36	A1	2533	G	C4-N9-C1'	6.18	134.53	126.50
36	A1	2611	U	N3-C4-C5	6.18	118.31	114.60
36	A1	2952	G	C8-N9-C4	6.18	108.87	106.40
68	Be	27	ARG	NE-CZ-NH2	-6.18	117.21	120.30
36	A5	2399	A	C8-N9-C4	6.18	108.27	105.80
36	A1	922	U	C6-N1-C2	-6.18	117.29	121.00
36	A1	776	U	C2-N3-C4	-6.18	123.30	127.00
36	A1	2798	C	C5-C4-N4	6.18	124.52	120.20
38	A4	50	C	C6-N1-C2	-6.18	117.83	120.30
80	A6	1329	A	C5-C6-N6	-6.18	118.76	123.70
36	A5	1301	A	C5-C6-N6	-6.18	118.76	123.70
36	A1	1001	G	C8-N9-C4	-6.17	103.93	106.40
36	A1	2357	A	C5-C6-N6	-6.17	118.76	123.70
36	A1	2663	G	N3-C4-C5	-6.17	125.51	128.60
36	A5	32	U	C6-N1-C2	-6.17	117.30	121.00
36	A5	722	G	N9-C4-C5	6.17	107.87	105.40
36	A5	734	C	N1-C2-O2	6.17	122.61	118.90
36	A5	1134	G	C6-N1-C2	-6.17	121.39	125.10
36	A1	1187	C	N1-C2-N3	6.17	123.52	119.20
36	A1	1294	A	N9-C4-C5	6.17	108.27	105.80
36	A5	87	U	N3-C4-O4	-6.17	115.08	119.40
36	A5	1525	G	C4-N9-C1'	6.17	134.52	126.50
1	A2	734	A	N1-C6-N6	6.17	122.30	118.60
36	A1	546	C	C5-C6-N1	6.17	124.09	121.00
38	A4	39	G	N1-C6-O6	-6.17	116.20	119.90
80	A6	603	U	C2-N3-C4	-6.17	123.30	127.00
36	A5	408	A	N1-C2-N3	6.17	132.39	129.30
36	A5	3330	A	C6-N1-C2	-6.17	114.90	118.60
80	A6	44	U	N3-C4-O4	-6.17	115.08	119.40
36	A1	1118	C	C5-C6-N1	-6.17	117.92	121.00
36	A1	2380	U	N3-C4-C5	6.17	118.30	114.60
36	A1	2635	A	C5-N7-C8	-6.17	100.81	103.90
36	A1	3317	U	C5-C4-O4	6.17	129.60	125.90
80	A6	956	C	C5-C6-N1	-6.17	117.92	121.00
80	A6	1480	G	C8-N9-C4	-6.17	103.93	106.40
80	A6	1595	U	N1-C2-O2	6.17	127.12	122.80
36	A1	278	U	N1-C2-N3	6.17	118.60	114.90
36	A5	2228	A	C8-N9-C4	-6.17	103.33	105.80
36	A5	3266	G	C8-N9-C4	-6.17	103.93	106.40
36	A1	889	U	N3-C4-O4	-6.17	115.08	119.40
36	A5	1931	U	C5-C6-N1	-6.17	119.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1227	C	C5-C6-N1	6.16	124.08	121.00
80	A6	778	G	N3-C4-N9	6.16	129.70	126.00
80	A6	956	C	C6-N1-C2	6.16	122.77	120.30
36	A5	386	A	C4-C5-N7	6.16	113.78	110.70
36	A5	753	C	C5-C4-N4	-6.16	115.89	120.20
37	A7	46	A	C8-N9-C4	-6.16	103.33	105.80
36	A1	1142	G	C6-N1-C2	-6.16	121.40	125.10
38	A4	85	G	C6-C5-N7	-6.16	126.70	130.40
80	A6	1433	G	C8-N9-C4	-6.16	103.94	106.40
36	A5	590	G	C5-C6-N1	6.16	114.58	111.50
36	A5	600	G	C6-C5-N7	-6.16	126.70	130.40
36	A5	949	C	C5-C6-N1	-6.16	117.92	121.00
36	A5	1064	A	C8-N9-C4	6.16	108.26	105.80
1	A2	1258	U	C4-C5-C6	6.16	123.39	119.70
36	A1	2302	G	N3-C2-N2	6.16	124.21	119.90
80	A6	306	U	C6-N1-C2	6.16	124.69	121.00
36	A5	42	C	C2-N3-C4	6.16	122.98	119.90
36	A5	999	G	C2-N3-C4	6.16	114.98	111.90
36	A5	1007	U	C2-N3-C4	-6.16	123.30	127.00
36	A5	2381	G	N1-C6-O6	-6.16	116.20	119.90
36	A5	2858	U	N1-C2-N3	6.16	118.59	114.90
1	A2	36	C	N3-C4-N4	6.16	122.31	118.00
1	A2	704	C	C6-N1-C1'	-6.16	113.41	120.80
36	A5	2396	G	C8-N9-C4	-6.16	103.94	106.40
36	A1	61	A	N9-C4-C5	-6.16	103.34	105.80
36	A1	203	G	N1-C6-O6	-6.16	116.21	119.90
36	A1	641	C	N1-C2-O2	-6.16	115.21	118.90
36	A1	1392	G	C5-C6-N1	6.16	114.58	111.50
36	A1	2816	G	N3-C2-N2	6.16	124.21	119.90
78	Bo	74	CYS	CA-CB-SG	6.16	125.08	114.00
80	A6	1614	A	C6-C5-N7	-6.16	127.99	132.30
36	A5	351	A	C5-C6-N6	-6.16	118.78	123.70
36	A5	1381	A	C2-N3-C4	-6.16	107.52	110.60
36	A5	1591	G	C5-C6-N1	6.16	114.58	111.50
36	A5	3272	C	C6-N1-C2	6.16	122.76	120.30
36	A5	3358	U	N3-C2-O2	-6.16	117.89	122.20
36	A1	1336	U	C5-C4-O4	6.15	129.59	125.90
36	A1	1916	U	C6-N1-C2	6.15	124.69	121.00
36	A1	2973	G	C5-C6-O6	-6.15	124.91	128.60
1	A2	1490	C	C2-N1-C1'	6.15	125.57	118.80
36	A1	284	A	C8-N9-C4	-6.15	103.34	105.80
36	A1	1114	U	N1-C2-N3	-6.15	111.21	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2307	G	N1-C6-O6	-6.15	116.21	119.90
36	A5	1148	G	C5-C6-N1	6.15	114.58	111.50
36	A5	2757	U	N1-C2-O2	-6.15	118.49	122.80
36	A5	3228	C	N3-C2-O2	-6.15	117.59	121.90
36	A5	3345	G	N3-C2-N2	-6.15	115.59	119.90
36	A1	1778	G	C4-N9-C1'	6.15	134.49	126.50
36	A1	2867	C	C6-N1-C2	-6.15	117.84	120.30
80	A6	1481	C	N3-C4-C5	-6.15	119.44	121.90
80	A6	1723	U	N1-C2-N3	6.15	118.59	114.90
36	A5	822	G	N3-C4-N9	-6.15	122.31	126.00
36	A5	917	A	C8-N9-C4	-6.15	103.34	105.80
36	A5	2824	G	N3-C4-C5	-6.15	125.53	128.60
36	A1	1546	A	C4-C5-N7	-6.15	107.63	110.70
36	A1	2704	A	C5-C6-N6	6.15	128.62	123.70
36	A5	924	G	N3-C2-N2	-6.15	115.60	119.90
36	A1	272	G	C8-N9-C4	6.14	108.86	106.40
80	A6	947	U	N1-C2-O2	-6.14	118.50	122.80
80	A6	1631	A	C8-N9-C4	6.14	108.26	105.80
36	A5	2207	A	C5-N7-C8	-6.14	100.83	103.90
36	A1	672	A	C4-C5-N7	6.14	113.77	110.70
36	A1	1624	G	C8-N9-C4	-6.14	103.94	106.40
36	A1	2794	G	C8-N9-C4	-6.14	103.94	106.40
36	A5	102	C	N3-C4-N4	6.14	122.30	118.00
36	A5	2347	U	N3-C4-C5	6.14	118.29	114.60
1	A2	1781	A	C5-C6-N6	6.14	128.61	123.70
36	A5	1772	U	N3-C2-O2	-6.14	117.90	122.20
36	A1	1155	C	C5-C6-N1	6.14	124.07	121.00
36	A1	3089	C	N3-C4-C5	6.14	124.36	121.90
38	A4	2	A	C8-N9-C4	-6.14	103.34	105.80
80	A6	1122	G	N3-C4-C5	6.14	131.67	128.60
80	A6	1730	A	N1-C6-N6	6.14	122.28	118.60
36	A5	1303	A	C2-N3-C4	6.14	113.67	110.60
36	A5	2728	G	C6-N1-C2	-6.14	121.42	125.10
36	A5	2928	C	C6-N1-C2	-6.14	117.84	120.30
36	A1	606	C	C6-N1-C2	-6.14	117.84	120.30
36	A5	370	U	N1-C2-N3	6.14	118.58	114.90
36	A5	1162	U	C2-N3-C4	-6.14	123.32	127.00
36	A1	30	G	N3-C2-N2	6.14	124.19	119.90
80	A6	194	U	N1-C2-O2	6.14	127.10	122.80
80	A6	558	U	C5-C6-N1	6.14	125.77	122.70
80	A6	1241	G	C2-N3-C4	-6.14	108.83	111.90
36	A5	2775	U	C5-C4-O4	6.14	129.58	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2978	U	C2-N3-C4	-6.14	123.32	127.00
21	CT	89	ARG	NE-CZ-NH1	6.13	123.37	120.30
36	A5	1872	C	C4-C5-C6	6.13	120.47	117.40
1	A2	335	U	N1-C2-O2	-6.13	118.51	122.80
36	A1	574	U	C2-N3-C4	-6.13	123.32	127.00
80	A6	1347	U	C5-C6-N1	-6.13	119.63	122.70
36	A5	1165	A	C8-N9-C4	6.13	108.25	105.80
36	A5	3098	G	N1-C6-O6	-6.13	116.22	119.90
52	DO	117[A]	ARG	NE-CZ-NH2	-6.13	117.23	120.30
52	DO	117[B]	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A2	627	C	C5-C4-N4	-6.13	115.91	120.20
36	A1	340	C	N1-C2-N3	6.13	123.49	119.20
36	A1	1163	A	C5-N7-C8	-6.13	100.83	103.90
36	A1	1343	A	C2-N3-C4	-6.13	107.53	110.60
68	Be	105	ARG	NE-CZ-NH2	-6.13	117.23	120.30
80	A6	1515	A	C8-N9-C4	-6.13	103.35	105.80
36	A5	3068	U	N1-C2-N3	6.13	118.58	114.90
36	A5	3266	G	C4-C5-N7	-6.13	108.35	110.80
38	A8	79	A	N9-C4-C5	-6.13	103.35	105.80
1	A2	781	U	C2-N1-C1'	6.13	125.06	117.70
36	A5	933	A	C2-N3-C4	-6.13	107.53	110.60
36	A5	2371	G	C8-N9-C4	6.13	108.85	106.40
1	A2	852	C	C5-C6-N1	6.13	124.06	121.00
1	A2	865	A	N1-C6-N6	-6.13	114.92	118.60
1	A2	1746	A	C8-N9-C4	6.13	108.25	105.80
36	A1	862	U	C5-C6-N1	6.13	125.76	122.70
36	A1	1149	G	N1-C6-O6	6.13	123.58	119.90
36	A1	2306	C	C2-N1-C1'	6.13	125.54	118.80
36	A5	909	G	C5-N7-C8	6.13	107.36	104.30
36	A5	2939	G	N7-C8-N9	-6.13	110.04	113.10
36	A1	1025	A	C8-N9-C4	-6.13	103.35	105.80
36	A1	1139	G	N1-C6-O6	-6.13	116.22	119.90
36	A1	2376	G	N3-C2-N2	-6.13	115.61	119.90
36	A1	2629	U	C5-C4-O4	6.13	129.58	125.90
36	A1	3318	G	C8-N9-C1'	-6.13	119.03	127.00
80	A6	1459	C	N1-C2-O2	-6.13	115.22	118.90
36	A5	2632	G	N9-C4-C5	6.13	107.85	105.40
36	A5	3101	G	N1-C6-O6	-6.13	116.22	119.90
1	A2	932	U	C5-C4-O4	6.12	129.57	125.90
36	A1	658	G	C8-N9-C1'	-6.12	119.04	127.00
36	A5	2176	U	N1-C2-N3	6.12	118.58	114.90
36	A1	650	C	C4-C5-C6	6.12	120.46	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1377	G	C4-C5-C6	-6.12	115.13	118.80
36	A1	2663	G	C2-N3-C4	6.12	114.96	111.90
36	A1	3049	A	N1-C6-N6	6.12	122.27	118.60
36	A1	3242	G	C8-N9-C4	-6.12	103.95	106.40
36	A5	33	G	C6-N1-C2	-6.12	121.43	125.10
36	A5	1114	U	N3-C4-C5	6.12	118.27	114.60
36	A5	3150	A	C2-N3-C4	-6.12	107.54	110.60
1	A2	1099	U	C5-C6-N1	6.12	125.76	122.70
36	A1	966	U	N3-C4-O4	-6.12	115.11	119.40
36	A1	1120	A	C6-N1-C2	-6.12	114.93	118.60
36	A1	1386	A	N1-C2-N3	6.12	132.36	129.30
45	BG	158	ASP	N-CA-C	6.12	127.53	111.00
36	A5	1719	G	N1-C6-O6	6.12	123.57	119.90
36	A1	638	C	N3-C4-C5	6.12	124.35	121.90
80	A6	1509	C	N3-C2-O2	-6.12	117.62	121.90
36	A5	2830	G	C6-N1-C2	-6.12	121.43	125.10
36	A5	3138	U	C5-C4-O4	-6.12	122.23	125.90
80	A6	15	U	C5-C4-O4	-6.12	122.23	125.90
36	A5	2359	C	C5-C6-N1	-6.12	117.94	121.00
36	A1	862	U	C5-C4-O4	-6.12	122.23	125.90
36	A5	386	A	N9-C4-C5	-6.12	103.35	105.80
38	A4	113	U	C2-N3-C4	-6.12	123.33	127.00
80	A6	997	G	N1-C6-O6	-6.12	116.23	119.90
36	A5	1044	U	N3-C4-C5	6.12	118.27	114.60
36	A1	2394	G	C5-C6-O6	-6.11	124.93	128.60
36	A5	1323	G	C8-N9-C4	-6.11	103.95	106.40
36	A1	797	U	C2-N3-C4	-6.11	123.33	127.00
36	A1	1000	C	C2-N1-C1'	6.11	125.52	118.80
80	A6	341	A	C8-N9-C4	-6.11	103.36	105.80
36	A5	367	A	N3-C4-N9	-6.11	122.51	127.40
36	A5	2395	G	C4-C5-N7	-6.11	108.36	110.80
36	A1	1183	C	N1-C2-O2	-6.11	115.23	118.90
37	A3	3	U	C5-C6-N1	-6.11	119.64	122.70
38	A4	21	C	C5-C6-N1	-6.11	117.94	121.00
80	A6	1299	G	N3-C4-N9	6.11	129.67	126.00
36	A5	880	G	C5-C6-N1	6.11	114.56	111.50
36	A5	2353	G	N3-C4-N9	6.11	129.67	126.00
1	A2	1346	A	N7-C8-N9	6.11	116.86	113.80
36	A5	2650	U	N3-C4-O4	-6.11	115.12	119.40
1	A2	1514	U	N3-C2-O2	-6.11	117.92	122.20
36	A1	919	U	C2-N3-C4	-6.11	123.33	127.00
36	A1	2957	G	N7-C8-N9	-6.11	110.05	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	3110	C	C2-N3-C4	-6.11	116.85	119.90
36	A1	1467	A	C8-N9-C4	-6.11	103.36	105.80
36	A1	2705	A	C2-N3-C4	6.11	113.65	110.60
36	A1	2726	C	C4-C5-C6	6.11	120.45	117.40
36	A1	3312	U	C5-C6-N1	-6.11	119.65	122.70
38	A4	25	G	N9-C4-C5	6.11	107.84	105.40
36	A5	785	G	C2-N3-C4	6.11	114.95	111.90
36	A5	2930	A	C8-N9-C1'	6.11	138.69	127.70
36	A5	3086	A	C8-N9-C4	6.11	108.24	105.80
36	A1	1836	C	C6-N1-C2	6.10	122.74	120.30
36	A1	2372	A	N9-C4-C5	6.10	108.24	105.80
56	BS	51	VAL	CB-CA-C	-6.10	99.80	111.40
36	A5	933	A	C6-N1-C2	-6.10	114.94	118.60
80	A6	1295	G	N1-C6-O6	6.10	123.56	119.90
36	A5	673	U	C2-N3-C4	-6.10	123.34	127.00
36	A5	1119	C	N1-C2-O2	-6.10	115.24	118.90
36	A1	2148	U	C5-C4-O4	-6.10	122.24	125.90
36	A5	2646	C	N1-C2-O2	-6.10	115.24	118.90
36	A1	702	C	N1-C2-N3	6.10	123.47	119.20
36	A1	1505	C	C2-N3-C4	-6.10	116.85	119.90
36	A5	1124	U	N3-C4-C5	6.10	118.26	114.60
36	A5	1206	G	N3-C4-C5	-6.10	125.55	128.60
38	A8	15	G	C5-C6-N1	6.10	114.55	111.50
1	A2	621	A	C8-N9-C4	6.10	108.24	105.80
1	A2	1473	U	C5-C4-O4	6.10	129.56	125.90
1	A2	1596	C	C2-N1-C1'	6.10	125.51	118.80
36	A5	216	G	C6-C5-N7	-6.10	126.74	130.40
36	A5	516	A	N1-C6-N6	6.10	122.26	118.60
36	A1	941	G	C2-N3-C4	6.09	114.95	111.90
36	A1	2160	G	C6-C5-N7	-6.09	126.74	130.40
36	A1	2944	U	C4-C5-C6	-6.09	116.04	119.70
36	A5	1469	C	C4-C5-C6	6.09	120.45	117.40
36	A5	2833	A	C5-C6-N1	6.09	120.75	117.70
36	A1	617	G	N1-C2-N3	6.09	127.56	123.90
40	DB	205	VAL	CB-CA-C	-6.09	99.82	111.40
1	A2	266	A	N1-C6-N6	6.09	122.25	118.60
1	A2	1749	A	C8-N9-C4	6.09	108.24	105.80
36	A1	1103	A	C2-N3-C4	6.09	113.65	110.60
80	A6	1121	C	C6-N1-C2	6.09	122.74	120.30
80	A6	1244	A	C8-N9-C4	-6.09	103.36	105.80
80	A6	1482	C	C6-N1-C2	6.09	122.74	120.30
80	A6	1662	G	C5-C6-N1	6.09	114.55	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1909	A	N1-C2-N3	-6.09	126.25	129.30
36	A5	2386	A	C5-C6-N6	-6.09	118.83	123.70
36	A5	2749	G	N1-C2-N3	-6.09	120.25	123.90
1	A2	192	U	N3-C2-O2	-6.09	117.94	122.20
80	A6	682	C	C5-C6-N1	6.09	124.04	121.00
36	A5	1652	G	C8-N9-C4	6.09	108.84	106.40
36	A5	2134	G	C2-N3-C4	6.09	114.94	111.90
36	A5	2358	A	C8-N9-C4	6.09	108.24	105.80
36	A5	2620	G	N1-C6-O6	-6.09	116.25	119.90
36	A1	1133	A	N7-C8-N9	-6.09	110.76	113.80
36	A5	935	U	C5-C4-O4	-6.09	122.25	125.90
36	A5	2865	U	C2-N1-C1'	6.09	125.01	117.70
36	A1	1122	U	N3-C4-O4	-6.09	115.14	119.40
36	A1	2306	C	N3-C4-N4	-6.09	113.74	118.00
36	A1	2758	A	C2-N3-C4	6.09	113.64	110.60
36	A5	1147	G	C6-C5-N7	6.09	134.05	130.40
36	A5	2368	A	N1-C6-N6	-6.09	114.95	118.60
36	A1	302	U	C5-C6-N1	-6.08	119.66	122.70
36	A1	511	G	N1-C6-O6	-6.08	116.25	119.90
36	A1	670	C	C2-N3-C4	-6.08	116.86	119.90
36	A1	1329	U	C3'-C2'-C1'	6.08	106.37	101.50
80	A6	84	A	N1-C6-N6	-6.08	114.95	118.60
36	A5	282	G	N9-C4-C5	6.08	107.83	105.40
1	A2	61	A	C8-N9-C4	-6.08	103.37	105.80
36	A1	1472	U	C5-C6-N1	-6.08	119.66	122.70
80	A6	1792	G	C6-C5-N7	-6.08	126.75	130.40
36	A5	341	G	N1-C6-O6	6.08	123.55	119.90
38	A8	14	C	C2-N3-C4	-6.08	116.86	119.90
36	A1	371	G	N3-C2-N2	6.08	124.16	119.90
36	A1	1145	G	C5-N7-C8	6.08	107.34	104.30
36	A1	3242	G	C4-C5-C6	-6.08	115.15	118.80
36	A5	125	C	N3-C4-N4	-6.08	113.74	118.00
36	A1	1170	A	N1-C2-N3	-6.08	126.26	129.30
36	A1	2749	G	C6-C5-N7	-6.08	126.75	130.40
36	A5	1929	G	N9-C4-C5	-6.08	102.97	105.40
36	A5	2730	G	N3-C4-N9	-6.08	122.35	126.00
38	A8	47	C	N1-C2-O2	6.08	122.55	118.90
36	A5	2392	C	N3-C4-C5	6.08	124.33	121.90
1	A2	1057	U	C2-N1-C1'	6.08	124.99	117.70
36	A1	1155	C	C6-N1-C2	-6.08	117.87	120.30
36	A1	1724	U	N3-C2-O2	-6.08	117.95	122.20
36	A1	2177	G	N3-C4-N9	6.08	129.65	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2393	G	N1-C6-O6	6.08	123.55	119.90
36	A1	2434	U	C4-C5-C6	6.08	123.34	119.70
36	A5	1666	G	C5-C6-O6	6.08	132.25	128.60
36	A5	2128	C	C2-N3-C4	-6.08	116.86	119.90
36	A5	2791	G	N1-C6-O6	6.08	123.55	119.90
36	A1	1494	U	N3-C4-C5	6.07	118.24	114.60
36	A1	1719	G	C5-C6-O6	-6.07	124.96	128.60
36	A1	2770	G	N7-C8-N9	6.07	116.14	113.10
37	A7	40	C	C4-C5-C6	6.07	120.44	117.40
1	A2	377	G	N3-C4-N9	-6.07	122.36	126.00
80	A6	337	G	C5-C6-O6	-6.07	124.96	128.60
80	A6	1304	G	N3-C4-N9	6.07	129.64	126.00
36	A5	1136	A	N1-C2-N3	-6.07	126.26	129.30
36	A5	1192	C	C2-N3-C4	-6.07	116.86	119.90
51	BN	38	ARG	NE-CZ-NH1	6.07	123.33	120.30
36	A5	3020	U	C5-C4-O4	-6.07	122.26	125.90
36	A5	3382	U	N3-C2-O2	-6.07	117.95	122.20
36	A1	1481	A	C5-N7-C8	-6.07	100.86	103.90
36	A5	66	A	N9-C4-C5	-6.07	103.37	105.80
36	A5	2954	U	C5-C4-O4	-6.07	122.26	125.90
36	A1	509	U	C2-N3-C4	-6.07	123.36	127.00
36	A1	1145	G	N3-C2-N2	6.07	124.15	119.90
80	A6	36	C	C2-N3-C4	-6.07	116.87	119.90
80	A6	563	U	C5-C6-N1	-6.07	119.67	122.70
80	A6	1749	A	C5-N7-C8	-6.07	100.87	103.90
36	A5	976	U	N3-C2-O2	-6.07	117.95	122.20
36	A5	2764	C	N3-C4-C5	6.07	124.33	121.90
36	A1	694	C	N3-C4-C5	6.07	124.33	121.90
15	CN	114	ARG	NE-CZ-NH1	6.07	123.33	120.30
36	A5	1438	U	C2-N1-C1'	6.07	124.98	117.70
36	A1	2649	A	N1-C2-N3	-6.06	126.27	129.30
36	A1	3377	G	N3-C4-N9	6.06	129.64	126.00
80	A6	387	A	C2-N3-C4	6.06	113.63	110.60
36	A5	1902	G	N7-C8-N9	-6.06	110.07	113.10
36	A1	331	G	C2-N3-C4	6.06	114.93	111.90
36	A1	718	G	C2-N3-C4	-6.06	108.87	111.90
36	A1	1474	A	N1-C2-N3	6.06	132.33	129.30
36	A1	1743	G	C8-N9-C4	6.06	108.83	106.40
36	A1	2380	U	N1-C2-N3	6.06	118.54	114.90
80	A6	1428	G	C8-N9-C4	-6.06	103.97	106.40
36	A5	80	G	N1-C6-O6	-6.06	116.26	119.90
36	A5	883	A	N7-C8-N9	-6.06	110.77	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1808	G	N1-C6-O6	6.06	123.54	119.90
36	A5	1042	U	N3-C2-O2	-6.06	117.96	122.20
36	A1	1092	C	C6-N1-C2	-6.06	117.88	120.30
36	A1	2349	U	N3-C4-C5	6.06	118.23	114.60
46	BH	166	ARG	NE-CZ-NH2	6.06	123.33	120.30
80	A6	906	A	C2-N3-C4	-6.06	107.57	110.60
80	A6	1473	U	C5-C4-O4	6.06	129.54	125.90
80	A6	1754	A	N1-C6-N6	-6.06	114.96	118.60
36	A5	1222	G	P-O3'-C3'	6.06	126.97	119.70
36	A5	2353	G	C6-C5-N7	-6.06	126.76	130.40
36	A5	3245	A	N9-C4-C5	-6.06	103.38	105.80
1	A2	397	A	N1-C6-N6	-6.06	114.97	118.60
1	A2	719	U	C5-C6-N1	6.06	125.73	122.70
36	A1	388	G	C8-N9-C4	-6.06	103.98	106.40
38	A4	10	A	C6-N1-C2	-6.06	114.97	118.60
36	A5	920	A	N7-C8-N9	-6.06	110.77	113.80
36	A5	3382	U	C6-N1-C1'	-6.06	112.72	121.20
1	A2	557	G	N3-C4-N9	6.05	129.63	126.00
80	A6	799	A	C8-N9-C4	-6.05	103.38	105.80
80	A6	1473	U	C6-N1-C2	-6.05	117.37	121.00
36	A5	555	U	N3-C4-O4	6.05	123.64	119.40
36	A5	1168	U	N3-C4-O4	-6.05	115.16	119.40
36	A5	2415	C	N3-C4-C5	6.05	124.32	121.90
36	A5	2887	A	C6-N1-C2	6.05	122.23	118.60
36	A5	2911	A	C8-N9-C4	-6.05	103.38	105.80
1	A2	1192	C	N3-C2-O2	6.05	126.14	121.90
36	A1	46	U	N3-C2-O2	-6.05	117.96	122.20
36	A1	677	A	N1-C6-N6	6.05	122.23	118.60
36	A1	1379	G	C2-N3-C4	-6.05	108.87	111.90
38	A4	5	U	N1-C2-O2	-6.05	118.56	122.80
36	A5	311	C	N3-C4-C5	6.05	124.32	121.90
36	A5	2730	G	C5-N7-C8	-6.05	101.27	104.30
36	A5	2830	G	N3-C2-N2	-6.05	115.66	119.90
36	A5	3309	G	C5-C6-N1	6.05	114.53	111.50
52	DO	117[A]	ARG	CG-CD-NE	-6.05	99.09	111.80
52	DO	117[B]	ARG	CG-CD-NE	-6.05	99.09	111.80
36	A1	1175	C	N3-C4-C5	6.05	124.32	121.90
36	A1	1820	U	P-O3'-C3'	6.05	126.96	119.70
80	A6	623	A	C8-N9-C4	6.05	108.22	105.80
36	A5	927	C	N3-C4-C5	6.05	124.32	121.90
36	A5	1301	A	N9-C4-C5	-6.05	103.38	105.80
36	A5	1582	C	C6-N1-C2	-6.05	117.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1897	G	C5-C6-N1	6.05	114.53	111.50
36	A5	3182	G	C5-C6-O6	6.05	132.23	128.60
51	DN	96	ARG	NE-CZ-NH1	6.05	123.32	120.30
80	A6	1481	C	C3'-C2'-C1'	-6.05	96.66	101.50
36	A5	811	U	C4-C5-C6	6.05	123.33	119.70
36	A5	1869	C	C2-N3-C4	-6.05	116.88	119.90
36	A1	1450	G	C8-N9-C4	6.05	108.82	106.40
36	A1	2528	G	N3-C4-C5	6.05	131.62	128.60
80	A6	429	G	C4-C5-N7	-6.05	108.38	110.80
38	A8	42	G	N7-C8-N9	-6.05	110.08	113.10
36	A1	290	G	C2-N3-C4	6.04	114.92	111.90
36	A5	1518	U	N3-C2-O2	-6.04	117.97	122.20
1	A2	1121	C	C5-C6-N1	-6.04	117.98	121.00
36	A1	659	G	N1-C2-N2	-6.04	110.76	116.20
36	A1	1894	U	N3-C4-C5	6.04	118.23	114.60
36	A1	2161	G	N3-C4-C5	-6.04	125.58	128.60
36	A1	2930	A	C4-C5-N7	-6.04	107.68	110.70
1	A2	349	U	C4-C5-C6	6.04	123.33	119.70
1	A2	557	G	C6-C5-N7	-6.04	126.78	130.40
36	A1	2174	G	N1-C2-N3	6.04	127.53	123.90
36	A1	3228	C	C2-N1-C1'	6.04	125.44	118.80
80	A6	358	U	N1-C2-O2	-6.04	118.57	122.80
80	A6	640	U	C5-C6-N1	-6.04	119.68	122.70
80	A6	1164	G	C8-N9-C4	6.04	108.82	106.40
36	A5	424	G	N1-C6-O6	-6.04	116.28	119.90
36	A5	2837	A	N7-C8-N9	-6.04	110.78	113.80
36	A1	1800	A	N1-C6-N6	-6.04	114.98	118.60
11	CJ	3	ARG	NE-CZ-NH2	6.04	123.32	120.30
36	A5	2980	U	C6-N1-C2	-6.04	117.38	121.00
36	A5	3211	C	C4-C5-C6	6.04	120.42	117.40
1	A2	445	A	C2-N3-C4	6.04	113.62	110.60
1	A2	719	U	N1-C2-O2	6.04	127.03	122.80
36	A1	1347	U	N3-C2-O2	-6.04	117.97	122.20
36	A5	2993	G	N3-C4-N9	6.04	129.62	126.00
1	A2	1246	C	N3-C4-N4	-6.04	113.78	118.00
36	A1	630	A	C5-C6-N1	6.04	120.72	117.70
36	A1	1807	G	N3-C4-C5	-6.04	125.58	128.60
36	A1	2353	G	C6-C5-N7	-6.04	126.78	130.40
36	A1	2406	C	C4-C5-C6	6.04	120.42	117.40
69	Bf	67	MET	CG-SD-CE	-6.04	90.54	100.20
36	A5	1000	C	C6-N1-C2	-6.04	117.89	120.30
36	A1	3048	A	N7-C8-N9	6.03	116.82	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A4	58	G	C8-N9-C4	6.03	108.81	106.40
36	A5	813	G	N9-C4-C5	6.03	107.81	105.40
36	A5	3003	G	C4-C5-C6	-6.03	115.18	118.80
36	A5	3148	U	N3-C4-C5	6.03	118.22	114.60
80	A6	1572	G	C6-C5-N7	-6.03	126.78	130.40
36	A5	1368	U	C6-N1-C2	6.03	124.62	121.00
1	A2	538	A	N1-C2-N3	-6.03	126.28	129.30
1	A2	1450	U	C5-C4-O4	6.03	129.52	125.90
36	A1	907	G	N7-C8-N9	6.03	116.12	113.10
36	A1	1312	C	N1-C2-O2	-6.03	115.28	118.90
36	A1	1175	C	C5-C4-N4	-6.03	115.98	120.20
36	A1	1881	A	N9-C4-C5	-6.03	103.39	105.80
37	A3	98	C	C4-C5-C6	6.03	120.41	117.40
64	Ba	66	ALA	N-CA-C	-6.03	94.72	111.00
36	A5	1184	A	C2-N3-C4	-6.03	107.59	110.60
36	A5	3318	G	N1-C6-O6	-6.03	116.28	119.90
36	A1	2187	G	N9-C4-C5	-6.03	102.99	105.40
36	A1	2620	G	C5-C6-O6	-6.03	124.98	128.60
36	A1	2902	A	C2-N3-C4	-6.03	107.59	110.60
36	A5	1117	G	C5-C6-O6	-6.03	124.98	128.60
36	A5	1128	U	C5-C6-N1	-6.03	119.69	122.70
36	A5	2361	A	C5-N7-C8	6.03	106.91	103.90
36	A5	3343	G	N1-C2-N2	-6.03	110.78	116.20
1	A2	144	U	N1-C2-N3	6.03	118.52	114.90
36	A1	39	A	N7-C8-N9	-6.03	110.79	113.80
36	A1	2129	U	C6-N1-C2	-6.03	117.39	121.00
36	A1	2941	A	C8-N9-C4	6.03	108.21	105.80
38	A4	14	C	C2-N3-C4	-6.03	116.89	119.90
80	A6	1550	A	N1-C6-N6	6.03	122.22	118.60
36	A5	2364	G	N3-C4-C5	-6.03	125.59	128.60
36	A5	2920	U	N1-C2-N3	6.03	118.52	114.90
36	A1	639	G	N9-C4-C5	-6.02	102.99	105.40
36	A5	341	G	N1-C2-N2	6.02	121.62	116.20
36	A1	934	G	C5-C6-N1	6.02	114.51	111.50
36	A1	3006	A	N1-C6-N6	6.02	122.21	118.60
36	A5	226	C	C5-C4-N4	-6.02	115.98	120.20
36	A5	520	U	N1-C2-N3	6.02	118.51	114.90
36	A5	795	G	C2-N3-C4	6.02	114.91	111.90
1	A2	1000	C	C5-C4-N4	6.02	124.42	120.20
36	A5	884	A	C4-C5-C6	-6.02	113.99	117.00
36	A1	1335	C	C2-N3-C4	-6.02	116.89	119.90
36	A1	2284	C	N1-C2-N3	6.02	123.41	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2844	C	N1-C2-O2	6.02	122.51	118.90
1	A2	75	U	C2-N1-C1'	6.02	124.92	117.70
1	A2	377	G	N1-C6-O6	6.02	123.51	119.90
1	A2	389	G	N3-C4-C5	-6.02	125.59	128.60
1	A2	1387	G	C5-C6-O6	-6.02	124.99	128.60
36	A1	81	C	N3-C4-C5	6.02	124.31	121.90
36	A1	700	C	N3-C4-C5	6.02	124.31	121.90
80	A6	879	G	C5-C6-O6	6.02	132.21	128.60
36	A5	2108	C	N3-C4-N4	-6.02	113.79	118.00
36	A5	2976	A	N7-C8-N9	-6.02	110.79	113.80
36	A5	3095	U	N3-C4-C5	6.02	118.21	114.60
1	A2	831	U	C6-N1-C2	-6.02	117.39	121.00
36	A1	50	U	N1-C2-O2	-6.02	118.59	122.80
36	A1	1152	G	C6-N1-C2	-6.02	121.49	125.10
38	A4	96	A	N1-C6-N6	6.02	122.21	118.60
80	A6	820	U	N3-C2-O2	6.02	126.41	122.20
36	A5	912	G	N3-C4-N9	6.02	129.61	126.00
1	A2	404	G	N9-C4-C5	-6.01	102.99	105.40
36	A1	197	G	N3-C2-N2	-6.01	115.69	119.90
36	A1	906	A	C5-C6-N1	6.01	120.71	117.70
36	A1	2979	U	N3-C4-O4	-6.01	115.19	119.40
38	A4	51	G	C5-C6-O6	-6.01	124.99	128.60
80	A6	1111	G	C4-C5-N7	6.01	113.20	110.80
36	A5	517	G	N1-C2-N3	6.01	127.51	123.90
36	A5	822	G	N3-C2-N2	-6.01	115.69	119.90
76	Dm	97	ARG	NE-CZ-NH2	-6.01	117.29	120.30
36	A1	968	G	N7-C8-N9	6.01	116.11	113.10
36	A1	2417	U	N1-C2-N3	6.01	118.51	114.90
36	A5	2939	G	C5-N7-C8	6.01	107.31	104.30
36	A5	3140	G	C5-N7-C8	-6.01	101.29	104.30
36	A1	405	U	N3-C4-C5	6.01	118.21	114.60
36	A1	1484	U	P-O3'-C3'	6.01	126.91	119.70
36	A1	1522	U	C2-N3-C4	-6.01	123.39	127.00
36	A1	2638	C	N1-C2-O2	6.01	122.51	118.90
36	A1	2692	A	C8-N9-C4	-6.01	103.39	105.80
80	A6	1781	A	C5-C6-N6	6.01	128.51	123.70
36	A1	867	G	N9-C4-C5	6.01	107.80	105.40
36	A1	1409	G	C6-C5-N7	6.01	134.00	130.40
36	A1	1604	G	C8-N9-C1'	-6.01	119.19	127.00
36	A1	933	A	C8-N9-C4	-6.01	103.40	105.80
36	A1	987	U	C5-C6-N1	-6.01	119.70	122.70
36	A1	1174	G	C4-C5-N7	6.01	113.20	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	3212	C	N3-C4-C5	6.01	124.30	121.90
80	A6	375	U	N3-C4-C5	6.01	118.20	114.60
47	DI	83	ASP	CB-CG-OD1	-6.01	112.89	118.30
36	A1	1017	C	C5-C6-N1	6.01	124.00	121.00
36	A1	1433	A	C5-C6-N6	-6.01	118.89	123.70
36	A1	2168	A	N7-C8-N9	-6.01	110.80	113.80
36	A1	2879	C	C2-N3-C4	6.01	122.90	119.90
80	A6	150	U	N3-C4-O4	-6.01	115.20	119.40
36	A5	1242	G	C4-N9-C1'	6.01	134.31	126.50
36	A5	1340	G	N7-C8-N9	-6.01	110.10	113.10
36	A5	2724	U	C5-C4-O4	6.01	129.50	125.90
36	A5	2911	A	N1-C2-N3	-6.01	126.30	129.30
1	A2	1753	A	C8-N9-C4	6.00	108.20	105.80
36	A1	290	G	N1-C6-O6	-6.00	116.30	119.90
36	A5	1858	A	C4-C5-C6	6.00	120.00	117.00
1	A2	1157	A	C8-N9-C4	-6.00	103.40	105.80
36	A1	92	G	C5-C6-N1	6.00	114.50	111.50
36	A1	1941	C	N1-C2-O2	-6.00	115.30	118.90
36	A1	2990	G	N3-C4-C5	-6.00	125.60	128.60
36	A5	595	G	N1-C6-O6	-6.00	116.30	119.90
36	A5	1371	G	C6-N1-C2	-6.00	121.50	125.10
36	A5	3187	A	N7-C8-N9	-6.00	110.80	113.80
36	A1	2916	U	C4-C5-C6	6.00	123.30	119.70
36	A1	3214	U	C6-N1-C2	-6.00	117.40	121.00
36	A5	392	G	C5-C6-O6	-6.00	125.00	128.60
36	A5	641	C	C5-C4-N4	6.00	124.40	120.20
36	A5	903	U	C5-C6-N1	-6.00	119.70	122.70
36	A5	2381	G	C5-C6-O6	6.00	132.20	128.60
36	A1	1399	A	C8-N9-C4	6.00	108.20	105.80
36	A1	3225	C	C5-C6-N1	-6.00	118.00	121.00
80	A6	631	G	C8-N9-C4	-6.00	104.00	106.40
36	A5	701	G	C4-C5-N7	-6.00	108.40	110.80
36	A5	2603	G	C5-N7-C8	-6.00	101.30	104.30
36	A5	3369	G	C6-N1-C2	-6.00	121.50	125.10
1	A2	1601	G	C5-C6-N1	6.00	114.50	111.50
80	A6	1568	C	C2-N1-C1'	6.00	125.40	118.80
36	A5	1110	U	N3-C4-O4	-6.00	115.20	119.40
36	A5	1378	U	C6-N1-C2	6.00	124.60	121.00
36	A5	2346	C	N1-C2-O2	-6.00	115.30	118.90
40	DB	232	ARG	NE-CZ-NH2	-6.00	117.30	120.30
36	A1	440	A	C8-N9-C4	-6.00	103.40	105.80
80	A6	1594	G	N3-C4-N9	6.00	129.60	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	DO	13[B]	ASP	C-N-CA	6.00	136.69	121.70
36	A1	1374	G	N1-C2-N2	-5.99	110.81	116.20
38	A4	28	C	C4-C5-C6	5.99	120.40	117.40
80	A6	1186	U	C5-C6-N1	-5.99	119.70	122.70
36	A5	619	A	N1-C6-N6	-5.99	115.00	118.60
36	A5	994	G	C8-N9-C4	5.99	108.80	106.40
38	A8	100	U	C5-C4-O4	-5.99	122.30	125.90
36	A1	1870	C	C6-N1-C2	5.99	122.70	120.30
36	A1	2794	G	N1-C6-O6	-5.99	116.31	119.90
36	A5	1047	A	C5-C6-N1	5.99	120.70	117.70
36	A5	2370	G	C5-C6-N1	5.99	114.50	111.50
36	A5	2908	G	C5-C6-N1	-5.99	108.50	111.50
1	A2	274	G	C4-N9-C1'	5.99	134.29	126.50
1	A2	1643	U	C5-C6-N1	-5.99	119.70	122.70
36	A1	919	U	N3-C4-O4	-5.99	115.21	119.40
36	A1	1362	G	C5-C6-O6	-5.99	125.00	128.60
36	A1	2514	U	C5-C6-N1	-5.99	119.70	122.70
36	A5	2116	G	C6-C5-N7	-5.99	126.81	130.40
36	A5	3028	G	N3-C4-N9	5.99	129.59	126.00
36	A5	3343	G	N3-C2-N2	5.99	124.09	119.90
36	A1	802	C	C2-N1-C1'	5.99	125.39	118.80
80	A6	337	G	C5-C6-N1	-5.99	108.51	111.50
80	A6	1129	U	N3-C4-C5	5.99	118.19	114.60
36	A5	2526	C	N1-C2-O2	5.99	122.49	118.90
36	A1	384	A	N9-C4-C5	-5.99	103.41	105.80
59	BV	80	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A2	1417	A	N1-C6-N6	5.99	122.19	118.60
36	A1	931	C	C5-C4-N4	5.99	124.39	120.20
36	A1	1831	U	N3-C2-O2	-5.99	118.01	122.20
80	A6	1440	C	N3-C4-N4	5.99	122.19	118.00
36	A5	283	G	C4-C5-N7	5.99	113.19	110.80
36	A1	1369	A	N3-C4-C5	5.98	130.99	126.80
37	A3	103	A	N9-C4-C5	-5.98	103.41	105.80
36	A5	3341	U	C5-C6-N1	5.98	125.69	122.70
47	DI	57	LEU	CA-CB-CG	5.98	129.06	115.30
1	A2	554	C	N1-C2-O2	5.98	122.49	118.90
36	A1	1425	U	C5-C4-O4	5.98	129.49	125.90
36	A1	2193	U	C5-C6-N1	-5.98	119.71	122.70
36	A1	3046	A	N9-C4-C5	5.98	108.19	105.80
36	A5	1808	G	C8-N9-C4	5.98	108.79	106.40
36	A5	3298	C	C4-C5-C6	5.98	120.39	117.40
38	A8	63	G	N1-C6-O6	-5.98	116.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	106	U	C6-N1-C2	-5.98	117.41	121.00
1	A2	829	A	C8-N9-C4	-5.98	103.41	105.80
36	A1	78	U	C5-C6-N1	-5.98	119.71	122.70
36	A1	716	A	C5-C6-N6	-5.98	118.92	123.70
36	A1	2387	A	N1-C6-N6	-5.98	115.01	118.60
36	A1	2608	G	N1-C6-O6	-5.98	116.31	119.90
80	A6	1745	G	N9-C4-C5	-5.98	103.01	105.40
36	A5	351	A	N1-C6-N6	5.98	122.19	118.60
36	A5	2426	U	N3-C4-O4	-5.98	115.21	119.40
36	A5	2617	U	N3-C4-C5	5.98	118.19	114.60
50	DM	135	LEU	CA-CB-CG	5.98	129.06	115.30
1	A2	628	G	C5-C6-O6	5.98	132.19	128.60
36	A1	2171	G	C2-N3-C4	5.98	114.89	111.90
36	A5	892	U	C2-N3-C4	-5.98	123.41	127.00
1	A2	360	A	N1-C6-N6	5.98	122.19	118.60
1	A2	1768	G	C4-N9-C1'	-5.98	118.73	126.50
36	A5	2952	G	C6-N1-C2	-5.98	121.51	125.10
36	A1	67	A	C4-C5-C6	5.98	119.99	117.00
36	A1	1492	G	N7-C8-N9	-5.98	110.11	113.10
80	A6	416	A	N1-C6-N6	5.98	122.19	118.60
80	A6	1090	C	N1-C2-O2	-5.98	115.31	118.90
36	A1	32	U	C2-N3-C4	-5.97	123.42	127.00
36	A1	1584	U	N3-C4-O4	-5.97	115.22	119.40
36	A1	1796	G	N9-C4-C5	5.97	107.79	105.40
36	A1	1899	G	N7-C8-N9	5.97	116.09	113.10
36	A1	2547	A	N9-C4-C5	-5.97	103.41	105.80
36	A5	416	A	N9-C4-C5	5.97	108.19	105.80
36	A5	1171	G	N7-C8-N9	5.97	116.09	113.10
36	A5	2318	U	N3-C4-O4	-5.97	115.22	119.40
36	A5	2365	C	C5-C6-N1	-5.97	118.01	121.00
36	A5	2753	G	N7-C8-N9	5.97	116.09	113.10
36	A5	3013	U	N3-C2-O2	-5.97	118.02	122.20
36	A1	923	C	N1-C2-O2	-5.97	115.32	118.90
36	A1	941	G	C5-C6-N1	5.97	114.49	111.50
36	A1	2640	A	C6-N1-C2	-5.97	115.02	118.60
36	A1	3377	G	C6-N1-C2	-5.97	121.52	125.10
38	A4	101	U	N3-C2-O2	-5.97	118.02	122.20
80	A6	622	A	C4-C5-C6	5.97	119.99	117.00
80	A6	1120	U	C2-N3-C4	-5.97	123.42	127.00
80	A6	1519	U	N3-C2-O2	-5.97	118.02	122.20
36	A5	419	G	C8-N9-C4	5.97	108.79	106.40
36	A5	3112	G	N1-C6-O6	5.97	123.48	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	802	C	C4-C5-C6	5.97	120.39	117.40
36	A1	124	U	N1-C2-O2	5.97	126.98	122.80
36	A1	614	C	C2-N3-C4	-5.97	116.92	119.90
36	A1	3015	G	N3-C4-C5	-5.97	125.61	128.60
36	A1	3090	U	N1-C2-O2	-5.97	118.62	122.80
36	A5	2329	C	N3-C4-N4	-5.97	113.82	118.00
51	DN	172	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	A2	1000	C	N3-C2-O2	-5.97	117.72	121.90
1	A2	382	C	C2-N3-C4	-5.97	116.92	119.90
1	A2	1119	G	C5-C6-O6	5.97	132.18	128.60
1	A2	1455	G	N9-C4-C5	5.97	107.79	105.40
1	A2	1745	G	C6-N1-C2	-5.97	121.52	125.10
36	A1	439	C	C6-N1-C1'	-5.97	113.64	120.80
38	A4	10	A	N1-C6-N6	-5.97	115.02	118.60
36	A5	987	U	N3-C2-O2	-5.97	118.02	122.20
36	A5	1910	A	C5-C6-N1	5.97	120.68	117.70
36	A5	2167	A	N9-C4-C5	5.97	108.19	105.80
36	A5	2421	U	N1-C2-O2	-5.97	118.62	122.80
36	A5	2917	G	N3-C4-C5	-5.97	125.62	128.60
36	A5	3192	U	C2-N3-C4	-5.97	123.42	127.00
36	A5	3222	U	N3-C2-O2	-5.97	118.02	122.20
1	A2	1121	C	N3-C4-C5	-5.96	119.51	121.90
14	CM	62	LEU	CA-CB-CG	5.96	129.02	115.30
36	A5	679	U	C5-C4-O4	5.96	129.48	125.90
36	A5	873	C	P-O3'-C3'	5.96	126.86	119.70
36	A5	1323	G	N9-C4-C5	5.96	107.79	105.40
36	A5	1725	C	C5-C4-N4	5.96	124.38	120.20
36	A5	1739	U	C5-C4-O4	5.96	129.48	125.90
37	A7	96	U	C2-N1-C1'	5.96	124.86	117.70
1	A2	1600	A	C5-N7-C8	-5.96	100.92	103.90
36	A1	1337	A	C2-N3-C4	5.96	113.58	110.60
36	A5	594	U	C5-C6-N1	5.96	125.68	122.70
36	A5	2411	U	N3-C4-C5	5.96	118.18	114.60
36	A5	2799	A	C2-N3-C4	-5.96	107.62	110.60
1	A2	1521	G	N3-C4-N9	5.96	129.58	126.00
36	A1	2794	G	C5-C6-O6	5.96	132.18	128.60
36	A5	1305	U	N3-C4-O4	5.96	123.57	119.40
36	A5	3216	G	C4-C5-C6	5.96	122.38	118.80
50	DM	106	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A2	794	U	C2-N1-C1'	5.96	124.85	117.70
36	A1	417	A	N9-C4-C5	-5.96	103.42	105.80
36	A5	2166	A	N1-C6-N6	5.96	122.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	554	C	C2-N3-C4	-5.96	116.92	119.90
36	A5	2323	G	N1-C6-O6	-5.96	116.33	119.90
36	A5	3351	U	N3-C2-O2	-5.96	118.03	122.20
36	A1	340	C	C5-C4-N4	5.96	124.37	120.20
36	A1	1060	U	N3-C4-C5	5.96	118.17	114.60
80	A6	687	G	C4-N9-C1'	-5.96	118.76	126.50
36	A5	3075	G	C4-C5-N7	-5.96	108.42	110.80
73	Dj	21	ARG	NE-CZ-NH2	-5.96	117.32	120.30
36	A5	2250	G	N1-C6-O6	-5.96	116.33	119.90
36	A5	3333	G	N9-C4-C5	-5.96	103.02	105.40
47	DI	7	ARG	NE-CZ-NH1	-5.96	117.32	120.30
36	A1	49	A	C2-N3-C4	-5.95	107.62	110.60
36	A1	950	G	N3-C2-N2	5.95	124.07	119.90
36	A1	1010	G	C8-N9-C4	-5.95	104.02	106.40
39	BA	122	ASP	CB-CG-OD2	5.95	123.66	118.30
36	A5	1190	A	N1-C6-N6	-5.95	115.03	118.60
36	A5	2917	G	N1-C6-O6	5.95	123.47	119.90
36	A5	3064	U	N3-C2-O2	-5.95	118.03	122.20
54	DQ	99	THR	N-CA-C	5.95	127.08	111.00
36	A1	2852	C	C6-N1-C2	5.95	122.68	120.30
36	A5	2552	C	C5-C4-N4	5.95	124.37	120.20
26	AY	44	LEU	CA-CB-CG	5.95	128.99	115.30
36	A1	200	C	N1-C2-O2	5.95	122.47	118.90
36	A1	783	A	C2-N3-C4	-5.95	107.62	110.60
80	A6	1720	G	C6-C5-N7	-5.95	126.83	130.40
36	A5	1678	G	C5-C6-N1	5.95	114.48	111.50
36	A5	2167	A	N1-C6-N6	-5.95	115.03	118.60
36	A5	2410	U	N3-C4-C5	5.95	118.17	114.60
36	A5	2730	G	N3-C4-C5	5.95	131.57	128.60
36	A5	2851	A	N7-C8-N9	-5.95	110.83	113.80
1	A2	781	U	N1-C2-O2	5.95	126.96	122.80
36	A1	413	U	C5-C4-O4	-5.95	122.33	125.90
36	A1	651	G	C5-N7-C8	5.95	107.28	104.30
36	A1	1332	A	N9-C4-C5	-5.95	103.42	105.80
36	A1	2948	C	C2-N3-C4	-5.95	116.93	119.90
36	A1	3001	C	C5-C6-N1	-5.95	118.03	121.00
36	A1	3130	A	C8-N9-C4	-5.95	103.42	105.80
36	A5	655	C	C6-N1-C2	-5.95	117.92	120.30
36	A5	2349	U	C4-C5-C6	-5.95	116.13	119.70
36	A5	2792	A	C8-N9-C4	-5.95	103.42	105.80
36	A5	337	G	N1-C6-O6	-5.95	116.33	119.90
36	A5	1548	C	N1-C2-O2	-5.95	115.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	542	A	C6-C5-N7	-5.95	128.14	132.30
36	A1	173	G	C4-N9-C1'	5.95	134.23	126.50
37	A3	91	G	C2-N3-C4	-5.95	108.93	111.90
80	A6	1792	G	C4-C5-N7	5.95	113.18	110.80
36	A5	359	U	C6-N1-C2	5.95	124.57	121.00
36	A5	1753	G	C2-N3-C4	5.95	114.87	111.90
36	A5	2416	U	N3-C2-O2	-5.95	118.04	122.20
36	A5	3395	G	N3-C4-C5	5.95	131.57	128.60
80	A6	553	G	N1-C2-N3	5.94	127.47	123.90
80	A6	1662	G	N1-C6-O6	-5.94	116.33	119.90
36	A5	3240	C	N3-C4-N4	-5.94	113.84	118.00
1	A2	1796	C	C4-C5-C6	5.94	120.37	117.40
36	A5	971	G	N1-C2-N3	-5.94	120.33	123.90
36	A5	974	G	C8-N9-C1'	-5.94	119.28	127.00
36	A5	1035	G	C4-N9-C1'	5.94	134.22	126.50
36	A5	1772	U	C5-C4-O4	5.94	129.47	125.90
36	A5	2758	A	N3-C4-C5	-5.94	122.64	126.80
1	A2	1582	U	C6-N1-C2	5.94	124.56	121.00
80	A6	59	C	N1-C2-O2	5.94	122.47	118.90
80	A6	1003	A	C8-N9-C4	5.94	108.18	105.80
36	A5	39	A	N3-C4-N9	5.94	132.15	127.40
36	A5	546	C	N3-C2-O2	-5.94	117.74	121.90
36	A5	708	G	C8-N9-C4	-5.94	104.02	106.40
36	A5	968	G	C4-C5-N7	5.94	113.18	110.80
36	A1	1144	U	C2-N3-C4	-5.94	123.44	127.00
36	A1	2888	U	C2-N3-C4	-5.94	123.44	127.00
36	A5	83	U	C2-N1-C1'	5.94	124.83	117.70
36	A5	182	U	C5-C6-N1	5.94	125.67	122.70
36	A5	2130	G	N1-C2-N2	-5.94	110.86	116.20
36	A1	960	U	C5-C6-N1	-5.94	119.73	122.70
36	A1	1152	G	C4-C5-N7	5.94	113.17	110.80
36	A1	1202	A	C5-C6-N1	-5.94	114.73	117.70
36	A1	2680	A	N1-C2-N3	5.94	132.27	129.30
37	A3	103	A	N1-C6-N6	5.94	122.16	118.60
80	A6	87	C	C6-N1-C2	-5.94	117.92	120.30
80	A6	1638	G	N1-C6-O6	-5.94	116.34	119.90
36	A5	386	A	C5-C6-N6	-5.94	118.95	123.70
36	A5	2421	U	N1-C2-N3	5.94	118.46	114.90
36	A5	2607	G	N1-C6-O6	-5.94	116.34	119.90
37	A7	25	G	C5-C6-O6	-5.94	125.04	128.60
1	A2	279	G	C8-N9-C4	-5.94	104.03	106.40
36	A1	1164	G	N1-C2-N2	-5.94	110.86	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1928	G	N3-C4-N9	-5.94	122.44	126.00
36	A5	1181	U	C6-N1-C2	5.94	124.56	121.00
36	A5	2424	A	C5-C6-N6	-5.94	118.95	123.70
1	A2	1097	U	C2-N1-C1'	5.93	124.82	117.70
36	A1	3361	G	N3-C4-N9	5.93	129.56	126.00
36	A5	1699	A	N1-C6-N6	5.93	122.16	118.60
36	A5	2184	U	N3-C2-O2	-5.93	118.05	122.20
36	A1	78	U	N1-C2-N3	5.93	118.46	114.90
36	A1	637	C	C5-C4-N4	5.93	124.35	120.20
36	A1	1717	U	N3-C2-O2	-5.93	118.05	122.20
41	BC	212	ASP	CB-CG-OD1	5.93	123.64	118.30
36	A5	216	G	C5-C6-O6	-5.93	125.04	128.60
36	A5	416	A	C8-N9-C4	-5.93	103.43	105.80
36	A5	749	C	N3-C4-C5	-5.93	119.53	121.90
36	A5	1456	A	C8-N9-C4	5.93	108.17	105.80
36	A5	2405	C	N3-C2-O2	-5.93	117.75	121.90
36	A5	2518	C	C2-N3-C4	-5.93	116.93	119.90
36	A5	3269	U	N3-C2-O2	-5.93	118.05	122.20
36	A5	1175	C	N3-C4-C5	5.93	124.27	121.90
1	A2	393	C	N3-C4-C5	5.93	124.27	121.90
36	A1	2328	U	N3-C2-O2	-5.93	118.05	122.20
41	BC	189	ALA	C-N-CA	-5.93	109.85	122.30
80	A6	1149	G	N1-C2-N2	-5.93	110.86	116.20
36	A5	283	G	N1-C6-O6	5.93	123.46	119.90
36	A5	1307	G	P-O3'-C3'	5.93	126.82	119.70
36	A5	2988	C	N1-C2-N3	5.93	123.35	119.20
37	A7	92	A	N9-C4-C5	-5.93	103.43	105.80
1	A2	1537	C	C5-C6-N1	5.93	123.96	121.00
36	A1	1472	U	C2-N3-C4	-5.93	123.44	127.00
36	A1	1489	A	C5-C6-N6	-5.93	118.96	123.70
80	A6	1085	G	N3-C2-N2	5.93	124.05	119.90
36	A5	667	C	C2-N1-C1'	-5.93	112.28	118.80
36	A5	2639	G	C6-C5-N7	-5.93	126.84	130.40
36	A5	2849	C	C6-N1-C2	-5.93	117.93	120.30
1	A2	703	G	C8-N9-C4	-5.93	104.03	106.40
80	A6	49	C	C5-C4-N4	-5.93	116.05	120.20
80	A6	272	U	N1-C2-O2	5.93	126.95	122.80
38	A8	12	A	N7-C8-N9	5.93	116.76	113.80
38	A8	33	A	C8-N9-C4	5.93	108.17	105.80
36	A1	2768	U	N3-C2-O2	-5.92	118.05	122.20
80	A6	826	U	C6-N1-C2	-5.92	117.44	121.00
80	A6	1428	G	C5-C6-O6	5.92	132.16	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1122	U	N3-C2-O2	-5.92	118.05	122.20
36	A5	1369	A	N1-C6-N6	5.92	122.16	118.60
36	A5	2687	G	C5-C6-N1	5.92	114.46	111.50
36	A5	2965	U	N1-C2-O2	-5.92	118.65	122.80
36	A5	3120	C	N3-C4-C5	-5.92	119.53	121.90
36	A5	3215	A	C8-N9-C4	5.92	108.17	105.80
44	DF	191	VAL	C-N-CA	-5.92	109.86	122.30
1	A2	538	A	C4-C5-C6	-5.92	114.04	117.00
1	A2	1188	G	C5-C6-O6	-5.92	125.05	128.60
36	A1	794	U	N3-C2-O2	-5.92	118.06	122.20
36	A1	1881	A	C5-C6-N6	-5.92	118.96	123.70
36	A1	3175	U	C5-C6-N1	-5.92	119.74	122.70
38	A4	94	C	C6-N1-C2	5.92	122.67	120.30
36	A5	2709	C	N3-C4-C5	5.92	124.27	121.90
38	A8	99	C	N3-C4-C5	5.92	124.27	121.90
38	A4	145	U	C5-C6-N1	-5.92	119.74	122.70
36	A5	1438	U	N3-C2-O2	-5.92	118.06	122.20
36	A5	1866	C	N3-C2-O2	5.92	126.04	121.90
36	A1	301	G	C6-C5-N7	5.92	133.95	130.40
36	A1	635	G	C4-C5-N7	5.92	113.17	110.80
36	A1	860	G	N3-C2-N2	-5.92	115.76	119.90
36	A1	885	U	C4-C5-C6	5.92	123.25	119.70
36	A1	1434	G	N3-C4-C5	-5.92	125.64	128.60
36	A1	2942	C	N3-C2-O2	5.92	126.04	121.90
36	A5	965	A	N3-C4-C5	-5.92	122.66	126.80
36	A5	2692	A	C5-C6-N6	5.92	128.43	123.70
36	A5	2943	G	N1-C2-N2	-5.92	110.87	116.20
37	A7	12	U	C5-C4-O4	-5.92	122.35	125.90
38	A8	24	G	N3-C2-N2	5.92	124.04	119.90
40	DB	114	VAL	CB-CA-C	-5.92	100.15	111.40
36	A1	392	G	C8-N9-C4	5.92	108.77	106.40
36	A1	899	U	N3-C2-O2	-5.92	118.06	122.20
36	A1	1443	G	C4-C5-N7	5.92	113.17	110.80
36	A1	1733	G	N3-C4-N9	5.92	129.55	126.00
36	A1	3047	U	N1-C2-N3	5.92	118.45	114.90
37	A3	91	G	N1-C2-N3	5.92	127.45	123.90
36	A5	1882	G	N9-C4-C5	5.92	107.77	105.40
36	A5	3326	G	N1-C6-O6	-5.92	116.35	119.90
36	A1	1327	C	C5-C6-N1	5.92	123.96	121.00
80	A6	555	A	C3'-C2'-C1'	-5.92	96.77	101.50
36	A5	590	G	C5-C6-O6	-5.92	125.05	128.60
36	A5	2347	U	C2-N3-C4	-5.92	123.45	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	151	G	N1-C6-O6	-5.91	116.35	119.90
36	A1	1929	G	N3-C4-C5	5.91	131.56	128.60
36	A1	2383	C	N1-C2-O2	-5.91	115.35	118.90
40	BB	10	ARG	CB-CA-C	-5.91	98.57	110.40
80	A6	144	U	N1-C2-N3	5.91	118.45	114.90
80	A6	422	G	C8-N9-C4	-5.91	104.03	106.40
36	A5	1178	G	C5-N7-C8	-5.91	101.34	104.30
42	DD	248	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A2	13	C	N3-C4-C5	5.91	124.27	121.90
36	A1	970	A	N3-C4-N9	-5.91	122.67	127.40
36	A1	2816	G	C4-C5-N7	5.91	113.17	110.80
36	A1	3090	U	C5-C6-N1	-5.91	119.74	122.70
36	A5	847	A	N7-C8-N9	-5.91	110.84	113.80
36	A5	3075	G	C5-C6-N1	-5.91	108.54	111.50
36	A1	667	C	N3-C4-N4	-5.91	113.86	118.00
36	A1	2798	C	N3-C4-C5	-5.91	119.54	121.90
80	A6	1640	C	C2-N3-C4	-5.91	116.94	119.90
36	A5	201	A	C2-N3-C4	-5.91	107.64	110.60
36	A5	365	A	C5-C6-N6	-5.91	118.97	123.70
36	A5	2931	C	C2-N3-C4	-5.91	116.94	119.90
36	A5	3055	U	N1-C2-O2	5.91	126.94	122.80
36	A1	2286	U	C4-C5-C6	5.91	123.25	119.70
80	A6	356	G	C5-N7-C8	5.91	107.25	104.30
80	A6	542	A	C4-C5-C6	5.91	119.95	117.00
80	A6	991	G	C5-C6-O6	-5.91	125.05	128.60
36	A5	587	U	C5-C6-N1	-5.91	119.75	122.70
36	A5	2114	C	N1-C2-N3	5.91	123.34	119.20
41	DC	84	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A2	1274	C	C4-C5-C6	5.91	120.35	117.40
36	A1	388	G	N9-C4-C5	5.91	107.76	105.40
80	A6	471	A	N1-C6-N6	-5.91	115.06	118.60
80	A6	901	G	C5-N7-C8	-5.91	101.35	104.30
80	A6	1458	G	C6-C5-N7	-5.91	126.86	130.40
80	A6	1472	C	C2-N3-C4	-5.91	116.95	119.90
36	A5	894	G	N3-C4-N9	5.91	129.54	126.00
36	A5	3277	U	C6-N1-C2	-5.91	117.46	121.00
36	A1	329	U	N1-C2-O2	-5.90	118.67	122.80
36	A1	340	C	C6-N1-C2	-5.90	117.94	120.30
36	A1	2957	G	C5-N7-C8	5.90	107.25	104.30
80	A6	945	U	N1-C2-O2	5.90	126.93	122.80
1	A2	1387	G	C4-C5-N7	5.90	113.16	110.80
36	A1	52	A	N1-C6-N6	5.90	122.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	939	U	N1-C2-N3	5.90	118.44	114.90
36	A1	2210	G	N1-C6-O6	-5.90	116.36	119.90
49	BL	141	ALA	N-CA-C	-5.90	95.06	111.00
80	A6	976	G	N3-C2-N2	5.90	124.03	119.90
80	A6	1766	A	C5-C6-N1	-5.90	114.75	117.70
1	A2	192	U	N1-C2-O2	5.90	126.93	122.80
36	A1	1838	G	N9-C4-C5	-5.90	103.04	105.40
36	A5	2410	U	N3-C4-O4	-5.90	115.27	119.40
36	A1	1191	U	C4-C5-C6	5.90	123.24	119.70
36	A1	2631	U	N3-C4-C5	5.90	118.14	114.60
80	A6	65	A	C5-N7-C8	-5.90	100.95	103.90
36	A5	1189	C	C6-N1-C2	5.90	122.66	120.30
36	A5	2409	G	N7-C8-N9	5.90	116.05	113.10
36	A1	1073	U	N1-C2-O2	-5.90	118.67	122.80
36	A1	2289	U	C4-C5-C6	5.90	123.24	119.70
36	A1	2595	A	C6-C5-N7	-5.90	128.17	132.30
80	A6	280	U	N1-C2-O2	5.90	126.93	122.80
36	A5	2148	U	N3-C2-O2	5.90	126.33	122.20
36	A5	2320	A	N1-C6-N6	-5.90	115.06	118.60
36	A5	2366	C	C6-N1-C1'	-5.90	113.72	120.80
36	A5	2617	U	C6-N1-C2	5.90	124.54	121.00
36	A5	3075	G	C4-C5-C6	5.90	122.34	118.80
36	A1	23	A	N1-C6-N6	5.90	122.14	118.60
36	A1	98	G	C2-N3-C4	-5.90	108.95	111.90
36	A1	1137	C	N3-C4-C5	5.90	124.26	121.90
36	A1	1489	A	N1-C2-N3	5.90	132.25	129.30
36	A1	1514	G	C8-N9-C4	-5.90	104.04	106.40
36	A1	2825	C	C2-N3-C4	5.90	122.85	119.90
80	A6	1476	C	C6-N1-C2	-5.90	117.94	120.30
36	A5	2426	U	N3-C2-O2	-5.90	118.07	122.20
1	A2	1503	A	C5-N7-C8	-5.89	100.95	103.90
36	A1	1174	G	N9-C4-C5	-5.89	103.04	105.40
36	A1	1269	U	N1-C2-O2	5.89	126.93	122.80
36	A1	1329	U	C2-N3-C4	-5.89	123.46	127.00
36	A1	1386	A	C5-C6-N1	5.89	120.65	117.70
36	A1	1444	G	C4-C5-N7	5.89	113.16	110.80
36	A1	1556	C	C2-N1-C1'	5.89	125.28	118.80
36	A1	3215	A	C8-N9-C4	5.89	108.16	105.80
52	BO	3[B]	SER	O-C-N	5.89	132.13	122.70
36	A1	347	G	N9-C4-C5	-5.89	103.04	105.40
36	A1	2816	G	C8-N9-C4	5.89	108.76	106.40
36	A1	3045	G	C2-N3-C4	5.89	114.85	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	640	U	N3-C2-O2	-5.89	118.08	122.20
36	A5	426	G	N7-C8-N9	-5.89	110.15	113.10
36	A5	874	U	C5-C6-N1	-5.89	119.75	122.70
36	A5	2188	A	N7-C8-N9	-5.89	110.85	113.80
36	A5	2915	U	N3-C2-O2	-5.89	118.08	122.20
36	A5	2992	U	N3-C2-O2	-5.89	118.08	122.20
59	DV	33	ASN	CB-CA-C	-5.89	98.62	110.40
36	A1	2142	A	N3-C4-N9	5.89	132.11	127.40
38	A4	10	A	C5-C6-N1	5.89	120.65	117.70
36	A5	1586	G	N3-C4-C5	-5.89	125.66	128.60
36	A5	2292	U	C2-N3-C4	-5.89	123.47	127.00
36	A5	3088	G	C5-N7-C8	-5.89	101.36	104.30
36	A1	361	A	C5-C6-N1	5.89	120.64	117.70
36	A1	2293	C	C2-N3-C4	-5.89	116.95	119.90
36	A5	345	G	C6-N1-C2	-5.89	121.57	125.10
36	A5	509	U	N1-C2-N3	5.89	118.43	114.90
36	A5	1311	G	N1-C2-N3	-5.89	120.37	123.90
1	A2	308	C	C2-N3-C4	-5.89	116.96	119.90
1	A2	1314	U	N3-C2-O2	-5.89	118.08	122.20
36	A5	1206	G	C4-C5-N7	-5.89	108.44	110.80
36	A1	351	A	N7-C8-N9	-5.89	110.86	113.80
36	A1	922	U	C5-C4-O4	5.89	129.43	125.90
36	A1	1802	C	C5-C4-N4	-5.89	116.08	120.20
80	A6	184	C	C6-N1-C2	5.89	122.65	120.30
80	A6	465	G	C8-N9-C4	5.89	108.75	106.40
1	A2	416	A	C8-N9-C4	5.88	108.15	105.80
36	A1	2203	U	C6-N1-C2	-5.88	117.47	121.00
36	A1	2933	A	C4-C5-N7	5.88	113.64	110.70
38	A4	36	G	N1-C6-O6	-5.88	116.37	119.90
36	A5	874	U	N3-C4-O4	-5.88	115.28	119.40
36	A5	1481	A	N3-C4-C5	-5.88	122.68	126.80
36	A5	1834	U	C6-N1-C2	5.88	124.53	121.00
36	A5	1892	G	N3-C2-N2	-5.88	115.78	119.90
36	A5	2118	C	N1-C2-O2	5.88	122.43	118.90
36	A5	2271	A	N1-C6-N6	-5.88	115.07	118.60
36	A5	2843	U	C2-N1-C1'	5.88	124.76	117.70
38	A8	55	U	N3-C4-C5	-5.88	111.07	114.60
36	A1	1198	C	C6-N1-C2	-5.88	117.95	120.30
36	A1	1928	G	N3-C4-C5	5.88	131.54	128.60
38	A4	1	A	C5-C6-N6	-5.88	118.99	123.70
36	A5	2113	A	C8-N9-C4	5.88	108.15	105.80
36	A1	1056	U	C5-C6-N1	5.88	125.64	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	5	U	N3-C4-C5	-5.88	111.07	114.60
80	A6	999	U	N1-C2-O2	5.88	126.92	122.80
36	A5	993	G	C8-N9-C4	-5.88	104.05	106.40
36	A5	1317	A	N3-C4-N9	5.88	132.10	127.40
36	A5	2549	G	C4-N9-C1'	5.88	134.15	126.50
36	A1	3058	U	C6-N1-C1'	-5.88	112.97	121.20
36	A5	591	G	N3-C4-N9	5.88	129.53	126.00
36	A5	3226	A	N1-C2-N3	-5.88	126.36	129.30
1	A2	997	G	N9-C4-C5	-5.88	103.05	105.40
36	A1	157	A	C6-N1-C2	-5.88	115.07	118.60
36	A1	359	U	N3-C4-C5	5.88	118.13	114.60
36	A1	617	G	C6-N1-C2	-5.88	121.57	125.10
36	A1	825	U	N3-C4-O4	-5.88	115.29	119.40
36	A1	1124	U	N1-C2-O2	5.88	126.92	122.80
36	A1	1269	U	C2-N1-C1'	5.88	124.75	117.70
36	A1	2325	G	C8-N9-C4	-5.88	104.05	106.40
80	A6	13	C	C5-C6-N1	-5.88	118.06	121.00
80	A6	1641	C	N1-C2-O2	-5.88	115.37	118.90
31	Cd	36	LEU	CA-CB-CG	5.88	128.82	115.30
36	A5	908	G	C8-N9-C1'	-5.88	119.36	127.00
36	A5	2745	G	C5-C6-O6	-5.88	125.07	128.60
36	A5	2893	C	C4-C5-C6	5.88	120.34	117.40
36	A1	663	C	C5-C4-N4	-5.88	116.09	120.20
36	A1	875	G	C6-C5-N7	5.88	133.93	130.40
36	A1	953	G	N3-C4-C5	5.88	131.54	128.60
36	A1	3077	A	N9-C4-C5	5.88	108.15	105.80
38	A4	6	U	C2-N3-C4	-5.88	123.47	127.00
80	A6	1739	C	N1-C2-O2	-5.88	115.38	118.90
36	A5	861	C	N1-C2-O2	-5.88	115.37	118.90
36	A5	2961	G	N7-C8-N9	5.88	116.04	113.10
1	A2	1776	A	N9-C4-C5	5.88	108.15	105.80
36	A1	905	U	C5-C6-N1	-5.88	119.76	122.70
36	A1	98	G	N1-C2-N2	-5.87	110.91	116.20
36	A1	214	G	C5-N7-C8	5.87	107.24	104.30
36	A1	975	C	N1-C2-O2	-5.87	115.38	118.90
80	A6	114	C	C2-N1-C1'	5.87	125.26	118.80
80	A6	1654	G	N1-C2-N3	5.87	127.42	123.90
36	A5	1043	C	C5-C6-N1	-5.87	118.06	121.00
36	A5	2910	A	N1-C6-N6	-5.87	115.08	118.60
1	A2	1479	A	N1-C6-N6	5.87	122.12	118.60
36	A1	142	C	N3-C4-N4	5.87	122.11	118.00
80	A6	385	A	C4-C5-N7	-5.87	107.76	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1798	U	C2-N1-C1'	5.87	124.74	117.70
49	DL	46	ILE	CG1-CB-CG2	-5.87	98.49	111.40
36	A1	696	C	N1-C2-O2	5.87	122.42	118.90
36	A1	1434	G	C5-N7-C8	5.87	107.23	104.30
36	A1	1719	G	C4-C5-N7	5.87	113.15	110.80
36	A1	2370	G	C5-C6-O6	-5.87	125.08	128.60
36	A5	1838	G	N7-C8-N9	-5.87	110.17	113.10
36	A5	1907	C	C5-C6-N1	5.87	123.94	121.00
36	A5	3112	G	C5-C6-O6	-5.87	125.08	128.60
1	A2	1542	G	C5-C6-O6	5.87	132.12	128.60
36	A1	504	A	N7-C8-N9	-5.87	110.87	113.80
36	A1	901	G	N1-C6-O6	5.87	123.42	119.90
36	A1	2623	G	N1-C2-N2	-5.87	110.92	116.20
36	A1	251	G	C8-N9-C1'	-5.87	119.38	127.00
36	A1	776	U	N3-C2-O2	-5.87	118.09	122.20
36	A1	1298	C	C6-N1-C2	-5.87	117.95	120.30
36	A1	1300	G	N7-C8-N9	-5.87	110.17	113.10
36	A1	2131	A	N1-C6-N6	5.87	122.12	118.60
36	A1	2775	U	C5-C6-N1	-5.87	119.77	122.70
79	Bp	71	VAL	CB-CA-C	-5.87	100.26	111.40
36	A5	593	C	C2-N1-C1'	5.87	125.25	118.80
36	A5	2641	U	N1-C2-O2	-5.87	118.69	122.80
36	A5	2744	U	C5-C6-N1	-5.87	119.77	122.70
36	A1	1778	G	C6-C5-N7	-5.86	126.88	130.40
36	A1	2669	G	N1-C2-N3	5.86	127.42	123.90
80	A6	298	C	C6-N1-C2	-5.86	117.95	120.30
36	A5	1495	U	N3-C4-C5	-5.86	111.08	114.60
36	A5	2145	A	C5-C6-N1	5.86	120.63	117.70
36	A5	3216	G	N1-C2-N3	5.86	127.42	123.90
1	A2	1745	G	C6-C5-N7	-5.86	126.88	130.40
80	A6	1037	C	C2-N1-C1'	-5.86	112.35	118.80
36	A5	2346	C	C5-C4-N4	-5.86	116.10	120.20
1	A2	628	G	N1-C2-N2	-5.86	110.92	116.20
36	A1	80	G	N1-C6-O6	-5.86	116.38	119.90
36	A1	1791	C	C2-N3-C4	-5.86	116.97	119.90
36	A1	2819	A	C6-N1-C2	-5.86	115.08	118.60
36	A1	3259	U	C2-N3-C4	-5.86	123.48	127.00
36	A5	2248	C	C5-C6-N1	-5.86	118.07	121.00
36	A5	2792	A	C2-N3-C4	5.86	113.53	110.60
36	A5	3340	G	N1-C6-O6	-5.86	116.38	119.90
36	A1	86	G	C5-N7-C8	5.86	107.23	104.30
36	A1	148	G	N1-C6-O6	5.86	123.42	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	815	G	N7-C8-N9	5.86	116.03	113.10
36	A5	2338	C	N3-C4-C5	-5.86	119.56	121.90
36	A1	639	G	C5-C6-O6	-5.86	125.09	128.60
36	A1	1388	U	C2-N3-C4	-5.86	123.49	127.00
36	A1	2541	U	C6-N1-C1'	-5.86	113.00	121.20
80	A6	1130	G	C6-N1-C2	-5.86	121.59	125.10
80	A6	1594	G	C8-N9-C4	5.86	108.74	106.40
36	A5	2314	U	C6-N1-C1'	-5.86	113.00	121.20
36	A5	2531	C	C6-N1-C1'	-5.86	113.77	120.80
36	A5	3296	A	C8-N9-C4	5.86	108.14	105.80
36	A1	343	U	C5-C6-N1	-5.86	119.77	122.70
36	A1	1431	G	C8-N9-C4	5.86	108.74	106.40
36	A1	2877	G	C5-C6-O6	5.86	132.11	128.60
80	A6	1320	U	C2-N1-C1'	5.86	124.73	117.70
80	A6	1490	C	C6-N1-C2	-5.86	117.96	120.30
36	A5	1911	A	C2-N3-C4	-5.86	107.67	110.60
36	A5	2711	C	C4-C5-C6	5.86	120.33	117.40
36	A1	857	G	C4-C5-N7	5.85	113.14	110.80
80	A6	1304	G	C4-C5-N7	5.85	113.14	110.80
36	A5	795	G	C5-N7-C8	5.85	107.23	104.30
1	A2	611	U	N1-C2-O2	-5.85	118.70	122.80
36	A5	376	G	N1-C6-O6	-5.85	116.39	119.90
36	A5	1429	G	C2-N3-C4	-5.85	108.97	111.90
36	A5	1437	C	C2-N1-C1'	5.85	125.24	118.80
36	A5	1495	U	C2-N1-C1'	5.85	124.72	117.70
36	A5	3113	A	C5-C6-N1	5.85	120.63	117.70
36	A1	2418	G	C5-C6-N1	5.85	114.42	111.50
36	A5	1136	A	C2-N3-C4	5.85	113.53	110.60
36	A1	2369	G	C5-C6-O6	-5.85	125.09	128.60
36	A1	2611	U	N3-C4-O4	-5.85	115.31	119.40
80	A6	389	G	N3-C4-N9	5.85	129.51	126.00
4	CC	113	LEU	CA-CB-CG	5.85	128.75	115.30
36	A5	2643	A	N1-C2-N3	-5.85	126.38	129.30
36	A1	926	A	N1-C2-N3	-5.85	126.38	129.30
36	A1	1510	G	C6-C5-N7	-5.85	126.89	130.40
77	Bn	9	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A2	21	U	N3-C2-O2	-5.84	118.11	122.20
1	A2	810	G	N1-C6-O6	5.84	123.41	119.90
1	A2	1536	G	C4-N9-C1'	5.84	134.10	126.50
36	A1	1610	G	N1-C6-O6	5.84	123.41	119.90
36	A1	2127	U	N1-C2-O2	-5.84	118.71	122.80
36	A1	2193	U	C2-N3-C4	-5.84	123.49	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2547	A	C8-N9-C1'	-5.84	117.18	127.70
38	A4	120	C	N1-C2-O2	-5.84	115.39	118.90
80	A6	757	A	C8-N9-C4	5.84	108.14	105.80
36	A5	2141	U	N3-C2-O2	-5.84	118.11	122.20
36	A5	2361	A	N3-C4-N9	5.84	132.07	127.40
36	A5	3019	U	N3-C4-C5	5.84	118.11	114.60
36	A1	363	G	C6-N1-C2	-5.84	121.59	125.10
36	A1	2298	U	C6-N1-C2	5.84	124.51	121.00
36	A1	2602	G	C5-N7-C8	5.84	107.22	104.30
38	A4	125	U	C6-N1-C1'	-5.84	113.02	121.20
36	A5	1490	A	C2-N3-C4	-5.84	107.68	110.60
36	A5	3241	G	C4-C5-N7	5.84	113.14	110.80
1	A2	1340	U	C5-C4-O4	5.84	129.41	125.90
36	A1	959	C	N3-C2-O2	5.84	125.99	121.90
36	A1	1387	G	C5-C6-O6	5.84	132.10	128.60
36	A1	1907	C	N3-C4-C5	-5.84	119.56	121.90
36	A1	2522	G	C4-N9-C1'	5.84	134.09	126.50
36	A1	2626	A	C5-C6-N1	-5.84	114.78	117.70
36	A1	2756	C	N3-C4-N4	5.84	122.09	118.00
80	A6	376	C	C2-N3-C4	-5.84	116.98	119.90
80	A6	1340	U	N1-C2-O2	5.84	126.89	122.80
36	A5	994	G	C6-N1-C2	-5.84	121.59	125.10
36	A5	1477	A	N1-C2-N3	5.84	132.22	129.30
36	A5	1902	G	C5-C6-N1	5.84	114.42	111.50
36	A5	1939	G	N1-C2-N2	-5.84	110.94	116.20
36	A5	2381	G	C2-N3-C4	5.84	114.82	111.90
38	A4	57	C	C5-C6-N1	-5.84	118.08	121.00
38	A4	73	U	C4-C5-C6	-5.84	116.20	119.70
56	BS	117	ARG	NE-CZ-NH1	-5.84	117.38	120.30
36	A5	1086	C	N1-C2-O2	5.84	122.40	118.90
36	A5	1181	U	C2-N3-C4	-5.84	123.50	127.00
36	A5	1917	C	C2-N3-C4	-5.84	116.98	119.90
36	A5	2838	A	C6-N1-C2	-5.84	115.10	118.60
36	A5	3224	G	N1-C6-O6	-5.84	116.40	119.90
36	A5	3373	U	C5-C6-N1	-5.84	119.78	122.70
80	A6	96	G	C8-N9-C4	-5.84	104.06	106.40
80	A6	359	A	N3-C4-C5	5.84	130.89	126.80
36	A5	741	U	C2-N3-C4	5.84	130.50	127.00
36	A5	2976	A	C8-N9-C4	5.84	108.14	105.80
36	A5	3100	U	N1-C2-O2	5.84	126.89	122.80
36	A1	2200	U	N3-C4-C5	-5.84	111.10	114.60
36	A1	3316	A	C5-N7-C8	-5.84	100.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2305	G	N1-C2-N2	-5.84	110.95	116.20
36	A5	2846	U	C5-C6-N1	-5.84	119.78	122.70
36	A5	3212	C	C5-C6-N1	-5.84	118.08	121.00
80	A6	240	U	N3-C2-O2	-5.83	118.12	122.20
80	A6	355	G	C5-N7-C8	5.83	107.22	104.30
80	A6	1540	G	N1-C6-O6	-5.83	116.40	119.90
80	A6	1658	G	C5-C6-O6	5.83	132.10	128.60
36	A1	3092	C	C5-C6-N1	-5.83	118.08	121.00
51	BN	105	ARG	NE-CZ-NH2	-5.83	117.38	120.30
64	Ba	115	LYS	C-N-CA	-5.83	110.05	122.30
36	A5	680	G	N3-C2-N2	5.83	123.98	119.90
36	A5	1485	G	N3-C4-C5	-5.83	125.68	128.60
1	A2	542	A	C4-C5-N7	5.83	113.61	110.70
44	BF	110	ARG	NE-CZ-NH2	-5.83	117.39	120.30
80	A6	1014	G	N1-C2-N2	-5.83	110.95	116.20
36	A5	272	G	C2-N3-C4	-5.83	108.98	111.90
36	A5	966	U	C2-N1-C1'	5.83	124.70	117.70
36	A5	1133	A	N1-C2-N3	-5.83	126.39	129.30
36	A5	1247	U	C5-C6-N1	5.83	125.62	122.70
36	A5	3267	A	N1-C2-N3	5.83	132.22	129.30
1	A2	1291	G	N3-C2-N2	-5.83	115.82	119.90
36	A1	1144	U	N3-C4-O4	-5.83	115.32	119.40
36	A1	1586	G	N1-C2-N2	-5.83	110.95	116.20
38	A4	25	G	N1-C6-O6	-5.83	116.40	119.90
36	A5	795	G	N1-C2-N3	-5.83	120.40	123.90
36	A5	815	G	N9-C4-C5	5.83	107.73	105.40
37	A7	5	G	C8-N9-C4	5.83	108.73	106.40
36	A1	66	A	C8-N9-C4	5.83	108.13	105.80
36	A1	100	A	C2-N3-C4	-5.83	107.69	110.60
36	A1	1615	C	C5-C6-N1	-5.83	118.09	121.00
36	A1	1849	C	N3-C2-O2	5.83	125.98	121.90
36	A1	2737	C	N1-C2-O2	-5.83	115.40	118.90
36	A1	3227	A	C2-N3-C4	-5.83	107.69	110.60
37	A3	83	U	N3-C4-C5	5.83	118.10	114.60
80	A6	858	G	C4-N9-C1'	5.83	134.08	126.50
36	A5	153	U	C5-C4-O4	5.83	129.40	125.90
36	A5	968	G	C8-N9-C4	5.83	108.73	106.40
36	A5	1669	C	C6-N1-C2	5.83	122.63	120.30
36	A5	3130	A	C6-N1-C2	-5.83	115.10	118.60
36	A1	3077	A	C4-C5-C6	5.83	119.91	117.00
36	A5	432	G	C2-N3-C4	-5.83	108.99	111.90
36	A1	1190	A	C2-N3-C4	5.83	113.51	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2640	A	N1-C6-N6	-5.83	115.11	118.60
36	A5	96	G	N1-C2-N3	5.83	127.40	123.90
36	A5	1607	U	C2-N3-C4	-5.83	123.50	127.00
36	A5	2920	U	C4-C5-C6	5.83	123.19	119.70
36	A5	3095	U	C2-N3-C4	-5.83	123.50	127.00
37	A7	106	U	C5-C6-N1	-5.83	119.79	122.70
36	A1	743	C	N3-C4-C5	5.82	124.23	121.90
36	A1	2647	A	C2-N3-C4	5.82	113.51	110.60
36	A1	2990	G	N9-C4-C5	5.82	107.73	105.40
36	A1	3111	U	N1-C2-O2	5.82	126.88	122.80
80	A6	1458	G	C4-N9-C1'	5.82	134.07	126.50
36	A5	2584	G	C4-C5-N7	5.82	113.13	110.80
36	A5	2817	A	C2-N3-C4	5.82	113.51	110.60
38	A8	16	G	N1-C2-N3	5.82	127.39	123.90
36	A1	46	U	C5-C4-O4	5.82	129.39	125.90
36	A1	929	A	C6-N1-C2	-5.82	115.11	118.60
36	A1	1175	C	C5-C6-N1	-5.82	118.09	121.00
36	A1	3192	U	C5-C6-N1	-5.82	119.79	122.70
38	A4	10	A	C8-N9-C4	-5.82	103.47	105.80
80	A6	560	U	N3-C4-O4	5.82	123.47	119.40
36	A5	1116	G	C5-C6-O6	5.82	132.09	128.60
1	A2	294	C	C6-N1-C2	5.82	122.63	120.30
1	A2	1291	G	N3-C4-N9	-5.82	122.51	126.00
36	A1	1589	A	N9-C4-C5	-5.82	103.47	105.80
36	A1	2299	A	N1-C2-N3	5.82	132.21	129.30
38	A4	79	A	N7-C8-N9	5.82	116.71	113.80
80	A6	419	G	N1-C6-O6	-5.82	116.41	119.90
36	A5	2516	U	C5-C4-O4	-5.82	122.41	125.90
40	DB	19	ARG	NE-CZ-NH2	-5.82	117.39	120.30
36	A1	159	A	N9-C4-C5	-5.82	103.47	105.80
36	A5	2846	U	C2-N3-C4	-5.82	123.51	127.00
36	A1	1950	U	C5-C6-N1	5.82	125.61	122.70
36	A1	2130	G	N1-C2-N2	-5.82	110.97	116.20
36	A1	3140	G	C8-N9-C1'	-5.82	119.44	127.00
36	A1	3312	U	N1-C2-N3	5.82	118.39	114.90
44	BF	215	GLY	N-CA-C	-5.82	98.56	113.10
56	BS	115	ARG	NE-CZ-NH1	5.82	123.21	120.30
80	A6	1788	G	C4-C5-N7	-5.82	108.47	110.80
36	A5	798	G	C5-C6-N1	5.82	114.41	111.50
36	A5	2370	G	N1-C2-N3	5.82	127.39	123.90
1	A2	1666	U	C6-N1-C2	-5.82	117.51	121.00
36	A1	388	G	N3-C2-N2	-5.82	115.83	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	859	G	N1-C6-O6	5.82	123.39	119.90
36	A1	973	A	N1-C2-N3	5.82	132.21	129.30
36	A1	2960	C	N1-C2-O2	-5.82	115.41	118.90
36	A1	3278	C	C2-N1-C1'	5.82	125.20	118.80
80	A6	341	A	N9-C4-C5	5.82	108.13	105.80
80	A6	1037	C	C5-C6-N1	-5.82	118.09	121.00
36	A5	689	U	N3-C4-O4	-5.82	115.33	119.40
36	A5	916	G	N3-C4-N9	-5.82	122.51	126.00
36	A5	1045	C	N1-C2-N3	5.82	123.27	119.20
36	A5	1127	G	C5-C6-N1	5.82	114.41	111.50
36	A5	2971	A	C2-N3-C4	5.82	113.51	110.60
36	A5	3099	C	C4-C5-C6	5.82	120.31	117.40
36	A1	1948	G	N1-C6-O6	5.81	123.39	119.90
80	A6	1509	C	N1-C2-O2	5.81	122.39	118.90
36	A5	404	G	N3-C2-N2	-5.81	115.83	119.90
36	A5	2920	U	N1-C2-O2	-5.81	118.73	122.80
1	A2	344	A	N1-C6-N6	-5.81	115.11	118.60
36	A1	1137	C	N1-C2-O2	-5.81	115.41	118.90
36	A1	1523	U	C5-C4-O4	-5.81	122.41	125.90
36	A1	1947	G	N3-C4-C5	5.81	131.51	128.60
36	A1	2385	G	N3-C4-C5	5.81	131.51	128.60
36	A1	2816	G	N9-C4-C5	-5.81	103.08	105.40
36	A1	2980	U	C6-N1-C2	-5.81	117.51	121.00
36	A5	432	G	C4-C5-N7	5.81	113.12	110.80
36	A5	2335	G	N1-C6-O6	-5.81	116.41	119.90
36	A5	2510	U	C2-N1-C1'	-5.81	110.73	117.70
36	A5	3152	U	C6-N1-C2	5.81	124.49	121.00
36	A1	857	G	C4-C5-C6	-5.81	115.31	118.80
36	A1	1151	U	C6-N1-C2	-5.81	117.51	121.00
36	A1	1232	C	C6-N1-C2	-5.81	117.98	120.30
1	A2	92	A	N1-C6-N6	-5.81	115.11	118.60
1	A2	581	U	C6-N1-C1'	-5.81	113.07	121.20
36	A1	804	C	C2-N3-C4	-5.81	117.00	119.90
36	A1	908	G	C4-N9-C1'	5.81	134.05	126.50
67	Bd	64	VAL	CB-CA-C	-5.81	100.36	111.40
80	A6	647	G	N3-C2-N2	-5.81	115.83	119.90
36	A5	1158	A	C4-C5-N7	5.81	113.61	110.70
36	A5	1415	U	C5-C6-N1	-5.81	119.80	122.70
36	A5	1494	U	N3-C2-O2	5.81	126.27	122.20
1	A2	1633	A	N3-C4-C5	-5.81	122.73	126.80
36	A1	649	A	N1-C6-N6	-5.81	115.12	118.60
36	A1	796	U	C5-C4-O4	-5.81	122.42	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	901	G	C8-N9-C4	5.81	108.72	106.40
36	A1	1396	C	C6-N1-C2	5.81	122.62	120.30
36	A1	2965	U	N3-C4-C5	5.81	118.08	114.60
80	A6	102	U	N1-C2-N3	5.81	118.38	114.90
80	A6	767	U	N1-C2-N3	5.81	118.39	114.90
80	A6	1755	A	C4-C5-N7	5.81	113.60	110.70
36	A5	1210	U	N3-C4-O4	-5.81	115.33	119.40
1	A2	934	C	C6-N1-C1'	-5.81	113.83	120.80
36	A1	3049	A	C4-C5-C6	5.81	119.90	117.00
49	BL	63	VAL	CB-CA-C	-5.81	100.37	111.40
80	A6	858	G	C6-C5-N7	-5.81	126.92	130.40
36	A5	35	A	C8-N9-C4	5.81	108.12	105.80
36	A5	590	G	C5-N7-C8	-5.81	101.40	104.30
36	A5	1438	U	C6-N1-C2	-5.81	117.52	121.00
36	A1	864	G	C6-N1-C2	-5.80	121.62	125.10
36	A1	2281	A	C2-N3-C4	-5.80	107.70	110.60
36	A1	2417	U	N1-C2-O2	-5.80	118.74	122.80
36	A1	3201	C	C6-N1-C2	-5.80	117.98	120.30
80	A6	1075	C	N3-C2-O2	5.80	125.96	121.90
36	A5	1129	A	C2-N3-C4	5.80	113.50	110.60
36	A5	2327	U	N3-C4-C5	5.80	118.08	114.60
36	A5	2692	A	C5-N7-C8	5.80	106.80	103.90
1	A2	1324	G	C8-N9-C1'	5.80	134.54	127.00
36	A5	1889	G	N3-C4-C5	-5.80	125.70	128.60
1	A2	732	G	C4-C5-N7	5.80	113.12	110.80
36	A1	304	G	N9-C4-C5	5.80	107.72	105.40
36	A1	376	G	N9-C4-C5	5.80	107.72	105.40
36	A1	835	G	O4'-C1'-N9	5.80	112.84	108.20
36	A5	25	U	N1-C2-O2	-5.80	118.74	122.80
36	A5	332	C	C5-C6-N1	-5.80	118.10	121.00
36	A5	801	A	C6-N1-C2	5.80	122.08	118.60
36	A5	979	U	N1-C2-O2	5.80	126.86	122.80
49	DL	76	THR	N-CA-CB	5.80	121.32	110.30
36	A1	730	C	C5-C6-N1	-5.80	118.10	121.00
36	A1	851	C	N3-C4-N4	5.80	122.06	118.00
36	A1	2961	G	C8-N9-C4	-5.80	104.08	106.40
80	A6	5	U	C4-C5-C6	5.80	123.18	119.70
80	A6	151	G	N3-C2-N2	-5.80	115.84	119.90
36	A5	2147	A	C5-C6-N6	-5.80	119.06	123.70
36	A1	24	G	N1-C2-N3	5.80	127.38	123.90
36	A1	892	U	N3-C4-C5	5.80	118.08	114.60
73	Bj	65	ARG	NE-CZ-NH1	5.80	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	43	A	N1-C6-N6	-5.80	115.12	118.60
36	A5	3388	C	N3-C2-O2	-5.80	117.84	121.90
1	A2	1241	G	C8-N9-C4	-5.80	104.08	106.40
1	A2	1324	G	N9-C4-C5	5.80	107.72	105.40
36	A1	786	A	C4-C5-N7	-5.80	107.80	110.70
36	A1	994	G	N7-C8-N9	-5.80	110.20	113.10
36	A1	1081	U	N1-C2-N3	-5.80	111.42	114.90
36	A1	2939	G	N3-C2-N2	-5.80	115.84	119.90
36	A1	3377	G	C5-C6-O6	-5.80	125.12	128.60
36	A5	706	A	C5-C6-N6	-5.80	119.06	123.70
36	A5	798	G	C5-C6-O6	-5.80	125.12	128.60
36	A5	1297	C	C5-C4-N4	-5.80	116.14	120.20
1	A2	811	A	C8-N9-C4	-5.79	103.48	105.80
80	A6	470	A	C5-N7-C8	-5.79	101.00	103.90
80	A6	557	G	N1-C6-O6	-5.79	116.42	119.90
80	A6	1145	U	N3-C4-O4	5.79	123.46	119.40
36	A5	1060	U	C2-N3-C4	-5.79	123.52	127.00
36	A5	2770	G	C2-N3-C4	5.79	114.80	111.90
36	A1	1340	G	C5-C6-N1	5.79	114.40	111.50
36	A1	1929	G	C5-C6-O6	-5.79	125.12	128.60
38	A4	81	U	C6-N1-C1'	5.79	129.31	121.20
63	BZ	135	ARG	NE-CZ-NH2	5.79	123.20	120.30
80	A6	272	U	C2-N1-C1'	5.79	124.65	117.70
80	A6	553	G	C6-N1-C2	-5.79	121.62	125.10
80	A6	768	C	C5-C4-N4	-5.79	116.14	120.20
80	A6	1414	U	N3-C2-O2	-5.79	118.14	122.20
36	A5	523	A	C5-C6-N6	5.79	128.34	123.70
36	A5	2207	A	N7-C8-N9	5.79	116.70	113.80
36	A5	2306	C	C2-N1-C1'	5.79	125.17	118.80
36	A5	2835	U	N1-C2-N3	5.79	118.38	114.90
1	A2	460	A	N1-C6-N6	-5.79	115.12	118.60
1	A2	1416	G	C8-N9-C4	-5.79	104.08	106.40
36	A1	582	G	C8-N9-C4	-5.79	104.08	106.40
36	A1	2188	A	C8-N9-C4	5.79	108.12	105.80
36	A1	2298	U	N1-C2-N3	5.79	118.38	114.90
36	A1	2299	A	C5-N7-C8	5.79	106.80	103.90
80	A6	1510	U	N3-C4-C5	-5.79	111.12	114.60
36	A5	159	A	C8-N9-C4	5.79	108.12	105.80
36	A5	1512	U	C5-C6-N1	-5.79	119.80	122.70
36	A5	3102	G	C5-C6-O6	5.79	132.07	128.60
36	A5	3285	C	C2-N1-C1'	5.79	125.17	118.80
36	A1	1407	A	C5-N7-C8	5.79	106.80	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1607	U	P-O3'-C3'	5.79	126.65	119.70
36	A5	3218	A	N7-C8-N9	5.79	116.69	113.80
1	A2	1198	G	N7-C8-N9	5.79	116.00	113.10
36	A1	23	A	C5-C6-N6	-5.79	119.07	123.70
36	A1	2177	G	N3-C4-C5	-5.79	125.70	128.60
36	A1	2434	U	N3-C2-O2	-5.79	118.15	122.20
36	A1	2763	U	C4-C5-C6	5.79	123.17	119.70
13	CL	120	GLY	N-CA-C	-5.79	98.63	113.10
36	A5	1322	U	N3-C4-C5	5.79	118.07	114.60
36	A5	2899	C	C5-C6-N1	-5.79	118.11	121.00
1	A2	1131	A	N7-C8-N9	-5.79	110.91	113.80
36	A1	1420	C	C6-N1-C2	-5.79	117.98	120.30
38	A8	7	U	C5-C6-N1	-5.79	119.81	122.70
56	DS	155	ARG	CG-CD-NE	5.79	123.95	111.80
1	A2	1129	U	N3-C4-O4	-5.79	115.35	119.40
36	A1	299	G	N3-C2-N2	5.79	123.95	119.90
36	A1	922	U	C2-N1-C1'	5.79	124.64	117.70
36	A1	1303	A	C4-C5-C6	-5.79	114.11	117.00
36	A1	1327	C	N3-C4-C5	5.79	124.22	121.90
80	A6	1122	G	C4-N9-C1'	-5.79	118.98	126.50
80	A6	1521	G	C2-N3-C4	5.79	114.79	111.90
36	A5	1044	U	C2-N3-C4	-5.79	123.53	127.00
36	A5	1159	A	N3-C4-C5	5.79	130.85	126.80
36	A5	1369	A	N9-C4-C5	-5.79	103.49	105.80
36	A5	2926	A	C2-N3-C4	5.79	113.49	110.60
36	A5	3000	A	C5-C6-N6	-5.79	119.07	123.70
36	A5	3141	A	C4-C5-C6	5.79	119.89	117.00
36	A5	3375	A	N1-C2-N3	-5.79	126.41	129.30
36	A1	269	G	C2-N3-C4	5.78	114.79	111.90
36	A1	2607	G	N1-C6-O6	-5.78	116.43	119.90
36	A5	1116	G	N3-C4-C5	-5.78	125.71	128.60
36	A5	2706	G	C2-N3-C4	5.78	114.79	111.90
36	A1	341	G	C5-C6-O6	-5.78	125.13	128.60
36	A5	2549	G	N1-C6-O6	5.78	123.37	119.90
1	A2	1602	C	C6-N1-C2	5.78	122.61	120.30
36	A1	356	C	N3-C4-C5	5.78	124.21	121.90
36	A1	598	A	N1-C6-N6	5.78	122.07	118.60
36	A1	814	U	C2-N3-C4	-5.78	123.53	127.00
36	A1	2148	U	C2-N3-C4	-5.78	123.53	127.00
41	BC	139	GLY	N-CA-C	-5.78	98.65	113.10
80	A6	613	G	N3-C2-N2	5.78	123.95	119.90
36	A5	289	A	C5-C6-N1	5.78	120.59	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	524	U	N1-C2-O2	-5.78	118.75	122.80
36	A5	2412	G	N9-C4-C5	5.78	107.71	105.40
36	A5	2665	U	C2-N3-C4	5.78	130.47	127.00
36	A1	2408	U	C5-C4-O4	-5.78	122.43	125.90
80	A6	1120	U	C5-C6-N1	-5.78	119.81	122.70
36	A5	427	C	C2-N3-C4	-5.78	117.01	119.90
36	A1	2165	G	C5-N7-C8	-5.78	101.41	104.30
36	A5	666	A	C8-N9-C4	5.78	108.11	105.80
1	A2	339	C	N1-C2-O2	-5.78	115.43	118.90
36	A1	499	G	C5-C6-O6	5.78	132.06	128.60
36	A1	968	G	N3-C4-C5	-5.78	125.71	128.60
80	A6	153	G	N3-C4-N9	-5.78	122.53	126.00
80	A6	418	G	C8-N9-C1'	-5.78	119.49	127.00
80	A6	622	A	N1-C6-N6	-5.78	115.14	118.60
36	A5	365	A	N1-C6-N6	5.78	122.06	118.60
36	A5	526	C	C5-C4-N4	-5.78	116.16	120.20
36	A1	3270	U	N3-C4-C5	5.77	118.06	114.60
1	A2	1370	U	N3-C2-O2	-5.77	118.16	122.20
36	A1	212	G	N3-C4-N9	5.77	129.46	126.00
36	A1	1747	G	C4-C5-N7	5.77	113.11	110.80
36	A1	2227	C	N1-C2-O2	-5.77	115.44	118.90
36	A1	2361	A	C2-N3-C4	5.77	113.49	110.60
36	A5	1193	A	C2-N3-C4	-5.77	107.71	110.60
36	A5	1206	G	C2-N3-C4	5.77	114.79	111.90
1	A2	570	A	N3-C4-C5	-5.77	122.76	126.80
36	A1	1591	G	N1-C6-O6	-5.77	116.44	119.90
80	A6	1749	A	C5-C6-N6	-5.77	119.08	123.70
36	A5	411	U	N1-C2-N3	5.77	118.36	114.90
36	A5	1904	C	N1-C2-O2	5.77	122.36	118.90
36	A5	2774	C	N1-C2-O2	-5.77	115.44	118.90
36	A1	505	G	N9-C4-C5	5.77	107.71	105.40
36	A1	968	G	C6-C5-N7	-5.77	126.94	130.40
36	A1	1192	C	N1-C2-O2	5.77	122.36	118.90
36	A1	1458	U	C6-N1-C2	5.77	124.46	121.00
36	A1	1665	C	C5-C4-N4	-5.77	116.16	120.20
36	A1	2343	C	C6-N1-C2	5.77	122.61	120.30
36	A1	2728	G	C2-N3-C4	5.77	114.78	111.90
1	A2	1339	C	C6-N1-C2	-5.77	117.99	120.30
36	A1	44	U	N3-C4-O4	-5.77	115.36	119.40
36	A1	420	G	N1-C2-N2	-5.77	111.01	116.20
36	A1	658	G	C5-C6-N1	-5.77	108.62	111.50
36	A1	947	G	N3-C2-N2	5.77	123.94	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2805	G	N3-C4-N9	5.77	129.46	126.00
36	A1	2989	U	C2-N3-C4	-5.77	123.54	127.00
80	A6	1241	G	N3-C4-C5	5.77	131.48	128.60
36	A5	1208	U	N1-C2-N3	5.77	118.36	114.90
36	A5	3088	G	N7-C8-N9	5.77	115.98	113.10
1	A2	1614	A	C4-C5-C6	5.77	119.88	117.00
36	A1	1379	G	N1-C2-N2	-5.77	111.01	116.20
36	A1	2279	A	C8-N9-C4	5.77	108.11	105.80
36	A5	3076	C	N3-C2-O2	-5.77	117.86	121.90
38	A8	104	A	N1-C6-N6	5.77	122.06	118.60
1	A2	1112	G	C6-N1-C2	-5.76	121.64	125.10
36	A1	2525	G	C3'-C2'-C1'	-5.76	96.89	101.50
36	A1	2653	C	C2-N3-C4	-5.76	117.02	119.90
80	A6	1028	C	C5-C6-N1	-5.76	118.12	121.00
36	A5	1116	G	C4-C5-C6	5.76	122.26	118.80
36	A5	1524	A	N1-C2-N3	5.76	132.18	129.30
36	A5	2329	C	C5-C4-N4	5.76	124.23	120.20
36	A5	3131	U	C5-C4-O4	-5.76	122.44	125.90
1	A2	144	U	N1-C2-O2	5.76	126.83	122.80
36	A5	2320	A	N3-C4-N9	-5.76	122.79	127.40
1	A2	1027	A	C8-N9-C4	-5.76	103.50	105.80
36	A1	1432	C	N1-C2-N3	5.76	123.23	119.20
36	A1	1447	G	N3-C4-N9	-5.76	122.54	126.00
36	A1	1905	G	C5-C6-O6	-5.76	125.14	128.60
36	A1	2623	G	N9-C4-C5	-5.76	103.10	105.40
36	A1	3092	C	C2-N1-C1'	-5.76	112.46	118.80
52	DO	197[B]	PHE	O-C-N	5.76	133.00	123.20
80	A6	1772	C	N1-C2-O2	-5.76	115.44	118.90
36	A5	706	A	N1-C2-N3	-5.76	126.42	129.30
36	A5	1126	G	C2-N3-C4	-5.76	109.02	111.90
36	A5	1724	U	C2-N1-C1'	5.76	124.61	117.70
36	A5	2129	U	N3-C4-C5	5.76	118.06	114.60
36	A5	2342	U	N3-C2-O2	-5.76	118.17	122.20
1	A2	377	G	N1-C2-N2	5.76	121.38	116.20
1	A2	1274	C	C5-C4-N4	5.76	124.23	120.20
80	A6	1324	G	N3-C2-N2	-5.76	115.87	119.90
36	A5	1888	U	N1-C2-N3	5.76	118.36	114.90
36	A5	3316	A	N1-C6-N6	5.76	122.06	118.60
36	A1	2357	A	C6-N1-C2	-5.76	115.15	118.60
36	A1	2752	U	N3-C2-O2	-5.76	118.17	122.20
36	A5	1846	C	N3-C2-O2	-5.76	117.87	121.90
36	A5	2305	G	C6-C5-N7	-5.76	126.95	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2337	C	C2-N3-C4	-5.76	117.02	119.90
1	A2	169	A	C8-N9-C4	5.75	108.10	105.80
36	A5	2335	G	N9-C4-C5	5.75	107.70	105.40
36	A5	3298	C	C2-N3-C4	-5.75	117.02	119.90
1	A2	971	A	C5-C6-N1	-5.75	114.82	117.70
36	A1	1747	G	C5-N7-C8	-5.75	101.42	104.30
36	A1	3046	A	C2-N3-C4	5.75	113.48	110.60
80	A6	1681	A	N1-C6-N6	5.75	122.05	118.60
36	A5	518	G	C8-N9-C4	5.75	108.70	106.40
36	A5	1931	U	C6-N1-C1'	5.75	129.25	121.20
1	A2	158	U	N3-C2-O2	-5.75	118.17	122.20
1	A2	864	U	N1-C2-N3	5.75	118.35	114.90
80	A6	1124	A	N9-C4-C5	-5.75	103.50	105.80
36	A1	702	C	C5-C4-N4	-5.75	116.17	120.20
36	A5	2747	A	N9-C4-C5	5.75	108.10	105.80
1	A2	639	U	N3-C4-O4	-5.75	115.38	119.40
36	A1	368	G	C2-N3-C4	-5.75	109.03	111.90
36	A1	984	G	N1-C2-N2	-5.75	111.03	116.20
36	A1	1167	U	C2-N3-C4	-5.75	123.55	127.00
53	BP	24	VAL	CB-CA-C	-5.75	100.48	111.40
80	A6	99	C	C2-N1-C1'	5.75	125.12	118.80
80	A6	1164	G	C5-C6-N1	5.75	114.37	111.50
36	A5	591	G	C8-N9-C4	5.75	108.70	106.40
36	A5	1143	A	C5-N7-C8	-5.75	101.03	103.90
36	A5	2192	C	C4-C5-C6	5.75	120.27	117.40
36	A5	3212	C	N1-C2-O2	-5.75	115.45	118.90
38	A8	31	G	N7-C8-N9	-5.75	110.23	113.10
36	A1	817	A	N1-C2-N3	5.75	132.17	129.30
36	A1	1904	C	N3-C2-O2	5.75	125.92	121.90
36	A1	2571	U	N1-C2-O2	5.75	126.82	122.80
36	A1	3204	C	C5-C6-N1	-5.75	118.13	121.00
36	A1	3218	A	N3-C4-N9	-5.75	122.80	127.40
80	A6	677	G	C4-N9-C1'	-5.75	119.03	126.50
36	A5	911	C	C2-N3-C4	-5.75	117.03	119.90
36	A5	1512	U	C4-C5-C6	5.75	123.15	119.70
36	A5	1553	U	N3-C2-O2	5.75	126.22	122.20
36	A1	1669	C	N1-C2-O2	-5.75	115.45	118.90
36	A5	613	G	N1-C6-O6	-5.75	116.45	119.90
36	A5	1128	U	N1-C2-N3	5.75	118.35	114.90
38	A8	17	A	C5-C6-N6	-5.75	119.10	123.70
1	A2	1169	G	N3-C4-C5	-5.74	125.73	128.60
36	A1	1377	G	C2-N3-C4	5.74	114.77	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1091	A	C5-N7-C8	-5.74	101.03	103.90
36	A5	3301	U	C6-N1-C2	5.74	124.45	121.00
36	A1	187	A	N3-C4-N9	5.74	131.99	127.40
36	A1	2117	A	C5-C6-N6	5.74	128.29	123.70
38	A4	135	G	C8-N9-C4	-5.74	104.10	106.40
36	A5	363	G	N9-C4-C5	5.74	107.70	105.40
36	A5	382	U	N1-C2-N3	5.74	118.34	114.90
36	A5	3123	A	N9-C4-C5	-5.74	103.50	105.80
1	A2	527	A	C8-N9-C4	-5.74	103.50	105.80
36	A1	804	C	C2-N1-C1'	-5.74	112.49	118.80
36	A1	1391	C	C5-C6-N1	-5.74	118.13	121.00
80	A6	944	A	N7-C8-N9	5.74	116.67	113.80
36	A5	88	A	C5-C6-N1	-5.74	114.83	117.70
36	A1	87	U	C2-N3-C4	-5.74	123.56	127.00
36	A1	1143	A	C4-C5-N7	5.74	113.57	110.70
36	A1	1314	C	C2-N3-C4	-5.74	117.03	119.90
80	A6	524	U	N3-C2-O2	-5.74	118.18	122.20
80	A6	901	G	C6-C5-N7	-5.74	126.96	130.40
36	A5	201	A	C5-C6-N1	-5.74	114.83	117.70
36	A5	216	G	C4-C5-N7	5.74	113.10	110.80
36	A5	672	A	N1-C6-N6	5.74	122.04	118.60
36	A5	3047	U	C2-N3-C4	-5.74	123.56	127.00
36	A5	3339	A	C5-C6-N6	-5.74	119.11	123.70
1	A2	1354	G	N3-C4-C5	-5.74	125.73	128.60
36	A1	1130	A	N1-C6-N6	5.74	122.04	118.60
80	A6	988	A	C8-N9-C4	-5.74	103.50	105.80
36	A1	1778	G	N7-C8-N9	5.74	115.97	113.10
36	A1	2815	G	N1-C2-N2	-5.74	111.04	116.20
36	A5	3241	G	C5-C6-O6	-5.74	125.16	128.60
40	DB	266	ARG	NE-CZ-NH1	5.74	123.17	120.30
75	DI	45	ARG	NE-CZ-NH2	-5.74	117.43	120.30
80	A6	448	C	N1-C2-O2	-5.73	115.46	118.90
36	A5	1113	G	N7-C8-N9	-5.73	110.23	113.10
38	A8	106	C	N3-C4-C5	5.73	124.19	121.90
78	Bo	87	ARG	NE-CZ-NH1	-5.73	117.43	120.30
47	DI	139	ARG	NE-CZ-NH1	5.73	123.17	120.30
80	A6	798	C	N3-C4-C5	5.73	124.19	121.90
36	A5	2148	U	C5-C4-O4	-5.73	122.46	125.90
80	A6	1489	U	N3-C4-O4	-5.73	115.39	119.40
36	A5	666	A	C2-N3-C4	-5.73	107.73	110.60
36	A5	1035	G	C8-N9-C1'	-5.73	119.55	127.00
36	A5	1242	G	N3-C4-N9	5.73	129.44	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2906	C	N3-C4-C5	-5.73	119.61	121.90
37	A7	47	C	C2-N3-C4	-5.73	117.04	119.90
1	A2	1776	A	N1-C6-N6	-5.73	115.16	118.60
36	A1	689	U	C2-N1-C1'	5.73	124.57	117.70
36	A1	1101	G	C2-N3-C4	-5.73	109.04	111.90
38	A4	102	U	C2-N3-C4	-5.73	123.56	127.00
36	A5	1443	G	C5-C6-N1	-5.73	108.64	111.50
36	A5	1445	U	C2-N3-C4	-5.73	123.56	127.00
36	A5	1832	C	C5-C4-N4	-5.73	116.19	120.20
36	A5	2422	C	N3-C2-O2	-5.73	117.89	121.90
36	A5	2658	G	N7-C8-N9	-5.73	110.24	113.10
36	A1	435	C	C2-N1-C1'	-5.73	112.50	118.80
80	A6	96	G	N9-C4-C5	5.73	107.69	105.40
36	A5	224	C	N3-C2-O2	-5.73	117.89	121.90
36	A5	1045	C	N1-C2-O2	-5.73	115.46	118.90
36	A5	2736	A	C5-C6-N6	5.73	128.28	123.70
40	DB	21	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A2	1421	A	C8-N9-C4	5.72	108.09	105.80
27	AZ	95	HIS	N-CA-C	5.72	126.46	111.00
36	A1	670	C	C5-C6-N1	-5.72	118.14	121.00
36	A1	2728	G	C5-C6-N1	5.72	114.36	111.50
80	A6	396	G	N9-C4-C5	-5.72	103.11	105.40
36	A5	920	A	C8-N9-C4	5.72	108.09	105.80
36	A5	2142	A	N3-C4-N9	5.72	131.98	127.40
36	A5	3197	G	N3-C4-N9	-5.72	122.56	126.00
36	A1	120	G	C8-N9-C4	5.72	108.69	106.40
36	A1	591	G	C6-C5-N7	-5.72	126.97	130.40
36	A1	2348	A	N1-C2-N3	5.72	132.16	129.30
80	A6	571	G	N3-C4-N9	-5.72	122.57	126.00
36	A5	1856	C	C6-N1-C2	-5.72	118.01	120.30
36	A1	2748	A	N1-C2-N3	5.72	132.16	129.30
36	A1	3054	U	C5-C6-N1	-5.72	119.84	122.70
36	A5	1512	U	C2-N3-C4	-5.72	123.57	127.00
36	A5	2827	U	N3-C2-O2	-5.72	118.19	122.20
38	A8	28	C	C4-C5-C6	-5.72	114.54	117.40
36	A1	311	C	C6-N1-C2	5.72	122.59	120.30
36	A1	434	U	N3-C4-C5	5.72	118.03	114.60
36	A1	658	G	C4-C5-N7	-5.72	108.51	110.80
36	A1	1100	U	C5-C6-N1	-5.72	119.84	122.70
36	A5	2108	C	N3-C4-C5	5.72	124.19	121.90
1	A2	142	G	N1-C6-O6	5.72	123.33	119.90
36	A5	1159	A	C6-N1-C2	5.72	122.03	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2361	A	C5-C6-N1	5.72	120.56	117.70
36	A5	2978	U	N1-C2-N3	5.72	118.33	114.90
54	DQ	50	LYS	CD-CE-NZ	5.72	124.85	111.70
36	A1	2817	A	N3-C4-C5	-5.72	122.80	126.80
80	A6	137	U	C2-N1-C1'	5.72	124.56	117.70
80	A6	1274	C	N3-C4-N4	-5.72	114.00	118.00
80	A6	1781	A	C4-C5-C6	5.72	119.86	117.00
36	A5	2619	G	C5-C6-N1	5.72	114.36	111.50
36	A1	811	U	N1-C2-N3	5.71	118.33	114.90
36	A1	994	G	C8-N9-C4	5.71	108.69	106.40
36	A1	1160	C	C5-C4-N4	5.71	124.20	120.20
36	A1	2142	A	C8-N9-C4	-5.71	103.51	105.80
36	A1	2533	G	C8-N9-C1'	-5.71	119.57	127.00
80	A6	922	G	C5-C6-N1	5.71	114.36	111.50
80	A6	1136	U	C5-C4-O4	-5.71	122.47	125.90
36	A5	760	G	C5-C6-O6	-5.71	125.17	128.60
36	A5	884	A	N1-C6-N6	-5.71	115.17	118.60
36	A5	1371	G	N7-C8-N9	-5.71	110.24	113.10
36	A5	2392	C	C5-C6-N1	-5.71	118.14	121.00
36	A5	3259	U	C5-C6-N1	5.71	125.56	122.70
36	A1	755	A	C2-N3-C4	-5.71	107.74	110.60
36	A1	773	G	N1-C6-O6	-5.71	116.47	119.90
36	A1	959	C	C2-N3-C4	-5.71	117.04	119.90
36	A1	1333	C	C6-N1-C2	-5.71	118.02	120.30
36	A1	1582	C	C6-N1-C1'	5.71	127.66	120.80
36	A1	1586	G	N3-C2-N2	5.71	123.90	119.90
36	A1	3149	G	N3-C2-N2	-5.71	115.90	119.90
37	A3	82	G	C2-N3-C4	-5.71	109.04	111.90
80	A6	1	U	C5-C6-N1	5.71	125.56	122.70
80	A6	163	G	N1-C2-N3	5.71	127.33	123.90
36	A5	670	C	C2-N3-C4	-5.71	117.04	119.90
36	A5	1159	A	C5-N7-C8	-5.71	101.04	103.90
38	A8	23	U	C4-C5-C6	5.71	123.13	119.70
47	DI	21	ARG	NE-CZ-NH1	5.71	123.16	120.30
36	A1	2906	C	C2-N3-C4	-5.71	117.05	119.90
36	A1	3269	U	N1-C2-O2	5.71	126.80	122.80
36	A5	3365	U	C6-N1-C2	-5.71	117.57	121.00
36	A1	280	U	C5-C4-O4	-5.71	122.47	125.90
80	A6	136	C	C2-N1-C1'	5.71	125.08	118.80
80	A6	541	A	C3'-C2'-C1'	-5.71	96.93	101.50
36	A5	270	U	N3-C2-O2	-5.71	118.20	122.20
36	A5	1364	C	C5-C6-N1	-5.71	118.14	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2730	G	N3-C2-N2	-5.71	115.90	119.90
36	A5	2804	A	C8-N9-C4	5.71	108.08	105.80
36	A5	2979	U	N3-C2-O2	5.71	126.20	122.20
36	A1	333	G	C4-C5-N7	-5.71	108.52	110.80
37	A3	83	U	C5-C6-N1	-5.71	119.85	122.70
53	BP	131	ARG	NE-CZ-NH2	5.71	123.15	120.30
36	A5	2320	A	N9-C4-C5	5.71	108.08	105.80
53	DP	24	VAL	CB-CA-C	-5.71	100.56	111.40
36	A1	2882	U	C2-N3-C4	-5.71	123.58	127.00
36	A5	563	U	N3-C2-O2	-5.71	118.21	122.20
1	A2	92	A	C6-N1-C2	-5.70	115.18	118.60
1	A2	831	U	C2-N1-C1'	5.70	124.55	117.70
1	A2	1075	C	N3-C2-O2	5.70	125.89	121.90
36	A1	517	G	C5-N7-C8	-5.70	101.45	104.30
36	A1	1374	G	C6-C5-N7	-5.70	126.98	130.40
36	A1	1392	G	N9-C4-C5	-5.70	103.12	105.40
36	A1	1932	A	C5-C6-N1	5.70	120.55	117.70
36	A1	2571	U	N3-C2-O2	-5.70	118.21	122.20
36	A1	2634	U	C5-C6-N1	-5.70	119.85	122.70
80	A6	826	U	C2-N1-C1'	5.70	124.55	117.70
36	A5	1163	A	C5-C6-N1	5.70	120.55	117.70
36	A5	2836	C	C5-C4-N4	5.70	124.19	120.20
36	A1	2329	C	C6-N1-C1'	5.70	127.64	120.80
36	A1	3137	C	C5-C6-N1	5.70	123.85	121.00
80	A6	1025	A	C5-C6-N1	-5.70	114.85	117.70
36	A5	2293	C	N1-C2-O2	5.70	122.32	118.90
36	A5	2866	U	C2-N3-C4	-5.70	123.58	127.00
1	A2	612	U	N3-C4-O4	-5.70	115.41	119.40
1	A2	1489	U	N3-C2-O2	-5.70	118.21	122.20
36	A1	859	G	N9-C4-C5	-5.70	103.12	105.40
36	A1	2310	U	C6-N1-C2	-5.70	117.58	121.00
36	A1	2606	G	N3-C2-N2	5.70	123.89	119.90
36	A5	2552	C	N3-C4-N4	-5.70	114.01	118.00
36	A1	967	A	N1-C6-N6	-5.70	115.18	118.60
36	A1	1141	C	N3-C4-C5	-5.70	119.62	121.90
36	A1	1787	A	N7-C8-N9	-5.70	110.95	113.80
73	Bj	72	ARG	NE-CZ-NH1	5.70	123.15	120.30
80	A6	1015	U	C2-N3-C4	5.70	130.42	127.00
36	A5	971	G	N9-C4-C5	5.70	107.68	105.40
36	A5	1840	U	N1-C2-O2	5.70	126.79	122.80
36	A1	2202	C	C5-C6-N1	-5.70	118.15	121.00
36	A1	2735	U	N3-C4-O4	-5.70	115.41	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A8	20	U	C5-C6-N1	-5.70	119.85	122.70
1	A2	539	G	C5-N7-C8	-5.70	101.45	104.30
36	A1	3071	U	N1-C2-O2	-5.70	118.81	122.80
80	A6	11	A	C8-N9-C4	5.70	108.08	105.80
80	A6	1127	G	C6-N1-C2	-5.70	121.68	125.10
36	A5	665	A	N9-C4-C5	-5.70	103.52	105.80
36	A5	3006	A	N9-C4-C5	5.70	108.08	105.80
54	DQ	127	LEU	CA-CB-CG	5.70	128.40	115.30
1	A2	741	C	N1-C2-O2	-5.69	115.48	118.90
80	A6	1643	U	N3-C4-O4	-5.69	115.41	119.40
36	A5	1639	C	C6-N1-C2	-5.69	118.02	120.30
1	A2	1282	U	N1-C2-N3	5.69	118.32	114.90
36	A1	1514	G	N3-C4-C5	-5.69	125.75	128.60
36	A1	2571	U	C2-N1-C1'	5.69	124.53	117.70
36	A1	2760	C	N3-C4-C5	-5.69	119.62	121.90
80	A6	411	C	N3-C2-O2	-5.69	117.92	121.90
36	A5	276	U	C4-C5-C6	5.69	123.11	119.70
36	A5	1466	G	N3-C4-N9	-5.69	122.58	126.00
36	A5	1589	A	C5-C6-N1	5.69	120.55	117.70
36	A5	1652	G	C4-C5-N7	-5.69	108.52	110.80
36	A5	2330	C	C4-C5-C6	5.69	120.25	117.40
36	A1	87	U	N3-C4-O4	-5.69	115.42	119.40
36	A1	233	C	C6-N1-C2	5.69	122.58	120.30
36	A1	655	C	C2-N3-C4	-5.69	117.06	119.90
36	A1	678	G	C5-C6-O6	-5.69	125.19	128.60
36	A1	1331	U	C2-N3-C4	-5.69	123.59	127.00
36	A1	1507	G	C4-C5-N7	-5.69	108.52	110.80
36	A1	2438	A	C8-N9-C4	5.69	108.08	105.80
36	A1	2865	U	C2-N3-C4	-5.69	123.59	127.00
62	BY	60	ARG	NE-CZ-NH1	-5.69	117.45	120.30
80	A6	1421	A	C8-N9-C4	5.69	108.08	105.80
36	A5	2400	G	C4-C5-N7	5.69	113.08	110.80
38	A8	26	U	C2-N1-C1'	5.69	124.53	117.70
38	A8	34	U	C5-C6-N1	-5.69	119.86	122.70
46	DH	151	VAL	CB-CA-C	-5.69	100.59	111.40
52	DO	163[B]	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A2	92	A	N3-C4-C5	-5.69	122.82	126.80
1	A2	494	U	N3-C2-O2	-5.69	118.22	122.20
36	A1	272	G	C5-N7-C8	5.69	107.14	104.30
36	A1	1502	C	C4-C5-C6	5.69	120.25	117.40
36	A5	582	G	N1-C6-O6	-5.69	116.49	119.90
36	A1	3052	G	N1-C6-O6	-5.69	116.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	24	G	C5-C6-O6	-5.69	125.19	128.60
36	A5	580	C	N3-C4-C5	-5.69	119.62	121.90
36	A5	1726	C	C5-C6-N1	-5.69	118.16	121.00
36	A5	1849	C	N3-C2-O2	-5.69	117.92	121.90
36	A5	3200	G	C5-C6-O6	-5.69	125.19	128.60
36	A1	2984	C	C5-C4-N4	5.69	124.18	120.20
36	A1	3010	U	N3-C2-O2	-5.69	118.22	122.20
80	A6	864	U	C2-N1-C1'	5.69	124.52	117.70
36	A5	2123	G	C5-C6-N1	5.69	114.34	111.50
38	A8	95	G	C4-N9-C1'	-5.69	119.11	126.50
1	A2	1781	A	C5-C6-N1	-5.68	114.86	117.70
36	A1	2147	A	C5-C6-N6	-5.68	119.15	123.70
36	A1	3110	C	N1-C2-O2	5.68	122.31	118.90
36	A1	3188	G	N3-C4-N9	5.68	129.41	126.00
36	A1	3235	C	C6-N1-C2	-5.68	118.03	120.30
36	A1	3293	U	C5-C4-O4	-5.68	122.49	125.90
38	A4	113	U	C6-N1-C1'	5.68	129.16	121.20
36	A5	79	U	C5-C4-O4	-5.68	122.49	125.90
37	A7	8	G	C8-N9-C4	-5.68	104.13	106.40
36	A1	68	C	N3-C2-O2	-5.68	117.92	121.90
80	A6	1143	A	C2-N3-C4	5.68	113.44	110.60
80	A6	1572	G	C5-N7-C8	-5.68	101.46	104.30
36	A5	1429	G	C6-C5-N7	-5.68	126.99	130.40
36	A5	1458	U	N3-C4-C5	5.68	118.01	114.60
36	A1	70	A	C8-N9-C4	5.68	108.07	105.80
36	A1	1191	U	C2-N3-C4	-5.68	123.59	127.00
36	A1	1209	G	N3-C4-C5	-5.68	125.76	128.60
36	A1	2749	G	N1-C6-O6	5.68	123.31	119.90
80	A6	66	U	C4-C5-C6	5.68	123.11	119.70
80	A6	385	A	N7-C8-N9	-5.68	110.96	113.80
36	A5	1159	A	N9-C4-C5	-5.68	103.53	105.80
36	A5	1371	G	C5-N7-C8	5.68	107.14	104.30
36	A5	1448	U	C4-C5-C6	5.68	123.11	119.70
37	A7	103	A	C5-C6-N6	-5.68	119.16	123.70
1	A2	1361	U	N3-C2-O2	-5.68	118.22	122.20
1	A2	1749	A	C4-C5-N7	5.68	113.54	110.70
36	A1	574	U	N3-C4-C5	5.68	118.01	114.60
80	A6	1118	G	C6-N1-C2	-5.68	121.69	125.10
36	A5	39	A	C2-N3-C4	5.68	113.44	110.60
36	A5	3290	G	N7-C8-N9	5.68	115.94	113.10
37	A7	38	U	C2-N1-C1'	5.68	124.52	117.70
36	A1	62	A	C5-C6-N6	-5.68	119.16	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2772	C	C5-C6-N1	5.68	123.84	121.00
36	A1	2944	U	N3-C4-O4	-5.68	115.42	119.40
36	A1	885	U	N3-C2-O2	-5.68	118.23	122.20
36	A1	1170	A	C6-N1-C2	5.68	122.00	118.60
80	A6	1600	A	N3-C4-C5	5.68	130.77	126.80
36	A5	413	U	N1-C2-N3	5.68	118.31	114.90
36	A5	1405	U	C2-N3-C4	-5.68	123.59	127.00
36	A5	2197	C	C2-N1-C1'	-5.68	112.56	118.80
36	A5	2584	G	C5-C6-O6	-5.68	125.19	128.60
36	A5	2892	A	N1-C6-N6	-5.68	115.19	118.60
36	A5	2988	C	N3-C4-C5	-5.68	119.63	121.90
36	A5	3020	U	N3-C2-O2	5.68	126.17	122.20
1	A2	1458	G	C4-N9-C1'	5.67	133.88	126.50
36	A1	588	G	N3-C4-N9	5.67	129.41	126.00
36	A1	643	U	C2-N1-C1'	-5.67	110.89	117.70
36	A1	2403	G	N3-C4-N9	5.67	129.40	126.00
38	A8	95	G	C8-N9-C1'	5.67	134.38	127.00
52	DO	23[B]	ILE	C-N-CA	-5.67	107.51	121.70
36	A1	417	A	C2-N3-C4	-5.67	107.76	110.60
36	A1	1156	C	C6-N1-C2	5.67	122.57	120.30
80	A6	109	G	N7-C8-N9	-5.67	110.26	113.10
80	A6	194	U	N3-C2-O2	-5.67	118.23	122.20
36	A5	334	A	C2-N3-C4	5.67	113.44	110.60
36	A5	819	U	N3-C4-O4	5.67	123.37	119.40
1	A2	507	U	C6-N1-C2	-5.67	117.60	121.00
36	A1	1417	G	N7-C8-N9	-5.67	110.27	113.10
36	A1	1546	A	C5-C6-N6	5.67	128.24	123.70
36	A5	2326	A	C2-N3-C4	5.67	113.44	110.60
38	A8	113	U	C6-N1-C1'	-5.67	113.26	121.20
80	A6	389	G	N3-C4-C5	-5.67	125.77	128.60
80	A6	987	G	N1-C6-O6	5.67	123.30	119.90
80	A6	1421	A	N9-C4-C5	-5.67	103.53	105.80
36	A5	953	G	N3-C4-N9	-5.67	122.60	126.00
36	A5	1314	C	N3-C4-C5	5.67	124.17	121.90
36	A5	2733	A	C2-N3-C4	-5.67	107.77	110.60
38	A8	109	A	C8-N9-C4	-5.67	103.53	105.80
36	A1	86	G	C4-C5-N7	-5.67	108.53	110.80
36	A1	652	G	N1-C6-O6	-5.67	116.50	119.90
36	A1	658	G	N3-C4-C5	-5.67	125.77	128.60
36	A1	1919	G	C8-N9-C4	-5.67	104.13	106.40
80	A6	328	A	N9-C4-C5	5.67	108.07	105.80
36	A5	248	U	C2-N1-C1'	5.67	124.50	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	998	A	N1-C2-N3	5.67	132.13	129.30
36	A5	1127	G	N9-C4-C5	-5.67	103.13	105.40
36	A5	1940	G	C8-N9-C4	5.67	108.67	106.40
36	A5	2848	G	C4-C5-C6	5.67	122.20	118.80
1	A2	279	G	N7-C8-N9	5.67	115.93	113.10
36	A1	1434	G	C4-C5-N7	-5.67	108.53	110.80
36	A1	3228	C	N1-C2-O2	5.67	122.30	118.90
80	A6	814	A	N7-C8-N9	5.67	116.63	113.80
36	A5	905	U	N3-C4-O4	5.67	123.37	119.40
36	A5	958	C	N3-C4-C5	5.67	124.17	121.90
36	A5	1321	G	N1-C6-O6	5.67	123.30	119.90
36	A5	2748	A	C5-C6-N6	-5.67	119.17	123.70
36	A5	2832	C	C6-N1-C2	5.67	122.57	120.30
36	A5	2979	U	C5-C6-N1	-5.67	119.87	122.70
41	DC	136	LEU	CA-CB-CG	5.67	128.34	115.30
36	A1	324	A	N1-C2-N3	5.67	132.13	129.30
36	A1	2967	A	C5-N7-C8	5.67	106.73	103.90
36	A1	3096	C	C2-N3-C4	-5.67	117.07	119.90
36	A1	1156	C	N1-C2-O2	5.66	122.30	118.90
36	A1	1858	A	C4-C5-C6	5.66	119.83	117.00
36	A1	3060	C	N3-C2-O2	5.66	125.86	121.90
36	A5	65	A	P-O3'-C3'	5.66	126.50	119.70
36	A5	824	C	N3-C4-C5	-5.66	119.64	121.90
36	A5	948	C	N3-C4-N4	5.66	121.97	118.00
36	A5	1525	G	C8-N9-C1'	-5.66	119.64	127.00
36	A5	2191	U	C5-C6-N1	-5.66	119.87	122.70
36	A5	2865	U	N1-C2-O2	5.66	126.76	122.80
36	A5	3285	C	N1-C2-O2	5.66	122.30	118.90
36	A1	1003	A	C4-C5-C6	5.66	119.83	117.00
36	A1	2197	C	C4-C5-C6	-5.66	114.57	117.40
73	Bj	73	ARG	NE-CZ-NH1	5.66	123.13	120.30
80	A6	1764	C	N3-C4-N4	-5.66	114.04	118.00
1	A2	810	G	C4-C5-N7	5.66	113.06	110.80
36	A1	22	G	N1-C6-O6	-5.66	116.50	119.90
36	A1	969	C	N3-C4-C5	5.66	124.16	121.90
36	A1	1349	G	N3-C4-C5	-5.66	125.77	128.60
36	A1	1381	A	N1-C6-N6	5.66	122.00	118.60
36	A1	1518	U	C4-C5-C6	5.66	123.10	119.70
36	A1	2385	G	C2-N3-C4	-5.66	109.07	111.90
36	A1	2888	U	C5-C6-N1	-5.66	119.87	122.70
36	A5	39	A	C5-N7-C8	5.66	106.73	103.90
36	A5	114	A	N1-C6-N6	5.66	122.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	326	U	C4-C5-C6	-5.66	116.30	119.70
36	A5	1284	C	C5-C6-N1	5.66	123.83	121.00
36	A5	3010	U	N3-C4-O4	-5.66	115.44	119.40
36	A1	192	C	C2-N1-C1'	5.66	125.02	118.80
36	A1	435	C	N3-C2-O2	5.66	125.86	121.90
36	A1	2306	C	C5-C6-N1	5.66	123.83	121.00
36	A1	3204	C	N3-C4-N4	-5.66	114.04	118.00
38	A4	145	U	C2-N3-C4	-5.66	123.61	127.00
36	A5	769	G	N7-C8-N9	-5.66	110.27	113.10
36	A5	2951	G	C5-C6-N1	5.66	114.33	111.50
1	A2	712	G	C8-N9-C4	-5.66	104.14	106.40
36	A1	1309	U	N3-C4-O4	5.66	123.36	119.40
36	A5	2400	G	N1-C6-O6	5.66	123.29	119.90
36	A1	2121	G	N1-C6-O6	-5.66	116.51	119.90
36	A5	1285	G	N7-C8-N9	-5.66	110.27	113.10
36	A5	2293	C	C2-N1-C1'	5.66	125.02	118.80
36	A5	3006	A	C8-N9-C4	-5.66	103.54	105.80
36	A5	3054	U	N3-C4-C5	-5.66	111.21	114.60
38	A4	9	A	N1-C6-N6	-5.65	115.21	118.60
36	A5	625	G	C8-N9-C4	-5.65	104.14	106.40
1	A2	1644	C	N1-C2-O2	-5.65	115.51	118.90
36	A1	824	C	N3-C4-N4	-5.65	114.04	118.00
36	A1	1428	A	C8-N9-C4	-5.65	103.54	105.80
38	A4	88	A	N1-C6-N6	5.65	121.99	118.60
38	A4	103	G	C8-N9-C4	-5.65	104.14	106.40
52	BO	3[B]	SER	CA-C-N	-5.65	104.77	117.20
36	A5	1300	G	C6-C5-N7	-5.65	127.01	130.40
36	A1	197	G	N1-C2-N2	5.65	121.29	116.20
36	A1	1196	C	C6-N1-C2	5.65	122.56	120.30
36	A1	1349	G	N3-C4-N9	5.65	129.39	126.00
36	A5	1603	A	N9-C4-C5	5.65	108.06	105.80
37	A7	80	G	N3-C4-N9	5.65	129.39	126.00
1	A2	627	C	N1-C2-O2	-5.65	115.51	118.90
1	A2	1600	A	C4-C5-N7	5.65	113.53	110.70
36	A5	925	A	N1-C6-N6	5.65	121.99	118.60
36	A5	2237	C	N3-C2-O2	-5.65	117.95	121.90
36	A5	2341	A	C5-N7-C8	5.65	106.72	103.90
36	A5	2415	C	C6-N1-C2	5.65	122.56	120.30
36	A5	2904	U	C2-N3-C4	-5.65	123.61	127.00
36	A1	2257	C	C6-N1-C2	-5.65	118.04	120.30
36	A1	2368	A	N1-C2-N3	5.65	132.12	129.30
41	BC	230	VAL	CB-CA-C	-5.65	100.67	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	339	C	C6-N1-C2	-5.65	118.04	120.30
36	A5	880	G	C2-N3-C4	5.65	114.72	111.90
36	A1	1002	A	C4-C5-C6	-5.65	114.18	117.00
36	A1	1048	A	C4-C5-C6	-5.65	114.18	117.00
36	A1	1168	U	N3-C2-O2	-5.65	118.25	122.20
36	A1	1770	G	N7-C8-N9	5.65	115.92	113.10
36	A1	2142	A	C4-C5-C6	5.65	119.82	117.00
36	A1	3373	U	C6-N1-C2	5.65	124.39	121.00
36	A5	2955	U	N1-C2-N3	5.65	118.29	114.90
36	A1	304	G	N1-C2-N3	-5.64	120.51	123.90
36	A1	2282	U	N3-C4-C5	5.64	117.99	114.60
36	A1	2885	C	C5-C6-N1	-5.64	118.18	121.00
38	A4	113	U	C2-N1-C1'	-5.64	110.93	117.70
80	A6	587	C	C2-N3-C4	-5.64	117.08	119.90
36	A5	1434	G	C1'-O4'-C4'	-5.64	105.38	109.90
36	A5	1883	A	C8-N9-C4	-5.64	103.54	105.80
1	A2	355	G	N3-C4-C5	-5.64	125.78	128.60
1	A2	402	C	C2-N1-C1'	-5.64	112.59	118.80
36	A1	1125	U	C5-C6-N1	-5.64	119.88	122.70
36	A1	1483	G	N3-C2-N2	5.64	123.85	119.90
36	A1	2920	U	C5-C6-N1	-5.64	119.88	122.70
80	A6	940	A	C2-N3-C4	-5.64	107.78	110.60
80	A6	1620	C	N3-C2-O2	-5.64	117.95	121.90
36	A5	53	G	N3-C2-N2	5.64	123.85	119.90
36	A5	1210	U	N1-C2-O2	5.64	126.75	122.80
36	A5	1832	C	C6-N1-C2	5.64	122.56	120.30
80	A6	194	U	C5-C6-N1	5.64	125.52	122.70
36	A5	1192	C	C5-C6-N1	-5.64	118.18	121.00
36	A5	1331	U	C5-C4-O4	-5.64	122.52	125.90
1	A2	382	C	N3-C4-C5	5.64	124.16	121.90
36	A1	686	G	C5-C6-O6	5.64	131.98	128.60
36	A1	1169	A	N3-C4-N9	5.64	131.91	127.40
36	A1	2679	A	C4-C5-C6	5.64	119.82	117.00
38	A4	53	A	N3-C4-C5	-5.64	122.85	126.80
36	A5	1370	G	N3-C4-N9	5.64	129.38	126.00
36	A5	3007	U	C5-C4-O4	-5.64	122.52	125.90
1	A2	1782	A	C4-C5-N7	-5.64	107.88	110.70
36	A1	44	U	C2-N3-C4	-5.64	123.62	127.00
36	A1	1514	G	N1-C2-N2	-5.64	111.13	116.20
80	A6	310	C	C2-N3-C4	-5.64	117.08	119.90
80	A6	612	U	C5-C4-O4	5.64	129.28	125.90
36	A5	574	U	C5-C4-O4	-5.64	122.52	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2257	C	N1-C2-O2	5.64	122.28	118.90
36	A5	2816	G	C4-N9-C1'	-5.64	119.17	126.50
64	Da	46	ASP	N-CA-C	-5.64	95.78	111.00
36	A1	34	A	C5-C6-N6	-5.63	119.19	123.70
36	A1	109	A	N1-C6-N6	-5.63	115.22	118.60
36	A1	157	A	N1-C2-N3	5.63	132.12	129.30
36	A1	880	G	N1-C6-O6	-5.63	116.52	119.90
36	A1	970	A	C2-N3-C4	-5.63	107.78	110.60
36	A1	3065	G	N7-C8-N9	-5.63	110.28	113.10
36	A1	3105	U	N3-C4-C5	5.63	117.98	114.60
36	A1	3343	G	N3-C2-N2	5.63	123.84	119.90
36	A5	873	C	C4-C5-C6	5.63	120.22	117.40
36	A1	2787	G	N3-C4-C5	-5.63	125.78	128.60
24	CW	129	VAL	CB-CA-C	-5.63	100.70	111.40
36	A5	634	C	C2-N3-C4	-5.63	117.08	119.90
36	A5	1909	A	C4-C5-C6	-5.63	114.18	117.00
36	A1	1849	C	N1-C2-O2	-5.63	115.52	118.90
80	A6	993	A	C8-N9-C4	-5.63	103.55	105.80
36	A5	825	U	N3-C4-O4	-5.63	115.46	119.40
36	A5	2277	C	N1-C2-O2	5.63	122.28	118.90
36	A5	2631	U	N1-C2-O2	-5.63	118.86	122.80
36	A5	2717	U	C2-N3-C4	-5.63	123.62	127.00
36	A5	3200	G	N3-C2-N2	-5.63	115.96	119.90
36	A1	3142	A	C2-N3-C4	-5.63	107.78	110.60
36	A5	359	U	C5-C6-N1	-5.63	119.89	122.70
36	A5	2389	C	C5-C4-N4	-5.63	116.26	120.20
1	A2	498	G	N3-C4-C5	-5.63	125.79	128.60
36	A1	279	U	N1-C2-N3	5.63	118.28	114.90
36	A1	1444	G	N9-C4-C5	-5.63	103.15	105.40
36	A1	2369	G	C4-N9-C1'	5.63	133.82	126.50
36	A1	3269	U	N3-C4-O4	-5.63	115.46	119.40
80	A6	158	U	P-O3'-C3'	5.63	126.45	119.70
36	A5	842	G	N1-C6-O6	5.63	123.28	119.90
36	A5	916	G	N9-C4-C5	5.63	107.65	105.40
36	A5	3313	U	N3-C4-O4	-5.63	115.46	119.40
43	DE	31	ARG	NE-CZ-NH2	-5.63	117.49	120.30
36	A1	933	A	N7-C8-N9	5.63	116.61	113.80
36	A1	1126	G	C8-N9-C4	5.63	108.65	106.40
36	A1	1439	U	C2-N3-C4	-5.63	123.62	127.00
36	A1	1834	U	C2-N1-C1'	-5.63	110.95	117.70
36	A1	2145	A	C5-C6-N1	5.63	120.51	117.70
38	A4	85	G	N3-C4-C5	-5.63	125.79	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1173	C	C6-N1-C2	-5.63	118.05	120.30
36	A5	355	A	N1-C6-N6	5.63	121.98	118.60
36	A5	946	U	N1-C2-O2	5.63	126.74	122.80
36	A5	1146	C	C2-N3-C4	-5.63	117.09	119.90
36	A5	1163	A	C4-C5-N7	-5.63	107.89	110.70
36	A5	1381	A	N9-C4-C5	-5.63	103.55	105.80
1	A2	397	A	C5-C6-N6	5.62	128.20	123.70
1	A2	1052	U	N3-C2-O2	-5.62	118.26	122.20
36	A1	418	A	C2-N3-C4	-5.62	107.79	110.60
36	A1	1849	C	C5-C4-N4	-5.62	116.26	120.20
38	A4	31	G	N3-C2-N2	5.62	123.84	119.90
80	A6	84	A	C5-N7-C8	5.62	106.71	103.90
36	A5	636	C	C2-N3-C4	-5.62	117.09	119.90
36	A5	1365	G	N1-C2-N3	5.62	127.28	123.90
36	A1	1156	C	C5-C6-N1	-5.62	118.19	121.00
36	A1	1357	G	C6-C5-N7	-5.62	127.03	130.40
36	A1	1451	C	C5-C6-N1	-5.62	118.19	121.00
36	A5	2434	U	C2-N3-C4	-5.62	123.63	127.00
1	A2	951	A	C8-N9-C4	5.62	108.05	105.80
36	A1	313	A	N1-C2-N3	5.62	132.11	129.30
36	A1	2882	U	N3-C4-C5	5.62	117.97	114.60
80	A6	153	G	N3-C4-C5	5.62	131.41	128.60
80	A6	968	U	C4-C5-C6	-5.62	116.33	119.70
36	A5	966	U	N3-C4-C5	5.62	117.97	114.60
36	A5	2188	A	N1-C2-N3	5.62	132.11	129.30
36	A5	2606	G	C4-C5-C6	5.62	122.17	118.80
38	A8	15	G	C5-C6-O6	-5.62	125.23	128.60
1	A2	74	U	C3'-C2'-C1'	-5.62	97.00	101.50
1	A2	1052	U	N1-C2-O2	5.62	126.73	122.80
36	A1	1065	A	C5-N7-C8	5.62	106.71	103.90
36	A1	1294	A	C2-N3-C4	5.62	113.41	110.60
36	A1	2528	G	C8-N9-C4	5.62	108.65	106.40
80	A6	129	U	N1-C2-N3	5.62	118.27	114.90
80	A6	472	U	C2-N3-C4	-5.62	123.63	127.00
36	A5	1845	G	N7-C8-N9	-5.62	110.29	113.10
36	A5	1914	G	N1-C6-O6	-5.62	116.53	119.90
36	A5	2217	U	N3-C2-O2	-5.62	118.27	122.20
37	A7	25	G	N1-C2-N2	5.62	121.26	116.20
36	A1	1329	U	C6-N1-C2	-5.62	117.63	121.00
36	A5	2719	U	N1-C2-O2	-5.62	118.87	122.80
36	A5	2744	U	C5-C4-O4	5.62	129.27	125.90
1	A2	1745	G	N3-C4-C5	-5.62	125.79	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	470	A	C8-N9-C4	-5.62	103.55	105.80
80	A6	711	U	C2-N1-C1'	5.62	124.44	117.70
36	A5	666	A	N7-C8-N9	-5.62	110.99	113.80
36	A5	1206	G	C5-C6-O6	5.62	131.97	128.60
36	A5	2616	C	N3-C4-C5	5.62	124.15	121.90
36	A5	2742	C	N3-C4-C5	5.62	124.15	121.90
1	A2	444	C	C2-N3-C4	5.61	122.71	119.90
1	A2	1119	G	N9-C4-C5	5.61	107.65	105.40
36	A1	794	U	N1-C2-N3	5.61	118.27	114.90
36	A5	180	C	C6-N1-C2	-5.61	118.05	120.30
36	A5	3197	G	N3-C2-N2	-5.61	115.97	119.90
68	De	105	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A2	109	G	C5-C6-O6	-5.61	125.23	128.60
36	A1	23	A	C2-N3-C4	5.61	113.41	110.60
36	A1	1788	C	C5-C4-N4	-5.61	116.27	120.20
36	A1	2819	A	C5-N7-C8	5.61	106.71	103.90
36	A1	3294	A	N7-C8-N9	5.61	116.61	113.80
80	A6	825	U	N3-C2-O2	5.61	126.13	122.20
36	A5	1485	G	C4-C5-N7	-5.61	108.56	110.80
36	A5	2116	G	C4-C5-C6	5.61	122.17	118.80
36	A5	2180	G	N3-C2-N2	5.61	123.83	119.90
36	A5	2363	A	N7-C8-N9	5.61	116.61	113.80
1	A2	453	U	C5-C4-O4	5.61	129.27	125.90
36	A1	2639	G	C5-C6-N1	5.61	114.31	111.50
36	A1	3137	C	C6-N1-C2	-5.61	118.06	120.30
80	A6	51	A	N1-C2-N3	5.61	132.10	129.30
36	A5	145	G	N9-C4-C5	5.61	107.64	105.40
36	A5	217	U	C2-N3-C4	-5.61	123.63	127.00
36	A5	903	U	N1-C2-O2	5.61	126.73	122.80
36	A5	1744	G	C5-C6-N1	5.61	114.31	111.50
36	A5	2249	G	C8-N9-C4	-5.61	104.16	106.40
36	A5	2870	C	C5-C4-N4	5.61	124.13	120.20
50	DM	77	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A2	1646	C	C6-N1-C2	-5.61	118.06	120.30
36	A1	3269	U	C6-N1-C2	-5.61	117.63	121.00
80	A6	96	G	N1-C2-N3	5.61	127.27	123.90
36	A5	909	G	N1-C6-O6	-5.61	116.53	119.90
36	A5	1510	G	N1-C2-N3	5.61	127.27	123.90
36	A5	3003	G	C5-N7-C8	-5.61	101.50	104.30
36	A5	3219	G	N3-C2-N2	5.61	123.83	119.90
37	A7	38	U	N3-C4-C5	5.61	117.97	114.60
38	A8	100	U	C2-N1-C1'	5.61	124.43	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1761	U	N3-C4-C5	-5.61	111.24	114.60
36	A1	1360	C	C5-C6-N1	-5.61	118.20	121.00
36	A1	2606	G	N3-C4-N9	5.61	129.36	126.00
80	A6	553	G	C4-N9-C1'	5.61	133.79	126.50
80	A6	1423	U	N1-C2-O2	-5.61	118.88	122.80
36	A5	280	U	N3-C4-C5	5.61	117.96	114.60
36	A5	282	G	C2'-C3'-O3'	5.61	122.67	113.70
36	A5	1307	G	N1-C6-O6	-5.61	116.53	119.90
36	A5	1451	C	C2-N3-C4	-5.61	117.10	119.90
36	A5	1773	C	C5-C6-N1	-5.61	118.20	121.00
36	A5	2630	C	N1-C2-O2	-5.61	115.54	118.90
37	A7	5	G	C5-C6-N1	-5.61	108.70	111.50
44	DF	229	PHE	CB-CG-CD1	5.61	124.73	120.80
1	A2	401	A	N1-C6-N6	5.61	121.96	118.60
1	A2	1642	G	N3-C4-C5	-5.61	125.80	128.60
36	A1	649	A	C2-N3-C4	-5.61	107.80	110.60
36	A1	1391	C	C4-C5-C6	5.61	120.20	117.40
36	A1	1448	U	C5-C4-O4	-5.61	122.54	125.90
36	A1	2227	C	C3'-C2'-C1'	-5.61	97.02	101.50
36	A1	2390	A	C5-C6-N6	-5.61	119.22	123.70
41	BC	327	LEU	CA-CB-CG	5.61	128.19	115.30
80	A6	359	A	C8-N9-C4	5.61	108.04	105.80
80	A6	1773	C	C2-N3-C4	5.61	122.70	119.90
36	A5	2683	U	C2-N1-C1'	5.61	124.43	117.70
1	A2	966	A	N9-C4-C5	-5.60	103.56	105.80
36	A1	62	A	N3-C4-N9	5.60	131.88	127.40
36	A1	317	A	C8-N9-C4	-5.60	103.56	105.80
36	A1	651	G	C2-N3-C4	5.60	114.70	111.90
80	A6	1534	G	N3-C4-C5	-5.60	125.80	128.60
36	A5	106	A	C8-N9-C4	5.60	108.04	105.80
1	A2	131	C	C5-C6-N1	5.60	123.80	121.00
1	A2	380	U	N1-C2-O2	5.60	126.72	122.80
36	A1	412	G	C8-N9-C4	-5.60	104.16	106.40
36	A1	634	C	C2-N1-C1'	-5.60	112.64	118.80
36	A5	934	G	N1-C2-N2	5.60	121.24	116.20
36	A5	1942	U	N3-C4-O4	5.60	123.32	119.40
36	A1	2430	A	N1-C2-N3	5.60	132.10	129.30
80	A6	1100	G	N3-C4-C5	-5.60	125.80	128.60
36	A5	1601	U	N1-C2-N3	-5.60	111.54	114.90
36	A5	1942	U	N1-C2-N3	5.60	118.26	114.90
36	A5	3173	G	C5-C6-N1	5.60	114.30	111.50
1	A2	1153	G	N1-C6-O6	-5.60	116.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	147	U	N3-C2-O2	-5.60	118.28	122.20
36	A1	1548	C	C6-N1-C2	-5.60	118.06	120.30
36	A1	2860	U	C5-C6-N1	5.60	125.50	122.70
36	A1	2933	A	C5-N7-C8	-5.60	101.10	103.90
36	A1	3029	A	C8-N9-C4	-5.60	103.56	105.80
80	A6	272	U	P-O3'-C3'	5.60	126.42	119.70
80	A6	624	G	N7-C8-N9	-5.60	110.30	113.10
80	A6	1343	U	N3-C4-O4	5.60	123.32	119.40
36	A5	347	G	C8-N9-C4	5.60	108.64	106.40
36	A5	635	G	N1-C2-N2	5.60	121.24	116.20
36	A5	658	G	N1-C6-O6	5.60	123.26	119.90
38	A8	37	A	N1-C6-N6	-5.60	115.24	118.60
1	A2	1749	A	N3-C4-C5	5.60	130.72	126.80
36	A1	52	A	C5-C6-N1	-5.60	114.90	117.70
36	A1	631	U	C5-C6-N1	-5.60	119.90	122.70
25	CX	132	LEU	CB-CG-CD1	-5.60	101.48	111.00
36	A5	796	U	N1-C2-O2	5.60	126.72	122.80
36	A5	950	G	N9-C4-C5	-5.60	103.16	105.40
36	A5	1343	A	C8-N9-C4	-5.60	103.56	105.80
36	A5	2828	G	N1-C6-O6	-5.60	116.54	119.90
36	A5	2889	C	N3-C4-N4	-5.60	114.08	118.00
36	A1	1796	G	N1-C6-O6	-5.60	116.54	119.90
80	A6	390	G	N3-C4-C5	-5.60	125.80	128.60
11	CJ	99	LEU	CA-CB-CG	5.60	128.17	115.30
36	A1	148	G	C6-C5-N7	-5.59	127.04	130.40
36	A1	890	C	N3-C4-N4	-5.59	114.08	118.00
36	A1	2646	C	C2-N3-C4	-5.59	117.10	119.90
80	A6	512	A	N9-C4-C5	-5.59	103.56	105.80
36	A5	369	A	N1-C6-N6	-5.59	115.24	118.60
36	A5	911	C	C4-C5-C6	5.59	120.20	117.40
36	A5	1844	C	N1-C2-N3	5.59	123.12	119.20
1	A2	1445	G	N1-C6-O6	5.59	123.26	119.90
1	A2	1796	C	C6-N1-C2	-5.59	118.06	120.30
36	A1	97	U	C2-N1-C1'	-5.59	110.99	117.70
36	A1	2623	G	C8-N9-C4	5.59	108.64	106.40
1	A2	453	U	C6-N1-C1'	-5.59	113.37	121.20
1	A2	852	C	C4-C5-C6	-5.59	114.60	117.40
1	A2	1145	U	N1-C2-O2	-5.59	118.89	122.80
36	A1	416	A	C4-C5-N7	-5.59	107.91	110.70
36	A1	2633	U	N3-C4-O4	-5.59	115.49	119.40
36	A1	3056	U	N1-C2-N3	5.59	118.25	114.90
40	BB	305	ILE	CB-CA-C	-5.59	100.42	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	432	G	N9-C4-C5	5.59	107.64	105.40
36	A5	1171	G	C8-N9-C4	-5.59	104.16	106.40
36	A5	3140	G	C6-C5-N7	-5.59	127.05	130.40
68	De	4	LEU	C-N-CA	-5.59	98.52	122.00
1	A2	334	G	N3-C4-C5	5.59	131.40	128.60
36	A1	34	A	N1-C6-N6	5.59	121.95	118.60
36	A1	658	G	C4-C5-C6	5.59	122.15	118.80
36	A1	1224	C	C6-N1-C2	-5.59	118.06	120.30
36	A1	2547	A	C4-N9-C1'	5.59	136.36	126.30
37	A3	21	G	C8-N9-C4	5.59	108.64	106.40
80	A6	359	A	C6-C5-N7	5.59	136.21	132.30
36	A5	1315	U	C6-N1-C1'	-5.59	113.38	121.20
36	A5	3252	G	C8-N9-C4	5.59	108.64	106.40
37	A7	46	A	N9-C4-C5	5.59	108.04	105.80
1	A2	1633	A	C4-C5-N7	-5.59	107.91	110.70
36	A1	903	U	N1-C2-N3	5.59	118.25	114.90
36	A5	637	C	C5-C6-N1	-5.59	118.21	121.00
36	A5	743	C	C6-N1-C2	-5.59	118.06	120.30
36	A5	1872	C	N3-C2-O2	-5.59	117.99	121.90
37	A7	79	A	N7-C8-N9	5.59	116.59	113.80
1	A2	1279	C	C6-N1-C2	-5.59	118.06	120.30
36	A1	126	U	N1-C2-N3	5.59	118.25	114.90
36	A1	726	G	N7-C8-N9	5.59	115.89	113.10
36	A1	974	G	C4-N9-C1'	5.59	133.76	126.50
36	A1	3052	G	N9-C4-C5	5.59	107.64	105.40
36	A1	3188	G	C8-N9-C1'	-5.59	119.74	127.00
80	A6	102	U	N3-C4-O4	5.59	123.31	119.40
80	A6	1260	U	N3-C2-O2	-5.59	118.29	122.20
36	A5	363	G	C4-C5-N7	-5.59	108.56	110.80
36	A5	546	C	C6-N1-C2	-5.59	118.07	120.30
36	A5	1207	G	N1-C6-O6	-5.59	116.55	119.90
36	A5	1926	C	N1-C2-O2	-5.59	115.55	118.90
36	A1	47	C	N3-C4-C5	-5.58	119.67	121.90
36	A1	154	U	N3-C4-O4	-5.58	115.49	119.40
36	A1	2305	G	N3-C4-N9	5.58	129.35	126.00
36	A5	1754	G	N1-C2-N2	-5.58	111.17	116.20
36	A5	2999	U	C5-C6-N1	-5.58	119.91	122.70
63	DZ	135	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A2	1456	C	N1-C2-N3	5.58	123.11	119.20
36	A1	332	C	C2-N3-C4	-5.58	117.11	119.90
36	A1	420	G	N3-C2-N2	5.58	123.81	119.90
36	A1	776	U	N3-C4-C5	-5.58	111.25	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1409	G	C4-C5-N7	-5.58	108.57	110.80
36	A1	2161	G	N9-C4-C5	5.58	107.63	105.40
36	A1	2950	G	C5-C6-N1	5.58	114.29	111.50
62	BY	126	LEU	CA-CB-CG	5.58	128.14	115.30
80	A6	254	A	C8-N9-C4	5.58	108.03	105.80
36	A5	340	C	N1-C2-N3	5.58	123.11	119.20
36	A5	960	U	C4-C5-C6	5.58	123.05	119.70
45	DG	69	LEU	CA-CB-CG	5.58	128.14	115.30
1	A2	74	U	C1'-O4'-C4'	-5.58	105.44	109.90
36	A1	592	A	C8-N9-C4	5.58	108.03	105.80
36	A1	960	U	C5-C4-O4	-5.58	122.55	125.90
36	A1	2173	U	N1-C2-O2	-5.58	118.89	122.80
37	A3	68	C	C6-N1-C2	5.58	122.53	120.30
80	A6	99	C	C5-C4-N4	-5.58	116.29	120.20
10	CI	58	LEU	CB-CG-CD1	-5.58	101.51	111.00
36	A5	911	C	C5-C6-N1	-5.58	118.21	121.00
36	A5	1144	U	C2-N3-C4	-5.58	123.65	127.00
36	A5	2343	C	C5-C4-N4	-5.58	116.29	120.20
1	A2	42	G	C8-N9-C4	5.58	108.63	106.40
1	A2	1536	G	C8-N9-C1'	-5.58	119.75	127.00
36	A1	345	G	C6-N1-C2	-5.58	121.75	125.10
36	A1	2343	C	C5-C6-N1	-5.58	118.21	121.00
36	A1	2552	C	N1-C2-O2	5.58	122.25	118.90
40	BB	316	GLU	N-CA-C	5.58	126.07	111.00
80	A6	687	G	N3-C4-C5	5.58	131.39	128.60
36	A5	234	G	N1-C6-O6	5.58	123.25	119.90
36	A5	405	U	C5-C4-O4	-5.58	122.55	125.90
36	A5	1403	C	C2-N3-C4	-5.58	117.11	119.90
36	A1	20	A	N1-C6-N6	-5.58	115.25	118.60
36	A1	206	G	C2-N3-C4	5.58	114.69	111.90
36	A1	1548	C	N3-C4-N4	5.58	121.91	118.00
36	A1	2200	U	C5-C6-N1	5.58	125.49	122.70
36	A1	2740	A	C8-N9-C4	-5.58	103.57	105.80
36	A1	3173	G	N7-C8-N9	5.58	115.89	113.10
36	A5	2239	G	N3-C2-N2	5.58	123.80	119.90
36	A5	3287	U	N3-C2-O2	-5.58	118.30	122.20
36	A1	350	C	N1-C2-N3	5.58	123.10	119.20
36	A1	835	G	N7-C8-N9	-5.58	110.31	113.10
36	A1	1110	U	C4-C5-C6	-5.58	116.35	119.70
36	A1	2138	A	N7-C8-N9	5.58	116.59	113.80
36	A5	1797	A	C4-C5-N7	-5.58	107.91	110.70
36	A5	2307	G	N3-C2-N2	5.58	123.80	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2729	U	C4-C5-C6	-5.58	116.35	119.70
37	A7	1	G	C6-C5-N7	-5.58	127.05	130.40
38	A8	147	U	N3-C4-C5	5.58	117.95	114.60
78	Do	41	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A2	1650	U	C5-C6-N1	-5.58	119.91	122.70
36	A1	1439	U	N1-C2-N3	5.58	118.25	114.90
36	A1	2642	A	N3-C4-C5	5.58	130.70	126.80
36	A1	3328	G	N7-C8-N9	5.58	115.89	113.10
80	A6	352	A	N3-C4-C5	5.58	130.70	126.80
80	A6	1665	U	C4-C5-C6	-5.58	116.36	119.70
36	A5	21	G	N3-C4-C5	5.58	131.39	128.60
36	A5	1183	C	N3-C4-C5	5.58	124.13	121.90
36	A5	2974	U	C5-C4-O4	5.58	129.25	125.90
1	A2	1280	C	C4-C5-C6	5.57	120.19	117.40
18	AQ	69	VAL	CB-CA-C	-5.57	100.81	111.40
36	A1	2435	G	N3-C4-C5	-5.57	125.81	128.60
80	A6	13	C	C4-C5-C6	5.57	120.19	117.40
80	A6	1763	A	C8-N9-C4	5.57	108.03	105.80
36	A5	1586	G	C6-N1-C2	-5.57	121.76	125.10
36	A5	2642	A	C8-N9-C4	5.57	108.03	105.80
36	A5	2830	G	N1-C6-O6	-5.57	116.56	119.90
38	A8	13	A	C5-N7-C8	-5.57	101.11	103.90
36	A1	425	G	N1-C2-N3	5.57	127.24	123.90
36	A5	2914	G	N1-C6-O6	-5.57	116.56	119.90
36	A1	44	U	C2-N1-C1'	-5.57	111.02	117.70
36	A1	2678	A	C5-C6-N6	5.57	128.16	123.70
70	Bg	71	THR	CB-CA-C	-5.57	96.56	111.60
80	A6	356	G	N7-C8-N9	-5.57	110.31	113.10
36	A5	436	A	C4-C5-N7	5.57	113.48	110.70
36	A5	935	U	C2-N3-C4	-5.57	123.66	127.00
36	A5	1365	G	C4-N9-C1'	5.57	133.74	126.50
36	A5	3152	U	C5-C6-N1	-5.57	119.91	122.70
36	A1	1480	G	C6-C5-N7	-5.57	127.06	130.40
36	A1	2692	A	C6-C5-N7	-5.57	128.40	132.30
36	A5	2139	A	C5-C6-N6	5.57	128.16	123.70
1	A2	542	A	C8-N9-C4	-5.57	103.57	105.80
36	A1	142	C	C5-C6-N1	5.57	123.78	121.00
36	A1	226	C	C2-N3-C4	-5.57	117.12	119.90
36	A1	2513	U	C3'-C2'-C1'	5.57	105.95	101.50
38	A4	85	G	C5-C6-O6	-5.57	125.26	128.60
80	A6	1153	G	N3-C4-C5	5.57	131.38	128.60
80	A6	1745	G	C8-N9-C4	5.57	108.63	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2287	C	C6-N1-C2	-5.57	118.07	120.30
36	A5	2605	G	C2-N3-C4	5.57	114.68	111.90
36	A5	367	A	N3-C4-C5	5.57	130.69	126.80
36	A5	2975	U	N3-C4-O4	-5.57	115.50	119.40
38	A8	12	A	C4-C5-C6	-5.57	114.22	117.00
36	A1	1899	G	C8-N9-C4	-5.56	104.17	106.40
36	A1	2134	G	C5-C6-N1	5.56	114.28	111.50
36	A1	2137	U	N3-C4-O4	5.56	123.30	119.40
36	A5	1670	C	C6-N1-C2	5.56	122.53	120.30
36	A5	1909	A	N1-C6-N6	-5.56	115.26	118.60
1	A2	1277	G	N3-C4-N9	-5.56	122.66	126.00
36	A1	431	U	N3-C2-O2	-5.56	118.31	122.20
36	A1	1930	A	C2-N3-C4	-5.56	107.82	110.60
36	A1	3013	U	C5-C6-N1	5.56	125.48	122.70
80	A6	580	A	N9-C4-C5	5.56	108.03	105.80
36	A5	957	C	C5-C6-N1	-5.56	118.22	121.00
36	A5	1170	A	C8-N9-C4	5.56	108.03	105.80
36	A5	2975	U	C4-C5-C6	-5.56	116.36	119.70
36	A5	3010	U	C5-C4-O4	5.56	129.24	125.90
80	A6	1361	U	C2-N1-C1'	5.56	124.37	117.70
36	A5	33	G	C5-C6-N1	5.56	114.28	111.50
36	A5	728	G	N7-C8-N9	-5.56	110.32	113.10
38	A8	112	U	C6-N1-C1'	5.56	128.99	121.20
1	A2	1486	G	C6-C5-N7	-5.56	127.06	130.40
36	A1	212	G	C8-N9-C4	5.56	108.62	106.40
36	A1	290	G	N1-C2-N3	-5.56	120.56	123.90
36	A1	1802	C	N3-C2-O2	5.56	125.79	121.90
36	A1	2130	G	N3-C2-N2	5.56	123.79	119.90
36	A1	2821	C	N3-C4-C5	-5.56	119.68	121.90
36	A5	648	C	C2-N1-C1'	5.56	124.92	118.80
36	A5	2327	U	C2-N1-C1'	-5.56	111.03	117.70
36	A5	3059	G	C8-N9-C4	5.56	108.62	106.40
37	A7	69	C	N3-C4-C5	5.56	124.12	121.90
36	A1	105	C	C5-C6-N1	-5.56	118.22	121.00
36	A1	787	G	C4-C5-N7	-5.56	108.58	110.80
36	A1	2131	A	C2-N3-C4	-5.56	107.82	110.60
36	A1	3171	U	C6-N1-C2	5.56	124.33	121.00
36	A1	3362	A	C8-N9-C1'	-5.56	117.70	127.70
36	A5	42	C	N1-C2-O2	5.56	122.23	118.90
36	A5	335	G	N1-C6-O6	-5.56	116.57	119.90
36	A5	1658	G	N1-C6-O6	-5.56	116.56	119.90
36	A5	1670	C	C5-C4-N4	-5.56	116.31	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1773	C	C4-C5-C6	5.56	120.18	117.40
36	A5	1901	A	C6-C5-N7	-5.56	128.41	132.30
36	A1	1841	A	C8-N9-C4	-5.56	103.58	105.80
36	A5	1444	G	C8-N9-C4	5.56	108.62	106.40
36	A5	1905	G	N1-C6-O6	-5.56	116.57	119.90
1	A2	435	C	C2-N3-C4	5.55	122.68	119.90
80	A6	110	U	N1-C2-O2	5.55	126.69	122.80
80	A6	1235	C	C6-N1-C2	-5.55	118.08	120.30
36	A5	715	A	C5-C6-N1	5.55	120.48	117.70
36	A1	2371	G	N1-C6-O6	5.55	123.23	119.90
36	A5	1360	C	C2-N3-C4	-5.55	117.12	119.90
36	A5	2158	A	C6-N1-C2	-5.55	115.27	118.60
36	A5	2293	C	C5-C4-N4	-5.55	116.31	120.20
1	A2	696	C	C6-N1-C2	-5.55	118.08	120.30
1	A2	1127	G	N9-C4-C5	5.55	107.62	105.40
1	A2	1636	C	N3-C4-N4	5.55	121.89	118.00
36	A1	65	A	P-O3'-C3'	5.55	126.36	119.70
36	A1	695	C	C5-C4-N4	5.55	124.09	120.20
36	A1	1131	G	N1-C2-N2	-5.55	111.20	116.20
36	A1	1158	A	C5-C6-N6	-5.55	119.26	123.70
80	A6	54	C	N3-C4-C5	5.55	124.12	121.90
80	A6	987	G	N1-C2-N2	5.55	121.20	116.20
36	A5	367	A	C5-C6-N6	5.55	128.14	123.70
36	A5	3055	U	C2-N1-C1'	5.55	124.36	117.70
36	A1	880	G	C4-N9-C1'	-5.55	119.29	126.50
36	A1	1365	G	N3-C4-C5	-5.55	125.83	128.60
36	A1	1480	G	C8-N9-C1'	-5.55	119.78	127.00
36	A1	2645	G	C6-N1-C2	-5.55	121.77	125.10
36	A1	2806	U	N1-C2-N3	5.55	118.23	114.90
36	A1	2814	G	N9-C4-C5	-5.55	103.18	105.40
36	A1	3362	A	N9-C4-C5	-5.55	103.58	105.80
80	A6	750	U	C6-N1-C2	5.55	124.33	121.00
36	A5	431	U	C2-N3-C4	-5.55	123.67	127.00
36	A5	914	A	N1-C2-N3	5.55	132.07	129.30
36	A5	2658	G	N3-C2-N2	-5.55	116.02	119.90
36	A5	2717	U	N3-C2-O2	-5.55	118.31	122.20
36	A5	3179	U	N3-C4-C5	5.55	117.93	114.60
36	A1	2940	A	C5-N7-C8	5.55	106.67	103.90
80	A6	2	A	C8-N9-C4	5.55	108.02	105.80
36	A5	3336	A	C4-C5-C6	5.55	119.77	117.00
1	A2	1560	U	N1-C2-O2	5.55	126.68	122.80
36	A1	579	G	N1-C6-O6	-5.55	116.57	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	98	G	C8-N9-C4	5.55	108.62	106.40
36	A5	1086	C	C5-C6-N1	5.55	123.77	121.00
36	A5	1847	A	C2-N3-C4	-5.55	107.83	110.60
36	A5	3395	G	N1-C6-O6	5.55	123.23	119.90
36	A1	2273	G	C4-N9-C1'	-5.54	119.29	126.50
36	A5	1305	U	C6-N1-C2	5.54	124.33	121.00
36	A5	3103	A	C5-C6-N1	5.54	120.47	117.70
1	A2	258	C	N3-C4-C5	5.54	124.12	121.90
1	A2	342	C	C6-N1-C2	5.54	122.52	120.30
36	A1	51	A	N1-C6-N6	5.54	121.93	118.60
36	A1	1869	C	N1-C2-O2	5.54	122.23	118.90
80	A6	385	A	C5-C6-N6	5.54	128.13	123.70
37	A7	1	G	N3-C4-N9	5.54	129.33	126.00
64	Da	17	ALA	C-N-CA	-5.54	110.66	122.30
1	A2	115	G	N1-C6-O6	5.54	123.22	119.90
1	A2	144	U	C5-C4-O4	5.54	129.22	125.90
1	A2	613	G	N1-C6-O6	-5.54	116.58	119.90
36	A1	639	G	C2-N3-C4	-5.54	109.13	111.90
36	A1	949	C	C2-N3-C4	-5.54	117.13	119.90
36	A1	2773	C	C5-C4-N4	-5.54	116.32	120.20
80	A6	647	G	C8-N9-C4	-5.54	104.18	106.40
36	A5	347	G	N7-C8-N9	-5.54	110.33	113.10
36	A5	395	A	N7-C8-N9	5.54	116.57	113.80
36	A5	1125	U	N3-C4-O4	-5.54	115.52	119.40
36	A5	1189	C	N3-C2-O2	5.54	125.78	121.90
36	A5	1215	U	N3-C2-O2	5.54	126.08	122.20
36	A5	1441	G	C5-C6-N1	5.54	114.27	111.50
36	A5	2706	G	N3-C4-C5	-5.54	125.83	128.60
36	A5	3326	G	C5-C6-O6	5.54	131.93	128.60
36	A1	2340	U	C4-C5-C6	-5.54	116.38	119.70
36	A1	3375	A	C4-C5-C6	5.54	119.77	117.00
36	A5	1843	C	C5-C6-N1	5.54	123.77	121.00
36	A5	3052	G	C4-N9-C1'	-5.54	119.30	126.50
52	DO	23[B]	ILE	CA-C-N	-5.54	105.01	117.20
1	A2	323	A	N9-C4-C5	5.54	108.02	105.80
36	A1	970	A	N9-C4-C5	5.54	108.02	105.80
36	A5	390	G	N9-C4-C5	-5.54	103.19	105.40
36	A5	1797	A	C8-N9-C4	5.54	108.02	105.80
36	A5	1906	G	C2-N3-C4	-5.54	109.13	111.90
36	A1	362	U	N3-C4-O4	-5.54	115.52	119.40
36	A5	1380	G	C8-N9-C4	5.54	108.61	106.40
36	A5	1724	U	N3-C2-O2	-5.54	118.32	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1741	A	N7-C8-N9	5.54	116.57	113.80
36	A1	1910	A	N9-C4-C5	-5.54	103.58	105.80
36	A1	3193	C	N1-C2-O2	-5.54	115.58	118.90
43	BE	64	LEU	CA-CB-CG	5.54	128.03	115.30
80	A6	306	U	C5-C4-O4	-5.54	122.58	125.90
36	A5	46	U	C2-N3-C4	5.54	130.32	127.00
36	A5	1165	A	N7-C8-N9	-5.54	111.03	113.80
36	A5	1305	U	C6-N1-C1'	-5.54	113.45	121.20
36	A5	2289	U	C5-C4-O4	5.54	129.22	125.90
36	A5	2309	A	C8-N9-C4	5.54	108.01	105.80
36	A5	2335	G	C6-N1-C2	-5.54	121.78	125.10
36	A1	847	A	C4-C5-N7	5.53	113.47	110.70
36	A1	1048	A	C2-N3-C4	5.53	113.37	110.60
36	A5	1887	A	N9-C4-C5	-5.53	103.59	105.80
36	A5	2870	C	C2-N1-C1'	-5.53	112.71	118.80
36	A1	2350	C	C5-C6-N1	-5.53	118.23	121.00
1	A2	36	C	C5-C4-N4	-5.53	116.33	120.20
1	A2	1129	U	C2-N3-C4	-5.53	123.68	127.00
1	A2	1503	A	N7-C8-N9	5.53	116.56	113.80
36	A1	45	A	N7-C8-N9	-5.53	111.03	113.80
36	A1	56	G	C4-C5-N7	5.53	113.01	110.80
36	A1	810	A	N9-C4-C5	5.53	108.01	105.80
36	A1	926	A	C4-C5-C6	-5.53	114.23	117.00
36	A1	3203	U	N3-C2-O2	-5.53	118.33	122.20
36	A5	266	A	N1-C2-N3	5.53	132.06	129.30
36	A5	285	A	C8-N9-C4	-5.53	103.59	105.80
36	A5	517	G	C4-C5-C6	5.53	122.12	118.80
36	A5	953	G	N3-C4-C5	5.53	131.37	128.60
36	A5	954	U	C6-N1-C2	-5.53	117.68	121.00
36	A5	2966	G	C5-C6-N1	5.53	114.27	111.50
36	A5	2996	U	C6-N1-C1'	-5.53	113.46	121.20
80	A6	1400	A	C2-N3-C4	5.53	113.36	110.60
36	A5	969	C	C5-C6-N1	-5.53	118.24	121.00
36	A1	190	U	N3-C4-O4	-5.53	115.53	119.40
36	A1	642	U	N3-C4-C5	-5.53	111.28	114.60
36	A1	1415	U	N3-C4-O4	-5.53	115.53	119.40
80	A6	1678	A	C8-N9-C4	-5.53	103.59	105.80
36	A5	39	A	N7-C8-N9	-5.53	111.04	113.80
36	A5	814	U	N1-C2-N3	-5.53	111.58	114.90
36	A5	3394	U	N3-C4-O4	-5.53	115.53	119.40
38	A8	87	G	C5-C6-O6	-5.53	125.28	128.60
36	A1	1421	G	C8-N9-C4	5.53	108.61	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	359	U	N3-C4-C5	5.53	117.92	114.60
36	A5	844	G	N7-C8-N9	-5.53	110.34	113.10
36	A5	1178	G	N7-C8-N9	5.53	115.86	113.10
36	A5	1295	G	C5-C6-O6	5.53	131.92	128.60
36	A5	2182	A	C4-C5-C6	-5.53	114.24	117.00
36	A5	3064	U	N1-C2-N3	5.53	118.22	114.90
1	A2	1614	A	C6-C5-N7	-5.52	128.43	132.30
36	A1	795	G	N7-C8-N9	-5.52	110.34	113.10
36	A1	1211	U	N3-C4-C5	5.52	117.91	114.60
80	A6	1170	G	C8-N9-C1'	-5.52	119.82	127.00
1	A2	145	A	N9-C4-C5	5.52	108.01	105.80
1	A2	386	G	C4-C5-N7	-5.52	108.59	110.80
36	A1	620	U	N1-C2-N3	5.52	118.21	114.90
36	A1	1335	C	C5-C6-N1	-5.52	118.24	121.00
72	Bi	27	SER	N-CA-C	-5.52	96.09	111.00
80	A6	96	G	C5-C6-O6	5.52	131.91	128.60
80	A6	418	G	C4-C5-C6	5.52	122.11	118.80
80	A6	1292	G	N1-C6-O6	5.52	123.21	119.90
80	A6	1340	U	C5-C4-O4	5.52	129.21	125.90
36	A5	1938	U	C5-C6-N1	-5.52	119.94	122.70
36	A5	2172	A	N1-C6-N6	5.52	121.91	118.60
36	A5	2346	C	N3-C4-C5	5.52	124.11	121.90
36	A5	2549	G	N7-C8-N9	5.52	115.86	113.10
36	A5	2699	G	N3-C4-N9	5.52	129.31	126.00
38	A8	104	A	N1-C2-N3	-5.52	126.54	129.30
36	A1	34	A	C5-N7-C8	-5.52	101.14	103.90
36	A1	1543	G	C5-C6-O6	-5.52	125.29	128.60
36	A1	2376	G	C4-N9-C1'	5.52	133.68	126.50
1	A2	639	U	N3-C4-C5	5.52	117.91	114.60
36	A1	346	C	C5-C6-N1	-5.52	118.24	121.00
36	A1	386	A	C8-N9-C1'	-5.52	117.77	127.70
36	A1	658	G	N1-C6-O6	5.52	123.21	119.90
36	A1	1917	C	C6-N1-C2	5.52	122.51	120.30
80	A6	767	U	N3-C2-O2	-5.52	118.34	122.20
36	A5	419	G	C4-C5-N7	5.52	113.01	110.80
36	A5	1441	G	C5-N7-C8	5.52	107.06	104.30
36	A5	1869	C	C6-N1-C2	5.52	122.51	120.30
36	A5	2607	G	C8-N9-C4	-5.52	104.19	106.40
64	Da	4	ARG	NE-CZ-NH1	-5.52	117.54	120.30
36	A1	408	A	C5-C6-N6	5.52	128.11	123.70
36	A1	1507	G	N3-C4-C5	-5.52	125.84	128.60
36	A1	3138	U	C5-C6-N1	-5.52	119.94	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	633	U	N1-C2-N3	-5.52	111.59	114.90
80	A6	1401	A	N1-C6-N6	-5.52	115.29	118.60
80	A6	1773	C	N3-C2-O2	5.52	125.76	121.90
36	A5	590	G	C8-N9-C4	-5.52	104.19	106.40
36	A5	2843	U	N3-C2-O2	-5.52	118.34	122.20
36	A5	3042	U	N1-C2-N3	5.52	118.21	114.90
80	A6	756	A	C5-N7-C8	-5.52	101.14	103.90
36	A5	1007	U	C6-N1-C2	5.52	124.31	121.00
36	A5	1869	C	N3-C4-C5	5.52	124.11	121.90
1	A2	599	A	C5-N7-C8	5.51	106.66	103.90
59	BV	80	ARG	NE-CZ-NH1	5.51	123.06	120.30
80	A6	409	C	C5-C4-N4	-5.51	116.34	120.20
36	A5	1183	C	C5-C6-N1	-5.51	118.24	121.00
80	A6	387	A	C4-C5-N7	-5.51	107.94	110.70
36	A5	1176	C	C4-C5-C6	5.51	120.16	117.40
36	A5	2654	C	C2-N3-C4	-5.51	117.14	119.90
36	A1	220	G	N3-C4-N9	5.51	129.31	126.00
36	A1	1537	A	C2-N3-C4	-5.51	107.84	110.60
36	A1	2184	U	C5-C4-O4	-5.51	122.59	125.90
36	A1	3114	A	C8-N9-C4	5.51	108.00	105.80
36	A1	3355	U	C2-N1-C1'	5.51	124.31	117.70
80	A6	146	U	N3-C2-O2	-5.51	118.34	122.20
80	A6	1269	U	C5-C4-O4	5.51	129.21	125.90
36	A5	631	U	N1-C2-O2	5.51	126.66	122.80
36	A5	1878	G	C4-N9-C1'	5.51	133.66	126.50
36	A5	2396	G	N1-C6-O6	-5.51	116.59	119.90
36	A1	437	G	C4-N9-C1'	-5.51	119.34	126.50
36	A1	910	G	C8-N9-C4	-5.51	104.20	106.40
36	A1	2618	G	C2-N3-C4	5.51	114.66	111.90
36	A1	2794	G	N9-C4-C5	5.51	107.60	105.40
38	A4	14	C	N3-C4-C5	5.51	124.10	121.90
36	A5	745	C	N1-C2-O2	-5.51	115.59	118.90
36	A5	1178	G	C6-N1-C2	-5.51	121.79	125.10
36	A5	1338	C	C4-C5-C6	5.51	120.16	117.40
48	BJ	112	LEU	CA-CB-CG	5.51	127.97	115.30
36	A5	1841	A	C8-N9-C4	-5.51	103.60	105.80
36	A5	2177	G	C8-N9-C4	-5.51	104.20	106.40
36	A5	2777	G	C8-N9-C4	-5.51	104.20	106.40
36	A5	3318	G	C4-C5-N7	-5.51	108.60	110.80
37	A7	8	G	N3-C2-N2	5.51	123.76	119.90
36	A1	347	G	N1-C6-O6	5.51	123.20	119.90
36	A1	1497	C	C6-N1-C2	-5.51	118.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2891	U	N3-C4-C5	5.51	117.90	114.60
36	A1	3201	C	N3-C2-O2	-5.51	118.05	121.90
80	A6	418	G	N1-C6-O6	5.51	123.20	119.90
80	A6	1177	C	C2-N1-C1'	-5.51	112.74	118.80
36	A5	666	A	N1-C2-N3	5.51	132.05	129.30
36	A5	1140	G	C5-C6-N1	5.51	114.25	111.50
36	A5	2134	G	N3-C4-N9	5.51	129.30	126.00
36	A5	2665	U	C4-C5-C6	-5.51	116.40	119.70
36	A5	3043	C	N3-C4-N4	-5.51	114.15	118.00
1	A2	838	G	N7-C8-N9	-5.50	110.35	113.10
36	A1	2819	A	N3-C4-C5	-5.50	122.95	126.80
54	BQ	66	ARG	NE-CZ-NH1	-5.50	117.55	120.30
80	A6	681	U	N3-C2-O2	-5.50	118.35	122.20
36	A5	96	G	C4-C5-N7	-5.50	108.60	110.80
36	A5	1115	G	C6-N1-C2	-5.50	121.80	125.10
36	A5	2181	C	C6-N1-C2	-5.50	118.10	120.30
1	A2	1024	U	N1-C2-O2	5.50	126.65	122.80
1	A2	1207	C	C6-N1-C2	5.50	122.50	120.30
36	A1	1144	U	N3-C2-O2	-5.50	118.35	122.20
36	A1	1475	A	C5-C6-N1	5.50	120.45	117.70
36	A1	2252	A	N7-C8-N9	5.50	116.55	113.80
36	A1	2257	C	C5-C4-N4	5.50	124.05	120.20
36	A1	2358	A	N7-C8-N9	-5.50	111.05	113.80
36	A1	2795	U	C5-C6-N1	-5.50	119.95	122.70
80	A6	1650	U	C5-C6-N1	-5.50	119.95	122.70
36	A5	3350	C	C6-N1-C2	-5.50	118.10	120.30
36	A1	437	G	N3-C4-C5	5.50	131.35	128.60
36	A1	1411	C	N3-C4-C5	5.50	124.10	121.90
36	A1	2286	U	C5-C6-N1	-5.50	119.95	122.70
39	BA	247	ARG	NE-CZ-NH1	5.50	123.05	120.30
80	A6	425	A	N1-C6-N6	-5.50	115.30	118.60
80	A6	1078	C	N3-C4-N4	-5.50	114.15	118.00
36	A5	1792	C	C4-C5-C6	5.50	120.15	117.40
36	A5	2344	U	C2-N3-C4	-5.50	123.70	127.00
36	A5	2369	G	C8-N9-C4	5.50	108.60	106.40
37	A7	101	G	N9-C4-C5	-5.50	103.20	105.40
36	A1	49	A	C6-N1-C2	5.50	121.90	118.60
36	A1	637	C	N3-C4-N4	-5.50	114.15	118.00
36	A1	2323	G	N3-C2-N2	5.50	123.75	119.90
36	A5	54	C	N3-C4-N4	-5.50	114.15	118.00
1	A2	393	C	C2-N3-C4	-5.50	117.15	119.90
36	A1	898	U	C5-C6-N1	-5.50	119.95	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1049	C	C5-C6-N1	5.50	123.75	121.00
36	A5	1931	U	C5-C4-O4	5.50	129.20	125.90
1	A2	995	A	C8-N9-C4	5.50	108.00	105.80
36	A1	224	C	C6-N1-C2	-5.50	118.10	120.30
36	A1	672	A	C6-C5-N7	-5.50	128.45	132.30
36	A1	1824	U	N3-C2-O2	-5.50	118.35	122.20
36	A1	1923	C	C5-C6-N1	-5.50	118.25	121.00
80	A6	622	A	N3-C4-C5	-5.50	122.95	126.80
80	A6	1573	A	C2-N3-C4	5.50	113.35	110.60
36	A5	1508	C	N1-C2-O2	5.50	122.20	118.90
36	A1	1041	U	C6-N1-C2	5.50	124.30	121.00
36	A1	1578	C	C5-C6-N1	5.50	123.75	121.00
36	A1	1646	G	N1-C6-O6	5.50	123.20	119.90
36	A1	2290	C	N3-C2-O2	-5.50	118.05	121.90
36	A1	2819	A	C4-C5-C6	5.50	119.75	117.00
36	A1	3101	G	C6-C5-N7	5.50	133.70	130.40
36	A5	1495	U	C6-N1-C2	-5.50	117.70	121.00
36	A5	1937	U	C5-C6-N1	-5.50	119.95	122.70
1	A2	938	G	N1-C2-N2	-5.49	111.26	116.20
1	A2	1270	G	C2-N3-C4	5.49	114.65	111.90
36	A1	965	A	N9-C4-C5	5.49	108.00	105.80
36	A1	2422	C	N3-C2-O2	-5.49	118.06	121.90
41	BC	76	ARG	CG-CD-NE	-5.49	100.26	111.80
80	A6	1455	G	C4-C5-N7	-5.49	108.60	110.80
36	A5	1365	G	N1-C2-N2	-5.49	111.26	116.20
36	A5	2112	U	C6-N1-C2	-5.49	117.70	121.00
36	A5	3028	G	N3-C2-N2	5.49	123.75	119.90
1	A2	829	A	C2-N3-C4	5.49	113.35	110.60
1	A2	1462	G	C5-C6-O6	-5.49	125.31	128.60
36	A1	106	A	N1-C2-N3	5.49	132.05	129.30
36	A1	929	A	C4-C5-C6	5.49	119.75	117.00
38	A8	19	C	N3-C4-C5	-5.49	119.70	121.90
38	A8	156	U	C5-C6-N1	5.49	125.45	122.70
1	A2	42	G	N7-C8-N9	-5.49	110.36	113.10
1	A2	566	C	N3-C2-O2	-5.49	118.06	121.90
36	A1	606	C	N3-C4-C5	-5.49	119.70	121.90
36	A1	694	C	C2-N3-C4	-5.49	117.15	119.90
47	BI	24	ARG	NE-CZ-NH2	-5.49	117.56	120.30
54	BQ	38	ARG	NE-CZ-NH2	-5.49	117.56	120.30
80	A6	448	C	N1-C2-N3	5.49	123.04	119.20
36	A5	620	U	C2-N1-C1'	5.49	124.29	117.70
37	A7	8	G	N1-C2-N2	-5.49	111.26	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	Da	9	ARG	NE-CZ-NH1	-5.49	117.56	120.30
36	A1	1345	G	C4-N9-C1'	5.49	133.63	126.50
80	A6	351	C	C6-N1-C1'	-5.49	114.22	120.80
36	A5	3387	U	N1-C2-O2	5.49	126.64	122.80
1	A2	380	U	N3-C2-O2	-5.49	118.36	122.20
36	A1	740	G	N1-C6-O6	-5.49	116.61	119.90
36	A1	1326	A	N7-C8-N9	-5.49	111.06	113.80
36	A1	2126	A	C2-N3-C4	5.49	113.34	110.60
80	A6	557	G	N3-C4-C5	-5.49	125.86	128.60
36	A5	828	A	N1-C6-N6	-5.49	115.31	118.60
36	A5	2109	U	N3-C4-O4	-5.49	115.56	119.40
1	A2	972	G	C4-C5-N7	-5.49	108.61	110.80
36	A1	332	C	C5-C6-N1	-5.49	118.26	121.00
36	A1	514	G	N1-C2-N3	5.49	127.19	123.90
36	A1	947	G	N1-C6-O6	-5.49	116.61	119.90
36	A1	1681	U	N1-C2-O2	5.49	126.64	122.80
36	A1	2957	G	C8-N9-C4	5.49	108.59	106.40
80	A6	72	A	N1-C6-N6	-5.49	115.31	118.60
80	A6	542	A	C5-N7-C8	-5.49	101.16	103.90
36	A5	3341	U	N3-C2-O2	-5.49	118.36	122.20
36	A5	3350	C	C5-C6-N1	5.49	123.74	121.00
1	A2	992	A	C4-C5-N7	5.48	113.44	110.70
36	A1	1802	C	N3-C4-N4	5.48	121.84	118.00
68	Be	105	ARG	NE-CZ-NH1	5.48	123.04	120.30
80	A6	1354	G	N7-C8-N9	5.48	115.84	113.10
1	A2	1455	G	C4-C5-C6	5.48	122.09	118.80
36	A1	1133	A	C5-C6-N1	5.48	120.44	117.70
36	A1	3149	G	N3-C4-N9	-5.48	122.71	126.00
80	A6	782	U	N3-C2-O2	-5.48	118.36	122.20
36	A5	411	U	C2-N3-C4	-5.48	123.71	127.00
36	A5	997	A	N7-C8-N9	5.48	116.54	113.80
36	A5	2321	A	C5-C6-N1	5.48	120.44	117.70
36	A5	2728	G	N1-C2-N2	5.48	121.13	116.20
1	A2	377	G	C4-N9-C1'	-5.48	119.38	126.50
36	A1	45	A	C5-N7-C8	5.48	106.64	103.90
36	A1	2730	G	C5-C6-N1	-5.48	108.76	111.50
36	A1	3244	A	C8-N9-C4	5.48	107.99	105.80
80	A6	751	G	N3-C4-C5	-5.48	125.86	128.60
36	A5	25	U	N1-C2-N3	5.48	118.19	114.90
36	A5	229	G	N1-C6-O6	5.48	123.19	119.90
37	A7	90	U	C6-N1-C2	5.48	124.29	121.00
36	A1	334	A	N1-C6-N6	5.48	121.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2756	C	C6-N1-C2	-5.48	118.11	120.30
36	A5	3336	A	C5-C6-N1	-5.48	114.96	117.70
37	A7	37	G	N9-C4-C5	-5.48	103.21	105.40
36	A1	2135	U	N1-C2-O2	5.48	126.64	122.80
36	A1	2272	G	N1-C6-O6	5.48	123.19	119.90
80	A6	1308	G	N1-C6-O6	5.48	123.19	119.90
37	A7	105	C	N3-C4-C5	-5.48	119.71	121.90
1	A2	42	G	N1-C6-O6	-5.48	116.61	119.90
36	A1	1330	A	C4-C5-N7	5.47	113.44	110.70
36	A1	1877	U	C5-C6-N1	-5.47	119.96	122.70
36	A1	2361	A	N3-C4-C5	-5.47	122.97	126.80
36	A1	2770	G	C8-N9-C4	-5.47	104.21	106.40
36	A1	3109	G	C5-C6-O6	-5.47	125.32	128.60
36	A5	961	C	C4-C5-C6	5.47	120.14	117.40
38	A8	43	A	C8-N9-C4	-5.47	103.61	105.80
36	A1	1331	U	C6-N1-C1'	-5.47	113.54	121.20
36	A1	2329	C	C2-N1-C1'	-5.47	112.78	118.80
38	A4	60	U	C2-N3-C4	-5.47	123.72	127.00
36	A5	282	G	N7-C8-N9	5.47	115.84	113.10
36	A5	1187	C	N3-C4-N4	-5.47	114.17	118.00
36	A5	2430	A	N1-C2-N3	5.47	132.04	129.30
36	A5	3015	G	N1-C6-O6	-5.47	116.62	119.90
36	A1	634	C	N1-C2-O2	5.47	122.18	118.90
36	A1	3192	U	N3-C4-C5	5.47	117.88	114.60
36	A5	810	A	C5-C6-N6	5.47	128.08	123.70
1	A2	703	G	N7-C8-N9	5.47	115.83	113.10
36	A1	2309	A	C8-N9-C4	5.47	107.99	105.80
36	A1	2550	U	C4-C5-C6	5.47	122.98	119.70
36	A1	2990	G	C5-N7-C8	5.47	107.03	104.30
36	A1	3000	A	C2-N3-C4	-5.47	107.86	110.60
6	CE	77	ARG	NE-CZ-NH1	5.47	123.03	120.30
36	A5	996	A	C5-C6-N1	5.47	120.43	117.70
36	A5	1191	U	C5-C6-N1	-5.47	119.97	122.70
69	Df	91	ALA	N-CA-CB	5.47	117.76	110.10
36	A5	2119	A	C6-N1-C2	-5.47	115.32	118.60
36	A5	2800	G	C4-C5-N7	-5.47	108.61	110.80
1	A2	1386	G	C4-C5-N7	-5.47	108.61	110.80
1	A2	1491	U	N3-C2-O2	-5.47	118.37	122.20
36	A1	1459	C	C5-C6-N1	-5.47	118.27	121.00
80	A6	639	U	N3-C4-O4	-5.47	115.57	119.40
80	A6	790	U	N3-C2-O2	-5.47	118.37	122.20
36	A5	422	A	C8-N9-C4	5.47	107.99	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A7	82	G	N9-C4-C5	5.47	107.59	105.40
1	A2	1097	U	C6-N1-C1'	-5.46	113.55	121.20
1	A2	1754	A	N3-C4-C5	5.46	130.63	126.80
36	A1	200	C	C2-N1-C1'	5.46	124.81	118.80
36	A1	1307	G	C8-N9-C4	-5.46	104.21	106.40
36	A1	1926	C	C2-N3-C4	-5.46	117.17	119.90
36	A1	2384	A	N9-C4-C5	-5.46	103.61	105.80
36	A1	3029	A	C6-C5-N7	-5.46	128.47	132.30
80	A6	1078	C	C5-C4-N4	5.46	124.03	120.20
36	A5	809	G	C5-N7-C8	5.46	107.03	104.30
36	A5	811	U	N1-C2-N3	5.46	118.18	114.90
36	A1	2782	U	C5-C4-O4	5.46	129.18	125.90
36	A5	98	G	N9-C4-C5	-5.46	103.22	105.40
36	A5	3215	A	C5-C6-N1	-5.46	114.97	117.70
36	A1	1119	C	N3-C2-O2	-5.46	118.08	121.90
36	A1	2786	G	N9-C4-C5	5.46	107.58	105.40
36	A5	1190	A	C5-N7-C8	5.46	106.63	103.90
36	A5	1380	G	C2-N3-C4	-5.46	109.17	111.90
36	A5	2608	G	N1-C6-O6	-5.46	116.62	119.90
36	A5	2808	A	C6-C5-N7	-5.46	128.48	132.30
36	A5	2948	C	N3-C4-C5	5.46	124.08	121.90
36	A1	1868	G	C6-C5-N7	-5.46	127.12	130.40
36	A1	2408	U	C2-N1-C1'	5.46	124.25	117.70
36	A1	2662	G	C2-N3-C4	-5.46	109.17	111.90
36	A1	2902	A	N1-C6-N6	5.46	121.88	118.60
80	A6	991	G	C5-C6-N1	5.46	114.23	111.50
80	A6	1097	U	P-O3'-C3'	5.46	126.25	119.70
49	DL	47	ALA	C-N-CD	5.46	139.87	128.40
1	A2	1185	U	C6-N1-C1'	-5.46	113.56	121.20
36	A1	1081	U	C2-N1-C1'	5.46	124.25	117.70
80	A6	1019	A	C8-N9-C4	5.46	107.98	105.80
80	A6	1111	G	C6-C5-N7	-5.46	127.12	130.40
36	A5	1239	C	C6-N1-C2	-5.46	118.12	120.30
1	A2	1027	A	C5-N7-C8	-5.46	101.17	103.90
36	A1	280	U	C5-C6-N1	5.46	125.43	122.70
36	A1	1528	G	N9-C4-C5	5.46	107.58	105.40
36	A1	1949	G	N1-C6-O6	5.46	123.17	119.90
36	A1	2368	A	C8-N9-C4	-5.46	103.62	105.80
36	A1	2855	U	C5-C6-N1	-5.46	119.97	122.70
80	A6	1284	C	N3-C2-O2	-5.46	118.08	121.90
80	A6	1654	G	C6-N1-C2	-5.46	121.83	125.10
80	A6	1678	A	N7-C8-N9	5.46	116.53	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	414	U	N3-C4-O4	5.46	123.22	119.40
36	A5	2904	U	N1-C2-N3	5.46	118.17	114.90
37	A7	105	C	C2-N3-C4	5.46	122.63	119.90
52	DO	197[B]	PHE	CA-C-N	-5.46	105.29	116.20
36	A5	41	G	C6-C5-N7	-5.46	127.13	130.40
36	A5	2379	U	N1-C2-N3	5.46	118.17	114.90
36	A1	1906	G	N1-C6-O6	5.45	123.17	119.90
36	A1	3110	C	N3-C2-O2	-5.45	118.08	121.90
80	A6	300	A	C8-N9-C4	5.45	107.98	105.80
80	A6	426	G	N3-C4-N9	5.45	129.27	126.00
80	A6	1642	G	C5-C6-N1	5.45	114.23	111.50
36	A5	879	U	C6-N1-C1'	-5.45	113.57	121.20
36	A5	1045	C	C2-N3-C4	-5.45	117.17	119.90
36	A5	1242	G	N3-C4-C5	-5.45	125.87	128.60
36	A5	2632	G	N1-C2-N3	-5.45	120.63	123.90
38	A8	17	A	C5-N7-C8	-5.45	101.17	103.90
38	A8	103	G	C5-C6-N1	5.45	114.23	111.50
36	A1	708	G	C4-C5-N7	5.45	112.98	110.80
36	A1	1591	G	C5-C6-O6	5.45	131.87	128.60
36	A1	3007	U	C4-C5-C6	5.45	122.97	119.70
36	A5	266	A	C4-C5-C6	5.45	119.73	117.00
36	A5	2524	A	N3-C4-C5	5.45	130.62	126.80
36	A5	3035	A	C8-N9-C4	5.45	107.98	105.80
36	A5	3302	U	N3-C4-C5	5.45	117.87	114.60
36	A1	797	U	C5-C6-N1	-5.45	119.97	122.70
36	A1	1100	U	N1-C2-O2	-5.45	118.98	122.80
36	A1	3172	A	N1-C6-N6	5.45	121.87	118.60
38	A4	125	U	N3-C2-O2	-5.45	118.38	122.20
80	A6	1332	C	N1-C2-O2	5.45	122.17	118.90
37	A7	61	G	C8-N9-C4	5.45	108.58	106.40
37	A7	100	C	N3-C4-C5	5.45	124.08	121.90
36	A1	748	U	N3-C4-C5	5.45	117.87	114.60
36	A1	785	G	N3-C4-N9	5.45	129.27	126.00
36	A1	1791	C	N3-C4-C5	5.45	124.08	121.90
36	A1	3127	A	C8-N9-C4	-5.45	103.62	105.80
38	A4	23	U	N1-C2-O2	-5.45	118.99	122.80
80	A6	30	G	N9-C4-C5	5.45	107.58	105.40
36	A5	341	G	C5-N7-C8	-5.45	101.58	104.30
36	A5	1176	C	C6-N1-C2	5.45	122.48	120.30
36	A1	2850	G	C8-N9-C1'	-5.45	119.92	127.00
36	A5	844	G	C8-N9-C4	5.45	108.58	106.40
36	A5	1127	G	N3-C4-N9	5.45	129.27	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2958	A	N1-C6-N6	-5.45	115.33	118.60
36	A5	3263	G	N1-C6-O6	-5.45	116.63	119.90
37	A7	19	C	N3-C4-C5	5.45	124.08	121.90
1	A2	1662	G	C8-N9-C4	-5.45	104.22	106.40
36	A1	283	G	C8-N9-C1'	-5.45	119.92	127.00
36	A1	2400	G	N3-C2-N2	-5.45	116.09	119.90
36	A5	1306	G	C5-C6-N1	5.45	114.22	111.50
36	A5	2754	G	N3-C4-N9	5.45	129.27	126.00
36	A1	416	A	N9-C4-C5	5.44	107.98	105.80
36	A1	2805	G	N3-C4-C5	-5.44	125.88	128.60
80	A6	403	G	N9-C4-C5	-5.44	103.22	105.40
36	A5	63	A	N9-C4-C5	-5.44	103.62	105.80
36	A5	648	C	C4-C5-C6	5.44	120.12	117.40
36	A5	2522	G	N9-C4-C5	-5.44	103.22	105.40
41	DC	73	ARG	CB-CG-CD	-5.44	97.44	111.60
1	A2	264	G	N3-C4-N9	-5.44	122.73	126.00
36	A1	821	U	N1-C2-O2	5.44	126.61	122.80
36	A1	859	G	C5-C6-N1	-5.44	108.78	111.50
36	A1	2414	G	N3-C2-N2	-5.44	116.09	119.90
36	A1	2727	A	N3-C4-C5	-5.44	122.99	126.80
36	A1	3192	U	C2-N3-C4	-5.44	123.73	127.00
80	A6	1306	C	C6-N1-C2	-5.44	118.12	120.30
36	A5	277	G	C5-C6-O6	5.44	131.87	128.60
36	A5	498	A	N1-C6-N6	-5.44	115.33	118.60
36	A5	516	A	C5-C6-N6	-5.44	119.35	123.70
36	A5	1335	C	C6-N1-C2	-5.44	118.12	120.30
36	A5	2123	G	N3-C4-C5	-5.44	125.88	128.60
1	A2	1330	G	C4-N9-C1'	-5.44	119.43	126.50
36	A1	104	G	N9-C4-C5	-5.44	103.22	105.40
36	A1	649	A	N7-C8-N9	-5.44	111.08	113.80
36	A1	2178	A	C5-C6-N1	-5.44	114.98	117.70
36	A5	339	C	C6-N1-C2	-5.44	118.12	120.30
36	A5	2433	U	C5-C6-N1	-5.44	119.98	122.70
36	A5	3052	G	C6-C5-N7	5.44	133.66	130.40
36	A5	3083	G	N1-C2-N3	5.44	127.16	123.90
1	A2	529	A	C8-N9-C4	5.44	107.98	105.80
36	A1	121	A	N7-C8-N9	-5.44	111.08	113.80
36	A1	1514	G	C5-C6-N1	5.44	114.22	111.50
1	A2	42	G	C5-C6-N1	5.44	114.22	111.50
1	A2	1458	G	C8-N9-C1'	-5.44	119.93	127.00
36	A1	794	U	C6-N1-C2	-5.44	117.74	121.00
36	A1	2996	U	C2-N1-C1'	5.44	124.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	647	G	C5-N7-C8	-5.44	101.58	104.30
80	A6	1537	C	N3-C2-O2	5.44	125.71	121.90
36	A5	519	A	C6-C5-N7	-5.44	128.49	132.30
36	A5	3112	G	C8-N9-C4	5.44	108.58	106.40
36	A5	3143	C	N3-C2-O2	5.44	125.71	121.90
36	A1	1269	U	N3-C2-O2	-5.44	118.39	122.20
36	A1	1503	A	N3-C4-N9	-5.44	123.05	127.40
36	A1	1858	A	C8-N9-C1'	-5.44	117.92	127.70
36	A1	3326	G	C8-N9-C4	5.44	108.58	106.40
36	A5	2197	C	C6-N1-C1'	5.44	127.32	120.80
36	A5	2757	U	C5-C4-O4	-5.44	122.64	125.90
36	A1	25	U	N3-C4-O4	5.43	123.20	119.40
36	A1	504	A	C2-N3-C4	-5.43	107.88	110.60
36	A1	864	G	N3-C2-N2	5.43	123.70	119.90
36	A1	1313	G	C4-C5-N7	5.43	112.97	110.80
36	A1	1882	G	N3-C4-N9	-5.43	122.74	126.00
36	A1	2553	U	C5-C6-N1	-5.43	119.98	122.70
36	A1	3055	U	C5-C4-O4	-5.43	122.64	125.90
36	A1	3245	A	C5-N7-C8	-5.43	101.18	103.90
70	Bg	8	ARG	NE-CZ-NH2	-5.43	117.58	120.30
80	A6	720	G	C2-N3-C4	5.43	114.62	111.90
36	A5	1041	U	C5-C6-N1	-5.43	119.98	122.70
36	A5	2323	G	C8-N9-C4	-5.43	104.23	106.40
36	A5	2386	A	C5-N7-C8	-5.43	101.18	103.90
36	A5	3049	A	C8-N9-C4	5.43	107.97	105.80
36	A1	76	G	N3-C4-C5	-5.43	125.88	128.60
36	A1	1658	G	N1-C6-O6	-5.43	116.64	119.90
36	A1	2129	U	N3-C2-O2	-5.43	118.40	122.20
36	A1	2621	G	C8-N9-C4	-5.43	104.23	106.40
37	A3	96	U	C2-N3-C4	-5.43	123.74	127.00
38	A4	23	U	C2-N3-C4	-5.43	123.74	127.00
80	A6	381	C	C2-N3-C4	-5.43	117.18	119.90
80	A6	1028	C	C2-N3-C4	-5.43	117.18	119.90
4	CC	229	LEU	CA-CB-CG	5.43	127.80	115.30
36	A5	2634	U	N3-C2-O2	5.43	126.00	122.20
36	A5	3064	U	C2-N3-C4	-5.43	123.74	127.00
36	A5	3366	G	N1-C6-O6	-5.43	116.64	119.90
64	Da	28	HIS	CB-CA-C	-5.43	99.54	110.40
36	A1	628	A	N1-C6-N6	5.43	121.86	118.60
36	A1	3142	A	C5-N7-C8	-5.43	101.18	103.90
36	A5	923	C	C5-C6-N1	-5.43	118.28	121.00
38	A8	11	C	N1-C2-O2	5.43	122.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1560	U	C6-N1-C2	-5.43	117.74	121.00
36	A1	347	G	C8-N9-C1'	-5.43	119.94	127.00
37	A3	53	U	N1-C2-N3	5.43	118.16	114.90
52	BO	3[B]	SER	C-N-CA	-5.43	108.13	121.70
80	A6	153	G	C2-N3-C4	-5.43	109.19	111.90
36	A5	591	G	C6-C5-N7	-5.43	127.14	130.40
36	A5	706	A	N9-C4-C5	-5.43	103.63	105.80
36	A5	1359	C	N3-C4-N4	5.43	121.80	118.00
36	A5	2355	G	C5-C6-O6	-5.43	125.34	128.60
36	A5	2635	A	N1-C6-N6	-5.43	115.34	118.60
37	A7	1	G	C8-N9-C1'	-5.43	119.94	127.00
37	A7	93	C	N3-C4-C5	5.43	124.07	121.90
1	A2	396	G	C5-C6-O6	-5.43	125.34	128.60
1	A2	767	U	N3-C2-O2	-5.43	118.40	122.20
36	A1	105	C	N1-C2-N3	5.43	123.00	119.20
36	A1	967	A	C8-N9-C4	5.43	107.97	105.80
36	A1	2366	C	C5-C6-N1	5.43	123.71	121.00
80	A6	1724	U	N3-C4-C5	5.43	117.86	114.60
36	A5	2375	G	C4-C5-N7	5.43	112.97	110.80
36	A5	3031	G	C5-C6-O6	-5.43	125.34	128.60
1	A2	268	C	C6-N1-C2	-5.43	118.13	120.30
36	A1	892	U	N3-C4-O4	-5.43	115.60	119.40
36	A1	3048	A	C5-N7-C8	-5.43	101.19	103.90
80	A6	647	G	C2-N3-C4	-5.43	109.19	111.90
36	A5	1491	A	C4-C5-C6	5.43	119.71	117.00
36	A5	2149	A	N9-C4-C5	5.43	107.97	105.80
36	A5	2174	G	N1-C2-N3	5.43	127.16	123.90
36	A5	2549	G	C5-C6-N1	-5.43	108.79	111.50
1	A2	396	G	N1-C6-O6	5.42	123.16	119.90
1	A2	407	A	C5-N7-C8	5.42	106.61	103.90
36	A1	328	U	N1-C2-O2	5.42	126.60	122.80
36	A1	342	A	C8-N9-C4	5.42	107.97	105.80
36	A1	944	C	C5-C6-N1	5.42	123.71	121.00
36	A1	1385	C	C6-N1-C2	-5.42	118.13	120.30
36	A1	1658	G	N9-C4-C5	5.42	107.57	105.40
36	A1	1836	C	N3-C4-C5	5.42	124.07	121.90
36	A1	2359	C	N3-C4-C5	5.42	124.07	121.90
36	A5	930	U	N1-C2-O2	5.42	126.60	122.80
36	A5	1007	U	C5-C4-O4	-5.42	122.64	125.90
36	A5	1724	U	N1-C2-N3	5.42	118.16	114.90
36	A5	2385	G	C8-N9-C1'	5.42	134.05	127.00
36	A5	3115	C	N1-C2-N3	5.42	123.00	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	731	U	C5-C6-N1	-5.42	119.99	122.70
36	A1	1173	U	C6-N1-C2	5.42	124.25	121.00
36	A1	2647	A	C5-C6-N1	5.42	120.41	117.70
38	A4	78	G	N3-C2-N2	5.42	123.70	119.90
36	A5	2744	U	N3-C4-O4	-5.42	115.60	119.40
36	A5	3008	A	C8-N9-C4	5.42	107.97	105.80
36	A5	3377	G	C6-N1-C2	-5.42	121.85	125.10
37	A7	33	U	N1-C2-O2	5.42	126.60	122.80
36	A1	24	G	N7-C8-N9	-5.42	110.39	113.10
36	A1	370	U	C6-N1-C2	-5.42	117.75	121.00
36	A1	934	G	C2-N3-C4	5.42	114.61	111.90
36	A1	1496	C	C4-C5-C6	-5.42	114.69	117.40
56	DS	167	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A2	1679	G	C2-N3-C4	5.42	114.61	111.90
36	A1	582	G	C8-N9-C1'	5.42	134.05	127.00
80	A6	1124	A	C4-C5-C6	-5.42	114.29	117.00
36	A5	616	G	C2-N3-C4	5.42	114.61	111.90
36	A5	2257	C	C5-C6-N1	5.42	123.71	121.00
36	A1	376	G	N3-C4-C5	-5.42	125.89	128.60
36	A1	506	U	C2-N1-C1'	-5.42	111.20	117.70
36	A1	1518	U	N1-C2-O2	-5.42	119.01	122.80
36	A1	3112	G	N9-C4-C5	-5.42	103.23	105.40
80	A6	1649	G	N1-C6-O6	-5.42	116.65	119.90
36	A5	675	C	N1-C2-O2	-5.42	115.65	118.90
36	A5	1510	G	C2-N3-C4	-5.42	109.19	111.90
36	A5	1858	A	C4-N9-C1'	5.42	136.05	126.30
36	A5	2145	A	C6-N1-C2	-5.42	115.35	118.60
36	A5	2320	A	N7-C8-N9	-5.42	111.09	113.80
36	A5	2434	U	N3-C2-O2	-5.42	118.41	122.20
36	A5	2810	C	C6-N1-C2	-5.42	118.13	120.30
36	A5	2837	A	C8-N9-C4	5.42	107.97	105.80
36	A1	547	G	C3'-C2'-C1'	5.42	105.83	101.50
36	A1	1902	G	C4-N9-C1'	5.42	133.54	126.50
80	A6	336	G	C5-N7-C8	5.42	107.01	104.30
80	A6	491	C	C2-N1-C1'	5.42	124.76	118.80
36	A5	1081	U	C5-C6-N1	5.42	125.41	122.70
36	A5	3021	A	N1-C6-N6	-5.42	115.35	118.60
36	A5	1399	A	N9-C4-C5	-5.42	103.63	105.80
36	A5	3362	A	C4-C5-N7	5.42	113.41	110.70
1	A2	426	G	C4-N9-C1'	5.41	133.54	126.50
36	A1	3140	G	N3-C4-N9	5.41	129.25	126.00
36	A5	1427	U	N3-C4-O4	-5.41	115.61	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1538	G	N9-C4-C5	-5.41	103.23	105.40
36	A5	2377	G	N3-C4-C5	-5.41	125.89	128.60
1	A2	1146	G	C4-N9-C1'	5.41	133.53	126.50
36	A1	386	A	C4-C5-C6	5.41	119.71	117.00
36	A1	1447	G	C4-C5-N7	-5.41	108.64	110.80
40	BB	4	ARG	NE-CZ-NH2	-5.41	117.59	120.30
36	A5	1905	G	N9-C4-C5	5.41	107.56	105.40
36	A5	2980	U	N3-C2-O2	-5.41	118.41	122.20
36	A1	406	G	C4-N9-C1'	-5.41	119.47	126.50
36	A1	529	A	C8-N9-C4	-5.41	103.64	105.80
36	A1	2830	G	N9-C4-C5	5.41	107.56	105.40
36	A1	2975	U	N1-C2-O2	5.41	126.59	122.80
36	A5	632	G	C5-C6-N1	5.41	114.20	111.50
36	A5	1159	A	C4-C5-C6	-5.41	114.30	117.00
36	A5	2374	C	N3-C4-N4	-5.41	114.21	118.00
36	A5	2767	U	N3-C4-O4	-5.41	115.61	119.40
36	A1	1363	A	N1-C6-N6	-5.41	115.36	118.60
36	A1	1507	G	N1-C2-N3	5.41	127.14	123.90
36	A5	288	C	C6-N1-C2	5.41	122.46	120.30
36	A5	987	U	C5-C4-O4	5.41	129.15	125.90
36	A5	1144	U	C4-C5-C6	5.41	122.94	119.70
36	A5	1660	C	N1-C2-O2	-5.41	115.66	118.90
36	A1	1450	G	C5-C6-O6	-5.41	125.36	128.60
36	A1	2227	C	C2-N3-C4	-5.41	117.20	119.90
36	A1	2915	U	N3-C4-C5	5.41	117.84	114.60
80	A6	1241	G	C4-C5-N7	5.41	112.96	110.80
36	A5	1191	U	C4-C5-C6	5.41	122.94	119.70
1	A2	557	G	N1-C2-N2	-5.41	111.33	116.20
36	A1	22	G	C5-C6-N1	5.41	114.20	111.50
36	A1	1337	A	N1-C6-N6	-5.41	115.36	118.60
80	A6	372	G	N7-C8-N9	-5.41	110.40	113.10
80	A6	988	A	N9-C4-C5	5.41	107.96	105.80
80	A6	1541	G	C2-N3-C4	5.41	114.60	111.90
18	CQ	69	VAL	CB-CA-C	-5.41	101.13	111.40
36	A5	600	G	C4-N9-C1'	5.41	133.53	126.50
36	A5	646	A	N1-C2-N3	5.41	132.00	129.30
36	A5	1209	G	N1-C2-N2	5.41	121.06	116.20
36	A5	2242	A	N9-C4-C5	5.41	107.96	105.80
36	A5	2524	A	C5-C6-N1	-5.41	115.00	117.70
36	A5	848	A	N1-C2-N3	5.40	132.00	129.30
36	A5	1447	G	N7-C8-N9	5.40	115.80	113.10
36	A5	2665	U	N1-C2-O2	5.40	126.58	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	393	C	C5-C6-N1	-5.40	118.30	121.00
1	A2	469	C	N3-C2-O2	5.40	125.68	121.90
1	A2	1170	G	C6-C5-N7	-5.40	127.16	130.40
1	A2	1666	U	C5-C6-N1	5.40	125.40	122.70
36	A1	364	G	C5-N7-C8	-5.40	101.60	104.30
36	A1	931	C	N3-C2-O2	-5.40	118.12	121.90
36	A1	1377	G	N1-C6-O6	-5.40	116.66	119.90
36	A1	3230	G	C5-C6-N1	5.40	114.20	111.50
37	A3	97	A	N9-C4-C5	5.40	107.96	105.80
80	A6	232	U	N1-C2-O2	5.40	126.58	122.80
80	A6	1035	G	N7-C8-N9	-5.40	110.40	113.10
80	A6	1549	C	C4-C5-C6	5.40	120.10	117.40
36	A5	1925	U	N1-C2-N3	5.40	118.14	114.90
36	A5	2184	U	N3-C4-C5	5.40	117.84	114.60
36	A5	3350	C	N1-C2-O2	5.40	122.14	118.90
62	DY	14	LYS	CD-CE-NZ	5.40	124.13	111.70
1	A2	1768	G	C8-N9-C1'	5.40	134.02	127.00
36	A1	80	G	N1-C2-N2	-5.40	111.34	116.20
36	A1	89	A	C8-N9-C4	-5.40	103.64	105.80
36	A1	503	C	N3-C4-C5	5.40	124.06	121.90
36	A1	1382	G	N7-C8-N9	-5.40	110.40	113.10
36	A1	2835	U	C5-C6-N1	-5.40	120.00	122.70
36	A1	3345	G	C8-N9-C4	5.40	108.56	106.40
52	BO	104[B]	ILE	CA-C-N	-5.40	105.32	117.20
36	A5	852	U	N1-C2-N3	5.40	118.14	114.90
36	A5	1447	G	N9-C4-C5	5.40	107.56	105.40
36	A5	2794	G	C5-C6-O6	-5.40	125.36	128.60
36	A5	2894	C	C2-N3-C4	-5.40	117.20	119.90
39	DA	207	VAL	CB-CA-C	-5.40	101.14	111.40
18	AQ	40	GLU	C-N-CA	5.40	144.68	122.00
36	A5	1164	G	C2-N3-C4	-5.40	109.20	111.90
36	A5	3113	A	C6-N1-C2	-5.40	115.36	118.60
1	A2	523	G	N1-C6-O6	-5.40	116.66	119.90
1	A2	790	U	N1-C2-N3	5.40	118.14	114.90
1	A2	966	A	N7-C8-N9	-5.40	111.10	113.80
36	A1	637	C	C2-N3-C4	-5.40	117.20	119.90
36	A1	950	G	N9-C4-C5	-5.40	103.24	105.40
36	A1	2958	A	C6-C5-N7	5.40	136.08	132.30
36	A1	3256	G	N1-C2-N3	-5.40	120.66	123.90
38	A4	109	A	C5-C6-N6	-5.40	119.38	123.70
36	A5	1505	C	C4-C5-C6	5.40	120.10	117.40
36	A5	2148	U	N3-C4-C5	5.40	117.84	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2904	U	N3-C2-O2	-5.40	118.42	122.20
36	A1	158	G	N3-C4-N9	-5.40	122.76	126.00
36	A1	1482	A	C4-C5-N7	-5.40	108.00	110.70
36	A1	2197	C	C5-C6-N1	5.40	123.70	121.00
70	Bg	8	ARG	NE-CZ-NH1	5.40	123.00	120.30
36	A5	2655	U	N3-C4-C5	5.40	117.84	114.60
36	A1	1499	C	C6-N1-C2	-5.39	118.14	120.30
36	A1	1834	U	C5-C4-O4	5.39	129.14	125.90
38	A4	23	U	C5-C4-O4	-5.39	122.66	125.90
80	A6	1043	A	N1-C6-N6	5.39	121.84	118.60
80	A6	1198	G	C6-C5-N7	5.39	133.64	130.40
36	A5	339	C	C6-N1-C1'	5.39	127.27	120.80
36	A5	1808	G	C5-C6-O6	-5.39	125.36	128.60
1	A2	307	G	C8-N9-C4	5.39	108.56	106.40
36	A1	506	U	C2-N3-C4	-5.39	123.77	127.00
36	A1	653	A	C5-C6-N6	-5.39	119.39	123.70
36	A1	743	C	C5-C6-N1	-5.39	118.30	121.00
36	A1	1948	G	C8-N9-C1'	-5.39	119.99	127.00
36	A1	2787	G	C5-C6-N1	5.39	114.20	111.50
80	A6	366	A	C2-N3-C4	-5.39	107.90	110.60
80	A6	1484	G	N3-C4-C5	-5.39	125.90	128.60
36	A5	91	G	N9-C4-C5	5.39	107.56	105.40
1	A2	1361	U	C2-N1-C1'	5.39	124.17	117.70
36	A1	1053	A	C8-N9-C4	5.39	107.96	105.80
36	A1	2692	A	C4-C5-C6	5.39	119.69	117.00
38	A4	103	G	C5-C6-O6	5.39	131.84	128.60
36	A5	1396	C	C6-N1-C2	5.39	122.46	120.30
36	A5	3245	A	C4-C5-C6	5.39	119.69	117.00
1	A2	1192	C	N1-C2-O2	-5.39	115.67	118.90
36	A1	593	C	N1-C2-N3	5.39	122.97	119.20
36	A1	1654	A	N1-C2-N3	-5.39	126.61	129.30
36	A5	998	A	C5-N7-C8	5.39	106.59	103.90
36	A5	1389	G	C8-N9-C4	5.39	108.56	106.40
36	A5	2658	G	C8-N9-C4	5.39	108.56	106.40
36	A1	327	A	N1-C6-N6	5.39	121.83	118.60
36	A5	1170	A	N9-C4-C5	-5.39	103.64	105.80
1	A2	336	G	C6-C5-N7	-5.39	127.17	130.40
1	A2	1389	C	N3-C2-O2	-5.39	118.13	121.90
12	AK	63	TYR	N-CA-C	5.39	125.55	111.00
36	A1	412	G	N1-C2-N3	5.39	127.13	123.90
36	A1	1379	G	N1-C2-N3	5.39	127.13	123.90
36	A1	1610	G	C5-C6-N1	-5.39	108.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2685	C	N1-C2-O2	-5.39	115.67	118.90
36	A1	2963	C	N3-C4-C5	-5.39	119.75	121.90
36	A1	3107	U	N3-C2-O2	-5.39	118.43	122.20
80	A6	69	G	C8-N9-C4	5.39	108.56	106.40
21	CT	57	ARG	NE-CZ-NH1	5.39	122.99	120.30
36	A5	363	G	C5-N7-C8	5.39	106.99	104.30
36	A5	1534	A	C6-N1-C2	-5.39	115.37	118.60
36	A5	2399	A	C5-C6-N6	-5.39	119.39	123.70
36	A5	2820	A	N9-C4-C5	5.39	107.95	105.80
36	A5	2955	U	C6-N1-C2	-5.39	117.77	121.00
36	A5	3374	U	C6-N1-C2	5.39	124.23	121.00
36	A1	857	G	N9-C4-C5	-5.38	103.25	105.40
36	A1	1178	G	C5-C6-O6	5.38	131.83	128.60
36	A5	3193	C	C4-C5-C6	5.38	120.09	117.40
1	A2	719	U	C6-N1-C1'	-5.38	113.66	121.20
36	A1	3147	G	N1-C2-N2	-5.38	111.36	116.20
36	A1	3209	A	C4-C5-N7	5.38	113.39	110.70
36	A5	696	C	C2-N1-C1'	5.38	124.72	118.80
36	A5	2429	G	N9-C4-C5	5.38	107.55	105.40
36	A1	200	C	N3-C2-O2	-5.38	118.13	121.90
36	A1	339	C	C6-N1-C2	-5.38	118.15	120.30
36	A1	3362	A	O4'-C1'-N9	5.38	112.51	108.20
80	A6	1320	U	C5-C6-N1	5.38	125.39	122.70
80	A6	1615	C	N1-C2-O2	-5.38	115.67	118.90
36	A5	1192	C	N1-C2-N3	5.38	122.97	119.20
80	A6	418	G	C5-N7-C8	-5.38	101.61	104.30
1	A2	392	G	C5-C6-O6	-5.38	125.37	128.60
36	A1	1369	A	C6-N1-C2	5.38	121.83	118.60
36	A1	2426	U	C5-C4-O4	5.38	129.13	125.90
36	A5	388	G	N3-C2-N2	-5.38	116.14	119.90
36	A5	806	A	C8-N9-C4	5.38	107.95	105.80
36	A5	2621	G	N1-C2-N2	5.38	121.04	116.20
36	A1	66	A	N3-C4-C5	5.38	130.56	126.80
36	A1	324	A	C6-N1-C2	-5.38	115.37	118.60
36	A1	1819	U	C5-C6-N1	5.38	125.39	122.70
36	A1	1832	C	C2-N3-C4	-5.38	117.21	119.90
36	A1	2621	G	N1-C2-N2	5.38	121.04	116.20
36	A1	2981	U	C2-N3-C4	-5.38	123.77	127.00
38	A4	31	G	N3-C4-C5	5.38	131.29	128.60
80	A6	524	U	N3-C4-O4	-5.38	115.64	119.40
80	A6	814	A	C5-N7-C8	-5.38	101.21	103.90
36	A5	2393	G	C8-N9-C1'	-5.38	120.01	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	3243	A	C4-C5-C6	5.38	119.69	117.00
37	A7	48	U	C5-C6-N1	-5.38	120.01	122.70
43	DE	173	MET	CB-CG-SD	-5.38	96.27	112.40
80	A6	879	G	N9-C4-C5	5.38	107.55	105.40
36	A5	706	A	N1-C6-N6	5.38	121.83	118.60
1	A2	1324	G	N1-C2-N2	5.37	121.04	116.20
36	A1	1000	C	C5-C6-N1	5.37	123.69	121.00
36	A1	1308	A	N1-C2-N3	5.37	131.99	129.30
36	A1	1929	G	C4-C5-N7	5.37	112.95	110.80
36	A1	2148	U	C5-C6-N1	-5.37	120.01	122.70
36	A1	2156	C	C2-N3-C4	-5.37	117.21	119.90
36	A1	2400	G	C4-N9-C1'	-5.37	119.52	126.50
36	A1	2639	G	C6-N1-C2	-5.37	121.88	125.10
36	A1	3055	U	C6-N1-C1'	-5.37	113.68	121.20
80	A6	558	U	C6-N1-C1'	-5.37	113.68	121.20
36	A5	1804	A	C8-N9-C4	5.37	107.95	105.80
36	A5	1828	A	C8-N9-C4	-5.37	103.65	105.80
36	A5	1870	C	N1-C2-O2	-5.37	115.68	118.90
36	A5	1885	U	N1-C2-O2	-5.37	119.04	122.80
36	A5	1907	C	C6-N1-C1'	5.37	127.25	120.80
36	A5	2639	G	C6-N1-C2	-5.37	121.88	125.10
36	A5	3047	U	N3-C2-O2	-5.37	118.44	122.20
36	A5	3189	G	C6-N1-C2	-5.37	121.88	125.10
36	A5	3336	A	C2-N3-C4	-5.37	107.91	110.60
36	A5	3346	U	C5-C6-N1	-5.37	120.01	122.70
36	A1	386	A	C4-N9-C1'	5.37	135.97	126.30
36	A1	1773	C	C6-N1-C2	5.37	122.45	120.30
36	A1	2157	G	C2-N3-C4	5.37	114.59	111.90
36	A1	2275	A	C5-C6-N1	-5.37	115.01	117.70
36	A1	2722	U	C4-C5-C6	5.37	122.92	119.70
36	A1	2787	G	C6-N1-C2	-5.37	121.88	125.10
38	A4	1	A	N1-C6-N6	5.37	121.82	118.60
38	A4	41	A	N1-C2-N3	5.37	131.99	129.30
44	BF	100	ARG	NE-CZ-NH1	-5.37	117.61	120.30
36	A5	51	A	N1-C6-N6	5.37	121.82	118.60
36	A5	965	A	N1-C2-N3	-5.37	126.61	129.30
36	A5	2134	G	N3-C2-N2	5.37	123.66	119.90
36	A5	2376	G	C8-N9-C1'	-5.37	120.02	127.00
36	A5	3003	G	N3-C4-N9	-5.37	122.78	126.00
1	A2	1422	A	N7-C8-N9	-5.37	111.11	113.80
1	A2	1481	C	C5-C6-N1	5.37	123.69	121.00
36	A1	1556	C	N1-C2-O2	5.37	122.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	3083	G	C5-N7-C8	5.37	106.98	104.30
36	A1	3319	U	N1-C2-O2	5.37	126.56	122.80
21	CT	57	ARG	NE-CZ-NH2	-5.37	117.61	120.30
36	A5	799	G	C6-N1-C2	-5.37	121.88	125.10
36	A5	1409	G	N9-C4-C5	5.37	107.55	105.40
36	A5	1844	C	C6-N1-C2	-5.37	118.15	120.30
1	A2	864	U	C2-N1-C1'	5.37	124.14	117.70
36	A1	2288	G	C2-N3-C4	5.37	114.58	111.90
49	BL	57	VAL	N-CA-C	-5.37	96.51	111.00
80	A6	328	A	N1-C6-N6	-5.37	115.38	118.60
80	A6	385	A	C5-C6-N1	-5.37	115.02	117.70
80	A6	491	C	N1-C2-O2	5.37	122.12	118.90
80	A6	538	A	C8-N9-C4	-5.37	103.65	105.80
80	A6	1144	U	N3-C2-O2	-5.37	118.44	122.20
8	CG	108	VAL	CB-CA-C	-5.37	101.20	111.40
36	A5	1300	G	N1-C6-O6	5.37	123.12	119.90
36	A5	2915	U	N3-C4-O4	-5.37	115.64	119.40
36	A5	3043	C	N1-C2-O2	5.37	122.12	118.90
38	A8	6	U	C5-C4-O4	-5.37	122.68	125.90
38	A8	29	U	C5-C6-N1	-5.37	120.02	122.70
36	A5	76	G	N1-C6-O6	5.37	123.12	119.90
1	A2	1504	G	C5-C6-O6	5.37	131.82	128.60
1	A2	1762	A	N9-C4-C5	-5.37	103.65	105.80
10	AI	29	LEU	CA-CB-CG	5.37	127.64	115.30
29	Ab	29	ARG	NE-CZ-NH1	5.37	122.98	120.30
36	A1	126	U	C4-C5-C6	5.37	122.92	119.70
36	A1	972	A	C5-C6-N1	-5.37	115.02	117.70
36	A1	1372	C	N3-C4-C5	5.37	124.05	121.90
36	A1	2305	G	C4-N9-C1'	5.37	133.48	126.50
36	A1	3014	U	C5-C6-N1	-5.37	120.02	122.70
38	A4	151	C	N3-C4-C5	-5.37	119.75	121.90
36	A5	419	G	C5-C6-N1	5.37	114.18	111.50
36	A5	555	U	N1-C2-O2	-5.37	119.04	122.80
36	A5	1374	G	N1-C2-N2	-5.37	111.37	116.20
36	A5	2614	G	C4-N9-C1'	5.37	133.47	126.50
36	A5	3101	G	N1-C2-N2	-5.37	111.37	116.20
1	A2	628	G	N3-C4-C5	5.36	131.28	128.60
1	A2	1148	C	C6-N1-C2	5.36	122.45	120.30
36	A1	362	U	N3-C4-C5	5.36	117.82	114.60
36	A1	714	G	C8-N9-C4	5.36	108.55	106.40
36	A1	2273	G	C2-N3-C4	5.36	114.58	111.90
36	A1	2777	G	N7-C8-N9	5.36	115.78	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1297	G	N7-C8-N9	-5.36	110.42	113.10
36	A5	227	G	C5-C6-O6	-5.36	125.38	128.60
36	A5	356	C	C5-C6-N1	-5.36	118.32	121.00
36	A5	536	U	N3-C4-O4	-5.36	115.65	119.40
36	A5	1128	U	C2-N3-C4	-5.36	123.78	127.00
36	A5	2231	C	C2-N1-C1'	5.36	124.70	118.80
36	A5	3028	G	C8-N9-C1'	-5.36	120.03	127.00
36	A1	2809	C	N3-C4-C5	5.36	124.05	121.90
80	A6	477	A	N9-C4-C5	-5.36	103.66	105.80
37	A7	83	U	N3-C4-O4	-5.36	115.65	119.40
53	DP	127	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A2	554	C	C6-N1-C1'	-5.36	114.37	120.80
1	A2	1642	G	N3-C4-N9	5.36	129.22	126.00
36	A1	1445	U	C6-N1-C2	5.36	124.22	121.00
56	BS	115	ARG	NE-CZ-NH2	-5.36	117.62	120.30
80	A6	434	G	N1-C6-O6	-5.36	116.68	119.90
80	A6	991	G	C6-N1-C2	-5.36	121.88	125.10
80	A6	1085	G	N1-C2-N2	-5.36	111.38	116.20
36	A5	1838	G	C6-N1-C2	-5.36	121.88	125.10
36	A5	1889	G	C4-C5-N7	-5.36	108.66	110.80
36	A5	2609	A	N7-C8-N9	-5.36	111.12	113.80
36	A5	3179	U	N1-C2-O2	5.36	126.55	122.80
36	A5	322	U	C2-N3-C4	-5.36	123.78	127.00
36	A5	948	C	C4-C5-C6	5.36	120.08	117.40
36	A5	1312	C	C5-C4-N4	5.36	123.95	120.20
36	A5	1319	G	N1-C2-N2	-5.36	111.38	116.20
36	A5	2836	C	N1-C2-O2	-5.36	115.68	118.90
1	A2	350	U	C5-C6-N1	-5.36	120.02	122.70
1	A2	720	G	P-O3'-C3'	5.36	126.13	119.70
36	A1	367	A	C5-C6-N1	-5.36	115.02	117.70
36	A1	640	U	N1-C2-O2	5.36	126.55	122.80
36	A1	805	G	C5-C6-N1	5.36	114.18	111.50
36	A1	2674	A	N1-C6-N6	-5.36	115.39	118.60
36	A1	2871	G	N3-C4-C5	5.36	131.28	128.60
80	A6	3	U	N3-C4-O4	-5.36	115.65	119.40
80	A6	93	A	N9-C4-C5	-5.36	103.66	105.80
80	A6	146	U	N1-C2-O2	5.36	126.55	122.80
80	A6	1724	U	C5-C4-O4	-5.36	122.69	125.90
80	A6	1783	C	N3-C4-C5	-5.36	119.76	121.90
36	A5	408	A	C2-N3-C4	-5.36	107.92	110.60
36	A5	1143	A	C2-N3-C4	-5.36	107.92	110.60
36	A5	2369	G	N3-C2-N2	5.36	123.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2755	C	N1-C2-O2	-5.36	115.69	118.90
36	A5	3112	G	N7-C8-N9	-5.36	110.42	113.10
1	A2	932	U	C6-N1-C1'	5.36	128.70	121.20
1	A2	1524	A	N1-C6-N6	-5.36	115.39	118.60
36	A1	2345	A	C2-N3-C4	-5.36	107.92	110.60
80	A6	1458	G	C8-N9-C1'	-5.36	120.04	127.00
36	A5	3138	U	N3-C2-O2	5.36	125.95	122.20
36	A5	3246	G	N1-C6-O6	5.36	123.11	119.90
37	A7	115	G	C8-N9-C4	-5.36	104.26	106.40
1	A2	1769	U	C5-C4-O4	5.35	129.11	125.90
36	A1	701	G	C5-N7-C8	-5.35	101.62	104.30
36	A1	843	A	C8-N9-C4	5.35	107.94	105.80
36	A1	1362	G	N7-C8-N9	-5.35	110.42	113.10
80	A6	1100	G	N1-C2-N3	5.35	127.11	123.90
36	A1	73	C	C4-C5-C6	5.35	120.08	117.40
36	A1	1164	G	C2-N3-C4	-5.35	109.22	111.90
36	A1	1506	A	N1-C2-N3	5.35	131.98	129.30
36	A1	1512	U	N1-C2-N3	5.35	118.11	114.90
36	A1	2315	G	C5-C6-O6	5.35	131.81	128.60
36	A1	2884	C	C5-C4-N4	-5.35	116.45	120.20
80	A6	148	A	C8-N9-C4	-5.35	103.66	105.80
36	A5	14	U	N3-C4-C5	5.35	117.81	114.60
36	A5	590	G	C2-N3-C4	5.35	114.58	111.90
36	A5	702	C	N3-C4-C5	5.35	124.04	121.90
36	A5	1152	G	N9-C4-C5	5.35	107.54	105.40
36	A1	276	U	C2-N3-C4	-5.35	123.79	127.00
36	A1	1180	A	C4-C5-C6	5.35	119.68	117.00
36	A1	1472	U	C5-C4-O4	-5.35	122.69	125.90
36	A1	2244	A	N1-C6-N6	-5.35	115.39	118.60
36	A5	3227	A	C2-N3-C4	-5.35	107.92	110.60
38	A8	135	G	C4-C5-N7	-5.35	108.66	110.80
40	DB	4	ARG	NE-CZ-NH2	-5.35	117.62	120.30
36	A1	1183	C	C6-N1-C2	5.35	122.44	120.30
36	A1	2233	A	N1-C6-N6	-5.35	115.39	118.60
36	A1	3111	U	C6-N1-C2	5.35	124.21	121.00
38	A4	88	A	C4-C5-N7	5.35	113.38	110.70
80	A6	866	G	N1-C6-O6	-5.35	116.69	119.90
36	A5	283	G	C5-C6-O6	-5.35	125.39	128.60
36	A5	354	U	C5-C6-N1	-5.35	120.03	122.70
36	A5	372	A	N1-C6-N6	5.35	121.81	118.60
36	A5	564	G	C5-N7-C8	5.35	106.97	104.30
36	A5	688	G	N3-C4-N9	-5.35	122.79	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	810	A	C4-C5-N7	-5.35	108.03	110.70
36	A5	1838	G	C4-C5-N7	-5.35	108.66	110.80
36	A5	2342	U	N3-C4-C5	5.35	117.81	114.60
36	A5	2891	U	N1-C2-N3	5.35	118.11	114.90
36	A5	3368	U	C2-N1-C1'	-5.35	111.28	117.70
1	A2	313	U	C5-C4-O4	5.35	129.11	125.90
1	A2	343	C	C6-N1-C2	-5.35	118.16	120.30
17	AP	60	LEU	CA-CB-CG	5.35	127.60	115.30
36	A1	1388	U	N1-C2-O2	-5.35	119.06	122.80
80	A6	336	G	N7-C8-N9	-5.35	110.43	113.10
36	A5	909	G	N7-C8-N9	-5.35	110.43	113.10
36	A5	1321	G	C8-N9-C4	5.35	108.54	106.40
36	A5	1506	A	N9-C4-C5	5.35	107.94	105.80
36	A5	3055	U	C6-N1-C1'	-5.35	113.71	121.20
36	A5	3347	A	C8-N9-C4	5.35	107.94	105.80
36	A5	3078	U	C2-N1-C1'	5.35	124.11	117.70
1	A2	1461	C	C6-N1-C2	5.34	122.44	120.30
36	A1	715	A	C8-N9-C4	-5.34	103.66	105.80
36	A1	806	A	C8-N9-C4	5.34	107.94	105.80
36	A1	857	G	N1-C2-N2	-5.34	111.39	116.20
36	A1	2644	C	N1-C2-N3	5.34	122.94	119.20
80	A6	1227	A	P-O3'-C3'	5.34	126.11	119.70
80	A6	1400	A	C5-C6-N1	5.34	120.37	117.70
80	A6	1764	C	N3-C4-C5	5.34	124.04	121.90
36	A5	859	G	N3-C4-C5	-5.34	125.93	128.60
36	A5	1017	C	C2-N1-C1'	5.34	124.68	118.80
56	BS	117	ARG	NE-CZ-NH2	5.34	122.97	120.30
36	A5	1239	C	C2-N1-C1'	5.34	124.68	118.80
36	A5	1375	G	C8-N9-C4	-5.34	104.26	106.40
36	A5	1628	C	C6-N1-C2	-5.34	118.16	120.30
36	A1	582	G	N1-C6-O6	-5.34	116.69	119.90
36	A1	960	U	N3-C2-O2	5.34	125.94	122.20
36	A1	1113	G	N3-C2-N2	-5.34	116.16	119.90
36	A1	2278	C	C5-C4-N4	5.34	123.94	120.20
36	A1	2412	G	C8-N9-C4	-5.34	104.26	106.40
77	Bn	6	ARG	NE-CZ-NH2	-5.34	117.63	120.30
80	A6	124	A	C6-N1-C2	5.34	121.81	118.60
11	CJ	149	ARG	NE-CZ-NH1	5.34	122.97	120.30
36	A5	496	C	N3-C2-O2	-5.34	118.16	121.90
36	A5	1433	A	C6-N1-C2	5.34	121.81	118.60
36	A5	2261	G	N7-C8-N9	-5.34	110.43	113.10
36	A5	2319	U	C5-C6-N1	-5.34	120.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	3048	A	C6-N1-C2	-5.34	115.40	118.60
1	A2	1679	G	N1-C6-O6	-5.34	116.70	119.90
36	A1	115	A	C5-C6-N6	5.34	127.97	123.70
36	A1	867	G	C6-N1-C2	-5.34	121.90	125.10
36	A1	2377	G	C2-N3-C4	-5.34	109.23	111.90
36	A1	2719	U	C6-N1-C1'	5.34	128.67	121.20
80	A6	1329	A	C6-C5-N7	-5.34	128.56	132.30
80	A6	1419	G	C5-C6-N1	-5.34	108.83	111.50
36	A5	1129	A	C5-C6-N1	5.34	120.37	117.70
36	A5	2930	A	C5-C6-N1	5.34	120.37	117.70
36	A1	1187	C	C6-N1-C2	-5.34	118.17	120.30
36	A1	2710	C	C2-N3-C4	-5.34	117.23	119.90
36	A1	2965	U	C6-N1-C2	5.34	124.20	121.00
38	A8	3	A	C5-C6-N1	5.34	120.37	117.70
38	A8	87	G	C4-C5-N7	5.34	112.94	110.80
1	A2	527	A	N7-C8-N9	5.34	116.47	113.80
36	A1	318	A	N1-C6-N6	5.34	121.80	118.60
36	A1	857	G	C8-N9-C4	5.34	108.53	106.40
36	A1	2607	G	N3-C2-N2	5.34	123.64	119.90
36	A1	2786	G	C2-N3-C4	5.34	114.57	111.90
38	A4	121	U	C5-C4-O4	5.34	129.10	125.90
80	A6	542	A	C8-N9-C1'	-5.34	118.10	127.70
80	A6	1185	U	C2-N1-C1'	5.34	124.10	117.70
80	A6	1458	G	C4-C5-N7	5.34	112.94	110.80
36	A5	524	U	C2-N1-C1'	-5.34	111.30	117.70
36	A5	1376	C	C6-N1-C2	5.34	122.43	120.30
36	A5	2300	G	C5-C6-N1	5.34	114.17	111.50
36	A5	2361	A	N9-C4-C5	5.34	107.93	105.80
36	A1	109	A	C5-C6-N6	5.33	127.97	123.70
80	A6	1060	U	N3-C2-O2	-5.33	118.47	122.20
36	A5	509	U	N3-C4-C5	5.33	117.80	114.60
36	A5	514	G	N9-C4-C5	-5.33	103.27	105.40
36	A5	972	A	C4-C5-C6	5.33	119.67	117.00
36	A5	2636	A	N1-C6-N6	-5.33	115.40	118.60
36	A5	3247	G	C5-C6-O6	5.33	131.80	128.60
1	A2	274	G	C8-N9-C4	-5.33	104.27	106.40
1	A2	1145	U	N3-C2-O2	5.33	125.93	122.20
36	A1	1037	C	C6-N1-C2	-5.33	118.17	120.30
36	A1	1882	G	N9-C4-C5	5.33	107.53	105.40
36	A1	2932	U	N3-C4-O4	-5.33	115.67	119.40
41	BC	60	THR	CB-CA-C	-5.33	97.20	111.60
80	A6	411	C	C5-C6-N1	-5.33	118.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1230	A	N7-C8-N9	5.33	116.47	113.80
20	CS	15	LEU	CA-CB-CG	5.33	127.57	115.30
36	A5	90	C	C6-N1-C2	-5.33	118.17	120.30
36	A5	1906	G	C6-N1-C2	-5.33	121.90	125.10
36	A5	1927	G	C8-N9-C4	-5.33	104.27	106.40
36	A5	2167	A	C5-C6-N1	5.33	120.37	117.70
36	A1	18	G	C8-N9-C4	-5.33	104.27	106.40
36	A1	1142	G	C4-N9-C1'	5.33	133.43	126.50
36	A1	2362	C	N3-C4-N4	5.33	121.73	118.00
36	A1	2549	G	N3-C4-C5	-5.33	125.94	128.60
36	A1	3140	G	N3-C4-C5	-5.33	125.93	128.60
36	A1	3214	U	C4-C5-C6	5.33	122.90	119.70
80	A6	547	U	N3-C4-C5	5.33	117.80	114.60
80	A6	1110	G	C5-N7-C8	5.33	106.97	104.30
80	A6	1522	U	N1-C2-N3	5.33	118.10	114.90
36	A5	98	G	C4-C5-N7	5.33	112.93	110.80
36	A5	1150	A	C5-N7-C8	-5.33	101.23	103.90
1	A2	1052	U	C2-N1-C1'	5.33	124.10	117.70
36	A1	1124	U	C5-C4-O4	-5.33	122.70	125.90
36	A1	1607	U	P-O3'-C3'	5.33	126.10	119.70
36	A1	2411	U	N3-C4-O4	-5.33	115.67	119.40
80	A6	484	C	C2-N1-C1'	5.33	124.66	118.80
36	A5	2664	C	C4-C5-C6	-5.33	114.73	117.40
36	A1	1690	C	C4-C5-C6	5.33	120.06	117.40
36	A1	2244	A	N7-C8-N9	-5.33	111.14	113.80
36	A1	2912	G	C5-C6-N1	5.33	114.16	111.50
36	A1	3293	U	N3-C2-O2	5.33	125.93	122.20
37	A3	52	G	C3'-C2'-C1'	-5.33	97.24	101.50
80	A6	1130	G	N1-C2-N3	5.33	127.10	123.90
36	A5	1788	C	C4-C5-C6	5.33	120.06	117.40
36	A5	1869	C	C5-C6-N1	-5.33	118.33	121.00
36	A5	2639	G	N1-C6-O6	5.33	123.10	119.90
36	A5	3174	A	N1-C6-N6	5.33	121.80	118.60
36	A1	429	U	C5-C6-N1	-5.33	120.04	122.70
80	A6	1749	A	C6-C5-N7	-5.33	128.57	132.30
36	A5	800	G	N9-C4-C5	-5.33	103.27	105.40
36	A5	1307	G	N3-C2-N2	5.33	123.63	119.90
36	A5	1722	U	N1-C2-O2	-5.33	119.07	122.80
36	A5	1939	G	C8-N9-C1'	-5.33	120.08	127.00
36	A5	2897	A	C5-N7-C8	5.33	106.56	103.90
36	A5	2928	C	N3-C4-C5	-5.33	119.77	121.90
36	A5	3045	G	N3-C4-C5	-5.33	125.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	190	C	C6-N1-C2	5.33	122.43	120.30
1	A2	393	C	C2-N1-C1'	-5.33	112.94	118.80
1	A2	1315	U	C5-C4-O4	-5.33	122.70	125.90
1	A2	1778	G	N1-C6-O6	-5.33	116.70	119.90
36	A1	72	C	N1-C2-O2	-5.33	115.70	118.90
36	A1	280	U	C4-C5-C6	-5.33	116.50	119.70
36	A1	2730	G	C2-N3-C4	-5.33	109.24	111.90
36	A1	2786	G	C4-C5-N7	-5.33	108.67	110.80
36	A1	2814	G	C5-N7-C8	5.33	106.96	104.30
36	A5	1054	A	N9-C4-C5	-5.33	103.67	105.80
36	A5	2625	C	N3-C4-C5	5.33	124.03	121.90
36	A5	3045	G	C4-C5-N7	-5.33	108.67	110.80
36	A1	381	U	C5-C6-N1	-5.32	120.04	122.70
36	A1	994	G	C6-N1-C2	-5.32	121.91	125.10
36	A1	1743	G	N7-C8-N9	-5.32	110.44	113.10
36	A1	3181	C	C2-N3-C4	-5.32	117.24	119.90
40	BB	7	GLU	CB-CA-C	5.32	121.05	110.40
80	A6	232	U	C5-C6-N1	5.32	125.36	122.70
1	A2	323	A	N7-C8-N9	5.32	116.46	113.80
36	A1	1399	A	C5-C6-N1	-5.32	115.04	117.70
36	A1	1609	C	N3-C4-N4	5.32	121.73	118.00
36	A1	2165	G	C6-C5-N7	-5.32	127.21	130.40
80	A6	85	A	C8-N9-C4	-5.32	103.67	105.80
80	A6	1099	U	N3-C4-O4	-5.32	115.67	119.40
36	A5	3141	A	N1-C2-N3	5.32	131.96	129.30
1	A2	969	C	N3-C4-C5	5.32	124.03	121.90
36	A1	83	U	C6-N1-C2	5.32	124.19	121.00
36	A1	428	A	C6-N1-C2	-5.32	115.41	118.60
36	A1	963	G	N3-C4-N9	5.32	129.19	126.00
36	A1	1154	A	C5-C6-N1	-5.32	115.04	117.70
41	BC	235	LEU	CB-CG-CD2	-5.32	101.95	111.00
80	A6	958	U	N3-C2-O2	5.32	125.92	122.20
36	A5	1107	C	N3-C4-C5	5.32	124.03	121.90
36	A5	1131	G	N1-C2-N3	5.32	127.09	123.90
36	A5	1490	A	C6-C5-N7	-5.32	128.58	132.30
36	A5	2998	U	C2-N3-C4	-5.32	123.81	127.00
36	A1	1899	G	C4-C5-N7	5.32	112.93	110.80
36	A5	2976	A	C5-C6-N1	5.32	120.36	117.70
36	A5	3025	C	N3-C2-O2	-5.32	118.18	121.90
36	A5	3323	A	N1-C2-N3	5.32	131.96	129.30
1	A2	811	A	C4-N9-C1'	5.32	135.87	126.30
1	A2	1541	G	N3-C4-C5	-5.32	125.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1754	A	C4-C5-C6	-5.32	114.34	117.00
36	A1	635	G	N9-C4-C5	-5.32	103.27	105.40
36	A1	638	C	C2-N3-C4	-5.32	117.24	119.90
36	A1	682	U	N1-C2-N3	5.32	118.09	114.90
36	A1	1546	A	C5-C6-N1	-5.32	115.04	117.70
36	A1	2970	C	N1-C2-O2	-5.32	115.71	118.90
36	A1	2993	G	C6-C5-N7	5.32	133.59	130.40
36	A1	3375	A	N9-C4-C5	5.32	107.93	105.80
38	A4	107	G	C8-N9-C4	5.32	108.53	106.40
80	A6	163	G	C6-C5-N7	-5.32	127.21	130.40
36	A5	806	A	C6-N1-C2	5.32	121.79	118.60
36	A5	887	G	C4-C5-C6	5.32	121.99	118.80
36	A5	1161	G	C6-C5-N7	5.32	133.59	130.40
36	A5	1317	A	N9-C4-C5	-5.32	103.67	105.80
36	A5	1483	G	N1-C6-O6	-5.32	116.71	119.90
1	A2	214	G	C8-N9-C1'	5.32	133.91	127.00
1	A2	1537	C	C5-C4-N4	-5.32	116.48	120.20
36	A1	425	G	N7-C8-N9	5.32	115.76	113.10
36	A1	2134	G	N3-C4-N9	5.32	129.19	126.00
36	A1	2853	A	C6-C5-N7	-5.32	128.58	132.30
38	A4	77	A	C2-N3-C4	-5.32	107.94	110.60
54	BQ	179	ARG	NE-CZ-NH2	-5.32	117.64	120.30
80	A6	396	G	N3-C4-N9	5.32	129.19	126.00
36	A5	588	G	C5-C6-N1	5.32	114.16	111.50
36	A5	1346	G	C8-N9-C4	5.32	108.53	106.40
36	A5	1833	G	N1-C2-N2	-5.32	111.42	116.20
36	A5	2942	C	N1-C2-O2	-5.32	115.71	118.90
36	A5	3019	U	C6-N1-C2	5.32	124.19	121.00
36	A1	78	U	C4-C5-C6	5.31	122.89	119.70
36	A1	89	A	C4-C5-C6	5.31	119.66	117.00
1	A2	557	G	N3-C4-C5	-5.31	125.94	128.60
36	A1	276	U	N3-C2-O2	-5.31	118.48	122.20
36	A1	2634	U	N1-C2-O2	-5.31	119.08	122.80
36	A1	2977	G	C5-N7-C8	5.31	106.96	104.30
80	A6	65	A	C6-C5-N7	-5.31	128.58	132.30
80	A6	571	G	C8-N9-C4	-5.31	104.28	106.40
80	A6	1087	A	N1-C2-N3	5.31	131.96	129.30
36	A5	1011	A	C2-N3-C4	-5.31	107.94	110.60
36	A5	1786	G	N3-C4-C5	-5.31	125.94	128.60
36	A5	2987	A	N7-C8-N9	-5.31	111.14	113.80
36	A5	3307	A	C6-N1-C2	5.31	121.79	118.60
36	A5	3369	G	C5-C6-N1	5.31	114.16	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A8	126	A	N7-C8-N9	5.31	116.46	113.80
43	DE	26	ARG	NE-CZ-NH2	-5.31	117.64	120.30
36	A1	1331	U	C5-C4-O4	-5.31	122.71	125.90
36	A1	1524	A	N1-C2-N3	5.31	131.96	129.30
80	A6	1649	G	N1-C2-N2	-5.31	111.42	116.20
36	A5	1442	U	C2-N3-C4	-5.31	123.81	127.00
36	A5	1586	G	C6-C5-N7	-5.31	127.21	130.40
36	A1	31	C	C2-N3-C4	-5.31	117.25	119.90
36	A1	635	G	C6-N1-C2	-5.31	121.91	125.10
36	A1	1851	G	C4-C5-C6	5.31	121.99	118.80
36	A1	1851	G	N1-C2-N3	5.31	127.08	123.90
36	A1	2306	C	C2-N3-C4	5.31	122.55	119.90
36	A1	2862	U	C5-C6-N1	-5.31	120.05	122.70
36	A1	3041	U	C2-N3-C4	-5.31	123.81	127.00
36	A5	641	C	C6-N1-C2	-5.31	118.18	120.30
36	A5	969	C	C6-N1-C2	5.31	122.42	120.30
36	A5	1085	A	C4-C5-N7	5.31	113.36	110.70
36	A5	3110	C	C5-C6-N1	-5.31	118.34	121.00
1	A2	1524	A	N1-C2-N3	5.31	131.95	129.30
36	A1	785	G	C5-N7-C8	5.31	106.95	104.30
36	A1	2328	U	N1-C2-O2	5.31	126.52	122.80
36	A1	2644	C	C2-N3-C4	-5.31	117.25	119.90
80	A6	447	U	N3-C2-O2	-5.31	118.48	122.20
80	A6	794	U	N1-C2-O2	5.31	126.52	122.80
36	A5	147	U	C5-C4-O4	5.31	129.09	125.90
36	A5	3046	A	N1-C6-N6	-5.31	115.42	118.60
36	A5	3259	U	C6-N1-C2	-5.31	117.81	121.00
38	A4	140	G	N3-C4-C5	-5.31	125.95	128.60
80	A6	1241	G	C5-N7-C8	-5.31	101.65	104.30
80	A6	1457	C	C4-C5-C6	5.31	120.05	117.40
36	A5	799	G	C5-C6-N1	5.31	114.15	111.50
36	A5	1110	U	N1-C2-N3	-5.31	111.72	114.90
36	A5	2175	U	C2-N1-C1'	-5.31	111.33	117.70
36	A1	249	U	N3-C2-O2	-5.30	118.49	122.20
36	A1	626	U	N3-C4-C5	5.30	117.78	114.60
36	A1	1877	U	N3-C4-C5	5.30	117.78	114.60
37	A3	29	C	C6-N1-C2	-5.30	118.18	120.30
80	A6	944	A	C2-N3-C4	-5.30	107.95	110.60
20	CS	116	LEU	CA-CB-CG	5.30	127.50	115.30
36	A5	587	U	N3-C4-O4	-5.30	115.69	119.40
36	A5	637	C	C2-N3-C4	-5.30	117.25	119.90
36	A5	924	G	C5-C6-O6	-5.30	125.42	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2572	C	C6-N1-C1'	-5.30	114.44	120.80
36	A5	3173	G	C4-C5-N7	5.30	112.92	110.80
38	A8	95	G	N3-C4-N9	-5.30	122.82	126.00
80	A6	1244	A	C2-N3-C4	5.30	113.25	110.60
7	CF	70	VAL	CB-CA-C	-5.30	101.32	111.40
36	A5	1846	C	C6-N1-C2	5.30	122.42	120.30
24	AW	93	LEU	CA-CB-CG	5.30	127.49	115.30
36	A1	16	A	C2-N3-C4	-5.30	107.95	110.60
36	A1	428	A	N1-C2-N3	5.30	131.95	129.30
36	A1	1201	C	N3-C4-C5	-5.30	119.78	121.90
36	A1	1387	G	C5-C6-N1	-5.30	108.85	111.50
36	A1	1513	G	C5-C6-N1	5.30	114.15	111.50
36	A1	2147	A	C6-N1-C2	-5.30	115.42	118.60
36	A1	2311	G	C5-N7-C8	-5.30	101.65	104.30
80	A6	1035	G	C6-C5-N7	5.30	133.58	130.40
36	A5	1315	U	C6-N1-C2	5.30	124.18	121.00
36	A5	1378	U	N3-C4-C5	5.30	117.78	114.60
36	A5	2279	A	C2-N3-C4	-5.30	107.95	110.60
36	A5	3385	U	C5-C6-N1	-5.30	120.05	122.70
1	A2	583	C	C2-N1-C1'	5.30	124.63	118.80
36	A1	921	A	C5-C6-N6	-5.30	119.46	123.70
36	A1	1209	G	C4-C5-N7	-5.30	108.68	110.80
36	A1	1887	A	C2-N3-C4	-5.30	107.95	110.60
36	A1	2615	G	N3-C2-N2	-5.30	116.19	119.90
37	A3	96	U	N3-C4-C5	5.30	117.78	114.60
80	A6	1754	A	N9-C4-C5	5.30	107.92	105.80
36	A5	2632	G	N3-C2-N2	5.30	123.61	119.90
36	A5	2884	C	C5-C4-N4	-5.30	116.49	120.20
51	DN	174	ILE	CG1-CB-CG2	-5.30	99.74	111.40
1	A2	1119	G	N3-C4-C5	-5.30	125.95	128.60
36	A1	726	G	C8-N9-C4	-5.30	104.28	106.40
36	A1	2361	A	N7-C8-N9	5.30	116.45	113.80
36	A1	2940	A	C4-C5-N7	-5.30	108.05	110.70
36	A5	637	C	C6-N1-C1'	5.30	127.16	120.80
36	A5	961	C	C5-C6-N1	-5.30	118.35	121.00
36	A1	221	A	N1-C2-N3	5.30	131.95	129.30
36	A1	1929	G	N7-C8-N9	-5.30	110.45	113.10
80	A6	1272	U	N3-C4-C5	-5.30	111.42	114.60
36	A5	661	G	C5-C6-O6	5.30	131.78	128.60
36	A5	1741	A	N1-C2-N3	5.30	131.95	129.30
36	A5	2893	C	N3-C2-O2	5.30	125.61	121.90
37	A7	35	C	N1-C2-O2	-5.30	115.72	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	DY	103	LYS	CD-CE-NZ	-5.30	99.52	111.70
80	A6	1072	C	N3-C4-C5	5.29	124.02	121.90
36	A5	979	U	C2-N1-C1'	5.29	124.05	117.70
36	A5	2213	A	N7-C8-N9	-5.29	111.15	113.80
1	A2	1763	A	C5-N7-C8	-5.29	101.25	103.90
36	A1	895	A	C6-N1-C2	5.29	121.78	118.60
36	A1	2177	G	C6-N1-C2	-5.29	121.92	125.10
36	A1	2435	G	C2-N3-C4	5.29	114.55	111.90
36	A1	2678	A	C8-N9-C4	-5.29	103.68	105.80
36	A5	656	A	C5-N7-C8	5.29	106.55	103.90
36	A5	960	U	C6-N1-C1'	-5.29	113.79	121.20
36	A5	1050	U	C5-C4-O4	5.29	129.08	125.90
36	A5	1126	G	C5-C6-N1	-5.29	108.85	111.50
36	A5	1140	G	N3-C4-N9	5.29	129.18	126.00
36	A5	1846	C	N1-C2-N3	5.29	122.91	119.20
36	A5	1917	C	C4-C5-C6	5.29	120.05	117.40
36	A5	2359	C	N3-C4-N4	-5.29	114.30	118.00
37	A7	14	U	N1-C2-N3	5.29	118.08	114.90
1	A2	319	U	N1-C2-N3	-5.29	111.73	114.90
36	A1	817	A	N3-C4-C5	-5.29	123.10	126.80
54	BQ	138	LEU	CA-CB-CG	5.29	127.47	115.30
6	CE	38	LEU	CA-CB-CG	5.29	127.47	115.30
36	A5	381	U	C5-C6-N1	-5.29	120.05	122.70
36	A5	2279	A	C5-N7-C8	-5.29	101.25	103.90
36	A5	2525	G	C8-N9-C4	5.29	108.52	106.40
36	A5	2665	U	C5-C6-N1	5.29	125.35	122.70
36	A5	2721	A	N3-C4-C5	-5.29	123.10	126.80
36	A5	2882	U	N3-C4-O4	-5.29	115.69	119.40
1	A2	1086	A	C5-C6-N1	5.29	120.34	117.70
36	A1	517	G	C2-N3-C4	5.29	114.55	111.90
36	A1	2364	G	N1-C6-O6	5.29	123.07	119.90
36	A1	2400	G	N1-C6-O6	5.29	123.07	119.90
36	A5	1369	A	N1-C2-N3	-5.29	126.66	129.30
36	A5	2370	G	N3-C4-N9	5.29	129.17	126.00
1	A2	12	U	N3-C2-O2	-5.29	118.50	122.20
1	A2	1200	G	C8-N9-C4	-5.29	104.28	106.40
1	A2	1370	U	C2-N1-C1'	5.29	124.05	117.70
36	A1	794	U	C5-C4-O4	5.29	129.07	125.90
36	A1	931	C	N1-C2-N3	5.29	122.90	119.20
36	A1	1904	C	C5-C6-N1	5.29	123.64	121.00
36	A1	2651	G	N7-C8-N9	-5.29	110.46	113.10
46	BH	166	ARG	CG-CD-NE	5.29	122.91	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	296	U	N3-C4-C5	5.29	117.77	114.60
80	A6	420	A	C5-N7-C8	-5.29	101.26	103.90
80	A6	1000	C	N1-C2-N3	5.29	122.90	119.20
36	A5	905	U	C2-N3-C4	-5.29	123.83	127.00
36	A5	1220	U	C5-C6-N1	-5.29	120.06	122.70
1	A2	387	A	N1-C6-N6	-5.29	115.43	118.60
36	A1	639	G	C4-C5-C6	5.29	121.97	118.80
36	A1	1565	G	N7-C8-N9	5.29	115.74	113.10
36	A1	2395	G	C5-N7-C8	5.29	106.94	104.30
36	A1	2989	U	N1-C2-N3	5.29	118.07	114.90
36	A5	929	A	C5-N7-C8	5.29	106.54	103.90
36	A5	992	A	C8-N9-C4	5.29	107.92	105.80
36	A5	1929	G	C2-N3-C4	-5.29	109.26	111.90
36	A5	3171	U	C6-N1-C2	5.29	124.17	121.00
1	A2	151	G	C5-C6-N1	5.29	114.14	111.50
36	A1	811	U	C2-N3-C4	-5.29	123.83	127.00
36	A1	835	G	C5-C6-O6	-5.29	125.43	128.60
36	A1	3207	U	C6-N1-C1'	5.29	128.60	121.20
36	A5	406	G	O4'-C1'-N9	5.29	112.43	108.20
36	A5	975	C	N1-C2-N3	5.29	122.90	119.20
36	A5	1828	A	C2-N3-C4	-5.29	107.96	110.60
36	A5	2506	U	C5-C6-N1	5.29	125.34	122.70
36	A5	2648	G	N9-C4-C5	-5.29	103.29	105.40
1	A2	1520	U	C5-C6-N1	-5.28	120.06	122.70
36	A1	1587	A	C5-C6-N1	5.28	120.34	117.70
80	A6	251	A	C2-N3-C4	-5.28	107.96	110.60
80	A6	1466	G	C5-C6-N1	-5.28	108.86	111.50
12	CK	88	PRO	N-CA-CB	5.28	109.64	103.30
36	A5	1190	A	C4-N9-C1'	5.28	135.81	126.30
36	A5	1421	G	N3-C4-C5	5.28	131.24	128.60
36	A5	2374	C	C5-C4-N4	5.28	123.90	120.20
36	A5	1007	U	N3-C4-C5	5.28	117.77	114.60
36	A5	1445	U	N1-C2-O2	-5.28	119.10	122.80
36	A5	2549	G	C5-N7-C8	-5.28	101.66	104.30
1	A2	1200	G	N7-C8-N9	5.28	115.74	113.10
36	A1	355	A	C8-N9-C4	5.28	107.91	105.80
36	A1	796	U	N3-C2-O2	5.28	125.90	122.20
36	A1	1916	U	N3-C4-C5	5.28	117.77	114.60
36	A1	3208	G	N3-C2-N2	-5.28	116.20	119.90
36	A1	3334	U	N1-C2-N3	5.28	118.07	114.90
37	A3	120	C	C6-N1-C2	5.28	122.41	120.30
80	A6	1455	G	N3-C2-N2	-5.28	116.20	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2422	C	N3-C4-C5	5.28	124.01	121.90
36	A5	2763	U	C5-C4-O4	-5.28	122.73	125.90
36	A5	2956	A	C5-C6-N1	-5.28	115.06	117.70
36	A1	3101	G	N1-C6-O6	-5.28	116.73	119.90
36	A1	3103	A	C2-N3-C4	-5.28	107.96	110.60
36	A1	3127	A	N9-C4-C5	5.28	107.91	105.80
36	A5	1180	A	C2-N3-C4	-5.28	107.96	110.60
36	A5	2279	A	N1-C6-N6	5.28	121.77	118.60
1	A2	1334	U	N1-C2-N3	5.28	118.07	114.90
36	A1	702	C	N3-C4-N4	5.28	121.69	118.00
36	A1	811	U	C5-C6-N1	-5.28	120.06	122.70
36	A1	1005	G	C8-N9-C4	-5.28	104.29	106.40
36	A1	1369	A	C2-N3-C4	-5.28	107.96	110.60
36	A1	2124	G	C5-C6-O6	-5.28	125.43	128.60
36	A1	2192	C	C4-C5-C6	5.28	120.04	117.40
36	A1	3256	G	C2-N3-C4	5.28	114.54	111.90
38	A4	1	A	C5-N7-C8	-5.28	101.26	103.90
80	A6	800	U	C5-C4-O4	5.28	129.07	125.90
80	A6	1389	C	N1-C2-O2	5.28	122.07	118.90
80	A6	1780	G	C4-C5-N7	5.28	112.91	110.80
36	A5	35	A	N1-C2-N3	5.28	131.94	129.30
36	A5	1080	A	N1-C2-N3	5.28	131.94	129.30
36	A5	1500	G	N7-C8-N9	-5.28	110.46	113.10
36	A5	2144	A	N1-C6-N6	5.28	121.77	118.60
36	A5	2364	G	C4-C5-N7	-5.28	108.69	110.80
1	A2	1086	A	N1-C6-N6	-5.28	115.44	118.60
1	A2	1195	C	P-O3'-C3'	5.28	126.03	119.70
36	A1	600	G	C6-C5-N7	-5.28	127.23	130.40
36	A1	1132	C	N3-C2-O2	-5.28	118.21	121.90
36	A1	1517	G	C4-C5-N7	-5.28	108.69	110.80
36	A1	1660	C	N1-C2-O2	-5.28	115.73	118.90
36	A1	1899	G	C5-N7-C8	-5.28	101.66	104.30
36	A1	2209	U	C5-C6-N1	5.28	125.34	122.70
38	A4	60	U	N1-C2-N3	5.28	118.06	114.90
54	BQ	24	VAL	CB-CA-C	-5.28	101.38	111.40
80	A6	1456	C	C5-C6-N1	-5.28	118.36	121.00
80	A6	1547	A	N1-C6-N6	-5.28	115.44	118.60
51	DN	201	ARG	NE-CZ-NH1	5.28	122.94	120.30
36	A1	3147	G	N1-C6-O6	-5.27	116.74	119.90
80	A6	946	U	N3-C4-C5	-5.27	111.44	114.60
36	A5	1203	A	N1-C6-N6	5.27	121.77	118.60
36	A5	2755	C	C4-C5-C6	5.27	120.04	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A7	48	U	N3-C2-O2	5.27	125.89	122.20
1	A2	1170	G	C5-C6-O6	-5.27	125.44	128.60
36	A1	313	A	C6-N1-C2	-5.27	115.44	118.60
36	A1	344	A	C2-N3-C4	5.27	113.24	110.60
36	A1	1131	G	N9-C4-C5	-5.27	103.29	105.40
36	A1	1550	C	N1-C2-O2	-5.27	115.74	118.90
36	A1	1897	G	C4-C5-C6	5.27	121.96	118.80
36	A1	2413	A	C6-N1-C2	5.27	121.76	118.60
36	A1	3325	G	C4-C5-N7	-5.27	108.69	110.80
80	A6	1295	G	N3-C2-N2	-5.27	116.21	119.90
1	A2	1761	U	N1-C2-N3	5.27	118.06	114.90
36	A1	1182	A	N1-C6-N6	5.27	121.76	118.60
51	BN	85	THR	CB-CA-C	-5.27	97.37	111.60
1	A2	1614	A	N1-C6-N6	5.27	121.76	118.60
36	A1	1691	U	C5-C6-N1	-5.27	120.06	122.70
36	A1	1751	G	N1-C6-O6	-5.27	116.74	119.90
36	A1	1893	A	N9-C4-C5	5.27	107.91	105.80
36	A1	2413	A	C2-N3-C4	5.27	113.23	110.60
36	A1	2909	U	C4-C5-C6	5.27	122.86	119.70
42	BD	41	LYS	CD-CE-NZ	5.27	123.82	111.70
80	A6	1031	U	N3-C2-O2	5.27	125.89	122.20
80	A6	1094	G	N3-C4-C5	-5.27	125.97	128.60
80	A6	1423	U	C2-N3-C4	-5.27	123.84	127.00
36	A5	1714	A	C2-N3-C4	-5.27	107.97	110.60
36	A5	2158	A	C5-C6-N1	5.27	120.33	117.70
36	A5	2191	U	C4-C5-C6	5.27	122.86	119.70
36	A5	2321	A	C8-N9-C4	5.27	107.91	105.80
36	A5	2524	A	C2-N3-C4	-5.27	107.97	110.60
36	A5	2921	U	N1-C2-N3	5.27	118.06	114.90
36	A5	2928	C	C2-N1-C1'	5.27	124.60	118.80
36	A5	3052	G	C5-N7-C8	5.27	106.94	104.30
1	A2	1297	G	C4-N9-C1'	-5.27	119.65	126.50
36	A1	375	A	C5-N7-C8	-5.27	101.27	103.90
36	A1	761	A	N1-C2-N3	5.27	131.93	129.30
36	A1	1506	A	C8-N9-C4	-5.27	103.69	105.80
80	A6	1114	G	N3-C4-N9	5.27	129.16	126.00
36	A5	813	G	N3-C4-C5	-5.27	125.97	128.60
36	A5	1724	U	P-O3'-C3'	5.27	126.02	119.70
36	A5	2211	U	C6-N1-C2	-5.27	117.84	121.00
36	A5	2606	G	C6-C5-N7	-5.27	127.24	130.40
36	A5	2692	A	C4-C5-N7	-5.27	108.07	110.70
36	A5	3309	G	C2-N3-C4	5.27	114.53	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1227	C	C6-N1-C2	-5.27	118.19	120.30
36	A5	997	A	C8-N9-C4	-5.27	103.69	105.80
36	A5	2163	C	N3-C4-C5	5.27	124.01	121.90
1	A2	1245	G	N3-C4-N9	-5.26	122.84	126.00
36	A1	658	G	N3-C2-N2	-5.26	116.22	119.90
36	A1	1358	C	C6-N1-C2	5.26	122.41	120.30
80	A6	449	C	C5-C6-N1	-5.26	118.37	121.00
80	A6	1675	C	C4-C5-C6	5.26	120.03	117.40
36	A5	141	C	C6-N1-C2	-5.26	118.19	120.30
36	A5	186	U	N1-C2-O2	5.26	126.49	122.80
36	A5	1305	U	C5-C6-N1	-5.26	120.07	122.70
36	A5	1310	G	C5-C6-N1	5.26	114.13	111.50
36	A5	2798	C	N3-C4-C5	-5.26	119.79	121.90
36	A1	21	G	N3-C4-C5	-5.26	125.97	128.60
36	A1	1343	A	N1-C2-N3	5.26	131.93	129.30
36	A5	1939	G	C4-N9-C1'	5.26	133.34	126.50
37	A7	37	G	C8-N9-C4	5.26	108.50	106.40
1	A2	542	A	C5-C6-N1	-5.26	115.07	117.70
36	A1	1332	A	C6-N1-C2	5.26	121.76	118.60
36	A1	2214	A	C5-C6-N1	-5.26	115.07	117.70
36	A1	2286	U	C2-N3-C4	-5.26	123.84	127.00
36	A1	2415	C	N3-C4-C5	5.26	124.00	121.90
80	A6	358	U	N1-C2-N3	5.26	118.06	114.90
80	A6	769	A	N1-C6-N6	-5.26	115.44	118.60
80	A6	1455	G	C8-N9-C4	-5.26	104.30	106.40
25	CX	23	ARG	CG-CD-NE	5.26	122.85	111.80
36	A5	1137	C	N3-C4-C5	-5.26	119.80	121.90
15	AN	22	ALA	C-N-CA	5.26	144.09	122.00
36	A1	373	A	N1-C6-N6	-5.26	115.44	118.60
36	A1	2608	G	C8-N9-C4	5.26	108.50	106.40
40	BB	25	ILE	CB-CA-C	-5.26	101.08	111.60
80	A6	1634	C	N3-C2-O2	-5.26	118.22	121.90
36	A5	282	G	C5-C6-N1	-5.26	108.87	111.50
36	A5	2164	A	C4-C5-C6	5.26	119.63	117.00
36	A5	2790	A	C5-C6-N1	5.26	120.33	117.70
38	A8	147	U	C2-N3-C4	-5.26	123.84	127.00
1	A2	1542	G	N1-C6-O6	-5.26	116.75	119.90
36	A1	426	G	C8-N9-C1'	-5.26	120.17	127.00
36	A1	636	C	C4-C5-C6	5.26	120.03	117.40
36	A1	931	C	N3-C4-C5	5.26	124.00	121.90
36	A1	2940	A	N1-C2-N3	5.26	131.93	129.30
36	A1	3242	G	C4-C5-N7	-5.26	108.70	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A4	102	U	N1-C2-N3	5.26	118.06	114.90
36	A5	693	A	C5-C6-N6	5.26	127.91	123.70
1	A2	971	A	N1-C2-N3	5.26	131.93	129.30
1	A2	1600	A	N3-C4-C5	5.26	130.48	126.80
36	A1	1049	C	C2-N3-C4	-5.26	117.27	119.90
36	A1	1409	G	C5-C6-N1	5.26	114.13	111.50
37	A3	93	C	C2-N3-C4	-5.26	117.27	119.90
38	A4	151	C	C6-N1-C2	-5.26	118.20	120.30
80	A6	1317	C	C6-N1-C2	-5.26	118.20	120.30
36	A5	327	A	N1-C2-N3	-5.26	126.67	129.30
36	A5	1178	G	C5-C6-O6	-5.26	125.45	128.60
36	A5	1327	C	C5-C4-N4	5.26	123.88	120.20
36	A5	3294	A	N1-C2-N3	5.26	131.93	129.30
36	A1	301	G	C5-C6-O6	5.25	131.75	128.60
36	A1	984	G	C6-C5-N7	-5.25	127.25	130.40
36	A1	1171	G	C5-C6-N1	5.25	114.13	111.50
36	A5	1516	C	C4-C5-C6	5.25	120.03	117.40
41	DC	190	GLY	N-CA-C	5.25	126.24	113.10
36	A1	1389	G	N9-C4-C5	-5.25	103.30	105.40
36	A1	1431	G	N1-C6-O6	-5.25	116.75	119.90
36	A1	2606	G	C6-C5-N7	-5.25	127.25	130.40
36	A1	2619	G	C5-C6-N1	5.25	114.13	111.50
36	A5	413	U	C5-C4-O4	-5.25	122.75	125.90
36	A5	494	G	N1-C6-O6	-5.25	116.75	119.90
36	A5	515	C	C5-C4-N4	-5.25	116.52	120.20
36	A5	802	C	N3-C2-O2	-5.25	118.22	121.90
36	A5	1856	C	N3-C2-O2	-5.25	118.22	121.90
36	A5	2271	A	C6-C5-N7	5.25	135.98	132.30
36	A5	2724	U	N3-C4-O4	-5.25	115.72	119.40
36	A5	2965	U	N3-C4-O4	5.25	123.08	119.40
36	A5	3005	A	C8-N9-C4	-5.25	103.70	105.80
1	A2	972	G	N1-C6-O6	-5.25	116.75	119.90
1	A2	1648	A	N1-C6-N6	-5.25	115.45	118.60
36	A1	54	C	C4-C5-C6	-5.25	114.77	117.40
36	A1	1421	G	N7-C8-N9	-5.25	110.47	113.10
36	A1	1515	A	N1-C2-N3	5.25	131.93	129.30
36	A1	2805	G	C2-N3-C4	5.25	114.53	111.90
36	A1	3100	U	N3-C4-C5	-5.25	111.45	114.60
80	A6	1129	U	C6-N1-C2	5.25	124.15	121.00
8	CG	193	LEU	CA-CB-CG	5.25	127.38	115.30
36	A5	831	G	C5-C6-O6	-5.25	125.45	128.60
36	A5	1158	A	N9-C4-C5	-5.25	103.70	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1925	U	N3-C4-C5	5.25	117.75	114.60
36	A5	2979	U	N1-C2-N3	-5.25	111.75	114.90
36	A1	2381	G	C5-N7-C8	5.25	106.92	104.30
36	A1	2645	G	N3-C2-N2	-5.25	116.22	119.90
80	A6	864	U	N1-C2-N3	5.25	118.05	114.90
36	A5	365	A	C4-C5-N7	5.25	113.33	110.70
36	A5	1792	C	C5-C6-N1	-5.25	118.38	121.00
36	A1	655	C	N1-C2-N3	5.25	122.87	119.20
36	A1	804	C	C6-N1-C1'	5.25	127.10	120.80
36	A1	1807	G	N7-C8-N9	5.25	115.72	113.10
36	A1	2912	G	C5-C6-O6	-5.25	125.45	128.60
36	A1	2996	U	N3-C2-O2	-5.25	118.53	122.20
80	A6	576	G	N3-C4-C5	-5.25	125.97	128.60
5	CD	202	LEU	CA-CB-CG	5.25	127.37	115.30
36	A5	318	A	N1-C2-N3	-5.25	126.67	129.30
36	A5	2851	A	C2-N3-C4	-5.25	107.98	110.60
36	A5	3339	A	N1-C6-N6	5.25	121.75	118.60
52	DO	182[B]	SER	CA-C-N	5.25	128.75	117.20
36	A1	1156	C	N3-C2-O2	-5.25	118.23	121.90
41	BC	198	ARG	NE-CZ-NH2	-5.25	117.68	120.30
36	A5	1100	U	N3-C4-C5	5.25	117.75	114.60
36	A5	1208	U	N1-C2-O2	5.25	126.47	122.80
36	A5	1432	C	C2-N1-C1'	5.25	124.57	118.80
1	A2	582	U	C5-C6-N1	5.25	125.32	122.70
36	A1	1131	G	N3-C2-N2	5.25	123.57	119.90
36	A1	2644	C	N3-C2-O2	-5.25	118.23	121.90
68	Be	16	LYS	CD-CE-NZ	5.25	123.76	111.70
80	A6	106	U	N3-C4-C5	5.25	117.75	114.60
36	A5	496	C	N1-C2-O2	5.25	122.05	118.90
36	A5	928	C	C6-N1-C2	-5.25	118.20	120.30
36	A5	2207	A	C4-C5-N7	5.25	113.32	110.70
47	DI	99	ILE	CB-CA-C	-5.25	101.11	111.60
1	A2	1454	G	C4-C5-N7	-5.24	108.70	110.80
36	A1	801	A	C6-N1-C2	5.24	121.75	118.60
36	A1	1337	A	N1-C2-N3	-5.24	126.68	129.30
80	A6	876	G	C4-C5-C6	5.24	121.95	118.80
80	A6	1282	U	N3-C2-O2	5.24	125.87	122.20
36	A5	404	G	C4-C5-N7	-5.24	108.70	110.80
36	A5	1603	A	C5-C6-N1	-5.24	115.08	117.70
36	A5	1901	A	C8-N9-C1'	-5.24	118.26	127.70
38	A8	77	A	C2-N3-C4	-5.24	107.98	110.60
38	A8	79	A	C4-C5-N7	5.24	113.32	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	608	U	C5-C6-N1	-5.24	120.08	122.70
36	A1	1160	C	C2-N3-C4	5.24	122.52	119.90
36	A1	1549	U	C6-N1-C1'	-5.24	113.86	121.20
80	A6	1328	G	N9-C4-C5	-5.24	103.30	105.40
36	A5	3335	A	C5-N7-C8	-5.24	101.28	103.90
16	AO	107	ARG	NE-CZ-NH2	5.24	122.92	120.30
36	A1	111	C	C6-N1-C2	5.24	122.40	120.30
36	A1	158	G	C2-N3-C4	-5.24	109.28	111.90
36	A1	696	C	C4-C5-C6	-5.24	114.78	117.40
80	A6	232	U	N3-C2-O2	-5.24	118.53	122.20
80	A6	870	C	C5-C6-N1	-5.24	118.38	121.00
36	A5	218	G	N1-C6-O6	-5.24	116.75	119.90
36	A5	719	U	N3-C2-O2	-5.24	118.53	122.20
36	A5	1834	U	C5-C6-N1	-5.24	120.08	122.70
36	A5	2403	G	N3-C4-N9	5.24	129.14	126.00
36	A5	2604	U	N3-C4-C5	-5.24	111.45	114.60
1	A2	1148	C	N3-C4-C5	5.24	124.00	121.90
36	A1	1303	A	N1-C2-N3	-5.24	126.68	129.30
36	A1	2888	U	C6-N1-C2	5.24	124.14	121.00
36	A1	3072	C	N3-C2-O2	-5.24	118.23	121.90
36	A5	576	C	C2-N3-C4	-5.24	117.28	119.90
36	A5	1116	G	C5-C6-N1	-5.24	108.88	111.50
36	A5	1545	A	C8-N9-C4	5.24	107.90	105.80
36	A5	2852	C	N1-C2-O2	-5.24	115.76	118.90
37	A7	100	C	C2-N3-C4	-5.24	117.28	119.90
36	A1	53	G	C2-N3-C4	-5.24	109.28	111.90
36	A1	1848	G	N1-C2-N3	5.24	127.04	123.90
36	A1	2602	G	N7-C8-N9	-5.24	110.48	113.10
1	A2	1015	U	N1-C2-O2	5.24	126.47	122.80
80	A6	379	U	N1-C2-O2	-5.24	119.14	122.80
80	A6	561	G	C8-N9-C4	-5.24	104.31	106.40
36	A5	784	A	C4-C5-N7	5.24	113.32	110.70
36	A5	808	A	C6-N1-C2	5.24	121.74	118.60
36	A5	1325	U	N1-C2-N3	5.24	118.04	114.90
36	A5	2213	A	C5-N7-C8	5.24	106.52	103.90
38	A8	113	U	C5-C4-O4	-5.24	122.76	125.90
36	A5	568	G	N1-C6-O6	-5.23	116.76	119.90
36	A5	2344	U	N1-C2-N3	5.23	118.04	114.90
36	A5	3094	A	C5-N7-C8	5.23	106.52	103.90
37	A7	1	G	C4-C5-N7	5.23	112.89	110.80
1	A2	938	G	N3-C2-N2	5.23	123.56	119.90
1	A2	1258	U	N1-C2-N3	5.23	118.04	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1391	C	C2-N3-C4	-5.23	117.28	119.90
36	A1	2184	U	C6-N1-C1'	-5.23	113.87	121.20
36	A1	2533	G	N3-C4-C5	-5.23	125.98	128.60
36	A1	2606	G	C8-N9-C1'	-5.23	120.20	127.00
80	A6	794	U	N3-C2-O2	-5.23	118.54	122.20
36	A5	1693	C	N1-C2-O2	-5.23	115.76	118.90
36	A5	2118	C	C5-C4-N4	5.23	123.86	120.20
36	A5	2930	A	N1-C2-N3	-5.23	126.68	129.30
55	DR	42	ARG	NE-CZ-NH2	-5.23	117.68	120.30
36	A1	643	U	C5-C6-N1	5.23	125.32	122.70
36	A1	2169	G	N9-C4-C5	5.23	107.49	105.40
36	A1	2776	C	C5-C4-N4	-5.23	116.54	120.20
80	A6	484	C	C5-C4-N4	-5.23	116.54	120.20
80	A6	1274	C	C5-C4-N4	5.23	123.86	120.20
80	A6	1638	G	C4-C5-N7	-5.23	108.71	110.80
36	A5	432	G	N3-C2-N2	5.23	123.56	119.90
36	A5	804	C	C2-N1-C1'	-5.23	113.05	118.80
36	A5	1404	G	N1-C2-N2	-5.23	111.49	116.20
36	A5	1603	A	C4-C5-C6	5.23	119.61	117.00
36	A5	1655	G	C5-N7-C8	-5.23	101.69	104.30
36	A5	2897	A	N7-C8-N9	-5.23	111.19	113.80
48	DJ	10	ARG	NE-CZ-NH2	-5.23	117.69	120.30
54	DQ	178	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A2	440	U	N1-C2-O2	5.23	126.46	122.80
1	A2	1188	G	C8-N9-C4	5.23	108.49	106.40
36	A1	22	G	C6-N1-C2	-5.23	121.96	125.10
36	A1	806	A	N9-C4-C5	-5.23	103.71	105.80
38	A4	74	U	N1-C2-N3	5.23	118.04	114.90
80	A6	1605	G	N1-C6-O6	-5.23	116.76	119.90
36	A5	227	G	N1-C6-O6	5.23	123.04	119.90
1	A2	647	G	C8-N9-C4	-5.23	104.31	106.40
1	A2	971	A	C2-N3-C4	-5.23	107.99	110.60
1	A2	1116	A	N1-C6-N6	5.23	121.74	118.60
36	A1	72	C	C5-C6-N1	-5.23	118.39	121.00
36	A1	652	G	N3-C4-C5	-5.23	125.99	128.60
36	A1	1578	C	C6-N1-C2	-5.23	118.21	120.30
36	A1	2350	C	N1-C2-N3	5.23	122.86	119.20
36	A1	2887	A	C4-C5-N7	5.23	113.31	110.70
80	A6	1300	A	N1-C6-N6	-5.23	115.46	118.60
36	A5	299	G	C5-C6-N1	5.23	114.11	111.50
36	A5	333	G	C2-N3-C4	-5.23	109.29	111.90
36	A5	894	G	C4-C5-N7	5.23	112.89	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2772	C	P-O3'-C3'	5.23	125.97	119.70
1	A2	139	C	C4-C5-C6	5.23	120.01	117.40
36	A1	363	G	N1-C6-O6	5.23	123.04	119.90
36	A1	1878	G	N1-C6-O6	5.23	123.04	119.90
36	A1	2725	U	N3-C4-O4	-5.23	115.74	119.40
80	A6	1260	U	N1-C2-O2	5.23	126.46	122.80
36	A5	46	U	N1-C2-N3	-5.23	111.76	114.90
36	A5	75	G	C5-C6-N1	5.23	114.11	111.50
36	A5	903	U	N3-C4-C5	5.23	117.73	114.60
36	A5	2245	C	N1-C2-N3	5.23	122.86	119.20
64	Da	15	VAL	N-CA-C	-5.23	96.89	111.00
36	A1	378	A	C4-C5-C6	5.22	119.61	117.00
36	A1	1044	U	N3-C4-C5	5.22	117.73	114.60
37	A3	71	G	N3-C2-N2	5.22	123.56	119.90
80	A6	1681	A	C5-N7-C8	-5.22	101.29	103.90
80	A6	1730	A	C5-C6-N6	-5.22	119.52	123.70
36	A5	857	G	N1-C2-N2	-5.22	111.50	116.20
36	A5	1828	A	N7-C8-N9	5.22	116.41	113.80
36	A5	2391	G	C5-C6-O6	5.22	131.73	128.60
36	A5	3247	G	C4-C5-N7	-5.22	108.71	110.80
38	A8	121	U	N3-C2-O2	-5.22	118.54	122.20
1	A2	308	C	C6-N1-C2	5.22	122.39	120.30
1	A2	1363	U	N3-C2-O2	-5.22	118.54	122.20
1	A2	1462	G	N3-C4-N9	5.22	129.13	126.00
1	A2	1600	A	C6-C5-N7	-5.22	128.64	132.30
1	A2	1600	A	N1-C2-N3	5.22	131.91	129.30
36	A1	28	C	C5-C6-N1	-5.22	118.39	121.00
64	Ba	55	LYS	CD-CE-NZ	-5.22	99.69	111.70
36	A5	1114	U	C2-N3-C4	-5.22	123.87	127.00
36	A5	1733	G	C6-C5-N7	-5.22	127.27	130.40
36	A5	2148	U	N1-C2-N3	5.22	118.03	114.90
36	A1	335	G	N7-C8-N9	5.22	115.71	113.10
36	A1	346	C	N3-C2-O2	-5.22	118.25	121.90
36	A1	1313	G	C6-N1-C2	-5.22	121.97	125.10
80	A6	539	G	C2-N3-C4	-5.22	109.29	111.90
14	CM	58	LEU	CA-CB-CG	5.22	127.31	115.30
1	A2	137	U	N3-C2-O2	-5.22	118.55	122.20
1	A2	987	G	C8-N9-C4	5.22	108.49	106.40
1	A2	1293	U	N3-C2-O2	-5.22	118.55	122.20
36	A1	1337	A	C8-N9-C4	-5.22	103.71	105.80
36	A1	2190	U	N3-C4-C5	5.22	117.73	114.60
36	A1	2238	G	C5-C6-O6	-5.22	125.47	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2984	C	N3-C2-O2	-5.22	118.25	121.90
71	Bh	69	LEU	CA-CB-CG	5.22	127.30	115.30
80	A6	791	A	N7-C8-N9	5.22	116.41	113.80
80	A6	1310	U	N3-C4-O4	-5.22	115.75	119.40
36	A5	2139	A	N1-C6-N6	-5.22	115.47	118.60
36	A5	2228	A	N7-C8-N9	5.22	116.41	113.80
36	A5	2379	U	C5-C6-N1	-5.22	120.09	122.70
36	A5	3028	G	N1-C2-N2	-5.22	111.50	116.20
38	A8	109	A	C5-C6-N1	5.22	120.31	117.70
36	A5	197	G	C4-N9-C1'	5.22	133.28	126.50
36	A5	341	G	C4-C5-N7	5.22	112.89	110.80
36	A5	682	U	C2-N3-C4	-5.22	123.87	127.00
36	A5	972	A	C5-N7-C8	5.22	106.51	103.90
36	A5	1167	U	N3-C2-O2	5.22	125.85	122.20
1	A2	1611	A	C6-C5-N7	-5.22	128.65	132.30
36	A1	2953	U	C5-C6-N1	-5.22	120.09	122.70
36	A1	3298	C	N3-C2-O2	5.22	125.55	121.90
36	A5	815	G	N3-C4-C5	-5.22	125.99	128.60
36	A5	868	C	C6-N1-C2	5.22	122.39	120.30
36	A5	1149	G	C4-C5-N7	-5.22	108.71	110.80
36	A5	1324	U	N3-C2-O2	-5.22	118.55	122.20
36	A5	1604	G	N3-C4-C5	-5.22	125.99	128.60
36	A5	2716	U	C5-C4-O4	5.22	129.03	125.90
36	A5	2841	G	N3-C2-N2	5.22	123.55	119.90
37	A7	41	G	C4-C5-N7	5.22	112.89	110.80
36	A1	1010	G	C2-N3-C4	5.21	114.51	111.90
36	A1	1310	G	C4-C5-N7	5.21	112.89	110.80
36	A1	2279	A	N3-C4-N9	5.21	131.57	127.40
36	A1	2965	U	C5-C6-N1	-5.21	120.09	122.70
80	A6	300	A	N7-C8-N9	-5.21	111.19	113.80
36	A5	1527	C	N1-C2-O2	5.21	122.03	118.90
36	A5	2375	G	C5-N7-C8	-5.21	101.69	104.30
36	A5	2721	A	C5-C6-N1	5.21	120.31	117.70
1	A2	63	G	C5-C6-O6	5.21	131.73	128.60
80	A6	1108	G	N1-C6-O6	-5.21	116.77	119.90
80	A6	1522	U	C2-N1-C1'	-5.21	111.44	117.70
36	A5	84	U	N3-C4-O4	5.21	123.05	119.40
36	A5	307	A	N9-C4-C5	5.21	107.89	105.80
36	A5	625	G	N3-C4-N9	-5.21	122.87	126.00
36	A5	1153	A	C5-C6-N6	-5.21	119.53	123.70
36	A5	3106	A	C8-N9-C4	-5.21	103.72	105.80
1	A2	687	G	N3-C4-N9	-5.21	122.87	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	634	C	C5-C6-N1	-5.21	118.39	121.00
36	A1	880	G	C8-N9-C1'	5.21	133.77	127.00
36	A1	912	G	C5-C6-O6	-5.21	125.47	128.60
36	A1	1075	A	C8-N9-C4	5.21	107.89	105.80
36	A1	1173	U	N3-C4-O4	-5.21	115.75	119.40
36	A1	1640	G	C4-C5-N7	5.21	112.88	110.80
36	A1	2596	U	C5-C4-O4	-5.21	122.77	125.90
36	A1	2794	G	C8-N9-C1'	5.21	133.78	127.00
36	A1	3110	C	C2-N1-C1'	5.21	124.53	118.80
36	A1	3318	G	C4-C5-C6	5.21	121.93	118.80
80	A6	611	U	N1-C2-O2	-5.21	119.15	122.80
36	A5	410	U	C5-C6-N1	-5.21	120.09	122.70
36	A5	817	A	N9-C4-C5	5.21	107.89	105.80
36	A5	2629	U	C2-N3-C4	-5.21	123.87	127.00
38	A8	45	C	C4-C5-C6	5.21	120.01	117.40
1	A2	811	A	N3-C4-C5	-5.21	123.15	126.80
49	BL	36	ARG	NE-CZ-NH1	-5.21	117.69	120.30
36	A5	329	U	C6-N1-C2	5.21	124.13	121.00
37	A7	88	G	N1-C6-O6	-5.21	116.77	119.90
1	A2	7	G	N9-C4-C5	5.21	107.48	105.40
36	A1	1345	G	N7-C8-N9	5.21	115.70	113.10
36	A1	1780	G	C8-N9-C1'	-5.21	120.23	127.00
80	A6	628	G	N1-C6-O6	-5.21	116.78	119.90
80	A6	1000	C	C2-N3-C4	-5.21	117.30	119.90
80	A6	1123	C	N3-C4-C5	5.21	123.98	121.90
80	A6	1483	A	N1-C6-N6	5.21	121.72	118.60
80	A6	1665	U	C5-C6-N1	5.21	125.31	122.70
36	A5	1518	U	C4-C5-C6	-5.21	116.57	119.70
36	A5	2934	A	N1-C6-N6	-5.21	115.47	118.60
36	A5	3103	A	C6-N1-C2	-5.21	115.47	118.60
36	A5	3381	U	C5-C6-N1	-5.21	120.09	122.70
1	A2	1648	A	C5-C6-N1	5.21	120.30	117.70
36	A1	500	C	N1-C2-N3	5.21	122.84	119.20
36	A1	3042	U	C5-C6-N1	-5.21	120.10	122.70
36	A5	689	U	N3-C4-C5	5.21	117.72	114.60
36	A5	1013	G	C4-N9-C1'	5.21	133.27	126.50
36	A5	3098	G	N3-C2-N2	5.21	123.55	119.90
36	A5	3124	G	C4-C5-N7	-5.21	108.72	110.80
36	A5	3315	G	C4-C5-N7	-5.21	108.72	110.80
38	A8	99	C	C5-C6-N1	-5.21	118.40	121.00
1	A2	1784	C	N3-C4-C5	5.21	123.98	121.90
36	A5	1704	A	C8-N9-C4	5.21	107.88	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2732	G	C5-N7-C8	5.21	106.90	104.30
37	A7	40	C	C2-N3-C4	-5.21	117.30	119.90
1	A2	391	A	C4-C5-C6	-5.20	114.40	117.00
36	A1	1817	G	C4-N9-C1'	-5.20	119.74	126.50
36	A1	3203	U	N1-C2-O2	5.20	126.44	122.80
38	A4	137	C	C6-N1-C2	5.20	122.38	120.30
49	BL	27	ASP	CB-CG-OD2	5.20	122.98	118.30
80	A6	941	A	C5-C6-N6	5.20	127.86	123.70
36	A5	2386	A	C4-C5-N7	5.20	113.30	110.70
36	A1	1316	C	N1-C2-N3	5.20	122.84	119.20
36	A1	1419	A	C5-N7-C8	5.20	106.50	103.90
36	A5	1833	G	C5-C6-O6	5.20	131.72	128.60
37	A7	11	A	C5-C6-N1	-5.20	115.10	117.70
36	A1	338	A	N1-C6-N6	5.20	121.72	118.60
36	A1	641	C	C5-C6-N1	-5.20	118.40	121.00
36	A1	644	G	N3-C4-N9	-5.20	122.88	126.00
36	A1	1549	U	N3-C2-O2	-5.20	118.56	122.20
80	A6	1414	U	C2-N3-C4	-5.20	123.88	127.00
80	A6	1609	U	N1-C2-O2	-5.20	119.16	122.80
36	A5	735	A	N7-C8-N9	5.20	116.40	113.80
36	A5	861	C	N3-C4-N4	5.20	121.64	118.00
36	A5	1458	U	C5-C4-O4	-5.20	122.78	125.90
36	A5	1876	U	C6-N1-C2	-5.20	117.88	121.00
36	A5	3302	U	C5-C6-N1	-5.20	120.10	122.70
41	DC	98	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A2	149	C	C6-N1-C2	5.20	122.38	120.30
1	A2	1330	G	C8-N9-C1'	5.20	133.76	127.00
36	A1	39	A	N1-C6-N6	5.20	121.72	118.60
36	A1	343	U	C2-N3-C4	-5.20	123.88	127.00
36	A1	1082	U	N3-C2-O2	-5.20	118.56	122.20
36	A1	1481	A	C4-C5-C6	5.20	119.60	117.00
80	A6	452	A	C8-N9-C4	5.20	107.88	105.80
36	A5	881	C	C5-C6-N1	5.20	123.60	121.00
36	A5	999	G	C5-C6-N1	5.20	114.10	111.50
36	A5	1183	C	N3-C4-N4	-5.20	114.36	118.00
36	A5	2364	G	C8-N9-C4	-5.20	104.32	106.40
36	A5	2416	U	N1-C2-N3	5.20	118.02	114.90
36	A5	3075	G	C5-N7-C8	5.20	106.90	104.30
36	A5	3101	G	N3-C2-N2	5.20	123.54	119.90
36	A5	3177	G	C2-N3-C4	-5.20	109.30	111.90
37	A7	50	U	C6-N1-C2	-5.20	117.88	121.00
1	A2	192	U	C5-C6-N1	5.20	125.30	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1000	C	C6-N1-C2	5.20	122.38	120.30
36	A1	28	C	N1-C2-O2	5.20	122.02	118.90
36	A1	809	G	C5-C6-O6	-5.20	125.48	128.60
36	A1	864	G	N3-C4-N9	5.20	129.12	126.00
80	A6	108	A	C6-N1-C2	-5.20	115.48	118.60
36	A5	376	G	N3-C4-C5	-5.20	126.00	128.60
36	A5	559	A	C8-N9-C4	-5.20	103.72	105.80
36	A5	595	G	C5-C6-O6	5.20	131.72	128.60
36	A5	2632	G	C6-N1-C2	5.20	128.22	125.10
1	A2	577	G	C2-N3-C4	-5.20	109.30	111.90
36	A1	981	U	C5-C6-N1	5.20	125.30	122.70
36	A1	1362	G	N9-C4-C5	-5.20	103.32	105.40
36	A1	1857	C	N1-C2-N3	5.20	122.84	119.20
38	A4	48	A	C4-C5-C6	5.20	119.60	117.00
80	A6	1190	C	N3-C2-O2	5.20	125.54	121.90
36	A5	421	G	C5-C6-N1	5.20	114.10	111.50
36	A5	424	G	C5-C6-N1	5.20	114.10	111.50
36	A5	635	G	N3-C4-C5	5.20	131.20	128.60
36	A5	2349	U	N1-C2-O2	5.20	126.44	122.80
36	A5	2406	C	C4-C5-C6	5.20	120.00	117.40
36	A5	2737	C	N1-C2-O2	-5.20	115.78	118.90
38	A8	12	A	C8-N9-C4	-5.20	103.72	105.80
1	A2	871	G	N3-C4-N9	5.19	129.12	126.00
36	A1	2197	C	N1-C2-N3	-5.19	115.56	119.20
80	A6	628	G	C5-C6-O6	5.19	131.72	128.60
80	A6	1170	G	C4-N9-C1'	5.19	133.25	126.50
36	A5	1402	C	N1-C2-O2	5.19	122.02	118.90
36	A5	2960	C	C2-N3-C4	-5.19	117.30	119.90
36	A5	3373	U	C2-N3-C4	-5.19	123.88	127.00
1	A2	361	C	C5-C6-N1	5.19	123.60	121.00
1	A2	460	A	C4-C5-C6	-5.19	114.40	117.00
1	A2	555	A	N9-C4-C5	5.19	107.88	105.80
1	A2	605	A	C8-N9-C4	5.19	107.88	105.80
36	A1	3028	G	N3-C4-N9	5.19	129.12	126.00
36	A1	3180	A	N7-C8-N9	5.19	116.40	113.80
80	A6	1787	C	N3-C4-C5	-5.19	119.82	121.90
36	A5	267	G	N7-C8-N9	-5.19	110.50	113.10
36	A5	1597	C	N3-C4-C5	-5.19	119.82	121.90
36	A5	2112	U	N1-C2-N3	5.19	118.02	114.90
1	A2	380	U	C6-N1-C2	-5.19	117.89	121.00
36	A1	59	G	N9-C4-C5	-5.19	103.32	105.40
36	A1	271	C	N3-C2-O2	-5.19	118.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	614	C	C5-C6-N1	-5.19	118.41	121.00
36	A1	652	G	C5-C6-N1	5.19	114.10	111.50
36	A1	2937	G	C4-C5-N7	-5.19	108.72	110.80
36	A1	3355	U	C5-C6-N1	5.19	125.30	122.70
80	A6	691	C	C2-N1-C1'	5.19	124.51	118.80
80	A6	1185	U	N3-C2-O2	-5.19	118.57	122.20
36	A5	367	A	C2-N3-C4	-5.19	108.00	110.60
36	A5	418	A	C4-C5-C6	5.19	119.59	117.00
36	A5	943	U	C5-C4-O4	-5.19	122.79	125.90
36	A5	2193	U	N1-C2-N3	5.19	118.02	114.90
36	A5	2804	A	C2-N3-C4	-5.19	108.00	110.60
36	A5	3387	U	N3-C2-O2	-5.19	118.57	122.20
44	DF	232	ARG	NE-CZ-NH1	-5.19	117.70	120.30
36	A1	616	G	C6-N1-C2	-5.19	121.99	125.10
36	A1	1081	U	C5-C4-O4	-5.19	122.79	125.90
36	A1	1482	A	N3-C4-C5	-5.19	123.17	126.80
36	A5	1513	G	N1-C6-O6	-5.19	116.79	119.90
36	A5	3333	G	C4-C5-N7	5.19	112.88	110.80
1	A2	1245	G	N3-C4-C5	5.19	131.19	128.60
36	A1	586	C	N1-C2-O2	-5.19	115.79	118.90
36	A1	958	C	C2-N3-C4	-5.19	117.31	119.90
36	A1	1000	C	C4-C5-C6	-5.19	114.81	117.40
36	A1	1580	A	C3'-C2'-C1'	5.19	105.65	101.50
36	A1	2377	G	C5-C6-N1	-5.19	108.91	111.50
36	A1	2757	U	N1-C2-O2	-5.19	119.17	122.80
36	A1	2868	U	N3-C4-O4	-5.19	115.77	119.40
37	A3	96	U	C6-N1-C2	5.19	124.11	121.00
38	A4	36	G	N9-C4-C5	5.19	107.47	105.40
80	A6	95	G	N7-C8-N9	5.19	115.69	113.10
80	A6	113	U	N3-C2-O2	5.19	125.83	122.20
80	A6	610	G	N3-C4-N9	5.19	129.11	126.00
80	A6	613	G	N9-C4-C5	-5.19	103.33	105.40
36	A5	83	U	C6-N1-C1'	-5.19	113.94	121.20
36	A5	582	G	C4-C5-N7	-5.19	108.72	110.80
36	A5	872	U	N3-C4-O4	-5.19	115.77	119.40
36	A5	1485	G	N9-C4-C5	5.19	107.47	105.40
36	A5	2899	C	C2-N3-C4	-5.19	117.31	119.90
37	A7	51	A	C2-N3-C4	5.19	113.19	110.60
36	A1	187	A	C8-N9-C4	-5.19	103.73	105.80
80	A6	317	C	C5-C6-N1	-5.19	118.41	121.00
36	A5	340	C	N3-C2-O2	-5.19	118.27	121.90
36	A5	2695	A	C5-N7-C8	-5.19	101.31	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	445	A	N1-C2-N3	-5.18	126.71	129.30
36	A1	1420	C	C4-C5-C6	5.18	119.99	117.40
36	A1	2307	G	C5-N7-C8	5.18	106.89	104.30
36	A1	2831	G	N1-C6-O6	5.18	123.01	119.90
36	A5	2303	A	C5-C6-N1	5.18	120.29	117.70
36	A5	2724	U	N3-C2-O2	-5.18	118.57	122.20
36	A5	3107	U	N1-C2-O2	5.18	126.43	122.80
52	DO	27[B]	VAL	CA-C-N	5.18	128.61	117.20
63	DZ	121	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A2	139	C	P-O3'-C3'	5.18	125.92	119.70
1	A2	337	G	N3-C4-C5	-5.18	126.01	128.60
1	A2	704	C	C5-C6-N1	5.18	123.59	121.00
36	A1	90	C	C5-C6-N1	-5.18	118.41	121.00
37	A3	3	U	C2-N3-C4	-5.18	123.89	127.00
80	A6	997	G	C5-C6-O6	5.18	131.71	128.60
80	A6	1272	U	C5-C4-O4	5.18	129.01	125.90
80	A6	1396	U	C5-C6-N1	5.18	125.29	122.70
80	A6	1661	U	C2-N3-C4	-5.18	123.89	127.00
36	A5	28	C	C6-N1-C2	5.18	122.37	120.30
36	A5	926	A	C4-C5-C6	-5.18	114.41	117.00
36	A5	1120	A	N1-C6-N6	-5.18	115.49	118.60
36	A5	1205	A	C5-N7-C8	-5.18	101.31	103.90
36	A5	1242	G	C8-N9-C1'	-5.18	120.26	127.00
36	A5	1312	C	C6-N1-C1'	5.18	127.02	120.80
36	A5	1805	C	C6-N1-C2	5.18	122.37	120.30
36	A5	2942	C	C5-C4-N4	-5.18	116.57	120.20
36	A5	3048	A	C5-C6-N1	5.18	120.29	117.70
38	A8	32	C	N3-C2-O2	5.18	125.53	121.90
52	DO	16[B]	LEU	O-C-N	-5.18	114.39	123.20
1	A2	6	G	N3-C4-N9	5.18	129.11	126.00
36	A1	274	G	C5-C6-O6	5.18	131.71	128.60
36	A1	2727	A	N1-C6-N6	-5.18	115.49	118.60
80	A6	777	C	C6-N1-C2	-5.18	118.23	120.30
36	A1	500	C	N3-C2-O2	-5.18	118.27	121.90
36	A1	929	A	N9-C4-C5	5.18	107.87	105.80
36	A1	999	G	N3-C4-C5	-5.18	126.01	128.60
36	A1	1183	C	C5-C6-N1	-5.18	118.41	121.00
36	A5	39	A	N3-C4-C5	-5.18	123.17	126.80
36	A5	610	G	C5-C6-N1	5.18	114.09	111.50
36	A5	809	G	C8-N9-C4	5.18	108.47	106.40
36	A5	902	G	N7-C8-N9	-5.18	110.51	113.10
36	A5	2833	A	C6-C5-N7	5.18	135.93	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A7	90	U	C2-N3-C4	-5.18	123.89	127.00
38	A8	34	U	C2-N3-C4	-5.18	123.89	127.00
38	A8	109	A	C5-N7-C8	-5.18	101.31	103.90
68	De	33	ARG	NE-CZ-NH2	-5.18	117.71	120.30
36	A1	874	U	C6-N1-C2	5.18	124.11	121.00
36	A1	2363	A	C6-C5-N7	5.18	135.93	132.30
80	A6	1305	U	N1-C2-N3	5.18	118.01	114.90
41	DC	230	VAL	CB-CA-C	-5.18	101.56	111.40
1	A2	1171	A	N1-C6-N6	-5.18	115.49	118.60
1	A2	1245	G	C4-N9-C1'	-5.18	119.77	126.50
36	A1	726	G	C4-C5-N7	5.18	112.87	110.80
36	A1	2222	A	N1-C2-N3	5.18	131.89	129.30
36	A1	2341	A	C6-N1-C2	-5.18	115.49	118.60
36	A1	2733	A	N7-C8-N9	-5.18	111.21	113.80
36	A1	2953	U	N1-C2-O2	-5.18	119.18	122.80
36	A1	3176	G	N3-C2-N2	-5.18	116.28	119.90
80	A6	90	C	N3-C2-O2	-5.18	118.28	121.90
80	A6	109	G	C5-N7-C8	5.18	106.89	104.30
80	A6	110	U	N3-C2-O2	-5.18	118.58	122.20
80	A6	209	U	N1-C2-O2	-5.18	119.18	122.80
80	A6	1733	C	C6-N1-C2	-5.18	118.23	120.30
36	A5	80	G	C5-C6-O6	5.18	131.71	128.60
36	A5	1377	G	C8-N9-C4	-5.18	104.33	106.40
36	A5	2526	C	C6-N1-C1'	-5.18	114.59	120.80
36	A5	2884	C	N3-C4-N4	5.18	121.62	118.00
1	A2	1051	G	C8-N9-C1'	-5.17	120.27	127.00
36	A1	336	A	C2-N3-C4	5.17	113.19	110.60
36	A1	2686	A	N1-C6-N6	5.17	121.70	118.60
36	A1	2749	G	C4-C5-N7	5.17	112.87	110.80
43	BE	26	ARG	NE-CZ-NH2	-5.17	117.71	120.30
80	A6	583	C	C6-N1-C2	-5.17	118.23	120.30
80	A6	1020	A	C4-C5-C6	5.17	119.59	117.00
80	A6	1654	G	N3-C2-N2	-5.17	116.28	119.90
36	A5	114	A	C5-C6-N1	-5.17	115.11	117.70
36	A5	928	C	C2-N3-C4	-5.17	117.31	119.90
36	A5	2639	G	C4-C5-C6	5.17	121.90	118.80
36	A5	2693	C	N3-C4-N4	-5.17	114.38	118.00
36	A5	2858	U	C2-N1-C1'	5.17	123.91	117.70
36	A5	3173	G	N3-C4-N9	5.17	129.10	126.00
36	A1	1107	C	C5-C4-N4	-5.17	116.58	120.20
36	A1	2573	G	C8-N9-C4	-5.17	104.33	106.40
36	A1	3140	G	C4-N9-C1'	5.17	133.22	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	3306	U	C4-C5-C6	5.17	122.80	119.70
36	A5	2135	U	N3-C4-C5	5.17	117.70	114.60
36	A5	2584	G	N7-C8-N9	5.17	115.69	113.10
36	A1	282	G	P-O3'-C3'	5.17	125.91	119.70
36	A1	1335	C	C6-N1-C2	5.17	122.37	120.30
80	A6	464	A	C2-N3-C4	-5.17	108.02	110.60
80	A6	1428	G	N7-C8-N9	5.17	115.69	113.10
36	A5	102	C	C4-C5-C6	5.17	119.99	117.40
36	A5	434	U	N1-C2-O2	5.17	126.42	122.80
36	A5	852	U	N3-C2-O2	-5.17	118.58	122.20
36	A5	968	G	C6-N1-C2	5.17	128.20	125.10
36	A5	1004	U	N1-C2-N3	-5.17	111.80	114.90
36	A5	1633	C	N3-C4-C5	-5.17	119.83	121.90
36	A5	3107	U	N3-C4-O4	-5.17	115.78	119.40
1	A2	240	U	N1-C2-O2	5.17	126.42	122.80
36	A1	1940	G	N1-C6-O6	-5.17	116.80	119.90
36	A1	2740	A	N1-C6-N6	-5.17	115.50	118.60
36	A5	2169	G	N9-C4-C5	5.17	107.47	105.40
36	A5	2550	U	N3-C2-O2	-5.17	118.58	122.20
36	A5	2686	A	N1-C6-N6	5.17	121.70	118.60
36	A5	2716	U	N1-C2-N3	5.17	118.00	114.90
83	Dq	70	LEU	CA-CB-CG	5.17	127.19	115.30
1	A2	49	C	C6-N1-C2	-5.17	118.23	120.30
1	A2	783	G	C8-N9-C1'	-5.17	120.28	127.00
1	A2	1258	U	C5-C6-N1	-5.17	120.12	122.70
1	A2	1448	G	N1-C6-O6	-5.17	116.80	119.90
1	A2	1796	C	C5-C4-N4	5.17	123.82	120.20
36	A1	1507	G	N3-C4-N9	5.17	129.10	126.00
36	A1	2377	G	C6-N1-C2	5.17	128.20	125.10
80	A6	489	C	C2-N1-C1'	5.17	124.48	118.80
3	CB	106	THR	N-CA-CB	5.17	120.12	110.30
36	A5	149	U	N3-C2-O2	-5.17	118.58	122.20
36	A5	580	C	N1-C2-N3	5.17	122.82	119.20
36	A5	1466	G	N1-C6-O6	-5.17	116.80	119.90
36	A5	1845	G	C8-N9-C4	5.17	108.47	106.40
36	A5	2366	C	C2-N3-C4	5.17	122.48	119.90
36	A5	3309	G	C8-N9-C4	-5.17	104.33	106.40
37	A7	41	G	C5-C6-N1	5.17	114.08	111.50
52	DO	104[B]	ILE	CA-C-N	-5.17	105.83	117.20
64	Da	14	HIS	N-CA-C	-5.17	97.05	111.00
1	A2	815	G	C8-N9-C1'	5.17	133.72	127.00
1	A2	1503	A	C5-C6-N1	-5.17	115.12	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	654	C	C5-C6-N1	-5.17	118.42	121.00
36	A1	949	C	C4-C5-C6	5.17	119.98	117.40
36	A1	1154	A	C4-C5-C6	5.17	119.58	117.00
36	A1	1903	U	N3-C4-O4	-5.17	115.78	119.40
37	A3	22	A	C5-C6-N6	-5.17	119.57	123.70
80	A6	934	C	C2-N1-C1'	5.17	124.48	118.80
80	A6	1560	U	N1-C2-O2	5.17	126.42	122.80
36	A5	1695	U	N3-C2-O2	-5.17	118.58	122.20
36	A5	1872	C	N1-C2-N3	5.17	122.82	119.20
36	A5	2340	U	N3-C2-O2	-5.17	118.58	122.20
38	A8	14	C	N1-C2-O2	-5.17	115.80	118.90
1	A2	1093	A	C8-N9-C4	5.17	107.87	105.80
1	A2	1454	G	C5-N7-C8	5.17	106.88	104.30
36	A1	187	A	C4-C5-C6	5.17	119.58	117.00
36	A1	679	U	C5-C4-O4	5.17	129.00	125.90
80	A6	984	G	C8-N9-C4	5.17	108.47	106.40
36	A5	340	C	C4-C5-C6	5.17	119.98	117.40
36	A5	3018	C	C6-N1-C2	-5.17	118.23	120.30
36	A1	829	U	N1-C2-N3	5.16	118.00	114.90
36	A1	1006	A	C8-N9-C4	-5.16	103.73	105.80
36	A1	1051	U	N3-C4-O4	-5.16	115.78	119.40
36	A1	1131	G	C6-C5-N7	-5.16	127.30	130.40
36	A1	1857	C	C4-C5-C6	5.16	119.98	117.40
36	A1	2551	U	N1-C2-N3	5.16	118.00	114.90
80	A6	1258	U	N1-C2-O2	5.16	126.41	122.80
80	A6	1457	C	C5-C6-N1	-5.16	118.42	121.00
36	A5	110	G	C5-C6-N1	5.16	114.08	111.50
36	A5	234	G	C5-C6-O6	-5.16	125.50	128.60
36	A5	1205	A	C2-N3-C4	5.16	113.18	110.60
36	A5	1658	G	C5-C6-O6	5.16	131.70	128.60
36	A5	2560	C	N1-C2-O2	5.16	122.00	118.90
36	A5	2635	A	C8-N9-C4	-5.16	103.73	105.80
36	A5	3100	U	N3-C2-O2	-5.16	118.58	122.20
36	A5	3215	A	N9-C4-C5	-5.16	103.73	105.80
1	A2	1781	A	C4-C5-N7	-5.16	108.12	110.70
36	A1	1408	G	N1-C6-O6	-5.16	116.80	119.90
36	A1	2828	G	N1-C2-N3	-5.16	120.80	123.90
80	A6	1543	A	N1-C6-N6	5.16	121.70	118.60
36	A5	2565	U	C6-N1-C2	-5.16	117.90	121.00
36	A5	2731	U	N1-C2-N3	5.16	118.00	114.90
36	A5	2881	C	N1-C2-N3	5.16	122.81	119.20
1	A2	68	A	N7-C8-N9	5.16	116.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	342	A	C2-N3-C4	-5.16	108.02	110.60
36	A1	673	U	N3-C4-C5	5.16	117.70	114.60
36	A1	1143	A	N7-C8-N9	5.16	116.38	113.80
36	A1	1803	C	N3-C4-N4	5.16	121.61	118.00
36	A1	3042	U	N3-C4-O4	-5.16	115.79	119.40
36	A1	3378	C	C6-N1-C2	5.16	122.36	120.30
80	A6	54	C	C2-N3-C4	-5.16	117.32	119.90
80	A6	139	C	C5-C4-N4	5.16	123.81	120.20
80	A6	419	G	C5-C6-O6	5.16	131.70	128.60
36	A5	3202	G	C5-C6-O6	5.16	131.70	128.60
51	DN	172	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	A2	139	C	N1-C2-N3	5.16	122.81	119.20
1	A2	749	U	C5-C6-N1	5.16	125.28	122.70
1	A2	782	U	P-O3'-C3'	5.16	125.89	119.70
1	A2	1189	A	N7-C8-N9	-5.16	111.22	113.80
1	A2	1672	G	N3-C4-C5	-5.16	126.02	128.60
36	A1	2522	G	C8-N9-C1'	-5.16	120.29	127.00
36	A1	3302	U	N1-C2-N3	-5.16	111.81	114.90
36	A5	323	A	N1-C2-N3	5.16	131.88	129.30
36	A5	911	C	C5-C4-N4	-5.16	116.59	120.20
36	A5	2142	A	C5-C6-N6	-5.16	119.57	123.70
36	A5	2848	G	C4-N9-C1'	5.16	133.21	126.50
36	A5	3386	G	N1-C2-N3	5.16	127.00	123.90
37	A7	77	G	C6-C5-N7	-5.16	127.31	130.40
38	A8	8	C	N1-C2-N3	5.16	122.81	119.20
38	A8	24	G	C5-C6-O6	5.16	131.69	128.60
1	A2	140	A	C4-N9-C1'	5.16	135.58	126.30
36	A1	1848	G	C4-C5-N7	5.16	112.86	110.80
80	A6	308	C	C6-N1-C2	5.16	122.36	120.30
80	A6	406	U	C6-N1-C2	5.16	124.09	121.00
80	A6	416	A	N7-C8-N9	5.16	116.38	113.80
80	A6	677	G	C8-N9-C4	5.16	108.46	106.40
80	A6	1186	U	C2-N3-C4	-5.16	123.91	127.00
80	A6	1796	C	C4-C5-C6	5.16	119.98	117.40
37	A7	1	G	N7-C8-N9	5.16	115.68	113.10
37	A7	79	A	C8-N9-C4	-5.16	103.74	105.80
36	A1	596	C	C4-C5-C6	5.16	119.98	117.40
36	A1	659	G	N1-C6-O6	-5.16	116.81	119.90
76	Bm	106	ARG	NE-CZ-NH2	-5.16	117.72	120.30
36	A5	1476	G	N7-C8-N9	-5.16	110.52	113.10
36	A5	1607	U	N3-C4-O4	-5.16	115.79	119.40
36	A5	2272	G	O4'-C1'-N9	5.16	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2855	U	N3-C4-C5	5.16	117.69	114.60
36	A5	3321	C	C6-N1-C2	5.16	122.36	120.30
37	A7	120	C	C5-C6-N1	-5.16	118.42	121.00
36	A1	359	U	N3-C2-O2	-5.15	118.59	122.20
36	A5	985	U	C6-N1-C2	5.15	124.09	121.00
36	A5	996	A	N7-C8-N9	-5.15	111.22	113.80
36	A5	1087	G	N1-C6-O6	5.15	122.99	119.90
36	A5	1543	G	N1-C6-O6	-5.15	116.81	119.90
1	A2	1033	C	N3-C2-O2	-5.15	118.29	121.90
1	A2	1542	G	N9-C4-C5	5.15	107.46	105.40
1	A2	1736	G	C8-N9-C4	5.15	108.46	106.40
36	A1	398	A	N1-C2-N3	-5.15	126.72	129.30
36	A1	821	U	N3-C4-C5	5.15	117.69	114.60
36	A1	1416	C	N3-C4-C5	5.15	123.96	121.90
36	A1	1845	G	C5-C6-N1	5.15	114.08	111.50
36	A1	2240	G	C5-C6-O6	-5.15	125.51	128.60
80	A6	800	U	N3-C2-O2	-5.15	118.59	122.20
80	A6	1415	U	N3-C2-O2	-5.15	118.59	122.20
36	A5	1445	U	C6-N1-C2	5.15	124.09	121.00
36	A5	1832	C	C5-C6-N1	-5.15	118.42	121.00
36	A5	2396	G	C4-C5-N7	-5.15	108.74	110.80
1	A2	494	U	C2-N1-C1'	5.15	123.88	117.70
36	A1	112	U	C6-N1-C2	-5.15	117.91	121.00
36	A1	196	G	C5-C6-O6	-5.15	125.51	128.60
36	A1	2892	A	C5-C6-N6	5.15	127.82	123.70
38	A4	6	U	C5-C6-N1	-5.15	120.12	122.70
36	A5	2706	G	N1-C6-O6	-5.15	116.81	119.90
38	A8	23	U	N3-C2-O2	-5.15	118.59	122.20
1	A2	853	G	C4-C5-N7	5.15	112.86	110.80
80	A6	49	C	C2-N3-C4	-5.15	117.33	119.90
80	A6	637	C	C5-C4-N4	-5.15	116.60	120.20
36	A5	934	G	C8-N9-C1'	-5.15	120.31	127.00
36	A5	2351	U	N1-C2-O2	5.15	126.40	122.80
36	A5	2549	G	C8-N9-C1'	-5.15	120.31	127.00
1	A2	1270	G	N1-C6-O6	-5.15	116.81	119.90
36	A1	249	U	C6-N1-C2	-5.15	117.91	121.00
36	A1	592	A	N1-C6-N6	5.15	121.69	118.60
36	A1	774	G	N1-C6-O6	-5.15	116.81	119.90
36	A1	2647	A	N1-C6-N6	-5.15	115.51	118.60
36	A1	2754	G	N1-C2-N3	5.15	126.99	123.90
36	A1	2838	A	C2-N3-C4	-5.15	108.03	110.60
36	A5	216	G	N9-C4-C5	-5.15	103.34	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2634	U	N3-C4-O4	5.15	123.00	119.40
38	A8	95	G	N3-C4-C5	5.15	131.17	128.60
1	A2	766	U	N1-C2-O2	5.15	126.40	122.80
36	A1	223	U	C2-N3-C4	-5.15	123.91	127.00
80	A6	45	U	N3-C4-C5	5.15	117.69	114.60
80	A6	1020	A	N1-C2-N3	5.15	131.87	129.30
36	A5	420	G	C6-C5-N7	-5.15	127.31	130.40
36	A5	523	A	N1-C6-N6	-5.15	115.51	118.60
36	A5	1851	G	C4-N9-C1'	5.15	133.19	126.50
1	A2	944	A	C2-N3-C4	-5.14	108.03	110.60
1	A2	992	A	N7-C8-N9	5.14	116.37	113.80
36	A1	23	A	N3-C4-N9	5.14	131.51	127.40
36	A1	74	G	N3-C2-N2	-5.14	116.30	119.90
36	A1	557	A	C8-N9-C4	5.14	107.86	105.80
36	A1	793	C	N3-C4-N4	5.14	121.60	118.00
36	A1	2407	C	C4-C5-C6	5.14	119.97	117.40
80	A6	1428	G	N1-C6-O6	-5.14	116.81	119.90
80	A6	1722	A	N1-C6-N6	-5.14	115.51	118.60
36	A5	66	A	N7-C8-N9	-5.14	111.23	113.80
36	A5	1942	U	C4-C5-C6	5.14	122.79	119.70
36	A5	2280	A	C5-N7-C8	-5.14	101.33	103.90
37	A7	13	A	C8-N9-C4	-5.14	103.74	105.80
1	A2	432	G	C5-C6-N1	5.14	114.07	111.50
36	A1	126	U	C5-C6-N1	-5.14	120.13	122.70
36	A1	508	U	C2-N3-C4	-5.14	123.92	127.00
36	A1	1305	U	N3-C4-C5	5.14	117.69	114.60
36	A1	2326	A	C5-N7-C8	-5.14	101.33	103.90
36	A1	2638	C	N3-C4-C5	5.14	123.96	121.90
36	A1	3188	G	C2-N3-C4	5.14	114.47	111.90
80	A6	431	C	N3-C2-O2	-5.14	118.30	121.90
80	A6	691	C	N3-C2-O2	-5.14	118.30	121.90
36	A5	112	U	N3-C4-O4	5.14	123.00	119.40
36	A5	863	C	C5-C4-N4	5.14	123.80	120.20
38	A8	51	G	N3-C2-N2	-5.14	116.30	119.90
1	A2	712	G	N7-C8-N9	5.14	115.67	113.10
36	A1	1548	C	N3-C4-C5	-5.14	119.84	121.90
37	A3	4	U	C5-C4-O4	-5.14	122.81	125.90
80	A6	1033	C	N1-C2-O2	-5.14	115.82	118.90
36	A5	1013	G	N3-C4-C5	-5.14	126.03	128.60
1	A2	7	G	C5-C6-O6	5.14	131.68	128.60
36	A1	917	A	N9-C4-C5	5.14	107.86	105.80
36	A1	1770	G	C8-N9-C4	-5.14	104.34	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2176	U	N3-C4-O4	-5.14	115.80	119.40
73	Bj	21	ARG	NE-CZ-NH1	5.14	122.87	120.30
80	A6	138	A	N1-C6-N6	-5.14	115.52	118.60
80	A6	308	C	N3-C4-C5	5.14	123.96	121.90
80	A6	871	G	N3-C4-C5	-5.14	126.03	128.60
80	A6	1127	G	N1-C2-N3	5.14	126.98	123.90
80	A6	1735	U	N3-C4-O4	-5.14	115.80	119.40
36	A5	341	G	N3-C2-N2	-5.14	116.30	119.90
36	A5	1482	A	C8-N9-C4	-5.14	103.74	105.80
36	A5	2831	G	C2-N3-C4	5.14	114.47	111.90
36	A5	2877	G	C5-C6-O6	5.14	131.68	128.60
36	A5	3318	G	C5-C6-O6	5.14	131.68	128.60
36	A1	365	A	C6-C5-N7	-5.14	128.70	132.30
36	A1	580	C	N3-C2-O2	-5.14	118.30	121.90
36	A1	974	G	N3-C4-N9	5.14	129.08	126.00
36	A1	2152	A	C4-C5-N7	-5.14	108.13	110.70
80	A6	16	G	C8-N9-C4	5.14	108.45	106.40
36	A5	2122	G	N7-C8-N9	-5.14	110.53	113.10
1	A2	266	A	C2-N3-C4	-5.14	108.03	110.60
1	A2	1751	C	C2-N3-C4	-5.14	117.33	119.90
36	A1	1400	G	C8-N9-C1'	-5.14	120.32	127.00
36	A1	2634	U	C4-C5-C6	5.14	122.78	119.70
36	A1	3318	G	N7-C8-N9	5.14	115.67	113.10
37	A3	7	G	N3-C4-C5	-5.14	126.03	128.60
47	BI	7	ARG	NE-CZ-NH1	-5.14	117.73	120.30
36	A5	2145	A	N3-C4-C5	-5.14	123.20	126.80
36	A5	2246	G	C6-C5-N7	5.14	133.48	130.40
37	A7	75	G	N3-C2-N2	-5.14	116.31	119.90
1	A2	557	G	C5-C6-N1	-5.13	108.93	111.50
36	A1	625	G	N1-C6-O6	-5.13	116.82	119.90
36	A1	778	U	N3-C2-O2	-5.13	118.61	122.20
36	A1	1891	A	C4-N9-C1'	-5.13	117.06	126.30
36	A1	2371	G	C6-C5-N7	-5.13	127.32	130.40
36	A1	2776	C	C5-C6-N1	-5.13	118.43	121.00
36	A1	2866	U	C6-N1-C2	-5.13	117.92	121.00
36	A1	2905	U	N3-C2-O2	5.13	125.80	122.20
41	BC	82	THR	C-N-CA	-5.13	111.52	122.30
80	A6	1111	G	N9-C4-C5	-5.13	103.35	105.40
80	A6	1503	A	C8-N9-C4	-5.13	103.75	105.80
80	A6	1652	C	N3-C2-O2	-5.13	118.31	121.90
36	A5	1138	U	N3-C4-O4	-5.13	115.81	119.40
36	A5	1813	A	C8-N9-C4	-5.13	103.75	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	3173	G	C6-N1-C2	-5.13	122.02	125.10
36	A1	588	G	C6-N1-C2	-5.13	122.02	125.10
36	A1	994	G	C5-N7-C8	5.13	106.87	104.30
36	A1	2279	A	C6-C5-N7	-5.13	128.71	132.30
36	A1	2959	C	C6-N1-C2	-5.13	118.25	120.30
36	A1	3256	G	C4-C5-C6	-5.13	115.72	118.80
80	A6	1682	U	C5-C6-N1	5.13	125.27	122.70
36	A5	943	U	C6-N1-C2	5.13	124.08	121.00
36	A5	1938	U	N3-C4-C5	5.13	117.68	114.60
1	A2	142	G	C5-C6-N1	-5.13	108.93	111.50
1	A2	572	C	N3-C2-O2	-5.13	118.31	121.90
36	A1	819	U	N1-C2-N3	5.13	117.98	114.90
36	A1	2384	A	C8-N9-C4	5.13	107.85	105.80
80	A6	718	U	C2-N1-C1'	5.13	123.86	117.70
36	A5	146	U	C5-C6-N1	-5.13	120.14	122.70
36	A5	672	A	C5-C6-N6	-5.13	119.59	123.70
36	A5	1938	U	C2-N3-C4	-5.13	123.92	127.00
36	A5	2371	G	N7-C8-N9	-5.13	110.53	113.10
36	A5	2988	C	C5-C4-N4	5.13	123.79	120.20
36	A5	3186	A	N7-C8-N9	5.13	116.37	113.80
37	A7	116	C	C6-N1-C2	5.13	122.35	120.30
36	A1	1367	G	C4-C5-N7	5.13	112.85	110.80
75	B1	45	ARG	NE-CZ-NH2	-5.13	117.73	120.30
36	A5	2378	C	C2-N3-C4	5.13	122.47	119.90
1	A2	719	U	N3-C2-O2	-5.13	118.61	122.20
1	A2	1441	C	C6-N1-C2	5.13	122.35	120.30
36	A1	1496	C	C6-N1-C1'	-5.13	114.65	120.80
36	A1	1640	G	N1-C6-O6	5.13	122.98	119.90
36	A1	3036	G	N3-C4-C5	-5.13	126.04	128.60
38	A4	90	U	C6-N1-C2	5.13	124.08	121.00
38	A4	147	U	N3-C4-O4	5.13	122.99	119.40
80	A6	295	A	C8-N9-C4	5.13	107.85	105.80
80	A6	591	A	C8-N9-C4	5.13	107.85	105.80
80	A6	1031	U	C5-C6-N1	-5.13	120.14	122.70
80	A6	1661	U	C5-C6-N1	-5.13	120.14	122.70
36	A5	893	C	N3-C2-O2	5.13	125.49	121.90
36	A5	1938	U	C6-N1-C2	5.13	124.08	121.00
1	A2	866	G	C8-N9-C4	5.13	108.45	106.40
1	A2	1187	U	N3-C2-O2	-5.13	118.61	122.20
36	A1	899	U	C5-C4-O4	5.13	128.98	125.90
36	A1	1057	A	C8-N9-C4	5.13	107.85	105.80
36	A1	1404	G	N9-C4-C5	-5.13	103.35	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1588	A	C8-N9-C4	5.13	107.85	105.80
60	BW	97	LYS	C-N-CD	5.13	139.17	128.40
80	A6	32	U	N3-C2-O2	-5.13	118.61	122.20
36	A5	919	U	C5-C4-O4	-5.13	122.82	125.90
36	A5	1114	U	C5-C4-O4	-5.13	122.82	125.90
36	A5	1137	C	N3-C4-N4	5.13	121.59	118.00
36	A5	3074	G	N1-C2-N2	-5.13	111.58	116.20
53	DP	23	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A2	294	C	N1-C2-N3	-5.12	115.61	119.20
1	A2	994	G	C4-C5-N7	-5.12	108.75	110.80
36	A1	1565	G	C8-N9-C4	-5.12	104.35	106.40
36	A1	2960	C	C5-C6-N1	-5.12	118.44	121.00
36	A1	3242	G	C5-C6-O6	5.12	131.68	128.60
27	CZ	86	GLU	N-CA-C	-5.12	97.16	111.00
36	A5	973	A	C6-N1-C2	-5.12	115.53	118.60
36	A5	2305	G	N3-C4-N9	5.12	129.07	126.00
36	A1	32	U	C4-C5-C6	5.12	122.77	119.70
36	A1	267	G	C5-N7-C8	5.12	106.86	104.30
36	A1	419	G	N3-C2-N2	5.12	123.49	119.90
36	A1	829	U	C5-C6-N1	-5.12	120.14	122.70
36	A1	1923	C	C6-N1-C2	5.12	122.35	120.30
80	A6	1515	A	N9-C4-C5	5.12	107.85	105.80
36	A5	726	G	N7-C8-N9	5.12	115.66	113.10
36	A5	884	A	C8-N9-C1'	5.12	136.92	127.70
36	A5	2600	C	C2-N1-C1'	5.12	124.44	118.80
37	A7	89	G	C5-C6-N1	5.12	114.06	111.50
1	A2	885	G	N1-C6-O6	5.12	122.97	119.90
36	A1	101	G	C8-N9-C1'	-5.12	120.34	127.00
36	A1	437	G	C4-C5-C6	-5.12	115.73	118.80
36	A1	588	G	C2-N3-C4	5.12	114.46	111.90
36	A1	1851	G	C6-C5-N7	-5.12	127.33	130.40
36	A1	2650	U	N3-C4-O4	-5.12	115.81	119.40
36	A1	2868	U	N3-C4-C5	5.12	117.67	114.60
80	A6	879	G	N1-C6-O6	-5.12	116.83	119.90
36	A5	1822	C	C6-N1-C2	5.12	122.35	120.30
36	A5	2810	C	C2-N3-C4	-5.12	117.34	119.90
36	A5	2820	A	N3-C4-C5	-5.12	123.22	126.80
1	A2	502	U	C5-C6-N1	5.12	125.26	122.70
36	A1	374	A	N1-C2-N3	-5.12	126.74	129.30
36	A1	1118	C	N1-C2-N3	5.12	122.78	119.20
36	A1	2184	U	N1-C2-O2	5.12	126.38	122.80
36	A1	2364	G	C8-N9-C4	5.12	108.45	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2399	A	C2-N3-C4	5.12	113.16	110.60
36	A1	2977	G	C6-C5-N7	5.12	133.47	130.40
80	A6	1066	C	N3-C4-C5	-5.12	119.85	121.90
36	A5	1403	C	N3-C4-C5	5.12	123.95	121.90
36	A5	2344	U	N1-C2-O2	-5.12	119.22	122.80
1	A2	378	A	C4-C5-N7	5.12	113.26	110.70
10	AI	172	ARG	NE-CZ-NH2	-5.12	117.74	120.30
36	A1	1308	A	C4-C5-C6	5.12	119.56	117.00
36	A1	1363	A	C5-C6-N1	5.12	120.26	117.70
36	A1	2931	C	N3-C4-N4	5.12	121.58	118.00
36	A1	3078	U	N3-C2-O2	-5.12	118.62	122.20
36	A1	3119	U	C5-C4-O4	5.12	128.97	125.90
36	A5	887	G	N1-C2-N2	-5.12	111.59	116.20
36	A5	943	U	C2-N3-C4	-5.12	123.93	127.00
36	A5	1144	U	N3-C2-O2	-5.12	118.62	122.20
36	A5	1316	C	C5-C6-N1	5.12	123.56	121.00
36	A5	2278	C	P-O3'-C3'	5.12	125.84	119.70
1	A2	1321	A	N1-C6-N6	-5.12	115.53	118.60
36	A1	225	C	C5-C4-N4	-5.12	116.62	120.20
36	A5	1303	A	C8-N9-C4	5.12	107.85	105.80
36	A5	1901	A	N1-C6-N6	5.12	121.67	118.60
36	A5	2352	A	C5-N7-C8	5.12	106.46	103.90
1	A2	570	A	C2-N3-C4	5.12	113.16	110.60
1	A2	886	U	N3-C2-O2	-5.12	118.62	122.20
36	A1	267	G	N3-C4-C5	-5.12	126.04	128.60
36	A1	688	G	C5-C6-O6	5.12	131.67	128.60
36	A1	903	U	C4-C5-C6	5.12	122.77	119.70
36	A1	1116	G	N9-C4-C5	5.12	107.45	105.40
36	A1	1790	G	C8-N9-C4	-5.12	104.35	106.40
36	A1	2222	A	C4-C5-C6	5.12	119.56	117.00
36	A1	2616	C	N3-C4-C5	5.12	123.95	121.90
36	A1	2659	G	C8-N9-C4	5.12	108.45	106.40
36	A1	2679	A	N3-C4-C5	5.12	130.38	126.80
36	A1	2703	A	C8-N9-C4	-5.12	103.75	105.80
13	CL	122	ILE	N-CA-C	-5.12	97.19	111.00
36	A5	2745	G	C5-C6-N1	5.12	114.06	111.50
36	A5	2913	C	N3-C2-O2	-5.12	118.32	121.90
39	DA	242	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A2	1761	U	N3-C2-O2	-5.11	118.62	122.20
36	A1	518	G	C4-C5-N7	5.11	112.84	110.80
36	A1	639	G	C5-C6-N1	-5.11	108.94	111.50
36	A1	812	G	C8-N9-C4	-5.11	104.35	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2661	G	N1-C6-O6	5.11	122.97	119.90
36	A1	2859	U	N1-C2-O2	-5.11	119.22	122.80
38	A4	144	G	C8-N9-C4	5.11	108.45	106.40
80	A6	432	G	C8-N9-C4	-5.11	104.35	106.40
36	A5	433	A	C8-N9-C4	5.11	107.84	105.80
36	A5	802	C	N1-C2-N3	5.11	122.78	119.20
36	A5	2124	G	N7-C8-N9	-5.11	110.54	113.10
36	A5	3255	U	N3-C4-C5	5.11	117.67	114.60
1	A2	1782	A	C5-C6-N1	-5.11	115.14	117.70
80	A6	695	U	N3-C2-O2	-5.11	118.62	122.20
36	A5	2848	G	C8-N9-C4	-5.11	104.36	106.40
36	A5	3218	A	N3-C4-N9	-5.11	123.31	127.40
36	A1	672	A	C5-N7-C8	-5.11	101.34	103.90
36	A1	1787	A	C5-N7-C8	5.11	106.46	103.90
36	A1	1948	G	C6-C5-N7	-5.11	127.33	130.40
36	A1	2154	U	C2-N3-C4	-5.11	123.93	127.00
36	A1	2618	G	N1-C6-O6	-5.11	116.83	119.90
36	A1	3180	A	N3-C4-N9	-5.11	123.31	127.40
36	A1	3328	G	C5-N7-C8	-5.11	101.75	104.30
36	A1	3375	A	N1-C2-N3	5.11	131.85	129.30
38	A4	88	A	N9-C4-C5	-5.11	103.76	105.80
36	A5	1445	U	N3-C2-O2	5.11	125.78	122.20
38	A8	47	C	N3-C2-O2	-5.11	118.32	121.90
41	DC	60	THR	CB-CA-C	-5.11	97.80	111.60
36	A1	950	G	C8-N9-C4	5.11	108.44	106.40
36	A1	2160	G	N3-C4-N9	5.11	129.06	126.00
36	A1	2916	U	C5-C4-O4	-5.11	122.83	125.90
36	A5	3019	U	C5-C6-N1	-5.11	120.15	122.70
1	A2	20	G	N1-C2-N2	-5.11	111.60	116.20
36	A1	339	C	N1-C2-N3	5.11	122.78	119.20
36	A1	854	G	N1-C2-N3	5.11	126.96	123.90
36	A1	1942	U	N1-C2-N3	5.11	117.96	114.90
36	A1	2201	G	C4-C5-N7	5.11	112.84	110.80
36	A1	2382	G	N3-C4-C5	-5.11	126.05	128.60
36	A1	2830	G	N1-C2-N3	5.11	126.96	123.90
80	A6	383	G	C8-N9-C4	-5.11	104.36	106.40
80	A6	430	G	C6-N1-C2	-5.11	122.04	125.10
80	A6	695	U	C6-N1-C2	-5.11	117.94	121.00
36	A5	284	A	C8-N9-C4	-5.11	103.76	105.80
36	A5	1412	G	N9-C4-C5	5.11	107.44	105.40
36	A5	2290	C	N1-C2-O2	-5.11	115.83	118.90
36	A5	3259	U	N1-C2-N3	5.11	117.97	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	3294	A	C5-C6-N6	5.11	127.79	123.70
1	A2	422	G	C8-N9-C4	-5.11	104.36	106.40
1	A2	1096	C	C6-N1-C2	-5.11	118.26	120.30
1	A2	1376	C	C6-N1-C2	5.11	122.34	120.30
24	AW	104	LEU	CA-CB-CG	5.11	127.04	115.30
36	A1	354	U	C5-C6-N1	-5.11	120.15	122.70
36	A1	1461	A	C5-C6-N1	5.11	120.25	117.70
36	A1	1482	A	C4-C5-C6	5.11	119.55	117.00
36	A1	3144	G	C5-C6-N1	5.11	114.05	111.50
80	A6	403	G	C8-N9-C1'	-5.11	120.36	127.00
80	A6	624	G	C5-C6-N1	5.11	114.05	111.50
36	A5	2271	A	C5-C6-N6	5.11	127.78	123.70
36	A5	2364	G	C6-N1-C2	-5.11	122.04	125.10
36	A1	614	C	C6-N1-C2	5.10	122.34	120.30
36	A1	929	A	C4-C5-N7	-5.10	108.15	110.70
36	A1	1395	G	N3-C4-N9	5.10	129.06	126.00
36	A1	2275	A	N1-C2-N3	5.10	131.85	129.30
36	A5	3056	U	N1-C2-O2	-5.10	119.23	122.80
38	A8	100	U	C6-N1-C1'	-5.10	114.06	121.20
1	A2	597	G	C8-N9-C4	-5.10	104.36	106.40
36	A1	282	G	C2'-C3'-O3'	5.10	121.86	113.70
36	A1	2160	G	C4-C5-N7	5.10	112.84	110.80
36	A1	2727	A	N9-C4-C5	5.10	107.84	105.80
36	A1	2787	G	C8-N9-C4	-5.10	104.36	106.40
80	A6	543	C	C4-C5-C6	5.10	119.95	117.40
36	A5	437	G	C5-C6-O6	-5.10	125.54	128.60
36	A5	1468	A	N7-C8-N9	5.10	116.35	113.80
36	A5	3180	A	C6-N1-C2	-5.10	115.54	118.60
36	A5	3378	C	N3-C4-N4	-5.10	114.43	118.00
1	A2	564	G	C5-C6-O6	5.10	131.66	128.60
36	A1	643	U	N1-C2-O2	-5.10	119.23	122.80
36	A1	889	U	N1-C2-O2	5.10	126.37	122.80
36	A1	2200	U	C2-N1-C1'	5.10	123.82	117.70
80	A6	568	G	N1-C6-O6	-5.10	116.84	119.90
80	A6	820	U	N1-C2-N3	-5.10	111.84	114.90
36	A5	2830	G	C8-N9-C4	-5.10	104.36	106.40
37	A7	57	G	C5-C6-O6	5.10	131.66	128.60
36	A1	275	U	C4-C5-C6	-5.10	116.64	119.70
36	A1	2277	C	N3-C4-N4	-5.10	114.43	118.00
36	A1	3083	G	C5-C6-N1	5.10	114.05	111.50
37	A3	97	A	C8-N9-C4	-5.10	103.76	105.80
80	A6	118	U	C2-N3-C4	-5.10	123.94	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1120	U	N3-C4-C5	5.10	117.66	114.60
36	A5	2392	C	C2-N1-C1'	-5.10	113.19	118.80
51	BN	172	ARG	NE-CZ-NH1	-5.10	117.75	120.30
36	A5	2128	C	C6-N1-C2	-5.10	118.26	120.30
36	A5	2978	U	C5-C4-O4	5.10	128.96	125.90
36	A5	3241	G	N1-C6-O6	5.10	122.96	119.90
1	A2	1734	U	C5-C4-O4	5.10	128.96	125.90
36	A1	1183	C	N3-C2-O2	5.10	125.47	121.90
36	A5	583	G	C8-N9-C4	5.10	108.44	106.40
36	A5	2691	A	N1-C2-N3	5.10	131.85	129.30
60	DW	39	LEU	CA-CB-CG	5.10	127.02	115.30
1	A2	1431	C	C6-N1-C2	5.09	122.34	120.30
36	A1	51	A	N9-C4-C5	-5.09	103.76	105.80
36	A1	214	G	N7-C8-N9	-5.09	110.55	113.10
36	A1	718	G	N7-C8-N9	5.09	115.65	113.10
36	A1	1838	G	C4-C5-C6	5.09	121.86	118.80
36	A1	2363	A	C5-C6-N6	5.09	127.78	123.70
36	A1	2850	G	N3-C4-N9	5.09	129.06	126.00
36	A1	2969	A	N9-C4-C5	5.09	107.84	105.80
36	A1	3369	G	C5-C6-O6	-5.09	125.54	128.60
80	A6	543	C	N3-C4-N4	-5.09	114.43	118.00
80	A6	1527	C	C2-N1-C1'	-5.09	113.20	118.80
36	A5	102	C	N1-C2-O2	-5.09	115.84	118.90
36	A5	284	A	N1-C6-N6	-5.09	115.54	118.60
36	A5	613	G	C4-C5-N7	-5.09	108.76	110.80
36	A5	2518	C	C4-C5-C6	5.09	119.95	117.40
1	A2	810	G	C4-N9-C1'	5.09	133.12	126.50
37	A3	29	C	C5-C4-N4	5.09	123.77	120.20
36	A5	1100	U	C5-C4-O4	-5.09	122.84	125.90
1	A2	359	A	C4-C5-C6	-5.09	114.45	117.00
1	A2	647	G	C8-N9-C1'	5.09	133.62	127.00
36	A1	905	U	N1-C2-O2	-5.09	119.24	122.80
36	A1	983	A	C4-C5-C6	5.09	119.55	117.00
36	A1	1543	G	N1-C6-O6	5.09	122.95	119.90
36	A1	1617	G	N7-C8-N9	-5.09	110.56	113.10
36	A1	2163	C	C5-C6-N1	-5.09	118.45	121.00
36	A1	2368	A	C2-N3-C4	-5.09	108.05	110.60
36	A1	2979	U	C5-C4-O4	5.09	128.96	125.90
38	A4	39	G	C5-C6-O6	5.09	131.65	128.60
80	A6	1507	G	N1-C2-N2	-5.09	111.62	116.20
36	A5	183	G	C3'-C2'-C1'	-5.09	97.43	101.50
36	A5	436	A	N1-C2-N3	5.09	131.85	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	979	U	N1-C2-N3	-5.09	111.84	114.90
36	A5	1147	G	C5-C6-O6	5.09	131.66	128.60
36	A5	2317	A	C5-N7-C8	-5.09	101.35	103.90
36	A5	2866	U	N1-C2-N3	5.09	117.95	114.90
36	A5	3154	C	C6-N1-C2	-5.09	118.26	120.30
38	A8	31	G	C5-N7-C8	5.09	106.85	104.30
1	A2	111	U	C6-N1-C2	-5.09	117.95	121.00
36	A1	74	G	C8-N9-C4	-5.09	104.36	106.40
36	A1	218	G	N9-C4-C5	5.09	107.44	105.40
36	A1	1051	U	N1-C2-N3	5.09	117.95	114.90
36	A1	1452	A	N9-C4-C5	-5.09	103.76	105.80
36	A1	1919	G	N9-C4-C5	5.09	107.44	105.40
36	A1	3304	U	N1-C2-O2	-5.09	119.24	122.80
36	A1	3317	U	C5-C6-N1	5.09	125.25	122.70
80	A6	1792	G	C5-N7-C8	-5.09	101.75	104.30
36	A5	959	C	N3-C4-C5	5.09	123.94	121.90
36	A5	2136	C	C2-N3-C4	-5.09	117.36	119.90
36	A5	2283	G	C8-N9-C4	5.09	108.44	106.40
36	A5	2857	C	C5-C6-N1	-5.09	118.45	121.00
36	A5	3313	U	N1-C2-N3	5.09	117.95	114.90
1	A2	586	G	N1-C6-O6	-5.09	116.85	119.90
36	A1	1552	G	C5-C6-O6	-5.09	125.55	128.60
36	A1	2143	A	N1-C2-N3	5.09	131.84	129.30
36	A1	2206	G	C2-N3-C4	5.09	114.44	111.90
56	DS	167	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A2	553	G	C2-N3-C4	-5.09	109.36	111.90
36	A1	32	U	N1-C2-N3	5.09	117.95	114.90
36	A1	292	U	N1-C2-N3	5.09	117.95	114.90
36	A1	748	U	C5-C6-N1	-5.09	120.16	122.70
36	A1	1483	G	C5-C6-O6	5.09	131.65	128.60
36	A1	2349	U	N3-C2-O2	-5.09	118.64	122.20
37	A3	39	C	N1-C2-O2	5.09	121.95	118.90
80	A6	794	U	C5-C6-N1	5.09	125.24	122.70
80	A6	1641	C	C4-C5-C6	5.09	119.94	117.40
36	A5	95	A	C5-C6-N1	5.09	120.24	117.70
36	A5	2614	G	C2-N3-C4	-5.09	109.36	111.90
36	A1	1130	A	N3-C4-C5	-5.08	123.24	126.80
36	A1	1916	U	C2-N3-C4	-5.08	123.95	127.00
36	A5	2633	U	C2-N3-C4	-5.08	123.95	127.00
1	A2	132	U	C6-N1-C1'	5.08	128.32	121.20
1	A2	760	A	N1-C6-N6	5.08	121.65	118.60
36	A1	780	A	N1-C6-N6	-5.08	115.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	790	U	N1-C2-N3	5.08	117.95	114.90
36	A1	1049	C	C6-N1-C2	5.08	122.33	120.30
36	A1	1907	C	C5-C4-N4	5.08	123.76	120.20
36	A1	1947	G	C4-N9-C1'	-5.08	119.89	126.50
36	A1	2148	U	C6-N1-C2	5.08	124.05	121.00
36	A1	2549	G	C2-N3-C4	5.08	114.44	111.90
36	A1	2914	G	C4-N9-C1'	5.08	133.11	126.50
36	A1	3126	C	C5-C4-N4	5.08	123.76	120.20
37	A3	102	A	N9-C4-C5	-5.08	103.77	105.80
73	Bj	79	GLN	CB-CA-C	-5.08	100.23	110.40
80	A6	358	U	C2-N3-C4	-5.08	123.95	127.00
80	A6	381	C	N1-C2-N3	5.08	122.76	119.20
36	A5	1637	A	N1-C6-N6	-5.08	115.55	118.60
36	A5	1788	C	C6-N1-C2	-5.08	118.27	120.30
36	A5	2974	U	C5-C6-N1	-5.08	120.16	122.70
1	A2	1311	U	C6-N1-C2	5.08	124.05	121.00
36	A1	1890	U	C4-C5-C6	5.08	122.75	119.70
36	A1	2310	U	C5-C4-O4	5.08	128.95	125.90
36	A1	2329	C	N3-C2-O2	5.08	125.46	121.90
41	BC	328	ASN	N-CA-C	5.08	124.72	111.00
43	BE	77	ARG	NE-CZ-NH2	-5.08	117.76	120.30
69	Bf	49	ILE	CB-CA-C	-5.08	101.44	111.60
80	A6	87	C	N1-C2-N3	5.08	122.76	119.20
36	A5	1439	U	C5-C4-O4	-5.08	122.85	125.90
36	A5	1473	G	C8-N9-C4	5.08	108.43	106.40
36	A5	2857	C	C2-N3-C4	-5.08	117.36	119.90
36	A5	2883	U	N1-C2-N3	5.08	117.95	114.90
36	A5	2941	A	C8-N9-C4	5.08	107.83	105.80
36	A5	3010	U	N1-C2-O2	5.08	126.36	122.80
36	A5	3066	U	N1-C2-O2	5.08	126.36	122.80
36	A1	1307	G	C5-C6-N1	5.08	114.04	111.50
36	A5	1412	G	N3-C2-N2	-5.08	116.34	119.90
36	A1	1482	A	C5-N7-C8	5.08	106.44	103.90
36	A1	2395	G	C2-N3-C4	5.08	114.44	111.90
36	A1	2945	G	N9-C4-C5	-5.08	103.37	105.40
36	A1	3102	G	N1-C6-O6	-5.08	116.85	119.90
38	A4	4	C	C2-N3-C4	-5.08	117.36	119.90
38	A4	46	G	C4-N9-C1'	5.08	133.10	126.50
36	A5	622	A	C4-C5-N7	5.08	113.24	110.70
36	A5	860	G	N3-C4-C5	-5.08	126.06	128.60
36	A5	958	C	C6-N1-C2	5.08	122.33	120.30
36	A5	2190	U	N3-C2-O2	-5.08	118.65	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	2293	C	N3-C2-O2	-5.08	118.34	121.90
36	A5	3132	C	C6-N1-C2	5.08	122.33	120.30
36	A1	699	A	C2-N3-C4	-5.08	108.06	110.60
36	A1	2327	U	N1-C2-N3	5.08	117.95	114.90
80	A6	1156	C	C6-N1-C2	5.08	122.33	120.30
80	A6	1743	U	C2-N3-C4	-5.08	123.95	127.00
36	A5	2198	A	C8-N9-C4	5.08	107.83	105.80
36	A5	3310	A	C5-N7-C8	5.08	106.44	103.90
37	A3	89	G	C5-C6-O6	-5.08	125.55	128.60
38	A4	12	A	N1-C6-N6	-5.08	115.56	118.60
80	A6	1027	A	N9-C4-C5	5.08	107.83	105.80
36	A5	1077	U	N1-C2-O2	-5.08	119.25	122.80
36	A5	1100	U	C6-N1-C2	5.08	124.05	121.00
36	A5	1851	G	C8-N9-C1'	-5.08	120.40	127.00
36	A5	2748	A	C5-C6-N1	5.08	120.24	117.70
36	A5	3127	A	C5-C6-N6	5.08	127.76	123.70
1	A2	638	U	C2-N3-C4	-5.07	123.96	127.00
36	A1	117	U	N1-C2-O2	-5.07	119.25	122.80
36	A1	2551	U	N3-C4-O4	-5.07	115.85	119.40
38	A4	41	A	C6-N1-C2	-5.07	115.56	118.60
80	A6	569	C	C6-N1-C2	-5.07	118.27	120.30
80	A6	1489	U	C2-N3-C4	-5.07	123.96	127.00
36	A5	1301	A	C6-C5-N7	-5.07	128.75	132.30
36	A5	1432	C	N3-C2-O2	-5.07	118.35	121.90
36	A5	2138	A	C5-C6-N1	-5.07	115.16	117.70
36	A5	3130	A	C4-C5-C6	5.07	119.54	117.00
36	A5	3273	A	C5-N7-C8	-5.07	101.36	103.90
1	A2	1596	C	N1-C2-O2	5.07	121.94	118.90
80	A6	909	U	N1-C2-O2	-5.07	119.25	122.80
36	A5	2162	U	C5-C6-N1	-5.07	120.16	122.70
1	A2	63	G	N1-C6-O6	-5.07	116.86	119.90
1	A2	158	U	N1-C2-O2	5.07	126.35	122.80
1	A2	26	A	C8-N9-C4	-5.07	103.77	105.80
36	A1	395	A	C8-N9-C4	-5.07	103.77	105.80
36	A1	574	U	C5-C6-N1	-5.07	120.17	122.70
36	A1	3135	U	C6-N1-C2	5.07	124.04	121.00
56	BS	12	ARG	N-CA-C	5.07	124.69	111.00
1	A2	335	U	N3-C2-O2	5.07	125.75	122.20
36	A1	651	G	C4-N9-C1'	5.07	133.09	126.50
36	A1	2917	G	C5-N7-C8	5.07	106.83	104.30
80	A6	22	A	N7-C8-N9	-5.07	111.27	113.80
80	A6	1299	G	C4-N9-C1'	5.07	133.09	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	874	U	C2-N1-C1'	-5.07	111.62	117.70
36	A5	1142	G	N3-C2-N2	5.07	123.45	119.90
36	A5	1804	A	N1-C6-N6	5.07	121.64	118.60
36	A5	2407	C	N3-C2-O2	5.07	125.45	121.90
37	A7	83	U	C6-N1-C1'	5.07	128.29	121.20
1	A2	1643	U	C2-N3-C4	-5.07	123.96	127.00
15	AN	114	ARG	NE-CZ-NH1	5.07	122.83	120.30
36	A1	340	C	N1-C2-O2	5.07	121.94	118.90
36	A1	808	A	C5-N7-C8	5.07	106.43	103.90
36	A1	1770	G	C4-N9-C1'	5.07	133.09	126.50
36	A1	2280	A	C4-C5-N7	5.07	113.23	110.70
36	A1	2866	U	N1-C2-N3	5.07	117.94	114.90
80	A6	802	G	C5-C6-O6	-5.07	125.56	128.60
80	A6	922	G	N1-C6-O6	-5.07	116.86	119.90
80	A6	1772	C	C2-N3-C4	-5.07	117.37	119.90
36	A5	1241	U	C5-C6-N1	5.07	125.23	122.70
36	A5	2386	A	N1-C6-N6	5.07	121.64	118.60
36	A5	2805	G	C5-C6-N1	5.07	114.03	111.50
36	A5	3377	G	C6-C5-N7	-5.07	127.36	130.40
1	A2	1536	G	N3-C4-C5	-5.06	126.07	128.60
36	A1	1215	U	N1-C2-O2	-5.06	119.25	122.80
36	A1	2644	C	C6-N1-C2	-5.06	118.28	120.30
44	BF	177	GLY	N-CA-C	-5.06	100.44	113.10
80	A6	1031	U	C2-N1-C1'	-5.06	111.62	117.70
36	A5	1451	C	C6-N1-C2	5.06	122.33	120.30
36	A5	3030	G	C5-C6-N1	-5.06	108.97	111.50
1	A2	704	C	N3-C2-O2	-5.06	118.36	121.90
1	A2	1354	G	C8-N9-C4	-5.06	104.38	106.40
36	A1	1791	C	C5-C6-N1	-5.06	118.47	121.00
71	Bh	31	LEU	CA-CB-CG	5.06	126.94	115.30
80	A6	37	U	N3-C2-O2	5.06	125.74	122.20
80	A6	99	C	C6-N1-C1'	-5.06	114.72	120.80
80	A6	575	C	N3-C4-C5	-5.06	119.88	121.90
80	A6	691	C	N1-C2-O2	5.06	121.94	118.90
4	CC	107	SER	N-CA-C	-5.06	97.33	111.00
36	A5	346	C	N3-C4-C5	5.06	123.92	121.90
36	A5	1414	G	C2-N3-C4	-5.06	109.37	111.90
36	A5	3137	C	N3-C4-N4	-5.06	114.46	118.00
36	A5	3191	G	N7-C8-N9	-5.06	110.57	113.10
37	A7	35	C	C6-N1-C2	5.06	122.33	120.30
37	A7	35	C	N3-C4-C5	5.06	123.92	121.90
1	A2	73	U	C1'-O4'-C4'	-5.06	105.85	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1541	G	C2-N3-C4	5.06	114.43	111.90
36	A5	2662	G	N3-C4-C5	-5.06	126.07	128.60
1	A2	927	C	C6-N1-C2	-5.06	118.28	120.30
36	A1	223	U	C5-C6-N1	-5.06	120.17	122.70
36	A1	431	U	N1-C2-N3	5.06	117.94	114.90
36	A1	620	U	C3'-C2'-C1'	5.06	105.55	101.50
36	A1	959	C	C5-C4-N4	-5.06	116.66	120.20
36	A1	1640	G	C5-C6-O6	-5.06	125.56	128.60
37	A3	94	C	C5-C4-N4	-5.06	116.66	120.20
38	A4	30	C	C6-N1-C2	-5.06	118.28	120.30
38	A4	31	G	C2-N3-C4	-5.06	109.37	111.90
80	A6	1005	A	C2-N3-C4	-5.06	108.07	110.60
80	A6	1246	C	N1-C2-O2	5.06	121.94	118.90
36	A5	627	U	N3-C2-O2	-5.06	118.66	122.20
36	A5	880	G	C6-N1-C2	-5.06	122.06	125.10
36	A5	2593	A	P-O3'-C3'	5.06	125.77	119.70
36	A5	2754	G	N3-C4-C5	-5.06	126.07	128.60
44	DF	177	GLY	N-CA-C	-5.06	100.45	113.10
1	A2	1649	G	N1-C2-N3	5.06	126.94	123.90
36	A1	37	U	N3-C2-O2	5.06	125.74	122.20
36	A1	695	C	C6-N1-C2	5.06	122.32	120.30
36	A1	2142	A	N9-C4-C5	5.06	107.82	105.80
37	A3	109	G	N9-C4-C5	5.06	107.42	105.40
36	A5	2371	G	N1-C2-N2	-5.06	111.65	116.20
80	A6	1119	G	N1-C6-O6	-5.06	116.87	119.90
36	A5	813	G	C4-N9-C1'	5.06	133.07	126.50
1	A2	1605	G	N1-C2-N2	-5.05	111.65	116.20
36	A1	351	A	C2-N3-C4	-5.05	108.07	110.60
36	A1	1150	A	N3-C4-N9	-5.05	123.36	127.40
36	A1	1187	C	C2-N3-C4	-5.05	117.37	119.90
36	A1	1313	G	C5-C6-N1	5.05	114.03	111.50
36	A1	1838	G	C5-C6-N1	-5.05	108.97	111.50
36	A1	2751	G	N1-C6-O6	5.05	122.93	119.90
36	A5	578	A	C2-N3-C4	5.05	113.13	110.60
36	A5	1461	A	C8-N9-C4	5.05	107.82	105.80
36	A5	1660	C	C2-N3-C4	-5.05	117.37	119.90
36	A5	2207	A	C5-C6-N1	-5.05	115.17	117.70
36	A5	2309	A	N1-C6-N6	5.05	121.63	118.60
36	A5	2919	A	C5-C6-N6	5.05	127.74	123.70
36	A5	3217	C	C2-N1-C1'	-5.05	113.24	118.80
38	A8	88	A	N1-C6-N6	5.05	121.63	118.60
80	A6	65	A	C8-N9-C4	5.05	107.82	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1039	A	O4'-C1'-N9	5.05	112.24	108.20
36	A5	524	U	C2-N3-C4	-5.05	123.97	127.00
36	A5	2731	U	C5-C6-N1	-5.05	120.17	122.70
36	A5	2951	G	C8-N9-C4	5.05	108.42	106.40
36	A5	3195	U	N1-C2-O2	5.05	126.34	122.80
1	A2	312	A	C8-N9-C4	-5.05	103.78	105.80
1	A2	819	G	P-O3'-C3'	5.05	125.76	119.70
1	A2	972	G	C5-N7-C8	5.05	106.83	104.30
36	A1	68	C	N3-C4-C5	-5.05	119.88	121.90
36	A1	545	U	C5-C6-N1	5.05	125.22	122.70
36	A1	2281	A	N3-C4-C5	5.05	130.34	126.80
36	A1	2829	U	N1-C2-O2	5.05	126.34	122.80
38	A4	26	U	C5-C6-N1	-5.05	120.17	122.70
80	A6	359	A	C8-N9-C1'	5.05	136.79	127.70
37	A7	41	G	C5-C6-O6	-5.05	125.57	128.60
38	A8	17	A	C6-C5-N7	-5.05	128.76	132.30
36	A1	1589	A	O4'-C1'-N9	-5.05	104.16	108.20
36	A1	2169	G	C5-N7-C8	5.05	106.83	104.30
36	A1	2692	A	N7-C8-N9	5.05	116.33	113.80
36	A1	2899	C	C5-C4-N4	-5.05	116.67	120.20
38	A4	29	U	C5-C6-N1	-5.05	120.17	122.70
80	A6	1289	U	N3-C4-O4	5.05	122.94	119.40
36	A5	1192	C	N3-C2-O2	-5.05	118.36	121.90
36	A5	1348	U	C5-C6-N1	5.05	125.22	122.70
36	A5	1726	C	C6-N1-C2	5.05	122.32	120.30
36	A5	2263	C	N3-C2-O2	-5.05	118.36	121.90
36	A5	2541	U	N1-C2-O2	5.05	126.33	122.80
36	A5	2696	A	C5-C6-N6	5.05	127.74	123.70
36	A5	2931	C	N1-C2-O2	-5.05	115.87	118.90
80	A6	970	A	C4-C5-C6	-5.05	114.48	117.00
36	A5	1338	C	N1-C2-O2	-5.05	115.87	118.90
36	A5	2944	U	N1-C2-O2	5.05	126.33	122.80
33	Af	138	ARG	NE-CZ-NH2	-5.05	117.78	120.30
36	A1	696	C	N3-C4-N4	-5.05	114.47	118.00
36	A1	938	C	N1-C2-N3	5.05	122.73	119.20
36	A1	2573	G	N7-C8-N9	5.05	115.62	113.10
36	A1	2718	U	N3-C2-O2	-5.05	118.67	122.20
36	A1	3174	A	N7-C8-N9	5.05	116.32	113.80
37	A3	101	G	N9-C4-C5	-5.05	103.38	105.40
80	A6	101	U	N3-C4-O4	-5.05	115.87	119.40
36	A5	41	G	N1-C2-N2	5.05	120.74	116.20
36	A5	1015	U	C2-N3-C4	5.05	130.03	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1480	G	N3-C4-N9	5.05	129.03	126.00
37	A7	14	U	C2-N3-C4	-5.05	123.97	127.00
47	DI	69	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	A2	1148	C	N1-C2-O2	5.04	121.93	118.90
1	A2	1600	A	N1-C6-N6	5.04	121.63	118.60
36	A1	722	G	C8-N9-C4	-5.04	104.38	106.40
36	A1	2892	A	C4-C5-N7	-5.04	108.18	110.70
80	A6	102	U	C2-N3-C4	-5.04	123.97	127.00
36	A5	367	A	C6-N1-C2	5.04	121.63	118.60
36	A5	2353	G	C4-C5-N7	5.04	112.82	110.80
36	A5	2701	U	N3-C4-O4	5.04	122.93	119.40
1	A2	440	U	N3-C4-O4	-5.04	115.87	119.40
36	A1	584	G	C4-C5-N7	-5.04	108.78	110.80
80	A6	1573	A	C5-C6-N1	5.04	120.22	117.70
36	A5	1303	A	N7-C8-N9	-5.04	111.28	113.80
36	A5	2110	G	C4-C5-N7	5.04	112.82	110.80
36	A5	2407	C	N3-C4-N4	5.04	121.53	118.00
37	A7	20	A	N1-C6-N6	5.04	121.63	118.60
37	A7	83	U	C5-C4-O4	5.04	128.93	125.90
1	A2	6	G	N1-C2-N2	-5.04	111.66	116.20
1	A2	192	U	C6-N1-C2	-5.04	117.97	121.00
36	A1	342	A	C5-C6-N1	-5.04	115.18	117.70
36	A1	1317	A	C2-N3-C4	5.04	113.12	110.60
36	A1	1839	A	N1-C2-N3	5.04	131.82	129.30
36	A1	2273	G	C6-C5-N7	5.04	133.43	130.40
36	A1	2408	U	N3-C4-O4	5.04	122.93	119.40
36	A1	2804	A	C8-N9-C4	-5.04	103.78	105.80
36	A1	3256	G	C6-C5-N7	5.04	133.43	130.40
80	A6	305	C	N3-C4-C5	-5.04	119.88	121.90
80	A6	310	C	C5-C6-N1	-5.04	118.48	121.00
36	A5	1887	A	C6-C5-N7	-5.04	128.77	132.30
36	A5	3189	G	C8-N9-C4	5.04	108.42	106.40
73	Dj	5	THR	C-N-CD	5.04	138.99	128.40
1	A2	1722	A	N1-C6-N6	-5.04	115.58	118.60
6	AE	164	LEU	CA-CB-CG	5.04	126.89	115.30
36	A1	1510	G	N9-C4-C5	-5.04	103.38	105.40
36	A1	2247	G	N3-C2-N2	-5.04	116.37	119.90
36	A1	3372	A	C6-N1-C2	-5.04	115.58	118.60
36	A5	2965	U	C5-C6-N1	-5.04	120.18	122.70
36	A1	218	G	C8-N9-C4	-5.04	104.39	106.40
36	A1	577	C	N1-C2-O2	-5.04	115.88	118.90
36	A1	800	G	C6-N1-C2	5.04	128.12	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	935	U	C2-N3-C4	-5.04	123.98	127.00
36	A1	1216	C	C6-N1-C1'	5.04	126.85	120.80
36	A1	2211	U	C5-C6-N1	5.04	125.22	122.70
36	A1	2795	U	N3-C2-O2	-5.04	118.67	122.20
36	A1	2823	G	C6-C5-N7	5.04	133.42	130.40
37	A3	33	U	N3-C2-O2	-5.04	118.67	122.20
80	A6	234	G	N3-C4-C5	-5.04	126.08	128.60
80	A6	605	A	N7-C8-N9	-5.04	111.28	113.80
36	A5	356	C	C6-N1-C2	5.04	122.32	120.30
36	A5	1902	G	N9-C4-C5	-5.04	103.39	105.40
36	A5	2167	A	N3-C4-C5	-5.04	123.27	126.80
36	A5	2531	C	N3-C2-O2	-5.04	118.37	121.90
37	A7	88	G	N9-C4-C5	5.04	107.42	105.40
55	DR	97	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A2	270	C	C2-N1-C1'	5.04	124.34	118.80
1	A2	802	G	N3-C4-C5	-5.04	126.08	128.60
36	A1	868	C	C5-C4-N4	5.04	123.73	120.20
36	A1	2395	G	N1-C6-O6	-5.04	116.88	119.90
80	A6	20	G	N3-C4-C5	5.04	131.12	128.60
80	A6	363	G	C4-C5-N7	5.04	112.81	110.80
36	A5	587	U	C6-N1-C2	5.04	124.02	121.00
36	A5	998	A	C4-C5-N7	-5.04	108.18	110.70
36	A5	2215	A	N1-C6-N6	5.04	121.62	118.60
36	A5	2284	C	C2-N1-C1'	5.04	124.34	118.80
36	A5	2606	G	N1-C2-N2	-5.04	111.67	116.20
36	A5	2774	C	N3-C4-N4	5.04	121.53	118.00
36	A5	2935	U	N1-C2-O2	5.04	126.33	122.80
36	A5	3145	C	C5-C4-N4	-5.04	116.67	120.20
1	A2	345	U	N1-C2-N3	5.04	117.92	114.90
1	A2	498	G	C4-N9-C1'	5.04	133.05	126.50
36	A1	2360	C	N1-C2-N3	5.04	122.72	119.20
36	A1	2551	U	N3-C2-O2	-5.04	118.68	122.20
36	A1	2811	A	C6-N1-C2	-5.04	115.58	118.60
36	A1	2878	G	C6-N1-C2	-5.04	122.08	125.10
37	A3	14	U	N3-C2-O2	5.04	125.72	122.20
80	A6	101	U	C5-C4-O4	5.04	128.92	125.90
80	A6	342	C	C6-N1-C2	5.04	122.31	120.30
80	A6	394	C	N3-C4-C5	-5.04	119.89	121.90
80	A6	583	C	C2-N1-C1'	5.04	124.34	118.80
36	A5	1178	G	N3-C2-N2	-5.04	116.38	119.90
36	A5	1314	C	C4-C5-C6	5.04	119.92	117.40
36	A5	1704	A	C2-N3-C4	-5.04	108.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	1832	C	N3-C4-C5	5.04	123.92	121.90
36	A5	2271	A	C5-N7-C8	5.04	106.42	103.90
36	A5	2280	A	N3-C4-C5	5.04	130.32	126.80
36	A5	3351	U	N1-C2-O2	5.04	126.33	122.80
1	A2	1220	C	C6-N1-C2	5.03	122.31	120.30
36	A1	271	C	N1-C2-O2	5.03	121.92	118.90
36	A1	1170	A	N1-C6-N6	5.03	121.62	118.60
36	A1	2174	G	C6-C5-N7	-5.03	127.38	130.40
36	A1	2621	G	C4-C5-N7	-5.03	108.79	110.80
36	A1	2788	C	N3-C2-O2	5.03	125.42	121.90
38	A4	15	G	C5-N7-C8	5.03	106.82	104.30
36	A5	282	G	P-O3'-C3'	5.03	125.74	119.70
36	A5	982	C	C4-C5-C6	-5.03	114.88	117.40
36	A5	2317	A	C6-C5-N7	-5.03	128.78	132.30
36	A5	2430	A	C4-C5-C6	5.03	119.52	117.00
36	A5	2674	A	N7-C8-N9	-5.03	111.28	113.80
36	A5	2958	A	C4-N9-C1'	-5.03	117.24	126.30
36	A5	3028	G	N9-C4-C5	-5.03	103.39	105.40
36	A5	2280	A	C8-N9-C4	5.03	107.81	105.80
11	AJ	175	ARG	NE-CZ-NH1	5.03	122.81	120.30
36	A1	28	C	C2-N3-C4	-5.03	117.39	119.90
36	A1	2170	U	N1-C2-N3	5.03	117.92	114.90
37	A3	80	G	N3-C4-C5	-5.03	126.08	128.60
38	A4	55	U	C6-N1-C2	-5.03	117.98	121.00
38	A4	149	A	N1-C6-N6	-5.03	115.58	118.60
36	A5	2623	G	N3-C4-N9	5.03	129.02	126.00
36	A5	2821	C	N1-C2-O2	-5.03	115.88	118.90
36	A5	3191	G	C5-N7-C8	5.03	106.81	104.30
37	A7	26	C	N1-C2-N3	5.03	122.72	119.20
54	DQ	3	ILE	CB-CA-C	-5.03	101.54	111.60
1	A2	1051	G	C4-N9-C1'	5.03	133.04	126.50
1	A2	1679	G	N3-C2-N2	5.03	123.42	119.90
36	A1	304	G	C4-C5-N7	-5.03	108.79	110.80
36	A1	1520	G	C4-C5-N7	-5.03	108.79	110.80
36	A1	1807	G	C4-N9-C1'	5.03	133.04	126.50
36	A1	2380	U	N1-C2-O2	-5.03	119.28	122.80
36	A5	940	G	C5-C6-N1	5.03	114.02	111.50
36	A5	1040	A	C2-N3-C4	-5.03	108.08	110.60
36	A5	3209	A	O4'-C1'-N9	5.03	112.22	108.20
36	A1	1178	G	N1-C6-O6	-5.03	116.88	119.90
36	A1	1357	G	N1-C6-O6	5.03	122.92	119.90
36	A1	2965	U	C2-N3-C4	-5.03	123.98	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A4	140	G	C4-C5-N7	-5.03	108.79	110.80
80	A6	512	A	C3'-C2'-C1'	-5.03	97.48	101.50
36	A5	16	A	C5-C6-N1	5.03	120.21	117.70
36	A5	584	G	N1-C6-O6	-5.03	116.88	119.90
36	A5	1660	C	N1-C2-N3	5.03	122.72	119.20
36	A5	2337	C	C5-C6-N1	-5.03	118.49	121.00
36	A5	3212	C	N1-C2-N3	5.03	122.72	119.20
1	A2	555	A	N3-C4-C5	-5.03	123.28	126.80
1	A2	914	G	C4-N9-C1'	5.03	133.03	126.50
25	AX	111	GLY	N-CA-C	-5.03	100.54	113.10
36	A1	425	G	N1-C2-N2	-5.03	111.68	116.20
36	A1	2383	C	C6-N1-C2	5.03	122.31	120.30
36	A1	2752	U	C5-C6-N1	-5.03	120.19	122.70
41	BC	246	ARG	CG-CD-NE	-5.03	101.25	111.80
64	Ba	12	ARG	NE-CZ-NH1	5.03	122.81	120.30
80	A6	1269	U	C6-N1-C2	-5.03	117.98	121.00
80	A6	1428	G	N9-C4-C5	5.03	107.41	105.40
36	A5	98	G	C5-C6-O6	-5.03	125.58	128.60
36	A5	1906	G	C5-C6-O6	-5.03	125.58	128.60
36	A5	2742	C	C2-N3-C4	-5.03	117.39	119.90
36	A5	2813	A	C5-C6-N6	5.03	127.72	123.70
36	A5	2945	G	C5-C6-O6	-5.03	125.58	128.60
36	A5	3049	A	N1-C6-N6	5.03	121.61	118.60
36	A5	3246	G	C5-C6-O6	-5.03	125.58	128.60
37	A7	96	U	N3-C4-C5	5.03	117.62	114.60
1	A2	404	G	N1-C6-O6	5.02	122.91	119.90
36	A1	411	U	C5-C6-N1	-5.02	120.19	122.70
36	A1	808	A	C6-C5-N7	5.02	135.82	132.30
36	A1	1493	G	N3-C4-N9	-5.02	122.99	126.00
36	A1	1899	G	N3-C2-N2	5.02	123.42	119.90
36	A1	2154	U	C2-N1-C1'	5.02	123.73	117.70
80	A6	96	G	C2-N3-C4	-5.02	109.39	111.90
36	A5	949	C	N1-C2-N3	5.02	122.72	119.20
36	A5	1481	A	C4-C5-C6	5.02	119.51	117.00
36	A5	2647	A	N1-C2-N3	5.02	131.81	129.30
38	A8	79	A	N1-C6-N6	5.02	121.61	118.60
1	A2	1568	C	P-O3'-C3'	5.02	125.73	119.70
1	A2	1629	G	N1-C2-N2	-5.02	111.68	116.20
36	A1	869	G	N3-C4-N9	5.02	129.01	126.00
36	A1	995	U	C5-C6-N1	5.02	125.21	122.70
36	A1	1372	C	C5-C6-N1	-5.02	118.49	121.00
36	A1	2249	G	C6-N1-C2	-5.02	122.09	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2541	U	N1-C2-O2	5.02	126.31	122.80
36	A1	2924	U	N3-C4-O4	-5.02	115.88	119.40
36	A1	3212	C	C2-N3-C4	-5.02	117.39	119.90
36	A1	3218	A	C2-N3-C4	-5.02	108.09	110.60
49	BL	76	THR	N-CA-CB	5.02	119.84	110.30
80	A6	531	C	C6-N1-C2	-5.02	118.29	120.30
80	A6	972	G	N7-C8-N9	-5.02	110.59	113.10
36	A5	191	U	C2-N1-C1'	-5.02	111.67	117.70
36	A5	391	A	C8-N9-C4	5.02	107.81	105.80
36	A5	2306	C	C5-C6-N1	5.02	123.51	121.00
36	A1	1306	G	N3-C2-N2	-5.02	116.39	119.90
36	A1	2314	U	N3-C4-O4	5.02	122.92	119.40
36	A5	530	G	N9-C4-C5	5.02	107.41	105.40
1	A2	1600	A	C3'-C2'-C1'	-5.02	97.48	101.50
1	A2	1791	A	C5-C6-N1	5.02	120.21	117.70
36	A1	406	G	C6-N1-C2	5.02	128.11	125.10
36	A1	2204	C	C6-N1-C2	-5.02	118.29	120.30
36	A1	2642	A	N3-C4-N9	-5.02	123.38	127.40
36	A1	2770	G	C5-N7-C8	-5.02	101.79	104.30
36	A1	2904	U	N3-C4-C5	5.02	117.61	114.60
36	A1	3098	G	N3-C2-N2	5.02	123.41	119.90
36	A5	609	G	C8-N9-C4	-5.02	104.39	106.40
36	A5	840	C	C4-C5-C6	5.02	119.91	117.40
36	A5	2353	G	N3-C4-C5	-5.02	126.09	128.60
36	A5	3048	A	C5-C6-N6	-5.02	119.69	123.70
59	DV	87	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A2	1441	C	C5-C6-N1	-5.02	118.49	121.00
36	A1	357	A	C5-C6-N1	5.02	120.21	117.70
36	A1	2316	G	N1-C6-O6	5.02	122.91	119.90
36	A1	2381	G	C8-N9-C4	5.02	108.41	106.40
80	A6	805	U	N3-C4-C5	-5.02	111.59	114.60
36	A5	432	G	N1-C2-N2	-5.02	111.68	116.20
36	A5	1004	U	C5-C4-O4	5.02	128.91	125.90
36	A5	2179	C	N3-C2-O2	5.02	125.41	121.90
36	A5	2343	C	N1-C2-O2	-5.02	115.89	118.90
36	A5	2393	G	N7-C8-N9	-5.02	110.59	113.10
36	A5	2878	G	C5-C6-N1	5.02	114.01	111.50
36	A5	3266	G	N3-C4-N9	-5.02	122.99	126.00
38	A8	40	A	N7-C8-N9	5.02	116.31	113.80
33	Af	106	TYR	N-CA-C	-5.02	97.46	111.00
36	A1	634	C	N3-C4-N4	-5.02	114.49	118.00
36	A1	1501	U	C5-C6-N1	5.02	125.21	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	3088	G	C5-N7-C8	5.02	106.81	104.30
80	A6	1550	A	C4-C5-N7	5.02	113.21	110.70
36	A5	1932	A	N1-C2-N3	5.02	131.81	129.30
36	A5	2323	G	C5-C6-O6	5.02	131.61	128.60
36	A5	2972	G	N1-C2-N2	-5.02	111.69	116.20
36	A1	1366	A	C2-N3-C4	5.01	113.11	110.60
36	A1	1382	G	N1-C6-O6	5.01	122.91	119.90
36	A1	1855	U	C2-N1-C1'	5.01	123.72	117.70
36	A1	2117	A	C4-C5-N7	-5.01	108.19	110.70
36	A1	2350	C	N3-C2-O2	-5.01	118.39	121.90
62	BY	112	ASP	CB-CG-OD1	5.01	122.81	118.30
36	A5	916	G	C6-N1-C2	5.01	128.11	125.10
36	A5	1463	U	C5-C4-O4	-5.01	122.89	125.90
36	A5	1872	C	C2-N3-C4	-5.01	117.39	119.90
36	A5	2379	U	C2-N3-C4	-5.01	123.99	127.00
36	A5	2808	A	C8-N9-C1'	-5.01	118.67	127.70
36	A5	3241	G	C6-C5-N7	-5.01	127.39	130.40
38	A8	4	C	C6-N1-C2	-5.01	118.29	120.30
38	A8	99	C	C2-N3-C4	-5.01	117.39	119.90
48	DJ	92	ARG	NE-CZ-NH1	5.01	122.81	120.30
36	A5	2349	U	N3-C4-O4	-5.01	115.89	119.40
36	A5	2369	G	N3-C4-N9	5.01	129.01	126.00
1	A2	613	G	N3-C2-N2	5.01	123.41	119.90
1	A2	1324	G	N3-C4-C5	5.01	131.11	128.60
1	A2	1780	G	N1-C6-O6	5.01	122.91	119.90
36	A1	582	G	N1-C2-N2	5.01	120.71	116.20
36	A1	1100	U	N1-C2-N3	5.01	117.91	114.90
36	A1	1157	G	C5-C6-O6	5.01	131.61	128.60
36	A1	2904	U	C4-C5-C6	-5.01	116.69	119.70
80	A6	381	C	N3-C4-N4	-5.01	114.49	118.00
80	A6	1200	G	N3-C4-N9	-5.01	122.99	126.00
80	A6	1747	G	C2-N3-C4	-5.01	109.39	111.90
36	A5	1078	U	N3-C2-O2	5.01	125.71	122.20
36	A5	2847	A	C5-C6-N6	5.01	127.71	123.70
1	A2	158	U	P-O3'-C3'	5.01	125.71	119.70
36	A1	375	A	C4-C5-N7	5.01	113.20	110.70
36	A1	431	U	C5-C6-N1	-5.01	120.20	122.70
36	A1	678	G	C2-N3-C4	5.01	114.41	111.90
36	A1	2117	A	N9-C4-C5	5.01	107.80	105.80
13	CL	128	CYS	N-CA-C	5.01	124.52	111.00
36	A5	820	A	N1-C2-N3	5.01	131.80	129.30
36	A5	880	G	C8-N9-C4	5.01	108.40	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A5	914	A	C2-N3-C4	-5.01	108.09	110.60
36	A5	1347	U	C2-N1-C1'	-5.01	111.69	117.70
1	A2	324	U	N1-C2-N3	5.01	117.91	114.90
36	A1	1377	G	N3-C2-N2	5.01	123.41	119.90
36	A1	2276	G	N1-C2-N3	-5.01	120.89	123.90
36	A1	2411	U	N3-C4-C5	5.01	117.61	114.60
36	A1	3362	A	C6-N1-C2	-5.01	115.59	118.60
1	A2	902	G	N1-C6-O6	5.01	122.90	119.90
36	A1	34	A	C4-C5-N7	5.01	113.20	110.70
36	A1	189	G	N3-C2-N2	5.01	123.41	119.90
36	A1	571	U	C5-C6-N1	-5.01	120.20	122.70
36	A1	637	C	P-O3'-C3'	5.01	125.71	119.70
36	A1	2409	G	N1-C2-N2	-5.01	111.69	116.20
36	A1	2504	U	C2-N1-C1'	5.01	123.71	117.70
36	A1	3172	A	N7-C8-N9	-5.01	111.30	113.80
36	A1	3361	G	N3-C2-N2	5.01	123.41	119.90
37	A3	15	C	N1-C2-O2	-5.01	115.90	118.90
38	A4	105	A	C6-N1-C2	5.01	121.60	118.60
39	BA	44	ILE	CB-CA-C	-5.01	101.59	111.60
47	BI	21	ARG	NE-CZ-NH1	-5.01	117.80	120.30
80	A6	980	G	C8-N9-C4	5.01	108.40	106.40
80	A6	1329	A	C4-C5-N7	5.01	113.20	110.70
36	A5	126	U	C2-N3-C4	-5.01	124.00	127.00
36	A5	270	U	N1-C2-O2	5.01	126.30	122.80
36	A5	628	A	C5-C6-N1	5.01	120.20	117.70
36	A5	2352	A	C4-C5-C6	5.01	119.50	117.00
36	A5	2361	A	N1-C6-N6	-5.01	115.60	118.60
36	A5	2375	G	N3-C2-N2	5.01	123.40	119.90
36	A5	3094	A	N7-C8-N9	-5.01	111.30	113.80
36	A5	3183	A	N1-C6-N6	5.01	121.60	118.60
38	A8	76	C	C2-N1-C1'	-5.01	113.29	118.80
1	A2	1215	C	N3-C2-O2	-5.00	118.40	121.90
17	AP	42	ARG	NE-CZ-NH1	5.00	122.80	120.30
36	A1	817	A	C4-C5-C6	5.00	119.50	117.00
1	A2	431	C	N3-C2-O2	-5.00	118.40	121.90
1	A2	1633	A	C8-N9-C4	-5.00	103.80	105.80
36	A1	2152	A	C6-C5-N7	5.00	135.80	132.30
36	A1	2294	U	N1-C2-N3	5.00	117.90	114.90
36	A1	2376	G	C5-C6-O6	-5.00	125.60	128.60
36	A1	3188	G	C4-N9-C1'	5.00	133.01	126.50
37	A3	2	G	N1-C6-O6	-5.00	116.90	119.90
37	A3	37	G	C5-C6-O6	-5.00	125.60	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	A6	1481	C	N3-C2-O2	-5.00	118.40	121.90
80	A6	1666	U	N1-C2-N3	5.00	117.90	114.90
36	A5	2994	A	N1-C2-N3	5.00	131.80	129.30
1	A2	1258	U	N1-C2-O2	5.00	126.30	122.80
1	A2	1432	U	C2-N1-C1'	-5.00	111.70	117.70
36	A1	225	C	N3-C4-N4	5.00	121.50	118.00
36	A1	633	C	C6-N1-C2	5.00	122.30	120.30
36	A1	1523	U	C2-N3-C4	-5.00	124.00	127.00
36	A1	1668	G	N1-C2-N3	5.00	126.90	123.90
36	A1	2168	A	N9-C4-C5	-5.00	103.80	105.80
36	A1	2736	A	N1-C2-N3	5.00	131.80	129.30
36	A1	3015	G	C2-N3-C4	5.00	114.40	111.90
36	A5	509	U	N3-C4-O4	-5.00	115.90	119.40

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	A1	1329	U	Sidechain
36	A1	406	G	Sidechain
36	A1	835	G	Sidechain
36	A5	2898	G	Sidechain
3	AB	131	ASP	Peptide
9	AH	131	PHE	Peptide
13	AL	127	GLN	Peptide
16	AO	124	ASP	Peptide
19	AR	22	PRO	Peptide
19	AR	85	VAL	Peptide
27	AZ	54	VAL	Peptide
27	AZ	93	SER	Peptide
27	AZ	96	SER	Peptide
29	Ab	42	ASN	Peptide
33	Af	105	TYR	Peptide
33	Af	138	ARG	Peptide
35	Ah	134	ASP	Sidechain
40	BB	172	ALA	Peptide
41	BC	318	LEU	Peptide
43	BE	129	GLU	Peptide
43	BE	51	ARG	Peptide
44	BF	157	ASN	Peptide
45	BG	158	ASP	Peptide
45	BG	30	THR	Peptide

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Mol	Chain	Res	Type	Group
45	BG	74	THR	Peptide
46	BH	21	LYS	Peptide
48	BJ	8	PRO	Peptide
52	BO	110[A]	PRO	Peptide
52	BO	110[B]	PRO	Peptide
57	BT	16	GLN	Peptide
65	Bb	19	ASN	Peptide
65	Bb	20	GLY	Peptide
67	Bd	110	GLU	Peptide
78	Bo	93	LEU	Peptide
2	CA	165	ARG	Peptide
5	CD	203	PRO	Peptide
7	CF	44	ASN	Peptide
7	CF	99	MET	Peptide
11	CJ	168	ARG	Peptide
11	CJ	88	GLU	Peptide
11	CJ	89	ASP	Peptide
16	CO	131	GLY	Peptide
17	CP	52	LYS	Peptide
18	CQ	41	PRO	Peptide
22	CU	70	THR	Peptide
25	CX	44	GLY	Peptide
27	CZ	85	LYS	Peptide
27	CZ	87	GLY	Peptide
33	Cf	102	VAL	Peptide
33	Cf	129	GLY	Peptide
39	DA	143	GLU	Peptide
39	DA	211	HIS	Peptide
41	DC	91	GLY	Peptide
42	DD	271	LYS	Peptide
43	DE	129	GLU	Peptide
44	DF	192	GLY	Peptide
44	DF	226	GLY	Peptide
52	DO	110[A]	PRO	Peptide
52	DO	68[B]	ARG	Peptide
56	DS	133	ALA	Peptide
59	DV	41	GLY	Peptide
62	DY	111	LEU	Peptide
63	DZ	101	PHE	Peptide
64	Da	26	ARG	Peptide
64	Da	66	ALA	Peptide
64	Da	75	LEU	Peptide

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Mol	Chain	Res	Type	Group
65	Db	19	ASN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	204/252 (81%)	143 (70%)	35 (17%)	26 (13%)	0	1
2	CA	204/252 (81%)	146 (72%)	33 (16%)	25 (12%)	0	1
3	AB	212/255 (83%)	133 (63%)	41 (19%)	38 (18%)	0	0
3	CB	214/255 (84%)	174 (81%)	25 (12%)	15 (7%)	1	6
4	AC	215/254 (85%)	187 (87%)	16 (7%)	12 (6%)	2	10
4	CC	215/254 (85%)	188 (87%)	14 (6%)	13 (6%)	1	9
5	AD	221/240 (92%)	180 (81%)	28 (13%)	13 (6%)	1	9
5	CD	221/240 (92%)	177 (80%)	23 (10%)	21 (10%)	0	3
6	AE	258/261 (99%)	201 (78%)	36 (14%)	21 (8%)	1	4
6	CE	258/261 (99%)	219 (85%)	19 (7%)	20 (8%)	1	4
7	AF	204/225 (91%)	154 (76%)	31 (15%)	19 (9%)	0	3
7	CF	204/225 (91%)	155 (76%)	32 (16%)	17 (8%)	1	4
8	AG	224/236 (95%)	190 (85%)	22 (10%)	12 (5%)	2	11
8	CG	216/236 (92%)	183 (85%)	21 (10%)	12 (6%)	2	10
9	AH	182/190 (96%)	127 (70%)	28 (15%)	27 (15%)	0	1
9	CH	184/190 (97%)	143 (78%)	23 (12%)	18 (10%)	0	2
10	AI	184/200 (92%)	155 (84%)	14 (8%)	15 (8%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CI	184/200 (92%)	160 (87%)	17 (9%)	7 (4%)	3	18
11	AJ	183/197 (93%)	152 (83%)	19 (10%)	12 (7%)	1	6
11	CJ	183/197 (93%)	152 (83%)	17 (9%)	14 (8%)	1	5
12	AK	94/105 (90%)	66 (70%)	18 (19%)	10 (11%)	0	2
12	CK	92/105 (88%)	59 (64%)	15 (16%)	18 (20%)	0	0
13	AL	153/156 (98%)	125 (82%)	19 (12%)	9 (6%)	1	9
13	CL	144/156 (92%)	118 (82%)	15 (10%)	11 (8%)	1	5
14	AM	122/143 (85%)	66 (54%)	23 (19%)	33 (27%)	0	0
14	CM	122/143 (85%)	60 (49%)	31 (25%)	31 (25%)	0	0
15	AN	148/151 (98%)	125 (84%)	15 (10%)	8 (5%)	2	11
15	CN	148/151 (98%)	129 (87%)	10 (7%)	9 (6%)	1	8
16	AO	125/137 (91%)	94 (75%)	16 (13%)	15 (12%)	0	1
16	CO	126/137 (92%)	101 (80%)	20 (16%)	5 (4%)	3	17
17	AP	122/142 (86%)	92 (75%)	15 (12%)	15 (12%)	0	1
17	CP	133/142 (94%)	91 (68%)	20 (15%)	22 (16%)	0	0
18	AQ	139/143 (97%)	114 (82%)	14 (10%)	11 (8%)	1	4
18	CQ	140/143 (98%)	122 (87%)	10 (7%)	8 (6%)	1	10
19	AR	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	0	2
19	CR	113/136 (83%)	92 (81%)	12 (11%)	9 (8%)	1	4
20	AS	143/146 (98%)	110 (77%)	19 (13%)	14 (10%)	0	2
20	CS	143/146 (98%)	111 (78%)	25 (18%)	7 (5%)	2	13
21	AT	141/144 (98%)	111 (79%)	18 (13%)	12 (8%)	1	4
21	CT	141/144 (98%)	125 (89%)	9 (6%)	7 (5%)	2	12
22	AU	105/121 (87%)	87 (83%)	13 (12%)	5 (5%)	2	13
22	CU	108/121 (89%)	81 (75%)	12 (11%)	15 (14%)	0	1
23	AV	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0	1
23	CV	85/87 (98%)	71 (84%)	7 (8%)	7 (8%)	1	4
24	AW	127/130 (98%)	114 (90%)	10 (8%)	3 (2%)	6	29
24	CW	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
25	AX	142/145 (98%)	111 (78%)	13 (9%)	18 (13%)	0	1
25	CX	142/145 (98%)	127 (89%)	13 (9%)	2 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	AY	132/135 (98%)	106 (80%)	13 (10%)	13 (10%)	0	2
26	CY	132/135 (98%)	100 (76%)	17 (13%)	15 (11%)	0	2
27	AZ	68/108 (63%)	46 (68%)	11 (16%)	11 (16%)	0	1
27	CZ	67/108 (62%)	50 (75%)	10 (15%)	7 (10%)	0	2
28	Aa	95/119 (80%)	57 (60%)	21 (22%)	17 (18%)	0	0
28	Ca	95/119 (80%)	67 (70%)	20 (21%)	8 (8%)	1	4
29	Ab	79/82 (96%)	62 (78%)	13 (16%)	4 (5%)	2	12
29	Cb	79/82 (96%)	62 (78%)	9 (11%)	8 (10%)	0	2
30	Ac	61/67 (91%)	47 (77%)	9 (15%)	5 (8%)	1	4
30	Cc	61/67 (91%)	41 (67%)	17 (28%)	3 (5%)	2	13
31	Ad	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	3	17
31	Cd	51/56 (91%)	45 (88%)	2 (4%)	4 (8%)	1	4
32	Ae	58/63 (92%)	49 (84%)	7 (12%)	2 (3%)	3	20
32	Ce	60/63 (95%)	45 (75%)	9 (15%)	6 (10%)	0	2
33	Af	50/152 (33%)	30 (60%)	9 (18%)	11 (22%)	0	0
33	Cf	50/152 (33%)	26 (52%)	13 (26%)	11 (22%)	0	0
34	Ag	316/319 (99%)	273 (86%)	30 (10%)	13 (4%)	3	16
34	Cg	316/319 (99%)	262 (83%)	38 (12%)	16 (5%)	2	12
35	Ah	120/273 (44%)	92 (77%)	17 (14%)	11 (9%)	1	3
39	BA	250/254 (98%)	230 (92%)	14 (6%)	6 (2%)	6	29
39	DA	250/254 (98%)	213 (85%)	30 (12%)	7 (3%)	5	25
40	BB	384/387 (99%)	333 (87%)	37 (10%)	14 (4%)	3	19
40	DB	384/387 (99%)	341 (89%)	34 (9%)	9 (2%)	6	30
41	BC	359/362 (99%)	304 (85%)	34 (10%)	21 (6%)	1	10
41	DC	359/362 (99%)	306 (85%)	32 (9%)	21 (6%)	1	10
42	BD	294/297 (99%)	242 (82%)	31 (10%)	21 (7%)	1	5
42	DD	292/297 (98%)	267 (91%)	19 (6%)	6 (2%)	7	33
43	BE	152/176 (86%)	137 (90%)	11 (7%)	4 (3%)	5	27
43	DE	153/176 (87%)	134 (88%)	15 (10%)	4 (3%)	5	27
44	BF	220/244 (90%)	200 (91%)	11 (5%)	9 (4%)	3	16
44	DF	221/244 (91%)	201 (91%)	15 (7%)	5 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BG	231/256 (90%)	186 (80%)	26 (11%)	19 (8%)	1	4
45	DG	229/256 (90%)	180 (79%)	28 (12%)	21 (9%)	1	3
46	BH	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	4	22
46	DH	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	7	33
47	BI	207/221 (94%)	181 (87%)	19 (9%)	7 (3%)	3	20
47	DI	209/221 (95%)	175 (84%)	22 (10%)	12 (6%)	1	10
48	BJ	167/174 (96%)	120 (72%)	26 (16%)	21 (13%)	0	1
48	DJ	167/174 (96%)	135 (81%)	19 (11%)	13 (8%)	1	4
49	BL	191/199 (96%)	161 (84%)	18 (9%)	12 (6%)	1	7
49	DL	192/199 (96%)	161 (84%)	20 (10%)	11 (6%)	1	10
50	BM	134/138 (97%)	117 (87%)	8 (6%)	9 (7%)	1	6
50	DM	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	22	60
51	BN	201/204 (98%)	184 (92%)	10 (5%)	7 (4%)	3	20
51	DN	201/204 (98%)	182 (90%)	13 (6%)	6 (3%)	4	24
52	BO	353/219 (161%)	332 (94%)	14 (4%)	7 (2%)	7	34
52	DO	352/219 (161%)	324 (92%)	18 (5%)	10 (3%)	5	25
53	BP	181/184 (98%)	155 (86%)	17 (9%)	9 (5%)	2	12
53	DP	153/184 (83%)	142 (93%)	9 (6%)	2 (1%)	12	45
54	BQ	183/186 (98%)	162 (88%)	17 (9%)	4 (2%)	6	31
54	DQ	183/186 (98%)	168 (92%)	9 (5%)	6 (3%)	4	21
55	BR	186/189 (98%)	170 (91%)	12 (6%)	4 (2%)	6	31
55	DR	186/189 (98%)	167 (90%)	16 (9%)	3 (2%)	9	40
56	BS	170/172 (99%)	154 (91%)	12 (7%)	4 (2%)	6	29
56	DS	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	64
57	BT	157/160 (98%)	140 (89%)	10 (6%)	7 (4%)	2	14
57	DT	157/160 (98%)	146 (93%)	9 (6%)	2 (1%)	12	45
58	BU	98/121 (81%)	75 (76%)	14 (14%)	9 (9%)	1	3
58	DU	96/121 (79%)	80 (83%)	13 (14%)	3 (3%)	4	23
59	BV	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	22	60
59	DV	134/137 (98%)	124 (92%)	8 (6%)	2 (2%)	10	42
60	BW	96/155 (62%)	69 (72%)	16 (17%)	11 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	DW	133/155 (86%)	106 (80%)	19 (14%)	8 (6%)	1	9
61	BX	119/142 (84%)	106 (89%)	11 (9%)	2 (2%)	9	39
61	DX	118/142 (83%)	103 (87%)	7 (6%)	8 (7%)	1	6
62	BY	124/127 (98%)	107 (86%)	15 (12%)	2 (2%)	9	40
62	DY	124/127 (98%)	107 (86%)	12 (10%)	5 (4%)	3	17
63	BZ	133/136 (98%)	114 (86%)	9 (7%)	10 (8%)	1	5
63	DZ	133/136 (98%)	107 (80%)	13 (10%)	13 (10%)	0	2
64	Ba	146/149 (98%)	120 (82%)	15 (10%)	11 (8%)	1	5
64	Da	146/149 (98%)	123 (84%)	18 (12%)	5 (3%)	3	20
65	Bb	56/59 (95%)	44 (79%)	9 (16%)	3 (5%)	2	11
65	Db	56/59 (95%)	44 (79%)	7 (12%)	5 (9%)	1	3
66	Bc	95/105 (90%)	86 (90%)	8 (8%)	1 (1%)	14	50
66	Dc	98/105 (93%)	87 (89%)	8 (8%)	3 (3%)	4	23
67	Bd	107/113 (95%)	94 (88%)	8 (8%)	5 (5%)	2	14
67	Dd	107/113 (95%)	88 (82%)	13 (12%)	6 (6%)	2	10
68	Be	125/130 (96%)	111 (89%)	10 (8%)	4 (3%)	4	22
68	De	125/130 (96%)	110 (88%)	9 (7%)	6 (5%)	2	13
69	Bf	104/107 (97%)	100 (96%)	2 (2%)	2 (2%)	8	36
69	Df	104/107 (97%)	96 (92%)	5 (5%)	3 (3%)	4	24
70	Bg	110/121 (91%)	97 (88%)	9 (8%)	4 (4%)	3	19
70	Dg	110/121 (91%)	93 (84%)	13 (12%)	4 (4%)	3	19
71	Bh	117/120 (98%)	99 (85%)	10 (8%)	8 (7%)	1	6
71	Dh	117/120 (98%)	99 (85%)	14 (12%)	4 (3%)	3	20
72	Bi	97/100 (97%)	75 (77%)	11 (11%)	11 (11%)	0	2
72	Di	97/100 (97%)	77 (79%)	13 (13%)	7 (7%)	1	5
73	Bj	85/88 (97%)	70 (82%)	12 (14%)	3 (4%)	3	20
73	Dj	85/88 (97%)	75 (88%)	8 (9%)	2 (2%)	6	29
74	Bk	75/78 (96%)	66 (88%)	8 (11%)	1 (1%)	12	45
74	Dk	75/78 (96%)	61 (81%)	10 (13%)	4 (5%)	2	11
75	Bl	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
75	Dl	48/51 (94%)	41 (85%)	6 (12%)	1 (2%)	7	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	Bm	50/128 (39%)	45 (90%)	3 (6%)	2 (4%)	3	17
76	Dm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	7	34
77	Bn	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
77	Dn	23/25 (92%)	22 (96%)	0	1 (4%)	2	15
78	Bo	103/106 (97%)	86 (84%)	13 (13%)	4 (4%)	3	17
78	Do	103/106 (97%)	90 (87%)	11 (11%)	2 (2%)	8	36
79	Bp	89/92 (97%)	77 (86%)	9 (10%)	3 (3%)	3	20
79	Dp	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
81	Ch	61/273 (22%)	38 (62%)	9 (15%)	14 (23%)	0	0
83	Dq	117/312 (38%)	93 (80%)	18 (15%)	6 (5%)	2	12
All	All	22511/24658 (91%)	18787 (84%)	2329 (10%)	1395 (6%)	1	8

All (1395) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AA	4	PRO
2	AA	29	VAL
2	AA	30	GLN
2	AA	39	ASN
2	AA	66	ALA
2	AA	95	ALA
2	AA	111	ILE
2	AA	191	ARG
2	AA	203	PHE
2	AA	205	ARG
3	AB	21	VAL
3	AB	26	ARG
3	AB	49	ASN
3	AB	58	SER
3	AB	60	ALA
3	AB	63	GLY
3	AB	113	MET
3	AB	116	LYS
3	AB	176	VAL
3	AB	177	GLN
3	AB	179	SER
3	AB	182	ALA
3	AB	206	PRO

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Mol	Chain	Res	Type
3	AB	221	PRO
4	AC	146	THR
4	AC	148	LEU
5	AD	4	LEU
5	AD	62	ASN
5	AD	65	ARG
5	AD	93	ASP
5	AD	211	PRO
5	AD	212	LYS
5	AD	216	PRO
5	AD	220	PRO
6	AE	104	ASP
6	AE	142	HIS
6	AE	153	ASN
6	AE	164	LEU
6	AE	260	GLY
7	AF	26	ALA
7	AF	39	GLU
7	AF	43	PHE
7	AF	63	GLN
7	AF	101	GLY
7	AF	153	GLY
7	AF	206	SER
8	AG	20	ASP
8	AG	25	ARG
8	AG	154	ARG
8	AG	173	PRO
8	AG	174	LYS
9	AH	31	SER
9	AH	36	ALA
9	AH	64	VAL
9	AH	67	LEU
9	AH	98	ILE
9	AH	105	THR
9	AH	111	LYS
9	AH	112	ARG
9	AH	131	PHE
9	AH	133	THR
9	AH	134	GLU
9	AH	155	ASP
10	AI	13	ALA
10	AI	22	ARG

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Mol	Chain	Res	Type
10	AI	147	ALA
10	AI	149	SER
11	AJ	98	ALA
11	AJ	100	LYS
11	AJ	118	LEU
11	AJ	121	SER
11	AJ	164	PHE
12	AK	60	SER
12	AK	81	ASN
12	AK	87	VAL
12	AK	88	PRO
12	AK	93	GLN
13	AL	7	VAL
13	AL	29	LYS
13	AL	133	LYS
14	AM	21	GLU
14	AM	25	GLU
14	AM	45	LEU
14	AM	55	GLY
14	AM	83	GLU
14	AM	87	PRO
14	AM	89	ILE
14	AM	90	LYS
14	AM	93	ASP
14	AM	126	TRP
15	AN	19	SER
15	AN	22	ALA
16	AO	38	THR
16	AO	39	ILE
16	AO	124	ASP
16	AO	125	SER
16	AO	126	THR
17	AP	29	SER
17	AP	54	ALA
17	AP	125	PRO
17	AP	126	VAL
18	AQ	41	PRO
18	AQ	58	ASP
18	AQ	59	LYS
18	AQ	114	ARG
18	AQ	116	LEU
18	AQ	138	PHE

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Mol	Chain	Res	Type
19	AR	6	THR
19	AR	26	LEU
19	AR	85	VAL
19	AR	86	PRO
19	AR	88	VAL
19	AR	96	SER
19	AR	124	VAL
20	AS	14	ILE
20	AS	25	ASN
20	AS	28	ILE
20	AS	60	GLU
20	AS	91	ASP
20	AS	92	ILE
21	AT	31	PRO
21	AT	53	TRP
21	AT	69	LYS
22	AU	118	VAL
23	AV	4	ASP
23	AV	7	GLN
23	AV	11	LEU
25	AX	3	LYS
25	AX	41	SER
25	AX	96	VAL
25	AX	114	LYS
25	AX	128	SER
25	AX	131	SER
25	AX	137	LYS
25	AX	138	GLU
25	AX	144	ARG
26	AY	32	ARG
26	AY	36	SER
26	AY	78	SER
27	AZ	38	HIS
27	AZ	39	ALA
27	AZ	43	ASP
27	AZ	44	GLN
27	AZ	54	VAL
27	AZ	71	ILE
27	AZ	88	ILE
28	Aa	19	LYS
28	Aa	45	VAL
28	Aa	46	GLU

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Mol	Chain	Res	Type
28	Aa	62	TYR
28	Aa	65	PRO
28	Aa	82	ARG
28	Aa	84	VAL
28	Aa	85	ARG
29	Ab	38	PRO
29	Ab	62	ILE
30	Ac	36	THR
30	Ac	51	ASN
31	Ad	8	PHE
32	Ae	47	VAL
33	Af	102	VAL
33	Af	103	LEU
33	Af	106	TYR
33	Af	111	GLU
33	Af	128	ALA
33	Af	148	TYR
34	Ag	51	ASP
34	Ag	160	GLU
34	Ag	318	ALA
35	Ah	47	ALA
35	Ah	52	PRO
35	Ah	85	SER
35	Ah	87	THR
39	BA	144	ASN
40	BB	3	HIS
40	BB	5	LYS
40	BB	140	ASP
40	BB	174	LYS
40	BB	300	ARG
40	BB	347	SER
40	BB	351	LEU
40	BB	385	LYS
41	BC	4	PRO
41	BC	268	ALA
41	BC	269	SER
41	BC	283	THR
41	BC	292	SER
41	BC	320	ASN
41	BC	338	LYS
41	BC	361	HIS
42	BD	20	PHE

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Mol	Chain	Res	Type
42	BD	58	LYS
42	BD	124	GLU
42	BD	125	VAL
42	BD	210	GLU
42	BD	233	ALA
42	BD	234	ASP
42	BD	258	LYS
42	BD	276	LYS
42	BD	293	LEU
42	BD	295	GLY
43	BE	6	ALA
44	BF	25	GLN
44	BF	26	VAL
44	BF	216	VAL
45	BG	25	PRO
45	BG	31	PRO
45	BG	36	ILE
45	BG	37	GLY
45	BG	156	ASP
46	BH	50	ASN
46	BH	109	ALA
47	BI	113	GLN
47	BI	207	GLU
47	BI	218	ALA
47	BI	219	ALA
48	BJ	8	PRO
48	BJ	11	ASP
48	BJ	12	LEU
48	BJ	74	PRO
48	BJ	94	ARG
48	BJ	165	GLN
49	BL	5	LYS
49	BL	47	ALA
49	BL	50	PRO
49	BL	129	ASN
49	BL	131	LYS
49	BL	193	ALA
50	BM	8	LYS
50	BM	9	ALA
50	BM	135	LEU
50	BM	136	ALA
51	BN	74	PRO

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Mol	Chain	Res	Type
51	BN	75	VAL
52	BO	3[B]	SER
52	BO	111[A]	PRO
52	BO	111[B]	PRO
53	BP	157	VAL
54	BQ	99	THR
55	BR	5	ARG
55	BR	47	ASN
56	BS	167	ARG
57	BT	124	VAL
57	BT	159	PHE
58	BU	107	PHE
60	BW	26	SER
60	BW	81	PRO
60	BW	86	SER
60	BW	97	LYS
61	BX	44	PRO
62	BY	84	LYS
63	BZ	17	ARG
63	BZ	59	ALA
63	BZ	125	GLY
63	BZ	128	GLN
63	BZ	129	TRP
64	Ba	66	ALA
64	Ba	76	ASP
66	Bc	100	ILE
67	Bd	5	LYS
67	Bd	6	ASP
67	Bd	7	VAL
67	Bd	83	GLU
67	Bd	84	ASP
68	Be	12	LYS
68	Be	27	ARG
68	Be	123	LYS
71	Bh	97	ALA
71	Bh	119	LYS
72	Bi	13	LYS
72	Bi	33	ALA
73	Bj	85	LYS
76	Bm	78	ILE
78	Bo	94	GLY
78	Bo	100	LYS

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Mol	Chain	Res	Type
2	CA	4	PRO
2	CA	8	ASP
2	CA	22	THR
2	CA	23	HIS
2	CA	44	GLY
2	CA	163	ASN
2	CA	164	ASN
2	CA	185	ARG
2	CA	187	ALA
2	CA	189	VAL
2	CA	203	PHE
2	CA	206	ASP
3	CB	26	ARG
3	CB	62	LYS
3	CB	81	PHE
3	CB	82	ARG
3	CB	147	ALA
3	CB	179	SER
3	CB	206	PRO
3	CB	210	ILE
3	CB	223	PHE
4	CC	91	ARG
4	CC	92	ALA
4	CC	107	SER
4	CC	248	SER
5	CD	4	LEU
5	CD	44	THR
5	CD	61	GLU
5	CD	91	VAL
5	CD	113	LEU
5	CD	115	ILE
5	CD	211	PRO
5	CD	212	LYS
5	CD	216	PRO
5	CD	217	ILE
5	CD	219	ALA
5	CD	220	PRO
6	CE	24	SER
6	CE	95	THR
6	CE	163	ASP
6	CE	164	LEU
6	CE	196	VAL

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Mol	Chain	Res	Type
7	CF	28	PRO
7	CF	39	GLU
7	CF	54	LYS
7	CF	58	LEU
7	CF	125	THR
7	CF	153	GLY
7	CF	184	PHE
8	CG	153	VAL
8	CG	173	PRO
8	CG	174	LYS
9	CH	10	SER
9	CH	11	GLN
9	CH	31	SER
9	CH	64	VAL
9	CH	67	LEU
9	CH	74	GLN
9	CH	110	GLN
9	CH	116	ARG
9	CH	131	PHE
9	CH	163	ASP
9	CH	185	ILE
10	CI	116	HIS
11	CJ	118	LEU
11	CJ	121	SER
11	CJ	168	ARG
12	CK	23	ALA
12	CK	79	TYR
12	CK	82	LEU
12	CK	83	PRO
12	CK	88	PRO
12	CK	92	ILE
12	CK	97	PRO
14	CM	21	GLU
14	CM	66	VAL
14	CM	83	GLU
14	CM	84	ASN
14	CM	85	LYS
14	CM	87	PRO
14	CM	89	ILE
14	CM	91	VAL
14	CM	93	ASP
14	CM	109	GLU

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Mol	Chain	Res	Type
15	CN	19	SER
15	CN	66	ILE
15	CN	87	ASP
16	CO	50	ALA
16	CO	126	THR
17	CP	9	LYS
17	CP	11	VAL
17	CP	51	SER
17	CP	52	LYS
17	CP	68	PRO
17	CP	125	PRO
17	CP	126	VAL
17	CP	127	ARG
17	CP	135	THR
18	CQ	42	GLU
18	CQ	115	THR
18	CQ	116	LEU
19	CR	88	VAL
19	CR	96	SER
19	CR	98	GLY
19	CR	104	ASN
19	CR	116	LYS
20	CS	91	ASP
20	CS	92	ILE
21	CT	29	GLU
21	CT	33	TYR
21	CT	34	VAL
22	CU	15	GLN
22	CU	17	GLN
22	CU	18	GLN
22	CU	49	ASN
22	CU	52	LYS
22	CU	96	PRO
22	CU	97	VAL
23	CV	78	LEU
25	CX	131	SER
26	CY	12	VAL
26	CY	30	PRO
26	CY	33	ALA
26	CY	35	VAL
26	CY	52	LYS
26	CY	68	LYS

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Mol	Chain	Res	Type
26	CY	121	THR
26	CY	123	LYS
27	CZ	44	GLN
27	CZ	85	LYS
27	CZ	104	ALA
28	Ca	28	LYS
28	Ca	46	GLU
28	Ca	47	ALA
28	Ca	63	ALA
29	Cb	20	LYS
29	Cb	38	PRO
29	Cb	60	SER
29	Cb	62	ILE
31	Cd	6	VAL
31	Cd	19	ARG
32	Ce	45	VAL
32	Ce	60	PRO
33	Cf	102	VAL
33	Cf	103	LEU
33	Cf	106	TYR
33	Cf	136	LYS
33	Cf	148	TYR
34	Cg	4	ASN
34	Cg	160	GLU
34	Cg	163	ASP
34	Cg	165	ASP
34	Cg	318	ALA
81	Ch	42	ALA
81	Ch	50	ASN
81	Ch	66	ALA
81	Ch	69	ARG
39	DA	96	LEU
40	DB	129	ALA
40	DB	140	ASP
40	DB	347	SER
41	DC	14	GLU
41	DC	15	ALA
41	DC	90	PHE
41	DC	145	ILE
41	DC	302	ALA
41	DC	311	HIS
41	DC	329	PRO

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Mol	Chain	Res	Type
41	DC	330	TYR
41	DC	361	HIS
42	DD	215	ASP
42	DD	260	PHE
43	DE	97	ASN
43	DE	98	VAL
44	DF	158	LYS
45	DG	25	PRO
45	DG	26	LEU
45	DG	34	PHE
45	DG	122	LYS
47	DI	25	ALA
47	DI	82	ARG
47	DI	170	LYS
47	DI	175	ASN
47	DI	187	ALA
48	DJ	8	PRO
48	DJ	10	ARG
48	DJ	12	LEU
48	DJ	94	ARG
48	DJ	95	ASN
48	DJ	108	GLU
48	DJ	115	LYS
48	DJ	167	TYR
49	DL	47	ALA
49	DL	129	ASN
49	DL	134	GLU
49	DL	150	PRO
50	DM	136	ALA
51	DN	49	ARG
51	DN	146	ALA
51	DN	147	ARG
52	DO	110[A]	PRO
52	DO	110[B]	PRO
52	DO	111[A]	PRO
52	DO	111[B]	PRO
52	DO	180[A]	SER
52	DO	180[B]	SER
52	DO	181[A]	ALA
52	DO	181[B]	ALA
54	DQ	41	ASP
54	DQ	99	THR

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Mol	Chain	Res	Type
55	DR	35	ALA
56	DS	2	ALA
57	DT	136	ARG
59	DV	42	SER
60	DW	26	SER
60	DW	71	ARG
60	DW	76	VAL
61	DX	24	LEU
61	DX	25	LYS
61	DX	40	LEU
61	DX	44	PRO
61	DX	45	LYS
62	DY	77	LYS
62	DY	83	ASP
62	DY	84	LYS
62	DY	125	LYS
62	DY	126	LEU
63	DZ	5	LEU
63	DZ	125	GLY
63	DZ	129	TRP
64	Da	76	ASP
65	Db	21	ILE
65	Db	23	LYS
65	Db	25	LYS
65	Db	39	PHE
66	Dc	100	ILE
66	Dc	104	LEU
67	Dd	7	VAL
67	Dd	45	GLY
67	Dd	84	ASP
68	De	4	LEU
68	De	5	PRO
68	De	27	ARG
69	Df	88	ASN
70	Dg	10	ARG
70	Dg	100	ILE
71	Dh	40	SER
71	Dh	82	ALA
72	Di	33	ALA
72	Di	63	ASN
72	Di	64	SER
72	Di	98	ARG

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Mol	Chain	Res	Type
73	Dj	87	SER
74	Dk	17	ARG
74	Dk	18	ALA
75	Dl	3	ALA
78	Do	78	LYS
2	AA	5	ALA
2	AA	49	ASN
2	AA	81	PHE
2	AA	94	GLY
2	AA	190	ASP
2	AA	194	PRO
2	AA	196	SER
3	AB	23	PRO
3	AB	55	LYS
3	AB	72	ASP
3	AB	79	HIS
3	AB	82	ARG
3	AB	93	GLY
3	AB	108	ASP
3	AB	148	ASN
3	AB	181	LEU
3	AB	207	LEU
4	AC	35	TRP
4	AC	203	LYS
4	AC	248	SER
5	AD	44	THR
5	AD	218	LEU
6	AE	12	LEU
6	AE	152	PRO
6	AE	157	ASN
6	AE	195	ILE
6	AE	245	LYS
7	AF	35	GLN
7	AF	45	LYS
7	AF	58	LEU
7	AF	127	GLN
7	AF	150	GLY
7	AF	223	SER
8	AG	24	ILE
8	AG	146	GLY
8	AG	152	ASP
8	AG	153	VAL

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Mol	Chain	Res	Type
9	AH	32	PRO
9	AH	104	ARG
9	AH	156	SER
9	AH	186	PRO
10	AI	40	ALA
10	AI	105	ASP
10	AI	120	THR
10	AI	199	LYS
11	AJ	134	ILE
11	AJ	167	ALA
11	AJ	171	ARG
12	AK	30	ALA
12	AK	64	TYR
12	AK	82	LEU
14	AM	54	ARG
14	AM	63	VAL
14	AM	66	VAL
14	AM	84	ASN
14	AM	91	VAL
14	AM	113	ARG
14	AM	128	ALA
15	AN	13	SER
15	AN	27	LYS
15	AN	28	LEU
15	AN	68	GLY
16	AO	40	ALA
16	AO	42	VAL
16	AO	46	MET
16	AO	50	ALA
16	AO	51	ASP
16	AO	114	ARG
17	AP	48	GLY
17	AP	51	SER
17	AP	101	ALA
18	AQ	40	GLU
18	AQ	113	ASP
19	AR	25	THR
20	AS	59	GLY
20	AS	61	LEU
20	AS	142	GLY
21	AT	11	ALA
21	AT	28	LEU

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Mol	Chain	Res	Type
21	AT	50	ALA
22	AU	17	GLN
23	AV	12	TYR
24	AW	66	ASN
25	AX	8	GLY
25	AX	97	ASP
26	AY	5	VAL
26	AY	11	LYS
27	AZ	73	GLY
28	Aa	36	ILE
28	Aa	63	ALA
28	Aa	75	VAL
28	Aa	86	VAL
29	Ab	63	LEU
30	Ac	35	ASP
30	Ac	61	ARG
31	Ad	34	TYR
33	Af	118	ARG
33	Af	127	GLY
34	Ag	3	SER
34	Ag	28	GLY
34	Ag	161	LYS
34	Ag	217	ASP
35	Ah	46	LYS
35	Ah	82	THR
35	Ah	89	ARG
35	Ah	140	ASP
39	BA	13	GLY
39	BA	70	ARG
40	BB	136	LYS
40	BB	138	ALA
41	BC	15	ALA
41	BC	107	ARG
41	BC	182	LEU
41	BC	232	SER
41	BC	311	HIS
41	BC	317	PRO
42	BD	137	ASP
42	BD	188	GLU
42	BD	209	GLU
42	BD	215	ASP
42	BD	292	ALA

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Mol	Chain	Res	Type
43	BE	97	ASN
43	BE	98	VAL
44	BF	24	GLU
44	BF	175	LYS
45	BG	39	ALA
45	BG	115	ALA
45	BG	159	PRO
45	BG	254	ASP
47	BI	194	GLY
48	BJ	9	MET
48	BJ	73	GLY
48	BJ	86	VAL
48	BJ	115	LYS
48	BJ	167	TYR
49	BL	136	GLU
49	BL	141	ALA
50	BM	10	SER
51	BN	144	ARG
51	BN	184	LYS
52	BO	17[A]	GLY
52	BO	17[B]	GLY
53	BP	164	LYS
53	BP	182	ILE
54	BQ	98	LYS
54	BQ	183	GLY
56	BS	2	ALA
56	BS	12	ARG
56	BS	13	ARG
57	BT	125	ALA
58	BU	11	ILE
58	BU	50	LEU
58	BU	51	GLY
58	BU	91	ASP
59	BV	82	ALA
61	BX	45	LYS
62	BY	92	GLY
64	Ba	47	LYS
64	Ba	57	GLY
64	Ba	121	VAL
70	Bg	74	ARG
70	Bg	77	GLY
71	Bh	90	ARG

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Mol	Chain	Res	Type
71	Bh	95	PHE
71	Bh	96	GLU
72	Bi	28	TYR
72	Bi	49	GLY
72	Bi	50	LEU
73	Bj	65	ARG
79	Bp	60	CYS
2	CA	29	VAL
2	CA	30	GLN
2	CA	95	ALA
2	CA	103	THR
2	CA	111	ILE
2	CA	158	VAL
2	CA	186	GLY
2	CA	191	ARG
2	CA	194	PRO
3	CB	93	GLY
3	CB	154	SER
3	CB	209	ASN
3	CB	224	ASP
4	CC	93	GLY
4	CC	106	ASP
4	CC	153	SER
4	CC	163	GLY
4	CC	164	SER
5	CD	45	LYS
5	CD	221	SER
6	CE	12	LEU
6	CE	104	ASP
7	CF	35	GLN
7	CF	36	ALA
7	CF	55	ASP
7	CF	100	ASN
7	CF	204	GLY
8	CG	25	ARG
8	CG	68	LEU
8	CG	152	ASP
8	CG	154	ARG
9	CH	87	ASP
9	CH	112	ARG
10	CI	62	THR
10	CI	115	ALA

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Mol	Chain	Res	Type
11	CJ	105	LEU
11	CJ	110	GLN
11	CJ	134	ILE
11	CJ	147	MET
11	CJ	169	PRO
12	CK	9	ASN
12	CK	32	HIS
12	CK	35	ILE
12	CK	81	ASN
12	CK	94	GLU
13	CL	114	ALA
13	CL	133	LYS
13	CL	144	ALA
14	CM	22	VAL
14	CM	58	LEU
14	CM	63	VAL
14	CM	103	LEU
14	CM	119	SER
14	CM	131	ASP
15	CN	60	VAL
15	CN	139	TRP
15	CN	140	LYS
17	CP	6	ASN
17	CP	10	ARG
17	CP	14	THR
17	CP	17	TYR
17	CP	131	ALA
17	CP	132	GLY
18	CQ	39	VAL
18	CQ	142	TYR
19	CR	63	LYS
19	CR	99	VAL
20	CS	60	GLU
20	CS	61	LEU
21	CT	26	GLY
22	CU	16	GLN
22	CU	100	VAL
23	CV	4	ASP
23	CV	43	GLY
23	CV	44	ARG
26	CY	34	ASN
26	CY	58	PHE

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Mol	Chain	Res	Type
27	CZ	38	HIS
28	Ca	62	TYR
29	Cb	57	GLU
30	Cc	61	ARG
30	Cc	62	GLU
32	Ce	47	VAL
32	Ce	51	ASN
32	Ce	61	SER
33	Cf	112	GLY
33	Cf	124	PRO
33	Cf	131	PHE
33	Cf	145	HIS
34	Cg	97	GLY
34	Cg	149	ASP
34	Cg	282	SER
81	Ch	46	LYS
81	Ch	47	ALA
81	Ch	48	ARG
81	Ch	63	ASP
81	Ch	65	THR
81	Ch	72	ARG
39	DA	24	GLN
39	DA	194	ASN
40	DB	235	THR
40	DB	293	ASN
41	DC	71	VAL
41	DC	190	GLY
41	DC	272	VAL
41	DC	345	GLU
41	DC	353	ALA
42	DD	125	VAL
42	DD	178	ASN
45	DG	81	THR
45	DG	121	SER
45	DG	188	THR
45	DG	203	VAL
45	DG	223	ALA
45	DG	240	ASN
46	DH	144	ILE
46	DH	189	GLU
47	DI	220	GLN
48	DJ	55	ARG

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Mol	Chain	Res	Type
49	DL	135	ALA
49	DL	141	ALA
51	DN	184	LYS
53	DP	66	SER
53	DP	67	ILE
54	DQ	91	ALA
54	DQ	167	SER
58	DU	49	ASN
58	DU	91	ASP
59	DV	41	GLY
60	DW	63	ILE
60	DW	77	LYS
63	DZ	17	ARG
63	DZ	93	LYS
63	DZ	130	PHE
63	DZ	134	LEU
64	Da	24	LYS
66	Dc	10	ILE
67	Dd	83	GLU
68	De	6	HIS
68	De	12	LYS
68	De	124	GLY
69	Df	91	ALA
71	Dh	119	LYS
77	Dn	23	ARG
83	Dq	47	GLY
83	Dq	198	PRO
2	AA	27	ARG
2	AA	103	THR
3	AB	35	PRO
3	AB	38	PHE
3	AB	62	LYS
3	AB	209	ASN
4	AC	106	ASP
4	AC	150	GLN
4	AC	235	LEU
5	AD	54	ARG
6	AE	200	ARG
7	AF	33	VAL
7	AF	156	ARG
9	AH	5	GLN
9	AH	29	ASN

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Mol	Chain	Res	Type
9	AH	74	GLN
9	AH	75	THR
9	AH	110	GLN
10	AI	41	LYS
10	AI	136	SER
10	AI	153	GLU
11	AJ	163	PRO
13	AL	4	GLU
13	AL	55	ASP
13	AL	146	ALA
13	AL	153	PHE
13	AL	154	ALA
14	AM	22	VAL
14	AM	81	ASP
14	AM	82	PRO
14	AM	85	LYS
14	AM	112	ALA
14	AM	135	MET
16	AO	18	ARG
16	AO	123	SER
17	AP	11	VAL
17	AP	22	LEU
17	AP	52	LYS
19	AR	83	GLN
19	AR	115	LEU
20	AS	10	SER
20	AS	80	LYS
20	AS	83	ALA
21	AT	25	GLN
22	AU	55	PRO
23	AV	2	GLU
23	AV	10	GLU
23	AV	15	ARG
25	AX	37	ALA
25	AX	40	SER
25	AX	89	ASN
26	AY	34	ASN
26	AY	51	GLU
26	AY	53	ASP
27	AZ	41	ILE
27	AZ	55	PRO
27	AZ	97	LYS

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Mol	Chain	Res	Type
28	Aa	66	LYS
33	Af	138	ARG
34	Ag	15	GLY
34	Ag	96	THR
34	Ag	98	GLU
39	BA	250	GLN
40	BB	4	ARG
41	BC	14	GLU
41	BC	16	THR
42	BD	112	LYS
45	BG	78	PHE
45	BG	122	LYS
46	BH	42	ASP
47	BI	195	ALA
48	BJ	140	ARG
48	BJ	169	ALA
48	BJ	173	ASP
49	BL	134	GLU
49	BL	166	ALA
50	BM	28	SER
50	BM	95	ALA
51	BN	145	ASP
53	BP	160	ALA
55	BR	53	LYS
55	BR	64	ARG
57	BT	114	ALA
58	BU	10	LYS
58	BU	44	GLU
60	BW	17	ARG
60	BW	77	LYS
63	BZ	16	GLY
63	BZ	35	SER
63	BZ	102	GLU
64	Ba	93	SER
70	Bg	46	ASP
70	Bg	98	GLN
71	Bh	4	VAL
71	Bh	91	ALA
72	Bi	34	SER
72	Bi	95	ALA
72	Bi	98	ARG
78	Bo	34	SER

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Mol	Chain	Res	Type
79	Bp	58	SER
4	CC	238	SER
5	CD	179	GLN
5	CD	180	GLY
6	CE	57	ASN
6	CE	94	ALA
6	CE	168	LYS
6	CE	171	ASP
7	CF	43	PHE
8	CG	142	ARG
8	CG	165	GLY
9	CH	133	THR
10	CI	101	ILE
10	CI	136	SER
10	CI	137	LYS
11	CJ	162	SER
13	CL	6	THR
13	CL	121	ASP
13	CL	132	SER
14	CM	25	GLU
14	CM	26	ASP
14	CM	82	PRO
14	CM	135	MET
15	CN	22	ALA
16	CO	114	ARG
17	CP	69	GLU
19	CR	86	PRO
20	CS	33	THR
22	CU	13	GLU
22	CU	51	VAL
22	CU	53	LYS
22	CU	119	ALA
26	CY	11	LYS
26	CY	51	GLU
26	CY	132	ARG
31	Cd	11	PRO
34	Cg	39	ASP
34	Cg	161	LYS
34	Cg	297	ASP
81	Ch	84	LYS
39	DA	56	ALA
39	DA	144	ASN

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Mol	Chain	Res	Type
39	DA	249	SER
40	DB	138	ALA
40	DB	155	ALA
41	DC	146	PRO
42	DD	270	LYS
43	DE	10	TYR
43	DE	32	ALA
45	DG	39	ALA
45	DG	123	GLN
45	DG	133	LYS
45	DG	237	ILE
47	DI	83	ASP
47	DI	101	LYS
47	DI	174	THR
47	DI	176	LEU
49	DL	101	ARG
49	DL	140	SER
51	DN	181	ASN
52	DO	12[A]	LYS
52	DO	12[B]	LYS
58	DU	48	GLY
60	DW	74	LYS
60	DW	134	GLN
61	DX	38	LEU
61	DX	47	ALA
61	DX	55	ASN
63	DZ	16	GLY
64	Da	47	LYS
67	Dd	5	LYS
67	Dd	86	LYS
70	Dg	79	SER
72	Di	34	SER
83	Dq	33	VAL
2	AA	33	GLN
2	AA	158	VAL
2	AA	164	ASN
2	AA	185	ARG
2	AA	189	VAL
3	AB	54	LEU
3	AB	61	LEU
3	AB	81	PHE
3	AB	112	SER

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Mol	Chain	Res	Type
3	AB	154	SER
3	AB	215	VAL
4	AC	39	THR
5	AD	217	ILE
6	AE	77	ARG
6	AE	80	THR
6	AE	163	ASP
6	AE	188	ASN
6	AE	193	GLY
7	AF	51	VAL
7	AF	79	ASN
8	AG	69	LEU
9	AH	13	PRO
9	AH	84	LYS
9	AH	132	PRO
10	AI	59	ARG
10	AI	152	ILE
12	AK	94	GLU
13	AL	145	ALA
14	AM	39	ASP
14	AM	68	GLU
14	AM	106	ILE
14	AM	107	ASP
14	AM	108	ARG
14	AM	129	GLU
14	AM	130	THR
15	AN	138	ASN
16	AO	69	ALA
18	AQ	142	TYR
19	AR	23	LYS
19	AR	72	LYS
21	AT	7	ARG
21	AT	23	GLN
21	AT	39	THR
23	AV	44	ARG
25	AX	92	CYS
25	AX	109	ARG
25	AX	112	LYS
26	AY	60	PHE
28	Aa	64	LEU
30	Ac	6	PRO
32	Ae	50	VAL

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Mol	Chain	Res	Type
33	Af	145	HIS
34	Ag	136	ILE
34	Ag	163	ASP
34	Ag	237	GLN
40	BB	386	ASP
41	BC	146	PRO
41	BC	233	LEU
42	BD	6	ASP
42	BD	252	ALA
42	BD	253	PHE
43	BE	95	GLY
44	BF	160	ARG
45	BG	157	VAL
45	BG	253	SER
46	BH	13	PRO
47	BI	24	ARG
48	BJ	95	ASN
48	BJ	108	GLU
48	BJ	114	ILE
48	BJ	117	ASP
51	BN	94	TYR
51	BN	149	ASN
53	BP	158	ALA
53	BP	161	ALA
53	BP	163	LYS
54	BQ	162	ALA
57	BT	12	ARG
58	BU	31	ALA
58	BU	49	ASN
60	BW	64	THR
63	BZ	103	GLN
64	Ba	96	LYS
65	Bb	32	LEU
68	Be	40	SER
71	Bh	27	GLU
73	Bj	25	ARG
74	Bk	33	LYS
78	Bo	15	LYS
79	Bp	51	ALA
2	CA	10	THR
4	CC	40	LYS
4	CC	150	GLN

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Mol	Chain	Res	Type
4	CC	235	LEU
5	CD	111	ASN
5	CD	144	ALA
6	CE	189	LEU
6	CE	245	LYS
7	CF	29	ILE
7	CF	101	GLY
7	CF	151	GLY
8	CG	2	LYS
8	CG	70	PRO
9	CH	66	SER
11	CJ	65	LYS
11	CJ	126	ARG
12	CK	30	ALA
12	CK	95	ARG
13	CL	7	VAL
13	CL	55	ASP
13	CL	61	THR
13	CL	129	ARG
14	CM	45	LEU
14	CM	64	SER
14	CM	81	ASP
14	CM	106	ILE
14	CM	118	ALA
14	CM	128	ALA
14	CM	129	GLU
16	CO	124	ASP
17	CP	7	ALA
17	CP	48	GLY
17	CP	75	PRO
20	CS	145	ARG
21	CT	25	GLN
21	CT	66	TYR
22	CU	19	ILE
23	CV	10	GLU
25	CX	101	GLU
26	CY	53	ASP
27	CZ	103	ARG
28	Ca	15	ARG
28	Ca	35	ALA
28	Ca	59	TYR
29	Cb	58	SER

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Mol	Chain	Res	Type
32	Ce	54	ARG
33	Cf	138	ARG
34	Cg	298	GLY
81	Ch	43	ASP
81	Ch	64	LYS
39	DA	143	GLU
40	DB	333	LYS
41	DC	233	LEU
41	DC	306	THR
41	DC	331	ALA
41	DC	342	LYS
42	DD	124	GLU
44	DF	191	VAL
45	DG	206	GLU
46	DH	167	VAL
47	DI	207	GLU
49	DL	60	ALA
49	DL	76	THR
51	DN	48	ALA
55	DR	147	ALA
60	DW	25	ASP
63	DZ	34	LYS
63	DZ	36	HIS
64	Da	121	VAL
70	Dg	99	LYS
73	Dj	85	LYS
74	Dk	8	ILE
83	Dq	102	SER
3	AB	64	ARG
4	AC	36	VAL
5	AD	59	LEU
6	AE	233	LYS
7	AF	21	THR
7	AF	64	VAL
9	AH	73	VAL
9	AH	185	ILE
11	AJ	162	SER
14	AM	101	ALA
17	AP	38	PRO
21	AT	29	GLU
22	AU	49	ASN
23	AV	46	ILE

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Mol	Chain	Res	Type
23	AV	49	GLU
24	AW	67	GLY
24	AW	83	ILE
25	AX	70	LYS
26	AY	6	THR
26	AY	47	VAL
29	Ab	51	GLN
35	Ah	53	ARG
35	Ah	102	THR
39	BA	35	ALA
39	BA	251	LYS
41	BC	5	GLN
44	BF	178	ILE
45	BG	47	SER
46	BH	2	LYS
46	BH	107	ASP
48	BJ	24	GLY
48	BJ	111	ASP
48	BJ	172	LEU
49	BL	130	GLY
49	BL	133	PRO
50	BM	6	ILE
50	BM	36	VAL
52	BO	187[A]	GLU
52	BO	187[B]	GLU
57	BT	18	ASP
60	BW	80	ARG
60	BW	89	LEU
64	Ba	56	VAL
64	Ba	117	ARG
65	Bb	53	ALA
69	Bf	59	VAL
72	Bi	3	VAL
76	Bm	79	GLU
3	CB	63	GLY
6	CE	90	ILE
6	CE	205	PHE
9	CH	12	ALA
9	CH	13	PRO
10	CI	78	ILE
11	CJ	115	LYS
11	CJ	119	ALA

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Mol	Chain	Res	Type
11	CJ	150	LEU
12	CK	10	LYS
14	CM	59	LEU
14	CM	107	ASP
14	CM	127	GLY
15	CN	43	LYS
15	CN	137	PRO
17	CP	49	MET
17	CP	130	ARG
17	CP	136	SER
20	CS	14	ILE
21	CT	28	LEU
27	CZ	54	VAL
27	CZ	70	LYS
29	Cb	21	LEU
29	Cb	63	LEU
30	Cc	37	SER
31	Cd	7	TRP
33	Cf	146	SER
34	Cg	217	ASP
34	Cg	228	LYS
81	Ch	51	ARG
41	DC	5	GLN
44	DF	229	PHE
45	DG	69	LEU
45	DG	120	LYS
45	DG	124	ASP
46	DH	110	LYS
48	DJ	111	ASP
48	DJ	153	LYS
49	DL	121	SER
54	DQ	98	LYS
55	DR	183	ALA
57	DT	20	ARG
63	DZ	7	ALA
64	Da	129	PHE
65	Db	24	PRO
72	Di	9	ILE
74	Dk	19	ASP
76	Dm	78	ILE
83	Dq	197	PHE
2	AA	139	VAL

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Mol	Chain	Res	Type
3	AB	78	ASP
3	AB	210	ILE
6	AE	3	ARG
6	AE	53	LYS
8	AG	132	ARG
9	AH	11	GLN
10	AI	10	LYS
10	AI	186	GLY
11	AJ	132	ARG
15	AN	60	VAL
17	AP	10	ARG
17	AP	23	GLU
17	AP	69	GLU
17	AP	130	ARG
20	AS	7	GLU
20	AS	34	THR
22	AU	117	VAL
26	AY	58	PHE
26	AY	77	ASN
28	Aa	10	ARG
35	Ah	88	ARG
40	BB	155	ALA
40	BB	317	ILE
41	BC	72	ALA
42	BD	259	LYS
44	BF	164	SER
45	BG	75	ILE
53	BP	162	GLU
60	BW	67	VAL
60	BW	76	VAL
64	Ba	91	LEU
65	Bb	21	ILE
69	Bf	91	ALA
72	Bi	21	THR
72	Bi	94	ILE
2	CA	109	ASN
2	CA	139	VAL
3	CB	21	VAL
6	CE	194	THR
12	CK	3	MET
12	CK	24	LYS
12	CK	31	LYS

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Mol	Chain	Res	Type
13	CL	146	ALA
14	CM	115	VAL
18	CQ	40	GLU
19	CR	120	SER
23	CV	6	GLY
34	Cg	153	GLN
40	DB	187	SER
41	DC	328	ASN
44	DF	157	ASN
45	DG	202	GLU
47	DI	204	GLY
48	DJ	114	ILE
63	DZ	29	HIS
71	Dh	83	LYS
6	AE	234	PRO
11	AJ	117	GLY
16	AO	48	VAL
18	AQ	97	VAL
64	Ba	29	PRO
5	CD	203	PRO
8	CG	69	LEU
9	CH	32	PRO
18	CQ	97	VAL
44	DF	178	ILE
45	DG	190	VAL
83	Dq	196	VAL
2	AA	117	GLU
14	AM	40	GLY
28	Aa	50	VAL
28	Aa	59	TYR
44	BF	91	GLY
45	BG	158	ASP
5	CD	43	PRO
22	CU	118	VAL
23	CV	77	GLY
63	DZ	103	GLN
72	Di	3	VAL
78	Do	31	GLY
3	AB	197	ILE
4	AC	145	GLY
18	AQ	29	ILE
21	AT	100	ILE

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Mol	Chain	Res	Type
33	Af	147	VAL
45	BG	116	VAL
45	BG	119	GLY
45	BG	135	GLY
63	BZ	36	HIS
2	CA	94	GLY
6	CE	150	PRO
6	CE	195	ILE
7	CF	152	GLY
16	CO	131	GLY
34	Cg	15	GLY
45	DG	73	PRO
48	DJ	118	PRO
54	DQ	42	ALA
6	AE	45	ILE
8	AG	70	PRO
12	AK	89	GLY
14	AM	117	GLY
41	BC	131	VAL
53	BP	84	PRO
5	CD	163	PRO
6	CE	260	GLY
18	CQ	4	VAL
26	CY	29	HIS
69	Df	59	VAL
4	AC	163	GLY
57	BT	123	GLY
6	CE	30	ARG

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	
2	AA	164/210 (78%)	122 (74%)	42 (26%)	0	3
2	CA	165/210 (79%)	131 (79%)	34 (21%)	1	6
3	AB	191/224 (85%)	137 (72%)	54 (28%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CB	192/224 (86%)	148 (77%)	44 (23%)	1	4
4	AC	176/205 (86%)	130 (74%)	46 (26%)	0	2
4	CC	176/205 (86%)	133 (76%)	43 (24%)	0	3
5	AD	182/195 (93%)	138 (76%)	44 (24%)	0	3
5	CD	182/195 (93%)	140 (77%)	42 (23%)	1	4
6	AE	221/222 (100%)	166 (75%)	55 (25%)	0	3
6	CE	221/222 (100%)	178 (80%)	43 (20%)	1	7
7	AF	173/191 (91%)	137 (79%)	36 (21%)	1	5
7	CF	173/191 (91%)	132 (76%)	41 (24%)	1	3
8	AG	188/201 (94%)	149 (79%)	39 (21%)	1	6
8	CG	187/201 (93%)	143 (76%)	44 (24%)	1	3
9	AH	165/170 (97%)	124 (75%)	41 (25%)	0	3
9	CH	165/170 (97%)	127 (77%)	38 (23%)	1	4
10	AI	150/161 (93%)	118 (79%)	32 (21%)	1	5
10	CI	150/161 (93%)	117 (78%)	33 (22%)	1	4
11	AJ	158/166 (95%)	117 (74%)	41 (26%)	0	2
11	CJ	158/166 (95%)	124 (78%)	34 (22%)	1	5
12	AK	77/98 (79%)	58 (75%)	19 (25%)	0	3
12	CK	73/98 (74%)	56 (77%)	17 (23%)	1	4
13	AL	129/137 (94%)	105 (81%)	24 (19%)	1	8
13	CL	129/137 (94%)	100 (78%)	29 (22%)	1	4
14	AM	88/119 (74%)	55 (62%)	33 (38%)	0	0
14	CM	88/119 (74%)	55 (62%)	33 (38%)	0	0
15	AN	127/128 (99%)	91 (72%)	36 (28%)	0	2
15	CN	127/128 (99%)	103 (81%)	24 (19%)	1	8
16	AO	81/105 (77%)	57 (70%)	24 (30%)	0	1
16	CO	97/105 (92%)	71 (73%)	26 (27%)	0	2
17	AP	101/118 (86%)	82 (81%)	19 (19%)	1	8
17	CP	103/118 (87%)	81 (79%)	22 (21%)	1	5
18	AQ	117/119 (98%)	84 (72%)	33 (28%)	0	2
18	CQ	118/119 (99%)	92 (78%)	26 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AR	94/124 (76%)	70 (74%)	24 (26%)	0	3
19	CR	92/124 (74%)	74 (80%)	18 (20%)	1	7
20	AS	128/129 (99%)	87 (68%)	41 (32%)	0	1
20	CS	128/129 (99%)	98 (77%)	30 (23%)	1	4
21	AT	115/116 (99%)	84 (73%)	31 (27%)	0	2
21	CT	115/116 (99%)	88 (76%)	27 (24%)	1	3
22	AU	100/114 (88%)	71 (71%)	29 (29%)	0	2
22	CU	103/114 (90%)	69 (67%)	34 (33%)	0	1
23	AV	74/74 (100%)	56 (76%)	18 (24%)	0	3
23	CV	74/74 (100%)	57 (77%)	17 (23%)	1	4
24	AW	110/111 (99%)	84 (76%)	26 (24%)	1	3
24	CW	110/111 (99%)	96 (87%)	14 (13%)	4	19
25	AX	119/120 (99%)	97 (82%)	22 (18%)	1	8
25	CX	119/120 (99%)	101 (85%)	18 (15%)	3	14
26	AY	112/113 (99%)	84 (75%)	28 (25%)	0	3
26	CY	112/113 (99%)	90 (80%)	22 (20%)	1	7
27	AZ	61/89 (68%)	43 (70%)	18 (30%)	0	1
27	CZ	61/89 (68%)	44 (72%)	17 (28%)	0	2
28	Aa	83/101 (82%)	65 (78%)	18 (22%)	1	5
28	Ca	83/101 (82%)	68 (82%)	15 (18%)	1	9
29	Ab	70/71 (99%)	62 (89%)	8 (11%)	5	24
29	Cb	70/71 (99%)	57 (81%)	13 (19%)	1	8
30	Ac	56/60 (93%)	38 (68%)	18 (32%)	0	1
30	Cc	56/60 (93%)	38 (68%)	18 (32%)	0	1
31	Ad	47/49 (96%)	38 (81%)	9 (19%)	1	8
31	Cd	47/49 (96%)	36 (77%)	11 (23%)	1	4
32	Ae	51/54 (94%)	43 (84%)	8 (16%)	2	13
32	Ce	53/54 (98%)	37 (70%)	16 (30%)	0	1
33	Af	43/112 (38%)	32 (74%)	11 (26%)	0	3
33	Cf	43/112 (38%)	32 (74%)	11 (26%)	0	3
34	Ag	259/262 (99%)	222 (86%)	37 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	Cg	260/262 (99%)	226 (87%)	34 (13%)	4	18
35	Ah	97/195 (50%)	74 (76%)	23 (24%)	1	3
39	BA	193/196 (98%)	160 (83%)	33 (17%)	2	10
39	DA	192/196 (98%)	154 (80%)	38 (20%)	1	7
40	BB	321/323 (99%)	240 (75%)	81 (25%)	0	3
40	DB	321/323 (99%)	251 (78%)	70 (22%)	1	5
41	BC	288/289 (100%)	227 (79%)	61 (21%)	1	5
41	DC	288/289 (100%)	222 (77%)	66 (23%)	1	4
42	BD	244/245 (100%)	189 (78%)	55 (22%)	1	4
42	DD	243/245 (99%)	195 (80%)	48 (20%)	1	7
43	BE	134/153 (88%)	116 (87%)	18 (13%)	4	17
43	DE	135/153 (88%)	115 (85%)	20 (15%)	3	14
44	BF	186/205 (91%)	165 (89%)	21 (11%)	6	24
44	DF	187/205 (91%)	158 (84%)	29 (16%)	2	13
45	BG	187/208 (90%)	151 (81%)	36 (19%)	1	8
45	DG	177/208 (85%)	138 (78%)	39 (22%)	1	4
46	BH	171/171 (100%)	131 (77%)	40 (23%)	1	4
46	DH	171/171 (100%)	132 (77%)	39 (23%)	1	4
47	BI	177/187 (95%)	143 (81%)	34 (19%)	1	8
47	DI	179/187 (96%)	142 (79%)	37 (21%)	1	6
48	BJ	147/150 (98%)	111 (76%)	36 (24%)	0	3
48	DJ	147/150 (98%)	114 (78%)	33 (22%)	1	4
49	BL	154/159 (97%)	123 (80%)	31 (20%)	1	6
49	DL	154/159 (97%)	124 (80%)	30 (20%)	1	7
50	BM	107/109 (98%)	84 (78%)	23 (22%)	1	5
50	DM	108/109 (99%)	84 (78%)	24 (22%)	1	4
51	BN	175/176 (99%)	146 (83%)	29 (17%)	2	11
51	DN	175/176 (99%)	142 (81%)	33 (19%)	1	8
52	BO	323/179 (180%)	276 (85%)	47 (15%)	3	15
52	DO	323/179 (180%)	267 (83%)	56 (17%)	2	10
53	BP	140/146 (96%)	109 (78%)	31 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	DP	125/146 (86%)	103 (82%)	22 (18%)	2	10
54	BQ	150/151 (99%)	126 (84%)	24 (16%)	2	12
54	DQ	150/151 (99%)	124 (83%)	26 (17%)	2	10
55	BR	153/154 (99%)	116 (76%)	37 (24%)	0	3
55	DR	153/154 (99%)	121 (79%)	32 (21%)	1	5
56	BS	156/156 (100%)	127 (81%)	29 (19%)	1	8
56	DS	156/156 (100%)	123 (79%)	33 (21%)	1	5
57	BT	136/137 (99%)	103 (76%)	33 (24%)	0	3
57	DT	136/137 (99%)	109 (80%)	27 (20%)	1	7
58	BU	87/107 (81%)	73 (84%)	14 (16%)	2	12
58	DU	85/107 (79%)	62 (73%)	23 (27%)	0	2
59	BV	104/105 (99%)	88 (85%)	16 (15%)	2	13
59	DV	104/105 (99%)	96 (92%)	8 (8%)	13	42
60	BW	57/129 (44%)	49 (86%)	8 (14%)	3	16
60	DW	100/129 (78%)	85 (85%)	15 (15%)	3	14
61	BX	104/118 (88%)	78 (75%)	26 (25%)	0	3
61	DX	104/118 (88%)	81 (78%)	23 (22%)	1	4
62	BY	109/110 (99%)	87 (80%)	22 (20%)	1	6
62	DY	109/110 (99%)	85 (78%)	24 (22%)	1	4
63	BZ	115/116 (99%)	88 (76%)	27 (24%)	1	3
63	DZ	115/116 (99%)	89 (77%)	26 (23%)	1	4
64	Ba	118/119 (99%)	97 (82%)	21 (18%)	2	9
64	Da	118/119 (99%)	95 (80%)	23 (20%)	1	7
65	Bb	46/47 (98%)	36 (78%)	10 (22%)	1	5
65	Db	46/47 (98%)	35 (76%)	11 (24%)	0	3
66	Bc	81/88 (92%)	63 (78%)	18 (22%)	1	4
66	Dc	84/88 (96%)	68 (81%)	16 (19%)	1	8
67	Bd	92/97 (95%)	73 (79%)	19 (21%)	1	6
67	Dd	94/97 (97%)	73 (78%)	21 (22%)	1	4
68	Be	109/111 (98%)	87 (80%)	22 (20%)	1	6
68	De	109/111 (98%)	89 (82%)	20 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	Bf	90/91 (99%)	77 (86%)	13 (14%)	3	15
69	Df	90/91 (99%)	79 (88%)	11 (12%)	5	21
70	Bg	95/103 (92%)	70 (74%)	25 (26%)	0	2
70	Dg	95/103 (92%)	71 (75%)	24 (25%)	0	3
71	Bh	104/105 (99%)	79 (76%)	25 (24%)	0	3
71	Dh	103/105 (98%)	77 (75%)	26 (25%)	0	3
72	Bi	81/82 (99%)	58 (72%)	23 (28%)	0	2
72	Di	80/82 (98%)	51 (64%)	29 (36%)	0	1
73	Bj	70/71 (99%)	56 (80%)	14 (20%)	1	7
73	Dj	70/71 (99%)	53 (76%)	17 (24%)	0	3
74	Bk	68/69 (99%)	48 (71%)	20 (29%)	0	1
74	Dk	67/69 (97%)	53 (79%)	14 (21%)	1	5
75	Bl	45/46 (98%)	36 (80%)	9 (20%)	1	7
75	Dl	45/46 (98%)	34 (76%)	11 (24%)	0	3
76	Bm	47/116 (40%)	37 (79%)	10 (21%)	1	5
76	Dm	47/116 (40%)	34 (72%)	13 (28%)	0	2
77	Bn	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	Dn	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Bo	90/91 (99%)	68 (76%)	22 (24%)	0	3
78	Do	90/91 (99%)	74 (82%)	16 (18%)	2	9
79	Bp	71/72 (99%)	56 (79%)	15 (21%)	1	5
79	Dp	71/72 (99%)	61 (86%)	10 (14%)	3	16
81	Ch	54/199 (27%)	38 (70%)	16 (30%)	0	1
83	Dq	105/233 (45%)	76 (72%)	29 (28%)	0	2
All	All	19013/20583 (92%)	14917 (78%)	4096 (22%)	1	5

All (4096) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	7	PHE
2	AA	10	THR
2	AA	24	LEU
2	AA	27	ARG
2	AA	29	VAL

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Mol	Chain	Res	Type
2	AA	33	GLN
2	AA	34	GLU
2	AA	37	VAL
2	AA	43	ASP
2	AA	45	VAL
2	AA	47	VAL
2	AA	50	VAL
2	AA	57	LEU
2	AA	59	LEU
2	AA	62	ARG
2	AA	76	ILE
2	AA	79	ARG
2	AA	84	ARG
2	AA	87	LEU
2	AA	88	LYS
2	AA	96	THR
2	AA	101	ARG
2	AA	103	THR
2	AA	110	TYR
2	AA	111	ILE
2	AA	114	SER
2	AA	117	GLU
2	AA	119	ARG
2	AA	123	VAL
2	AA	131	GLN
2	AA	135	GLU
2	AA	140	ASN
2	AA	154	GLU
2	AA	157	ASP
2	AA	162	CYS
2	AA	168	HIS
2	AA	172	LEU
2	AA	177	LEU
2	AA	184	LEU
2	AA	185	ARG
2	AA	196	SER
2	AA	197	ILE
3	AB	21	VAL
3	AB	22	ASP
3	AB	36	SER
3	AB	38	PHE
3	AB	47	LEU

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Mol	Chain	Res	Type
3	AB	54	LEU
3	AB	55	LYS
3	AB	58	SER
3	AB	61	LEU
3	AB	65	VAL
3	AB	68	VAL
3	AB	70	LEU
3	AB	73	LEU
3	AB	77	GLU
3	AB	78	ASP
3	AB	80	SER
3	AB	81	PHE
3	AB	83	LYS
3	AB	85	LYS
3	AB	89	ASP
3	AB	94	LYS
3	AB	96	LEU
3	AB	97	LEU
3	AB	105	PHE
3	AB	108	ASP
3	AB	109	LYS
3	AB	110	LEU
3	AB	115	ARG
3	AB	117	TRP
3	AB	124	ASN
3	AB	131	ASP
3	AB	135	LEU
3	AB	146	GLN
3	AB	148	ASN
3	AB	149	GLN
3	AB	154	SER
3	AB	166	LYS
3	AB	170	GLU
3	AB	177	GLN
3	AB	179	SER
3	AB	180	THR
3	AB	181	LEU
3	AB	183	GLN
3	AB	184	LEU
3	AB	193	ILE
3	AB	202	LYS
3	AB	214	LYS

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Mol	Chain	Res	Type
3	AB	215	VAL
3	AB	218	LEU
3	AB	219	LYS
3	AB	220	GLN
3	AB	223	PHE
3	AB	225	VAL
3	AB	228	LEU
4	AC	41	LEU
4	AC	50	ILE
4	AC	53	ILE
4	AC	58	LEU
4	AC	64	LYS
4	AC	70	ASP
4	AC	71	THR
4	AC	72	LEU
4	AC	73	LEU
4	AC	76	LEU
4	AC	77	GLN
4	AC	80	VAL
4	AC	87	GLN
4	AC	89	GLN
4	AC	90	THR
4	AC	95	ARG
4	AC	96	THR
4	AC	97	ARG
4	AC	106	ASP
4	AC	111	VAL
4	AC	117	THR
4	AC	119	LYS
4	AC	130	ILE
4	AC	134	LEU
4	AC	137	ILE
4	AC	139	ILE
4	AC	140	ARG
4	AC	141	ARG
4	AC	146	THR
4	AC	148	LEU
4	AC	159	THR
4	AC	166	THR
4	AC	174	ARG
4	AC	185	LYS
4	AC	187	LEU

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Mol	Chain	Res	Type
4	AC	201	ASN
4	AC	206	THR
4	AC	208	GLU
4	AC	221	THR
4	AC	222	TYR
4	AC	224	PHE
4	AC	226	THR
4	AC	237	VAL
4	AC	240	LEU
4	AC	245	ASP
4	AC	246	GLU
5	AD	4	LEU
5	AD	5	ILE
5	AD	7	LYS
5	AD	21	LEU
5	AD	23	GLU
5	AD	29	LEU
5	AD	37	VAL
5	AD	39	VAL
5	AD	53	THR
5	AD	57	ASP
5	AD	65	ARG
5	AD	66	ILE
5	AD	81	PRO
5	AD	84	ILE
5	AD	89	GLU
5	AD	90	ARG
5	AD	92	GLN
5	AD	93	ASP
5	AD	94	ARG
5	AD	96	LEU
5	AD	105	MET
5	AD	117	ARG
5	AD	127	MET
5	AD	129	SER
5	AD	134	CYS
5	AD	141	LYS
5	AD	142	LEU
5	AD	146	ARG
5	AD	151	LYS
5	AD	158	ILE
5	AD	170	THR

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Mol	Chain	Res	Type
5	AD	172	THR
5	AD	176	LEU
5	AD	178	ARG
5	AD	181	VAL
5	AD	182	LEU
5	AD	187	LYS
5	AD	190	ARG
5	AD	204	ASP
5	AD	210	GLU
5	AD	215	GLU
5	AD	220	PRO
5	AD	221	SER
5	AD	222	VAL
6	AE	7	LYS
6	AE	9	LEU
6	AE	12	LEU
6	AE	23	LEU
6	AE	26	CYS
6	AE	38	LEU
6	AE	39	ARG
6	AE	45	ILE
6	AE	48	LEU
6	AE	56	LEU
6	AE	59	ARG
6	AE	62	LYS
6	AE	67	GLN
6	AE	68	ARG
6	AE	70	VAL
6	AE	72	VAL
6	AE	77	ARG
6	AE	92	LEU
6	AE	95	THR
6	AE	105	VAL
6	AE	116	ASP
6	AE	117	GLU
6	AE	123	LEU
6	AE	126	VAL
6	AE	129	VAL
6	AE	131	LEU
6	AE	133	LYS
6	AE	146	THR
6	AE	153	ASN

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Mol	Chain	Res	Type
6	AE	155	LYS
6	AE	158	ASP
6	AE	164	LEU
6	AE	166	SER
6	AE	176	ASP
6	AE	180	LEU
6	AE	182	TYR
6	AE	187	ARG
6	AE	192	ILE
6	AE	197	HIS
6	AE	198	LYS
6	AE	206	ASP
6	AE	211	LYS
6	AE	215	ASP
6	AE	220	THR
6	AE	222	LEU
6	AE	226	PHE
6	AE	227	VAL
6	AE	237	SER
6	AE	240	LYS
6	AE	242	LYS
6	AE	246	LEU
6	AE	248	ILE
6	AE	258	GLN
6	AE	259	GLN
6	AE	261	LEU
7	AF	21	THR
7	AF	23	VAL
7	AF	24	VAL
7	AF	25	LEU
7	AF	27	THR
7	AF	32	GLU
7	AF	41	LYS
7	AF	42	LEU
7	AF	43	PHE
7	AF	45	LYS
7	AF	53	VAL
7	AF	63	GLN
7	AF	65	ARG
7	AF	68	ILE
7	AF	70	VAL
7	AF	76	ARG

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Mol	Chain	Res	Type
7	AF	79	ASN
7	AF	84	LYS
7	AF	89	ILE
7	AF	93	LEU
7	AF	94	THR
7	AF	117	THR
7	AF	119	ASP
7	AF	130	ILE
7	AF	146	THR
7	AF	147	THR
7	AF	156	ARG
7	AF	157	ARG
7	AF	160	VAL
7	AF	162	VAL
7	AF	163	SER
7	AF	193	THR
7	AF	203	LYS
7	AF	206	SER
7	AF	216	GLU
7	AF	225	ARG
8	AG	21	GLU
8	AG	25	ARG
8	AG	45	PHE
8	AG	58	LYS
8	AG	59	GLN
8	AG	69	LEU
8	AG	70	PRO
8	AG	71	THR
8	AG	76	LEU
8	AG	78	THR
8	AG	79	LYS
8	AG	82	SER
8	AG	98	ARG
8	AG	105	ASP
8	AG	109	LEU
8	AG	115	LYS
8	AG	120	GLU
8	AG	124	LEU
8	AG	126	ASP
8	AG	127	THR
8	AG	129	VAL
8	AG	132	ARG

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Mol	Chain	Res	Type
8	AG	133	LEU
8	AG	137	ARG
8	AG	143	LYS
8	AG	150	GLU
8	AG	151	ASP
8	AG	154	ARG
8	AG	155	ASP
8	AG	162	VAL
8	AG	170	THR
8	AG	175	ILE
8	AG	176	GLN
8	AG	177	ARG
8	AG	179	VAL
8	AG	211	LEU
8	AG	212	LEU
8	AG	217	SER
8	AG	223	LYS
9	AH	9	LEU
9	AH	25	VAL
9	AH	37	GLU
9	AH	38	LEU
9	AH	42	GLN
9	AH	46	ILE
9	AH	50	ASP
9	AH	51	VAL
9	AH	60	ILE
9	AH	66	SER
9	AH	67	LEU
9	AH	70	PHE
9	AH	71	HIS
9	AH	74	GLN
9	AH	75	THR
9	AH	77	LEU
9	AH	78	THR
9	AH	79	ARG
9	AH	80	GLU
9	AH	85	PHE
9	AH	87	ASP
9	AH	97	ARG
9	AH	103	SER
9	AH	105	THR
9	AH	109	VAL

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Mol	Chain	Res	Type
9	AH	110	GLN
9	AH	114	ARG
9	AH	116	ARG
9	AH	117	THR
9	AH	126	LEU
9	AH	131	PHE
9	AH	143	LEU
9	AH	144	VAL
9	AH	148	LYS
9	AH	154	LEU
9	AH	162	ILE
9	AH	167	GLU
9	AH	181	ILE
9	AH	184	GLU
9	AH	185	ILE
9	AH	187	SER
10	AI	6	ASP
10	AI	7	SER
10	AI	8	ARG
10	AI	14	THR
10	AI	20	GLN
10	AI	21	PHE
10	AI	26	LYS
10	AI	28	GLU
10	AI	29	LEU
10	AI	36	THR
10	AI	46	VAL
10	AI	49	ARG
10	AI	58	LEU
10	AI	76	THR
10	AI	103	GLN
10	AI	107	THR
10	AI	120	THR
10	AI	121	LEU
10	AI	123	LYS
10	AI	135	LYS
10	AI	137	LYS
10	AI	138	ASN
10	AI	140	GLU
10	AI	142	LYS
10	AI	151	LYS
10	AI	152	ILE

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Mol	Chain	Res	Type
10	AI	154	SER
10	AI	155	SER
10	AI	164	ARG
10	AI	184	LEU
10	AI	196	LEU
10	AI	199	LYS
11	AJ	3	ARG
11	AJ	6	ARG
11	AJ	7	THR
11	AJ	13	SER
11	AJ	14	THR
11	AJ	22	SER
11	AJ	28	LEU
11	AJ	39	LYS
11	AJ	46	SER
11	AJ	49	LEU
11	AJ	54	ARG
11	AJ	60	LEU
11	AJ	78	ARG
11	AJ	79	ARG
11	AJ	82	ARG
11	AJ	88	GLU
11	AJ	89	ASP
11	AJ	92	LYS
11	AJ	93	LEU
11	AJ	94	ASP
11	AJ	96	VAL
11	AJ	97	LEU
11	AJ	99	LEU
11	AJ	101	VAL
11	AJ	105	LEU
11	AJ	109	LEU
11	AJ	110	GLN
11	AJ	111	THR
11	AJ	120	LYS
11	AJ	130	THR
11	AJ	133	HIS
11	AJ	134	ILE
11	AJ	138	LYS
11	AJ	149	ARG
11	AJ	151	ASP
11	AJ	161	THR

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Mol	Chain	Res	Type
11	AJ	171	ARG
11	AJ	172	VAL
11	AJ	174	ARG
11	AJ	175	ARG
11	AJ	182	GLU
12	AK	1	MET
12	AK	7	ASP
12	AK	8	ARG
12	AK	13	GLN
12	AK	20	VAL
12	AK	27	PHE
12	AK	29	GLN
12	AK	31	LYS
12	AK	32	HIS
12	AK	46	LEU
12	AK	49	LEU
12	AK	50	THR
12	AK	55	VAL
12	AK	56	LYS
12	AK	71	GLU
12	AK	76	LEU
12	AK	78	GLU
12	AK	80	LEU
12	AK	82	LEU
13	AL	3	THR
13	AL	7	VAL
13	AL	21	ASN
13	AL	27	THR
13	AL	29	LYS
13	AL	30	ARG
13	AL	40	LEU
13	AL	43	LYS
13	AL	44	THR
13	AL	54	ILE
13	AL	56	LYS
13	AL	67	ARG
13	AL	69	LYS
13	AL	74	THR
13	AL	79	LYS
13	AL	80	MET
13	AL	83	THR
13	AL	99	ARG

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Mol	Chain	Res	Type
13	AL	109	VAL
13	AL	123	VAL
13	AL	131	ILE
13	AL	136	ARG
13	AL	140	VAL
13	AL	141	LYS
14	AM	25	GLU
14	AM	28	LEU
14	AM	33	ARG
14	AM	36	LEU
14	AM	43	ARG
14	AM	45	LEU
14	AM	50	LYS
14	AM	53	THR
14	AM	58	LEU
14	AM	59	LEU
14	AM	61	VAL
14	AM	62	LEU
14	AM	63	VAL
14	AM	71	ILE
14	AM	74	LEU
14	AM	75	VAL
14	AM	83	GLU
14	AM	85	LYS
14	AM	88	LEU
14	AM	89	ILE
14	AM	97	LEU
14	AM	103	LEU
14	AM	116	VAL
14	AM	119	SER
14	AM	121	VAL
14	AM	125	ASN
14	AM	126	TRP
14	AM	129	GLU
14	AM	132	GLU
14	AM	135	MET
14	AM	138	GLU
14	AM	139	HIS
14	AM	140	PHE
15	AN	3	ARG
15	AN	4	MET
15	AN	9	LYS

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Mol	Chain	Res	Type
15	AN	12	SER
15	AN	16	ILE
15	AN	21	ASN
15	AN	27	LYS
15	AN	33	VAL
15	AN	36	GLN
15	AN	39	LYS
15	AN	42	ARG
15	AN	45	LEU
15	AN	50	ILE
15	AN	56	ASP
15	AN	58	HIS
15	AN	60	VAL
15	AN	64	ARG
15	AN	66	ILE
15	AN	67	THR
15	AN	76	LYS
15	AN	77	SER
15	AN	83	GLU
15	AN	84	ILE
15	AN	88	LEU
15	AN	94	LYS
15	AN	97	SER
15	AN	102	LEU
15	AN	105	ASN
15	AN	109	LYS
15	AN	114	ARG
15	AN	115	LEU
15	AN	125	LEU
15	AN	145	THR
15	AN	149	LEU
15	AN	150	VAL
15	AN	151	ASN
16	AO	13	VAL
16	AO	14	PHE
16	AO	16	VAL
16	AO	20	TYR
16	AO	24	ASN
16	AO	26	THR
16	AO	29	HIS
16	AO	31	THR
16	AO	39	ILE

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Mol	Chain	Res	Type
16	AO	42	VAL
16	AO	43	THR
16	AO	51	ASP
16	AO	92	LYS
16	AO	99	GLN
16	AO	102	LEU
16	AO	103	ARG
16	AO	107	ARG
16	AO	108	SER
16	AO	118	VAL
16	AO	123	SER
16	AO	124	ASP
16	AO	125	SER
16	AO	133	ARG
16	AO	137	LEU
17	AP	14	THR
17	AP	22	LEU
17	AP	24	LYS
17	AP	26	LEU
17	AP	31	GLU
17	AP	35	LYS
17	AP	40	ARG
17	AP	44	ARG
17	AP	47	ARG
17	AP	50	THR
17	AP	52	LYS
17	AP	69	GLU
17	AP	86	VAL
17	AP	92	SER
17	AP	100	LYS
17	AP	110	GLU
17	AP	121	ILE
17	AP	125	PRO
17	AP	130	ARG
18	AQ	4	VAL
18	AQ	14	LYS
18	AQ	17	THR
18	AQ	23	LYS
18	AQ	26	LYS
18	AQ	28	LEU
18	AQ	36	ILE
18	AQ	44	LEU

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Mol	Chain	Res	Type
18	AQ	45	ARG
18	AQ	52	LEU
18	AQ	53	LEU
18	AQ	54	LEU
18	AQ	57	LEU
18	AQ	59	LYS
18	AQ	63	ILE
18	AQ	66	ARG
18	AQ	68	ARG
18	AQ	69	VAL
18	AQ	76	SER
18	AQ	90	VAL
18	AQ	94	GLN
18	AQ	98	ASP
18	AQ	101	SER
18	AQ	106	LYS
18	AQ	115	THR
18	AQ	118	ILE
18	AQ	123	ARG
18	AQ	127	LYS
18	AQ	128	LYS
18	AQ	136	SER
18	AQ	137	ARG
18	AQ	138	PHE
18	AQ	141	SER
19	AR	5	ARG
19	AR	25	THR
19	AR	26	LEU
19	AR	29	GLN
19	AR	30	THR
19	AR	34	LEU
19	AR	36	ASP
19	AR	38	ILE
19	AR	44	LYS
19	AR	46	LEU
19	AR	49	LYS
19	AR	54	THR
19	AR	69	ILE
19	AR	72	LYS
19	AR	73	LEU
19	AR	78	ARG
19	AR	83	GLN

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Mol	Chain	Res	Type
19	AR	84	TYR
19	AR	87	GLU
19	AR	105	GLN
19	AR	107	SER
19	AR	113	LEU
19	AR	115	LEU
19	AR	119	LEU
20	AS	3	LEU
20	AS	5	VAL
20	AS	8	GLN
20	AS	11	PHE
20	AS	12	GLN
20	AS	13	HIS
20	AS	14	ILE
20	AS	15	LEU
20	AS	17	LEU
20	AS	20	THR
20	AS	21	ASN
20	AS	26	ILE
20	AS	28	ILE
20	AS	34	THR
20	AS	38	VAL
20	AS	40	ARG
20	AS	46	VAL
20	AS	53	ASP
20	AS	54	LEU
20	AS	57	ARG
20	AS	60	GLU
20	AS	61	LEU
20	AS	71	GLN
20	AS	74	GLN
20	AS	77	THR
20	AS	80	LYS
20	AS	81	ILE
20	AS	86	LEU
20	AS	89	GLN
20	AS	92	ILE
20	AS	93	THR
20	AS	107	SER
20	AS	108	LYS
20	AS	110	ARG
20	AS	116	LEU

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Mol	Chain	Res	Type
20	AS	119	ILE
20	AS	132	ARG
20	AS	136	GLN
20	AS	138	THR
20	AS	140	THR
20	AS	143	ARG
21	AT	4	VAL
21	AT	6	VAL
21	AT	13	ASP
21	AT	18	TYR
21	AT	22	LEU
21	AT	25	GLN
21	AT	28	LEU
21	AT	30	VAL
21	AT	33	TYR
21	AT	34	VAL
21	AT	35	ASP
21	AT	36	ILE
21	AT	37	VAL
21	AT	57	ARG
21	AT	63	ARG
21	AT	67	MET
21	AT	68	ARG
21	AT	84	LYS
21	AT	86	ARG
21	AT	88	VAL
21	AT	89	ARG
21	AT	92	LYS
21	AT	94	ILE
21	AT	103	LYS
21	AT	111	ILE
21	AT	126	GLU
21	AT	130	ARG
21	AT	131	ASP
21	AT	132	LEU
21	AT	134	ARG
21	AT	144	GLU
22	AU	15	GLN
22	AU	17	GLN
22	AU	18	GLN
22	AU	20	ILE
22	AU	22	ILE

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Mol	Chain	Res	Type
22	AU	23	ARG
22	AU	27	THR
22	AU	30	LYS
22	AU	31	VAL
22	AU	34	LEU
22	AU	35	GLU
22	AU	42	VAL
22	AU	47	GLN
22	AU	48	HIS
22	AU	51	VAL
22	AU	57	ARG
22	AU	58	LEU
22	AU	60	THR
22	AU	61	LYS
22	AU	66	SER
22	AU	74	GLU
22	AU	76	SER
22	AU	81	THR
22	AU	88	LYS
22	AU	89	ARG
22	AU	99	ILE
22	AU	103	ILE
22	AU	108	ILE
22	AU	121	ASN
23	AV	1	MET
23	AV	2	GLU
23	AV	3	ASN
23	AV	5	LYS
23	AV	7	GLN
23	AV	11	LEU
23	AV	25	LYS
23	AV	41	GLU
23	AV	49	GLU
23	AV	50	TYR
23	AV	52	THR
23	AV	60	ARG
23	AV	62	ARG
23	AV	68	SER
23	AV	69	LEU
23	AV	74	GLN
23	AV	76	ASP
23	AV	80	LYS

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Mol	Chain	Res	Type
24	AW	3	ARG
24	AW	6	VAL
24	AW	7	LEU
24	AW	23	ARG
24	AW	24	GLN
24	AW	25	VAL
24	AW	27	ILE
24	AW	30	SER
24	AW	43	LYS
24	AW	53	ILE
24	AW	56	HIS
24	AW	65	LEU
24	AW	66	ASN
24	AW	69	LEU
24	AW	74	VAL
24	AW	76	SER
24	AW	83	ILE
24	AW	87	GLU
24	AW	93	LEU
24	AW	98	GLN
24	AW	103	ILE
24	AW	104	LEU
24	AW	105	THR
24	AW	114	GLU
24	AW	121	VAL
24	AW	129	VAL
25	AX	7	ARG
25	AX	9	LEU
25	AX	14	LYS
25	AX	18	HIS
25	AX	19	ARG
25	AX	28	ASN
25	AX	40	SER
25	AX	60	GLU
25	AX	82	LYS
25	AX	84	THR
25	AX	103	LEU
25	AX	107	PHE
25	AX	109	ARG
25	AX	110	LYS
25	AX	114	LYS
25	AX	117	ILE

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Mol	Chain	Res	Type
25	AX	131	SER
25	AX	133	LEU
25	AX	137	LYS
25	AX	138	GLU
25	AX	140	LYS
25	AX	144	ARG
26	AY	17	LEU
26	AY	29	HIS
26	AY	32	ARG
26	AY	34	ASN
26	AY	44	LEU
26	AY	46	GLU
26	AY	47	VAL
26	AY	49	LYS
26	AY	51	GLU
26	AY	52	LYS
26	AY	57	VAL
26	AY	61	ARG
26	AY	62	THR
26	AY	75	VAL
26	AY	84	LYS
26	AY	88	THR
26	AY	93	ARG
26	AY	96	LEU
26	AY	99	LYS
26	AY	102	LYS
26	AY	105	ARG
26	AY	112	LYS
26	AY	123	LYS
26	AY	124	ARG
26	AY	127	LYS
26	AY	128	LYS
26	AY	129	VAL
26	AY	135	ASP
27	AZ	38	HIS
27	AZ	42	LEU
27	AZ	49	ARG
27	AZ	50	ILE
27	AZ	58	ARG
27	AZ	59	TYR
27	AZ	69	LEU
27	AZ	71	ILE

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Mol	Chain	Res	Type
27	AZ	75	LEU
27	AZ	77	ARG
27	AZ	80	LEU
27	AZ	85	LYS
27	AZ	92	ILE
27	AZ	93	SER
27	AZ	95	HIS
27	AZ	96	SER
27	AZ	100	ILE
27	AZ	105	THR
28	Aa	12	LYS
28	Aa	36	ILE
28	Aa	41	ILE
28	Aa	44	ILE
28	Aa	45	VAL
28	Aa	53	LEU
28	Aa	58	VAL
28	Aa	61	GLU
28	Aa	64	LEU
28	Aa	66	LYS
28	Aa	67	THR
28	Aa	69	ASN
28	Aa	70	LYS
28	Aa	82	ARG
28	Aa	83	ILE
28	Aa	85	ARG
28	Aa	86	VAL
28	Aa	90	GLU
29	Ab	3	LEU
29	Ab	4	VAL
29	Ab	20	LYS
29	Ab	29	ARG
29	Ab	33	LEU
29	Ab	34	ASP
29	Ab	41	LEU
29	Ab	67	THR
30	Ac	5	THR
30	Ac	13	ILE
30	Ac	14	LYS
30	Ac	15	VAL
30	Ac	19	THR
30	Ac	32	PHE

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Mol	Chain	Res	Type
30	Ac	33	LEU
30	Ac	34	GLU
30	Ac	38	ARG
30	Ac	39	THR
30	Ac	49	ARG
30	Ac	52	ASP
30	Ac	57	MET
30	Ac	58	GLU
30	Ac	59	SER
30	Ac	62	GLU
30	Ac	64	ARG
30	Ac	65	ARG
31	Ad	6	VAL
31	Ad	8	PHE
31	Ad	22	ARG
31	Ad	25	SER
31	Ad	30	LEU
31	Ad	32	ARG
31	Ad	36	LEU
31	Ad	39	CYS
31	Ad	48	ASN
32	Ae	20	LYS
32	Ae	25	GLU
32	Ae	26	LYS
32	Ae	28	LYS
32	Ae	29	LYS
32	Ae	42	ARG
32	Ae	48	THR
32	Ae	50	VAL
33	Af	102	VAL
33	Af	108	VAL
33	Af	120	GLU
33	Af	121	CYS
33	Af	125	THR
33	Af	130	VAL
33	Af	137	ASP
33	Af	140	TYR
33	Af	146	SER
33	Af	147	VAL
33	Af	151	ASN
34	Ag	6	VAL
34	Ag	7	LEU

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Mol	Chain	Res	Type
34	Ag	8	VAL
34	Ag	46	LYS
34	Ag	48	THR
34	Ag	51	ASP
34	Ag	52	GLN
34	Ag	59	ARG
34	Ag	71	CYS
34	Ag	76	ASP
34	Ag	87	LYS
34	Ag	88	THR
34	Ag	94	VAL
34	Ag	96	THR
34	Ag	112	SER
34	Ag	117	LYS
34	Ag	118	LYS
34	Ag	129	LYS
34	Ag	134	TRP
34	Ag	136	ILE
34	Ag	137	LYS
34	Ag	141	LEU
34	Ag	149	ASP
34	Ag	153	GLN
34	Ag	165	ASP
34	Ag	166	SER
34	Ag	188	ILE
34	Ag	199	ILE
34	Ag	207	ASP
34	Ag	221	MET
34	Ag	238	ASP
34	Ag	250	TYR
34	Ag	266	ASP
34	Ag	268	GLN
34	Ag	292	LEU
34	Ag	300	THR
34	Ag	317	THR
35	Ah	28	SER
35	Ah	34	LYS
35	Ah	46	LYS
35	Ah	51	ARG
35	Ah	61	ILE
35	Ah	64	LYS
35	Ah	65	THR

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Mol	Chain	Res	Type
35	Ah	68	ARG
35	Ah	75	ASP
35	Ah	78	ASP
35	Ah	82	THR
35	Ah	84	LYS
35	Ah	88	ARG
35	Ah	89	ARG
35	Ah	94	HIS
35	Ah	96	ARG
35	Ah	97	THR
35	Ah	100	THR
35	Ah	102	THR
35	Ah	105	LYS
35	Ah	112	ASP
35	Ah	130	GLU
35	Ah	139	GLU
39	BA	10	LYS
39	BA	18	SER
39	BA	20	THR
39	BA	30	ARG
39	BA	32	LEU
39	BA	44	ILE
39	BA	45	VAL
39	BA	48	ILE
39	BA	62	VAL
39	BA	70	ARG
39	BA	72	ARG
39	BA	74	GLU
39	BA	88	ILE
39	BA	95	SER
39	BA	101	VAL
39	BA	104	LEU
39	BA	116	VAL
39	BA	157	VAL
39	BA	165	VAL
39	BA	177	LYS
39	BA	179	LEU
39	BA	180	LEU
39	BA	181	LYS
39	BA	190	ARG
39	BA	191	LEU
39	BA	202	VAL

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Mol	Chain	Res	Type
39	BA	204	MET
39	BA	207	VAL
39	BA	219	ILE
39	BA	225	ILE
39	BA	227	ARG
39	BA	230	VAL
39	BA	247	ARG
40	BB	2	SER
40	BB	7	GLU
40	BB	10	ARG
40	BB	17	LEU
40	BB	19	ARG
40	BB	20	LYS
40	BB	25	ILE
40	BB	30	LYS
40	BB	37	ARG
40	BB	39	LYS
40	BB	47	LEU
40	BB	50	LYS
40	BB	56	ILE
40	BB	73	VAL
40	BB	79	VAL
40	BB	84	VAL
40	BB	85	VAL
40	BB	90	VAL
40	BB	100	ARG
40	BB	103	THR
40	BB	105	VAL
40	BB	110	LEU
40	BB	111	SER
40	BB	114	VAL
40	BB	116	ARG
40	BB	121	ASN
40	BB	134	SER
40	BB	139	GLN
40	BB	146	ARG
40	BB	148	LEU
40	BB	150	ARG
40	BB	153	LYS
40	BB	156	SER
40	BB	162	VAL
40	BB	166	ILE

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Mol	Chain	Res	Type
40	BB	167	ARG
40	BB	169	THR
40	BB	173	GLN
40	BB	183	LEU
40	BB	187	SER
40	BB	188	ILE
40	BB	192	VAL
40	BB	196	ARG
40	BB	200	GLU
40	BB	202	THR
40	BB	205	VAL
40	BB	206	ASP
40	BB	210	GLU
40	BB	221	THR
40	BB	229	VAL
40	BB	232	ARG
40	BB	235	THR
40	BB	238	LEU
40	BB	241	LYS
40	BB	242	THR
40	BB	244	ARG
40	BB	264	VAL
40	BB	281	LYS
40	BB	300	ARG
40	BB	301	THR
40	BB	305	ILE
40	BB	308	MET
40	BB	319	ASN
40	BB	320	ASP
40	BB	324	VAL
40	BB	325	LYS
40	BB	328	ILE
40	BB	332	ARG
40	BB	338	LEU
40	BB	341	SER
40	BB	344	THR
40	BB	347	SER
40	BB	349	LYS
40	BB	352	GLU
40	BB	355	SER
40	BB	361	THR
40	BB	364	LYS

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Mol	Chain	Res	Type
40	BB	372	THR
40	BB	380	MET
40	BB	385	LYS
40	BB	387	LEU
41	BC	4	PRO
41	BC	22	LEU
41	BC	25	VAL
41	BC	40	THR
41	BC	47	ARG
41	BC	53	SER
41	BC	60	THR
41	BC	71	VAL
41	BC	73	ARG
41	BC	74	ILE
41	BC	93	MET
41	BC	99	MET
41	BC	122	THR
41	BC	124	SER
41	BC	133	SER
41	BC	136	LEU
41	BC	138	ARG
41	BC	144	LYS
41	BC	148	ILE
41	BC	150	LEU
41	BC	152	VAL
41	BC	156	LEU
41	BC	170	LYS
41	BC	172	VAL
41	BC	177	ASP
41	BC	179	LEU
41	BC	185	LYS
41	BC	187	LEU
41	BC	188	ARG
41	BC	193	LYS
41	BC	200	THR
41	BC	203	ARG
41	BC	206	LEU
41	BC	220	ARG
41	BC	222	VAL
41	BC	230	VAL
41	BC	233	LEU
41	BC	246	ARG

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Mol	Chain	Res	Type
41	BC	258	LEU
41	BC	259	ASP
41	BC	267	VAL
41	BC	283	THR
41	BC	287	THR
41	BC	289	ILE
41	BC	295	ILE
41	BC	306	THR
41	BC	307	GLN
41	BC	313	LEU
41	BC	319	LYS
41	BC	323	VAL
41	BC	332	LYS
41	BC	333	VAL
41	BC	339	LEU
41	BC	343	LYS
41	BC	345	GLU
41	BC	346	LYS
41	BC	349	THR
41	BC	350	LYS
41	BC	354	VAL
41	BC	356	THR
41	BC	358	THR
42	BD	4	GLN
42	BD	5	LYS
42	BD	8	LYS
42	BD	9	SER
42	BD	10	SER
42	BD	15	ARG
42	BD	22	ARG
42	BD	23	ARG
42	BD	35	ARG
42	BD	41	LYS
42	BD	50	ARG
42	BD	64	ILE
42	BD	68	THR
42	BD	69	ILE
42	BD	81	HIS
42	BD	85	ARG
42	BD	89	THR
42	BD	92	LEU
42	BD	93	THR

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Mol	Chain	Res	Type
42	BD	95	TRP
42	BD	105	ILE
42	BD	109	THR
42	BD	115	LEU
42	BD	118	THR
42	BD	123	GLU
42	BD	131	LEU
42	BD	135	VAL
42	BD	137	ASP
42	BD	140	ARG
42	BD	144	VAL
42	BD	146	LEU
42	BD	148	ILE
42	BD	151	GLN
42	BD	152	ARG
42	BD	154	THR
42	BD	155	THR
42	BD	163	LEU
42	BD	177	GLU
42	BD	185	PHE
42	BD	187	THR
42	BD	188	GLU
42	BD	196	ARG
42	BD	211	LEU
42	BD	222	LEU
42	BD	231	ILE
42	BD	232	ASP
42	BD	254	LYS
42	BD	257	GLU
42	BD	259	LYS
42	BD	263	GLU
42	BD	264	GLN
42	BD	273	ARG
42	BD	277	LEU
42	BD	280	GLU
42	BD	293	LEU
43	BE	5	LYS
43	BE	15	VAL
43	BE	18	LEU
43	BE	21	THR
43	BE	52	VAL
43	BE	64	LEU

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Mol	Chain	Res	Type
43	BE	65	ILE
43	BE	78	ARG
43	BE	79	VAL
43	BE	84	VAL
43	BE	89	THR
43	BE	93	VAL
43	BE	94	GLU
43	BE	108	LYS
43	BE	129	GLU
43	BE	134	ARG
43	BE	152	THR
43	BE	175	LYS
44	BF	24	GLU
44	BF	25	GLN
44	BF	38	LYS
44	BF	56	GLU
44	BF	77	VAL
44	BF	82	LYS
44	BF	92	ILE
44	BF	93	ASN
44	BF	98	LYS
44	BF	110	ARG
44	BF	121	LYS
44	BF	124	LEU
44	BF	143	THR
44	BF	151	ARG
44	BF	179	LEU
44	BF	184	LEU
44	BF	208	SER
44	BF	216	VAL
44	BF	229	PHE
44	BF	239	LEU
44	BF	244	ASN
45	BG	26	LEU
45	BG	27	THR
45	BG	36	ILE
45	BG	41	GLN
45	BG	47	SER
45	BG	50	VAL
45	BG	61	GLN
45	BG	63	LYS
45	BG	74	THR

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Mol	Chain	Res	Type
45	BG	79	GLN
45	BG	81	THR
45	BG	82	LEU
45	BG	84	ARG
45	BG	90	THR
45	BG	92	LYS
45	BG	110	THR
45	BG	118	GLU
45	BG	132	VAL
45	BG	136	LEU
45	BG	150	LEU
45	BG	156	ASP
45	BG	160	ILE
45	BG	163	VAL
45	BG	169	LEU
45	BG	181	LYS
45	BG	185	ARG
45	BG	203	VAL
45	BG	204	ARG
45	BG	214	LEU
45	BG	216	SER
45	BG	238	LEU
45	BG	241	LYS
45	BG	246	MET
45	BG	248	LYS
45	BG	251	LYS
45	BG	254	ASP
46	BH	4	ILE
46	BH	5	GLN
46	BH	9	GLN
46	BH	18	VAL
46	BH	20	ILE
46	BH	22	SER
46	BH	24	ILE
46	BH	33	THR
46	BH	36	LYS
46	BH	41	ILE
46	BH	48	VAL
46	BH	49	ASN
46	BH	52	LEU
46	BH	62	ARG
46	BH	68	LEU

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Mol	Chain	Res	Type
46	BH	69	ARG
46	BH	70	THR
46	BH	80	THR
46	BH	82	VAL
46	BH	91	ARG
46	BH	123	ILE
46	BH	132	VAL
46	BH	135	GLU
46	BH	137	SER
46	BH	138	THR
46	BH	139	ASN
46	BH	147	SER
46	BH	151	VAL
46	BH	152	GLU
46	BH	157	ASN
46	BH	161	LEU
46	BH	162	GLN
46	BH	164	ILE
46	BH	168	ARG
46	BH	172	ILE
46	BH	173	ARG
46	BH	177	ASP
46	BH	189	GLU
46	BH	190	ASP
46	BH	191	LEU
47	BI	3	ARG
47	BI	19	LYS
47	BI	24	ARG
47	BI	26	VAL
47	BI	30	LYS
47	BI	32	ARG
47	BI	33	ILE
47	BI	36	LEU
47	BI	40	LYS
47	BI	42	THR
47	BI	48	LEU
47	BI	52	LEU
47	BI	57	LEU
47	BI	63	GLU
47	BI	77	THR
47	BI	78	THR
47	BI	87	LEU

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Mol	Chain	Res	Type
47	BI	90	ARG
47	BI	99	ILE
47	BI	116	ARG
47	BI	128	ARG
47	BI	129	VAL
47	BI	130	ASP
47	BI	139	ARG
47	BI	140	THR
47	BI	156	ARG
47	BI	163	GLN
47	BI	165	ILE
47	BI	174	THR
47	BI	185	ARG
47	BI	191	LYS
47	BI	197	VAL
47	BI	203	LYS
47	BI	207	GLU
48	BJ	6	GLN
48	BJ	7	ASN
48	BJ	9	MET
48	BJ	10	ARG
48	BJ	12	LEU
48	BJ	13	LYS
48	BJ	16	LYS
48	BJ	19	LEU
48	BJ	26	SER
48	BJ	31	THR
48	BJ	34	SER
48	BJ	44	THR
48	BJ	46	VAL
48	BJ	55	ARG
48	BJ	65	ILE
48	BJ	70	THR
48	BJ	80	LEU
48	BJ	82	ARG
48	BJ	84	LEU
48	BJ	94	ARG
48	BJ	106	ILE
48	BJ	107	ASP
48	BJ	112	LEU
48	BJ	115	LYS
48	BJ	119	SER

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Mol	Chain	Res	Type
48	BJ	120	ILE
48	BJ	122	ILE
48	BJ	130	VAL
48	BJ	134	PRO
48	BJ	138	VAL
48	BJ	140	ARG
48	BJ	142	LYS
48	BJ	158	ASP
48	BJ	161	SER
48	BJ	166	LYS
48	BJ	172	LEU
49	BL	5	LYS
49	BL	13	HIS
49	BL	15	ARG
49	BL	23	LYS
49	BL	46	ILE
49	BL	51	LEU
49	BL	54	LEU
49	BL	55	ARG
49	BL	58	VAL
49	BL	59	ARG
49	BL	63	VAL
49	BL	67	ARG
49	BL	69	VAL
49	BL	85	LEU
49	BL	91	ARG
49	BL	100	ARG
49	BL	107	GLU
49	BL	114	GLN
49	BL	115	ARG
49	BL	124	ILE
49	BL	131	LYS
49	BL	136	GLU
49	BL	140	SER
49	BL	147	ILE
49	BL	164	GLU
49	BL	168	ARG
49	BL	171	ARG
49	BL	180	ARG
49	BL	182	ILE
49	BL	190	LYS
49	BL	194	GLU

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Mol	Chain	Res	Type
50	BM	5	SER
50	BM	8	LYS
50	BM	13	ARG
50	BM	20	VAL
50	BM	25	LYS
50	BM	27	GLN
50	BM	50	LYS
50	BM	53	VAL
50	BM	58	ILE
50	BM	64	VAL
50	BM	66	THR
50	BM	72	LEU
50	BM	82	SER
50	BM	90	VAL
50	BM	92	GLU
50	BM	102	LYS
50	BM	106	ARG
50	BM	108	ARG
50	BM	113	THR
50	BM	125	LYS
50	BM	126	GLN
50	BM	130	THR
50	BM	135	LEU
51	BN	10	LEU
51	BN	15	GLN
51	BN	18	VAL
51	BN	19	LEU
51	BN	20	ARG
51	BN	22	LEU
51	BN	27	VAL
51	BN	38	ARG
51	BN	49	ARG
51	BN	50	ARG
51	BN	68	ARG
51	BN	80	THR
51	BN	85	THR
51	BN	89	VAL
51	BN	92	LEU
51	BN	96	ARG
51	BN	97	SER
51	BN	98	LEU
51	BN	105	ARG

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Mol	Chain	Res	Type
51	BN	109	ARG
51	BN	117	ASN
51	BN	131	GLU
51	BN	133	ILE
51	BN	151	ILE
51	BN	155	VAL
51	BN	182	ASN
51	BN	183	THR
51	BN	190	THR
51	BN	198	SER
52	BO	3[B]	SER
52	BO	12[A]	LYS
52	BO	12[B]	LYS
52	BO	16[B]	LEU
52	BO	22[A]	VAL
52	BO	22[B]	THR
52	BO	25[A]	LYS
52	BO	25[B]	LYS
52	BO	34[A]	VAL
52	BO	34[B]	VAL
52	BO	58[A]	LEU
52	BO	58[B]	LEU
52	BO	59[A]	ARG
52	BO	59[B]	ARG
52	BO	67[A]	THR
52	BO	67[B]	THR
52	BO	78[A]	ARG
52	BO	78[B]	ARG
52	BO	80[B]	LEU
52	BO	84[A]	LEU
52	BO	85[A]	ARG
52	BO	85[B]	ARG
52	BO	106[A]	GLU
52	BO	106[B]	GLU
52	BO	110[A]	PRO
52	BO	110[B]	PRO
52	BO	116[A]	LYS
52	BO	116[B]	LYS
52	BO	117[A]	ARG
52	BO	117[B]	ARG
52	BO	122[A]	GLN
52	BO	122[B]	GLN

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Mol	Chain	Res	Type
52	BO	124[A]	LEU
52	BO	124[B]	LEU
52	BO	126[A]	VAL
52	BO	126[B]	VAL
52	BO	128[A]	ARG
52	BO	128[B]	ARG
52	BO	142[A]	SER
52	BO	142[B]	SER
52	BO	143[A]	THR
52	BO	143[B]	THR
52	BO	163[B]	ARG
52	BO	175[A]	THR
52	BO	175[B]	THR
52	BO	182[A]	ASN
52	BO	186[B]	SER
53	BP	3	ARG
53	BP	9	THR
53	BP	23	ARG
53	BP	24	VAL
53	BP	29	THR
53	BP	32	THR
53	BP	36	ILE
53	BP	52	LEU
53	BP	53	ASP
53	BP	56	ARG
53	BP	67	ILE
53	BP	69	ARG
53	BP	70	THR
53	BP	78	VAL
53	BP	94	LEU
53	BP	111	LYS
53	BP	112	LEU
53	BP	114	VAL
53	BP	120	ASN
53	BP	123	PRO
53	BP	126	ARG
53	BP	127	ARG
53	BP	136	ILE
53	BP	142	SER
53	BP	144	SER
53	BP	153	LYS
53	BP	166	VAL

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Mol	Chain	Res	Type
53	BP	171	ARG
53	BP	173	ARG
53	BP	180	LYS
53	BP	181	ARG
54	BQ	3	ILE
54	BQ	17	THR
54	BQ	24	VAL
54	BQ	26	LEU
54	BQ	32	LEU
54	BQ	34	THR
54	BQ	41	ASP
54	BQ	46	LYS
54	BQ	49	LEU
54	BQ	57	ILE
54	BQ	64	VAL
54	BQ	69	ARG
54	BQ	74	GLU
54	BQ	81	VAL
54	BQ	86	THR
54	BQ	88	THR
54	BQ	93	ILE
54	BQ	98	LYS
54	BQ	113	LYS
54	BQ	135	GLN
54	BQ	138	LEU
54	BQ	150	VAL
54	BQ	168	THR
54	BQ	180	ARG
55	BR	5	ARG
55	BR	8	LYS
55	BR	10	LEU
55	BR	20	ARG
55	BR	22	VAL
55	BR	25	ASP
55	BR	29	THR
55	BR	30	SER
55	BR	41	ILE
55	BR	43	LYS
55	BR	49	THR
55	BR	52	LYS
55	BR	60	LYS
55	BR	71	ARG

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Mol	Chain	Res	Type
55	BR	74	ARG
55	BR	81	ARG
55	BR	86	GLU
55	BR	91	SER
55	BR	98	ARG
55	BR	99	LEU
55	BR	100	ARG
55	BR	103	ARG
55	BR	104	ARG
55	BR	106	LEU
55	BR	108	LYS
55	BR	115	ILE
55	BR	116	ASP
55	BR	128	LYS
55	BR	135	LYS
55	BR	138	LEU
55	BR	144	GLN
55	BR	153	LYS
55	BR	164	LEU
55	BR	165	LYS
55	BR	175	GLN
55	BR	177	VAL
55	BR	182	ASP
56	BS	1	MET
56	BS	12	ARG
56	BS	13	ARG
56	BS	17	GLU
56	BS	40	ARG
56	BS	45	LEU
56	BS	51	VAL
56	BS	58	ILE
56	BS	61	ILE
56	BS	71	LYS
56	BS	80	ARG
56	BS	87	THR
56	BS	97	VAL
56	BS	100	VAL
56	BS	105	THR
56	BS	115	ARG
56	BS	117	ARG
56	BS	130	GLU
56	BS	132	THR

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Mol	Chain	Res	Type
56	BS	137	ARG
56	BS	138	GLN
56	BS	142	GLN
56	BS	155	ARG
56	BS	160	THR
56	BS	162	THR
56	BS	166	LYS
56	BS	167	ARG
56	BS	169	SER
56	BS	172	TYR
57	BT	4	SER
57	BT	9	SER
57	BT	12	ARG
57	BT	25	VAL
57	BT	26	HIS
57	BT	27	LEU
57	BT	28	SER
57	BT	32	LYS
57	BT	55	LYS
57	BT	75	ILE
57	BT	78	LYS
57	BT	79	MET
57	BT	80	VAL
57	BT	83	ARG
57	BT	88	ARG
57	BT	89	LEU
57	BT	96	ILE
57	BT	102	ARG
57	BT	103	GLN
57	BT	104	GLU
57	BT	118	GLU
57	BT	124	VAL
57	BT	126	VAL
57	BT	127	GLN
57	BT	128	LEU
57	BT	139	ARG
57	BT	143	THR
57	BT	144	GLU
57	BT	146	ASN
57	BT	149	GLN
57	BT	158	THR
57	BT	159	PHE

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Mol	Chain	Res	Type
57	BT	160	ILE
58	BU	10	LYS
58	BU	27	VAL
58	BU	29	ASP
58	BU	38	ILE
58	BU	39	ASP
58	BU	43	VAL
58	BU	49	ASN
58	BU	52	ASN
58	BU	61	THR
58	BU	66	VAL
58	BU	82	LYS
58	BU	88	GLN
58	BU	93	ILE
58	BU	100	THR
59	BV	13	ILE
59	BV	32	ARG
59	BV	33	ASN
59	BV	45	ARG
59	BV	48	ARG
59	BV	63	LYS
59	BV	64	LYS
59	BV	69	LEU
59	BV	73	VAL
59	BV	74	MET
59	BV	83	LYS
59	BV	84	SER
59	BV	102	ILE
59	BV	115	THR
59	BV	120	LYS
59	BV	125	LEU
60	BW	4	GLU
60	BW	5	ILE
60	BW	19	THR
60	BW	25	ASP
60	BW	34	SER
60	BW	39	LEU
60	BW	54	LEU
60	BW	63	ILE
61	BX	27	ARG
61	BX	34	LEU
61	BX	36	LYS

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Mol	Chain	Res	Type
61	BX	37	THR
61	BX	38	LEU
61	BX	39	LYS
61	BX	40	LEU
61	BX	45	LYS
61	BX	48	SER
61	BX	63	ILE
61	BX	71	THR
61	BX	73	MET
61	BX	75	LYS
61	BX	85	GLN
61	BX	86	VAL
61	BX	92	LYS
61	BX	105	VAL
61	BX	108	LEU
61	BX	109	LYS
61	BX	115	ARG
61	BX	125	ARG
61	BX	127	THR
61	BX	133	LEU
61	BX	135	ILE
61	BX	139	ILE
61	BX	142	ILE
62	BY	3	LYS
62	BY	8	VAL
62	BY	13	ARG
62	BY	17	LYS
62	BY	37	LYS
62	BY	40	ARG
62	BY	45	ILE
62	BY	50	ILE
62	BY	51	ARG
62	BY	56	VAL
62	BY	57	LEU
62	BY	74	TYR
62	BY	76	LEU
62	BY	80	VAL
62	BY	90	VAL
62	BY	94	SER
62	BY	95	VAL
62	BY	97	ILE
62	BY	105	VAL

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Mol	Chain	Res	Type
62	BY	115	ARG
62	BY	122	LYS
62	BY	125	LYS
63	BZ	14	VAL
63	BZ	15	ARG
63	BZ	17	ARG
63	BZ	24	VAL
63	BZ	34	LYS
63	BZ	43	VAL
63	BZ	46	ILE
63	BZ	53	VAL
63	BZ	54	THR
63	BZ	64	LYS
63	BZ	72	ILE
63	BZ	75	VAL
63	BZ	80	LEU
63	BZ	81	LEU
63	BZ	83	THR
63	BZ	86	THR
63	BZ	87	LEU
63	BZ	90	GLU
63	BZ	92	PHE
63	BZ	97	SER
63	BZ	99	GLU
63	BZ	102	GLU
63	BZ	103	GLN
63	BZ	109	GLU
63	BZ	121	ARG
63	BZ	127	ASN
63	BZ	134	LEU
64	Ba	6	THR
64	Ba	7	LYS
64	Ba	8	THR
64	Ba	10	LYS
64	Ba	12	ARG
64	Ba	16	SER
64	Ba	29	PRO
64	Ba	42	ARG
64	Ba	47	LYS
64	Ba	60	TYR
64	Ba	76	ASP
64	Ba	78	LEU

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Mol	Chain	Res	Type
64	Ba	84	GLU
64	Ba	91	LEU
64	Ba	92	LYS
64	Ba	96	LYS
64	Ba	115	LYS
64	Ba	120	ASN
64	Ba	130	VAL
64	Ba	133	LEU
64	Ba	139	ARG
65	Bb	14	ARG
65	Bb	22	LYS
65	Bb	23	LYS
65	Bb	25	LYS
65	Bb	28	LYS
65	Bb	33	LYS
65	Bb	35	VAL
65	Bb	38	LYS
65	Bb	50	THR
65	Bb	59	LYS
66	Bc	16	LEU
66	Bc	30	THR
66	Bc	32	LYS
66	Bc	34	LEU
66	Bc	36	GLN
66	Bc	40	LYS
66	Bc	48	THR
66	Bc	52	ARG
66	Bc	54	SER
66	Bc	61	MET
66	Bc	79	THR
66	Bc	83	LYS
66	Bc	87	VAL
66	Bc	93	LEU
66	Bc	97	ASP
66	Bc	99	ASP
66	Bc	100	ILE
66	Bc	103	THR
67	Bd	6	ASP
67	Bd	8	VAL
67	Bd	13	THR
67	Bd	16	LEU
67	Bd	26	LYS

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Mol	Chain	Res	Type
67	Bd	28	ARG
67	Bd	31	ARG
67	Bd	46	THR
67	Bd	47	ASP
67	Bd	53	PRO
67	Bd	55	LEU
67	Bd	64	VAL
67	Bd	68	GLU
67	Bd	79	ARG
67	Bd	82	GLU
67	Bd	86	LYS
67	Bd	94	GLU
67	Bd	102	LYS
67	Bd	106	THR
68	Be	4	LEU
68	Be	18	LYS
68	Be	19	ARG
68	Be	27	ARG
68	Be	33	ARG
68	Be	51	SER
68	Be	54	LYS
68	Be	61	LYS
68	Be	62	LYS
68	Be	73	THR
68	Be	75	LEU
68	Be	76	VAL
68	Be	82	LEU
68	Be	84	THR
68	Be	85	LEU
68	Be	87	MET
68	Be	103	LYS
68	Be	106	VAL
68	Be	109	LEU
68	Be	125	ARG
68	Be	126	LEU
68	Be	128	LEU
69	Bf	10	LYS
69	Bf	15	SER
69	Bf	20	LYS
69	Bf	28	SER
69	Bf	31	LYS
69	Bf	49	ILE

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Mol	Chain	Res	Type
69	Bf	59	VAL
69	Bf	60	ARG
69	Bf	70	LYS
69	Bf	80	VAL
69	Bf	92	LYS
69	Bf	98	VAL
69	Bf	106	ASN
70	Bg	3	GLN
70	Bg	5	VAL
70	Bg	8	ARG
70	Bg	20	ILE
70	Bg	21	LYS
70	Bg	23	VAL
70	Bg	24	LYS
70	Bg	29	ILE
70	Bg	33	GLN
70	Bg	38	LEU
70	Bg	44	CYS
70	Bg	51	LEU
70	Bg	52	GLN
70	Bg	56	THR
70	Bg	58	ARG
70	Bg	65	VAL
70	Bg	71	THR
70	Bg	72	VAL
70	Bg	74	ARG
70	Bg	86	LYS
70	Bg	88	ARG
70	Bg	95	ILE
70	Bg	99	LYS
70	Bg	102	LYS
70	Bg	104	VAL
71	Bh	15	GLU
71	Bh	20	GLN
71	Bh	21	LEU
71	Bh	27	GLU
71	Bh	28	LEU
71	Bh	38	ARG
71	Bh	44	ILE
71	Bh	45	LYS
71	Bh	46	THR
71	Bh	48	ARG

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Mol	Chain	Res	Type
71	Bh	49	LYS
71	Bh	50	SER
71	Bh	71	LYS
71	Bh	73	LYS
71	Bh	74	LYS
71	Bh	81	ARG
71	Bh	85	THR
71	Bh	89	ARG
71	Bh	100	VAL
71	Bh	101	THR
71	Bh	104	GLN
71	Bh	105	ARG
71	Bh	107	LYS
71	Bh	115	LYS
71	Bh	119	LYS
72	Bi	11	LEU
72	Bi	17	VAL
72	Bi	18	THR
72	Bi	21	THR
72	Bi	25	LYS
72	Bi	26	ILE
72	Bi	29	LYS
72	Bi	34	SER
72	Bi	36	ARG
72	Bi	42	SER
72	Bi	45	ARG
72	Bi	57	LEU
72	Bi	58	ILE
72	Bi	60	LEU
72	Bi	62	ARG
72	Bi	64	SER
72	Bi	68	ARG
72	Bi	70	ARG
72	Bi	76	ARG
72	Bi	81	THR
72	Bi	88	GLU
72	Bi	90	MET
72	Bi	99	ARG
73	Bj	3	LYS
73	Bj	5	THR
73	Bj	17	THR
73	Bj	24	ARG

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Mol	Chain	Res	Type
73	Bj	25	ARG
73	Bj	33	THR
73	Bj	36	SER
73	Bj	37	CYS
73	Bj	59	THR
73	Bj	67	LEU
73	Bj	75	LYS
73	Bj	80	THR
73	Bj	82	SER
73	Bj	84	SER
74	Bk	3	ARG
74	Bk	5	ILE
74	Bk	6	THR
74	Bk	8	ILE
74	Bk	12	LEU
74	Bk	19	ASP
74	Bk	24	THR
74	Bk	31	LEU
74	Bk	32	ASN
74	Bk	41	THR
74	Bk	45	VAL
74	Bk	46	ARG
74	Bk	48	SER
74	Bk	50	SER
74	Bk	53	THR
74	Bk	64	LYS
74	Bk	65	LEU
74	Bk	67	GLN
74	Bk	72	THR
74	Bk	77	ARG
75	Bl	5	LYS
75	Bl	6	SER
75	Bl	21	ARG
75	Bl	23	LEU
75	Bl	27	ILE
75	Bl	34	THR
75	Bl	36	ARG
75	Bl	45	ARG
75	Bl	51	ILE
76	Bm	77	ILE
76	Bm	78	ILE
76	Bm	79	GLU

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Mol	Chain	Res	Type
76	Bm	83	LYS
76	Bm	85	LEU
76	Bm	108	THR
76	Bm	112	LYS
76	Bm	113	ARG
76	Bm	114	LYS
76	Bm	127	LEU
77	Bn	4	LYS
77	Bn	6	ARG
77	Bn	9	ARG
77	Bn	10	THR
77	Bn	11	ARG
77	Bn	16	LYS
77	Bn	19	LYS
77	Bn	21	ARG
78	Bo	2	VAL
78	Bo	3	ASN
78	Bo	8	ARG
78	Bo	17	CYS
78	Bo	26	THR
78	Bo	29	LYS
78	Bo	34	SER
78	Bo	35	LEU
78	Bo	47	GLN
78	Bo	60	LYS
78	Bo	66	LYS
78	Bo	72	LEU
78	Bo	76	LYS
78	Bo	79	THR
78	Bo	80	ARG
78	Bo	83	LEU
78	Bo	84	THR
78	Bo	93	LEU
78	Bo	99	GLN
78	Bo	100	LYS
78	Bo	104	LEU
78	Bo	105	GLN
79	Bp	5	THR
79	Bp	6	LYS
79	Bp	11	THR
79	Bp	24	ARG
79	Bp	32	GLN

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Mol	Chain	Res	Type
79	Bp	45	LYS
79	Bp	48	LYS
79	Bp	49	ARG
79	Bp	56	THR
79	Bp	59	CYS
79	Bp	60	CYS
79	Bp	73	THR
79	Bp	78	THR
79	Bp	84	ARG
79	Bp	91	GLU
2	CA	6	THR
2	CA	9	LEU
2	CA	12	GLU
2	CA	21	ASN
2	CA	29	VAL
2	CA	30	GLN
2	CA	31	VAL
2	CA	41	ARG
2	CA	45	VAL
2	CA	49	ASN
2	CA	50	VAL
2	CA	57	LEU
2	CA	59	LEU
2	CA	62	ARG
2	CA	76	ILE
2	CA	88	LYS
2	CA	96	THR
2	CA	103	THR
2	CA	110	TYR
2	CA	124	THR
2	CA	131	GLN
2	CA	139	VAL
2	CA	146	LEU
2	CA	151	SER
2	CA	154	GLU
2	CA	167	LYS
2	CA	172	LEU
2	CA	180	GLU
2	CA	183	ARG
2	CA	185	ARG
2	CA	188	LEU
2	CA	189	VAL

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Mol	Chain	Res	Type
2	CA	196	SER
2	CA	198	MET
3	CB	21	VAL
3	CB	22	ASP
3	CB	33	LYS
3	CB	36	SER
3	CB	37	THR
3	CB	40	ASN
3	CB	47	LEU
3	CB	51	SER
3	CB	55	LYS
3	CB	61	LEU
3	CB	62	LYS
3	CB	65	VAL
3	CB	70	LEU
3	CB	73	LEU
3	CB	81	PHE
3	CB	83	LYS
3	CB	85	LYS
3	CB	89	ASP
3	CB	90	GLU
3	CB	105	PHE
3	CB	106	THR
3	CB	108	ASP
3	CB	116	LYS
3	CB	125	VAL
3	CB	126	THR
3	CB	129	THR
3	CB	137	ILE
3	CB	154	SER
3	CB	159	SER
3	CB	170	GLU
3	CB	173	THR
3	CB	177	GLN
3	CB	180	THR
3	CB	181	LEU
3	CB	184	LEU
3	CB	203	ASP
3	CB	204	ILE
3	CB	212	VAL
3	CB	213	ARG
3	CB	214	LYS

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Mol	Chain	Res	Type
3	CB	215	VAL
3	CB	219	LYS
3	CB	222	LYS
3	CB	234	GLU
4	CC	41	LEU
4	CC	50	ILE
4	CC	53	ILE
4	CC	54	GLU
4	CC	55	GLU
4	CC	58	LEU
4	CC	69	ILE
4	CC	71	THR
4	CC	72	LEU
4	CC	73	LEU
4	CC	76	LEU
4	CC	77	GLN
4	CC	81	MET
4	CC	83	ILE
4	CC	89	GLN
4	CC	90	THR
4	CC	91	ARG
4	CC	94	GLN
4	CC	95	ARG
4	CC	97	ARG
4	CC	106	ASP
4	CC	111	VAL
4	CC	130	ILE
4	CC	139	ILE
4	CC	140	ARG
4	CC	141	ARG
4	CC	146	THR
4	CC	148	LEU
4	CC	150	GLN
4	CC	159	THR
4	CC	164	SER
4	CC	170	ILE
4	CC	185	LYS
4	CC	194	GLU
4	CC	206	THR
4	CC	207	LEU
4	CC	218	ILE
4	CC	225	LEU

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Mol	Chain	Res	Type
4	CC	229	LEU
4	CC	233	GLN
4	CC	240	LEU
4	CC	245	ASP
4	CC	248	SER
5	CD	4	LEU
5	CD	5	ILE
5	CD	7	LYS
5	CD	9	ARG
5	CD	10	LYS
5	CD	11	LEU
5	CD	21	LEU
5	CD	37	VAL
5	CD	39	VAL
5	CD	40	ARG
5	CD	41	VAL
5	CD	45	LYS
5	CD	53	THR
5	CD	55	THR
5	CD	59	LEU
5	CD	65	ARG
5	CD	66	ILE
5	CD	67	ASN
5	CD	69	LEU
5	CD	76	ARG
5	CD	84	ILE
5	CD	93	ASP
5	CD	94	ARG
5	CD	115	ILE
5	CD	116	ARG
5	CD	117	ARG
5	CD	127	MET
5	CD	142	LEU
5	CD	143	ARG
5	CD	146	ARG
5	CD	150	MET
5	CD	158	ILE
5	CD	162	GLN
5	CD	170	THR
5	CD	172	THR
5	CD	178	ARG
5	CD	202	LEU

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Mol	Chain	Res	Type
5	CD	204	ASP
5	CD	208	ILE
5	CD	212	LYS
5	CD	213	GLU
5	CD	223	LYS
6	CE	6	LYS
6	CE	7	LYS
6	CE	9	LEU
6	CE	12	LEU
6	CE	23	LEU
6	CE	38	LEU
6	CE	39	ARG
6	CE	42	LEU
6	CE	48	LEU
6	CE	49	ARG
6	CE	50	ASN
6	CE	51	ARG
6	CE	67	GLN
6	CE	70	VAL
6	CE	71	LYS
6	CE	95	THR
6	CE	97	GLU
6	CE	102	VAL
6	CE	105	VAL
6	CE	106	LYS
6	CE	113	ARG
6	CE	116	ASP
6	CE	123	LEU
6	CE	131	LEU
6	CE	147	ILE
6	CE	148	ARG
6	CE	160	VAL
6	CE	176	ASP
6	CE	180	LEU
6	CE	181	VAL
6	CE	182	TYR
6	CE	184	THR
6	CE	187	ARG
6	CE	219	VAL
6	CE	221	ARG
6	CE	222	LEU
6	CE	223	ASN

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Mol	Chain	Res	Type
6	CE	227	VAL
6	CE	236	ILE
6	CE	237	SER
6	CE	245	LYS
6	CE	246	LEU
6	CE	261	LEU
7	CF	23	VAL
7	CF	25	LEU
7	CF	27	THR
7	CF	32	GLU
7	CF	33	VAL
7	CF	38	THR
7	CF	39	GLU
7	CF	41	LYS
7	CF	50	GLU
7	CF	63	GLN
7	CF	64	VAL
7	CF	65	ARG
7	CF	68	ILE
7	CF	70	VAL
7	CF	76	ARG
7	CF	84	LYS
7	CF	89	ILE
7	CF	92	ARG
7	CF	93	LEU
7	CF	94	THR
7	CF	109	LYS
7	CF	112	ARG
7	CF	114	ILE
7	CF	125	THR
7	CF	128	ASN
7	CF	147	THR
7	CF	148	ARG
7	CF	156	ARG
7	CF	157	ARG
7	CF	162	VAL
7	CF	167	ARG
7	CF	170	GLN
7	CF	187	ILE
7	CF	190	ILE
7	CF	194	LEU
7	CF	203	LYS

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Mol	Chain	Res	Type
7	CF	208	SER
7	CF	212	LYS
7	CF	213	LYS
7	CF	216	GLU
7	CF	225	ARG
8	CG	6	SER
8	CG	12	SER
8	CG	17	GLU
8	CG	20	ASP
8	CG	21	GLU
8	CG	25	ARG
8	CG	30	LYS
8	CG	31	ARG
8	CG	44	GLU
8	CG	46	LYS
8	CG	51	LYS
8	CG	71	THR
8	CG	73	ILE
8	CG	76	LEU
8	CG	78	THR
8	CG	79	LYS
8	CG	81	VAL
8	CG	89	ASP
8	CG	93	LYS
8	CG	108	VAL
8	CG	109	LEU
8	CG	111	LEU
8	CG	115	LYS
8	CG	120	GLU
8	CG	121	LEU
8	CG	122	GLU
8	CG	126	ASP
8	CG	127	THR
8	CG	128	THR
8	CG	132	ARG
8	CG	137	ARG
8	CG	143	LYS
8	CG	150	GLU
8	CG	151	ASP
8	CG	153	VAL
8	CG	155	ASP
8	CG	168	THR

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Mol	Chain	Res	Type
8	CG	169	TYR
8	CG	170	THR
8	CG	176	GLN
8	CG	179	VAL
8	CG	193	LEU
8	CG	212	LEU
8	CG	215	ARG
9	CH	11	GLN
9	CH	14	THR
9	CH	24	PHE
9	CH	28	GLU
9	CH	33	GLU
9	CH	35	LYS
9	CH	39	ARG
9	CH	41	LEU
9	CH	42	GLN
9	CH	49	ILE
9	CH	51	VAL
9	CH	67	LEU
9	CH	77	LEU
9	CH	78	THR
9	CH	79	ARG
9	CH	81	LEU
9	CH	86	GLN
9	CH	87	ASP
9	CH	97	ARG
9	CH	105	THR
9	CH	106	SER
9	CH	108	GLN
9	CH	110	GLN
9	CH	114	ARG
9	CH	116	ARG
9	CH	117	THR
9	CH	118	LEU
9	CH	122	HIS
9	CH	126	LEU
9	CH	134	GLU
9	CH	135	ILE
9	CH	136	VAL
9	CH	143	LEU
9	CH	144	VAL
9	CH	181	ILE

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Mol	Chain	Res	Type
9	CH	182	VAL
9	CH	185	ILE
9	CH	187	SER
10	CI	5	ARG
10	CI	18	ARG
10	CI	25	ARG
10	CI	29	LEU
10	CI	36	THR
10	CI	46	VAL
10	CI	47	ARG
10	CI	58	LEU
10	CI	59	ARG
10	CI	60	ILE
10	CI	61	GLU
10	CI	62	THR
10	CI	64	ASN
10	CI	66	SER
10	CI	74	LYS
10	CI	76	THR
10	CI	77	ARG
10	CI	78	ILE
10	CI	82	VAL
10	CI	89	GLU
10	CI	110	ARG
10	CI	111	GLN
10	CI	120	THR
10	CI	138	ASN
10	CI	141	ARG
10	CI	151	LYS
10	CI	152	ILE
10	CI	153	GLU
10	CI	155	SER
10	CI	158	SER
10	CI	183	ILE
10	CI	184	LEU
10	CI	199	LYS
11	CJ	3	ARG
11	CJ	7	THR
11	CJ	22	SER
11	CJ	28	LEU
11	CJ	33	GLU
11	CJ	39	LYS

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Mol	Chain	Res	Type
11	CJ	45	ILE
11	CJ	48	GLN
11	CJ	49	LEU
11	CJ	78	ARG
11	CJ	82	ARG
11	CJ	90	LYS
11	CJ	93	LEU
11	CJ	101	VAL
11	CJ	105	LEU
11	CJ	109	LEU
11	CJ	110	GLN
11	CJ	111	THR
11	CJ	115	LYS
11	CJ	120	LYS
11	CJ	130	THR
11	CJ	134	ILE
11	CJ	140	ILE
11	CJ	142	ASN
11	CJ	145	SER
11	CJ	149	ARG
11	CJ	151	ASP
11	CJ	161	THR
11	CJ	171	ARG
11	CJ	172	VAL
11	CJ	175	ARG
11	CJ	179	ARG
11	CJ	180	LYS
11	CJ	186	GLU
12	CK	3	MET
12	CK	5	LYS
12	CK	13	GLN
12	CK	15	LEU
12	CK	20	VAL
12	CK	21	VAL
12	CK	26	ASP
12	CK	27	PHE
12	CK	33	GLU
12	CK	36	ASP
12	CK	40	LEU
12	CK	55	VAL
12	CK	57	THR
12	CK	71	GLU

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Mol	Chain	Res	Type
12	CK	74	GLU
12	CK	76	LEU
12	CK	77	ARG
13	CL	3	THR
13	CL	5	LEU
13	CL	10	GLU
13	CL	21	ASN
13	CL	26	LYS
13	CL	27	THR
13	CL	30	ARG
13	CL	31	THR
13	CL	32	LYS
13	CL	33	ARG
13	CL	40	LEU
13	CL	44	THR
13	CL	47	THR
13	CL	56	LYS
13	CL	60	PHE
13	CL	67	ARG
13	CL	72	THR
13	CL	74	THR
13	CL	80	MET
13	CL	83	THR
13	CL	96	LYS
13	CL	98	ASN
13	CL	109	VAL
13	CL	123	VAL
13	CL	128	CYS
13	CL	129	ARG
13	CL	131	ILE
13	CL	138	ASN
13	CL	140	VAL
14	CM	25	GLU
14	CM	28	LEU
14	CM	36	LEU
14	CM	39	ASP
14	CM	43	ARG
14	CM	52	LEU
14	CM	58	LEU
14	CM	59	LEU
14	CM	61	VAL
14	CM	62	LEU

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Mol	Chain	Res	Type
14	CM	63	VAL
14	CM	65	SER
14	CM	66	VAL
14	CM	71	ILE
14	CM	74	LEU
14	CM	75	VAL
14	CM	83	GLU
14	CM	85	LYS
14	CM	88	LEU
14	CM	89	ILE
14	CM	91	VAL
14	CM	97	LEU
14	CM	103	LEU
14	CM	116	VAL
14	CM	121	VAL
14	CM	129	GLU
14	CM	132	GLU
14	CM	134	SER
14	CM	135	MET
14	CM	136	ILE
14	CM	138	GLU
14	CM	139	HIS
14	CM	140	PHE
15	CN	13	SER
15	CN	14	SER
15	CN	16	ILE
15	CN	20	ARG
15	CN	21	ASN
15	CN	27	LYS
15	CN	28	LEU
15	CN	39	LYS
15	CN	64	ARG
15	CN	66	ILE
15	CN	70	LYS
15	CN	76	LYS
15	CN	80	LEU
15	CN	84	ILE
15	CN	86	GLU
15	CN	87	ASP
15	CN	88	LEU
15	CN	104	ARG
15	CN	114	ARG

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Mol	Chain	Res	Type
15	CN	115	LEU
15	CN	125	LEU
15	CN	127	ARG
15	CN	134	VAL
15	CN	138	ASN
16	CO	16	VAL
16	CO	18	ARG
16	CO	20	TYR
16	CO	26	THR
16	CO	28	VAL
16	CO	31	THR
16	CO	33	LEU
16	CO	34	SER
16	CO	51	ASP
16	CO	52	ARG
16	CO	62	LEU
16	CO	65	GLN
16	CO	71	CYS
16	CO	79	VAL
16	CO	81	VAL
16	CO	84	ARG
16	CO	92	LYS
16	CO	102	LEU
16	CO	103	ARG
16	CO	107	ARG
16	CO	114	ARG
16	CO	119	THR
16	CO	124	ASP
16	CO	125	SER
16	CO	127	ARG
16	CO	137	LEU
17	CP	12	PHE
17	CP	21	ASP
17	CP	22	LEU
17	CP	24	LYS
17	CP	27	GLU
17	CP	36	LEU
17	CP	43	ARG
17	CP	44	ARG
17	CP	61	ARG
17	CP	69	GLU
17	CP	71	GLU

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Mol	Chain	Res	Type
17	CP	72	LYS
17	CP	77	ARG
17	CP	92	SER
17	CP	104	GLN
17	CP	107	ILE
17	CP	110	GLU
17	CP	121	ILE
17	CP	122	THR
17	CP	124	THR
17	CP	125	PRO
17	CP	127	ARG
18	CQ	17	THR
18	CQ	23	LYS
18	CQ	28	LEU
18	CQ	34	SER
18	CQ	37	THR
18	CQ	40	GLU
18	CQ	43	ILE
18	CQ	47	LYS
18	CQ	48	VAL
18	CQ	53	LEU
18	CQ	54	LEU
18	CQ	57	LEU
18	CQ	63	ILE
18	CQ	68	ARG
18	CQ	69	VAL
18	CQ	81	ILE
18	CQ	90	VAL
18	CQ	94	GLN
18	CQ	98	ASP
18	CQ	113	ASP
18	CQ	114	ARG
18	CQ	117	LEU
18	CQ	123	ARG
18	CQ	128	LYS
18	CQ	137	ARG
18	CQ	141	SER
19	CR	3	ARG
19	CR	8	THR
19	CR	19	ARG
19	CR	31	ASN
19	CR	34	LEU

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Mol	Chain	Res	Type
19	CR	38	ILE
19	CR	46	LEU
19	CR	47	ARG
19	CR	54	THR
19	CR	66	VAL
19	CR	69	ILE
19	CR	78	ARG
19	CR	83	GLN
19	CR	85	VAL
19	CR	88	VAL
19	CR	89	SER
19	CR	104	ASN
19	CR	113	LEU
20	CS	2	SER
20	CS	3	LEU
20	CS	4	VAL
20	CS	5	VAL
20	CS	6	GLN
20	CS	10	SER
20	CS	13	HIS
20	CS	15	LEU
20	CS	17	LEU
20	CS	18	LEU
20	CS	26	ILE
20	CS	27	LYS
20	CS	28	ILE
20	CS	34	THR
20	CS	36	LYS
20	CS	38	VAL
20	CS	40	ARG
20	CS	55	HIS
20	CS	61	LEU
20	CS	63	GLN
20	CS	68	ARG
20	CS	85	PHE
20	CS	89	GLN
20	CS	94	ASP
20	CS	100	THR
20	CS	116	LEU
20	CS	119	ILE
20	CS	136	GLN
20	CS	138	THR

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Mol	Chain	Res	Type
20	CS	144	ARG
21	CT	6	VAL
21	CT	13	ASP
21	CT	22	LEU
21	CT	23	GLN
21	CT	27	LYS
21	CT	28	LEU
21	CT	30	VAL
21	CT	34	VAL
21	CT	36	ILE
21	CT	39	THR
21	CT	57	ARG
21	CT	68	ARG
21	CT	71	VAL
21	CT	75	LYS
21	CT	88	VAL
21	CT	89	ARG
21	CT	111	ILE
21	CT	123	ARG
21	CT	126	GLU
21	CT	131	ASP
21	CT	132	LEU
21	CT	135	ILE
21	CT	139	THR
21	CT	140	LEU
21	CT	141	GLU
21	CT	142	GLU
21	CT	144	GLU
22	CU	12	GLN
22	CU	15	GLN
22	CU	22	ILE
22	CU	23	ARG
22	CU	26	LEU
22	CU	27	THR
22	CU	30	LYS
22	CU	31	VAL
22	CU	39	SER
22	CU	44	ASN
22	CU	47	GLN
22	CU	51	VAL
22	CU	52	LYS
22	CU	57	ARG

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Mol	Chain	Res	Type
22	CU	60	THR
22	CU	63	LEU
22	CU	70	THR
22	CU	72	ASN
22	CU	74	GLU
22	CU	77	LYS
22	CU	81	THR
22	CU	88	LYS
22	CU	89	ARG
22	CU	96	PRO
22	CU	99	ILE
22	CU	102	ARG
22	CU	103	ILE
22	CU	104	THR
22	CU	105	GLN
22	CU	108	ILE
22	CU	113	ASP
22	CU	115	GLU
22	CU	116	VAL
22	CU	118	VAL
23	CV	1	MET
23	CV	2	GLU
23	CV	5	LYS
23	CV	10	GLU
23	CV	11	LEU
23	CV	12	TYR
23	CV	25	LYS
23	CV	32	VAL
23	CV	38	LYS
23	CV	41	GLU
23	CV	52	THR
23	CV	62	ARG
23	CV	68	SER
23	CV	69	LEU
23	CV	78	LEU
23	CV	81	ASN
23	CV	86	SER
24	CW	7	LEU
24	CW	23	ARG
24	CW	25	VAL
24	CW	26	LEU
24	CW	43	LYS

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Mol	Chain	Res	Type
24	CW	65	LEU
24	CW	68	ARG
24	CW	74	VAL
24	CW	88	LYS
24	CW	93	LEU
24	CW	98	GLN
24	CW	103	ILE
24	CW	117	ARG
24	CW	129	VAL
25	CX	9	LEU
25	CX	14	LYS
25	CX	17	VAL
25	CX	19	ARG
25	CX	20	ARG
25	CX	23	ARG
25	CX	31	LYS
25	CX	40	SER
25	CX	55	GLU
25	CX	73	ARG
25	CX	83	VAL
25	CX	84	THR
25	CX	96	VAL
25	CX	100	ASP
25	CX	103	LEU
25	CX	107	PHE
25	CX	109	ARG
25	CX	133	LEU
26	CY	6	THR
26	CY	10	ARG
26	CY	13	ILE
26	CY	14	SER
26	CY	21	LYS
26	CY	26	ASP
26	CY	29	HIS
26	CY	36	SER
26	CY	37	LYS
26	CY	43	LYS
26	CY	44	LEU
26	CY	49	LYS
26	CY	51	GLU
26	CY	62	THR
26	CY	77	ASN

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Mol	Chain	Res	Type
26	CY	78	SER
26	CY	83	LYS
26	CY	88	THR
26	CY	100	VAL
26	CY	105	ARG
26	CY	128	LYS
26	CY	135	ASP
27	CZ	37	GLN
27	CZ	41	ILE
27	CZ	43	ASP
27	CZ	45	GLU
27	CZ	46	LYS
27	CZ	51	LEU
27	CZ	53	GLU
27	CZ	57	TYR
27	CZ	60	VAL
27	CZ	70	LYS
27	CZ	71	ILE
27	CZ	81	ARG
27	CZ	86	GLU
27	CZ	93	SER
27	CZ	97	LYS
27	CZ	102	THR
27	CZ	105	THR
28	Ca	4	LYS
28	Ca	10	ARG
28	Ca	26	CYS
28	Ca	34	LYS
28	Ca	41	ILE
28	Ca	44	ILE
28	Ca	50	VAL
28	Ca	53	LEU
28	Ca	55	GLU
28	Ca	67	THR
28	Ca	76	SER
28	Ca	82	ARG
28	Ca	85	ARG
28	Ca	89	ARG
28	Ca	98	PRO
29	Cb	17	ARG
29	Cb	22	LYS
29	Cb	34	ASP

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Mol	Chain	Res	Type
29	Cb	41	LEU
29	Cb	43	ILE
29	Cb	44	THR
29	Cb	52	THR
29	Cb	55	THR
29	Cb	61	THR
29	Cb	72	LYS
29	Cb	77	THR
29	Cb	78	SER
29	Cb	81	ARG
30	Cc	5	THR
30	Cc	7	VAL
30	Cc	11	LYS
30	Cc	14	LYS
30	Cc	16	LEU
30	Cc	19	THR
30	Cc	22	ARG
30	Cc	30	VAL
30	Cc	32	PHE
30	Cc	33	LEU
30	Cc	35	ASP
30	Cc	36	THR
30	Cc	40	ILE
30	Cc	49	ARG
30	Cc	54	LEU
30	Cc	62	GLU
30	Cc	64	ARG
30	Cc	65	ARG
31	Cd	4	GLU
31	Cd	10	HIS
31	Cd	16	LYS
31	Cd	25	SER
31	Cd	30	LEU
31	Cd	32	ARG
31	Cd	36	LEU
31	Cd	40	ARG
31	Cd	53	ASN
31	Cd	54	LYS
31	Cd	56	ARG
32	Ce	4	VAL
32	Ce	13	LYS
32	Ce	23	LYS

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Mol	Chain	Res	Type
32	Ce	26	LYS
32	Ce	28	LYS
32	Ce	29	LYS
32	Ce	36	LYS
32	Ce	39	LEU
32	Ce	41	THR
32	Ce	44	PHE
32	Ce	45	VAL
32	Ce	47	VAL
32	Ce	50	VAL
32	Ce	53	LYS
32	Ce	54	ARG
32	Ce	56	MET
33	Cf	102	VAL
33	Cf	106	TYR
33	Cf	107	LYS
33	Cf	108	VAL
33	Cf	113	LYS
33	Cf	115	THR
33	Cf	135	HIS
33	Cf	140	TYR
33	Cf	141	CYS
33	Cf	146	SER
33	Cf	151	ASN
34	Cg	22	SER
34	Cg	25	THR
34	Cg	29	GLN
34	Cg	40	LYS
34	Cg	52	GLN
34	Cg	59	ARG
34	Cg	65	SER
34	Cg	76	ASP
34	Cg	96	THR
34	Cg	136	ILE
34	Cg	145	LEU
34	Cg	153	GLN
34	Cg	168	THR
34	Cg	176	LYS
34	Cg	184	ASN
34	Cg	188	ILE
34	Cg	199	ILE
34	Cg	202	LEU

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Mol	Chain	Res	Type
34	Cg	222	LEU
34	Cg	228	LYS
34	Cg	232	TYR
34	Cg	250	TYR
34	Cg	256	THR
34	Cg	264	SER
34	Cg	266	ASP
34	Cg	272	ASP
34	Cg	274	LEU
34	Cg	278	PHE
34	Cg	297	ASP
34	Cg	308	ASN
34	Cg	309	VAL
34	Cg	310	ILE
34	Cg	312	VAL
34	Cg	319	ASN
81	Ch	23	LYS
81	Ch	28	SER
81	Ch	34	LYS
81	Ch	43	ASP
81	Ch	45	SER
81	Ch	46	LYS
81	Ch	48	ARG
81	Ch	49	LYS
81	Ch	50	ASN
81	Ch	53	ARG
81	Ch	61	ILE
81	Ch	64	LYS
81	Ch	74	LYS
81	Ch	75	ASP
81	Ch	77	THR
81	Ch	82	THR
39	DA	15	ILE
39	DA	23	ARG
39	DA	32	LEU
39	DA	41	ILE
39	DA	44	ILE
39	DA	45	VAL
39	DA	46	LYS
39	DA	48	ILE
39	DA	61	VAL
39	DA	62	VAL

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Mol	Chain	Res	Type
39	DA	71	LEU
39	DA	96	LEU
39	DA	101	VAL
39	DA	112	ILE
39	DA	113	VAL
39	DA	114	SER
39	DA	119	LYS
39	DA	134	VAL
39	DA	137	ILE
39	DA	142	ASP
39	DA	147	ARG
39	DA	155	LYS
39	DA	158	ILE
39	DA	169	ILE
39	DA	179	LEU
39	DA	180	LEU
39	DA	181	LYS
39	DA	193	ARG
39	DA	202	VAL
39	DA	207	VAL
39	DA	215	ASN
39	DA	224	THR
39	DA	226	SER
39	DA	227	ARG
39	DA	230	VAL
39	DA	241	ARG
39	DA	243	THR
39	DA	246	LEU
40	DB	3	HIS
40	DB	4	ARG
40	DB	10	ARG
40	DB	17	LEU
40	DB	19	ARG
40	DB	20	LYS
40	DB	21	ARG
40	DB	24	SER
40	DB	30	LYS
40	DB	43	LEU
40	DB	47	LEU
40	DB	50	LYS
40	DB	56	ILE
40	DB	67	PHE

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Mol	Chain	Res	Type
40	DB	70	ARG
40	DB	77	THR
40	DB	79	VAL
40	DB	81	THR
40	DB	84	VAL
40	DB	85	VAL
40	DB	89	VAL
40	DB	100	ARG
40	DB	103	THR
40	DB	114	VAL
40	DB	116	ARG
40	DB	139	GLN
40	DB	146	ARG
40	DB	148	LEU
40	DB	150	ARG
40	DB	153	LYS
40	DB	157	VAL
40	DB	169	THR
40	DB	175	LYS
40	DB	183	LEU
40	DB	187	SER
40	DB	188	ILE
40	DB	192	VAL
40	DB	196	ARG
40	DB	202	THR
40	DB	205	VAL
40	DB	213	GLU
40	DB	221	THR
40	DB	229	VAL
40	DB	232	ARG
40	DB	235	THR
40	DB	236	LYS
40	DB	238	LEU
40	DB	242	THR
40	DB	248	LYS
40	DB	252	ILE
40	DB	284	ARG
40	DB	291	GLU
40	DB	297	SER
40	DB	301	THR
40	DB	304	THR
40	DB	308	MET

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Mol	Chain	Res	Type
40	DB	322	ILE
40	DB	324	VAL
40	DB	328	ILE
40	DB	332	ARG
40	DB	338	LEU
40	DB	340	LYS
40	DB	346	THR
40	DB	347	SER
40	DB	355	SER
40	DB	361	THR
40	DB	367	LYS
40	DB	369	ARG
40	DB	380	MET
40	DB	382	THR
41	DC	2	SER
41	DC	7	THR
41	DC	16	THR
41	DC	18	ASN
41	DC	25	VAL
41	DC	27	SER
41	DC	52	VAL
41	DC	53	SER
41	DC	55	LYS
41	DC	71	VAL
41	DC	85	SER
41	DC	93	MET
41	DC	99	MET
41	DC	112	LYS
41	DC	120	TYR
41	DC	122	THR
41	DC	136	LEU
41	DC	138	ARG
41	DC	144	LYS
41	DC	145	ILE
41	DC	150	LEU
41	DC	153	SER
41	DC	156	LEU
41	DC	158	SER
41	DC	160	GLN
41	DC	161	LYS
41	DC	170	LYS
41	DC	176	SER

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Mol	Chain	Res	Type
41	DC	177	ASP
41	DC	179	LEU
41	DC	182	LEU
41	DC	186	LYS
41	DC	187	LEU
41	DC	198	ARG
41	DC	203	ARG
41	DC	206	LEU
41	DC	220	ARG
41	DC	222	VAL
41	DC	230	VAL
41	DC	246	ARG
41	DC	258	LEU
41	DC	259	ASP
41	DC	265	GLU
41	DC	267	VAL
41	DC	283	THR
41	DC	287	THR
41	DC	289	ILE
41	DC	290	ILE
41	DC	300	ARG
41	DC	307	GLN
41	DC	313	LEU
41	DC	319	LYS
41	DC	323	VAL
41	DC	327	LEU
41	DC	333	VAL
41	DC	339	LEU
41	DC	342	LYS
41	DC	345	GLU
41	DC	349	THR
41	DC	354	VAL
41	DC	356	THR
41	DC	357	GLU
41	DC	358	THR
41	DC	359	LEU
41	DC	360	LYS
41	DC	362	ASP
42	DD	4	GLN
42	DD	5	LYS
42	DD	13	SER
42	DD	34	LYS

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Mol	Chain	Res	Type
42	DD	35	ARG
42	DD	41	LYS
42	DD	51	LEU
42	DD	65	ILE
42	DD	68	THR
42	DD	70	THR
42	DD	74	VAL
42	DD	81	HIS
42	DD	89	THR
42	DD	93	THR
42	DD	110	LEU
42	DD	112	LYS
42	DD	113	LEU
42	DD	118	THR
42	DD	124	GLU
42	DD	130	GLU
42	DD	131	LEU
42	DD	133	GLU
42	DD	136	GLU
42	DD	146	LEU
42	DD	148	ILE
42	DD	152	ARG
42	DD	155	THR
42	DD	164	LYS
42	DD	185	PHE
42	DD	186	GLU
42	DD	189	GLU
42	DD	190	ILE
42	DD	191	ASP
42	DD	194	LEU
42	DD	205	SER
42	DD	211	LEU
42	DD	218	ARG
42	DD	227	LEU
42	DD	232	ASP
42	DD	251	PRO
42	DD	254	LYS
42	DD	258	LYS
42	DD	259	LYS
42	DD	262	LYS
42	DD	268	GLU
42	DD	273	ARG

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Mol	Chain	Res	Type
42	DD	275	THR
42	DD	282	ARG
43	DE	5	LYS
43	DE	8	LYS
43	DE	20	LYS
43	DE	21	THR
43	DE	46	ARG
43	DE	50	LYS
43	DE	64	LEU
43	DE	65	ILE
43	DE	76	LEU
43	DE	78	ARG
43	DE	79	VAL
43	DE	89	THR
43	DE	93	VAL
43	DE	98	VAL
43	DE	99	GLU
43	DE	109	GLU
43	DE	143	LYS
43	DE	152	THR
43	DE	155	LEU
43	DE	162	SER
44	DF	22	THR
44	DF	24	GLU
44	DF	26	VAL
44	DF	39	GLU
44	DF	41	ARG
44	DF	45	LEU
44	DF	53	LYS
44	DF	54	GLU
44	DF	56	GLU
44	DF	60	ARG
44	DF	83	LEU
44	DF	88	ARG
44	DF	98	LYS
44	DF	101	LYS
44	DF	121	LYS
44	DF	124	LEU
44	DF	130	ILE
44	DF	156	ILE
44	DF	158	LYS
44	DF	159	GLN

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Mol	Chain	Res	Type
44	DF	173	LEU
44	DF	175	LYS
44	DF	179	LEU
44	DF	184	LEU
44	DF	196	LYS
44	DF	206	LYS
44	DF	219	LYS
44	DF	229	PHE
44	DF	239	LEU
45	DG	26	LEU
45	DG	41	GLN
45	DG	50	VAL
45	DG	68	ARG
45	DG	70	LYS
45	DG	74	THR
45	DG	79	GLN
45	DG	81	THR
45	DG	85	ASN
45	DG	89	GLU
45	DG	92	LYS
45	DG	95	ASN
45	DG	110	THR
45	DG	126	SER
45	DG	128	LYS
45	DG	136	LEU
45	DG	145	ASN
45	DG	146	LYS
45	DG	149	LYS
45	DG	150	LEU
45	DG	153	ILE
45	DG	160	ILE
45	DG	169	LEU
45	DG	172	LYS
45	DG	173	MET
45	DG	183	LYS
45	DG	185	ARG
45	DG	189	LEU
45	DG	208	GLU
45	DG	213	LYS
45	DG	214	LEU
45	DG	216	SER
45	DG	217	THR

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Mol	Chain	Res	Type
45	DG	219	ASP
45	DG	222	PHE
45	DG	230	LYS
45	DG	241	LYS
45	DG	245	LYS
45	DG	248	LYS
46	DH	4	ILE
46	DH	5	GLN
46	DH	6	THR
46	DH	18	VAL
46	DH	19	SER
46	DH	20	ILE
46	DH	31	ARG
46	DH	33	THR
46	DH	43	VAL
46	DH	44	THR
46	DH	52	LEU
46	DH	55	VAL
46	DH	62	ARG
46	DH	63	LYS
46	DH	68	LEU
46	DH	69	ARG
46	DH	70	THR
46	DH	80	THR
46	DH	82	VAL
46	DH	92	TYR
46	DH	106	LYS
46	DH	121	LYS
46	DH	123	ILE
46	DH	129	ARG
46	DH	130	ASP
46	DH	132	VAL
46	DH	133	THR
46	DH	134	ILE
46	DH	138	THR
46	DH	144	ILE
46	DH	151	VAL
46	DH	157	ASN
46	DH	161	LEU
46	DH	162	GLN
46	DH	164	ILE
46	DH	169	ASN

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Mol	Chain	Res	Type
46	DH	177	ASP
46	DH	179	ILE
46	DH	191	LEU
47	DI	4	ARG
47	DI	24	ARG
47	DI	26	VAL
47	DI	36	LEU
47	DI	42	THR
47	DI	52	LEU
47	DI	57	LEU
47	DI	58	GLU
47	DI	63	GLU
47	DI	71	CYS
47	DI	74	LYS
47	DI	76	MET
47	DI	78	THR
47	DI	83	ASP
47	DI	87	LEU
47	DI	91	VAL
47	DI	99	ILE
47	DI	129	VAL
47	DI	139	ARG
47	DI	140	THR
47	DI	143	SER
47	DI	144	ASN
47	DI	145	LYS
47	DI	153	ARG
47	DI	163	GLN
47	DI	167	LEU
47	DI	169	LYS
47	DI	174	THR
47	DI	177	ASP
47	DI	178	ARG
47	DI	185	ARG
47	DI	200	LEU
47	DI	206	LEU
47	DI	211	ARG
47	DI	212	GLU
47	DI	215	GLU
47	DI	217	PHE
48	DJ	10	ARG
48	DJ	12	LEU

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Mol	Chain	Res	Type
48	DJ	13	LYS
48	DJ	16	LYS
48	DJ	22	SER
48	DJ	29	ARG
48	DJ	30	LEU
48	DJ	31	THR
48	DJ	34	SER
48	DJ	35	LYS
48	DJ	44	THR
48	DJ	46	VAL
48	DJ	80	LEU
48	DJ	87	LYS
48	DJ	92	ARG
48	DJ	94	ARG
48	DJ	106	ILE
48	DJ	107	ASP
48	DJ	112	LEU
48	DJ	114	ILE
48	DJ	129	VAL
48	DJ	130	VAL
48	DJ	132	ASN
48	DJ	137	ARG
48	DJ	138	VAL
48	DJ	140	ARG
48	DJ	142	LYS
48	DJ	147	THR
48	DJ	158	ASP
48	DJ	159	THR
48	DJ	160	VAL
48	DJ	161	SER
48	DJ	165	GLN
49	DL	45	LYS
49	DL	46	ILE
49	DL	54	LEU
49	DL	55	ARG
49	DL	59	ARG
49	DL	63	VAL
49	DL	67	ARG
49	DL	68	LYS
49	DL	69	VAL
49	DL	73	ARG
49	DL	85	LEU

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Mol	Chain	Res	Type
49	DL	100	ARG
49	DL	107	GLU
49	DL	114	GLN
49	DL	115	ARG
49	DL	118	GLU
49	DL	121	SER
49	DL	123	ILE
49	DL	124	ILE
49	DL	128	ARG
49	DL	131	LYS
49	DL	152	THR
49	DL	154	VAL
49	DL	157	ARG
49	DL	164	GLU
49	DL	171	ARG
49	DL	175	SER
49	DL	184	GLU
49	DL	189	GLU
49	DL	194	GLU
50	DM	3	THR
50	DM	10	SER
50	DM	13	ARG
50	DM	20	VAL
50	DM	24	LYS
50	DM	42	LYS
50	DM	53	VAL
50	DM	62	GLN
50	DM	63	VAL
50	DM	64	VAL
50	DM	72	LEU
50	DM	74	ARG
50	DM	80	THR
50	DM	82	SER
50	DM	92	GLU
50	DM	106	ARG
50	DM	107	GLU
50	DM	124	ARG
50	DM	126	GLN
50	DM	128	ARG
50	DM	130	THR
50	DM	132	LYS
50	DM	133	LYS

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Mol	Chain	Res	Type
50	DM	135	LEU
51	DN	5	LYS
51	DN	7	LEU
51	DN	8	GLU
51	DN	10	LEU
51	DN	12	ARG
51	DN	15	GLN
51	DN	18	VAL
51	DN	22	LEU
51	DN	24	ARG
51	DN	41	ARG
51	DN	49	ARG
51	DN	54	LYS
51	DN	68	ARG
51	DN	80	THR
51	DN	85	THR
51	DN	92	LEU
51	DN	93	LYS
51	DN	96	ARG
51	DN	97	SER
51	DN	104	GLU
51	DN	105	ARG
51	DN	109	ARG
51	DN	117	ASN
51	DN	134	LEU
51	DN	138	GLN
51	DN	153	ASP
51	DN	155	VAL
51	DN	159	ARG
51	DN	170	LYS
51	DN	184	LYS
51	DN	190	THR
51	DN	196	THR
51	DN	204	LYS
52	DO	3[A]	VAL
52	DO	3[B]	SER
52	DO	12[A]	LYS
52	DO	12[B]	LYS
52	DO	16[B]	LEU
52	DO	22[B]	THR
52	DO	27[B]	VAL
52	DO	34[A]	VAL

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Mol	Chain	Res	Type
52	DO	34[B]	VAL
52	DO	41[A]	LEU
52	DO	41[B]	LEU
52	DO	58[A]	LEU
52	DO	58[B]	LEU
52	DO	59[A]	ARG
52	DO	59[B]	ARG
52	DO	67[A]	THR
52	DO	67[B]	THR
52	DO	74[A]	ARG
52	DO	74[B]	ARG
52	DO	78[A]	ARG
52	DO	78[B]	ARG
52	DO	80[B]	LEU
52	DO	85[A]	ARG
52	DO	85[B]	ARG
52	DO	100[A]	GLU
52	DO	100[B]	GLU
52	DO	106[A]	GLU
52	DO	106[B]	GLU
52	DO	108[A]	ILE
52	DO	108[B]	ILE
52	DO	117[A]	ARG
52	DO	117[B]	ARG
52	DO	124[A]	LEU
52	DO	124[B]	LEU
52	DO	126[A]	VAL
52	DO	126[B]	VAL
52	DO	128[A]	ARG
52	DO	128[B]	ARG
52	DO	129[A]	LEU
52	DO	129[B]	LEU
52	DO	130[A]	LYS
52	DO	130[B]	LYS
52	DO	144[A]	SER
52	DO	144[B]	SER
52	DO	160[A]	ARG
52	DO	160[B]	ARG
52	DO	163[B]	ARG
52	DO	166[A]	GLU
52	DO	166[B]	GLU
52	DO	171[A]	LYS

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Mol	Chain	Res	Type
52	DO	171[B]	LYS
52	DO	175[A]	THR
52	DO	175[B]	THR
52	DO	182[A]	ASN
52	DO	184[A]	THR
52	DO	197[A]	LEU
53	DP	9	THR
53	DP	24	VAL
53	DP	29	THR
53	DP	31	GLU
53	DP	32	THR
53	DP	41	LEU
53	DP	52	LEU
53	DP	56	ARG
53	DP	69	ARG
53	DP	74	LYS
53	DP	78	VAL
53	DP	79	THR
53	DP	80	LYS
53	DP	89	LYS
53	DP	94	LEU
53	DP	103	GLU
53	DP	112	LEU
53	DP	114	VAL
53	DP	119	VAL
53	DP	126	ARG
53	DP	128	ARG
53	DP	138	LYS
54	DQ	3	ILE
54	DQ	7	SER
54	DQ	17	THR
54	DQ	24	VAL
54	DQ	26	LEU
54	DQ	31	LYS
54	DQ	32	LEU
54	DQ	34	THR
54	DQ	49	LEU
54	DQ	57	ILE
54	DQ	64	VAL
54	DQ	80	THR
54	DQ	81	VAL
54	DQ	86	THR

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Mol	Chain	Res	Type
54	DQ	93	ILE
54	DQ	98	LYS
54	DQ	100	THR
54	DQ	105	ARG
54	DQ	113	LYS
54	DQ	135	GLN
54	DQ	138	LEU
54	DQ	147	ARG
54	DQ	161	LYS
54	DQ	165	ILE
54	DQ	166	LEU
54	DQ	170	ARG
55	DR	5	ARG
55	DR	7	GLN
55	DR	10	LEU
55	DR	17	VAL
55	DR	20	ARG
55	DR	27	ASN
55	DR	29	THR
55	DR	36	ASN
55	DR	39	ASN
55	DR	43	LYS
55	DR	49	THR
55	DR	55	VAL
55	DR	56	THR
55	DR	63	THR
55	DR	70	LYS
55	DR	71	ARG
55	DR	74	ARG
55	DR	98	ARG
55	DR	99	LEU
55	DR	105	LEU
55	DR	106	LEU
55	DR	114	LYS
55	DR	126	GLU
55	DR	138	LEU
55	DR	152	GLU
55	DR	153	LYS
55	DR	158	GLU
55	DR	162	ARG
55	DR	164	LEU
55	DR	167	ARG

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Mol	Chain	Res	Type
55	DR	173	ARG
55	DR	180	LYS
56	DS	1	MET
56	DS	13	ARG
56	DS	15	PRO
56	DS	17	GLU
56	DS	21	GLU
56	DS	23	LYS
56	DS	40	ARG
56	DS	50	LYS
56	DS	51	VAL
56	DS	52	LYS
56	DS	61	ILE
56	DS	71	LYS
56	DS	74	ASN
56	DS	80	ARG
56	DS	87	THR
56	DS	96	ASP
56	DS	97	VAL
56	DS	100	VAL
56	DS	104	GLU
56	DS	105	THR
56	DS	115	ARG
56	DS	117	ARG
56	DS	130	GLU
56	DS	136	LYS
56	DS	146	LYS
56	DS	148	LEU
56	DS	149	LYS
56	DS	155	ARG
56	DS	161	LYS
56	DS	162	THR
56	DS	166	LYS
56	DS	169	SER
56	DS	172	TYR
57	DT	17	ARG
57	DT	25	VAL
57	DT	26	HIS
57	DT	27	LEU
57	DT	35	LYS
57	DT	36	VAL
57	DT	47	SER

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Mol	Chain	Res	Type
57	DT	55	LYS
57	DT	68	THR
57	DT	71	SER
57	DT	78	LYS
57	DT	80	VAL
57	DT	83	ARG
57	DT	88	ARG
57	DT	89	LEU
57	DT	96	ILE
57	DT	102	ARG
57	DT	104	GLU
57	DT	118	GLU
57	DT	126	VAL
57	DT	131	GLN
57	DT	135	PRO
57	DT	139	ARG
57	DT	143	THR
57	DT	149	GLN
57	DT	150	THR
57	DT	160	ILE
58	DU	13	LYS
58	DU	14	THR
58	DU	16	THR
58	DU	21	SER
58	DU	23	THR
58	DU	27	VAL
58	DU	28	PHE
58	DU	37	LEU
58	DU	39	ASP
58	DU	43	VAL
58	DU	50	LEU
58	DU	52	ASN
58	DU	54	VAL
58	DU	55	THR
58	DU	58	GLU
58	DU	61	THR
58	DU	62	VAL
58	DU	63	VAL
58	DU	68	THR
58	DU	90	ARG
58	DU	98	THR
58	DU	100	THR

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Mol	Chain	Res	Type
58	DU	105	LEU
59	DV	13	ILE
59	DV	14	SER
59	DV	48	ARG
59	DV	70	ARG
59	DV	88	ARG
59	DV	91	VAL
59	DV	110	LYS
59	DV	115	THR
60	DW	1	MET
60	DW	5	ILE
60	DW	25	ASP
60	DW	47	ARG
60	DW	56	ARG
60	DW	57	LYS
60	DW	63	ILE
60	DW	95	SER
60	DW	97	LYS
60	DW	100	VAL
60	DW	105	ARG
60	DW	107	GLU
60	DW	126	GLU
60	DW	127	LYS
60	DW	135	SER
61	DX	24	LEU
61	DX	27	ARG
61	DX	34	LEU
61	DX	37	THR
61	DX	38	LEU
61	DX	40	LEU
61	DX	56	ARG
61	DX	57	LEU
61	DX	63	ILE
61	DX	70	GLU
61	DX	71	THR
61	DX	73	MET
61	DX	74	LYS
61	DX	86	VAL
61	DX	101	GLU
61	DX	108	LEU
61	DX	109	LYS
61	DX	115	ARG

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Mol	Chain	Res	Type
61	DX	121	LYS
61	DX	125	ARG
61	DX	133	LEU
61	DX	135	ILE
61	DX	142	ILE
62	DY	12	ARG
62	DY	13	ARG
62	DY	14	LYS
62	DY	17	LYS
62	DY	37	LYS
62	DY	40	ARG
62	DY	43	TYR
62	DY	45	ILE
62	DY	50	ILE
62	DY	52	ARG
62	DY	57	LEU
62	DY	59	VAL
62	DY	66	GLN
62	DY	71	SER
62	DY	74	TYR
62	DY	76	LEU
62	DY	80	VAL
62	DY	83	ASP
62	DY	87	LYS
62	DY	94	SER
62	DY	95	VAL
62	DY	97	ILE
62	DY	103	LYS
62	DY	120	GLN
63	DZ	3	LYS
63	DZ	14	VAL
63	DZ	17	ARG
63	DZ	24	VAL
63	DZ	30	ASP
63	DZ	31	GLU
63	DZ	34	LYS
63	DZ	55	LYS
63	DZ	65	ARG
63	DZ	72	ILE
63	DZ	81	LEU
63	DZ	83	THR
63	DZ	86	THR

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Mol	Chain	Res	Type
63	DZ	89	VAL
63	DZ	93	LYS
63	DZ	95	VAL
63	DZ	99	GLU
63	DZ	100	THR
63	DZ	102	GLU
63	DZ	103	GLN
63	DZ	105	SER
63	DZ	121	ARG
63	DZ	126	LYS
63	DZ	127	ASN
63	DZ	134	LEU
63	DZ	135	ARG
64	Da	6	THR
64	Da	8	THR
64	Da	10	LYS
64	Da	12	ARG
64	Da	16	SER
64	Da	24	LYS
64	Da	34	MET
64	Da	42	ARG
64	Da	44	ASN
64	Da	47	LYS
64	Da	60	TYR
64	Da	78	LEU
64	Da	80	THR
64	Da	82	ILE
64	Da	85	ASP
64	Da	91	LEU
64	Da	97	GLU
64	Da	98	THR
64	Da	115	LYS
64	Da	128	ARG
64	Da	130	VAL
64	Da	132	LYS
64	Da	133	LEU
65	Db	14	ARG
65	Db	15	LYS
65	Db	21	ILE
65	Db	22	LYS
65	Db	26	THR
65	Db	33	LYS

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Mol	Chain	Res	Type
65	Db	38	LYS
65	Db	50	THR
65	Db	52	LYS
65	Db	58	LYS
65	Db	59	LYS
66	Dc	8	GLU
66	Dc	9	SER
66	Dc	18	ILE
66	Dc	19	LYS
66	Dc	30	THR
66	Dc	33	SER
66	Dc	34	LEU
66	Dc	40	LYS
66	Dc	41	LEU
66	Dc	48	THR
66	Dc	61	MET
66	Dc	68	TYR
66	Dc	86	ARG
66	Dc	87	VAL
66	Dc	99	ASP
66	Dc	100	ILE
67	Dd	6	ASP
67	Dd	8	VAL
67	Dd	13	THR
67	Dd	16	LEU
67	Dd	26	LYS
67	Dd	31	ARG
67	Dd	34	LYS
67	Dd	44	MET
67	Dd	55	LEU
67	Dd	61	LYS
67	Dd	76	SER
67	Dd	82	GLU
67	Dd	89	LEU
67	Dd	90	PHE
67	Dd	96	VAL
67	Dd	100	SER
67	Dd	102	LYS
67	Dd	104	LEU
67	Dd	105	GLN
67	Dd	106	THR
67	Dd	110	GLU

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Mol	Chain	Res	Type
68	De	4	LEU
68	De	14	THR
68	De	16	LYS
68	De	18	LYS
68	De	19	ARG
68	De	27	ARG
68	De	31	ASN
68	De	33	ARG
68	De	35	GLN
68	De	51	SER
68	De	61	LYS
68	De	73	THR
68	De	75	LEU
68	De	82	LEU
68	De	87	MET
68	De	91	THR
68	De	106	VAL
68	De	109	LEU
68	De	125	ARG
68	De	126	LEU
69	Df	4	SER
69	Df	10	LYS
69	Df	20	LYS
69	Df	28	SER
69	Df	31	LYS
69	Df	49	ILE
69	Df	70	LYS
69	Df	81	VAL
69	Df	84	THR
69	Df	98	VAL
69	Df	107	ILE
70	Dg	5	VAL
70	Dg	9	ARG
70	Dg	16	ARG
70	Dg	19	LYS
70	Dg	20	ILE
70	Dg	23	VAL
70	Dg	24	LYS
70	Dg	29	ILE
70	Dg	30	LEU
70	Dg	31	ARG
70	Dg	35	VAL

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Mol	Chain	Res	Type
70	Dg	36	LYS
70	Dg	44	CYS
70	Dg	54	ILE
70	Dg	58	ARG
70	Dg	65	VAL
70	Dg	70	LYS
70	Dg	79	SER
70	Dg	85	VAL
70	Dg	86	LYS
70	Dg	88	ARG
70	Dg	90	ILE
70	Dg	98	GLN
70	Dg	104	VAL
71	Dh	15	GLU
71	Dh	20	GLN
71	Dh	21	LEU
71	Dh	27	GLU
71	Dh	28	LEU
71	Dh	38	ARG
71	Dh	40	SER
71	Dh	45	LYS
71	Dh	47	VAL
71	Dh	48	ARG
71	Dh	57	VAL
71	Dh	62	GLN
71	Dh	66	VAL
71	Dh	69	LEU
71	Dh	79	ASP
71	Dh	81	ARG
71	Dh	84	LYS
71	Dh	85	THR
71	Dh	86	ARG
71	Dh	89	ARG
71	Dh	90	ARG
71	Dh	98	SER
71	Dh	100	VAL
71	Dh	101	THR
71	Dh	107	LYS
71	Dh	119	LYS
72	Di	3	VAL
72	Di	7	ILE
72	Di	9	ILE

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Mol	Chain	Res	Type
72	Di	11	LEU
72	Di	17	VAL
72	Di	18	THR
72	Di	21	THR
72	Di	26	ILE
72	Di	29	LYS
72	Di	34	SER
72	Di	36	ARG
72	Di	37	THR
72	Di	38	LYS
72	Di	43	LEU
72	Di	45	ARG
72	Di	57	LEU
72	Di	58	ILE
72	Di	60	LEU
72	Di	61	ILE
72	Di	66	GLU
72	Di	68	ARG
72	Di	74	LYS
72	Di	75	LYS
72	Di	76	ARG
72	Di	81	THR
72	Di	88	GLU
72	Di	90	MET
72	Di	94	ILE
72	Di	98	ARG
73	Dj	3	LYS
73	Dj	11	ARG
73	Dj	17	THR
73	Dj	25	ARG
73	Dj	33	THR
73	Dj	36	SER
73	Dj	44	THR
73	Dj	55	ARG
73	Dj	58	THR
73	Dj	59	THR
73	Dj	64	MET
73	Dj	65	ARG
73	Dj	67	LEU
73	Dj	68	LYS
73	Dj	75	LYS
73	Dj	80	THR

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Mol	Chain	Res	Type
73	Dj	84	SER
74	Dk	5	ILE
74	Dk	12	LEU
74	Dk	24	THR
74	Dk	31	LEU
74	Dk	39	ARG
74	Dk	41	THR
74	Dk	46	ARG
74	Dk	50	SER
74	Dk	53	THR
74	Dk	61	LYS
74	Dk	64	LYS
74	Dk	65	LEU
74	Dk	67	GLN
74	Dk	68	SER
75	Dl	11	GLN
75	Dl	15	LYS
75	Dl	17	LYS
75	Dl	21	ARG
75	Dl	23	LEU
75	Dl	27	ILE
75	Dl	29	LEU
75	Dl	41	ARG
75	Dl	45	ARG
75	Dl	47	THR
75	Dl	51	ILE
76	Dm	78	ILE
76	Dm	79	GLU
76	Dm	83	LYS
76	Dm	85	LEU
76	Dm	88	LYS
76	Dm	91	CYS
76	Dm	93	LYS
76	Dm	106	ARG
76	Dm	112	LYS
76	Dm	113	ARG
76	Dm	114	LYS
76	Dm	126	LYS
76	Dm	127	LEU
77	Dn	6	ARG
77	Dn	9	ARG
77	Dn	13	LEU

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Mol	Chain	Res	Type
77	Dn	16	LYS
77	Dn	21	ARG
77	Dn	23	ARG
77	Dn	24	SER
78	Do	7	THR
78	Do	8	ARG
78	Do	18	ARG
78	Do	46	LYS
78	Do	47	GLN
78	Do	61	LYS
78	Do	63	LYS
78	Do	71	ARG
78	Do	78	LYS
78	Do	79	THR
78	Do	83	LEU
78	Do	84	THR
78	Do	89	LYS
78	Do	93	LEU
78	Do	104	LEU
78	Do	105	GLN
79	Dp	3	LYS
79	Dp	24	ARG
79	Dp	42	CYS
79	Dp	48	LYS
79	Dp	49	ARG
79	Dp	54	ILE
79	Dp	56	THR
79	Dp	79	VAL
79	Dp	89	MET
79	Dp	90	VAL
83	Dq	4	ILE
83	Dq	5	ARG
83	Dq	10	GLU
83	Dq	30	VAL
83	Dq	32	ASN
83	Dq	39	HIS
83	Dq	42	ARG
83	Dq	44	GLU
83	Dq	51	VAL
83	Dq	52	LEU
83	Dq	55	LYS
83	Dq	57	THR

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Mol	Chain	Res	Type
83	Dq	67	LEU
83	Dq	68	SER
83	Dq	70	LEU
83	Dq	72	ASP
83	Dq	74	GLU
83	Dq	75	LYS
83	Dq	76	LEU
83	Dq	79	PHE
83	Dq	80	VAL
83	Dq	81	LYS
83	Dq	84	VAL
83	Dq	91	GLU
83	Dq	93	LEU
83	Dq	96	ILE
83	Dq	97	LYS
83	Dq	185	LEU
83	Dq	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
2	AA	168	HIS
3	AB	101	HIS
3	AB	146	GLN
3	AB	149	GLN
3	AB	177	GLN
4	AC	82	ASN
4	AC	89	GLN
4	AC	94	GLN
5	AD	179	GLN
6	AE	98	ASN
7	AF	104	ASN
7	AF	128	ASN
7	AF	170	GLN
10	AI	64	ASN
10	AI	103	GLN
11	AJ	110	GLN
11	AJ	131	GLN
13	AL	110	HIS
14	AM	125	ASN
18	AQ	62	ASN
18	AQ	74	HIS

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Mol	Chain	Res	Type
20	AS	89	GLN
21	AT	64	HIS
23	AV	74	GLN
24	AW	24	GLN
24	AW	80	ASN
27	AZ	95	HIS
31	Ad	48	ASN
31	Ad	53	ASN
35	Ah	108	GLN
39	BA	83	HIS
39	BA	132	ASN
39	BA	209	HIS
40	BB	3	HIS
41	BC	48	GLN
41	BC	114	ASN
41	BC	221	ASN
41	BC	311	HIS
42	BD	40	HIS
42	BD	63	GLN
43	BE	167	ASN
44	BF	225	GLN
44	BF	244	ASN
45	BG	38	GLN
45	BG	240	ASN
46	BH	50	ASN
47	BI	14	ASN
47	BI	144	ASN
48	BJ	109	HIS
51	BN	37	HIS
54	BQ	9	GLN
54	BQ	145	ASN
57	BT	16	GLN
57	BT	103	GLN
59	BV	33	ASN
59	BV	98	ASN
64	Ba	74	ASN
65	Bb	43	HIS
65	Bb	45	HIS
70	Bg	52	GLN
74	Bk	40	GLN
78	Bo	82	GLN
2	CA	23	HIS

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Mol	Chain	Res	Type
2	CA	49	ASN
3	CB	146	GLN
3	CB	153	HIS
4	CC	199	GLN
4	CC	250	GLN
6	CE	67	GLN
6	CE	142	HIS
6	CE	157	ASN
6	CE	216	ASN
7	CF	170	GLN
9	CH	89	HIS
9	CH	122	HIS
11	CJ	110	GLN
11	CJ	124	HIS
11	CJ	142	ASN
12	CK	29	GLN
12	CK	32	HIS
17	CP	103	ASN
18	CQ	77	GLN
18	CQ	83	GLN
19	CR	31	ASN
20	CS	90	ASN
21	CT	64	HIS
24	CW	12	ASN
26	CY	22	GLN
26	CY	34	ASN
29	Cb	19	HIS
32	Ce	17	GLN
34	Cg	182	ASN
34	Cg	184	ASN
39	DA	209	HIS
39	DA	215	ASN
41	DC	48	GLN
41	DC	114	ASN
41	DC	221	ASN
41	DC	291	ASN
42	DD	40	HIS
42	DD	63	GLN
42	DD	81	HIS
43	DE	167	ASN
44	DF	80	GLN
46	DH	102	ASN

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Mol	Chain	Res	Type
48	DJ	109	HIS
48	DJ	132	ASN
49	DL	19	GLN
50	DM	126	GLN
53	DP	55	GLN
54	DQ	9	GLN
57	DT	49	GLN
58	DU	40	HIS
59	DV	33	ASN
63	DZ	57	HIS
64	Da	44	ASN
69	Df	77	ASN
70	Dg	52	GLN
71	Dh	20	GLN
83	Dq	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1764/1800 (98%)	545 (30%)	86 (4%)
36	A1	3146/3396 (92%)	738 (23%)	127 (4%)
36	A5	3145/3396 (92%)	731 (23%)	129 (4%)
37	A3	120/121 (99%)	22 (18%)	3 (2%)
37	A7	120/121 (99%)	18 (15%)	0
38	A4	157/158 (99%)	38 (24%)	5 (3%)
38	A8	157/158 (99%)	32 (20%)	3 (1%)
80	A6	1766/1800 (98%)	499 (28%)	60 (3%)
All	All	10375/10950 (94%)	2623 (25%)	413 (3%)

All (2623) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	4	C
1	A2	8	U
1	A2	16	G
1	A2	20	G
1	A2	25	C
1	A2	26	A
1	A2	27	U
1	A2	34	G

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Mol	Chain	Res	Type
1	A2	39	A
1	A2	41	A
1	A2	42	G
1	A2	45	U
1	A2	46	A
1	A2	47	A
1	A2	50	C
1	A2	57	G
1	A2	60	U
1	A2	67	A
1	A2	68	A
1	A2	69	G
1	A2	72	A
1	A2	73	U
1	A2	74	U
1	A2	75	U
1	A2	76	A
1	A2	77	U
1	A2	78	A
1	A2	97	C
1	A2	100	A
1	A2	101	U
1	A2	104	A
1	A2	114	C
1	A2	126	A
1	A2	127	G
1	A2	131	C
1	A2	132	U
1	A2	133	U
1	A2	134	U
1	A2	135	A
1	A2	136	C
1	A2	137	U
1	A2	138	A
1	A2	139	C
1	A2	140	A
1	A2	141	U
1	A2	144	U
1	A2	145	A
1	A2	146	U
1	A2	153	G
1	A2	158	U

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Mol	Chain	Res	Type
1	A2	159	U
1	A2	175	G
1	A2	178	U
1	A2	179	A
1	A2	185	U
1	A2	186	C
1	A2	187	G
1	A2	188	A
1	A2	189	C
1	A2	190	C
1	A2	191	C
1	A2	192	U
1	A2	193	U
1	A2	194	U
1	A2	195	G
1	A2	196	G
1	A2	197	A
1	A2	198	A
1	A2	199	G
1	A2	200	A
1	A2	215	A
1	A2	218	A
1	A2	219	A
1	A2	223	U
1	A2	225	A
1	A2	226	A
1	A2	227	U
1	A2	228	G
1	A2	229	U
1	A2	233	C
1	A2	234	G
1	A2	235	G
1	A2	236	A
1	A2	238	U
1	A2	239	C
1	A2	240	U
1	A2	241	U
1	A2	242	U
1	A2	249	U
1	A2	250	C
1	A2	261	U
1	A2	262	U

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Mol	Chain	Res	Type
1	A2	265	A
1	A2	266	A
1	A2	271	A
1	A2	272	U
1	A2	274	G
1	A2	275	C
1	A2	276	C
1	A2	277	U
1	A2	278	U
1	A2	279	G
1	A2	280	U
1	A2	281	G
1	A2	288	A
1	A2	290	G
1	A2	299	A
1	A2	301	A
1	A2	306	U
1	A2	308	C
1	A2	309	C
1	A2	314	C
1	A2	316	A
1	A2	319	U
1	A2	320	U
1	A2	321	C
1	A2	322	G
1	A2	337	G
1	A2	338	C
1	A2	341	A
1	A2	348	U
1	A2	352	A
1	A2	359	A
1	A2	360	A
1	A2	361	C
1	A2	399	A
1	A2	400	A
1	A2	401	A
1	A2	402	C
1	A2	403	G
1	A2	404	G
1	A2	411	C
1	A2	416	A
1	A2	418	G

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Mol	Chain	Res	Type
1	A2	423	G
1	A2	424	C
1	A2	425	A
1	A2	426	G
1	A2	428	A
1	A2	434	G
1	A2	439	U
1	A2	444	C
1	A2	445	A
1	A2	446	A
1	A2	448	C
1	A2	467	G
1	A2	468	A
1	A2	470	A
1	A2	475	A
1	A2	477	A
1	A2	484	C
1	A2	485	A
1	A2	486	G
1	A2	487	G
1	A2	488	G
1	A2	493	U
1	A2	494	U
1	A2	495	C
1	A2	496	G
1	A2	497	G
1	A2	498	G
1	A2	499	U
1	A2	500	C
1	A2	502	U
1	A2	503	G
1	A2	504	U
1	A2	505	A
1	A2	506	A
1	A2	507	U
1	A2	508	U
1	A2	510	G
1	A2	511	A
1	A2	512	A
1	A2	513	U
1	A2	515	A
1	A2	516	G

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Mol	Chain	Res	Type
1	A2	519	C
1	A2	525	A
1	A2	527	A
1	A2	532	U
1	A2	538	A
1	A2	539	G
1	A2	540	G
1	A2	541	A
1	A2	542	A
1	A2	543	C
1	A2	544	A
1	A2	545	A
1	A2	548	G
1	A2	555	A
1	A2	556	A
1	A2	557	G
1	A2	558	U
1	A2	559	C
1	A2	565	C
1	A2	570	A
1	A2	575	C
1	A2	579	A
1	A2	580	A
1	A2	582	U
1	A2	583	C
1	A2	585	A
1	A2	594	A
1	A2	595	G
1	A2	597	G
1	A2	605	A
1	A2	607	G
1	A2	611	U
1	A2	619	A
1	A2	620	A
1	A2	622	A
1	A2	623	A
1	A2	624	G
1	A2	630	A
1	A2	639	U
1	A2	640	U
1	A2	650	U
1	A2	653	C

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Mol	Chain	Res	Type
1	A2	655	G
1	A2	656	G
1	A2	657	U
1	A2	658	C
1	A2	677	G
1	A2	679	U
1	A2	680	U
1	A2	684	A
1	A2	685	A
1	A2	686	C
1	A2	692	C
1	A2	694	U
1	A2	696	C
1	A2	697	C
1	A2	699	U
1	A2	700	C
1	A2	701	U
1	A2	702	G
1	A2	703	G
1	A2	704	C
1	A2	705	U
1	A2	706	A
1	A2	707	A
1	A2	709	C
1	A2	710	U
1	A2	712	G
1	A2	713	A
1	A2	714	G
1	A2	717	C
1	A2	718	U
1	A2	719	U
1	A2	720	G
1	A2	721	U
1	A2	722	G
1	A2	723	G
1	A2	725	U
1	A2	727	U
1	A2	728	U
1	A2	729	G
1	A2	730	G
1	A2	731	C
1	A2	732	G

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Mol	Chain	Res	Type
1	A2	733	A
1	A2	734	A
1	A2	735	C
1	A2	736	C
1	A2	737	A
1	A2	738	G
1	A2	742	U
1	A2	743	U
1	A2	745	U
1	A2	754	A
1	A2	755	A
1	A2	756	A
1	A2	758	U
1	A2	765	G
1	A2	766	U
1	A2	771	A
1	A2	774	A
1	A2	775	G
1	A2	778	G
1	A2	779	U
1	A2	780	A
1	A2	781	U
1	A2	782	U
1	A2	783	G
1	A2	784	C
1	A2	785	U
1	A2	787	G
1	A2	789	A
1	A2	793	A
1	A2	794	U
1	A2	795	U
1	A2	806	A
1	A2	811	A
1	A2	812	A
1	A2	813	U
1	A2	815	G
1	A2	816	G
1	A2	818	C
1	A2	819	G
1	A2	820	U
1	A2	821	U
1	A2	823	G

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Mol	Chain	Res	Type
1	A2	824	G
1	A2	829	A
1	A2	830	U
1	A2	831	U
1	A2	832	U
1	A2	833	U
1	A2	837	G
1	A2	838	G
1	A2	840	U
1	A2	846	G
1	A2	848	C
1	A2	849	C
1	A2	854	U
1	A2	862	A
1	A2	863	A
1	A2	864	U
1	A2	873	U
1	A2	876	G
1	A2	892	A
1	A2	896	U
1	A2	898	A
1	A2	912	U
1	A2	913	G
1	A2	914	G
1	A2	921	U
1	A2	928	U
1	A2	933	A
1	A2	935	U
1	A2	942	G
1	A2	944	A
1	A2	951	A
1	A2	959	U
1	A2	960	U
1	A2	961	U
1	A2	966	A
1	A2	968	U
1	A2	982	U
1	A2	988	A
1	A2	992	A
1	A2	993	A
1	A2	995	A
1	A2	997	G

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Mol	Chain	Res	Type
1	A2	1003	A
1	A2	1004	U
1	A2	1005	A
1	A2	1020	A
1	A2	1021	C
1	A2	1026	A
1	A2	1028	C
1	A2	1031	U
1	A2	1039	A
1	A2	1040	G
1	A2	1052	U
1	A2	1053	G
1	A2	1058	U
1	A2	1059	U
1	A2	1060	U
1	A2	1061	A
1	A2	1064	G
1	A2	1073	G
1	A2	1074	G
1	A2	1079	U
1	A2	1080	U
1	A2	1082	C
1	A2	1083	G
1	A2	1084	A
1	A2	1086	A
1	A2	1087	A
1	A2	1091	A
1	A2	1092	A
1	A2	1093	A
1	A2	1096	C
1	A2	1097	U
1	A2	1100	G
1	A2	1104	U
1	A2	1111	G
1	A2	1138	A
1	A2	1139	A
1	A2	1146	G
1	A2	1149	G
1	A2	1151	A
1	A2	1152	A
1	A2	1155	G
1	A2	1157	A

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Mol	Chain	Res	Type
1	A2	1158	C
1	A2	1160	A
1	A2	1162	C
1	A2	1167	G
1	A2	1185	U
1	A2	1188	G
1	A2	1191	U
1	A2	1194	A
1	A2	1196	A
1	A2	1197	C
1	A2	1199	G
1	A2	1200	G
1	A2	1202	A
1	A2	1207	C
1	A2	1208	A
1	A2	1217	A
1	A2	1218	G
1	A2	1219	A
1	A2	1221	A
1	A2	1226	A
1	A2	1227	A
1	A2	1228	G
1	A2	1229	G
1	A2	1235	C
1	A2	1243	G
1	A2	1244	A
1	A2	1245	G
1	A2	1250	U
1	A2	1251	U
1	A2	1257	U
1	A2	1258	U
1	A2	1260	U
1	A2	1269	U
1	A2	1286	U
1	A2	1301	U
1	A2	1314	U
1	A2	1315	U
1	A2	1321	A
1	A2	1329	A
1	A2	1337	A
1	A2	1339	C
1	A2	1340	U

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Mol	Chain	Res	Type
1	A2	1341	A
1	A2	1344	A
1	A2	1345	A
1	A2	1349	G
1	A2	1354	G
1	A2	1361	U
1	A2	1363	U
1	A2	1364	G
1	A2	1370	U
1	A2	1371	A
1	A2	1372	U
1	A2	1379	C
1	A2	1382	A
1	A2	1383	G
1	A2	1388	A
1	A2	1390	U
1	A2	1398	U
1	A2	1399	C
1	A2	1400	A
1	A2	1412	G
1	A2	1413	U
1	A2	1414	U
1	A2	1415	U
1	A2	1420	C
1	A2	1421	A
1	A2	1427	A
1	A2	1428	G
1	A2	1429	G
1	A2	1431	C
1	A2	1445	G
1	A2	1446	A
1	A2	1448	G
1	A2	1454	G
1	A2	1457	C
1	A2	1459	C
1	A2	1461	C
1	A2	1462	G
1	A2	1471	A
1	A2	1473	U
1	A2	1474	G
1	A2	1475	A
1	A2	1478	G

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Mol	Chain	Res	Type
1	A2	1482	C
1	A2	1486	G
1	A2	1488	G
1	A2	1489	U
1	A2	1490	C
1	A2	1491	U
1	A2	1492	A
1	A2	1493	A
1	A2	1499	G
1	A2	1500	C
1	A2	1506	G
1	A2	1514	U
1	A2	1516	A
1	A2	1518	C
1	A2	1521	G
1	A2	1523	G
1	A2	1524	A
1	A2	1535	U
1	A2	1536	G
1	A2	1537	C
1	A2	1538	U
1	A2	1539	G
1	A2	1540	G
1	A2	1557	U
1	A2	1559	A
1	A2	1569	A
1	A2	1573	A
1	A2	1574	G
1	A2	1575	G
1	A2	1584	G
1	A2	1590	G
1	A2	1601	G
1	A2	1616	G
1	A2	1619	C
1	A2	1624	C
1	A2	1625	C
1	A2	1631	A
1	A2	1635	A
1	A2	1649	G
1	A2	1657	U
1	A2	1658	G
1	A2	1663	G

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Mol	Chain	Res	Type
1	A2	1680	G
1	A2	1682	U
1	A2	1683	C
1	A2	1684	U
1	A2	1685	G
1	A2	1686	C
1	A2	1687	U
1	A2	1693	A
1	A2	1712	A
1	A2	1713	G
1	A2	1716	C
1	A2	1717	G
1	A2	1727	G
1	A2	1729	C
1	A2	1731	A
1	A2	1759	C
1	A2	1760	G
1	A2	1761	U
1	A2	1762	A
1	A2	1766	A
1	A2	1768	G
1	A2	1769	U
1	A2	1770	U
1	A2	1780	G
1	A2	1782	A
1	A2	1783	C
1	A2	1789	G
1	A2	1792	G
1	A2	1793	G
1	A2	1794	A
1	A2	1795	U
1	A2	1796	C
36	A1	13	A
36	A1	14	U
36	A1	16	A
36	A1	26	A
36	A1	40	A
36	A1	42	C
36	A1	43	A
36	A1	49	A
36	A1	59	G
36	A1	60	A

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Mol	Chain	Res	Type
36	A1	65	A
36	A1	66	A
36	A1	68	C
36	A1	74	G
36	A1	75	G
36	A1	76	G
36	A1	83	U
36	A1	92	G
36	A1	93	C
36	A1	99	A
36	A1	109	A
36	A1	110	G
36	A1	113	C
36	A1	121	A
36	A1	122	A
36	A1	133	U
36	A1	135	C
36	A1	136	G
36	A1	147	U
36	A1	154	U
36	A1	156	G
36	A1	157	A
36	A1	161	G
36	A1	166	C
36	A1	169	U
36	A1	170	G
36	A1	173	G
36	A1	182	U
36	A1	187	A
36	A1	190	U
36	A1	191	U
36	A1	192	C
36	A1	210	U
36	A1	214	G
36	A1	218	G
36	A1	219	A
36	A1	224	C
36	A1	234	G
36	A1	235	A
36	A1	238	A
36	A1	240	U
36	A1	241	G

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Mol	Chain	Res	Type
36	A1	243	G
36	A1	244	G
36	A1	245	U
36	A1	249	U
36	A1	250	U
36	A1	251	G
36	A1	252	U
36	A1	263	C
36	A1	265	A
36	A1	269	G
36	A1	282	G
36	A1	283	G
36	A1	286	U
36	A1	295	A
36	A1	296	A
36	A1	298	U
36	A1	301	G
36	A1	305	U
36	A1	307	A
36	A1	318	A
36	A1	323	A
36	A1	329	U
36	A1	338	A
36	A1	339	C
36	A1	349	A
36	A1	350	C
36	A1	351	A
36	A1	352	A
36	A1	370	U
36	A1	373	A
36	A1	376	G
36	A1	395	A
36	A1	397	A
36	A1	398	A
36	A1	399	A
36	A1	401	U
36	A1	402	A
36	A1	403	C
36	A1	421	G
36	A1	422	A
36	A1	439	C
36	A1	440	A

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Mol	Chain	Res	Type
36	A1	495	G
36	A1	517	G
36	A1	520	U
36	A1	521	A
36	A1	531	G
36	A1	535	G
36	A1	544	C
36	A1	546	C
36	A1	547	G
36	A1	548	G
36	A1	549	U
36	A1	550	A
36	A1	551	A
36	A1	552	G
36	A1	555	U
36	A1	556	U
36	A1	557	A
36	A1	558	U
36	A1	559	A
36	A1	578	A
36	A1	579	G
36	A1	585	A
36	A1	592	A
36	A1	600	G
36	A1	601	U
36	A1	603	A
36	A1	604	G
36	A1	609	G
36	A1	611	A
36	A1	619	A
36	A1	620	U
36	A1	621	A
36	A1	622	A
36	A1	625	G
36	A1	636	C
36	A1	637	C
36	A1	638	C
36	A1	649	A
36	A1	656	A
36	A1	660	A
36	A1	677	A
36	A1	681	U

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Mol	Chain	Res	Type
36	A1	683	U
36	A1	691	A
36	A1	705	A
36	A1	708	G
36	A1	712	G
36	A1	715	A
36	A1	716	A
36	A1	719	U
36	A1	720	A
36	A1	725	G
36	A1	726	G
36	A1	733	G
36	A1	758	C
36	A1	764	U
36	A1	765	C
36	A1	766	U
36	A1	767	U
36	A1	768	C
36	A1	776	U
36	A1	777	U
36	A1	781	G
36	A1	785	G
36	A1	786	A
36	A1	801	A
36	A1	806	A
36	A1	807	A
36	A1	817	A
36	A1	830	A
36	A1	849	C
36	A1	861	C
36	A1	871	U
36	A1	874	U
36	A1	879	U
36	A1	883	A
36	A1	896	A
36	A1	907	G
36	A1	908	G
36	A1	914	A
36	A1	916	G
36	A1	917	A
36	A1	921	A
36	A1	923	C

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Mol	Chain	Res	Type
36	A1	924	G
36	A1	925	A
36	A1	937	G
36	A1	944	C
36	A1	947	G
36	A1	959	C
36	A1	960	U
36	A1	974	G
36	A1	979	U
36	A1	980	A
36	A1	981	U
36	A1	982	C
36	A1	989	A
36	A1	994	G
36	A1	1001	G
36	A1	1002	A
36	A1	1003	A
36	A1	1006	A
36	A1	1010	G
36	A1	1014	U
36	A1	1015	U
36	A1	1016	C
36	A1	1017	C
36	A1	1018	G
36	A1	1020	G
36	A1	1021	G
36	A1	1024	G
36	A1	1025	A
36	A1	1029	G
36	A1	1032	C
36	A1	1036	A
36	A1	1037	C
36	A1	1047	A
36	A1	1049	C
36	A1	1052	U
36	A1	1057	A
36	A1	1064	A
36	A1	1065	A
36	A1	1071	U
36	A1	1072	G
36	A1	1079	A
36	A1	1081	U

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Mol	Chain	Res	Type
36	A1	1082	U
36	A1	1083	G
36	A1	1087	G
36	A1	1093	A
36	A1	1094	U
36	A1	1095	U
36	A1	1096	U
36	A1	1097	G
36	A1	1098	A
36	A1	1103	A
36	A1	1104	G
36	A1	1117	G
36	A1	1131	G
36	A1	1153	A
36	A1	1159	A
36	A1	1180	A
36	A1	1181	U
36	A1	1182	A
36	A1	1185	C
36	A1	1191	U
36	A1	1192	C
36	A1	1201	C
36	A1	1202	A
36	A1	1209	G
36	A1	1212	A
36	A1	1213	G
36	A1	1216	C
36	A1	1218	U
36	A1	1222	G
36	A1	1225	A
36	A1	1227	C
36	A1	1232	C
36	A1	1233	G
36	A1	1234	G
36	A1	1236	G
36	A1	1237	G
36	A1	1239	C
36	A1	1241	U
36	A1	1242	G
36	A1	1243	G
36	A1	1245	A
36	A1	1246	G

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Mol	Chain	Res	Type
36	A1	1248	C
36	A1	1249	G
36	A1	1251	A
36	A1	1258	U
36	A1	1262	G
36	A1	1263	A
36	A1	1264	G
36	A1	1265	U
36	A1	1266	G
36	A1	1267	U
36	A1	1269	U
36	A1	1270	A
36	A1	1271	A
36	A1	1272	C
36	A1	1274	A
36	A1	1277	C
36	A1	1278	A
36	A1	1279	C
36	A1	1280	C
36	A1	1281	G
36	A1	1285	G
36	A1	1287	A
36	A1	1292	C
36	A1	1307	G
36	A1	1308	A
36	A1	1309	U
36	A1	1312	C
36	A1	1313	G
36	A1	1325	U
36	A1	1329	U
36	A1	1330	A
36	A1	1345	G
36	A1	1348	U
36	A1	1349	G
36	A1	1351	U
36	A1	1352	A
36	A1	1353	U
36	A1	1355	A
36	A1	1356	U
36	A1	1357	G
36	A1	1366	A
36	A1	1386	A

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Mol	Chain	Res	Type
36	A1	1399	A
36	A1	1400	G
36	A1	1401	A
36	A1	1414	G
36	A1	1418	A
36	A1	1419	A
36	A1	1428	A
36	A1	1434	G
36	A1	1437	C
36	A1	1440	G
36	A1	1443	G
36	A1	1446	A
36	A1	1449	A
36	A1	1450	G
36	A1	1454	A
36	A1	1478	C
36	A1	1481	A
36	A1	1482	A
36	A1	1485	G
36	A1	1488	G
36	A1	1508	C
36	A1	1526	U
36	A1	1527	C
36	A1	1528	G
36	A1	1529	A
36	A1	1549	U
36	A1	1555	U
36	A1	1556	C
36	A1	1557	A
36	A1	1558	A
36	A1	1560	G
36	A1	1561	G
36	A1	1562	C
36	A1	1563	C
36	A1	1564	U
36	A1	1566	A
36	A1	1567	U
36	A1	1568	U
36	A1	1569	U
36	A1	1570	U
36	A1	1572	U
36	A1	1575	A

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Mol	Chain	Res	Type
36	A1	1576	G
36	A1	1577	G
36	A1	1579	C
36	A1	1581	C
36	A1	1582	C
36	A1	1583	A
36	A1	1587	A
36	A1	1589	A
36	A1	1593	A
36	A1	1607	U
36	A1	1608	C
36	A1	1620	U
36	A1	1629	U
36	A1	1643	A
36	A1	1645	U
36	A1	1655	G
36	A1	1657	C
36	A1	1683	A
36	A1	1705	U
36	A1	1716	U
36	A1	1717	U
36	A1	1724	U
36	A1	1725	C
36	A1	1736	G
36	A1	1742	U
36	A1	1746	U
36	A1	1750	A
36	A1	1751	G
36	A1	1752	A
36	A1	1760	A
36	A1	1761	C
36	A1	1762	C
36	A1	1765	U
36	A1	1766	G
36	A1	1767	C
36	A1	1770	G
36	A1	1779	C
36	A1	1780	G
36	A1	1781	C
36	A1	1797	A
36	A1	1806	A
36	A1	1807	G

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Mol	Chain	Res	Type
36	A1	1809	A
36	A1	1810	A
36	A1	1812	G
36	A1	1814	A
36	A1	1816	A
36	A1	1817	G
36	A1	1818	U
36	A1	1819	U
36	A1	1820	U
36	A1	1821	U
36	A1	1834	U
36	A1	1835	A
36	A1	1836	C
36	A1	1839	A
36	A1	1840	U
36	A1	1841	A
36	A1	1842	A
36	A1	1845	G
36	A1	1846	C
36	A1	1849	C
36	A1	1850	A
36	A1	1855	U
36	A1	1876	U
36	A1	1879	A
36	A1	1880	U
36	A1	1886	A
36	A1	1901	A
36	A1	1905	G
36	A1	1906	G
36	A1	1951	C
36	A1	1952	G
36	A1	1953	G
36	A1	1954	G
36	A1	1955	U
36	A1	2094	C
36	A1	2101	C
36	A1	2102	U
36	A1	2112	U
36	A1	2113	A
36	A1	2114	C
36	A1	2116	G
36	A1	2121	G

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Mol	Chain	Res	Type
36	A1	2122	G
36	A1	2130	G
36	A1	2131	A
36	A1	2140	U
36	A1	2148	U
36	A1	2158	A
36	A1	2163	C
36	A1	2169	G
36	A1	2170	U
36	A1	2187	G
36	A1	2188	A
36	A1	2193	U
36	A1	2201	G
36	A1	2205	U
36	A1	2206	G
36	A1	2208	A
36	A1	2209	U
36	A1	2210	G
36	A1	2213	A
36	A1	2223	A
36	A1	2228	A
36	A1	2244	A
36	A1	2249	G
36	A1	2250	G
36	A1	2252	A
36	A1	2253	G
36	A1	2255	A
36	A1	2256	A
36	A1	2262	A
36	A1	2263	C
36	A1	2272	G
36	A1	2273	G
36	A1	2278	C
36	A1	2281	A
36	A1	2282	U
36	A1	2283	G
36	A1	2284	C
36	A1	2288	G
36	A1	2291	A
36	A1	2293	C
36	A1	2299	A
36	A1	2304	C

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Mol	Chain	Res	Type
36	A1	2307	G
36	A1	2310	U
36	A1	2313	A
36	A1	2314	U
36	A1	2315	G
36	A1	2319	U
36	A1	2330	C
36	A1	2336	U
36	A1	2360	C
36	A1	2374	C
36	A1	2375	G
36	A1	2378	C
36	A1	2385	G
36	A1	2388	U
36	A1	2393	G
36	A1	2397	A
36	A1	2398	A
36	A1	2401	A
36	A1	2402	A
36	A1	2403	G
36	A1	2404	A
36	A1	2405	C
36	A1	2406	C
36	A1	2411	U
36	A1	2418	G
36	A1	2419	A
36	A1	2435	G
36	A1	2437	G
36	A1	2443	A
36	A1	2444	C
36	A1	2445	A
36	A1	2502	A
36	A1	2503	G
36	A1	2504	U
36	A1	2505	U
36	A1	2507	C
36	A1	2511	A
36	A1	2513	U
36	A1	2514	U
36	A1	2515	A
36	A1	2522	G
36	A1	2523	A

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Mol	Chain	Res	Type
36	A1	2525	G
36	A1	2526	C
36	A1	2529	A
36	A1	2531	C
36	A1	2532	U
36	A1	2533	G
36	A1	2534	G
36	A1	2537	U
36	A1	2538	U
36	A1	2539	C
36	A1	2540	A
36	A1	2541	U
36	A1	2542	U
36	A1	2543	U
36	A1	2545	C
36	A1	2547	A
36	A1	2548	C
36	A1	2549	G
36	A1	2552	C
36	A1	2553	U
36	A1	2554	A
36	A1	2555	G
36	A1	2561	A
36	A1	2568	C
36	A1	2569	A
36	A1	2570	U
36	A1	2571	U
36	A1	2572	C
36	A1	2573	G
36	A1	2576	G
36	A1	2581	U
36	A1	2582	C
36	A1	2585	G
36	A1	2586	G
36	A1	2593	A
36	A1	2594	C
36	A1	2606	G
36	A1	2607	G
36	A1	2614	G
36	A1	2626	A
36	A1	2637	A
36	A1	2652	U

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Mol	Chain	Res	Type
36	A1	2656	A
36	A1	2672	G
36	A1	2674	A
36	A1	2677	G
36	A1	2681	U
36	A1	2689	A
36	A1	2690	G
36	A1	2691	A
36	A1	2693	C
36	A1	2694	A
36	A1	2696	A
36	A1	2699	G
36	A1	2705	A
36	A1	2709	C
36	A1	2714	G
36	A1	2728	G
36	A1	2729	U
36	A1	2752	U
36	A1	2753	G
36	A1	2762	A
36	A1	2771	U
36	A1	2772	C
36	A1	2777	G
36	A1	2778	G
36	A1	2779	A
36	A1	2796	G
36	A1	2799	A
36	A1	2800	G
36	A1	2801	A
36	A1	2810	C
36	A1	2816	G
36	A1	2817	A
36	A1	2818	U
36	A1	2819	A
36	A1	2829	U
36	A1	2842	U
36	A1	2843	U
36	A1	2845	A
36	A1	2849	C
36	A1	2860	U
36	A1	2867	C
36	A1	2871	G

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Mol	Chain	Res	Type
36	A1	2872	A
36	A1	2873	U
36	A1	2875	U
36	A1	2878	G
36	A1	2879	C
36	A1	2882	U
36	A1	2887	A
36	A1	2889	C
36	A1	2896	A
36	A1	2897	A
36	A1	2898	G
36	A1	2899	C
36	A1	2914	G
36	A1	2923	U
36	A1	2927	C
36	A1	2935	U
36	A1	2936	A
36	A1	2937	G
36	A1	2942	C
36	A1	2945	G
36	A1	2947	G
36	A1	2957	G
36	A1	2971	A
36	A1	2983	C
36	A1	2990	G
36	A1	2992	U
36	A1	2996	U
36	A1	2997	G
36	A1	3006	A
36	A1	3012	A
36	A1	3056	U
36	A1	3057	U
36	A1	3058	U
36	A1	3059	G
36	A1	3078	U
36	A1	3079	U
36	A1	3086	A
36	A1	3087	A
36	A1	3092	C
36	A1	3113	A
36	A1	3119	U
36	A1	3122	A

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Mol	Chain	Res	Type
36	A1	3130	A
36	A1	3131	U
36	A1	3139	A
36	A1	3142	A
36	A1	3143	C
36	A1	3151	U
36	A1	3153	U
36	A1	3154	C
36	A1	3155	U
36	A1	3156	U
36	A1	3157	U
36	A1	3164	C
36	A1	3165	A
36	A1	3168	A
36	A1	3169	U
36	A1	3170	A
36	A1	3171	U
36	A1	3173	G
36	A1	3174	A
36	A1	3176	G
36	A1	3179	U
36	A1	3181	C
36	A1	3185	U
36	A1	3187	A
36	A1	3196	U
36	A1	3197	G
36	A1	3198	U
36	A1	3199	G
36	A1	3207	U
36	A1	3209	A
36	A1	3210	A
36	A1	3217	C
36	A1	3218	A
36	A1	3219	G
36	A1	3223	A
36	A1	3228	C
36	A1	3229	G
36	A1	3235	C
36	A1	3238	G
36	A1	3239	G
36	A1	3242	G
36	A1	3243	A

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Mol	Chain	Res	Type
36	A1	3245	A
36	A1	3246	G
36	A1	3247	G
36	A1	3253	G
36	A1	3256	G
36	A1	3259	U
36	A1	3265	C
36	A1	3269	U
36	A1	3270	U
36	A1	3272	C
36	A1	3273	A
36	A1	3276	G
36	A1	3279	A
36	A1	3281	U
36	A1	3286	G
36	A1	3287	U
36	A1	3289	G
36	A1	3294	A
36	A1	3295	A
36	A1	3303	G
36	A1	3304	U
36	A1	3307	A
36	A1	3313	U
36	A1	3316	A
36	A1	3317	U
36	A1	3318	G
36	A1	3319	U
36	A1	3320	A
36	A1	3328	G
36	A1	3330	A
36	A1	3331	U
36	A1	3332	U
36	A1	3333	G
36	A1	3335	A
36	A1	3336	A
36	A1	3341	U
36	A1	3342	A
36	A1	3345	G
36	A1	3347	A
36	A1	3348	G
36	A1	3349	C
36	A1	3350	C

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Mol	Chain	Res	Type
36	A1	3351	U
36	A1	3352	U
36	A1	3353	G
36	A1	3354	U
36	A1	3355	U
36	A1	3356	G
36	A1	3369	G
36	A1	3375	A
36	A1	3376	A
36	A1	3378	C
36	A1	3382	U
36	A1	3383	G
36	A1	3389	U
36	A1	3396	U
37	A3	7	G
37	A3	13	A
37	A3	14	U
37	A3	21	G
37	A3	22	A
37	A3	26	C
37	A3	42	A
37	A3	45	A
37	A3	51	A
37	A3	53	U
37	A3	54	U
37	A3	65	G
37	A3	73	C
37	A3	74	C
37	A3	76	A
37	A3	91	G
37	A3	95	A
37	A3	102	A
37	A3	103	A
37	A3	110	G
37	A3	112	G
37	A3	115	G
38	A4	34	U
38	A4	35	C
38	A4	47	C
38	A4	48	A
38	A4	51	G
38	A4	52	A

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Mol	Chain	Res	Type
38	A4	53	A
38	A4	59	A
38	A4	62	C
38	A4	63	G
38	A4	77	A
38	A4	79	A
38	A4	80	A
38	A4	81	U
38	A4	82	U
38	A4	83	C
38	A4	84	C
38	A4	85	G
38	A4	86	U
38	A4	87	G
38	A4	90	U
38	A4	92	A
38	A4	93	U
38	A4	95	G
38	A4	104	A
38	A4	106	C
38	A4	111	A
38	A4	113	U
38	A4	125	U
38	A4	126	A
38	A4	127	U
38	A4	128	U
38	A4	138	A
38	A4	151	C
38	A4	152	G
38	A4	155	A
38	A4	157	U
38	A4	158	U
80	A6	2	A
80	A6	4	C
80	A6	13	C
80	A6	17	C
80	A6	24	U
80	A6	25	C
80	A6	26	A
80	A6	27	U
80	A6	34	G
80	A6	42	G

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Mol	Chain	Res	Type
80	A6	47	A
80	A6	57	G
80	A6	60	U
80	A6	67	A
80	A6	68	A
80	A6	69	G
80	A6	72	A
80	A6	73	U
80	A6	74	U
80	A6	75	U
80	A6	76	A
80	A6	77	U
80	A6	101	U
80	A6	104	A
80	A6	111	U
80	A6	114	C
80	A6	115	G
80	A6	132	U
80	A6	137	U
80	A6	138	A
80	A6	140	A
80	A6	141	U
80	A6	144	U
80	A6	145	A
80	A6	146	U
80	A6	153	G
80	A6	158	U
80	A6	159	U
80	A6	161	U
80	A6	166	C
80	A6	175	G
80	A6	178	U
80	A6	179	A
80	A6	182	A
80	A6	184	C
80	A6	185	U
80	A6	187	G
80	A6	188	A
80	A6	190	C
80	A6	191	C
80	A6	192	U
80	A6	193	U

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Mol	Chain	Res	Type
80	A6	194	U
80	A6	195	G
80	A6	196	G
80	A6	197	A
80	A6	198	A
80	A6	199	G
80	A6	200	A
80	A6	215	A
80	A6	216	U
80	A6	217	A
80	A6	218	A
80	A6	219	A
80	A6	220	A
80	A6	221	A
80	A6	222	A
80	A6	226	A
80	A6	227	U
80	A6	228	G
80	A6	229	U
80	A6	230	C
80	A6	231	U
80	A6	232	U
80	A6	233	C
80	A6	234	G
80	A6	235	G
80	A6	238	U
80	A6	240	U
80	A6	241	U
80	A6	249	U
80	A6	250	C
80	A6	260	U
80	A6	261	U
80	A6	262	U
80	A6	265	A
80	A6	268	C
80	A6	271	A
80	A6	272	U
80	A6	273	G
80	A6	275	C
80	A6	277	U
80	A6	278	U
80	A6	280	U

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Mol	Chain	Res	Type
80	A6	281	G
80	A6	283	U
80	A6	287	G
80	A6	299	A
80	A6	301	A
80	A6	308	C
80	A6	314	C
80	A6	316	A
80	A6	319	U
80	A6	320	U
80	A6	321	C
80	A6	322	G
80	A6	323	A
80	A6	325	G
80	A6	337	G
80	A6	338	C
80	A6	341	A
80	A6	352	A
80	A6	359	A
80	A6	360	A
80	A6	361	C
80	A6	381	C
80	A6	393	C
80	A6	396	G
80	A6	400	A
80	A6	401	A
80	A6	402	C
80	A6	404	G
80	A6	416	A
80	A6	418	G
80	A6	424	C
80	A6	425	A
80	A6	426	G
80	A6	434	G
80	A6	439	U
80	A6	444	C
80	A6	446	A
80	A6	448	C
80	A6	454	U
80	A6	464	A
80	A6	468	A
80	A6	469	C

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Mol	Chain	Res	Type
80	A6	470	A
80	A6	475	A
80	A6	477	A
80	A6	480	G
80	A6	484	C
80	A6	486	G
80	A6	487	G
80	A6	488	G
80	A6	489	C
80	A6	490	C
80	A6	492	A
80	A6	493	U
80	A6	494	U
80	A6	495	C
80	A6	496	G
80	A6	497	G
80	A6	500	C
80	A6	501	U
80	A6	503	G
80	A6	504	U
80	A6	505	A
80	A6	506	A
80	A6	508	U
80	A6	510	G
80	A6	511	A
80	A6	512	A
80	A6	513	U
80	A6	515	A
80	A6	519	C
80	A6	527	A
80	A6	532	U
80	A6	535	A
80	A6	538	A
80	A6	539	G
80	A6	540	G
80	A6	541	A
80	A6	542	A
80	A6	543	C
80	A6	544	A
80	A6	548	G
80	A6	555	A
80	A6	556	A

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Mol	Chain	Res	Type
80	A6	557	G
80	A6	558	U
80	A6	559	C
80	A6	565	C
80	A6	566	C
80	A6	570	A
80	A6	574	G
80	A6	578	U
80	A6	579	A
80	A6	580	A
80	A6	582	U
80	A6	594	A
80	A6	595	G
80	A6	597	G
80	A6	609	U
80	A6	610	G
80	A6	617	U
80	A6	619	A
80	A6	620	A
80	A6	621	A
80	A6	622	A
80	A6	623	A
80	A6	630	A
80	A6	637	C
80	A6	639	U
80	A6	640	U
80	A6	645	C
80	A6	648	G
80	A6	651	G
80	A6	652	G
80	A6	653	C
80	A6	654	C
80	A6	655	G
80	A6	658	C
80	A6	676	G
80	A6	678	A
80	A6	679	U
80	A6	680	U
80	A6	681	U
80	A6	682	C
80	A6	683	C
80	A6	684	A

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Mol	Chain	Res	Type
80	A6	688	G
80	A6	691	C
80	A6	695	U
80	A6	696	C
80	A6	697	C
80	A6	698	U
80	A6	706	A
80	A6	710	U
80	A6	711	U
80	A6	714	G
80	A6	718	U
80	A6	719	U
80	A6	720	G
80	A6	721	U
80	A6	722	G
80	A6	723	G
80	A6	726	C
80	A6	730	G
80	A6	733	A
80	A6	734	A
80	A6	735	C
80	A6	742	U
80	A6	747	C
80	A6	751	G
80	A6	753	A
80	A6	754	A
80	A6	755	A
80	A6	756	A
80	A6	765	G
80	A6	766	U
80	A6	774	A
80	A6	775	G
80	A6	780	A
80	A6	781	U
80	A6	782	U
80	A6	783	G
80	A6	787	G
80	A6	789	A
80	A6	792	U
80	A6	793	A
80	A6	794	U
80	A6	806	A

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Mol	Chain	Res	Type
80	A6	811	A
80	A6	812	A
80	A6	815	G
80	A6	821	U
80	A6	823	G
80	A6	825	U
80	A6	826	U
80	A6	829	A
80	A6	830	U
80	A6	831	U
80	A6	832	U
80	A6	834	G
80	A6	835	U
80	A6	841	U
80	A6	850	A
80	A6	856	A
80	A6	863	A
80	A6	876	G
80	A6	886	U
80	A6	898	A
80	A6	913	G
80	A6	914	G
80	A6	916	U
80	A6	926	A
80	A6	928	U
80	A6	933	A
80	A6	935	U
80	A6	942	G
80	A6	949	C
80	A6	959	U
80	A6	960	U
80	A6	966	A
80	A6	967	A
80	A6	968	U
80	A6	969	C
80	A6	970	A
80	A6	971	A
80	A6	976	G
80	A6	991	G
80	A6	992	A
80	A6	993	A
80	A6	997	G

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Mol	Chain	Res	Type
80	A6	1004	U
80	A6	1005	A
80	A6	1021	C
80	A6	1026	A
80	A6	1028	C
80	A6	1031	U
80	A6	1039	A
80	A6	1040	G
80	A6	1042	G
80	A6	1052	U
80	A6	1053	G
80	A6	1057	U
80	A6	1058	U
80	A6	1059	U
80	A6	1060	U
80	A6	1061	A
80	A6	1062	A
80	A6	1063	U
80	A6	1066	C
80	A6	1067	C
80	A6	1074	G
80	A6	1082	C
80	A6	1083	G
80	A6	1091	A
80	A6	1092	A
80	A6	1096	C
80	A6	1097	U
80	A6	1098	U
80	A6	1099	U
80	A6	1100	G
80	A6	1101	G
80	A6	1109	G
80	A6	1138	A
80	A6	1139	A
80	A6	1151	A
80	A6	1154	G
80	A6	1158	C
80	A6	1159	C
80	A6	1160	A
80	A6	1162	C
80	A6	1167	G
80	A6	1185	U

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Mol	Chain	Res	Type
80	A6	1193	A
80	A6	1194	A
80	A6	1196	A
80	A6	1197	C
80	A6	1199	G
80	A6	1200	G
80	A6	1202	A
80	A6	1203	A
80	A6	1208	A
80	A6	1217	A
80	A6	1218	G
80	A6	1220	C
80	A6	1221	A
80	A6	1225	U
80	A6	1226	A
80	A6	1228	G
80	A6	1229	G
80	A6	1230	A
80	A6	1231	U
80	A6	1234	A
80	A6	1239	U
80	A6	1240	U
80	A6	1241	G
80	A6	1242	A
80	A6	1243	G
80	A6	1244	A
80	A6	1245	G
80	A6	1246	C
80	A6	1255	G
80	A6	1256	A
80	A6	1257	U
80	A6	1258	U
80	A6	1261	G
80	A6	1262	U
80	A6	1285	U
80	A6	1286	U
80	A6	1288	G
80	A6	1314	U
80	A6	1315	U
80	A6	1316	G
80	A6	1321	A
80	A6	1329	A

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Mol	Chain	Res	Type
80	A6	1331	A
80	A6	1343	U
80	A6	1344	A
80	A6	1345	A
80	A6	1346	A
80	A6	1354	G
80	A6	1361	U
80	A6	1363	U
80	A6	1364	G
80	A6	1371	A
80	A6	1372	U
80	A6	1373	C
80	A6	1379	C
80	A6	1390	U
80	A6	1398	U
80	A6	1399	C
80	A6	1400	A
80	A6	1402	G
80	A6	1413	U
80	A6	1414	U
80	A6	1415	U
80	A6	1425	A
80	A6	1427	A
80	A6	1428	G
80	A6	1429	G
80	A6	1433	G
80	A6	1445	G
80	A6	1446	A
80	A6	1448	G
80	A6	1449	U
80	A6	1457	C
80	A6	1458	G
80	A6	1459	C
80	A6	1461	C
80	A6	1471	A
80	A6	1481	C
80	A6	1482	C
80	A6	1486	G
80	A6	1489	U
80	A6	1490	C
80	A6	1491	U
80	A6	1492	A

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Mol	Chain	Res	Type
80	A6	1493	A
80	A6	1494	C
80	A6	1496	U
80	A6	1497	U
80	A6	1506	G
80	A6	1514	U
80	A6	1515	A
80	A6	1516	A
80	A6	1517	U
80	A6	1521	G
80	A6	1523	G
80	A6	1524	A
80	A6	1531	G
80	A6	1535	U
80	A6	1536	G
80	A6	1537	C
80	A6	1538	U
80	A6	1539	G
80	A6	1540	G
80	A6	1554	U
80	A6	1555	A
80	A6	1557	U
80	A6	1559	A
80	A6	1569	A
80	A6	1573	A
80	A6	1574	G
80	A6	1575	G
80	A6	1582	U
80	A6	1584	G
80	A6	1596	C
80	A6	1601	G
80	A6	1616	G
80	A6	1621	U
80	A6	1634	C
80	A6	1635	A
80	A6	1637	C
80	A6	1638	G
80	A6	1657	U
80	A6	1658	G
80	A6	1665	U
80	A6	1710	U
80	A6	1712	A

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Mol	Chain	Res	Type
80	A6	1715	G
80	A6	1716	C
80	A6	1717	G
80	A6	1723	U
80	A6	1727	G
80	A6	1731	A
80	A6	1736	G
80	A6	1755	A
80	A6	1759	C
80	A6	1760	G
80	A6	1766	A
80	A6	1767	G
80	A6	1769	U
80	A6	1770	U
80	A6	1779	U
80	A6	1780	G
80	A6	1782	A
80	A6	1783	C
80	A6	1784	C
80	A6	1789	G
80	A6	1792	G
80	A6	1793	G
80	A6	1794	A
80	A6	1795	U
80	A6	1796	C
80	A6	1799	U
80	A6	1800	A
36	A5	14	U
36	A5	15	C
36	A5	16	A
36	A5	26	A
36	A5	38	U
36	A5	40	A
36	A5	43	A
36	A5	49	A
36	A5	60	A
36	A5	65	A
36	A5	66	A
36	A5	74	G
36	A5	76	G
36	A5	77	A
36	A5	92	G

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Mol	Chain	Res	Type
36	A5	93	C
36	A5	96	G
36	A5	99	A
36	A5	109	A
36	A5	110	G
36	A5	111	C
36	A5	116	A
36	A5	121	A
36	A5	122	A
36	A5	133	U
36	A5	134	U
36	A5	135	C
36	A5	136	G
36	A5	146	U
36	A5	150	A
36	A5	152	U
36	A5	156	G
36	A5	157	A
36	A5	160	G
36	A5	166	C
36	A5	170	G
36	A5	171	G
36	A5	174	C
36	A5	178	U
36	A5	180	C
36	A5	182	U
36	A5	183	G
36	A5	184	U
36	A5	187	A
36	A5	190	U
36	A5	191	U
36	A5	200	C
36	A5	201	A
36	A5	210	U
36	A5	218	G
36	A5	219	A
36	A5	221	A
36	A5	235	A
36	A5	236	G
36	A5	238	A
36	A5	239	G
36	A5	240	U

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Mol	Chain	Res	Type
36	A5	242	C
36	A5	244	G
36	A5	248	U
36	A5	249	U
36	A5	250	U
36	A5	251	G
36	A5	252	U
36	A5	253	A
36	A5	254	A
36	A5	258	G
36	A5	259	C
36	A5	269	G
36	A5	283	G
36	A5	284	A
36	A5	286	U
36	A5	294	U
36	A5	295	A
36	A5	305	U
36	A5	322	U
36	A5	323	A
36	A5	329	U
36	A5	334	A
36	A5	339	C
36	A5	349	A
36	A5	350	C
36	A5	351	A
36	A5	352	A
36	A5	370	U
36	A5	376	G
36	A5	390	G
36	A5	395	A
36	A5	398	A
36	A5	399	A
36	A5	401	U
36	A5	402	A
36	A5	403	C
36	A5	421	G
36	A5	422	A
36	A5	436	A
36	A5	437	G
36	A5	438	A
36	A5	439	C

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Mol	Chain	Res	Type
36	A5	440	A
36	A5	441	U
36	A5	442	G
36	A5	443	G
36	A5	492	U
36	A5	493	G
36	A5	495	G
36	A5	520	U
36	A5	521	A
36	A5	531	G
36	A5	535	G
36	A5	538	G
36	A5	546	C
36	A5	547	G
36	A5	548	G
36	A5	551	A
36	A5	553	U
36	A5	555	U
36	A5	557	A
36	A5	559	A
36	A5	578	A
36	A5	579	G
36	A5	592	A
36	A5	594	U
36	A5	595	G
36	A5	600	G
36	A5	604	G
36	A5	609	G
36	A5	610	G
36	A5	611	A
36	A5	612	U
36	A5	619	A
36	A5	620	U
36	A5	621	A
36	A5	630	A
36	A5	636	C
36	A5	649	A
36	A5	653	A
36	A5	656	A
36	A5	660	A
36	A5	675	C
36	A5	677	A

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Mol	Chain	Res	Type
36	A5	681	U
36	A5	705	A
36	A5	708	G
36	A5	712	G
36	A5	715	A
36	A5	716	A
36	A5	719	U
36	A5	720	A
36	A5	725	G
36	A5	726	G
36	A5	735	A
36	A5	736	A
36	A5	750	G
36	A5	758	C
36	A5	766	U
36	A5	767	U
36	A5	768	C
36	A5	776	U
36	A5	777	U
36	A5	780	A
36	A5	781	G
36	A5	785	G
36	A5	786	A
36	A5	806	A
36	A5	809	G
36	A5	817	A
36	A5	830	A
36	A5	846	A
36	A5	851	C
36	A5	861	C
36	A5	862	U
36	A5	871	U
36	A5	874	U
36	A5	879	U
36	A5	891	G
36	A5	893	C
36	A5	896	A
36	A5	897	U
36	A5	907	G
36	A5	908	G
36	A5	914	A
36	A5	916	G

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Mol	Chain	Res	Type
36	A5	917	A
36	A5	921	A
36	A5	923	C
36	A5	924	G
36	A5	937	G
36	A5	944	C
36	A5	946	U
36	A5	947	G
36	A5	958	C
36	A5	959	C
36	A5	960	U
36	A5	974	G
36	A5	979	U
36	A5	980	A
36	A5	981	U
36	A5	983	A
36	A5	994	G
36	A5	1000	C
36	A5	1001	G
36	A5	1002	A
36	A5	1003	A
36	A5	1010	G
36	A5	1014	U
36	A5	1015	U
36	A5	1016	C
36	A5	1017	C
36	A5	1018	G
36	A5	1020	G
36	A5	1021	G
36	A5	1023	C
36	A5	1024	G
36	A5	1025	A
36	A5	1026	A
36	A5	1027	A
36	A5	1028	U
36	A5	1029	G
36	A5	1032	C
36	A5	1034	U
36	A5	1035	G
36	A5	1047	A
36	A5	1049	C
36	A5	1057	A

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Mol	Chain	Res	Type
36	A5	1064	A
36	A5	1065	A
36	A5	1071	U
36	A5	1072	G
36	A5	1081	U
36	A5	1082	U
36	A5	1085	A
36	A5	1093	A
36	A5	1094	U
36	A5	1095	U
36	A5	1096	U
36	A5	1097	G
36	A5	1098	A
36	A5	1103	A
36	A5	1104	G
36	A5	1117	G
36	A5	1131	G
36	A5	1153	A
36	A5	1159	A
36	A5	1160	C
36	A5	1174	G
36	A5	1178	G
36	A5	1179	A
36	A5	1180	A
36	A5	1181	U
36	A5	1182	A
36	A5	1191	U
36	A5	1192	C
36	A5	1193	A
36	A5	1201	C
36	A5	1209	G
36	A5	1213	G
36	A5	1222	G
36	A5	1223	A
36	A5	1232	C
36	A5	1233	G
36	A5	1236	G
36	A5	1237	G
36	A5	1239	C
36	A5	1241	U
36	A5	1242	G
36	A5	1243	G

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Mol	Chain	Res	Type
36	A5	1245	A
36	A5	1246	G
36	A5	1248	C
36	A5	1258	U
36	A5	1259	A
36	A5	1262	G
36	A5	1263	A
36	A5	1264	G
36	A5	1265	U
36	A5	1266	G
36	A5	1270	A
36	A5	1281	G
36	A5	1285	G
36	A5	1294	A
36	A5	1307	G
36	A5	1308	A
36	A5	1309	U
36	A5	1312	C
36	A5	1330	A
36	A5	1332	A
36	A5	1348	U
36	A5	1349	G
36	A5	1350	A
36	A5	1351	U
36	A5	1352	A
36	A5	1353	U
36	A5	1354	G
36	A5	1355	A
36	A5	1356	U
36	A5	1357	G
36	A5	1366	A
36	A5	1385	C
36	A5	1386	A
36	A5	1387	G
36	A5	1399	A
36	A5	1400	G
36	A5	1403	C
36	A5	1419	A
36	A5	1422	G
36	A5	1428	A
36	A5	1434	G
36	A5	1437	C

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Mol	Chain	Res	Type
36	A5	1440	G
36	A5	1446	A
36	A5	1450	G
36	A5	1460	A
36	A5	1481	A
36	A5	1482	A
36	A5	1490	A
36	A5	1495	U
36	A5	1502	C
36	A5	1503	A
36	A5	1508	C
36	A5	1527	C
36	A5	1541	G
36	A5	1542	G
36	A5	1549	U
36	A5	1554	U
36	A5	1555	U
36	A5	1556	C
36	A5	1557	A
36	A5	1560	G
36	A5	1561	G
36	A5	1562	C
36	A5	1563	C
36	A5	1565	G
36	A5	1566	A
36	A5	1567	U
36	A5	1568	U
36	A5	1569	U
36	A5	1570	U
36	A5	1571	A
36	A5	1572	U
36	A5	1574	C
36	A5	1575	A
36	A5	1576	G
36	A5	1577	G
36	A5	1578	C
36	A5	1580	A
36	A5	1581	C
36	A5	1582	C
36	A5	1583	A
36	A5	1587	A
36	A5	1589	A

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Mol	Chain	Res	Type
36	A5	1593	A
36	A5	1605	A
36	A5	1607	U
36	A5	1608	C
36	A5	1620	U
36	A5	1629	U
36	A5	1633	C
36	A5	1635	G
36	A5	1639	C
36	A5	1641	U
36	A5	1643	A
36	A5	1644	C
36	A5	1645	U
36	A5	1655	G
36	A5	1657	C
36	A5	1680	G
36	A5	1683	A
36	A5	1716	U
36	A5	1717	U
36	A5	1718	G
36	A5	1724	U
36	A5	1725	C
36	A5	1736	G
36	A5	1750	A
36	A5	1751	G
36	A5	1754	G
36	A5	1758	G
36	A5	1760	A
36	A5	1762	C
36	A5	1764	U
36	A5	1765	U
36	A5	1766	G
36	A5	1767	C
36	A5	1770	G
36	A5	1778	G
36	A5	1780	G
36	A5	1783	U
36	A5	1797	A
36	A5	1810	A
36	A5	1812	G
36	A5	1814	A
36	A5	1815	U

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Mol	Chain	Res	Type
36	A5	1816	A
36	A5	1817	G
36	A5	1818	U
36	A5	1820	U
36	A5	1821	U
36	A5	1835	A
36	A5	1841	A
36	A5	1842	A
36	A5	1846	C
36	A5	1849	C
36	A5	1850	A
36	A5	1855	U
36	A5	1871	U
36	A5	1876	U
36	A5	1878	G
36	A5	1879	A
36	A5	1880	U
36	A5	1905	G
36	A5	1906	G
36	A5	1909	A
36	A5	1918	C
36	A5	1927	G
36	A5	1940	G
36	A5	1953	G
36	A5	2100	A
36	A5	2101	C
36	A5	2102	U
36	A5	2112	U
36	A5	2113	A
36	A5	2114	C
36	A5	2121	G
36	A5	2122	G
36	A5	2128	C
36	A5	2131	A
36	A5	2134	G
36	A5	2139	A
36	A5	2144	A
36	A5	2158	A
36	A5	2169	G
36	A5	2170	U
36	A5	2171	G
36	A5	2192	C

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Mol	Chain	Res	Type
36	A5	2201	G
36	A5	2205	U
36	A5	2210	G
36	A5	2213	A
36	A5	2222	A
36	A5	2223	A
36	A5	2228	A
36	A5	2229	A
36	A5	2244	A
36	A5	2250	G
36	A5	2253	G
36	A5	2255	A
36	A5	2256	A
36	A5	2257	C
36	A5	2258	U
36	A5	2264	U
36	A5	2270	A
36	A5	2273	G
36	A5	2276	G
36	A5	2278	C
36	A5	2279	A
36	A5	2288	G
36	A5	2290	C
36	A5	2294	U
36	A5	2298	U
36	A5	2307	G
36	A5	2310	U
36	A5	2313	A
36	A5	2315	G
36	A5	2324	A
36	A5	2329	C
36	A5	2334	U
36	A5	2335	G
36	A5	2336	U
36	A5	2373	A
36	A5	2374	C
36	A5	2375	G
36	A5	2377	G
36	A5	2385	G
36	A5	2388	U
36	A5	2393	G
36	A5	2394	G

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Mol	Chain	Res	Type
36	A5	2396	G
36	A5	2397	A
36	A5	2398	A
36	A5	2400	G
36	A5	2401	A
36	A5	2402	A
36	A5	2403	G
36	A5	2404	A
36	A5	2405	C
36	A5	2406	C
36	A5	2411	U
36	A5	2418	G
36	A5	2435	G
36	A5	2436	U
36	A5	2437	G
36	A5	2438	A
36	A5	2439	A
36	A5	2440	G
36	A5	2441	A
36	A5	2443	A
36	A5	2504	U
36	A5	2505	U
36	A5	2506	U
36	A5	2507	C
36	A5	2508	U
36	A5	2510	U
36	A5	2511	A
36	A5	2512	C
36	A5	2513	U
36	A5	2514	U
36	A5	2515	A
36	A5	2518	C
36	A5	2523	A
36	A5	2524	A
36	A5	2526	C
36	A5	2530	G
36	A5	2531	C
36	A5	2532	U
36	A5	2534	G
36	A5	2538	U
36	A5	2539	C
36	A5	2540	A

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Mol	Chain	Res	Type
36	A5	2543	U
36	A5	2544	U
36	A5	2549	G
36	A5	2552	C
36	A5	2555	G
36	A5	2562	A
36	A5	2567	C
36	A5	2568	C
36	A5	2569	A
36	A5	2570	U
36	A5	2571	U
36	A5	2572	C
36	A5	2573	G
36	A5	2574	G
36	A5	2584	G
36	A5	2585	G
36	A5	2589	G
36	A5	2590	A
36	A5	2591	A
36	A5	2593	A
36	A5	2594	C
36	A5	2598	G
36	A5	2599	U
36	A5	2606	G
36	A5	2607	G
36	A5	2610	G
36	A5	2614	G
36	A5	2615	G
36	A5	2622	C
36	A5	2637	A
36	A5	2639	G
36	A5	2652	U
36	A5	2656	A
36	A5	2662	G
36	A5	2663	G
36	A5	2667	A
36	A5	2674	A
36	A5	2677	G
36	A5	2678	A
36	A5	2681	U
36	A5	2683	U
36	A5	2689	A

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Mol	Chain	Res	Type
36	A5	2691	A
36	A5	2694	A
36	A5	2696	A
36	A5	2714	G
36	A5	2723	U
36	A5	2728	G
36	A5	2729	U
36	A5	2752	U
36	A5	2753	G
36	A5	2762	A
36	A5	2771	U
36	A5	2772	C
36	A5	2773	C
36	A5	2776	C
36	A5	2777	G
36	A5	2778	G
36	A5	2779	A
36	A5	2796	G
36	A5	2799	A
36	A5	2800	G
36	A5	2801	A
36	A5	2810	C
36	A5	2817	A
36	A5	2818	U
36	A5	2819	A
36	A5	2822	U
36	A5	2829	U
36	A5	2839	G
36	A5	2844	C
36	A5	2845	A
36	A5	2853	A
36	A5	2871	G
36	A5	2872	A
36	A5	2873	U
36	A5	2875	U
36	A5	2887	A
36	A5	2889	C
36	A5	2896	A
36	A5	2897	A
36	A5	2898	G
36	A5	2899	C
36	A5	2904	U

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Mol	Chain	Res	Type
36	A5	2910	A
36	A5	2923	U
36	A5	2928	C
36	A5	2935	U
36	A5	2936	A
36	A5	2941	A
36	A5	2942	C
36	A5	2945	G
36	A5	2947	G
36	A5	2954	U
36	A5	2957	G
36	A5	2970	C
36	A5	2971	A
36	A5	2972	G
36	A5	2979	U
36	A5	2983	C
36	A5	2987	A
36	A5	2990	G
36	A5	2996	U
36	A5	2997	G
36	A5	3012	A
36	A5	3028	G
36	A5	3050	U
36	A5	3056	U
36	A5	3057	U
36	A5	3059	G
36	A5	3078	U
36	A5	3079	U
36	A5	3080	G
36	A5	3086	A
36	A5	3087	A
36	A5	3092	C
36	A5	3130	A
36	A5	3131	U
36	A5	3139	A
36	A5	3142	A
36	A5	3143	C
36	A5	3148	U
36	A5	3153	U
36	A5	3154	C
36	A5	3155	U
36	A5	3156	U

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Mol	Chain	Res	Type
36	A5	3157	U
36	A5	3158	G
36	A5	3159	C
36	A5	3164	C
36	A5	3165	A
36	A5	3166	C
36	A5	3168	A
36	A5	3171	U
36	A5	3172	A
36	A5	3173	G
36	A5	3174	A
36	A5	3175	U
36	A5	3176	G
36	A5	3177	G
36	A5	3179	U
36	A5	3180	A
36	A5	3181	C
36	A5	3187	A
36	A5	3195	U
36	A5	3196	U
36	A5	3207	U
36	A5	3217	C
36	A5	3218	A
36	A5	3219	G
36	A5	3222	U
36	A5	3223	A
36	A5	3224	G
36	A5	3227	A
36	A5	3229	G
36	A5	3238	G
36	A5	3245	A
36	A5	3246	G
36	A5	3247	G
36	A5	3251	U
36	A5	3253	G
36	A5	3259	U
36	A5	3260	G
36	A5	3269	U
36	A5	3270	U
36	A5	3273	A
36	A5	3275	U
36	A5	3276	G

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Mol	Chain	Res	Type
36	A5	3277	U
36	A5	3279	A
36	A5	3280	U
36	A5	3282	U
36	A5	3284	G
36	A5	3285	C
36	A5	3286	G
36	A5	3288	G
36	A5	3289	G
36	A5	3290	G
36	A5	3292	A
36	A5	3294	A
36	A5	3304	U
36	A5	3307	A
36	A5	3313	U
36	A5	3316	A
36	A5	3317	U
36	A5	3318	G
36	A5	3319	U
36	A5	3320	A
36	A5	3330	A
36	A5	3333	G
36	A5	3335	A
36	A5	3336	A
36	A5	3341	U
36	A5	3342	A
36	A5	3343	G
36	A5	3345	G
36	A5	3349	C
36	A5	3351	U
36	A5	3352	U
36	A5	3354	U
36	A5	3355	U
36	A5	3356	G
36	A5	3357	U
36	A5	3358	U
36	A5	3369	G
36	A5	3378	C
36	A5	3382	U
36	A5	3383	G
36	A5	3389	U
36	A5	3390	G

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Mol	Chain	Res	Type
36	A5	3393	U
36	A5	3396	U
37	A7	7	G
37	A7	22	A
37	A7	27	A
37	A7	33	U
37	A7	38	U
37	A7	42	A
37	A7	54	U
37	A7	61	G
37	A7	65	G
37	A7	66	A
37	A7	73	C
37	A7	74	C
37	A7	93	C
37	A7	101	G
37	A7	102	A
37	A7	103	A
37	A7	104	A
37	A7	112	G
38	A8	21	C
38	A8	34	U
38	A8	35	C
38	A8	48	A
38	A8	52	A
38	A8	53	A
38	A8	59	A
38	A8	62	C
38	A8	63	G
38	A8	79	A
38	A8	80	A
38	A8	81	U
38	A8	83	C
38	A8	84	C
38	A8	86	U
38	A8	87	G
38	A8	90	U
38	A8	95	G
38	A8	104	A
38	A8	105	A
38	A8	106	C
38	A8	111	A

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Mol	Chain	Res	Type
38	A8	113	U
38	A8	122	U
38	A8	125	U
38	A8	126	A
38	A8	127	U
38	A8	138	A
38	A8	152	G
38	A8	156	U
38	A8	157	U
38	A8	158	U

All (413) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	25	C
1	A2	45	U
1	A2	68	A
1	A2	73	U
1	A2	74	U
1	A2	76	A
1	A2	103	A
1	A2	114	C
1	A2	126	A
1	A2	130	C
1	A2	131	C
1	A2	132	U
1	A2	133	U
1	A2	136	C
1	A2	139	C
1	A2	144	U
1	A2	158	U
1	A2	187	G
1	A2	217	A
1	A2	218	A
1	A2	232	U
1	A2	239	C
1	A2	240	U
1	A2	278	U
1	A2	280	U
1	A2	320	U
1	A2	400	A

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Mol	Chain	Res	Type
1	A2	417	A
1	A2	484	C
1	A2	495	C
1	A2	497	G
1	A2	498	G
1	A2	499	U
1	A2	501	U
1	A2	503	G
1	A2	507	U
1	A2	512	A
1	A2	542	A
1	A2	543	C
1	A2	555	A
1	A2	558	U
1	A2	582	U
1	A2	685	A
1	A2	704	C
1	A2	720	G
1	A2	721	U
1	A2	734	A
1	A2	755	A
1	A2	781	U
1	A2	782	U
1	A2	794	U
1	A2	811	A
1	A2	815	G
1	A2	819	G
1	A2	823	G
1	A2	829	A
1	A2	913	G
1	A2	1051	G
1	A2	1058	U
1	A2	1081	A
1	A2	1137	A
1	A2	1157	A
1	A2	1187	U
1	A2	1195	C
1	A2	1196	A
1	A2	1207	C
1	A2	1226	A
1	A2	1234	A
1	A2	1244	A

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Mol	Chain	Res	Type
1	A2	1250	U
1	A2	1339	C
1	A2	1344	A
1	A2	1370	U
1	A2	1428	G
1	A2	1481	C
1	A2	1489	U
1	A2	1490	C
1	A2	1521	G
1	A2	1568	C
1	A2	1572	G
1	A2	1573	A
1	A2	1615	C
1	A2	1657	U
1	A2	1711	C
1	A2	1761	U
36	A1	13	A
36	A1	43	A
36	A1	65	A
36	A1	99	A
36	A1	169	U
36	A1	210	U
36	A1	223	U
36	A1	239	G
36	A1	282	G
36	A1	397	A
36	A1	439	C
36	A1	517	G
36	A1	547	G
36	A1	558	U
36	A1	588	G
36	A1	594	U
36	A1	619	A
36	A1	620	U
36	A1	637	C
36	A1	648	C
36	A1	715	A
36	A1	719	U
36	A1	726	G
36	A1	763	G
36	A1	764	U
36	A1	816	A

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Mol	Chain	Res	Type
36	A1	873	C
36	A1	896	A
36	A1	908	G
36	A1	916	G
36	A1	979	U
36	A1	981	U
36	A1	993	G
36	A1	1015	U
36	A1	1017	C
36	A1	1064	A
36	A1	1094	U
36	A1	1097	G
36	A1	1103	A
36	A1	1152	G
36	A1	1222	G
36	A1	1241	U
36	A1	1273	A
36	A1	1307	G
36	A1	1317	A
36	A1	1329	U
36	A1	1331	U
36	A1	1352	A
36	A1	1355	A
36	A1	1481	A
36	A1	1484	U
36	A1	1507	G
36	A1	1554	U
36	A1	1556	C
36	A1	1562	C
36	A1	1568	U
36	A1	1580	A
36	A1	1582	C
36	A1	1589	A
36	A1	1607	U
36	A1	1716	U
36	A1	1751	G
36	A1	1778	G
36	A1	1815	U
36	A1	1816	A
36	A1	1820	U
36	A1	1841	A
36	A1	1842	A

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Mol	Chain	Res	Type
36	A1	1846	C
36	A1	1849	C
36	A1	2101	C
36	A1	2112	U
36	A1	2116	G
36	A1	2209	U
36	A1	2227	C
36	A1	2249	G
36	A1	2281	A
36	A1	2372	A
36	A1	2373	A
36	A1	2374	C
36	A1	2403	G
36	A1	2418	G
36	A1	2501	U
36	A1	2513	U
36	A1	2522	G
36	A1	2525	G
36	A1	2537	U
36	A1	2538	U
36	A1	2541	U
36	A1	2552	C
36	A1	2554	A
36	A1	2585	G
36	A1	2593	A
36	A1	2689	A
36	A1	2704	A
36	A1	2728	G
36	A1	2752	U
36	A1	2772	C
36	A1	2801	A
36	A1	2817	A
36	A1	2818	U
36	A1	2867	C
36	A1	2887	A
36	A1	2896	A
36	A1	3056	U
36	A1	3078	U
36	A1	3121	U
36	A1	3139	A
36	A1	3156	U
36	A1	3169	U

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Mol	Chain	Res	Type
36	A1	3195	U
36	A1	3207	U
36	A1	3217	C
36	A1	3218	A
36	A1	3228	C
36	A1	3242	G
36	A1	3269	U
36	A1	3275	U
36	A1	3276	G
36	A1	3316	A
36	A1	3317	U
36	A1	3319	U
36	A1	3330	A
36	A1	3350	C
36	A1	3351	U
36	A1	3353	G
36	A1	3375	A
37	A3	13	A
37	A3	41	G
37	A3	52	G
38	A4	82	U
38	A4	85	G
38	A4	111	A
38	A4	125	U
38	A4	157	U
80	A6	25	C
80	A6	66	U
80	A6	72	A
80	A6	75	U
80	A6	76	A
80	A6	103	A
80	A6	114	C
80	A6	136	C
80	A6	139	C
80	A6	158	U
80	A6	187	G
80	A6	217	A
80	A6	240	U
80	A6	249	U
80	A6	272	U
80	A6	277	U
80	A6	352	A

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Mol	Chain	Res	Type
80	A6	400	A
80	A6	417	A
80	A6	468	A
80	A6	512	A
80	A6	542	A
80	A6	543	C
80	A6	555	A
80	A6	557	G
80	A6	558	U
80	A6	647	G
80	A6	651	G
80	A6	678	A
80	A6	681	U
80	A6	695	U
80	A6	697	C
80	A6	717	C
80	A6	755	A
80	A6	811	A
80	A6	815	G
80	A6	829	A
80	A6	834	G
80	A6	1051	G
80	A6	1058	U
80	A6	1081	A
80	A6	1097	U
80	A6	1098	U
80	A6	1196	A
80	A6	1227	A
80	A6	1238	A
80	A6	1244	A
80	A6	1255	G
80	A6	1344	A
80	A6	1481	C
80	A6	1490	C
80	A6	1491	U
80	A6	1535	U
80	A6	1568	C
80	A6	1572	G
80	A6	1573	A
80	A6	1615	C
80	A6	1620	C
80	A6	1637	C

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Mol	Chain	Res	Type
80	A6	1657	U
36	A5	43	A
36	A5	65	A
36	A5	93	C
36	A5	151	A
36	A5	169	U
36	A5	183	G
36	A5	217	U
36	A5	238	A
36	A5	282	G
36	A5	397	A
36	A5	436	A
36	A5	438	A
36	A5	439	C
36	A5	545	U
36	A5	546	C
36	A5	588	G
36	A5	611	A
36	A5	619	A
36	A5	647	A
36	A5	705	A
36	A5	715	A
36	A5	719	U
36	A5	726	G
36	A5	735	A
36	A5	765	C
36	A5	786	A
36	A5	816	A
36	A5	873	C
36	A5	896	A
36	A5	908	G
36	A5	916	G
36	A5	937	G
36	A5	979	U
36	A5	993	G
36	A5	1027	A
36	A5	1033	U
36	A5	1064	A
36	A5	1081	U
36	A5	1085	A
36	A5	1094	U
36	A5	1152	G

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Mol	Chain	Res	Type
36	A5	1181	U
36	A5	1192	C
36	A5	1222	G
36	A5	1236	G
36	A5	1238	C
36	A5	1239	C
36	A5	1241	U
36	A5	1284	C
36	A5	1307	G
36	A5	1317	A
36	A5	1329	U
36	A5	1331	U
36	A5	1352	A
36	A5	1355	A
36	A5	1434	G
36	A5	1481	A
36	A5	1507	G
36	A5	1514	G
36	A5	1554	U
36	A5	1560	G
36	A5	1568	U
36	A5	1574	C
36	A5	1580	A
36	A5	1589	A
36	A5	1607	U
36	A5	1716	U
36	A5	1724	U
36	A5	1815	U
36	A5	1816	A
36	A5	1817	G
36	A5	1819	U
36	A5	1841	A
36	A5	1842	A
36	A5	1849	C
36	A5	1878	G
36	A5	1879	A
36	A5	2101	C
36	A5	2112	U
36	A5	2116	G
36	A5	2204	C
36	A5	2209	U
36	A5	2249	G

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Mol	Chain	Res	Type
36	A5	2255	A
36	A5	2257	C
36	A5	2372	A
36	A5	2374	C
36	A5	2440	G
36	A5	2507	C
36	A5	2513	U
36	A5	2531	C
36	A5	2537	U
36	A5	2539	C
36	A5	2583	C
36	A5	2585	G
36	A5	2593	A
36	A5	2662	G
36	A5	2682	C
36	A5	2689	A
36	A5	2714	G
36	A5	2728	G
36	A5	2752	U
36	A5	2772	C
36	A5	2777	G
36	A5	2801	A
36	A5	2817	A
36	A5	2818	U
36	A5	2887	A
36	A5	2896	A
36	A5	2970	C
36	A5	2971	A
36	A5	2996	U
36	A5	3056	U
36	A5	3078	U
36	A5	3154	C
36	A5	3155	U
36	A5	3167	A
36	A5	3195	U
36	A5	3218	A
36	A5	3228	C
36	A5	3259	U
36	A5	3269	U
36	A5	3275	U
36	A5	3289	G
36	A5	3317	U

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Mol	Chain	Res	Type
36	A5	3330	A
36	A5	3340	G
36	A5	3341	U
36	A5	3357	U
38	A8	111	A
38	A8	126	A
38	A8	156	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3566 ligands modelled in this entry, 2221 are monoatomic - leaving 1345 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	$\# Z > 2$
86	OHX	CP	201	-	0,6,6	0.00	-	-		
86	OHX	A6	2022	-	0,6,6	0.00	-	-		
86	OHX	A1	3509	-	0,6,6	0.00	-	-		
86	OHX	A1	3800	-	0,6,6	0.00	-	-		
86	OHX	A5	3730	-	0,6,6	0.00	-	-		
86	OHX	A8	218	-	0,6,6	0.00	-	-		
86	OHX	A1	3763	-	0,6,6	0.00	-	-		
86	OHX	A5	3654	-	0,6,6	0.00	-	-		
86	OHX	A1	3510	-	0,6,6	0.00	-	-		
86	OHX	A5	3452	-	0,6,6	0.00	-	-		
86	OHX	A1	3448	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A5	3480	-	0,6,6	0.00	-	-		
86	OHX	A3	212	-	0,6,6	0.00	-	-		
86	OHX	A5	3819	-	0,6,6	0.00	-	-		
86	OHX	A1	3743	-	0,6,6	0.00	-	-		
86	OHX	A6	1924	-	0,6,6	0.00	-	-		
86	OHX	A2	2087	-	0,6,6	0.00	-	-		
86	OHX	A6	1975	-	0,6,6	0.00	-	-		
86	OHX	A1	3482	-	0,6,6	0.00	-	-		
86	OHX	Cd	101	-	0,6,6	0.00	-	-		
86	OHX	A5	3505	-	0,6,6	0.00	-	-		
86	OHX	A5	3507	-	0,6,6	0.00	-	-		
86	OHX	A5	3756	-	0,6,6	0.00	-	-		
86	OHX	A5	3670	-	0,6,6	0.00	-	-		
86	OHX	A1	3644	-	0,6,6	0.00	-	-		
86	OHX	A5	3586	-	0,6,6	0.00	-	-		
86	OHX	A6	2065	-	0,6,6	0.00	-	-		
86	OHX	A1	3440	-	0,6,6	0.00	-	-		
86	OHX	Ag	401	-	0,6,6	0.00	-	-		
86	OHX	A1	3430	-	0,6,6	0.00	-	-		
86	OHX	A7	212	-	0,6,6	0.00	-	-		
86	OHX	A1	3737	-	0,6,6	0.00	-	-		
86	OHX	A8	205	-	0,6,6	0.00	-	-		
86	OHX	A5	3682	-	0,6,6	0.00	-	-		
86	OHX	A5	3437	-	0,6,6	0.00	-	-		
86	OHX	A2	1905	-	0,6,6	0.00	-	-		
86	OHX	A6	2041	-	0,6,6	0.00	-	-		
86	OHX	A1	3692	-	0,6,6	0.00	-	-		
86	OHX	A1	3419	-	0,6,6	0.00	-	-		
86	OHX	A5	3661	-	0,6,6	0.00	-	-		
86	OHX	A2	1936	-	0,6,6	0.00	-	-		
86	OHX	A1	3651	-	0,6,6	0.00	-	-		
86	OHX	A5	3698	-	0,6,6	0.00	-	-		
86	OHX	A5	3765	-	0,6,6	0.00	-	-		
86	OHX	A1	3660	-	0,6,6	0.00	-	-		
86	OHX	A5	3423	-	0,6,6	0.00	-	-		
86	OHX	A5	3695	36	0,6,6	0.00	-	-		
86	OHX	A6	1908	-	0,6,6	0.00	-	-		
86	OHX	A5	3464	-	0,6,6	0.00	-	-		
86	OHX	A5	3580	-	0,6,6	0.00	-	-		
86	OHX	A2	2048	-	0,6,6	0.00	-	-		
86	OHX	A3	211	-	0,6,6	0.00	-	-		
86	OHX	A1	3567	-	0,6,6	0.00	-	-		
86	OHX	A5	3413	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A2	2042	-	0,6,6	0.00	-	-		
86	OHX	A5	3500	-	0,6,6	0.00	-	-		
86	OHX	A5	3785	-	0,6,6	0.00	-	-		
86	OHX	A2	2045	-	0,6,6	0.00	-	-		
86	OHX	A5	3629	-	0,6,6	0.00	-	-		
86	OHX	A1	3505	-	0,6,6	0.00	-	-		
86	OHX	A1	3507	-	0,6,6	0.00	-	-		
86	OHX	A1	3697	-	0,6,6	0.00	-	-		
86	OHX	A5	3565	-	0,6,6	0.00	-	-		
86	OHX	A5	3517	-	0,6,6	0.00	-	-		
86	OHX	A5	3561	-	0,6,6	0.00	-	-		
86	OHX	A5	3764	-	0,6,6	0.00	-	-		
86	OHX	A6	1988	-	0,6,6	0.00	-	-		
86	OHX	A2	2076	-	0,6,6	0.00	-	-		
86	OHX	A5	3783	-	0,6,6	0.00	-	-		
86	OHX	A1	3437	-	0,6,6	0.00	-	-		
86	OHX	A6	2047	-	0,6,6	0.00	-	-		
86	OHX	A6	2004	-	0,6,6	0.00	-	-		
86	OHX	A6	2053	-	0,6,6	0.00	-	-		
86	OHX	A5	3430	-	0,6,6	0.00	-	-		
86	OHX	A1	3678	-	0,6,6	0.00	-	-		
86	OHX	A5	3713	-	0,6,6	0.00	-	-		
86	OHX	A6	1994	-	0,6,6	0.00	-	-		
86	OHX	A5	3810	-	0,6,6	0.00	-	-		
86	OHX	A5	3572	-	0,6,6	0.00	-	-		
86	OHX	A5	3754	-	0,6,6	0.00	-	-		
86	OHX	A2	2008	-	0,6,6	0.00	-	-		
86	OHX	A5	3521	86	0,6,6	0.00	-	-		
86	OHX	A6	2061	-	0,6,6	0.00	-	-		
86	OHX	A5	3420	-	0,6,6	0.00	-	-		
86	OHX	A1	3593	-	0,6,6	0.00	-	-		
86	OHX	A5	3488	-	0,6,6	0.00	-	-		
86	OHX	A1	3539	-	0,6,6	0.00	-	-		
86	OHX	A5	3530	-	0,6,6	0.00	-	-		
86	OHX	A6	2064	-	0,6,6	0.00	-	-		
86	OHX	A1	3503	-	0,6,6	0.00	-	-		
86	OHX	A1	3585	-	0,6,6	0.00	-	-		
86	OHX	A1	3621	-	0,6,6	0.00	-	-		
86	OHX	A2	1977	-	0,6,6	0.00	-	-		
86	OHX	A5	3459	-	0,6,6	0.00	-	-		
86	OHX	A5	3436	-	0,6,6	0.00	-	-		
86	OHX	A6	1914	-	0,6,6	0.00	-	-		
86	OHX	A2	1935	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A2	2011	-	0,6,6	0.00	-	-		
86	OHX	A2	1973	-	0,6,6	0.00	-	-		
86	OHX	A5	3538	-	0,6,6	0.00	-	-		
86	OHX	A5	3704	-	0,6,6	0.00	-	-		
86	OHX	A2	2029	-	0,6,6	0.00	-	-		
86	OHX	A5	3593	-	0,6,6	0.00	-	-		
86	OHX	A2	1968	-	0,6,6	0.00	-	-		
86	OHX	A1	3764	-	0,6,6	0.00	-	-		
86	OHX	A1	3553	-	0,6,6	0.00	-	-		
86	OHX	DC	401	-	0,6,6	0.00	-	-		
86	OHX	A1	3435	-	0,6,6	0.00	-	-		
86	OHX	A4	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3716	-	0,6,6	0.00	-	-		
86	OHX	A4	206	-	0,6,6	0.00	-	-		
86	OHX	A5	3701	-	0,6,6	0.00	-	-		
86	OHX	A6	2094	-	0,6,6	0.00	-	-		
86	OHX	A5	3618	-	0,6,6	0.00	-	-		
86	OHX	A2	1929	-	0,6,6	0.00	-	-		
86	OHX	A6	1910	-	0,6,6	0.00	-	-		
86	OHX	A6	2019	-	0,6,6	0.00	-	-		
86	OHX	A5	3533	-	0,6,6	0.00	-	-		
86	OHX	A6	1996	-	0,6,6	0.00	-	-		
86	OHX	A5	3445	-	0,6,6	0.00	-	-		
86	OHX	A1	3680	-	0,6,6	0.00	-	-		
86	OHX	A5	3477	-	0,6,6	0.00	-	-		
86	OHX	A5	3714	-	0,6,6	0.00	-	-		
86	OHX	A5	3563	-	0,6,6	0.00	-	-		
86	OHX	A1	3806	-	0,6,6	0.00	-	-		
86	OHX	A5	3560	-	0,6,6	0.00	-	-		
86	OHX	A1	3782	-	0,6,6	0.00	-	-		
86	OHX	A8	206	-	0,6,6	0.00	-	-		
86	OHX	CJ	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3794	-	0,6,6	0.00	-	-		
86	OHX	A5	3440	-	0,6,6	0.00	-	-		
86	OHX	A1	3655	-	0,6,6	0.00	-	-		
86	OHX	A2	2034	-	0,6,6	0.00	-	-		
86	OHX	A1	3543	-	0,6,6	0.00	-	-		
86	OHX	A6	1969	-	0,6,6	0.00	-	-		
86	OHX	A2	1993	-	0,6,6	0.00	-	-		
86	OHX	A4	211	-	0,6,6	0.00	-	-		
86	OHX	A2	1963	-	0,6,6	0.00	-	-		
86	OHX	A2	1989	-	0,6,6	0.00	-	-		
86	OHX	A6	1951	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A5	3431	-	0,6,6	0.00	-	-		
86	OHX	A6	2042	-	0,6,6	0.00	-	-		
86	OHX	A5	3799	-	0,6,6	0.00	-	-		
86	OHX	A5	3700	-	0,6,6	0.00	-	-		
86	OHX	A2	2052	-	0,6,6	0.00	-	-		
86	OHX	A1	3716	-	0,6,6	0.00	-	-		
86	OHX	A5	3463	-	0,6,6	0.00	-	-		
86	OHX	Bj	101	-	0,6,6	0.00	-	-		
86	OHX	A5	3599	-	0,6,6	0.00	-	-		
86	OHX	A6	2030	-	0,6,6	0.00	-	-		
86	OHX	A5	3426	-	0,6,6	0.00	-	-		
86	OHX	A6	2089	-	0,6,6	0.00	-	-		
86	OHX	CY	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3609	-	0,6,6	0.00	-	-		
86	OHX	A5	3658	-	0,6,6	0.00	-	-		
86	OHX	A1	3513	-	0,6,6	0.00	-	-		
86	OHX	A1	3724	-	0,6,6	0.00	-	-		
86	OHX	A5	3633	-	0,6,6	0.00	-	-		
86	OHX	A1	3529	-	0,6,6	0.00	-	-		
86	OHX	A5	3717	-	0,6,6	0.00	-	-		
86	OHX	A1	3425	-	0,6,6	0.00	-	-		
86	OHX	A6	2016	-	0,6,6	0.00	-	-		
86	OHX	A1	3789	-	0,6,6	0.00	-	-		
86	OHX	A6	1912	-	0,6,6	0.00	-	-		
86	OHX	A1	3493	-	0,6,6	0.00	-	-		
86	OHX	A1	3623	-	0,6,6	0.00	-	-		
86	OHX	A5	3518	-	0,6,6	0.00	-	-		
86	OHX	A5	3502	-	0,6,6	0.00	-	-		
86	OHX	A6	1902	-	0,6,6	0.00	-	-		
86	OHX	A2	2051	-	0,6,6	0.00	-	-		
86	OHX	A5	3450	-	0,6,6	0.00	-	-		
86	OHX	A1	3638	-	0,6,6	0.00	-	-		
86	OHX	A7	209	-	0,6,6	0.00	-	-		
86	OHX	A6	1930	-	0,6,6	0.00	-	-		
86	OHX	A5	3577	-	0,6,6	0.00	-	-		
86	OHX	A5	3525	-	0,6,6	0.00	-	-		
86	OHX	A1	3711	-	0,6,6	0.00	-	-		
86	OHX	A1	3767	-	0,6,6	0.00	-	-		
86	OHX	A5	3778	-	0,6,6	0.00	-	-		
86	OHX	A5	3731	-	0,6,6	0.00	-	-		
86	OHX	A1	3735	-	0,6,6	0.00	-	-		
86	OHX	A1	3555	-	0,6,6	0.00	-	-		
86	OHX	A2	2057	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A5	3669	-	0,6,6	0.00	-	-		
86	OHX	A5	3564	-	0,6,6	0.00	-	-		
86	OHX	A2	1928	-	0,6,6	0.00	-	-		
86	OHX	A5	3476	-	0,6,6	0.00	-	-		
86	OHX	A6	1986	-	0,6,6	0.00	-	-		
86	OHX	A6	2005	-	0,6,6	0.00	-	-		
86	OHX	A5	3407	-	0,6,6	0.00	-	-		
86	OHX	A5	3481	-	0,6,6	0.00	-	-		
86	OHX	A5	3448	-	0,6,6	0.00	-	-		
86	OHX	A5	3676	-	0,6,6	0.00	-	-		
86	OHX	A6	2062	-	0,6,6	0.00	-	-		
86	OHX	A5	3539	-	0,6,6	0.00	-	-		
86	OHX	A5	3457	86	0,6,6	0.00	-	-		
86	OHX	DP	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3705	-	0,6,6	0.00	-	-		
86	OHX	A6	1959	-	0,6,6	0.00	-	-		
86	OHX	A2	1974	-	0,6,6	0.00	-	-		
86	OHX	A1	3408	-	0,6,6	0.00	-	-		
86	OHX	A2	1946	-	0,6,6	0.00	-	-		
86	OHX	A1	3661	-	0,6,6	0.00	-	-		
86	OHX	A5	3667	-	0,6,6	0.00	-	-		
86	OHX	A5	3462	-	0,6,6	0.00	-	-		
86	OHX	A5	3818	-	0,6,6	0.00	-	-		
86	OHX	A5	3487	-	0,6,6	0.00	-	-		
86	OHX	A2	1978	-	0,6,6	0.00	-	-		
86	OHX	A6	2007	-	0,6,6	0.00	-	-		
86	OHX	A1	3663	-	0,6,6	0.00	-	-		
86	OHX	A1	3579	-	0,6,6	0.00	-	-		
86	OHX	A1	3464	-	0,6,6	0.00	-	-		
86	OHX	A1	3694	-	0,6,6	0.00	-	-		
86	OHX	A1	3564	-	0,6,6	0.00	-	-		
86	OHX	A1	3681	-	0,6,6	0.00	-	-		
86	OHX	A1	3785	-	0,6,6	0.00	-	-		
86	OHX	A1	3809	-	0,6,6	0.00	-	-		
86	OHX	A1	3446	-	0,6,6	0.00	-	-		
86	OHX	A6	2013	-	0,6,6	0.00	-	-		
86	OHX	A1	3608	-	0,6,6	0.00	-	-		
86	OHX	A5	3645	-	0,6,6	0.00	-	-		
86	OHX	A5	3442	-	0,6,6	0.00	-	-		
86	OHX	A1	3461	-	0,6,6	0.00	-	-		
86	OHX	A5	3619	-	0,6,6	0.00	-	-		
86	OHX	A5	3509	-	0,6,6	0.00	-	-		
86	OHX	AN	201	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A2	1909	86	0,6,6	0.00	-	-		
86	OHX	A2	2065	-	0,6,6	0.00	-	-		
86	OHX	A1	3411	-	0,6,6	0.00	-	-		
86	OHX	A1	3793	-	0,6,6	0.00	-	-		
86	OHX	A5	3786	-	0,6,6	0.00	-	-		
86	OHX	A2	1990	-	0,6,6	0.00	-	-		
86	OHX	A5	3800	-	0,6,6	0.00	-	-		
86	OHX	A6	1936	-	0,6,6	0.00	-	-		
86	OHX	A1	3596	-	0,6,6	0.00	-	-		
86	OHX	A2	1907	-	0,6,6	0.00	-	-		
86	OHX	A5	3616	-	0,6,6	0.00	-	-		
86	OHX	A1	3418	-	0,6,6	0.00	-	-		
86	OHX	A2	2054	-	0,6,6	0.00	-	-		
86	OHX	A2	2258	-	0,6,6	0.00	-	-		
86	OHX	CL	201	-	0,6,6	0.00	-	-		
86	OHX	A6	1948	-	0,6,6	0.00	-	-		
86	OHX	A6	1992	-	0,6,6	0.00	-	-		
86	OHX	CY	202	-	0,6,6	0.00	-	-		
86	OHX	A5	3804	-	0,6,6	0.00	-	-		
86	OHX	A1	3768	-	0,6,6	0.00	-	-		
86	OHX	A8	216	-	0,6,6	0.00	-	-		
86	OHX	A5	3482	-	0,6,6	0.00	-	-		
86	OHX	A1	3523	-	0,6,6	0.00	-	-		
86	OHX	A1	3684	-	0,6,6	0.00	-	-		
86	OHX	A6	2045	-	0,6,6	0.00	-	-		
86	OHX	DB	401	-	0,6,6	0.00	-	-		
86	OHX	A5	3724	-	0,6,6	0.00	-	-		
86	OHX	A1	3572	-	0,6,6	0.00	-	-		
86	OHX	A6	1903	-	0,6,6	0.00	-	-		
86	OHX	A6	1983	-	0,6,6	0.00	-	-		
86	OHX	BP	202	-	0,6,6	0.00	-	-		
86	OHX	A1	3536	-	0,6,6	0.00	-	-		
86	OHX	A1	3591	-	0,6,6	0.00	-	-		
86	OHX	A2	1979	-	0,6,6	0.00	-	-		
86	OHX	A5	3737	86	0,6,6	0.00	-	-		
86	OHX	A1	3576	-	0,6,6	0.00	-	-		
86	OHX	A2	1985	-	0,6,6	0.00	-	-		
86	OHX	A5	3684	-	0,6,6	0.00	-	-		
86	OHX	A4	205	-	0,6,6	0.00	-	-		
86	OHX	A1	3765	-	0,6,6	0.00	-	-		
86	OHX	A1	3746	-	0,6,6	0.00	-	-		
86	OHX	A2	2015	-	0,6,6	0.00	-	-		
86	OHX	A2	1988	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A2	1955	-	0,6,6	0.00	-	-		
86	OHX	A5	3725	-	0,6,6	0.00	-	-		
86	OHX	A1	3753	-	0,6,6	0.00	-	-		
86	OHX	A1	3747	-	0,6,6	0.00	-	-		
86	OHX	A6	2034	-	0,6,6	0.00	-	-		
86	OHX	A1	3544	-	0,6,6	0.00	-	-		
86	OHX	A5	3735	-	0,6,6	0.00	-	-		
86	OHX	A6	2048	-	0,6,6	0.00	-	-		
86	OHX	A1	3618	-	0,6,6	0.00	-	-		
86	OHX	A5	3651	-	0,6,6	0.00	-	-		
86	OHX	A5	3573	-	0,6,6	0.00	-	-		
86	OHX	A2	2078	-	0,6,6	0.00	-	-		
86	OHX	A5	3547	-	0,6,6	0.00	-	-		
86	OHX	A5	3660	-	0,6,6	0.00	-	-		
86	OHX	A1	3475	-	0,6,6	0.00	-	-		
86	OHX	A5	3511	-	0,6,6	0.00	-	-		
86	OHX	A1	3741	-	0,6,6	0.00	-	-		
86	OHX	A5	3434	-	0,6,6	0.00	-	-		
86	OHX	A1	3445	-	0,6,6	0.00	-	-		
86	OHX	A1	3532	-	0,6,6	0.00	-	-		
86	OHX	A1	3784	-	0,6,6	0.00	-	-		
86	OHX	A5	3598	-	0,6,6	0.00	-	-		
86	OHX	A1	3455	-	0,6,6	0.00	-	-		
86	OHX	A1	3771	-	0,6,6	0.00	-	-		
86	OHX	A6	2100	-	0,6,6	0.00	-	-		
86	OHX	A1	3468	-	0,6,6	0.00	-	-		
86	OHX	A7	202	-	0,6,6	0.00	-	-		
86	OHX	A1	3560	-	0,6,6	0.00	-	-		
86	OHX	A5	3792	-	0,6,6	0.00	-	-		
86	OHX	A5	3762	-	0,6,6	0.00	-	-		
86	OHX	A5	3652	-	0,6,6	0.00	-	-		
86	OHX	A1	3478	-	0,6,6	0.00	-	-		
86	OHX	A2	1972	-	0,6,6	0.00	-	-		
86	OHX	A6	2027	-	0,6,6	0.00	-	-		
86	OHX	A1	3432	-	0,6,6	0.00	-	-		
86	OHX	A1	3466	-	0,6,6	0.00	-	-		
86	OHX	A8	219	-	0,6,6	0.00	-	-		
86	OHX	A5	3627	-	0,6,6	0.00	-	-		
86	OHX	A1	3687	-	0,6,6	0.00	-	-		
86	OHX	A5	3755	-	0,6,6	0.00	-	-		
86	OHX	A5	3472	-	0,6,6	0.00	-	-		
86	OHX	A5	3678	-	0,6,6	0.00	-	-		
86	OHX	A5	3607	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A4	204	-	0,6,6	0.00	-	-		
86	OHX	A5	3622	-	0,6,6	0.00	-	-		
86	OHX	A5	3489	-	0,6,6	0.00	-	-		
86	OHX	A1	3599	-	0,6,6	0.00	-	-		
86	OHX	A5	3673	-	0,6,6	0.00	-	-		
86	OHX	A1	3434	-	0,6,6	0.00	-	-		
86	OHX	A6	2037	-	0,6,6	0.00	-	-		
86	OHX	A6	2068	-	0,6,6	0.00	-	-		
86	OHX	A5	3620	-	0,6,6	0.00	-	-		
86	OHX	A5	3749	-	0,6,6	0.00	-	-		
86	OHX	A5	3796	-	0,6,6	0.00	-	-		
86	OHX	A1	3519	-	0,6,6	0.00	-	-		
86	OHX	A5	3646	-	0,6,6	0.00	-	-		
86	OHX	A5	3650	-	0,6,6	0.00	-	-		
86	OHX	A6	1916	-	0,6,6	0.00	-	-		
86	OHX	A6	2083	-	0,6,6	0.00	-	-		
86	OHX	A1	3615	-	0,6,6	0.00	-	-		
86	OHX	A6	1963	-	0,6,6	0.00	-	-		
86	OHX	A1	3670	-	0,6,6	0.00	-	-		
86	OHX	A1	3639	-	0,6,6	0.00	-	-		
86	OHX	A5	3781	-	0,6,6	0.00	-	-		
86	OHX	A5	3808	-	0,6,6	0.00	-	-		
86	OHX	A1	3548	-	0,6,6	0.00	-	-		
86	OHX	A1	3738	-	0,6,6	0.00	-	-		
86	OHX	A6	2091	-	0,6,6	0.00	-	-		
86	OHX	A1	3714	-	0,6,6	0.00	-	-		
86	OHX	A5	3550	-	0,6,6	0.00	-	-		
86	OHX	A5	3719	-	0,6,6	0.00	-	-		
86	OHX	A2	2049	-	0,6,6	0.00	-	-		
86	OHX	A1	3666	-	0,6,6	0.00	-	-		
86	OHX	Db	101	-	0,6,6	0.00	-	-		
86	OHX	A5	3484	-	0,6,6	0.00	-	-		
86	OHX	A1	3656	-	0,6,6	0.00	-	-		
86	OHX	A8	204	-	0,6,6	0.00	-	-		
86	OHX	A5	3768	-	0,6,6	0.00	-	-		
86	OHX	A3	204	-	0,6,6	0.00	-	-		
86	OHX	A6	2012	-	0,6,6	0.00	-	-		
86	OHX	A2	1948	-	0,6,6	0.00	-	-		
86	OHX	A5	3536	-	0,6,6	0.00	-	-		
86	OHX	A1	3749	-	0,6,6	0.00	-	-		
86	OHX	A1	3589	-	0,6,6	0.00	-	-		
86	OHX	A1	3629	-	0,6,6	0.00	-	-		
86	OHX	A2	2000	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A6	1942	-	0,6,6	0.00	-	-		
86	OHX	A1	3578	-	0,6,6	0.00	-	-		
86	OHX	A5	3552	-	0,6,6	0.00	-	-		
86	OHX	A1	3460	-	0,6,6	0.00	-	-		
86	OHX	A1	3780	-	0,6,6	0.00	-	-		
86	OHX	A6	1915	-	0,6,6	0.00	-	-		
86	OHX	DM	201	-	0,6,6	0.00	-	-		
86	OHX	A1	3417	-	0,6,6	0.00	-	-		
86	OHX	A1	3646	-	0,6,6	0.00	-	-		
86	OHX	A1	3587	-	0,6,6	0.00	-	-		
86	OHX	A1	3469	-	0,6,6	0.00	-	-		
86	OHX	A1	3588	-	0,6,6	0.00	-	-		
86	OHX	A2	1934	-	0,6,6	0.00	-	-		
86	OHX	A2	2066	-	0,6,6	0.00	-	-		
86	OHX	A2	1941	-	0,6,6	0.00	-	-		
86	OHX	A5	3689	-	0,6,6	0.00	-	-		
86	OHX	A5	3569	-	0,6,6	0.00	-	-		
86	OHX	A1	3577	-	0,6,6	0.00	-	-		
86	OHX	A5	3532	-	0,6,6	0.00	-	-		
86	OHX	A5	3455	-	0,6,6	0.00	-	-		
86	OHX	A1	3490	-	0,6,6	0.00	-	-		
86	OHX	A1	3801	86	0,6,6	0.00	-	-		
86	OHX	A2	2075	-	0,6,6	0.00	-	-		
86	OHX	A1	3754	-	0,6,6	0.00	-	-		
86	OHX	A6	1956	-	0,6,6	0.00	-	-		
86	OHX	A5	3784	-	0,6,6	0.00	-	-		
86	OHX	A2	1951	-	0,6,6	0.00	-	-		
86	OHX	A5	3628	-	0,6,6	0.00	-	-		
86	OHX	A5	3811	-	0,6,6	0.00	-	-		
86	OHX	A5	3540	-	0,6,6	0.00	-	-		
86	OHX	A1	3645	-	0,6,6	0.00	-	-		
86	OHX	A1	3402	-	0,6,6	0.00	-	-		
86	OHX	BI	302	-	0,6,6	0.00	-	-		
86	OHX	A1	3551	-	0,6,6	0.00	-	-		
86	OHX	A6	1974	-	0,6,6	0.00	-	-		
86	OHX	A6	2014	-	0,6,6	0.00	-	-		
86	OHX	A1	3755	-	0,6,6	0.00	-	-		
86	OHX	A5	3433	-	0,6,6	0.00	-	-		
86	OHX	A5	3432	-	0,6,6	0.00	-	-		
86	OHX	A1	3720	-	0,6,6	0.00	-	-		
86	OHX	A2	2080	-	0,6,6	0.00	-	-		
86	OHX	A5	3491	-	0,6,6	0.00	-	-		
86	OHX	A5	3634	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A3	203	-	0,6,6	0.00	-	-		
86	OHX	A5	3612	-	0,6,6	0.00	-	-		
86	OHX	A2	1966	-	0,6,6	0.00	-	-		
86	OHX	A6	1946	-	0,6,6	0.00	-	-		
86	OHX	A5	3740	-	0,6,6	0.00	-	-		
86	OHX	A1	3630	-	0,6,6	0.00	-	-		
86	OHX	A1	3584	-	0,6,6	0.00	-	-		
86	OHX	A4	213	-	0,6,6	0.00	-	-		
86	OHX	A2	2033	86	0,6,6	0.00	-	-		
86	OHX	A1	3561	-	0,6,6	0.00	-	-		
86	OHX	A6	2078	-	0,6,6	0.00	-	-		
86	OHX	A2	1938	-	0,6,6	0.00	-	-		
86	OHX	DC	402	-	0,6,6	0.00	-	-		
86	OHX	A6	2060	-	0,6,6	0.00	-	-		
86	OHX	A6	1964	-	0,6,6	0.00	-	-		
86	OHX	A2	1940	-	0,6,6	0.00	-	-		
86	OHX	A1	3667	-	0,6,6	0.00	-	-		
86	OHX	A5	3456	-	0,6,6	0.00	-	-		
86	OHX	A5	3501	-	0,6,6	0.00	-	-		
86	OHX	A2	2026	-	0,6,6	0.00	-	-		
86	OHX	A5	3738	-	0,6,6	0.00	-	-		
86	OHX	A2	2079	-	0,6,6	0.00	-	-		
86	OHX	A6	2058	-	0,6,6	0.00	-	-		
86	OHX	A6	2054	-	0,6,6	0.00	-	-		
86	OHX	A2	1986	-	0,6,6	0.00	-	-		
86	OHX	A5	3526	-	0,6,6	0.00	-	-		
86	OHX	A1	3586	-	0,6,6	0.00	-	-		
86	OHX	A1	3473	-	0,6,6	0.00	-	-		
86	OHX	A1	3632	-	0,6,6	0.00	-	-		
86	OHX	A6	2000	-	0,6,6	0.00	-	-		
86	OHX	A6	2056	-	0,6,6	0.00	-	-		
86	OHX	A5	3548	-	0,6,6	0.00	-	-		
86	OHX	A5	3761	-	0,6,6	0.00	-	-		
86	OHX	A5	3807	86	0,6,6	0.00	-	-		
86	OHX	A8	210	-	0,6,6	0.00	-	-		
86	OHX	A1	3474	-	0,6,6	0.00	-	-		
86	OHX	A2	1913	-	0,6,6	0.00	-	-		
86	OHX	A6	1907	-	0,6,6	0.00	-	-		
86	OHX	A1	3438	86	0,6,6	0.00	-	-		
86	OHX	A1	3613	-	0,6,6	0.00	-	-		
86	OHX	A5	3790	-	0,6,6	0.00	-	-		
86	OHX	A5	3666	-	0,6,6	0.00	-	-		
86	OHX	A5	3766	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A5	3624	-	0,6,6	0.00	-	-		
86	OHX	A6	1979	-	0,6,6	0.00	-	-		
86	OHX	A1	3740	-	0,6,6	0.00	-	-		
86	OHX	A2	1997	-	0,6,6	0.00	-	-		
86	OHX	A1	3580	-	0,6,6	0.00	-	-		
86	OHX	A1	3674	-	0,6,6	0.00	-	-		
86	OHX	A5	3474	-	0,6,6	0.00	-	-		
86	OHX	A1	3750	-	0,6,6	0.00	-	-		
86	OHX	A5	3441	-	0,6,6	0.00	-	-		
86	OHX	A2	1904	-	0,6,6	0.00	-	-		
86	OHX	A6	2066	-	0,6,6	0.00	-	-		
86	OHX	A6	2044	-	0,6,6	0.00	-	-		
86	OHX	A1	3665	-	0,6,6	0.00	-	-		
86	OHX	A6	1927	-	0,6,6	0.00	-	-		
86	OHX	A6	1991	-	0,6,6	0.00	-	-		
86	OHX	CG	302	-	0,6,6	0.00	-	-		
86	OHX	A5	3478	-	0,6,6	0.00	-	-		
86	OHX	A5	3718	-	0,6,6	0.00	-	-		
86	OHX	A1	3559	-	0,6,6	0.00	-	-		
86	OHX	A1	3518	-	0,6,6	0.00	-	-		
86	OHX	A1	3534	-	0,6,6	0.00	-	-		
86	OHX	A6	1973	-	0,6,6	0.00	-	-		
86	OHX	A1	3514	-	0,6,6	0.00	-	-		
86	OHX	A1	3627	-	0,6,6	0.00	-	-		
86	OHX	A1	3756	-	0,6,6	0.00	-	-		
86	OHX	A1	3472	-	0,6,6	0.00	-	-		
86	OHX	A6	2088	-	0,6,6	0.00	-	-		
86	OHX	A6	2046	-	0,6,6	0.00	-	-		
86	OHX	A6	1968	-	0,6,6	0.00	-	-		
86	OHX	A6	2035	-	0,6,6	0.00	-	-		
86	OHX	A5	3401	-	0,6,6	0.00	-	-		
86	OHX	A5	3822	-	0,6,6	0.00	-	-		
86	OHX	DQ	201	-	0,6,6	0.00	-	-		
86	OHX	A1	3562	-	0,6,6	0.00	-	-		
86	OHX	A6	1987	-	0,6,6	0.00	-	-		
86	OHX	A5	3574	-	0,6,6	0.00	-	-		
86	OHX	A1	3766	-	0,6,6	0.00	-	-		
86	OHX	A6	1901	-	0,6,6	0.00	-	-		
86	OHX	A2	2002	-	0,6,6	0.00	-	-		
86	OHX	A1	3643	-	0,6,6	0.00	-	-		
86	OHX	A5	3490	-	0,6,6	0.00	-	-		
86	OHX	A2	1961	-	0,6,6	0.00	-	-		
86	OHX	A1	3535	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A6	1966	-	0,6,6	0.00	-	-		
86	OHX	A1	3776	-	0,6,6	0.00	-	-		
86	OHX	A1	3581	-	0,6,6	0.00	-	-		
86	OHX	A2	1970	-	0,6,6	0.00	-	-		
86	OHX	A1	3452	-	0,6,6	0.00	-	-		
86	OHX	A3	202	-	0,6,6	0.00	-	-		
86	OHX	A1	3796	-	0,6,6	0.00	-	-		
86	OHX	A5	3746	-	0,6,6	0.00	-	-		
86	OHX	A5	3699	-	0,6,6	0.00	-	-		
86	OHX	A1	3604	-	0,6,6	0.00	-	-		
86	OHX	A6	2076	86	0,6,6	0.00	-	-		
86	OHX	A1	3467	-	0,6,6	0.00	-	-		
86	OHX	A6	1920	-	0,6,6	0.00	-	-		
86	OHX	DJ	201	-	0,6,6	0.00	-	-		
86	OHX	A1	3781	-	0,6,6	0.00	-	-		
86	OHX	A5	3753	-	0,6,6	0.00	-	-		
86	OHX	A1	3511	-	0,6,6	0.00	-	-		
86	OHX	A5	3497	-	0,6,6	0.00	-	-		
86	OHX	A1	3492	-	0,6,6	0.00	-	-		
86	OHX	A6	2077	-	0,6,6	0.00	-	-		
86	OHX	A6	2099	-	0,6,6	0.00	-	-		
86	OHX	A2	1903	-	0,6,6	0.00	-	-		
86	OHX	A5	3600	-	0,6,6	0.00	-	-		
86	OHX	A5	3504	-	0,6,6	0.00	-	-		
86	OHX	A1	3672	-	0,6,6	0.00	-	-		
86	OHX	A6	2026	-	0,6,6	0.00	-	-		
86	OHX	A1	3565	-	0,6,6	0.00	-	-		
86	OHX	A5	3553	-	0,6,6	0.00	-	-		
86	OHX	A5	3435	-	0,6,6	0.00	-	-		
86	OHX	A5	3493	-	0,6,6	0.00	-	-		
86	OHX	A1	3614	-	0,6,6	0.00	-	-		
86	OHX	A5	3444	-	0,6,6	0.00	-	-		
86	OHX	A6	1952	-	0,6,6	0.00	-	-		
86	OHX	A5	3791	-	0,6,6	0.00	-	-		
86	OHX	A6	2011	-	0,6,6	0.00	-	-		
86	OHX	A4	210	-	0,6,6	0.00	-	-		
86	OHX	A1	3520	-	0,6,6	0.00	-	-		
86	OHX	A2	1924	-	0,6,6	0.00	-	-		
86	OHX	A5	3782	-	0,6,6	0.00	-	-		
86	OHX	A5	3597	-	0,6,6	0.00	-	-		
86	OHX	A6	2096	-	0,6,6	0.00	-	-		
86	OHX	A1	3673	-	0,6,6	0.00	-	-		
86	OHX	A5	3815	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A1	3545	-	0,6,6	0.00	-	-		
86	OHX	A1	3422	-	0,6,6	0.00	-	-		
86	OHX	A5	3466	-	0,6,6	0.00	-	-		
86	OHX	A2	2023	-	0,6,6	0.00	-	-		
86	OHX	A2	1923	-	0,6,6	0.00	-	-		
86	OHX	A1	3528	-	0,6,6	0.00	-	-		
86	OHX	A6	2049	-	0,6,6	0.00	-	-		
86	OHX	A1	3732	-	0,6,6	0.00	-	-		
86	OHX	A5	3688	-	0,6,6	0.00	-	-		
86	OHX	A2	2027	-	0,6,6	0.00	-	-		
86	OHX	A5	3595	-	0,6,6	0.00	-	-		
86	OHX	A1	3689	-	0,6,6	0.00	-	-		
86	OHX	A1	3444	-	0,6,6	0.00	-	-		
86	OHX	BI	301	-	0,6,6	0.00	-	-		
86	OHX	BT	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3649	-	0,6,6	0.00	-	-		
86	OHX	DH	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3750	-	0,6,6	0.00	-	-		
86	OHX	A1	3628	-	0,6,6	0.00	-	-		
86	OHX	A1	3540	-	0,6,6	0.00	-	-		
86	OHX	A5	3636	-	0,6,6	0.00	-	-		
86	OHX	A2	1921	-	0,6,6	0.00	-	-		
86	OHX	A1	3420	-	0,6,6	0.00	-	-		
86	OHX	A1	3573	-	0,6,6	0.00	-	-		
86	OHX	A5	3557	-	0,6,6	0.00	-	-		
86	OHX	DD	301	-	0,6,6	0.00	-	-		
86	OHX	A1	3592	-	0,6,6	0.00	-	-		
86	OHX	A5	3568	-	0,6,6	0.00	-	-		
86	OHX	A5	3465	-	0,6,6	0.00	-	-		
86	OHX	A1	3563	-	0,6,6	0.00	-	-		
86	OHX	A4	212	-	0,6,6	0.00	-	-		
86	OHX	A5	3817	-	0,6,6	0.00	-	-		
86	OHX	A6	1934	-	0,6,6	0.00	-	-		
86	OHX	A5	3635	-	0,6,6	0.00	-	-		
86	OHX	A2	2020	-	0,6,6	0.00	-	-		
86	OHX	A1	3677	-	0,6,6	0.00	-	-		
86	OHX	A2	2038	-	0,6,6	0.00	-	-		
86	OHX	A2	1916	-	0,6,6	0.00	-	-		
86	OHX	A1	3728	-	0,6,6	0.00	-	-		
86	OHX	A2	1914	-	0,6,6	0.00	-	-		
86	OHX	A2	2039	-	0,6,6	0.00	-	-		
86	OHX	AP	201	-	0,6,6	0.00	-	-		
86	OHX	A6	2097	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A2	1911	-	0,6,6	0.00	-	-		
86	OHX	A1	3554	-	0,6,6	0.00	-	-		
86	OHX	A2	2086	-	0,6,6	0.00	-	-		
86	OHX	A5	3643	-	0,6,6	0.00	-	-		
86	OHX	A5	3542	-	0,6,6	0.00	-	-		
86	OHX	A1	3552	-	0,6,6	0.00	-	-		
86	OHX	A2	1939	-	0,6,6	0.00	-	-		
86	OHX	A5	3584	-	0,6,6	0.00	-	-		
86	OHX	A1	3810	-	0,6,6	0.00	-	-		
86	OHX	A5	3813	-	0,6,6	0.00	-	-		
86	OHX	A2	1994	-	0,6,6	0.00	-	-		
86	OHX	A1	3537	-	0,6,6	0.00	-	-		
86	OHX	A1	3625	-	0,6,6	0.00	-	-		
86	OHX	A1	3757	-	0,6,6	0.00	-	-		
86	OHX	A6	1984	-	0,6,6	0.00	-	-		
86	OHX	A8	212	-	0,6,6	0.00	-	-		
86	OHX	A1	3742	-	0,6,6	0.00	-	-		
86	OHX	A5	3460	-	0,6,6	0.00	-	-		
86	OHX	A7	204	-	0,6,6	0.00	-	-		
86	OHX	A1	3616	-	0,6,6	0.00	-	-		
86	OHX	A5	3664	-	0,6,6	0.00	-	-		
86	OHX	A6	1917	-	0,6,6	0.00	-	-		
86	OHX	A5	3653	-	0,6,6	0.00	-	-		
86	OHX	A2	2064	-	0,6,6	0.00	-	-		
86	OHX	A5	3615	-	0,6,6	0.00	-	-		
86	OHX	A1	3570	-	0,6,6	0.00	-	-		
86	OHX	A1	3671	-	0,6,6	0.00	-	-		
86	OHX	A1	3526	-	0,6,6	0.00	-	-		
86	OHX	A6	2057	-	0,6,6	0.00	-	-		
86	OHX	A5	3523	-	0,6,6	0.00	-	-		
86	OHX	A1	3761	-	0,6,6	0.00	-	-		
86	OHX	A5	3742	-	0,6,6	0.00	-	-		
86	OHX	A2	2012	-	0,6,6	0.00	-	-		
86	OHX	A5	3797	-	0,6,6	0.00	-	-		
86	OHX	A3	206	-	0,6,6	0.00	-	-		
86	OHX	A3	213	-	0,6,6	0.00	-	-		
86	OHX	A5	3496	-	0,6,6	0.00	-	-		
86	OHX	A2	2001	-	0,6,6	0.00	-	-		
86	OHX	A2	2036	-	0,6,6	0.00	-	-		
86	OHX	A5	3470	86	0,6,6	0.00	-	-		
86	OHX	A5	3656	-	0,6,6	0.00	-	-		
86	OHX	A5	3498	-	0,6,6	0.00	-	-		
86	OHX	BB	401	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A5	3694	-	0,6,6	0.00	-	-		
86	OHX	A6	1981	-	0,6,6	0.00	-	-		
86	OHX	CG	301	-	0,6,6	0.00	-	-		
86	OHX	A5	3495	-	0,6,6	0.00	-	-		
86	OHX	A1	3779	-	0,6,6	0.00	-	-		
86	OHX	A5	3446	-	0,6,6	0.00	-	-		
86	OHX	A5	3677	-	0,6,6	0.00	-	-		
86	OHX	A1	3491	-	0,6,6	0.00	-	-		
86	OHX	A1	3451	-	0,6,6	0.00	-	-		
86	OHX	A1	3590	-	0,6,6	0.00	-	-		
86	OHX	A6	2017	-	0,6,6	0.00	-	-		
86	OHX	A5	3610	-	0,6,6	0.00	-	-		
86	OHX	A1	3442	-	0,6,6	0.00	-	-		
86	OHX	A7	208	-	0,6,6	0.00	-	-		
86	OHX	A1	3634	-	0,6,6	0.00	-	-		
86	OHX	A1	3612	-	0,6,6	0.00	-	-		
86	OHX	A5	3458	-	0,6,6	0.00	-	-		
86	OHX	A5	3814	-	0,6,6	0.00	-	-		
86	OHX	A2	1932	-	0,6,6	0.00	-	-		
86	OHX	A1	3462	-	0,6,6	0.00	-	-		
86	OHX	A7	213	-	0,6,6	0.00	-	-		
86	OHX	CB	301	-	0,6,6	0.00	-	-		
86	OHX	A5	3723	-	0,6,6	0.00	-	-		
86	OHX	A5	3581	-	0,6,6	0.00	-	-		
86	OHX	A5	3777	-	0,6,6	0.00	-	-		
86	OHX	A1	3719	-	0,6,6	0.00	-	-		
86	OHX	A1	3699	-	0,6,6	0.00	-	-		
86	OHX	A6	1997	-	0,6,6	0.00	-	-		
86	OHX	A5	3732	36	0,6,6	0.00	-	-		
86	OHX	A1	3456	-	0,6,6	0.00	-	-		
86	OHX	A6	2038	-	0,6,6	0.00	-	-		
86	OHX	A2	2014	-	0,6,6	0.00	-	-		
86	OHX	A5	3588	-	0,6,6	0.00	-	-		
86	OHX	A2	2030	-	0,6,6	0.00	-	-		
86	OHX	A1	3727	-	0,6,6	0.00	-	-		
86	OHX	A1	3787	-	0,6,6	0.00	-	-		
86	OHX	A4	203	-	0,6,6	0.00	-	-		
86	OHX	A1	3788	-	0,6,6	0.00	-	-		
86	OHX	A1	3610	-	0,6,6	0.00	-	-		
86	OHX	A2	2084	-	0,6,6	0.00	-	-		
86	OHX	A6	2006	-	0,6,6	0.00	-	-		
86	OHX	A6	1999	-	0,6,6	0.00	-	-		
86	OHX	A1	3708	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A1	3575	-	0,6,6	0.00	-	-		
86	OHX	A1	3601	-	0,6,6	0.00	-	-		
86	OHX	A6	2084	-	0,6,6	0.00	-	-		
86	OHX	A5	3554	-	0,6,6	0.00	-	-		
86	OHX	A5	3576	-	0,6,6	0.00	-	-		
86	OHX	A6	2063	-	0,6,6	0.00	-	-		
86	OHX	A5	3747	-	0,6,6	0.00	-	-		
86	OHX	A5	3544	-	0,6,6	0.00	-	-		
86	OHX	A6	2008	-	0,6,6	0.00	-	-		
86	OHX	A6	2001	-	0,6,6	0.00	-	-		
86	OHX	A1	3436	-	0,6,6	0.00	-	-		
86	OHX	A1	3453	-	0,6,6	0.00	-	-		
86	OHX	A1	3598	-	0,6,6	0.00	-	-		
86	OHX	A5	3763	-	0,6,6	0.00	-	-		
86	OHX	A2	2056	-	0,6,6	0.00	-	-		
86	OHX	A2	2077	-	0,6,6	0.00	-	-		
86	OHX	A1	3424	-	0,6,6	0.00	-	-		
86	OHX	A1	3808	-	0,6,6	0.00	-	-		
86	OHX	A5	3537	-	0,6,6	0.00	-	-		
86	OHX	A6	1980	-	0,6,6	0.00	-	-		
86	OHX	A5	3757	-	0,6,6	0.00	-	-		
86	OHX	Bj	103	-	0,6,6	0.00	-	-		
86	OHX	A5	3771	-	0,6,6	0.00	-	-		
86	OHX	A1	3479	-	0,6,6	0.00	-	-		
86	OHX	A6	2015	-	0,6,6	0.00	-	-		
86	OHX	A5	3626	-	0,6,6	0.00	-	-		
86	OHX	A1	3401	-	0,6,6	0.00	-	-		
86	OHX	A2	2007	-	0,6,6	0.00	-	-		
86	OHX	A5	3468	-	0,6,6	0.00	-	-		
86	OHX	A2	2025	-	0,6,6	0.00	-	-		
86	OHX	A6	2043	-	0,6,6	0.00	-	-		
86	OHX	A5	3644	-	0,6,6	0.00	-	-		
86	OHX	A6	2069	-	0,6,6	0.00	-	-		
86	OHX	DB	402	-	0,6,6	0.00	-	-		
86	OHX	A6	2095	-	0,6,6	0.00	-	-		
86	OHX	A1	3759	-	0,6,6	0.00	-	-		
86	OHX	A5	3631	-	0,6,6	0.00	-	-		
86	OHX	A1	3685	-	0,6,6	0.00	-	-		
86	OHX	A1	3709	-	0,6,6	0.00	-	-		
86	OHX	A2	1959	-	0,6,6	0.00	-	-		
86	OHX	A2	1991	-	0,6,6	0.00	-	-		
86	OHX	A1	3657	-	0,6,6	0.00	-	-		
86	OHX	A5	3776	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A6	2092	-	0,6,6	0.00	-	-		
86	OHX	A2	2004	-	0,6,6	0.00	-	-		
86	OHX	A5	3648	-	0,6,6	0.00	-	-		
86	OHX	A5	3485	-	0,6,6	0.00	-	-		
86	OHX	A5	3419	-	0,6,6	0.00	-	-		
86	OHX	A1	3494	-	0,6,6	0.00	-	-		
86	OHX	A1	3423	-	0,6,6	0.00	-	-		
86	OHX	A5	3721	-	0,6,6	0.00	-	-		
86	OHX	A1	3649	-	0,6,6	0.00	-	-		
86	OHX	A5	3404	-	0,6,6	0.00	-	-		
86	OHX	A2	2046	-	0,6,6	0.00	-	-		
86	OHX	A2	2035	-	0,6,6	0.00	-	-		
86	OHX	CP	202	-	0,6,6	0.00	-	-		
86	OHX	A5	3541	-	0,6,6	0.00	-	-		
86	OHX	A5	3519	-	0,6,6	0.00	-	-		
86	OHX	A2	2070	-	0,6,6	0.00	-	-		
86	OHX	A6	1926	-	0,6,6	0.00	-	-		
86	OHX	A1	3799	-	0,6,6	0.00	-	-		
86	OHX	A6	1931	-	0,6,6	0.00	-	-		
86	OHX	A6	1950	-	0,6,6	0.00	-	-		
86	OHX	A1	3733	-	0,6,6	0.00	-	-		
86	OHX	A2	1901	-	0,6,6	0.00	-	-		
86	OHX	A1	3647	-	0,6,6	0.00	-	-		
86	OHX	A5	3639	-	0,6,6	0.00	-	-		
86	OHX	A1	3774	-	0,6,6	0.00	-	-		
86	OHX	A1	3730	-	0,6,6	0.00	-	-		
86	OHX	A5	3611	-	0,6,6	0.00	-	-		
86	OHX	A7	205	-	0,6,6	0.00	-	-		
86	OHX	A6	1978	-	0,6,6	0.00	-	-		
86	OHX	A8	213	-	0,6,6	0.00	-	-		
86	OHX	A1	3556	-	0,6,6	0.00	-	-		
86	OHX	A2	1920	-	0,6,6	0.00	-	-		
86	OHX	A8	207	-	0,6,6	0.00	-	-		
86	OHX	A1	3705	-	0,6,6	0.00	-	-		
86	OHX	A6	2033	-	0,6,6	0.00	-	-		
86	OHX	A5	3706	-	0,6,6	0.00	-	-		
86	OHX	A2	1971	-	0,6,6	0.00	-	-		
86	OHX	A5	3524	-	0,6,6	0.00	-	-		
86	OHX	A5	3774	-	0,6,6	0.00	-	-		
86	OHX	A6	1938	-	0,6,6	0.00	-	-		
86	OHX	A6	2059	-	0,6,6	0.00	-	-		
86	OHX	A5	3512	-	0,6,6	0.00	-	-		
86	OHX	A1	3606	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A5	3662	-	0,6,6	0.00	-	-		
86	OHX	Bo	201	-	0,6,6	0.00	-	-		
86	OHX	BI	304	-	0,6,6	0.00	-	-		
86	OHX	DA	302	-	0,6,6	0.00	-	-		
86	OHX	A2	1983	-	0,6,6	0.00	-	-		
86	OHX	A6	1940	-	0,6,6	0.00	-	-		
86	OHX	A1	3413	-	0,6,6	0.00	-	-		
86	OHX	A6	2071	-	0,6,6	0.00	-	-		
86	OHX	A7	207	-	0,6,6	0.00	-	-		
86	OHX	A1	3707	-	0,6,6	0.00	-	-		
86	OHX	A5	3583	-	0,6,6	0.00	-	-		
86	OHX	A1	3470	-	0,6,6	0.00	-	-		
86	OHX	A5	3621	-	0,6,6	0.00	-	-		
86	OHX	A1	3517	-	0,6,6	0.00	-	-		
86	OHX	A5	3696	-	0,6,6	0.00	-	-		
86	OHX	A5	3630	-	0,6,6	0.00	-	-		
86	OHX	A6	2039	-	0,6,6	0.00	-	-		
86	OHX	A5	3708	-	0,6,6	0.00	-	-		
86	OHX	A5	3601	-	0,6,6	0.00	-	-		
86	OHX	A1	3496	-	0,6,6	0.00	-	-		
86	OHX	A1	3557	-	0,6,6	0.00	-	-		
86	OHX	A5	3647	-	0,6,6	0.00	-	-		
86	OHX	A1	3617	-	0,6,6	0.00	-	-		
86	OHX	A5	3605	-	0,6,6	0.00	-	-		
86	OHX	A1	3501	-	0,6,6	0.00	-	-		
86	OHX	A1	3568	-	0,6,6	0.00	-	-		
86	OHX	A1	3574	-	0,6,6	0.00	-	-		
86	OHX	A1	3465	-	0,6,6	0.00	-	-		
86	OHX	A5	3453	-	0,6,6	0.00	-	-		
86	OHX	A1	3489	-	0,6,6	0.00	-	-		
86	OHX	A2	1982	-	0,6,6	0.00	-	-		
86	OHX	A1	3811	36	0,6,6	0.00	-	-		
86	OHX	A1	3713	-	0,6,6	0.00	-	-		
86	OHX	A5	3549	-	0,6,6	0.00	-	-		
86	OHX	A1	3803	-	0,6,6	0.00	-	-		
86	OHX	A5	3556	-	0,6,6	0.00	-	-		
86	OHX	A5	3702	-	0,6,6	0.00	-	-		
86	OHX	A2	1967	-	0,6,6	0.00	-	-		
86	OHX	A6	1918	-	0,6,6	0.00	-	-		
86	OHX	A5	3729	-	0,6,6	0.00	-	-		
86	OHX	DI	302	-	0,6,6	0.00	-	-		
86	OHX	A1	3744	-	0,6,6	0.00	-	-		
86	OHX	A5	3592	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A1	3403	-	0,6,6	0.00	-	-		
86	OHX	A1	3624	-	0,6,6	0.00	-	-		
86	OHX	A5	3769	-	0,6,6	0.00	-	-		
86	OHX	A2	2060	-	0,6,6	0.00	-	-		
86	OHX	A5	3710	-	0,6,6	0.00	-	-		
86	OHX	A6	2002	-	0,6,6	0.00	-	-		
86	OHX	A1	3717	-	0,6,6	0.00	-	-		
86	OHX	A6	1954	-	0,6,6	0.00	-	-		
86	OHX	A1	3664	-	0,6,6	0.00	-	-		
86	OHX	A5	3712	-	0,6,6	0.00	-	-		
86	OHX	A6	2010	-	0,6,6	0.00	-	-		
86	OHX	A1	3653	-	0,6,6	0.00	-	-		
86	OHX	A1	3546	-	0,6,6	0.00	-	-		
86	OHX	A1	3602	-	0,6,6	0.00	-	-		
86	OHX	A1	3516	-	0,6,6	0.00	-	-		
86	OHX	A2	2031	-	0,6,6	0.00	-	-		
86	OHX	A1	3802	86,36	0,6,6	0.00	-	-		
86	OHX	A8	214	-	0,6,6	0.00	-	-		
86	OHX	A5	3795	86	0,6,6	0.00	-	-		
86	OHX	Cg	401	-	0,6,6	0.00	-	-		
86	OHX	A2	2074	1	0,6,6	0.00	-	-		
86	OHX	A6	1949	-	0,6,6	0.00	-	-		
86	OHX	A5	3546	-	0,6,6	0.00	-	-		
86	OHX	A2	1984	-	0,6,6	0.00	-	-		
86	OHX	A2	2072	-	0,6,6	0.00	-	-		
86	OHX	A5	3683	-	0,6,6	0.00	-	-		
86	OHX	A6	1932	-	0,6,6	0.00	-	-		
86	OHX	A5	3770	-	0,6,6	0.00	-	-		
86	OHX	A6	1977	-	0,6,6	0.00	-	-		
86	OHX	A5	3638	-	0,6,6	0.00	-	-		
86	OHX	BI	303	-	0,6,6	0.00	-	-		
86	OHX	A1	3679	-	0,6,6	0.00	-	-		
86	OHX	A1	3431	-	0,6,6	0.00	-	-		
86	OHX	A1	3712	-	0,6,6	0.00	-	-		
86	OHX	A3	205	-	0,6,6	0.00	-	-		
86	OHX	A5	3403	-	0,6,6	0.00	-	-		
86	OHX	A5	3728	-	0,6,6	0.00	-	-		
86	OHX	A2	1915	-	0,6,6	0.00	-	-		
86	OHX	A5	3751	-	0,6,6	0.00	-	-		
86	OHX	A1	3669	-	0,6,6	0.00	-	-		
86	OHX	DO	201	-	0,6,6	0.00	-	-		
86	OHX	A1	3695	-	0,6,6	0.00	-	-		
86	OHX	A5	3451	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A6	2023	-	0,6,6	0.00	-	-		
86	OHX	A6	2024	-	0,6,6	0.00	-	-		
86	OHX	A5	3534	-	0,6,6	0.00	-	-		
86	OHX	A3	207	-	0,6,6	0.00	-	-		
86	OHX	A6	2087	-	0,6,6	0.00	-	-		
86	OHX	A7	203	-	0,6,6	0.00	-	-		
86	OHX	A1	3683	-	0,6,6	0.00	-	-		
86	OHX	A6	1962	-	0,6,6	0.00	-	-		
86	OHX	A2	2032	-	0,6,6	0.00	-	-		
86	OHX	A5	3657	-	0,6,6	0.00	-	-		
86	OHX	A5	3454	-	0,6,6	0.00	-	-		
86	OHX	A5	3663	-	0,6,6	0.00	-	-		
86	OHX	A1	3550	-	0,6,6	0.00	-	-		
86	OHX	A1	3659	-	0,6,6	0.00	-	-		
86	OHX	A5	3562	-	0,6,6	0.00	-	-		
86	OHX	A1	3652	-	0,6,6	0.00	-	-		
86	OHX	A5	3787	-	0,6,6	0.00	-	-		
86	OHX	A1	3739	-	0,6,6	0.00	-	-		
86	OHX	A4	202	-	0,6,6	0.00	-	-		
86	OHX	A6	2090	-	0,6,6	0.00	-	-		
86	OHX	A2	2040	-	0,6,6	0.00	-	-		
86	OHX	A5	3545	-	0,6,6	0.00	-	-		
86	OHX	A5	3535	-	0,6,6	0.00	-	-		
86	OHX	A1	3772	-	0,6,6	0.00	-	-		
86	OHX	A6	2025	-	0,6,6	0.00	-	-		
86	OHX	A1	3721	-	0,6,6	0.00	-	-		
86	OHX	A1	3778	-	0,6,6	0.00	-	-		
86	OHX	A5	3559	-	0,6,6	0.00	-	-		
86	OHX	A1	3607	-	0,6,6	0.00	-	-		
86	OHX	DR	201	-	0,6,6	0.00	-	-		
86	OHX	A1	3439	86	0,6,6	0.00	-	-		
86	OHX	A5	3590	-	0,6,6	0.00	-	-		
86	OHX	CN	201	-	0,6,6	0.00	-	-		
86	OHX	A2	1910	-	0,6,6	0.00	-	-		
86	OHX	A5	3697	-	0,6,6	0.00	-	-		
86	OHX	A2	2019	-	0,6,6	0.00	-	-		
86	OHX	A1	3688	-	0,6,6	0.00	-	-		
86	OHX	CI	301	-	0,6,6	0.00	-	-		
86	OHX	A4	214	-	0,6,6	0.00	-	-		
86	OHX	A5	3775	-	0,6,6	0.00	-	-		
86	OHX	A1	3522	-	0,6,6	0.00	-	-		
86	OHX	A1	3486	-	0,6,6	0.00	-	-		
86	OHX	A2	1902	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A6	1937	-	0,6,6	0.00	-	-		
86	OHX	A5	3492	86	0,6,6	0.00	-	-		
86	OHX	A5	3793	-	0,6,6	0.00	-	-		
86	OHX	A5	3447	-	0,6,6	0.00	-	-		
86	OHX	A1	3751	-	0,6,6	0.00	-	-		
86	OHX	A6	2072	-	0,6,6	0.00	-	-		
86	OHX	A6	1955	-	0,6,6	0.00	-	-		
86	OHX	A5	3672	-	0,6,6	0.00	-	-		
86	OHX	A6	1970	-	0,6,6	0.00	-	-		
86	OHX	A1	3752	-	0,6,6	0.00	-	-		
86	OHX	A1	3454	-	0,6,6	0.00	-	-		
86	OHX	A5	3703	-	0,6,6	0.00	-	-		
86	OHX	A1	3582	-	0,6,6	0.00	-	-		
86	OHX	BP	201	-	0,6,6	0.00	-	-		
86	OHX	A1	3524	-	0,6,6	0.00	-	-		
86	OHX	A5	3415	-	0,6,6	0.00	-	-		
86	OHX	A2	1999	-	0,6,6	0.00	-	-		
86	OHX	A5	3680	-	0,6,6	0.00	-	-		
86	OHX	A5	3687	-	0,6,6	0.00	-	-		
86	OHX	A1	3662	-	0,6,6	0.00	-	-		
86	OHX	A5	3727	-	0,6,6	0.00	-	-		
86	OHX	A5	3802	-	0,6,6	0.00	-	-		
86	OHX	A1	3760	-	0,6,6	0.00	-	-		
86	OHX	A6	1976	-	0,6,6	0.00	-	-		
86	OHX	A5	3591	-	0,6,6	0.00	-	-		
86	OHX	A2	1919	-	0,6,6	0.00	-	-		
86	OHX	A5	3709	-	0,6,6	0.00	-	-		
86	OHX	A2	1964	-	0,6,6	0.00	-	-		
86	OHX	DV	201	-	0,6,6	0.00	-	-		
86	OHX	A2	1980	-	0,6,6	0.00	-	-		
86	OHX	A2	2059	-	0,6,6	0.00	-	-		
86	OHX	A1	3531	-	0,6,6	0.00	-	-		
86	OHX	A1	3798	-	0,6,6	0.00	-	-		
86	OHX	A5	3758	-	0,6,6	0.00	-	-		
86	OHX	BB	402	-	0,6,6	0.00	-	-		
86	OHX	A1	3521	86	0,6,6	0.00	-	-		
86	OHX	A6	1971	-	0,6,6	0.00	-	-		
86	OHX	A6	1965	-	0,6,6	0.00	-	-		
86	OHX	A6	2036	-	0,6,6	0.00	-	-		
86	OHX	A5	3528	-	0,6,6	0.00	-	-		
86	OHX	A5	3566	-	0,6,6	0.00	-	-		
86	OHX	A5	3767	-	0,6,6	0.00	-	-		
86	OHX	A5	3429	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A1	3729	-	0,6,6	0.00	-	-		
86	OHX	A2	1998	-	0,6,6	0.00	-	-		
86	OHX	A1	3414	-	0,6,6	0.00	-	-		
86	OHX	A6	2003	-	0,6,6	0.00	-	-		
86	OHX	A5	3726	-	0,6,6	0.00	-	-		
86	OHX	A7	206	-	0,6,6	0.00	-	-		
86	OHX	A5	3671	-	0,6,6	0.00	-	-		
86	OHX	Dg	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3494	-	0,6,6	0.00	-	-		
86	OHX	Bb	101	-	0,6,6	0.00	-	-		
86	OHX	A1	3611	-	0,6,6	0.00	-	-		
86	OHX	A5	3428	-	0,6,6	0.00	-	-		
86	OHX	A2	1960	-	0,6,6	0.00	-	-		
86	OHX	A1	3702	-	0,6,6	0.00	-	-		
86	OHX	A1	3594	-	0,6,6	0.00	-	-		
86	OHX	Do	201	-	0,6,6	0.00	-	-		
86	OHX	A6	1923	-	0,6,6	0.00	-	-		
86	OHX	A1	3797	-	0,6,6	0.00	-	-		
86	OHX	A3	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3823	-	0,6,6	0.00	-	-		
86	OHX	A6	1933	-	0,6,6	0.00	-	-		
86	OHX	A5	3733	-	0,6,6	0.00	-	-		
86	OHX	A6	2085	-	0,6,6	0.00	-	-		
86	OHX	A8	217	-	0,6,6	0.00	-	-		
86	OHX	A1	3769	-	0,6,6	0.00	-	-		
86	OHX	Dj	104	-	0,6,6	0.00	-	-		
86	OHX	A1	3758	-	0,6,6	0.00	-	-		
86	OHX	A5	3805	-	0,6,6	0.00	-	-		
86	OHX	A6	2093	-	0,6,6	0.00	-	-		
86	OHX	A1	3597	-	0,6,6	0.00	-	-		
86	OHX	A1	3734	-	0,6,6	0.00	-	-		
86	OHX	A5	3499	-	0,6,6	0.00	-	-		
86	OHX	A1	3603	-	0,6,6	0.00	-	-		
86	OHX	A1	3566	-	0,6,6	0.00	-	-		
86	OHX	A6	1982	-	0,6,6	0.00	-	-		
86	OHX	A5	3773	-	0,6,6	0.00	-	-		
86	OHX	A5	3722	-	0,6,6	0.00	-	-		
86	OHX	A6	2075	-	0,6,6	0.00	-	-		
86	OHX	A1	3726	-	0,6,6	0.00	-	-		
86	OHX	A3	209	-	0,6,6	0.00	-	-		
86	OHX	A1	3696	-	0,6,6	0.00	-	-		
86	OHX	A5	3690	-	0,6,6	0.00	-	-		
86	OHX	A5	3625	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A1	3723	-	0,6,6	0.00	-	-		
86	OHX	A2	2047	-	0,6,6	0.00	-	-		
86	OHX	A1	3795	-	0,6,6	0.00	-	-		
86	OHX	A6	2082	-	0,6,6	0.00	-	-		
86	OHX	A1	3595	-	0,6,6	0.00	-	-		
86	OHX	A6	2020	-	0,6,6	0.00	-	-		
86	OHX	A2	1981	-	0,6,6	0.00	-	-		
86	OHX	A6	1919	86	0,6,6	0.00	-	-		
86	OHX	A2	2009	-	0,6,6	0.00	-	-		
86	OHX	A6	2086	-	0,6,6	0.00	-	-		
86	OHX	A2	1957	-	0,6,6	0.00	-	-		
86	OHX	A2	2018	-	0,6,6	0.00	-	-		
86	OHX	A5	3686	-	0,6,6	0.00	-	-		
86	OHX	A6	2098	-	0,6,6	0.00	-	-		
86	OHX	A1	3636	-	0,6,6	0.00	-	-		
86	OHX	A6	1939	-	0,6,6	0.00	-	-		
86	OHX	A8	208	-	0,6,6	0.00	-	-		
86	OHX	A6	1995	-	0,6,6	0.00	-	-		
86	OHX	Ad	101	-	0,6,6	0.00	-	-		
86	OHX	A5	3418	-	0,6,6	0.00	-	-		
86	OHX	A6	1993	-	0,6,6	0.00	-	-		
86	OHX	A5	3582	-	0,6,6	0.00	-	-		
86	OHX	A6	2031	-	0,5,6	0.00	-	-		
86	OHX	A1	3791	-	0,6,6	0.00	-	-		
86	OHX	A2	2037	-	0,6,6	0.00	-	-		
86	OHX	A1	3706	-	0,6,6	0.00	-	-		
86	OHX	A1	3698	-	0,6,6	0.00	-	-		
86	OHX	BA	301	-	0,6,6	0.00	-	-		
86	OHX	A5	3736	-	0,6,6	0.00	-	-		
86	OHX	A5	3779	-	0,6,6	0.00	-	-		
86	OHX	A1	3691	-	0,6,6	0.00	-	-		
86	OHX	A5	3748	-	0,6,6	0.00	-	-		
86	OHX	A5	3668	-	0,6,6	0.00	-	-		
86	OHX	A1	3620	-	0,6,6	0.00	-	-		
86	OHX	A1	3541	-	0,6,6	0.00	-	-		
86	OHX	A1	3650	-	0,6,6	0.00	-	-		
86	OHX	A1	3783	-	0,6,6	0.00	-	-		
86	OHX	A5	3531	-	0,6,6	0.00	-	-		
86	OHX	A5	3443	-	0,6,6	0.00	-	-		
86	OHX	A6	2074	-	0,6,6	0.00	-	-		
86	OHX	A6	2051	-	0,6,6	0.00	-	-		
86	OHX	A5	3798	-	0,6,6	0.00	-	-		
86	OHX	A6	1905	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A1	3477	-	0,6,6	0.00	-	-		
86	OHX	A2	2061	-	0,6,6	0.00	-	-		
86	OHX	A1	3619	-	0,6,6	0.00	-	-		
86	OHX	A2	2081	-	0,6,6	0.00	-	-		
86	OHX	A1	3609	-	0,6,6	0.00	-	-		
86	OHX	A5	3469	-	0,6,6	0.00	-	-		
86	OHX	A1	3484	-	0,6,6	0.00	-	-		
86	OHX	A7	210	-	0,6,6	0.00	-	-		
86	OHX	A1	3488	-	0,6,6	0.00	-	-		
86	OHX	A5	3637	-	0,6,6	0.00	-	-		
86	OHX	A5	3475	-	0,6,6	0.00	-	-		
86	OHX	A1	3786	-	0,6,6	0.00	-	-		
86	OHX	A5	3594	-	0,6,6	0.00	-	-		
86	OHX	A5	3516	-	0,6,6	0.00	-	-		
86	OHX	A6	2055	-	0,6,6	0.00	-	-		
86	OHX	A5	3596	-	0,6,6	0.00	-	-		
86	OHX	A1	3715	-	0,6,6	0.00	-	-		
86	OHX	A5	3789	-	0,6,6	0.00	-	-		
86	OHX	A2	1942	-	0,6,6	0.00	-	-		
86	OHX	A1	3748	-	0,6,6	0.00	-	-		
86	OHX	A1	3498	-	0,6,6	0.00	-	-		
86	OHX	A1	3449	-	0,6,6	0.00	-	-		
86	OHX	A2	2058	-	0,6,6	0.00	-	-		
86	OHX	A6	1906	-	0,6,6	0.00	-	-		
86	OHX	A2	1945	-	0,6,6	0.00	-	-		
86	OHX	A1	3443	-	0,6,6	0.00	-	-		
86	OHX	A5	3675	-	0,6,6	0.00	-	-		
86	OHX	A6	2018	-	0,6,6	0.00	-	-		
86	OHX	A1	3693	-	0,6,6	0.00	-	-		
86	OHX	A5	3642	-	0,6,6	0.00	-	-		
86	OHX	A5	3734	-	0,6,6	0.00	-	-		
86	OHX	A1	3533	-	0,6,6	0.00	-	-		
86	OHX	A2	2069	-	0,6,6	0.00	-	-		
86	OHX	A6	2040	-	0,6,6	0.00	-	-		
86	OHX	DI	301	-	0,6,6	0.00	-	-		
86	OHX	A1	3704	-	0,6,6	0.00	-	-		
86	OHX	A6	2009	-	0,6,6	0.00	-	-		
86	OHX	A1	3814	-	0,6,6	0.00	-	-		
86	OHX	A1	3703	-	0,6,6	0.00	-	-		
86	OHX	A4	207	-	0,6,6	0.00	-	-		
86	OHX	A5	3520	-	0,6,6	0.00	-	-		
86	OHX	A2	1947	-	0,6,6	0.00	-	-		
86	OHX	A2	1949	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A5	3679	-	0,6,6	0.00	-	-		
86	OHX	A6	1958	-	0,6,6	0.00	-	-		
86	OHX	A5	3427	-	0,6,6	0.00	-	-		
86	OHX	A5	3529	-	0,6,6	0.00	-	-		
86	OHX	A1	3415	-	0,6,6	0.00	-	-		
86	OHX	A1	3626	-	0,6,6	0.00	-	-		
86	OHX	DG	301	-	0,6,6	0.00	-	-		
86	OHX	A2	2053	-	0,6,6	0.00	-	-		
86	OHX	A6	1953	-	0,6,6	0.00	-	-		
86	OHX	A2	1933	-	0,6,6	0.00	-	-		
86	OHX	A2	1969	-	0,6,6	0.00	-	-		
86	OHX	A2	1922	-	0,6,6	0.00	-	-		
86	OHX	A2	2044	-	0,6,6	0.00	-	-		
86	OHX	A5	3405	-	0,6,6	0.00	-	-		
86	OHX	A3	208	-	0,6,6	0.00	-	-		
86	OHX	A1	3429	-	0,6,6	0.00	-	-		
86	OHX	A5	3417	-	0,6,6	0.00	-	-		
86	OHX	A5	3558	-	0,6,6	0.00	-	-		
86	OHX	A5	3659	-	0,6,6	0.00	-	-		
86	OHX	A6	1909	-	0,6,6	0.00	-	-		
86	OHX	A1	3506	-	0,6,6	0.00	-	-		
86	OHX	A6	2029	-	0,6,6	0.00	-	-		
86	OHX	A5	3640	-	0,6,6	0.00	-	-		
86	OHX	A1	3815	-	0,6,6	0.00	-	-		
86	OHX	A5	3632	-	0,6,6	0.00	-	-		
86	OHX	A5	3685	-	0,6,6	0.00	-	-		
86	OHX	A1	3600	-	0,6,6	0.00	-	-		
86	OHX	A5	3555	-	0,6,6	0.00	-	-		
86	OHX	A2	1925	-	0,6,6	0.00	-	-		
86	OHX	A1	3642	-	0,6,6	0.00	-	-		
86	OHX	A1	3777	-	0,6,6	0.00	-	-		
86	OHX	A6	2067	-	0,6,6	0.00	-	-		
86	OHX	A5	3772	-	0,6,6	0.00	-	-		
86	OHX	A1	3481	-	0,6,6	0.00	-	-		
86	OHX	A2	2024	-	0,6,6	0.00	-	-		
86	OHX	A2	1912	-	0,6,6	0.00	-	-		
86	OHX	BC	401	-	0,6,6	0.00	-	-		
86	OHX	A5	3692	-	0,6,6	0.00	-	-		
86	OHX	A1	3635	-	0,6,6	0.00	-	-		
86	OHX	A1	3718	-	0,6,6	0.00	-	-		
86	OHX	A5	3551	-	0,6,6	0.00	-	-		
86	OHX	A1	3463	-	0,6,6	0.00	-	-		
86	OHX	A2	2028	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A1	3426	-	0,6,6	0.00	-	-		
86	OHX	A1	3428	-	0,6,6	0.00	-	-		
86	OHX	A6	2081	-	0,6,6	0.00	-	-		
86	OHX	A5	3752	-	0,6,6	0.00	-	-		
86	OHX	A1	3658	-	0,6,6	0.00	-	-		
86	OHX	AC	301	-	0,6,6	0.00	-	-		
86	OHX	A1	3457	-	0,6,6	0.00	-	-		
86	OHX	A5	3665	-	0,6,6	0.00	-	-		
86	OHX	A2	1995	-	0,6,6	0.00	-	-		
86	OHX	A5	3483	-	0,6,6	0.00	-	-		
86	OHX	A6	1985	-	0,6,6	0.00	-	-		
86	OHX	A6	1998	-	0,6,6	0.00	-	-		
86	OHX	A5	3473	-	0,6,6	0.00	-	-		
86	OHX	A1	3409	-	0,6,6	0.00	-	-		
86	OHX	A5	3514	-	0,6,6	0.00	-	-		
86	OHX	A1	3807	-	0,6,6	0.00	-	-		
86	OHX	A1	3476	-	0,6,6	0.00	-	-		
86	OHX	A1	3525	-	0,6,6	0.00	-	-		
86	OHX	A1	3549	-	0,6,6	0.00	-	-		
86	OHX	A1	3773	-	0,6,6	0.00	-	-		
86	OHX	A6	2070	-	0,6,6	0.00	-	-		
86	OHX	A1	3731	-	0,6,6	0.00	-	-		
86	OHX	A1	3722	-	0,6,6	0.00	-	-		
86	OHX	A5	3821	-	0,6,6	0.00	-	-		
86	OHX	A1	3790	-	0,6,6	0.00	-	-		
86	OHX	A2	2021	-	0,6,6	0.00	-	-		
86	OHX	A5	3812	-	0,6,6	0.00	-	-		
86	OHX	AI	301	-	0,6,6	0.00	-	-		
86	OHX	A7	201	-	0,6,6	0.00	-	-		
86	OHX	A2	1937	-	0,6,6	0.00	-	-		
86	OHX	A2	2050	-	0,6,6	0.00	-	-		
86	OHX	A5	3506	-	0,6,6	0.00	-	-		
86	OHX	Bj	102	-	0,6,6	0.00	-	-		
86	OHX	A5	3570	-	0,6,6	0.00	-	-		
86	OHX	A1	3690	-	0,6,6	0.00	-	-		
86	OHX	A5	3471	-	0,6,6	0.00	-	-		
86	OHX	A1	3485	-	0,6,6	0.00	-	-		
86	OHX	A6	1922	-	0,6,6	0.00	-	-		
86	OHX	A5	3604	-	0,6,6	0.00	-	-		
86	OHX	A5	3707	-	0,6,6	0.00	-	-		
86	OHX	A8	211	-	0,6,6	0.00	-	-		
86	OHX	A2	2006	-	0,6,6	0.00	-	-		
86	OHX	A2	1918	86	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A1	3483	-	0,6,6	0.00	-	-		
86	OHX	A5	3467	-	0,6,6	0.00	-	-		
86	OHX	A1	3686	-	0,6,6	0.00	-	-		
86	OHX	A5	3513	-	0,6,6	0.00	-	-		
86	OHX	A2	1976	-	0,6,6	0.00	-	-		
86	OHX	A5	3674	-	0,6,6	0.00	-	-		
86	OHX	A1	3631	-	0,6,6	0.00	-	-		
86	OHX	A7	211	-	0,6,6	0.00	-	-		
86	OHX	A2	2063	-	0,6,6	0.00	-	-		
86	OHX	A6	1925	-	0,6,6	0.00	-	-		
86	OHX	A5	3515	-	0,6,6	0.00	-	-		
86	OHX	A5	3614	-	0,6,6	0.00	-	-		
86	OHX	A5	3617	-	0,6,6	0.00	-	-		
86	OHX	A1	3459	-	0,6,6	0.00	-	-		
86	OHX	A5	3803	-	0,6,6	0.00	-	-		
86	OHX	A1	3641	-	0,6,6	0.00	-	-		
86	OHX	A6	1957	-	0,6,6	0.00	-	-		
86	OHX	A2	2003	-	0,6,6	0.00	-	-		
86	OHX	A2	1944	-	0,6,6	0.00	-	-		
86	OHX	A1	3668	-	0,6,6	0.00	-	-		
86	OHX	A6	1972	-	0,6,6	0.00	-	-		
86	OHX	A2	1975	-	0,6,6	0.00	-	-		
86	OHX	A5	3402	-	0,6,6	0.00	-	-		
86	OHX	A2	2043	-	0,6,6	0.00	-	-		
86	OHX	A5	3508	-	0,6,6	0.00	-	-		
86	OHX	A1	3471	-	0,6,6	0.00	-	-		
86	OHX	A2	1992	-	0,6,6	0.00	-	-		
86	OHX	A8	215	-	0,6,6	0.00	-	-		
86	OHX	A6	1921	-	0,6,6	0.00	-	-		
86	OHX	A1	3497	-	0,6,6	0.00	-	-		
86	OHX	A2	2016	-	0,6,6	0.00	-	-		
86	OHX	A1	3407	-	0,6,6	0.00	-	-		
86	OHX	A1	3500	-	0,6,6	0.00	-	-		
86	OHX	Df	201	-	0,6,6	0.00	-	-		
86	OHX	A4	209	-	0,6,6	0.00	-	-		
86	OHX	A2	1950	-	0,6,6	0.00	-	-		
86	OHX	A1	3447	-	0,6,6	0.00	-	-		
86	OHX	A1	3504	-	0,6,6	0.00	-	-		
86	OHX	A1	3710	-	0,6,6	0.00	-	-		
86	OHX	BR	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3744	-	0,6,6	0.00	-	-		
86	OHX	A2	1930	-	0,6,6	0.00	-	-		
86	OHX	A5	3421	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A6	1911	-	0,6,6	0.00	-	-		
86	OHX	A1	3637	-	0,6,6	0.00	-	-		
86	OHX	A6	1944	-	0,6,6	0.00	-	-		
86	OHX	A6	2021	-	0,6,6	0.00	-	-		
86	OHX	A1	3804	-	0,6,6	0.00	-	-		
86	OHX	A5	3743	-	0,6,6	0.00	-	-		
86	OHX	A5	3801	-	0,6,6	0.00	-	-		
86	OHX	A5	3510	-	0,6,6	0.00	-	-		
86	OHX	A5	3820	-	0,6,6	0.00	-	-		
86	OHX	A6	1943	-	0,6,6	0.00	-	-		
86	OHX	A2	2041	-	0,6,6	0.00	-	-		
86	OHX	A5	3425	-	0,6,6	0.00	-	-		
86	OHX	A1	3605	-	0,6,6	0.00	-	-		
86	OHX	A6	1935	-	0,6,6	0.00	-	-		
86	OHX	A2	1926	-	0,6,6	0.00	-	-		
86	OHX	A2	1931	-	0,6,6	0.00	-	-		
86	OHX	A5	3623	-	0,6,6	0.00	-	-		
86	OHX	A2	1908	-	0,6,6	0.00	-	-		
86	OHX	A2	2068	-	0,6,6	0.00	-	-		
86	OHX	A1	3542	-	0,6,6	0.00	-	-		
86	OHX	A1	3530	-	0,6,6	0.00	-	-		
86	OHX	A1	3813	-	0,6,6	0.00	-	-		
86	OHX	A6	1929	-	0,6,6	0.00	-	-		
86	OHX	A2	2082	-	0,6,6	0.00	-	-		
86	OHX	A5	3641	-	0,6,6	0.00	-	-		
86	OHX	A1	3538	-	0,6,6	0.00	-	-		
86	OHX	A5	3711	-	0,6,6	0.00	-	-		
86	OHX	A2	2022	-	0,6,6	0.00	-	-		
86	OHX	Bf	201	-	0,6,6	0.00	-	-		
86	OHX	A2	1952	-	0,6,6	0.00	-	-		
86	OHX	A1	3762	-	0,6,6	0.00	-	-		
86	OHX	A8	203	-	0,6,6	0.00	-	-		
86	OHX	A5	3438	-	0,6,6	0.00	-	-		
86	OHX	A1	3725	-	0,6,6	0.00	-	-		
86	OHX	A8	209	-	0,6,6	0.00	-	-		
86	OHX	A5	3691	-	0,6,6	0.00	-	-		
86	OHX	A1	3427	-	0,6,6	0.00	-	-		
86	OHX	A1	3421	-	0,6,6	0.00	-	-		
86	OHX	A5	3585	-	0,6,6	0.00	-	-		
86	OHX	A1	3502	-	0,6,6	0.00	-	-		
86	OHX	De	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3606	-	0,6,6	0.00	-	-		
86	OHX	A2	2073	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A6	1941	-	0,6,6	0.00	-	-		
86	OHX	A1	3775	86	0,6,6	0.00	-	-		
86	OHX	A1	3547	-	0,6,6	0.00	-	-		
86	OHX	A5	3422	-	0,6,6	0.00	-	-		
86	OHX	A6	2032	-	0,6,6	0.00	-	-		
86	OHX	A2	1987	-	0,6,6	0.00	-	-		
86	OHX	A2	2071	-	0,6,6	0.00	-	-		
86	OHX	A1	3527	-	0,6,6	0.00	-	-		
86	OHX	A1	3682	-	0,6,6	0.00	-	-		
86	OHX	A6	1989	-	0,6,6	0.00	-	-		
86	OHX	A1	3558	-	0,6,6	0.00	-	-		
86	OHX	A1	3745	-	0,6,6	0.00	-	-		
86	OHX	A5	3578	-	0,6,6	0.00	-	-		
86	OHX	A1	3622	-	0,6,6	0.00	-	-		
86	OHX	A2	1953	-	0,6,6	0.00	-	-		
86	OHX	A6	2052	-	0,6,6	0.00	-	-		
86	OHX	A1	3640	-	0,6,6	0.00	-	-		
86	OHX	A6	1945	-	0,6,6	0.00	-	-		
86	OHX	A2	2013	-	0,6,6	0.00	-	-		
86	OHX	A1	3495	-	0,6,6	0.00	-	-		
86	OHX	AL	201	-	0,6,6	0.00	-	-		
86	OHX	A5	3780	-	0,6,6	0.00	-	-		
86	OHX	A6	2080	-	0,6,6	0.00	-	-		
86	OHX	A5	3720	-	0,6,6	0.00	-	-		
86	OHX	A1	3412	-	0,6,6	0.00	-	-		
86	OHX	A1	3805	-	0,6,6	0.00	-	-		
86	OHX	A6	1947	-	0,6,6	0.00	-	-		
86	OHX	A2	2083	-	0,6,6	0.00	-	-		
86	OHX	A5	3571	-	0,6,6	0.00	-	-		
86	OHX	A2	1954	-	0,6,6	0.00	-	-		
86	OHX	A2	1996	-	0,6,6	0.00	-	-		
86	OHX	A1	3654	-	0,6,6	0.00	-	-		
86	OHX	A2	1917	-	0,6,6	0.00	-	-		
86	OHX	A5	3543	-	0,6,6	0.00	-	-		
86	OHX	A5	3809	86	0,6,6	0.00	-	-		
86	OHX	A5	3439	-	0,6,6	0.00	-	-		
86	OHX	A1	3675	-	0,6,6	0.00	-	-		
86	OHX	A1	3512	-	0,6,6	0.00	-	-		
86	OHX	A5	3715	-	0,6,6	0.00	-	-		
86	OHX	A5	3608	-	0,6,6	0.00	-	-		
86	OHX	A1	3480	-	0,6,6	0.00	-	-		
86	OHX	A1	3676	-	0,6,6	0.00	-	-		
86	OHX	A5	3739	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A5	3414	-	0,6,6	0.00	-	-		
86	OHX	A5	3461	-	0,6,6	0.00	-	-		
86	OHX	BO	201	-	0,6,6	0.00	-	-		
86	OHX	A1	3648	-	0,6,6	0.00	-	-		
86	OHX	A3	210	-	0,6,6	0.00	-	-		
86	OHX	A5	3816	-	0,6,6	0.00	-	-		
86	OHX	A2	2055	-	0,6,6	0.00	-	-		
86	OHX	A5	3522	-	0,6,6	0.00	-	-		
86	OHX	A5	3449	-	0,6,6	0.00	-	-		
86	OHX	A2	1962	-	0,6,6	0.00	-	-		
86	OHX	A5	3486	-	0,6,6	0.00	-	-		
86	OHX	A1	3458	-	0,6,6	0.00	-	-		
86	OHX	A5	3503	-	0,6,6	0.00	-	-		
86	OHX	A1	3583	-	0,6,6	0.00	-	-		
86	OHX	A1	3633	-	0,6,6	0.00	-	-		
86	OHX	A5	3741	-	0,6,6	0.00	-	-		
86	OHX	Dh	201	-	0,6,6	0.00	-	-		
86	OHX	A6	2079	-	0,6,6	0.00	-	-		
86	OHX	A5	3745	-	0,6,6	0.00	-	-		
86	OHX	A1	3450	-	0,6,6	0.00	-	-		
86	OHX	A1	3770	-	0,6,6	0.00	-	-		
86	OHX	A6	1928	-	0,6,6	0.00	-	-		
86	OHX	A6	1913	-	0,6,6	0.00	-	-		
86	OHX	A2	2017	-	0,6,6	0.00	-	-		
86	OHX	A1	3416	-	0,6,6	0.00	-	-		
86	OHX	A2	2010	-	0,6,6	0.00	-	-		
86	OHX	A6	1967	-	0,6,6	0.00	-	-		
86	OHX	A1	3701	-	0,6,6	0.00	-	-		
86	OHX	A1	3812	-	0,6,6	0.00	-	-		
86	OHX	A1	3792	-	0,6,6	0.00	-	-		
86	OHX	A1	3487	-	0,6,6	0.00	-	-		
86	OHX	A6	2073	-	0,6,6	0.00	-	-		
86	OHX	A1	3571	-	0,6,6	0.00	-	-		
86	OHX	CS	201	-	0,6,6	0.00	-	-		
86	OHX	A6	2028	-	0,6,6	0.00	-	-		
86	OHX	A1	3736	-	0,6,6	0.00	-	-		
86	OHX	A5	3760	-	0,6,6	0.00	-	-		
86	OHX	A1	3441	-	0,6,6	0.00	-	-		
86	OHX	A6	1904	-	0,6,6	0.00	-	-		
86	OHX	A2	1958	-	0,6,6	0.00	-	-		
86	OHX	A5	3788	-	0,6,6	0.00	-	-		
86	OHX	A5	3806	-	0,6,6	0.00	-	-		
86	OHX	A5	3589	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	A2	1943	-	0,6,6	0.00	-	-		
86	OHX	A1	3816	-	0,6,6	0.00	-	-		
86	OHX	A4	208	-	0,6,6	0.00	-	-		
86	OHX	A5	3567	-	0,6,6	0.00	-	-		
86	OHX	BD	301	-	0,6,6	0.00	-	-		
86	OHX	A5	3655	-	0,6,6	0.00	-	-		
86	OHX	A2	2085	-	0,6,6	0.00	-	-		
86	OHX	A2	1956	-	0,6,6	0.00	-	-		
86	OHX	A5	3575	-	0,6,6	0.00	-	-		
86	OHX	A1	3515	-	0,6,6	0.00	-	-		
86	OHX	A4	215	-	0,6,6	0.00	-	-		
86	OHX	A1	3410	-	0,6,6	0.00	-	-		
86	OHX	BN	301	-	0,6,6	0.00	-	-		
86	OHX	A1	3700	-	0,6,6	0.00	-	-		
86	OHX	A6	2050	-	0,6,6	0.00	-	-		
86	OHX	A8	220	-	0,6,6	0.00	-	-		
86	OHX	A1	3569	-	0,6,6	0.00	-	-		
86	OHX	A5	3587	-	0,6,6	0.00	-	-		
86	OHX	A6	1961	-	0,6,6	0.00	-	-		
86	OHX	A2	2067	86	0,6,6	0.00	-	-		
86	OHX	A5	3406	-	0,6,6	0.00	-	-		
86	OHX	A1	3794	-	0,6,6	0.00	-	-		
86	OHX	A5	3424	-	0,6,6	0.00	-	-		
86	OHX	A5	3479	-	0,6,6	0.00	-	-		
86	OHX	A5	3693	-	0,6,6	0.00	-	-		
86	OHX	A6	1990	-	0,6,6	0.00	-	-		
86	OHX	A2	1906	-	0,6,6	0.00	-	-		
86	OHX	A2	1927	-	0,6,6	0.00	-	-		
86	OHX	A5	3527	-	0,6,6	0.00	-	-		
86	OHX	A5	3416	-	0,6,6	0.00	-	-		
86	OHX	A1	3508	-	0,6,6	0.00	-	-		
86	OHX	A2	2005	-	0,6,6	0.00	-	-		
86	OHX	A2	1965	-	0,6,6	0.00	-	-		
86	OHX	A5	3602	-	0,6,6	0.00	-	-		
86	OHX	A5	3613	-	0,6,6	0.00	-	-		
86	OHX	A8	202	-	0,6,6	0.00	-	-		
86	OHX	A5	3579	-	0,6,6	0.00	-	-		
86	OHX	A5	3759	-	0,6,6	0.00	-	-		
86	OHX	A6	1960	-	0,6,6	0.00	-	-		
86	OHX	A2	2062	-	0,6,6	0.00	-	-		
86	OHX	A1	3433	-	0,6,6	0.00	-	-		
86	OHX	A5	3681	-	0,6,6	0.00	-	-		
86	OHX	A1	3499	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	A5	3603	-	0,6,6	0.00	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

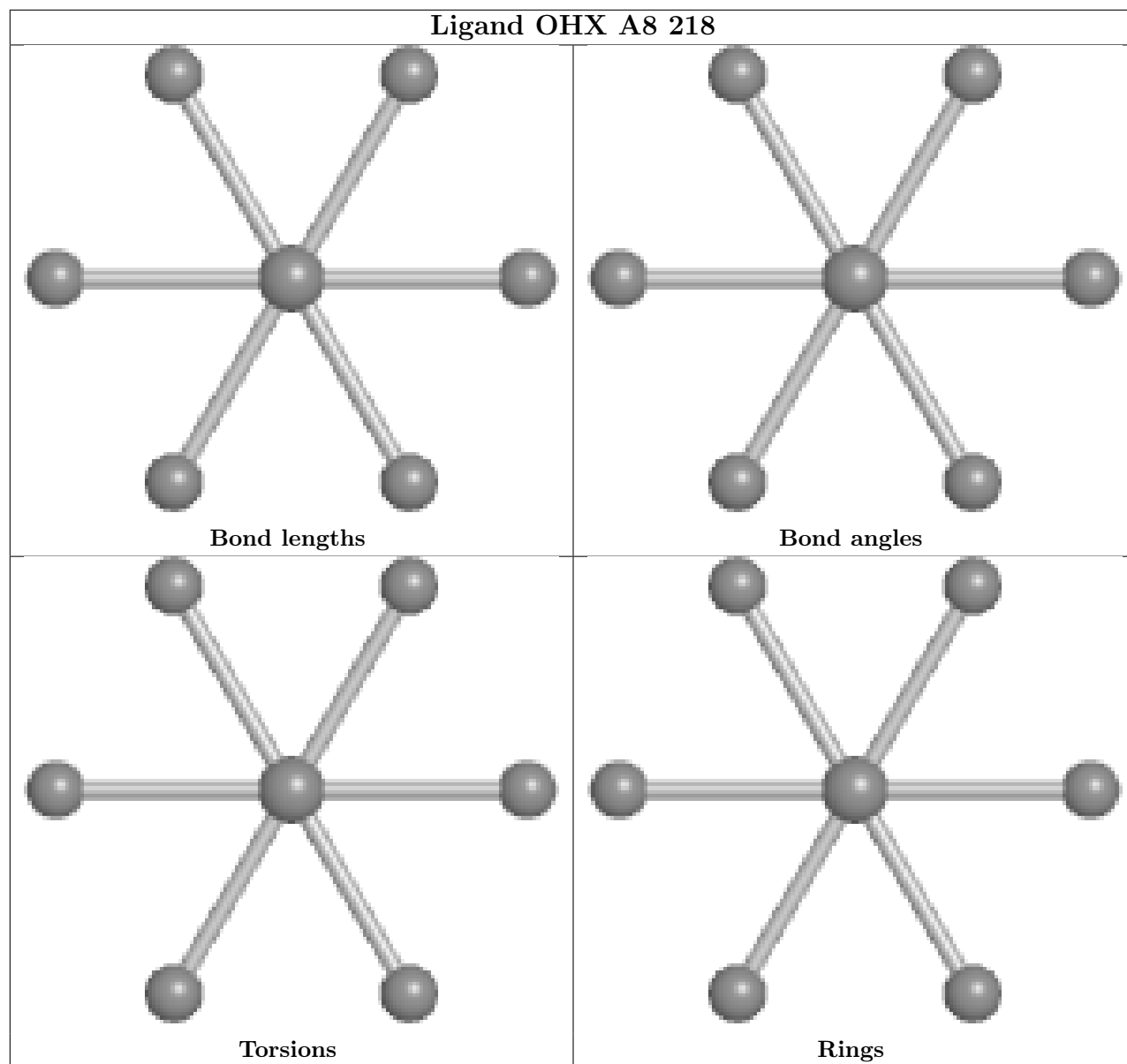
There are no torsion outliers.

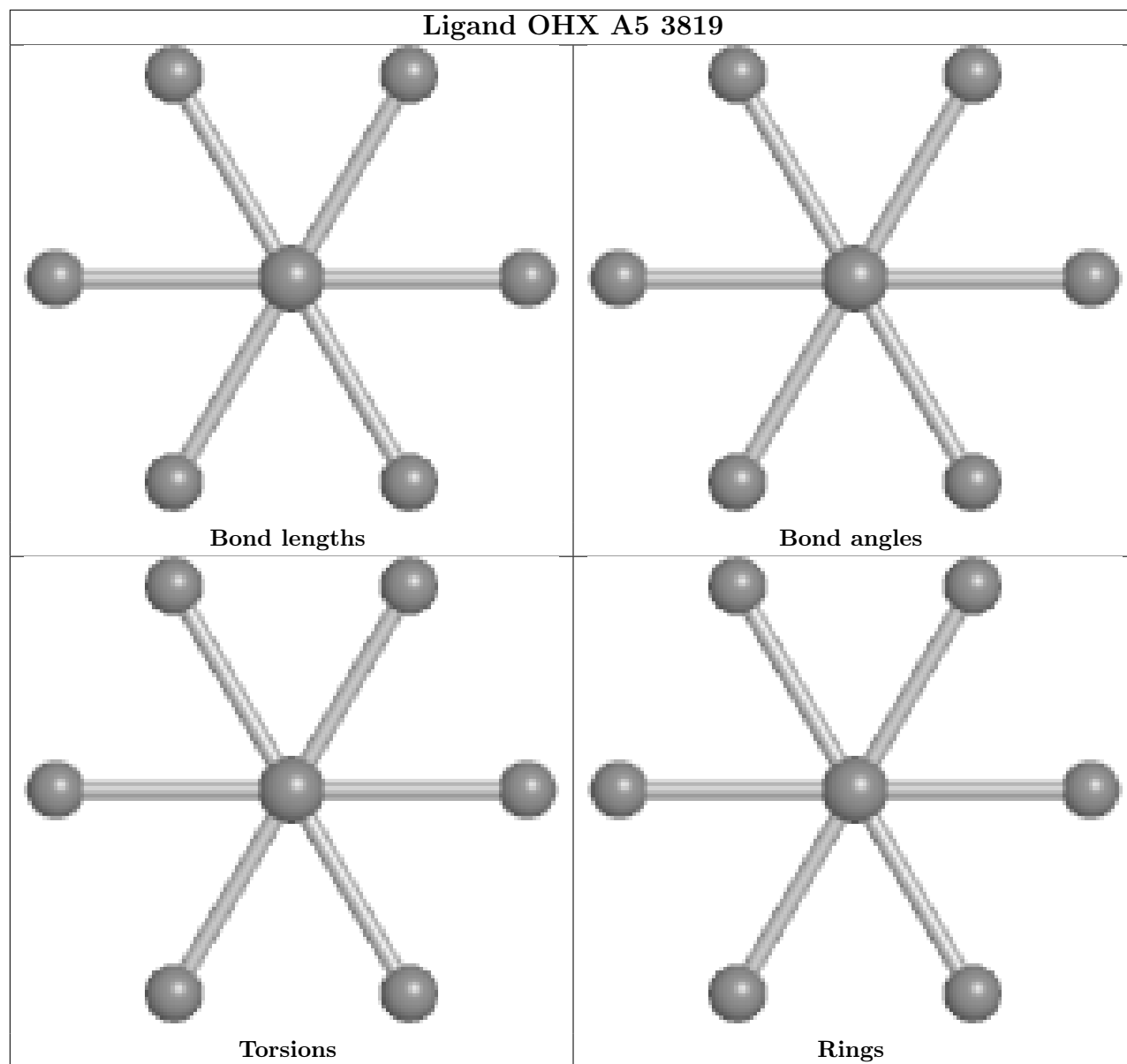
There are no ring outliers.

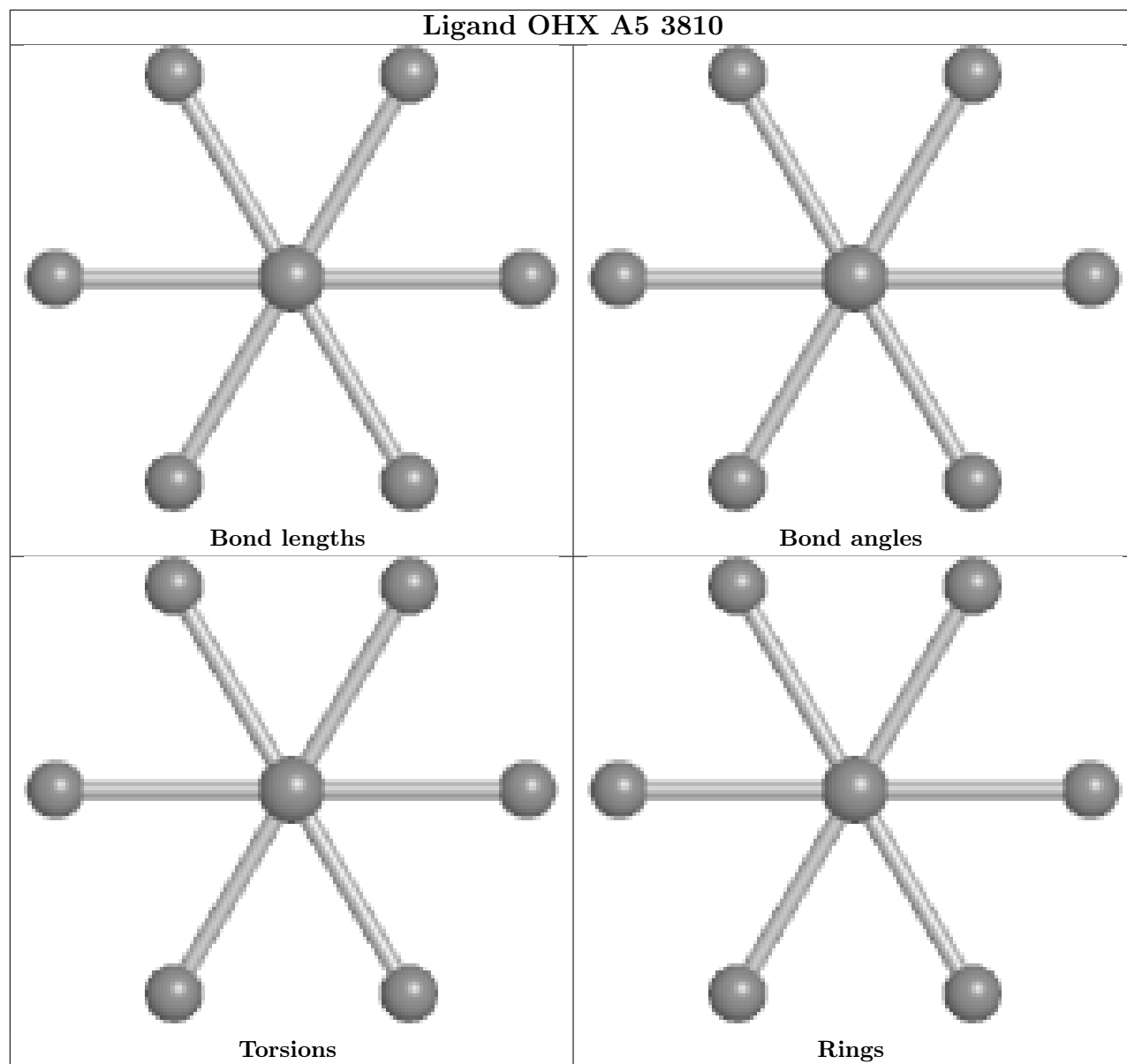
2 monomers are involved in 2 short contacts:

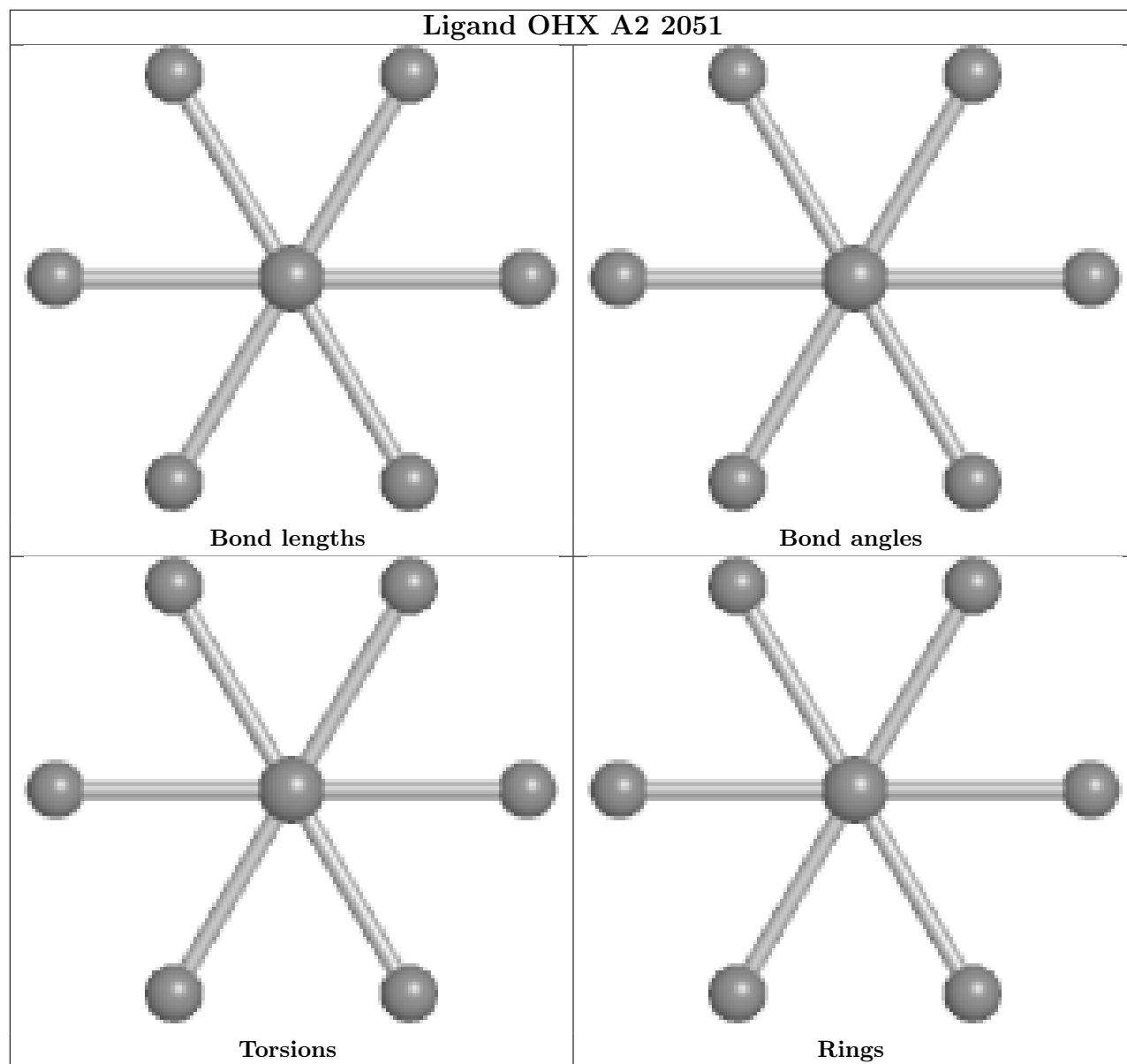
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	CG	301	OHX	0	1
86	A1	3788	OHX	0	1

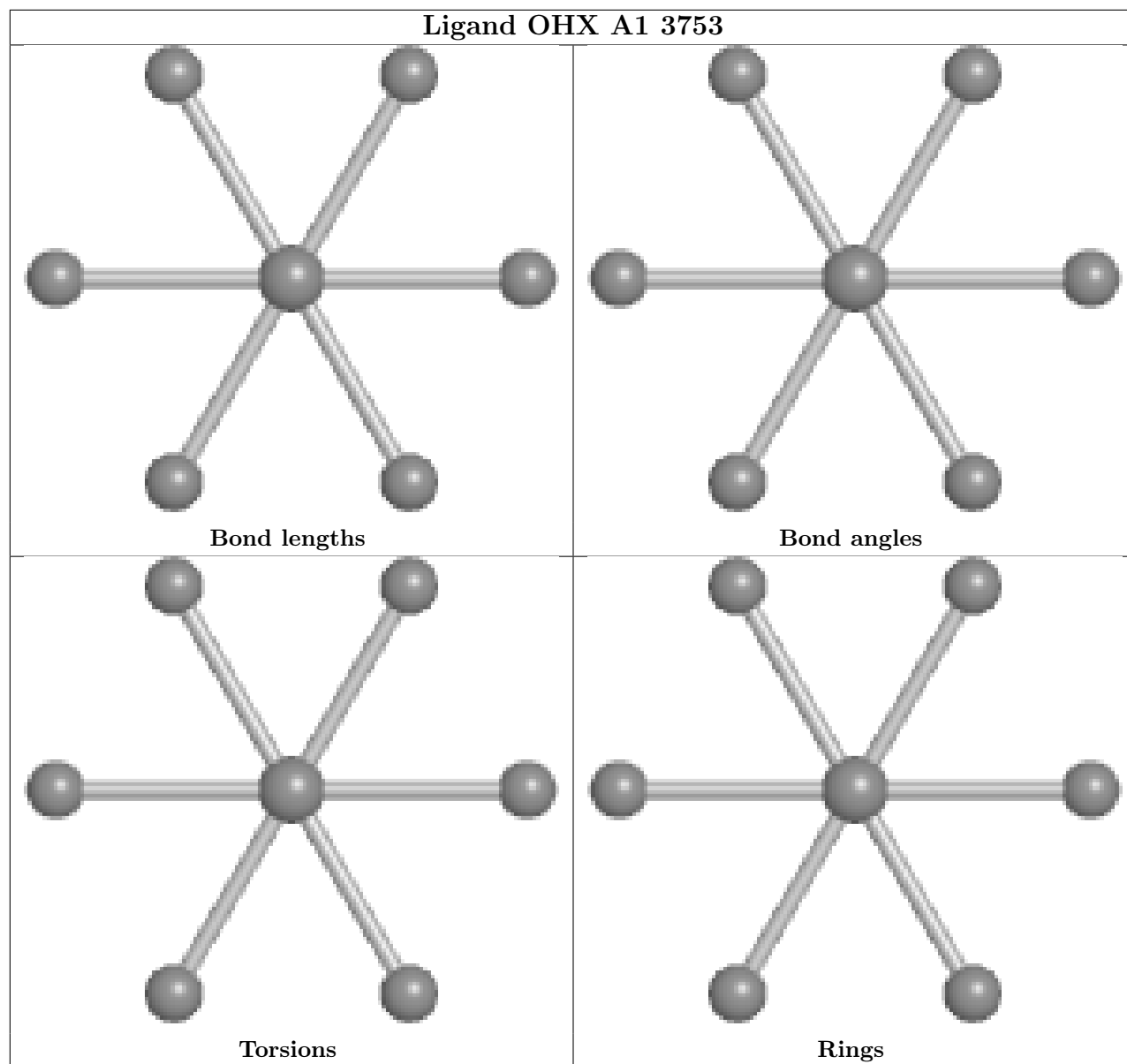
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

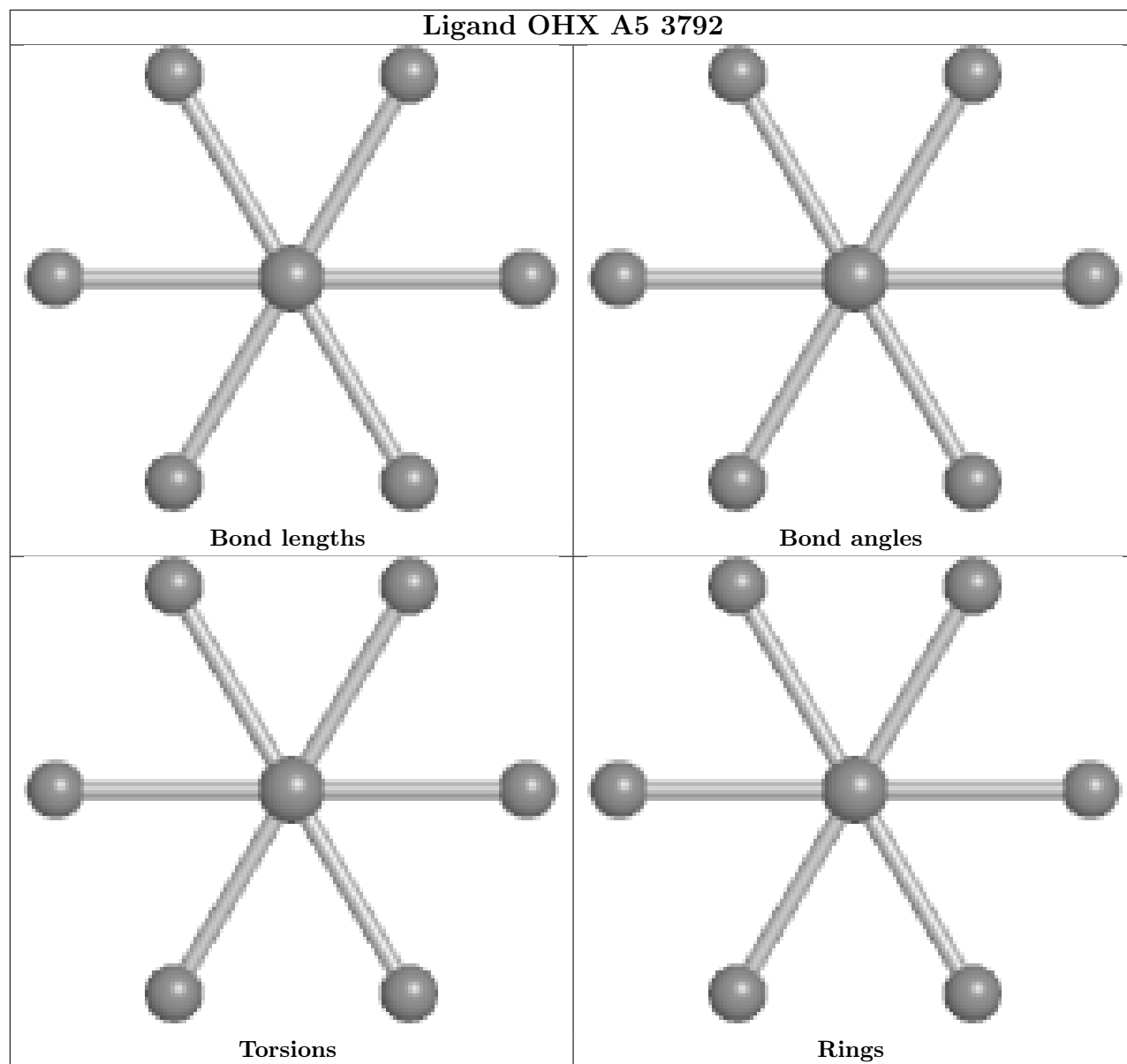


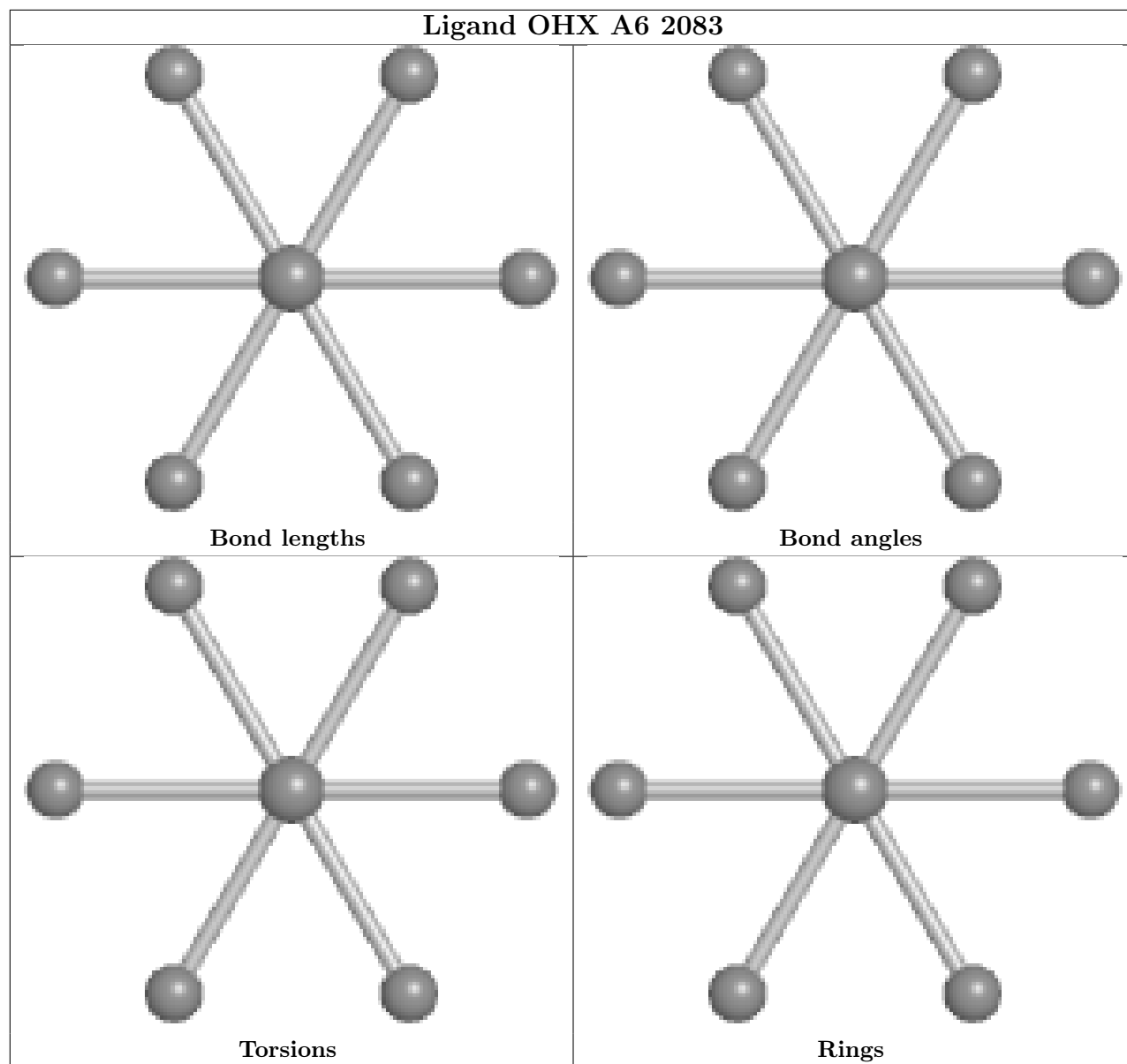


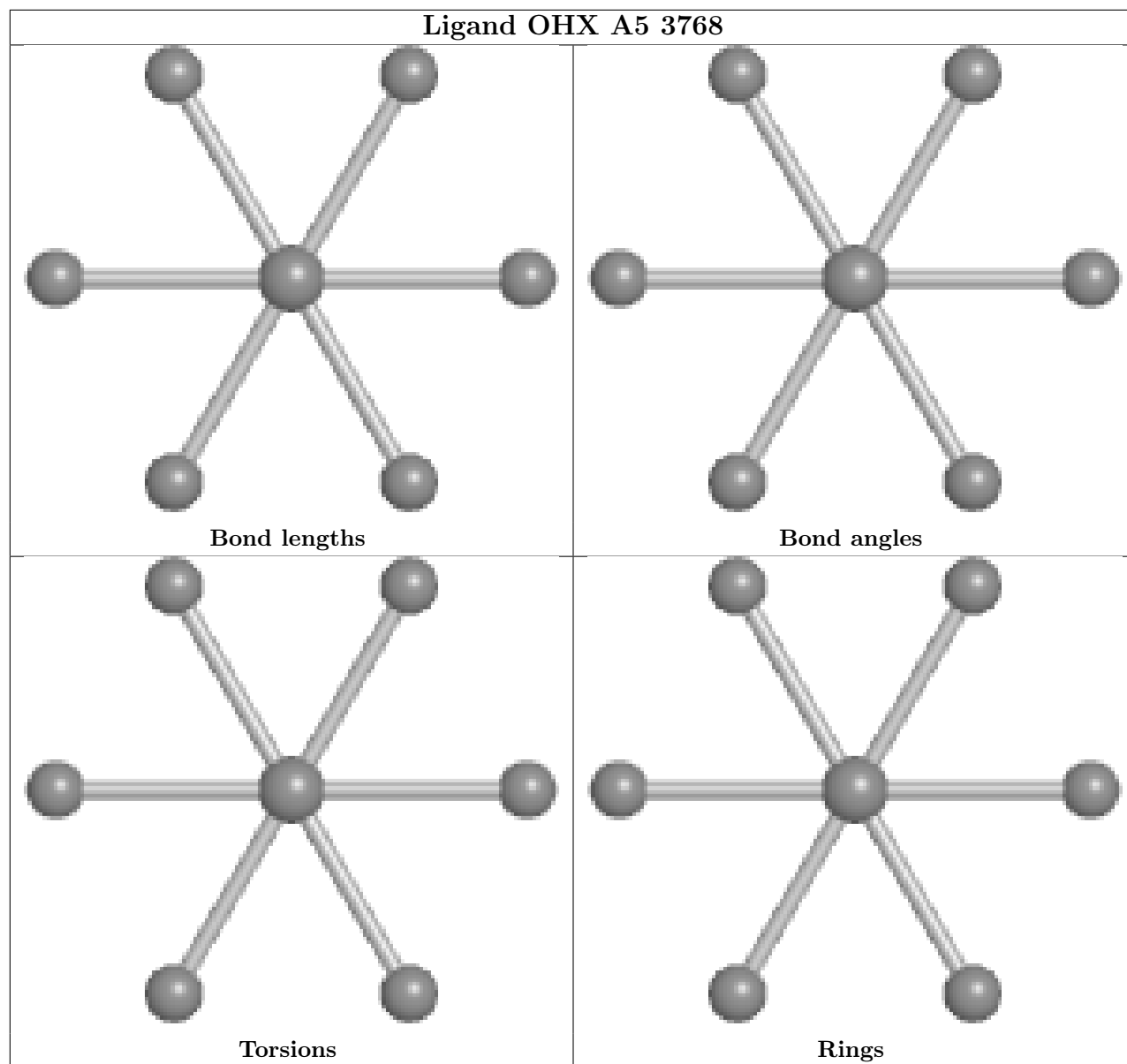


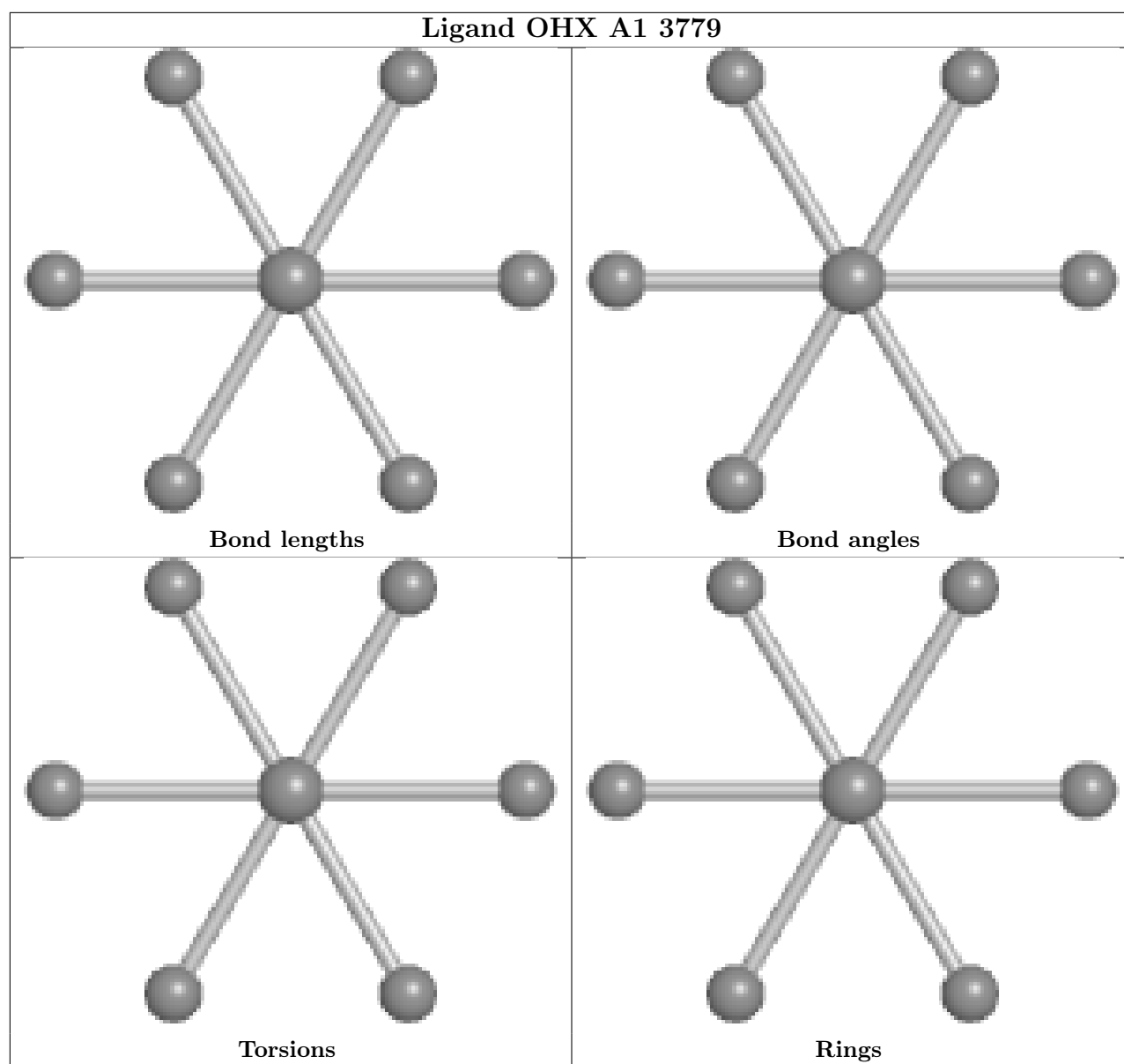


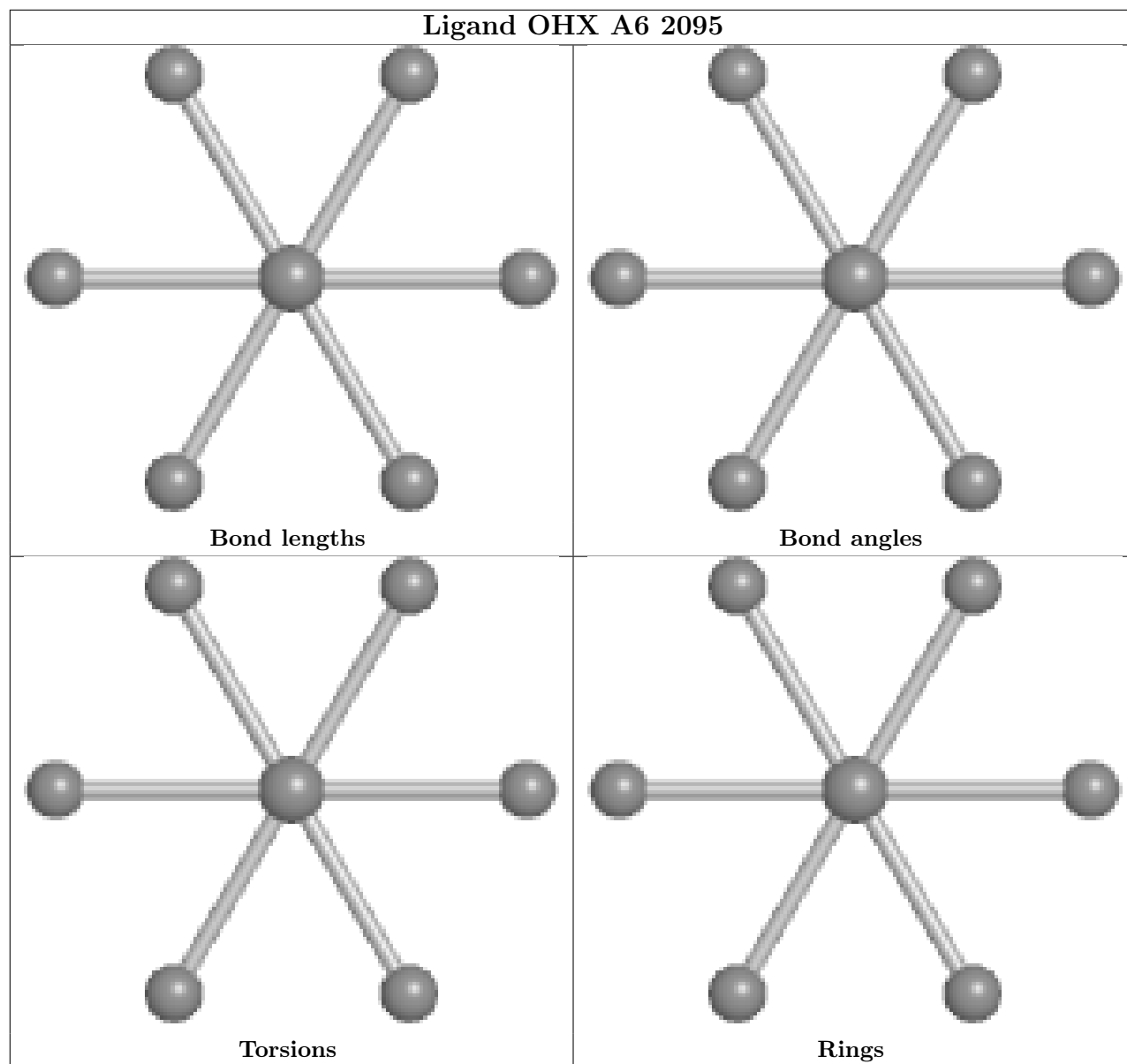


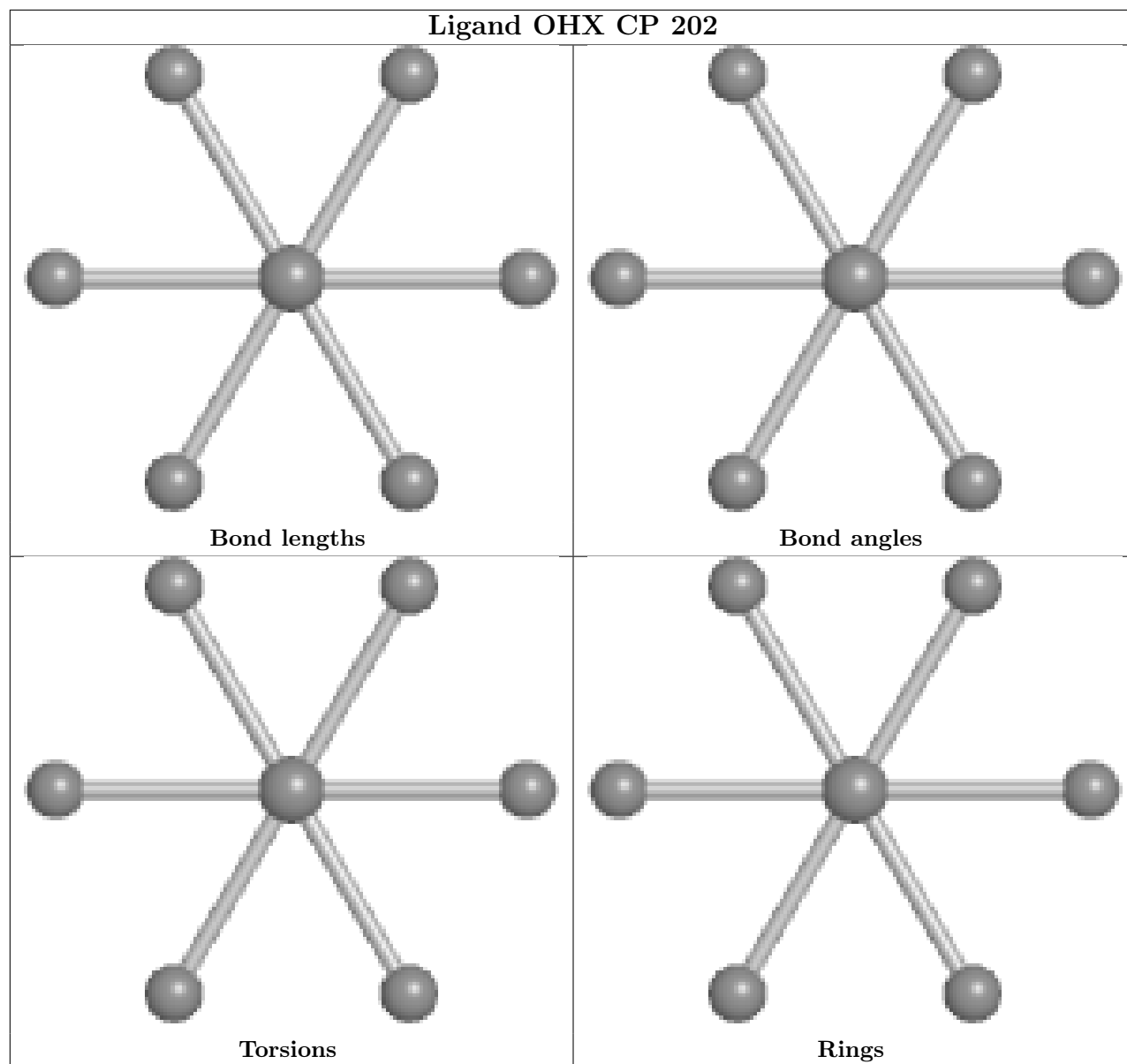


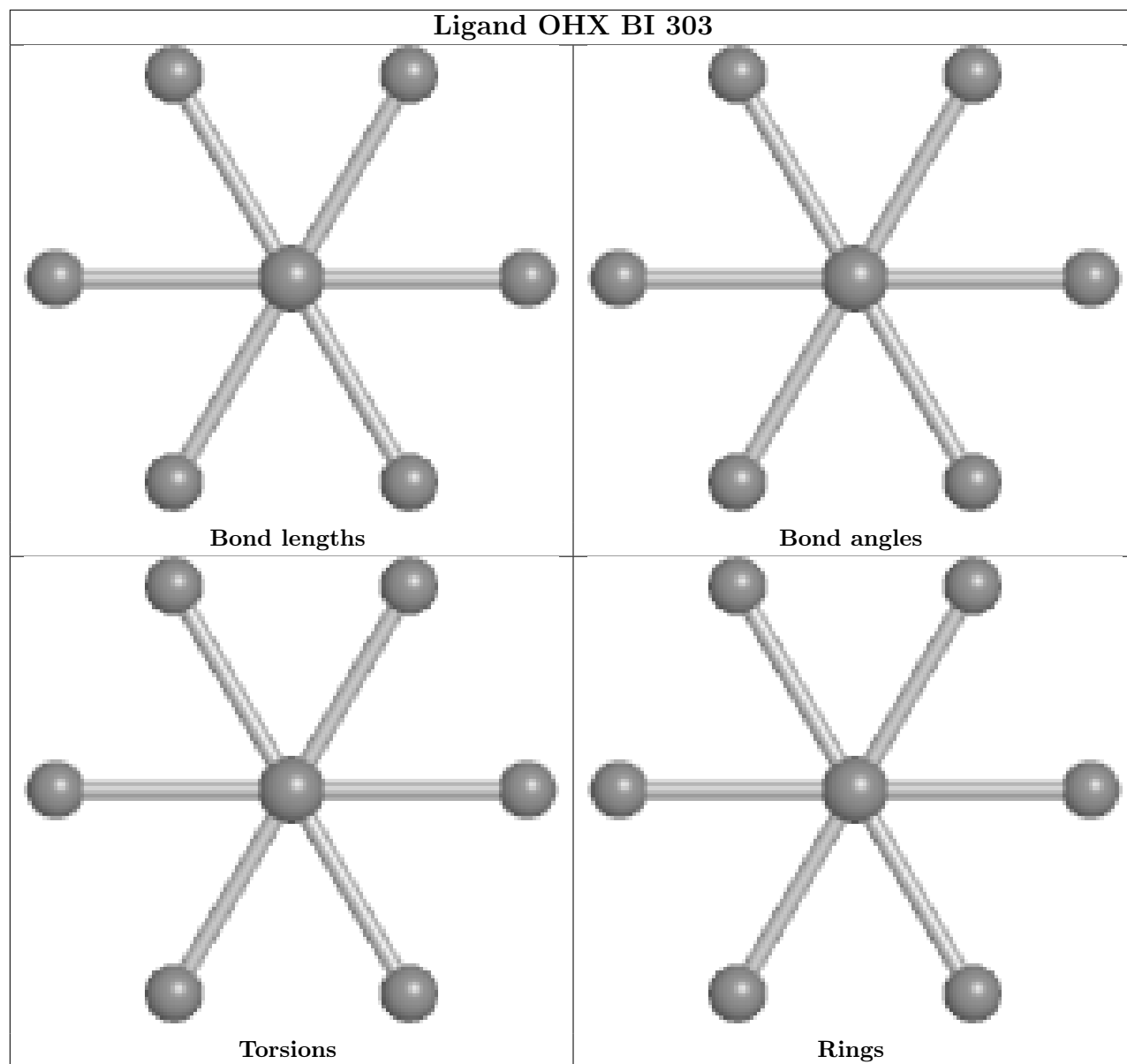


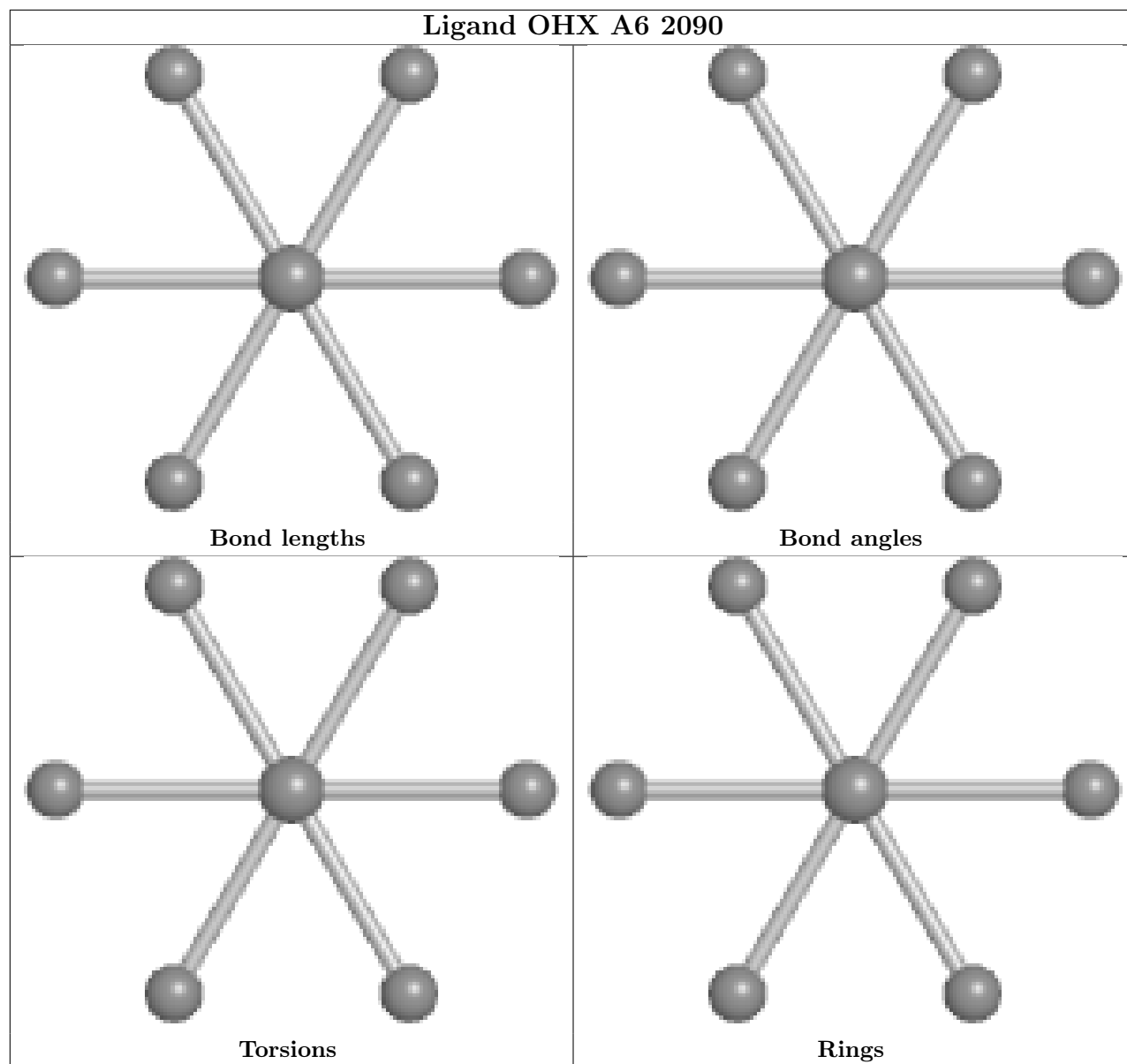


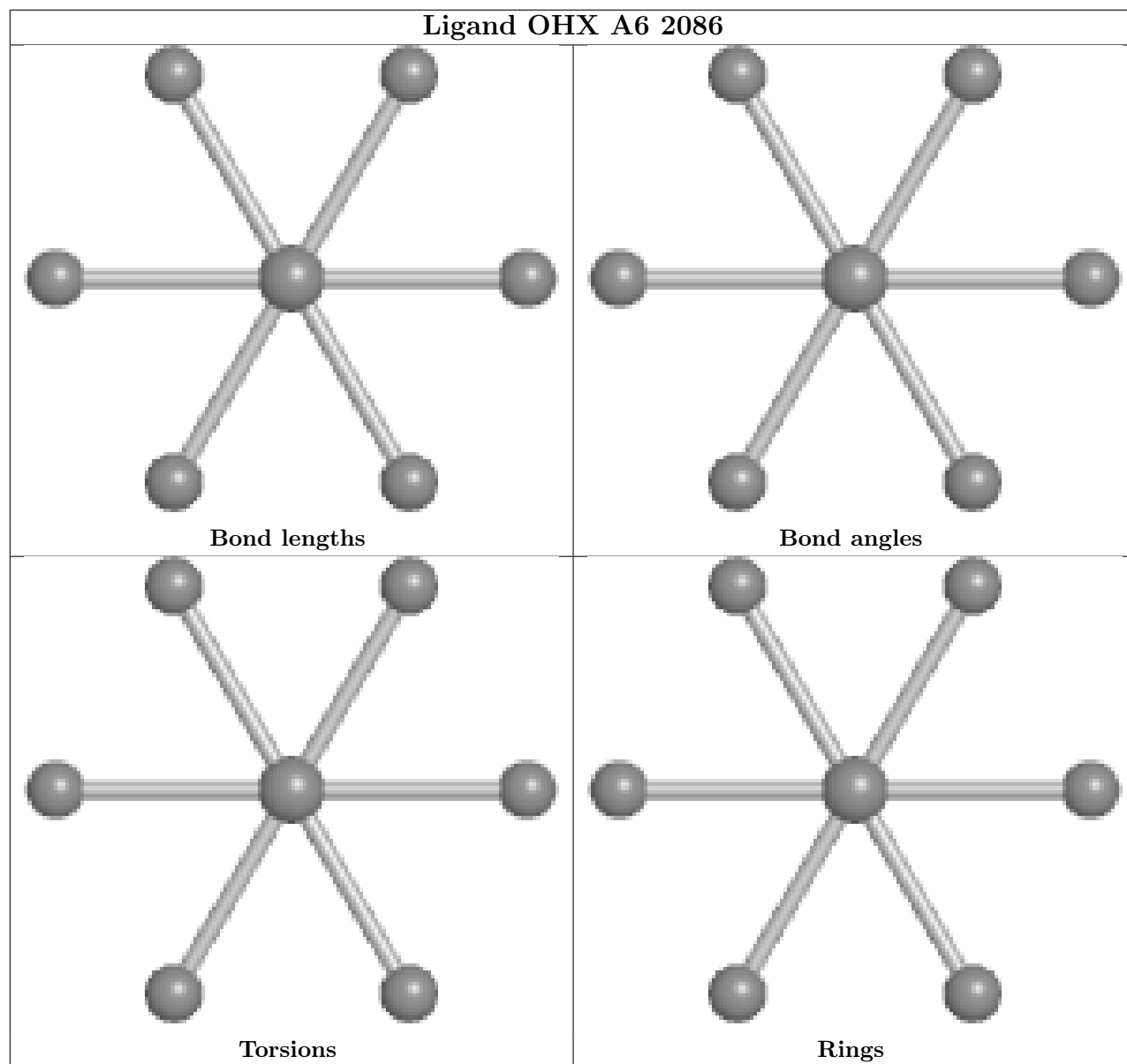


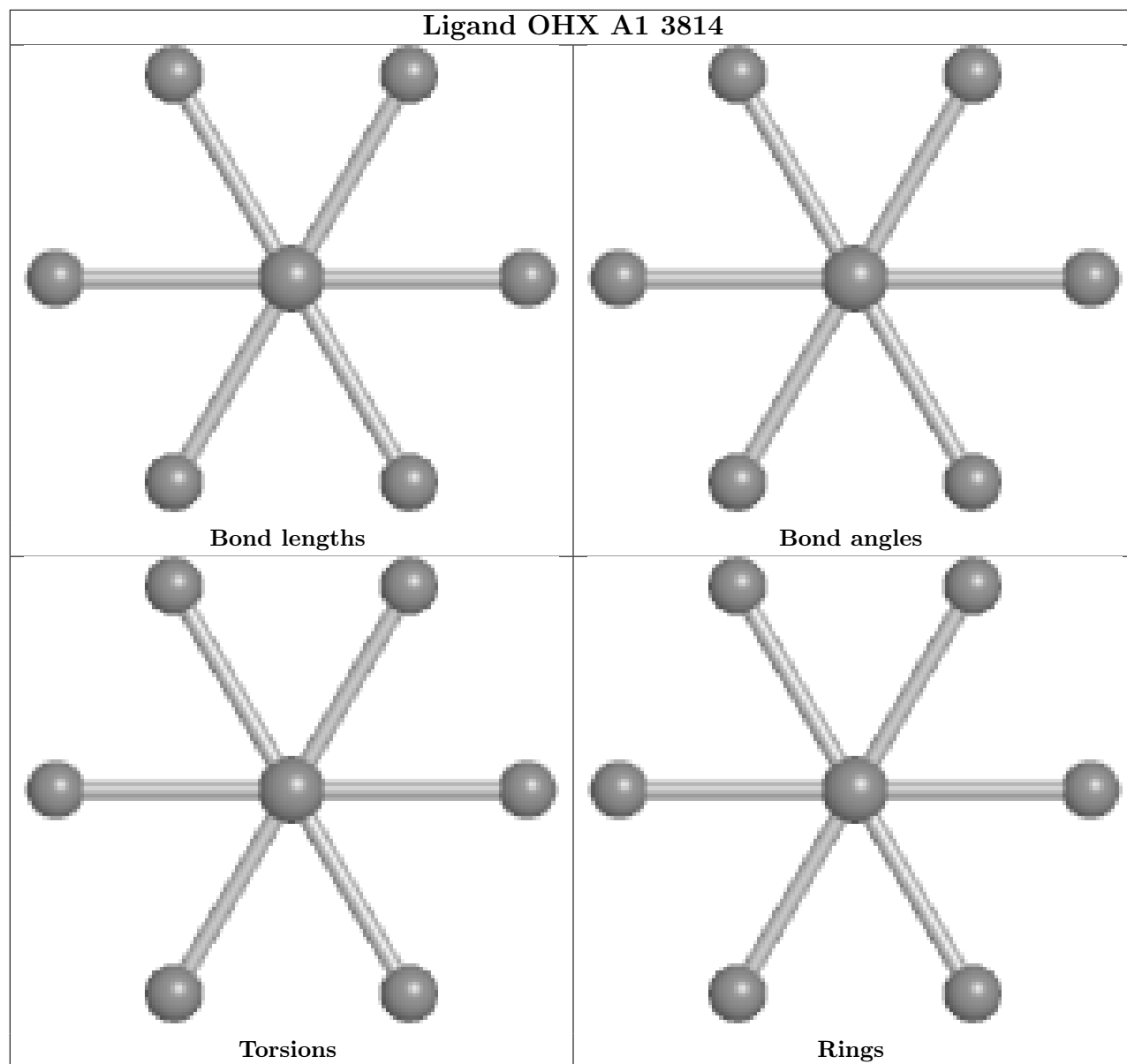


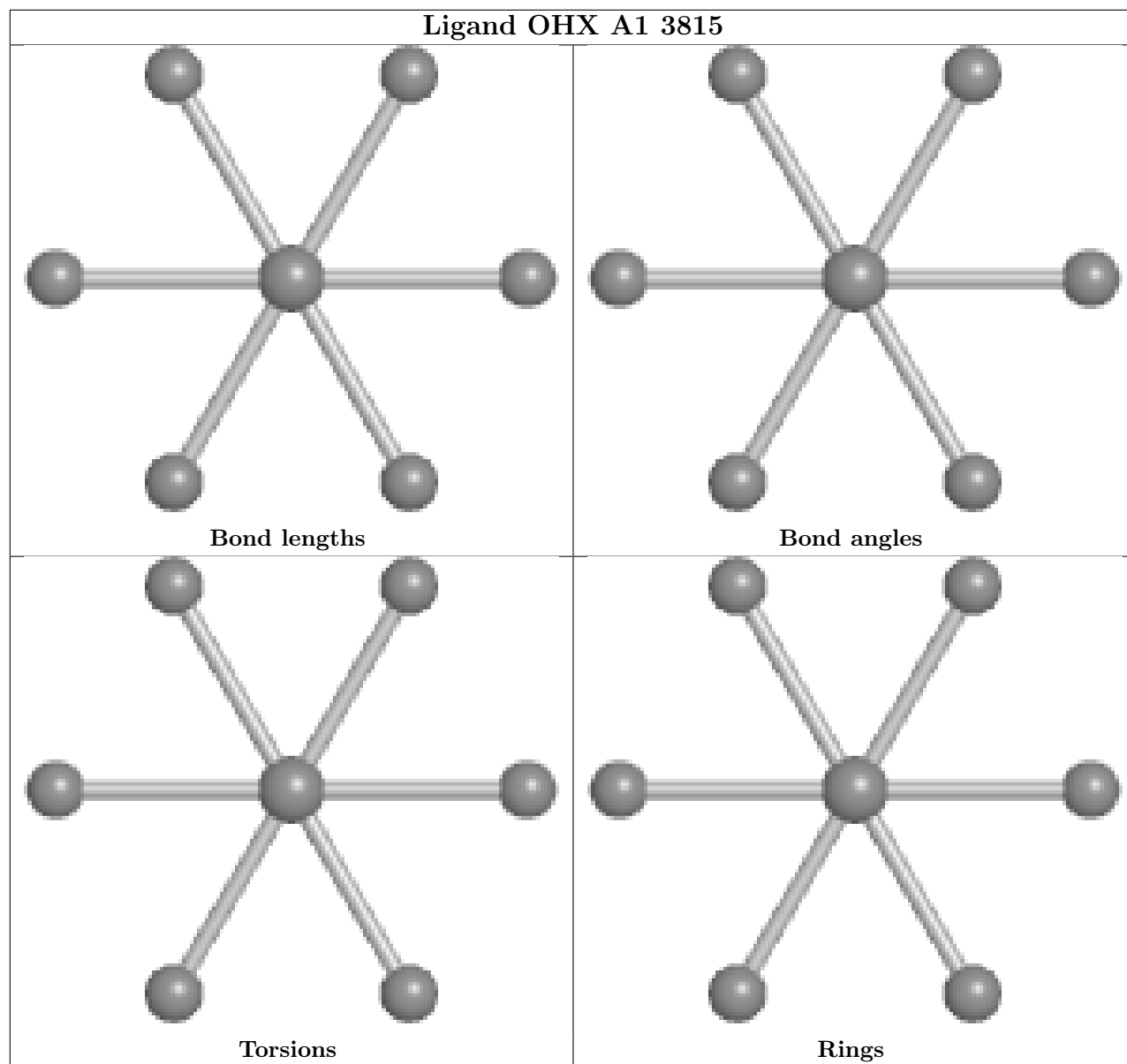


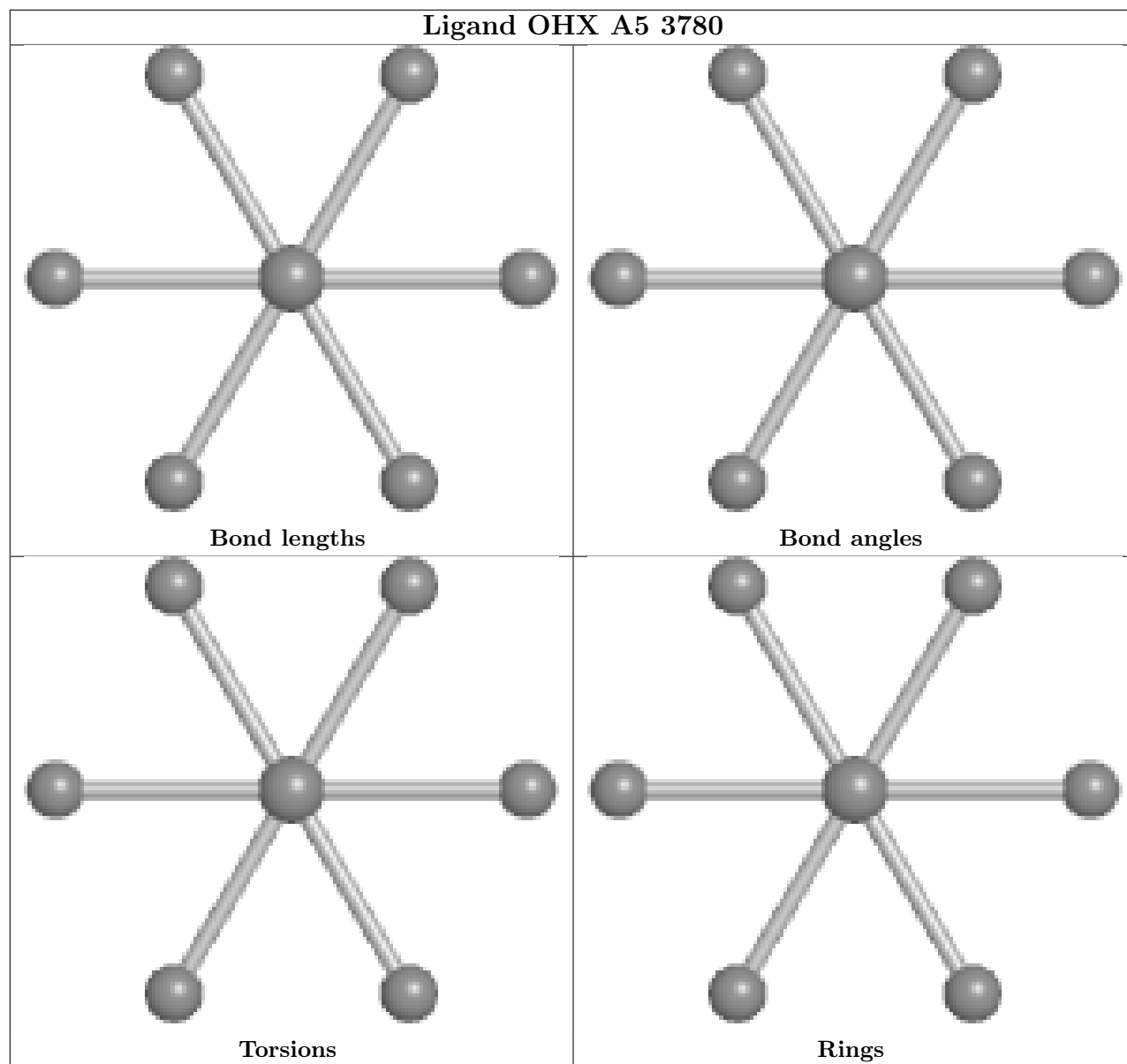


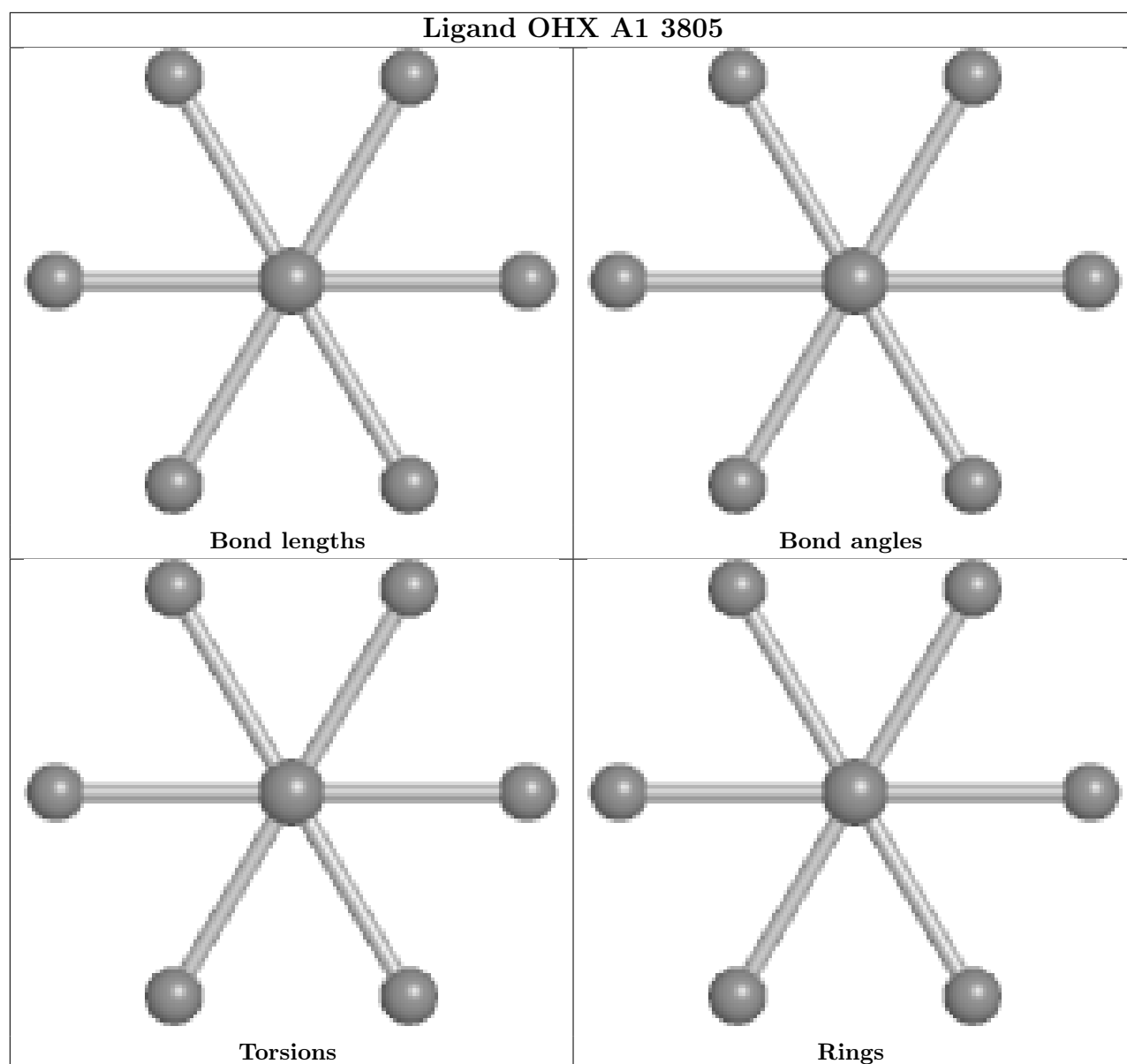












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A2	1767/1800 (98%)	0.00	39 (2%) 62 33	49, 88, 220, 373	0
2	AA	206/252 (81%)	0.20	5 (2%) 59 30	71, 111, 170, 202	0
2	CA	206/252 (81%)	0.14	2 (0%) 82 59	60, 90, 133, 228	0
3	AB	214/255 (83%)	0.64	28 (13%) 3 1	79, 144, 219, 256	0
3	CB	216/255 (84%)	0.04	0 100 100	59, 85, 127, 171	0
4	AC	217/254 (85%)	0.09	2 (0%) 84 63	60, 91, 130, 170	0
4	CC	217/254 (85%)	0.09	6 (2%) 53 25	50, 75, 127, 193	0
5	AD	223/240 (92%)	0.34	8 (3%) 42 17	69, 97, 154, 222	0
5	CD	223/240 (92%)	0.23	4 (1%) 68 40	56, 91, 144, 182	0
6	AE	260/261 (99%)	0.24	8 (3%) 49 21	60, 89, 131, 187	0
6	CE	260/261 (99%)	0.02	1 (0%) 92 79	48, 74, 112, 237	0
7	AF	206/225 (91%)	0.22	9 (4%) 34 13	72, 116, 160, 231	0
7	CF	206/225 (91%)	0.12	6 (2%) 51 23	53, 87, 143, 207	0
8	AG	226/236 (95%)	0.38	7 (3%) 49 21	58, 102, 153, 209	0
8	CG	218/236 (92%)	0.22	6 (2%) 53 25	49, 83, 140, 239	0
9	AH	184/190 (96%)	0.23	2 (1%) 80 56	75, 121, 178, 259	0
9	CH	186/190 (97%)	0.06	2 (1%) 80 56	64, 102, 162, 222	0
10	AI	188/200 (94%)	0.11	4 (2%) 63 34	48, 76, 132, 165	0
10	CI	188/200 (94%)	-0.01	0 100 100	41, 68, 116, 154	0
11	AJ	185/197 (93%)	0.69	13 (7%) 16 5	70, 101, 163, 231	0
11	CJ	185/197 (93%)	0.13	3 (1%) 72 44	55, 78, 138, 196	0
12	AK	96/105 (91%)	0.21	1 (1%) 82 59	71, 101, 164, 198	0
12	CK	96/105 (91%)	0.71	10 (10%) 6 2	77, 116, 163, 222	0
13	AL	155/156 (99%)	0.48	13 (8%) 11 3	48, 71, 176, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CL	146/156 (93%)	0.37	9 (6%) 20 7	41, 63, 134, 219	0
14	AM	124/143 (86%)	0.80	24 (19%) 1 0	97, 148, 209, 234	0
14	CM	124/143 (86%)	1.84	40 (32%) 0 0	121, 191, 250, 311	0
15	AN	150/151 (99%)	0.08	1 (0%) 87 69	57, 89, 127, 183	0
15	CN	150/151 (99%)	-0.22	0 100 100	49, 73, 109, 130	0
16	AO	127/137 (92%)	0.85	18 (14%) 2 1	61, 134, 179, 240	0
16	CO	128/137 (93%)	0.08	1 (0%) 86 65	50, 84, 118, 140	0
17	AP	124/142 (87%)	0.35	2 (1%) 72 44	68, 93, 167, 197	0
17	CP	135/142 (95%)	0.16	10 (7%) 14 4	61, 93, 166, 196	0
18	AQ	141/143 (98%)	0.67	12 (8%) 10 3	72, 100, 138, 155	0
18	CQ	142/143 (99%)	0.33	4 (2%) 53 25	53, 79, 121, 171	0
19	AR	120/136 (88%)	0.06	2 (1%) 70 41	66, 112, 180, 214	0
19	CR	117/136 (86%)	0.01	2 (1%) 70 41	58, 88, 142, 199	0
20	AS	145/146 (99%)	0.66	15 (10%) 6 2	57, 104, 156, 182	0
20	CS	145/146 (99%)	0.03	2 (1%) 75 49	56, 79, 138, 165	0
21	AT	143/144 (99%)	0.37	4 (2%) 53 25	73, 102, 147, 180	0
21	CT	143/144 (99%)	0.03	0 100 100	48, 74, 114, 181	0
22	AU	107/121 (88%)	0.69	10 (9%) 8 3	64, 102, 189, 226	0
22	CU	110/121 (90%)	0.83	12 (10%) 5 2	56, 93, 183, 243	0
23	AV	87/87 (100%)	0.13	0 100 100	75, 102, 151, 169	0
23	CV	87/87 (100%)	-0.03	1 (1%) 80 56	54, 79, 118, 185	0
24	AW	129/130 (99%)	0.03	0 100 100	58, 82, 103, 121	0
24	CW	129/130 (99%)	0.00	0 100 100	40, 62, 77, 98	0
25	AX	144/145 (99%)	0.24	1 (0%) 87 69	48, 68, 98, 150	0
25	CX	144/145 (99%)	-0.04	0 100 100	37, 53, 80, 139	0
26	AY	134/135 (99%)	0.29	3 (2%) 62 33	70, 106, 166, 216	0
26	CY	134/135 (99%)	0.06	3 (2%) 62 33	57, 84, 143, 191	0
27	AZ	70/108 (64%)	0.49	5 (7%) 16 5	88, 132, 172, 235	0
27	CZ	69/108 (63%)	0.30	5 (7%) 15 4	68, 103, 151, 196	0
28	Aa	97/119 (81%)	1.31	24 (24%) 0 0	69, 113, 206, 223	0
28	Ca	97/119 (81%)	0.27	1 (1%) 82 59	54, 79, 129, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	Ab	81/82 (98%)	0.22	3 (3%) 41 17	68, 102, 188, 225	0
29	Cb	81/82 (98%)	0.06	0 100 100	51, 85, 170, 203	0
30	Ac	63/67 (94%)	0.36	3 (4%) 30 11	86, 130, 182, 204	0
30	Cc	63/67 (94%)	0.54	6 (9%) 8 3	74, 107, 155, 180	0
31	Ad	53/56 (94%)	0.23	2 (3%) 40 16	64, 76, 106, 155	0
31	Cd	53/56 (94%)	0.35	3 (5%) 23 8	51, 69, 108, 168	0
32	Ae	60/63 (95%)	0.87	10 (16%) 1 0	56, 103, 179, 270	0
32	Ce	62/63 (98%)	0.09	4 (6%) 18 5	47, 84, 184, 218	0
33	Af	51/152 (33%)	0.56	5 (9%) 7 2	92, 138, 186, 202	0
33	Cf	51/152 (33%)	1.39	11 (21%) 0 0	113, 172, 222, 254	0
34	Ag	318/319 (99%)	0.21	10 (3%) 49 21	74, 113, 171, 237	0
34	Cg	318/319 (99%)	0.51	17 (5%) 26 10	73, 105, 158, 232	0
35	Ah	121/273 (44%)	0.39	6 (4%) 28 10	54, 99, 162, 212	0
36	A1	3149/3396 (92%)	0.03	23 (0%) 87 69	29, 54, 168, 351	0
36	A5	3150/3396 (92%)	0.06	36 (1%) 80 56	28, 52, 157, 346	0
37	A3	121/121 (100%)	-0.10	0 100 100	34, 72, 92, 118	0
37	A7	121/121 (100%)	0.03	0 100 100	31, 57, 74, 144	0
38	A4	158/158 (100%)	0.05	1 (0%) 89 72	37, 58, 112, 223	0
38	A8	158/158 (100%)	0.02	1 (0%) 89 72	39, 65, 128, 263	0
39	BA	252/254 (99%)	0.03	1 (0%) 92 79	27, 53, 78, 150	0
39	DA	252/254 (99%)	0.11	7 (2%) 53 25	29, 55, 83, 177	0
40	BB	386/387 (99%)	-0.05	1 (0%) 94 84	26, 58, 86, 187	0
40	DB	386/387 (99%)	-0.21	0 100 100	20, 44, 69, 188	0
41	BC	361/362 (99%)	-0.23	0 100 100	26, 50, 86, 132	0
41	DC	361/362 (99%)	-0.16	0 100 100	30, 56, 90, 136	0
42	BD	296/297 (99%)	-0.05	2 (0%) 87 69	47, 81, 132, 223	0
42	DD	294/297 (98%)	-0.07	2 (0%) 87 69	38, 58, 110, 205	0
43	BE	156/176 (88%)	-0.23	0 100 100	34, 52, 89, 152	0
43	DE	157/176 (89%)	-0.11	2 (1%) 77 51	37, 54, 97, 160	0
44	BF	222/244 (90%)	-0.23	1 (0%) 91 75	31, 46, 87, 247	0
44	DF	223/244 (91%)	-0.22	0 100 100	26, 44, 99, 196	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	BG	233/256 (91%)	-0.05	1 (0%) 92 79	52, 79, 148, 255	0
45	DG	231/256 (90%)	0.05	3 (1%) 77 51	63, 88, 132, 196	0
46	BH	191/191 (100%)	0.03	1 (0%) 91 75	44, 65, 99, 197	0
46	DH	191/191 (100%)	-0.26	1 (0%) 91 75	30, 47, 83, 206	0
47	BI	211/221 (95%)	-0.09	1 (0%) 91 75	37, 60, 121, 229	0
47	DI	213/221 (96%)	0.12	4 (1%) 66 37	34, 60, 106, 207	0
48	BJ	169/174 (97%)	0.18	2 (1%) 79 54	50, 84, 123, 151	0
48	DJ	169/174 (97%)	-0.11	0 100 100	40, 64, 98, 123	0
49	BL	193/199 (96%)	-0.22	0 100 100	30, 57, 126, 216	0
49	DL	194/199 (97%)	0.06	0 100 100	38, 69, 134, 174	0
50	BM	136/138 (98%)	-0.14	0 100 100	37, 55, 92, 132	0
50	DM	137/138 (99%)	-0.30	0 100 100	30, 47, 83, 153	0
51	BN	203/204 (99%)	-0.06	0 100 100	32, 52, 68, 92	0
51	DN	203/204 (99%)	0.09	0 100 100	37, 60, 82, 104	0
52	BO	217/219 (99%)	0.02	0 100 100	26, 51, 97, 114	40 (18%)
52	DO	217/219 (99%)	-0.00	0 100 100	22, 41, 91, 118	40 (18%)
53	BP	183/184 (99%)	0.23	7 (3%) 40 16	30, 49, 149, 224	0
53	DP	155/184 (84%)	-0.20	0 100 100	30, 44, 72, 161	0
54	BQ	185/186 (99%)	-0.17	0 100 100	33, 48, 68, 107	0
54	DQ	185/186 (99%)	-0.08	0 100 100	35, 54, 73, 125	0
55	BR	188/189 (99%)	0.00	3 (1%) 72 44	45, 71, 170, 201	0
55	DR	188/189 (99%)	-0.04	4 (2%) 63 34	36, 64, 142, 199	0
56	BS	172/172 (100%)	-0.06	2 (1%) 79 54	36, 51, 85, 123	0
56	DS	172/172 (100%)	-0.20	2 (1%) 79 54	26, 44, 72, 141	0
57	BT	159/160 (99%)	-0.18	0 100 100	33, 52, 111, 149	0
57	DT	159/160 (99%)	-0.13	0 100 100	30, 46, 97, 120	0
58	BU	100/121 (82%)	-0.02	3 (3%) 50 22	79, 108, 150, 180	0
58	DU	98/121 (80%)	0.36	7 (7%) 16 5	67, 97, 128, 168	0
59	BV	136/137 (99%)	-0.02	0 100 100	35, 57, 95, 182	0
59	DV	136/137 (99%)	-0.03	3 (2%) 62 33	26, 42, 78, 210	0
60	BW	98/155 (63%)	1.53	22 (22%) 0 0	47, 77, 244, 306	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	DW	135/155 (87%)	0.36	10 (7%) 14 4	36, 94, 192, 249	0
61	BX	121/142 (85%)	-0.03	1 (0%) 86 65	41, 68, 99, 152	0
61	DX	120/142 (84%)	0.07	1 (0%) 86 65	46, 71, 108, 135	0
62	BY	126/127 (99%)	-0.10	1 (0%) 86 65	38, 59, 91, 150	0
62	DY	126/127 (99%)	0.08	0 100 100	39, 66, 102, 168	0
63	BZ	135/136 (99%)	0.23	3 (2%) 62 33	68, 94, 138, 162	0
63	DZ	135/136 (99%)	0.23	3 (2%) 62 33	68, 103, 142, 170	0
64	Ba	148/149 (99%)	-0.07	0 100 100	26, 50, 89, 116	0
64	Da	148/149 (99%)	0.00	0 100 100	28, 55, 93, 142	0
65	Bb	58/59 (98%)	0.10	1 (1%) 70 41	33, 58, 119, 142	0
65	Db	58/59 (98%)	0.10	2 (3%) 45 19	35, 59, 123, 160	0
66	Bc	97/105 (92%)	-0.05	0 100 100	63, 88, 129, 171	0
66	Dc	100/105 (95%)	0.19	4 (4%) 38 15	59, 86, 154, 173	0
67	Bd	109/113 (96%)	0.12	3 (2%) 53 25	40, 66, 132, 202	0
67	Dd	109/113 (96%)	-0.08	0 100 100	34, 57, 126, 199	0
68	Be	127/130 (97%)	0.00	3 (2%) 59 30	22, 42, 65, 149	0
68	De	127/130 (97%)	-0.07	2 (1%) 72 44	25, 47, 77, 136	0
69	Bf	106/107 (99%)	-0.13	1 (0%) 84 63	30, 41, 73, 139	0
69	Df	106/107 (99%)	-0.15	0 100 100	27, 40, 75, 119	0
70	Bg	112/121 (92%)	0.29	3 (2%) 54 26	44, 71, 134, 197	0
70	Dg	112/121 (92%)	0.09	2 (1%) 68 40	41, 72, 139, 191	0
71	Bh	119/120 (99%)	-0.08	1 (0%) 86 65	42, 68, 104, 119	0
71	Dh	119/120 (99%)	0.07	1 (0%) 86 65	51, 75, 109, 149	0
72	Bi	99/100 (99%)	-0.03	0 100 100	45, 69, 111, 172	0
72	Di	99/100 (99%)	0.06	1 (1%) 82 59	57, 75, 116, 171	0
73	Bj	87/88 (98%)	0.06	1 (1%) 80 56	35, 45, 74, 216	0
73	Dj	87/88 (98%)	0.28	2 (2%) 60 31	30, 50, 91, 241	0
74	Bk	77/78 (98%)	-0.21	0 100 100	65, 95, 146, 168	0
74	Dk	77/78 (98%)	0.16	1 (1%) 77 51	64, 98, 138, 153	0
75	Bl	50/51 (98%)	0.23	0 100 100	37, 59, 80, 95	0
75	Dl	50/51 (98%)	0.19	1 (2%) 65 36	44, 59, 82, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	Bm	52/128 (40%)	0.01	2 (3%) 40 16	42, 55, 82, 139	0
76	Dm	52/128 (40%)	0.01	1 (1%) 66 37	30, 39, 68, 106	0
77	Bn	25/25 (100%)	0.49	1 (4%) 38 15	49, 62, 79, 94	0
77	Dn	25/25 (100%)	0.28	0 100 100	37, 55, 72, 99	0
78	Bo	105/106 (99%)	0.07	1 (0%) 82 59	35, 60, 97, 219	0
78	Do	105/106 (99%)	0.05	2 (1%) 66 37	37, 59, 101, 157	0
79	Bp	91/92 (98%)	-0.11	0 100 100	40, 61, 104, 126	0
79	Dp	91/92 (98%)	-0.07	1 (1%) 80 56	29, 60, 96, 111	0
80	A6	1769/1800 (98%)	0.02	32 (1%) 68 40	38, 72, 189, 360	0
81	Ch	63/273 (23%)	0.52	5 (7%) 12 4	50, 99, 156, 183	0
82	DK	0/155	-	-	-	-
83	Dq	120/312 (38%)	0.53	7 (5%) 23 7	70, 109, 166, 232	0
84	Dr	0/47	-	-	-	-
85	Ds	0/46	-	-	-	-
All	All	32947/35856 (91%)	0.09	713 (2%) 62 33	20, 71, 157, 373	80 (0%)

All (713) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	BW	76	VAL	21.3
16	AO	15	GLY	17.6
60	BW	75	THR	16.9
60	BW	86	SER	14.2
33	Cf	145	HIS	13.6
14	CM	20	ALA	13.6
13	CL	3	THR	13.2
53	BP	161	ALA	12.6
60	BW	85	ALA	11.9
1	A2	1693	A	11.4
36	A1	1955	U	11.1
14	CM	21	GLU	10.9
60	BW	84	GLY	10.5
40	BB	387	LEU	10.0
53	BP	184	ALA	9.8
3	AB	20	VAL	9.7
73	Dj	88	ALA	9.0
1	A2	1708	U	9.0
11	AJ	181	ALA	8.8

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Mol	Chain	Res	Type	RSRZ
47	DI	221	ALA	8.5
14	CM	22	VAL	8.2
1	A2	656	G	8.2
22	CU	98	GLN	8.2
36	A1	1350	A	7.9
1	A2	1692	G	7.9
78	Bo	106	PHE	7.9
14	CM	23	THR	7.9
71	Dh	120	ALA	7.8
28	Aa	62	TYR	7.7
14	CM	126	TRP	7.6
1	A2	1709	C	7.6
33	Af	145	HIS	7.4
33	Cf	110	ALA	7.3
12	CK	93	GLN	7.1
14	AM	85	LYS	7.1
12	CK	98	THR	7.1
14	CM	105	LYS	7.0
14	CM	85	LYS	6.9
14	CM	84	ASN	6.9
36	A5	2873	U	6.9
60	BW	69	LYS	6.8
83	Dq	192	ASP	6.8
13	AL	145	ALA	6.8
4	CC	90	THR	6.7
36	A1	1349	G	6.6
36	A5	2503	G	6.5
17	CP	4	ALA	6.5
36	A1	1351	U	6.4
66	Dc	6	SER	6.4
1	A2	134	U	6.3
36	A5	2506	U	6.3
1	A2	658	C	6.2
17	CP	135	THR	6.2
60	BW	88	ASP	6.2
32	Ae	46	ASN	6.2
34	Cg	2	ALA	6.1
73	Dj	87	SER	6.1
1	A2	1059	U	6.1
60	BW	89	LEU	6.0
22	AU	121	ASN	6.0
36	A5	1349	G	6.0

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Mol	Chain	Res	Type	RSRZ
47	DI	111	LEU	5.9
60	BW	83	THR	5.9
60	BW	90	ILE	5.8
39	DA	253	GLN	5.8
31	Cd	4	GLU	5.8
36	A5	1350	A	5.8
34	Cg	214	ALA	5.6
14	CM	56	GLU	5.6
1	A2	1711	C	5.5
73	Bj	87	SER	5.5
11	AJ	95	TYR	5.5
56	BS	1	MET	5.5
11	AJ	182	GLU	5.4
33	Cf	134	ASN	5.4
63	DZ	2	ALA	5.4
3	AB	26	ARG	5.4
42	DD	296	GLN	5.3
59	DV	2	SER	5.3
80	A6	493	U	5.3
1	A2	719	U	5.3
36	A5	1566	A	5.2
60	BW	87	LEU	5.2
3	AB	138	PHE	5.2
31	Ad	4	GLU	5.1
7	AF	152	GLY	5.1
80	A6	718	U	5.1
36	A5	2505	U	5.1
11	CJ	2	PRO	5.1
13	CL	2	SER	5.0
22	CU	121	ASN	5.0
36	A5	1025	A	5.0
22	CU	107	THR	5.0
10	AI	21	PHE	5.0
7	AF	37	GLN	5.0
34	Cg	3	SER	4.9
14	CM	128	ALA	4.9
11	AJ	2	PRO	4.9
27	AZ	88	ILE	4.9
29	Ab	38	PRO	4.9
35	Ah	88	ARG	4.8
1	A2	1690	G	4.7
60	BW	77	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
36	A1	1352	A	4.7
13	CL	5	LEU	4.7
60	BW	78	ALA	4.7
7	CF	37	GLN	4.6
8	CG	169	TYR	4.6
1	A2	135	A	4.6
38	A4	82	U	4.6
7	AF	36	ALA	4.5
29	Ab	41	LEU	4.5
14	CM	124	LYS	4.5
68	Be	128	LEU	4.5
32	Ae	61	SER	4.5
31	Cd	5	ASN	4.5
13	CL	145	ALA	4.5
80	A6	678	A	4.5
36	A5	1567	U	4.5
12	CK	94	GLU	4.4
18	AQ	143	ARG	4.4
2	CA	186	GLY	4.4
22	CU	18	GLN	4.4
27	AZ	71	ILE	4.4
20	AS	32	LEU	4.4
11	AJ	186	GLU	4.3
61	BX	24	LEU	4.3
1	A2	715	U	4.3
1	A2	913	G	4.3
61	DX	23	ALA	4.3
1	A2	657	U	4.3
80	A6	506	A	4.3
55	DR	184	LEU	4.3
53	BP	162	GLU	4.2
13	AL	148	LYS	4.2
36	A1	1569	U	4.2
81	Ch	83	LYS	4.2
53	BP	160	ALA	4.2
79	Dp	2	ALA	4.2
60	BW	95	SER	4.2
14	CM	123	VAL	4.2
2	AA	28	ASN	4.2
14	CM	125	ASN	4.2
47	DI	112	GLN	4.1
80	A6	494	U	4.1

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Mol	Chain	Res	Type	RSRZ
13	AL	146	ALA	4.1
62	BY	127	GLU	4.1
7	AF	41	LYS	4.1
36	A5	2504	U	4.1
16	AO	16	VAL	4.1
13	AL	2	SER	4.1
3	AB	46	THR	4.1
45	DG	120	LYS	4.1
32	Ae	54	ARG	4.1
17	AP	89	MET	4.1
9	CH	187	SER	4.1
34	Ag	102	ARG	4.0
60	DW	66	GLU	4.0
80	A6	1710	U	4.0
22	CU	105	GLN	4.0
17	CP	5	VAL	4.0
33	Af	143	LYS	4.0
13	CL	4	GLU	4.0
17	CP	136	SER	4.0
17	CP	134	THR	3.9
36	A1	1568	U	3.9
8	CG	216	LEU	3.9
39	DA	249	SER	3.9
18	AQ	20	ALA	3.9
28	Aa	63	ALA	3.9
60	DW	67	VAL	3.9
1	A2	1710	U	3.9
11	AJ	180	LYS	3.9
3	AB	25	THR	3.9
28	Aa	65	PRO	3.9
2	AA	44	GLY	3.8
1	A2	261	U	3.8
80	A6	679	U	3.8
59	DV	3	GLY	3.8
20	AS	145	ARG	3.8
11	AJ	3	ARG	3.8
1	A2	506	A	3.8
80	A6	495	C	3.8
18	AQ	141	SER	3.8
3	AB	94	LYS	3.7
60	DW	133	THR	3.7
16	AO	41	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
60	BW	68	ALA	3.7
1	A2	1691	A	3.7
14	CM	127	GLY	3.7
14	AM	137	MET	3.7
35	Ah	85	SER	3.7
36	A5	1352	A	3.7
3	AB	102	GLY	3.6
1	A2	495	C	3.6
13	AL	156	PHE	3.6
28	Aa	2	PRO	3.6
67	Bd	82	GLU	3.6
55	DR	187	GLU	3.6
13	AL	151	LYS	3.6
20	AS	2	SER	3.6
60	DW	68	ALA	3.6
34	Ag	319	ASN	3.6
14	CM	121	VAL	3.5
36	A1	2539	C	3.5
21	AT	71	VAL	3.5
60	DW	130	SER	3.5
1	A2	1370	U	3.5
36	A5	1351	U	3.5
20	AS	39	GLY	3.5
36	A5	1568	U	3.5
38	A8	81	U	3.5
13	AL	152	GLN	3.5
59	DV	4	ASN	3.5
1	A2	194	U	3.5
14	CM	41	LEU	3.5
36	A1	1952	G	3.5
14	CM	133	LEU	3.5
12	CK	25	LYS	3.5
28	Aa	8	ASN	3.4
32	Ce	63	GLN	3.4
16	AO	79	VAL	3.4
39	BA	253	GLN	3.4
36	A1	1566	A	3.4
18	AQ	29	ILE	3.4
36	A5	1580	A	3.4
1	A2	238	U	3.4
33	Cf	111	GLU	3.4
70	Bg	110	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
80	A6	658	C	3.4
35	Ah	89	ARG	3.3
14	CM	92	ALA	3.3
16	AO	27	PHE	3.3
18	AQ	132	LYS	3.3
53	BP	183	ALA	3.3
18	AQ	11	GLY	3.3
60	BW	94	ARG	3.3
80	A6	490	C	3.3
18	AQ	36	ILE	3.3
60	BW	67	VAL	3.3
27	CZ	86	GLU	3.3
32	Ae	53	LYS	3.3
30	Cc	65	ARG	3.3
26	CY	2	SER	3.3
36	A1	2873	U	3.3
16	AO	17	ALA	3.3
14	CM	33	ARG	3.2
22	AU	94	GLU	3.2
14	CM	59	LEU	3.2
20	AS	146	ALA	3.2
33	Cf	112	GLY	3.2
3	AB	21	VAL	3.2
76	Dm	128	LYS	3.2
20	AS	21	ASN	3.2
76	Bm	77	ILE	3.2
13	CL	30	ARG	3.2
20	CS	146	ALA	3.2
28	Aa	45	VAL	3.2
18	CQ	143	ARG	3.2
13	AL	30	ARG	3.2
28	Aa	20	PRO	3.2
56	DS	1	MET	3.2
4	CC	84	LYS	3.2
35	Ah	84	LYS	3.2
32	Ae	2	ALA	3.2
66	Dc	7	GLN	3.2
36	A5	1764	U	3.2
47	DI	103	LEU	3.2
14	AM	108	ARG	3.2
43	DE	129	GLU	3.1
67	Bd	79	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
4	AC	250	GLN	3.1
3	AB	131	ASP	3.1
28	Aa	98	PRO	3.1
80	A6	1708	U	3.1
12	CK	64	TYR	3.1
42	DD	270	LYS	3.1
14	CM	43	ARG	3.1
18	AQ	142	TYR	3.1
30	Cc	67	ARG	3.1
36	A1	1570	U	3.1
18	CQ	114	ARG	3.1
17	CP	7	ALA	3.1
44	BF	27	ALA	3.1
58	DU	52	ASN	3.1
36	A5	1581	C	3.1
80	A6	1371	A	3.1
66	Dc	105	ALA	3.1
19	CR	87	GLU	3.1
22	AU	105	GLN	3.1
80	A6	656	G	3.1
60	BW	66	GLU	3.1
3	AB	140	ILE	3.1
27	CZ	88	ILE	3.1
36	A5	1569	U	3.1
36	A5	2874	G	3.1
14	CM	62	LEU	3.0
14	CM	112	ALA	3.0
22	AU	19	ILE	3.0
14	CM	116	VAL	3.0
36	A1	2205	U	3.0
22	CU	99	ILE	3.0
8	AG	154	ARG	3.0
80	A6	676	G	3.0
3	AB	84	ILE	3.0
13	AL	3	THR	3.0
3	AB	101	HIS	3.0
5	CD	151	LYS	3.0
65	Bb	25	LYS	3.0
36	A5	2403	G	3.0
36	A5	2871	G	3.0
9	AH	98	ILE	3.0
20	AS	15	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
58	BU	9	GLN	3.0
21	AT	5	SER	2.9
22	AU	120	SER	2.9
16	AO	89	THR	2.9
3	AB	130	SER	2.9
26	AY	70	VAL	2.9
7	AF	43	PHE	2.9
81	Ch	52	PRO	2.9
8	AG	190	GLN	2.9
14	AM	62	LEU	2.9
28	Aa	18	VAL	2.9
81	Ch	50	ASN	2.9
13	CL	146	ALA	2.9
1	A2	493	U	2.9
36	A5	3275	U	2.9
34	Cg	92	TRP	2.9
14	AM	36	LEU	2.9
14	CM	31	VAL	2.9
33	Cf	147	VAL	2.9
34	Ag	51	ASP	2.9
20	AS	8	GLN	2.9
22	CU	17	GLN	2.9
39	DA	248	GLY	2.9
5	CD	86	LEU	2.8
22	CU	93	LEU	2.8
8	AG	175	ILE	2.8
22	CU	97	VAL	2.8
11	AJ	5	PRO	2.8
14	AM	141	SER	2.8
35	Ah	87	THR	2.8
32	Ce	62	VAL	2.8
60	BW	98	PRO	2.8
3	AB	29	TRP	2.8
36	A1	3155	U	2.8
1	A2	1686	C	2.8
1	A2	280	U	2.8
80	A6	487	G	2.8
80	A6	677	G	2.8
3	AB	47	LEU	2.8
14	CM	114	LYS	2.8
28	Aa	85	ARG	2.8
27	AZ	89	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
34	Cg	244	ALA	2.8
4	CC	89	GLN	2.8
12	CK	43	ILE	2.8
83	Dq	44	GLU	2.8
5	AD	218	LEU	2.8
20	AS	17	LEU	2.8
36	A5	2539	C	2.8
1	A2	718	U	2.7
36	A5	2971	A	2.7
1	A2	1688	U	2.7
18	AQ	66	ARG	2.7
27	AZ	69	LEU	2.7
67	Bd	4	LEU	2.7
14	CM	64	SER	2.7
33	Cf	104	SER	2.7
63	BZ	2	ALA	2.7
8	CG	133	LEU	2.7
14	AM	84	ASN	2.7
32	Ce	49	LEU	2.7
78	Do	106	PHE	2.7
5	AD	142	LEU	2.7
36	A1	1581	C	2.7
36	A5	1016	C	2.7
80	A6	1709	C	2.7
33	Af	148	TYR	2.7
56	DS	2	ALA	2.7
70	Bg	78	GLY	2.7
42	BD	293	LEU	2.7
32	Ae	42	ARG	2.7
81	Ch	53	ARG	2.7
18	CQ	142	TYR	2.7
14	CM	28	LEU	2.7
27	AZ	73	GLY	2.7
58	BU	108	TYR	2.7
3	AB	50	LYS	2.7
20	AS	19	ASN	2.7
3	AB	103	MET	2.7
8	CG	162	VAL	2.7
7	CF	154	ALA	2.7
17	CP	9	LYS	2.6
20	AS	18	LEU	2.6
13	AL	155	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
55	DR	181	ARG	2.6
33	Af	149	LYS	2.6
42	BD	296	GLN	2.6
6	AE	261	LEU	2.6
3	AB	106	THR	2.6
36	A5	1565	G	2.6
16	AO	82	LYS	2.6
12	CK	95	ARG	2.6
34	Cg	167	VAL	2.6
34	Cg	314	GLN	2.6
34	Cg	279	ALA	2.6
60	BW	74	LYS	2.6
71	Bh	120	ALA	2.6
1	A2	1362	U	2.6
36	A1	3154	C	2.6
8	AG	149	LYS	2.6
68	De	128	LEU	2.6
7	CF	155	ALA	2.6
16	AO	11	SER	2.6
14	AM	110	GLY	2.6
58	DU	14	THR	2.6
60	DW	69	LYS	2.6
16	AO	76	ILE	2.6
36	A1	1353	U	2.6
39	DA	250	GLN	2.6
32	Ae	51	ASN	2.6
18	AQ	54	LEU	2.6
34	Cg	165	ASP	2.6
48	BJ	11	ASP	2.6
5	AD	50	ILE	2.6
4	CC	92	ALA	2.5
28	Aa	49	ALA	2.5
45	BG	116	VAL	2.5
28	Aa	31	PRO	2.5
80	A6	721	U	2.5
20	AS	76	PRO	2.5
22	AU	20	ILE	2.5
28	Aa	61	GLU	2.5
12	CK	97	PRO	2.5
80	A6	239	C	2.5
7	AF	70	VAL	2.5
22	AU	53	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
60	DW	135	SER	2.5
6	AE	25	GLY	2.5
16	AO	75	GLY	2.5
58	DU	13	LYS	2.5
34	Cg	252	LEU	2.5
14	CM	82	PRO	2.5
2	CA	185	ARG	2.5
3	AB	132	ASP	2.5
34	Cg	319	ASN	2.5
33	Cf	125	THR	2.5
81	Ch	51	ARG	2.5
7	AF	71	ALA	2.5
27	CZ	50	ILE	2.5
55	BR	186	LYS	2.5
83	Dq	88	PHE	2.5
1	A2	716	C	2.5
14	AM	129	GLU	2.5
26	CY	133	ASN	2.5
7	CF	151	GLY	2.5
28	Aa	35	ALA	2.5
58	DU	33	TYR	2.5
3	AB	85	LYS	2.4
11	CJ	148	VAL	2.4
30	Ac	44	VAL	2.4
8	CG	22	HIS	2.4
14	AM	26	ASP	2.4
10	AI	200	LYS	2.4
22	AU	84	MET	2.4
3	AB	93	GLY	2.4
39	DA	247	ARG	2.4
14	AM	136	ILE	2.4
72	Di	100	HIS	2.4
29	Ab	32	PHE	2.4
14	AM	111	ASN	2.4
13	AL	4	GLU	2.4
1	A2	132	U	2.4
36	A5	1570	U	2.4
80	A6	657	U	2.4
9	CH	93	LEU	2.4
75	Dl	2	ALA	2.4
28	Aa	69	ASN	2.4
2	AA	40	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
27	CZ	37	GLN	2.4
45	DG	109	LEU	2.4
36	A5	2507	C	2.4
63	DZ	56	LYS	2.4
14	CM	25	GLU	2.4
28	Aa	46	GLU	2.4
14	CM	87	PRO	2.4
5	AD	143	ARG	2.4
46	DH	191	LEU	2.4
36	A1	2522	G	2.4
13	CL	116	ARG	2.4
47	BI	221	ALA	2.4
20	AS	69	ILE	2.4
4	CC	87	GLN	2.4
80	A6	1711	C	2.4
46	BH	134	ILE	2.4
83	Dq	100	ILE	2.4
3	AB	209	ASN	2.4
28	Aa	60	PRO	2.4
22	CU	104	THR	2.4
34	Ag	79	TYR	2.4
34	Cg	79	TYR	2.4
26	AY	125	LEU	2.4
6	AE	134	LYS	2.3
80	A6	719	U	2.3
17	AP	101	ALA	2.3
3	AB	184	LEU	2.3
14	AM	59	LEU	2.3
12	CK	92	ILE	2.3
43	DE	130	ILE	2.3
55	BR	170	ARG	2.3
17	CP	6	ASN	2.3
2	AA	185	ARG	2.3
13	AL	149	ALA	2.3
30	Cc	66	LEU	2.3
13	AL	147	GLY	2.3
6	AE	123	LEU	2.3
18	CQ	141	SER	2.3
80	A6	675	U	2.3
80	A6	653	C	2.3
1	A2	714	G	2.3
26	AY	132	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
4	CC	88	LYS	2.3
22	CU	14	GLN	2.3
33	Cf	151	ASN	2.3
36	A5	440	A	2.3
14	AM	32	LEU	2.3
34	Ag	115	ILE	2.3
6	AE	260	GLY	2.3
13	CL	147	GLY	2.3
1	A2	494	U	2.3
18	AQ	92	TYR	2.3
6	AE	22	LYS	2.3
14	AM	88	LEU	2.3
5	AD	217	ILE	2.3
14	CM	60	VAL	2.3
36	A5	1572	U	2.3
53	BP	157	VAL	2.3
7	AF	151	GLY	2.3
33	Cf	143	LYS	2.3
16	AO	114	ARG	2.3
3	AB	55	LYS	2.3
31	Ad	5	ASN	2.3
6	CE	261	LEU	2.3
36	A1	1103	A	2.3
60	DW	132	GLY	2.3
34	Cg	51	ASP	2.3
16	AO	103	ARG	2.3
27	CZ	71	ILE	2.3
12	CK	79	TYR	2.3
16	AO	13	VAL	2.3
34	Ag	253	ALA	2.3
1	A2	729	G	2.2
63	BZ	99	GLU	2.2
20	CS	18	LEU	2.2
39	DA	252	THR	2.2
80	A6	1491	U	2.2
80	A6	1399	C	2.2
14	CM	63	VAL	2.2
21	AT	50	ALA	2.2
22	AU	54	GLY	2.2
36	A1	2445	A	2.2
32	Ae	48	THR	2.2
80	A6	794	U	2.2

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Mol	Chain	Res	Type	RSRZ
3	AB	28	GLU	2.2
36	A5	2444	C	2.2
80	A6	491	C	2.2
7	CF	156	ARG	2.2
4	AC	34	GLY	2.2
32	Ce	2	ALA	2.2
28	Aa	17	HIS	2.2
28	Aa	66	LYS	2.2
14	CM	86	VAL	2.2
66	Dc	100	ILE	2.2
17	CP	103	ASN	2.2
20	AS	44	ASN	2.2
34	Cg	227	ALA	2.2
16	AO	80	HIS	2.2
30	Ac	67	ARG	2.2
8	AG	182	GLN	2.2
33	Af	151	ASN	2.2
3	AB	83	LYS	2.2
3	AB	216	LYS	2.2
16	AO	116	GLU	2.2
3	AB	104	ASP	2.2
28	Aa	83	ILE	2.2
7	CF	152	GLY	2.2
36	A1	1762	C	2.2
14	CM	137	MET	2.2
39	DA	143	GLU	2.2
11	AJ	87	SER	2.2
80	A6	1398	U	2.2
26	CY	134	ALA	2.2
58	BU	89	LEU	2.2
35	Ah	101	ASP	2.2
83	Dq	104	ARG	2.2
14	AM	28	LEU	2.2
14	AM	50	LYS	2.2
55	BR	173	ARG	2.2
34	Cg	121	MET	2.2
2	AA	32	HIS	2.2
10	AI	199	LYS	2.2
14	AM	128	ALA	2.2
32	Ae	45	VAL	2.2
33	Cf	108	VAL	2.2
17	CP	128	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
34	Ag	181	TRP	2.1
65	Db	22	LYS	2.2
65	Db	25	LYS	2.2
1	A2	711	U	2.1
1	A2	1687	U	2.1
70	Dg	33	GLN	2.1
7	AF	68	ILE	2.1
18	AQ	39	VAL	2.1
30	Cc	43	ASN	2.1
21	AT	80	TYR	2.1
10	AI	8	ARG	2.1
32	Ae	39	LEU	2.1
15	AN	61	THR	2.1
34	Cg	253	ALA	2.1
48	BJ	96	PHE	2.1
22	CU	102	ARG	2.1
30	Cc	9	LEU	2.1
5	AD	54	ARG	2.1
14	CM	113	ARG	2.1
63	DZ	4	PHE	2.1
60	DW	65	GLU	2.1
74	Dk	69	LEU	2.1
80	A6	651	G	2.1
1	A2	696	C	2.1
6	AE	54	TYR	2.1
28	Aa	68	TYR	2.1
36	A1	1567	U	2.1
8	CG	147	LEU	2.1
11	AJ	177	ALA	2.1
14	CM	26	ASP	2.1
55	DR	183	ALA	2.1
14	AM	83	GLU	2.1
36	A5	1564	U	2.1
31	Cd	6	VAL	2.1
34	Ag	43	ILE	2.1
83	Dq	80	VAL	2.1
28	Aa	64	LEU	2.1
76	Bm	128	LYS	2.1
56	BS	2	ALA	2.1
1	A2	492	A	2.1
34	Ag	313	TRP	2.1
28	Ca	11	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
34	Cg	53	LYS	2.1
36	A5	2538	U	2.1
11	AJ	179	ARG	2.1
58	DU	15	PHE	2.1
53	BP	156	ALA	2.1
14	CM	122	VAL	2.1
11	CJ	3	ARG	2.1
12	AK	66	TYR	2.1
60	BW	65	GLU	2.1
11	AJ	6	ARG	2.1
23	CV	44	ARG	2.1
34	Ag	3	SER	2.1
14	CM	74	LEU	2.1
36	A5	249	U	2.1
1	A2	717	C	2.1
5	AD	122	VAL	2.1
28	Aa	89	ARG	2.1
69	Bf	60	ARG	2.1
45	DG	121	SER	2.1
58	DU	11	ILE	2.1
19	AR	2	GLY	2.1
30	Ac	66	LEU	2.1
8	AG	156	PHE	2.1
68	De	16	LYS	2.1
36	A1	1764	U	2.1
36	A5	1763	U	2.1
60	BW	81	PRO	2.1
80	A6	501	U	2.1
6	AE	133	LYS	2.0
16	AO	78	ALA	2.0
58	DU	98	THR	2.0
68	Be	127	ALA	2.0
78	Do	54	THR	2.0
14	AM	89	ILE	2.0
20	AS	35	ILE	2.0
14	CM	40	GLY	2.0
5	CD	178	ARG	2.0
19	CR	62	GLN	2.0
14	AM	41	LEU	2.0
60	DW	129	LYS	2.0
25	AX	144	ARG	2.0
22	AU	87	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
14	AM	20	ALA	2.0
16	CO	112	ILE	2.0
28	Aa	67	THR	2.0
63	BZ	70	PRO	2.0
80	A6	194	U	2.0
11	AJ	97	LEU	2.0
77	Bn	25	LYS	2.0
14	AM	104	GLY	2.0
16	AO	44	GLY	2.0
19	AR	123	ASN	2.0
36	A5	1017	C	2.0
5	AD	179	GLN	2.0
8	AG	199	GLN	2.0
14	AM	107	ASP	2.0
68	Be	26	HIS	2.0
70	Bg	113	LYS	2.0
83	Dq	25	LEU	2.0
36	A5	1571	A	2.0
30	Cc	45	LYS	2.0
70	Dg	102	LYS	2.0
5	CD	142	LEU	2.0
9	AH	58	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	A2	2209	1/1	-0.15	0.41	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A2	2227	1/1	-0.10	0.19	106,106,106,106	0
87	MG	A1	4299	1/1	-0.05	0.41	84,84,84,84	0
87	MG	A5	4515	1/1	0.02	0.41	109,109,109,109	0
87	MG	A1	4230	1/1	0.08	0.38	91,91,91,91	0
87	MG	A6	2250	1/1	0.10	0.46	96,96,96,96	0
87	MG	A5	4203	1/1	0.12	0.29	82,82,82,82	0
87	MG	A5	4353	1/1	0.13	0.61	71,71,71,71	0
88	ZN	Ab	101	1/1	0.13	0.12	327,327,327,327	0
87	MG	A5	4099	1/1	0.14	0.30	93,93,93,93	0
87	MG	A1	4150	1/1	0.16	0.60	95,95,95,95	0
87	MG	A1	4481	1/1	0.18	0.32	97,97,97,97	0
87	MG	A6	2259	1/1	0.19	0.66	119,119,119,119	0
87	MG	A5	4177	1/1	0.19	0.42	65,65,65,65	0
87	MG	A5	4254	1/1	0.20	0.66	103,103,103,103	0
87	MG	A6	2316	1/1	0.21	0.58	112,112,112,112	0
87	MG	AB	301	1/1	0.23	0.33	98,98,98,98	0
87	MG	A1	4109	1/1	0.23	0.37	80,80,80,80	0
87	MG	A1	4147	1/1	0.24	0.34	73,73,73,73	0
87	MG	A1	4477	1/1	0.25	0.29	108,108,108,108	0
87	MG	A5	4478	1/1	0.25	0.37	81,81,81,81	0
87	MG	A5	4581	1/1	0.26	0.36	97,97,97,97	0
87	MG	A1	3921	1/1	0.26	0.26	87,87,87,87	0
87	MG	A1	3919	1/1	0.27	0.98	138,138,138,138	0
87	MG	A5	4552	1/1	0.27	0.30	84,84,84,84	0
87	MG	A1	3851	1/1	0.27	0.26	53,53,53,53	0
87	MG	DJ	202	1/1	0.27	0.28	81,81,81,81	0
87	MG	A5	4497	1/1	0.27	0.29	76,76,76,76	0
87	MG	A1	4448	1/1	0.29	0.33	66,66,66,66	0
87	MG	A2	2219	1/1	0.29	0.24	93,93,93,93	0
87	MG	A5	4485	1/1	0.30	0.61	77,77,77,77	0
87	MG	DM	203	1/1	0.31	0.28	94,94,94,94	0
87	MG	A1	4454	1/1	0.33	0.35	81,81,81,81	0
87	MG	A2	2221	1/1	0.34	0.34	83,83,83,83	0
87	MG	A1	4359	1/1	0.34	0.27	70,70,70,70	0
87	MG	A6	2308	1/1	0.34	0.40	81,81,81,81	0
87	MG	A1	4104	1/1	0.34	0.21	65,65,65,65	0
87	MG	A5	4320	1/1	0.34	0.24	117,117,117,117	0
87	MG	A1	4387	1/1	0.35	0.54	89,89,89,89	0
87	MG	A1	4495	1/1	0.35	0.45	109,109,109,109	0
87	MG	A1	4232	1/1	0.35	0.57	75,75,75,75	0
87	MG	A5	4207	1/1	0.35	0.38	102,102,102,102	0
87	MG	A2	2211	1/1	0.36	0.76	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A2	2156	1/1	0.36	0.33	70,70,70,70	0
87	MG	A8	237	1/1	0.37	0.27	85,85,85,85	0
87	MG	A5	4084	1/1	0.37	0.79	112,112,112,112	0
87	MG	A6	2337	1/1	0.38	0.29	127,127,127,127	0
87	MG	A2	2208	1/1	0.38	0.24	109,109,109,109	0
87	MG	A5	4576	1/1	0.38	0.31	77,77,77,77	0
87	MG	A1	4228	1/1	0.38	0.33	82,82,82,82	0
87	MG	AJ	201	1/1	0.39	0.29	82,82,82,82	0
87	MG	A5	4230	1/1	0.39	0.30	78,78,78,78	0
87	MG	A1	4369	1/1	0.39	0.27	85,85,85,85	0
87	MG	A6	2133	1/1	0.39	0.29	65,65,65,65	0
87	MG	A1	4501	1/1	0.40	1.01	103,103,103,103	0
87	MG	A5	4283	1/1	0.40	0.69	79,79,79,79	0
87	MG	A6	2255	1/1	0.40	0.30	81,81,81,81	0
87	MG	A6	2244	1/1	0.41	0.65	97,97,97,97	0
87	MG	A6	2278	1/1	0.41	0.72	64,64,64,64	0
87	MG	A5	4341	1/1	0.41	0.27	96,96,96,96	0
87	MG	A1	4325	1/1	0.41	0.31	67,67,67,67	0
87	MG	A1	4370	1/1	0.41	0.25	104,104,104,104	0
87	MG	A5	4318	1/1	0.43	0.15	83,83,83,83	0
87	MG	A5	4569	1/1	0.43	1.00	103,103,103,103	0
87	MG	A6	2249	1/1	0.44	0.22	71,71,71,71	0
87	MG	A5	4575	1/1	0.44	0.50	68,68,68,68	0
87	MG	A1	4478	1/1	0.44	0.25	100,100,100,100	0
87	MG	A1	4502	1/1	0.44	0.25	93,93,93,93	0
87	MG	CY	203	1/1	0.44	0.24	109,109,109,109	0
87	MG	A1	4256	1/1	0.44	0.18	86,86,86,86	0
87	MG	A6	2262	1/1	0.44	0.49	101,101,101,101	0
87	MG	A1	4364	1/1	0.44	0.23	92,92,92,92	0
87	MG	A1	4313	1/1	0.45	0.22	105,105,105,105	0
87	MG	A3	229	1/1	0.45	0.31	99,99,99,99	0
87	MG	A5	4543	1/1	0.45	0.18	78,78,78,78	0
87	MG	A5	4464	1/1	0.45	0.51	85,85,85,85	0
87	MG	A2	2166	1/1	0.45	0.34	90,90,90,90	0
87	MG	A5	4324	1/1	0.45	0.23	80,80,80,80	0
87	MG	A1	4155	1/1	0.46	0.73	88,88,88,88	0
87	MG	A5	3929	1/1	0.46	0.33	80,80,80,80	0
87	MG	A2	2254	1/1	0.46	0.22	61,61,61,61	0
87	MG	A1	4337	1/1	0.46	0.54	108,108,108,108	0
87	MG	A2	2222	1/1	0.46	0.64	103,103,103,103	0
87	MG	A3	230	1/1	0.47	0.48	85,85,85,85	0
87	MG	A6	2129	1/1	0.47	0.28	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4392	1/1	0.47	0.25	64,64,64,64	0
87	MG	A2	2092	1/1	0.47	0.24	69,69,69,69	0
87	MG	A6	2182	1/1	0.47	0.15	63,63,63,63	0
87	MG	A6	2312	1/1	0.47	0.38	85,85,85,85	0
87	MG	A1	4088	1/1	0.48	0.29	90,90,90,90	0
87	MG	A5	4479	1/1	0.48	0.38	64,64,64,64	0
87	MG	A2	2187	1/1	0.48	0.21	90,90,90,90	0
87	MG	A5	4414	1/1	0.48	1.28	101,101,101,101	0
87	MG	A1	3994	1/1	0.48	0.38	64,64,64,64	0
87	MG	A5	4493	1/1	0.49	0.24	76,76,76,76	0
87	MG	A1	4048	1/1	0.50	0.21	67,67,67,67	0
87	MG	Cd	102	1/1	0.50	0.24	75,75,75,75	0
87	MG	DB	413	1/1	0.50	0.34	101,101,101,101	0
87	MG	A2	2167	1/1	0.50	0.33	72,72,72,72	0
87	MG	A1	4274	1/1	0.50	0.37	87,87,87,87	0
87	MG	A2	2256	1/1	0.50	0.71	80,80,80,80	0
87	MG	A5	4263	1/1	0.51	0.27	72,72,72,72	0
87	MG	A1	4319	1/1	0.51	0.31	76,76,76,76	0
87	MG	A5	4503	1/1	0.51	0.33	72,72,72,72	0
87	MG	A1	4135	1/1	0.51	0.41	96,96,96,96	0
87	MG	A1	4239	1/1	0.51	0.28	60,60,60,60	0
87	MG	A5	4545	1/1	0.51	0.39	94,94,94,94	0
87	MG	A1	4241	1/1	0.51	0.38	74,74,74,74	0
87	MG	A5	4075	1/1	0.51	0.38	60,60,60,60	0
87	MG	A1	4249	1/1	0.51	0.34	73,73,73,73	0
87	MG	A5	4377	1/1	0.51	0.32	85,85,85,85	0
87	MG	A1	4184	1/1	0.51	0.36	81,81,81,81	0
87	MG	A1	4221	1/1	0.51	0.16	92,92,92,92	0
87	MG	A1	4288	1/1	0.51	0.38	81,81,81,81	0
87	MG	BV	201	1/1	0.51	0.22	95,95,95,95	0
87	MG	A1	3922	1/1	0.51	0.45	107,107,107,107	0
86	OHX	A6	2095	7/7	0.51	0.46	213,213,213,213	7
87	MG	A1	4047	1/1	0.52	0.24	98,98,98,98	0
87	MG	A5	4486	1/1	0.52	0.56	94,94,94,94	0
87	MG	AI	302	1/1	0.52	0.27	66,66,66,66	0
87	MG	A1	4273	1/1	0.52	0.42	85,85,85,85	0
87	MG	A5	4359	1/1	0.52	0.21	86,86,86,86	0
87	MG	A6	2317	1/1	0.52	0.94	82,82,82,82	0
87	MG	CQ	202	1/1	0.53	0.29	85,85,85,85	0
87	MG	A6	2293	1/1	0.53	0.21	78,78,78,78	0
87	MG	A1	4137	1/1	0.53	0.33	84,84,84,84	0
87	MG	DT	203	1/1	0.53	0.34	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4489	1/1	0.53	0.31	94,94,94,94	0
87	MG	A5	4518	1/1	0.54	1.25	144,144,144,144	0
87	MG	A5	3897	1/1	0.54	0.38	100,100,100,100	0
87	MG	A2	2181	1/1	0.54	0.17	79,79,79,79	0
87	MG	CF	302	1/1	0.54	0.25	73,73,73,73	0
86	OHX	A6	2083	7/7	0.54	0.64	214,214,214,214	7
87	MG	A1	4201	1/1	0.54	0.65	65,65,65,65	0
87	MG	A6	2209	1/1	0.54	0.23	79,79,79,79	0
87	MG	A1	4153	1/1	0.55	0.24	96,96,96,96	0
87	MG	A6	2296	1/1	0.55	2.16	119,119,119,119	0
86	OHX	A5	3817	7/7	0.55	0.19	205,205,205,205	7
87	MG	A6	2282	1/1	0.55	0.39	83,83,83,83	0
87	MG	A5	4251	1/1	0.55	0.38	85,85,85,85	0
87	MG	BS	202	1/1	0.56	0.35	84,84,84,84	0
87	MG	A1	3918	1/1	0.56	0.29	83,83,83,83	0
87	MG	A5	4214	1/1	0.56	0.32	66,66,66,66	0
87	MG	A6	2103	1/1	0.56	0.36	64,64,64,64	0
87	MG	A5	4495	1/1	0.56	0.31	88,88,88,88	0
87	MG	A5	4241	1/1	0.56	0.34	106,106,106,106	0
87	MG	A1	4213	1/1	0.56	0.19	79,79,79,79	0
87	MG	A2	2123	1/1	0.56	0.39	81,81,81,81	0
87	MG	A1	4103	1/1	0.56	0.24	74,74,74,74	0
87	MG	A1	4252	1/1	0.56	0.28	121,121,121,121	0
87	MG	A2	2236	1/1	0.56	0.10	100,100,100,100	0
87	MG	A1	3987	1/1	0.57	0.22	57,57,57,57	0
87	MG	A2	2231	1/1	0.57	0.32	75,75,75,75	0
87	MG	BQ	202	1/1	0.57	0.83	80,80,80,80	0
87	MG	A1	4395	1/1	0.57	0.16	97,97,97,97	0
87	MG	A6	2335	1/1	0.57	0.69	84,84,84,84	0
87	MG	A5	4349	1/1	0.57	1.82	79,79,79,79	0
87	MG	A1	4282	1/1	0.57	0.41	92,92,92,92	0
87	MG	A5	3826	1/1	0.58	0.45	63,63,63,63	0
87	MG	A2	2194	1/1	0.58	0.48	113,113,113,113	0
87	MG	A1	4301	1/1	0.58	0.13	118,118,118,118	0
87	MG	Ba	205	1/1	0.58	0.27	69,69,69,69	0
87	MG	A2	2147	1/1	0.58	0.20	93,93,93,93	0
87	MG	BA	302	1/1	0.59	0.40	63,63,63,63	0
87	MG	A6	2132	1/1	0.59	0.23	81,81,81,81	0
87	MG	A5	3920	1/1	0.59	0.31	83,83,83,83	0
87	MG	A1	4069	1/1	0.59	0.24	69,69,69,69	0
87	MG	A2	2135	1/1	0.59	0.12	54,54,54,54	0
87	MG	A7	228	1/1	0.59	0.44	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4233	1/1	0.59	0.24	79,79,79,79	0
87	MG	A6	2222	1/1	0.59	0.22	86,86,86,86	0
87	MG	A6	2240	1/1	0.59	0.21	95,95,95,95	0
87	MG	A2	2243	1/1	0.59	0.30	86,86,86,86	0
87	MG	A1	4059	1/1	0.59	0.43	84,84,84,84	0
87	MG	A5	4549	1/1	0.59	0.46	70,70,70,70	0
87	MG	A1	4420	1/1	0.60	0.61	73,73,73,73	0
87	MG	A6	2324	1/1	0.60	0.26	74,74,74,74	0
87	MG	A6	2334	1/1	0.60	0.36	72,72,72,72	0
87	MG	A5	4476	1/1	0.60	0.50	86,86,86,86	0
87	MG	A1	4141	1/1	0.60	0.40	53,53,53,53	0
87	MG	A5	4571	1/1	0.60	0.36	84,84,84,84	0
87	MG	A5	4312	1/1	0.60	0.39	87,87,87,87	0
87	MG	Ad	102	1/1	0.60	0.13	89,89,89,89	0
87	MG	A5	4146	1/1	0.60	0.25	80,80,80,80	0
87	MG	A1	3920	1/1	0.60	0.24	53,53,53,53	0
87	MG	A1	4291	1/1	0.60	0.18	112,112,112,112	0
87	MG	A6	2245	1/1	0.60	0.18	82,82,82,82	0
87	MG	A1	4244	1/1	0.60	0.32	52,52,52,52	0
87	MG	A1	4357	1/1	0.60	0.32	89,89,89,89	0
87	MG	A6	2169	1/1	0.60	0.33	77,77,77,77	0
87	MG	A5	4529	1/1	0.60	0.53	91,91,91,91	0
87	MG	A1	4465	1/1	0.61	0.37	92,92,92,92	0
87	MG	A5	3872	1/1	0.61	0.31	81,81,81,81	0
87	MG	A1	4222	1/1	0.61	0.25	73,73,73,73	0
87	MG	A1	4277	1/1	0.61	0.73	89,89,89,89	0
87	MG	A6	2134	1/1	0.61	0.35	67,67,67,67	0
87	MG	A6	2328	1/1	0.61	0.21	87,87,87,87	0
87	MG	BI	305	1/1	0.61	0.24	84,84,84,84	0
87	MG	A1	3928	1/1	0.61	0.43	88,88,88,88	0
87	MG	A5	4319	1/1	0.61	0.19	86,86,86,86	0
87	MG	A5	4492	1/1	0.61	0.42	73,73,73,73	0
87	MG	A6	2184	1/1	0.61	0.20	67,67,67,67	0
87	MG	A1	4190	1/1	0.61	0.27	98,98,98,98	0
87	MG	A5	4191	1/1	0.61	0.29	99,99,99,99	0
87	MG	DC	406	1/1	0.61	0.30	111,111,111,111	0
87	MG	A5	4502	1/1	0.61	0.28	84,84,84,84	0
86	OHX	BI	303	7/7	0.61	0.46	215,215,215,215	7
87	MG	DO	207	1/1	0.61	0.53	109,109,109,109	0
87	MG	A1	4058	1/1	0.61	0.27	97,97,97,97	0
87	MG	A2	2182	1/1	0.61	0.21	78,78,78,78	0
87	MG	BO	202	1/1	0.62	0.20	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	3991	1/1	0.62	0.40	52,52,52,52	0
87	MG	A2	2193	1/1	0.62	0.25	79,79,79,79	0
87	MG	A1	3898	1/1	0.62	0.23	64,64,64,64	0
87	MG	A5	4135	1/1	0.62	0.43	73,73,73,73	0
87	MG	A1	4087	1/1	0.62	0.25	67,67,67,67	0
87	MG	A2	2201	1/1	0.62	0.15	96,96,96,96	0
87	MG	A5	4179	1/1	0.62	0.23	71,71,71,71	0
87	MG	A5	4390	1/1	0.62	0.21	70,70,70,70	0
87	MG	DQ	202	1/1	0.62	0.28	88,88,88,88	0
87	MG	A6	2299	1/1	0.62	0.75	84,84,84,84	0
87	MG	A1	4089	1/1	0.62	0.18	89,89,89,89	0
88	ZN	Cb	101	1/1	0.62	0.33	305,305,305,305	0
87	MG	A1	4493	1/1	0.63	0.36	66,66,66,66	0
87	MG	A5	4067	1/1	0.63	0.33	61,61,61,61	0
86	OHX	A1	3779	7/7	0.63	0.46	164,164,164,164	7
87	MG	A5	4081	1/1	0.63	0.41	79,79,79,79	0
87	MG	A5	4244	1/1	0.63	0.17	82,82,82,82	0
86	OHX	A2	2082	7/7	0.63	0.23	225,225,225,225	7
87	MG	CS	203	1/1	0.63	0.12	71,71,71,71	0
87	MG	A1	4344	1/1	0.63	0.20	88,88,88,88	0
87	MG	A5	4267	1/1	0.63	0.28	88,88,88,88	0
87	MG	A1	4217	1/1	0.63	0.17	57,57,57,57	0
86	OHX	A5	3792	7/7	0.63	0.40	217,217,217,217	7
87	MG	A6	2332	1/1	0.63	0.41	80,80,80,80	0
87	MG	A1	4068	1/1	0.63	0.35	78,78,78,78	0
87	MG	A5	4482	1/1	0.63	0.73	79,79,79,79	0
87	MG	A6	2254	1/1	0.63	0.17	69,69,69,69	0
87	MG	A5	4253	1/1	0.64	0.28	75,75,75,75	0
87	MG	A1	4436	1/1	0.64	0.13	115,115,115,115	0
87	MG	A1	4447	1/1	0.64	0.58	104,104,104,104	0
87	MG	A5	4211	1/1	0.64	0.35	77,77,77,77	0
87	MG	A5	4162	1/1	0.64	0.20	70,70,70,70	0
87	MG	A5	4164	1/1	0.64	0.13	87,87,87,87	0
87	MG	A5	3839	1/1	0.64	0.19	48,48,48,48	0
87	MG	Dq	401	1/1	0.64	0.12	81,81,81,81	0
87	MG	A6	2187	1/1	0.64	0.23	64,64,64,64	0
87	MG	A5	4121	1/1	0.64	0.23	55,55,55,55	0
87	MG	A2	2168	1/1	0.65	0.28	78,78,78,78	0
87	MG	A5	4224	1/1	0.65	0.27	58,58,58,58	0
87	MG	DF	303	1/1	0.65	0.28	73,73,73,73	0
87	MG	A5	4561	1/1	0.65	0.58	111,111,111,111	0
87	MG	A5	4351	1/1	0.65	0.38	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4087	1/1	0.65	0.28	86,86,86,86	0
87	MG	A6	2128	1/1	0.65	0.36	81,81,81,81	0
87	MG	A2	2245	1/1	0.65	0.16	71,71,71,71	0
87	MG	A6	2333	1/1	0.65	1.27	99,99,99,99	0
87	MG	A5	3860	1/1	0.65	0.29	66,66,66,66	0
87	MG	A6	2158	1/1	0.65	0.46	66,66,66,66	0
87	MG	A5	4445	1/1	0.66	0.29	65,65,65,65	0
87	MG	A5	4556	1/1	0.66	0.31	73,73,73,73	0
87	MG	A1	3836	1/1	0.66	0.31	48,48,48,48	0
87	MG	A5	3965	1/1	0.66	0.38	64,64,64,64	0
87	MG	Bo	202	1/1	0.66	0.37	82,82,82,82	0
87	MG	Bo	203	1/1	0.66	0.38	79,79,79,79	0
87	MG	A2	2145	1/1	0.66	0.33	71,71,71,71	0
87	MG	A1	4281	1/1	0.66	0.23	74,74,74,74	0
87	MG	A7	226	1/1	0.66	0.19	74,74,74,74	0
87	MG	A2	2242	1/1	0.66	0.15	105,105,105,105	0
87	MG	A5	4347	1/1	0.66	0.26	78,78,78,78	0
87	MG	A1	4242	1/1	0.66	0.17	84,84,84,84	0
87	MG	A1	3932	1/1	0.66	0.29	30,30,30,30	0
87	MG	A5	4131	1/1	0.66	0.23	85,85,85,85	0
87	MG	DH	202	1/1	0.66	0.62	73,73,73,73	0
86	OHX	A2	2077	7/7	0.66	0.31	206,206,206,206	7
87	MG	A5	4375	1/1	0.66	0.82	65,65,65,65	0
87	MG	A2	2141	1/1	0.66	0.28	68,68,68,68	0
87	MG	A2	2207	1/1	0.66	0.34	76,76,76,76	0
87	MG	A1	4198	1/1	0.66	0.24	79,79,79,79	0
87	MG	De	203	1/1	0.66	1.56	109,109,109,109	0
87	MG	A5	4397	1/1	0.66	0.17	101,101,101,101	0
87	MG	A1	4404	1/1	0.66	0.28	80,80,80,80	0
88	ZN	Bo	205	1/1	0.66	0.14	209,209,209,209	0
87	MG	A5	4420	1/1	0.66	0.26	93,93,93,93	0
87	MG	A5	4334	1/1	0.67	0.11	109,109,109,109	0
87	MG	A5	4078	1/1	0.67	0.30	49,49,49,49	0
87	MG	A1	4492	1/1	0.67	0.21	100,100,100,100	0
86	OHX	BI	304	7/7	0.67	0.36	193,193,193,193	7
87	MG	A5	4086	1/1	0.67	0.28	59,59,59,59	0
87	MG	A1	3847	1/1	0.67	0.15	74,74,74,74	0
87	MG	A1	4156	1/1	0.67	0.24	75,75,75,75	0
87	MG	A1	4206	1/1	0.67	0.21	55,55,55,55	0
87	MG	A1	4057	1/1	0.67	0.25	63,63,63,63	0
87	MG	A5	4379	1/1	0.67	0.40	45,45,45,45	0
87	MG	A1	4368	1/1	0.67	0.71	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4138	1/1	0.67	0.39	77,77,77,77	0
87	MG	A5	3888	1/1	0.67	0.24	64,64,64,64	0
87	MG	A5	4157	1/1	0.67	0.19	56,56,56,56	0
87	MG	A6	2275	1/1	0.67	0.18	63,63,63,63	0
87	MG	A6	2195	1/1	0.67	0.32	93,93,93,93	0
87	MG	A1	4483	1/1	0.67	0.20	72,72,72,72	0
87	MG	A1	4290	1/1	0.67	0.25	69,69,69,69	0
87	MG	BI	307	1/1	0.67	2.09	81,81,81,81	0
87	MG	BN	304	1/1	0.67	0.33	80,80,80,80	0
87	MG	A1	4487	1/1	0.68	0.23	80,80,80,80	0
87	MG	A3	231	1/1	0.68	0.34	92,92,92,92	0
87	MG	Bj	107	1/1	0.68	0.44	101,101,101,101	0
87	MG	A6	2326	1/1	0.68	0.19	117,117,117,117	0
87	MG	A5	4217	1/1	0.68	0.40	83,83,83,83	0
87	MG	A1	3940	1/1	0.68	0.37	51,51,51,51	0
87	MG	BG	301	1/1	0.68	0.28	91,91,91,91	0
87	MG	A2	2111	1/1	0.68	0.18	69,69,69,69	0
87	MG	A5	4137	1/1	0.68	0.20	104,104,104,104	0
87	MG	AP	202	1/1	0.68	0.30	88,88,88,88	0
87	MG	A5	4364	1/1	0.68	0.23	76,76,76,76	0
87	MG	A6	2284	1/1	0.68	0.55	107,107,107,107	0
87	MG	A1	4207	1/1	0.68	0.17	85,85,85,85	0
87	MG	A5	4056	1/1	0.68	0.23	78,78,78,78	0
87	MG	A5	4382	1/1	0.68	0.62	99,99,99,99	0
87	MG	A1	4479	1/1	0.68	0.26	74,74,74,74	0
87	MG	BP	207	1/1	0.68	0.26	65,65,65,65	0
87	MG	A5	4540	1/1	0.68	0.21	94,94,94,94	0
87	MG	A1	4333	1/1	0.68	0.85	68,68,68,68	0
87	MG	A5	4315	1/1	0.68	0.24	106,106,106,106	0
87	MG	A5	4419	1/1	0.68	0.28	65,65,65,65	0
87	MG	A1	4450	1/1	0.68	0.24	68,68,68,68	0
87	MG	A5	4441	1/1	0.68	0.22	61,61,61,61	0
87	MG	A5	4399	1/1	0.69	0.27	64,64,64,64	0
87	MG	A5	4402	1/1	0.69	0.68	91,91,91,91	0
87	MG	A1	3894	1/1	0.69	0.33	43,43,43,43	0
87	MG	A5	4554	1/1	0.69	0.55	86,86,86,86	0
87	MG	A1	4284	1/1	0.69	0.29	87,87,87,87	0
87	MG	A5	4557	1/1	0.69	0.27	69,69,69,69	0
87	MG	A2	2224	1/1	0.69	0.20	77,77,77,77	0
87	MG	A5	3862	1/1	0.69	0.48	82,82,82,82	0
87	MG	A5	4330	1/1	0.69	0.19	86,86,86,86	0
87	MG	A5	4333	1/1	0.69	0.39	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4115	1/1	0.69	0.37	69,69,69,69	0
87	MG	A5	4338	1/1	0.69	0.31	93,93,93,93	0
87	MG	A2	2188	1/1	0.69	0.20	82,82,82,82	0
87	MG	A2	2191	1/1	0.69	0.23	91,91,91,91	0
87	MG	A8	235	1/1	0.69	0.79	79,79,79,79	0
87	MG	A6	2281	1/1	0.69	0.44	75,75,75,75	0
87	MG	A1	4507	1/1	0.69	0.30	90,90,90,90	0
87	MG	A5	4488	1/1	0.69	0.93	81,81,81,81	0
87	MG	A6	2243	1/1	0.69	0.27	74,74,74,74	0
87	MG	A5	3933	1/1	0.69	0.36	74,74,74,74	0
87	MG	DH	203	1/1	0.69	0.55	72,72,72,72	0
87	MG	A2	2152	1/1	0.69	0.28	88,88,88,88	0
87	MG	A5	4372	1/1	0.69	0.84	74,74,74,74	0
87	MG	A5	4256	1/1	0.69	0.69	81,81,81,81	0
87	MG	AN	202	1/1	0.69	0.13	63,63,63,63	0
87	MG	A5	4511	1/1	0.69	0.66	68,68,68,68	0
87	MG	A6	2246	1/1	0.69	0.41	78,78,78,78	0
87	MG	A1	4182	1/1	0.69	0.20	81,81,81,81	0
87	MG	A5	4285	1/1	0.69	0.57	68,68,68,68	0
87	MG	A4	242	1/1	0.69	0.21	81,81,81,81	0
87	MG	A1	3870	1/1	0.69	0.40	57,57,57,57	0
87	MG	A2	2226	1/1	0.70	0.40	87,87,87,87	0
87	MG	A2	2158	1/1	0.70	0.22	71,71,71,71	0
86	OHX	A1	3814	7/7	0.70	0.53	221,221,221,221	7
87	MG	A1	4258	1/1	0.70	0.18	67,67,67,67	0
87	MG	A6	2287	1/1	0.70	1.05	96,96,96,96	0
87	MG	A1	4422	1/1	0.70	0.24	68,68,68,68	0
87	MG	A5	4562	1/1	0.70	0.28	69,69,69,69	0
87	MG	A1	4431	1/1	0.70	0.36	59,59,59,59	0
87	MG	A6	2215	1/1	0.70	0.18	56,56,56,56	0
87	MG	A5	4323	1/1	0.70	0.34	64,64,64,64	0
87	MG	A2	2196	1/1	0.70	0.54	131,131,131,131	0
87	MG	Ba	207	1/1	0.70	0.81	89,89,89,89	0
87	MG	A7	221	1/1	0.70	0.30	82,82,82,82	0
87	MG	A5	4188	1/1	0.70	0.37	78,78,78,78	0
87	MG	A1	4175	1/1	0.70	0.09	69,69,69,69	0
87	MG	A5	4337	1/1	0.70	0.47	70,70,70,70	0
87	MG	B1	4500	1/1	0.70	0.53	77,77,77,77	0
87	MG	A1	3914	1/1	0.70	0.19	73,73,73,73	0
87	MG	A5	4491	1/1	0.70	0.57	82,82,82,82	0
87	MG	A5	3992	1/1	0.70	0.32	57,57,57,57	0
87	MG	A2	2237	1/1	0.70	0.16	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4451	1/1	0.70	0.44	75,75,75,75	0
87	MG	A2	2238	1/1	0.70	0.40	92,92,92,92	0
87	MG	DJ	203	1/1	0.70	0.26	80,80,80,80	0
86	OHX	A5	3819	7/7	0.70	0.56	238,238,238,238	7
87	MG	A2	2091	1/1	0.70	0.38	81,81,81,81	0
87	MG	A2	2170	1/1	0.70	0.41	88,88,88,88	0
87	MG	A2	2253	1/1	0.70	0.16	89,89,89,89	0
87	MG	A6	2267	1/1	0.70	0.24	72,72,72,72	0
87	MG	CP	203	1/1	0.70	0.63	63,63,63,63	0
87	MG	A1	4298	1/1	0.70	0.65	95,95,95,95	0
87	MG	A6	2276	1/1	0.70	0.36	105,105,105,105	0
87	MG	A5	4264	1/1	0.70	0.41	103,103,103,103	0
87	MG	A2	2139	1/1	0.71	0.19	81,81,81,81	0
87	MG	A5	4317	1/1	0.71	0.41	63,63,63,63	0
87	MG	A5	3871	1/1	0.71	0.24	56,56,56,56	0
87	MG	A6	2315	1/1	0.71	0.26	84,84,84,84	0
87	MG	A5	3880	1/1	0.71	0.26	45,45,45,45	0
87	MG	A5	4447	1/1	0.71	0.23	61,61,61,61	0
87	MG	A4	245	1/1	0.71	0.42	90,90,90,90	0
87	MG	A1	4176	1/1	0.71	0.07	84,84,84,84	0
87	MG	A5	3906	1/1	0.71	0.30	56,56,56,56	0
87	MG	A1	4035	1/1	0.71	0.12	59,59,59,59	0
87	MG	A1	4238	1/1	0.71	0.19	69,69,69,69	0
86	OHX	A1	3805	7/7	0.71	0.41	209,209,209,209	7
87	MG	A1	4187	1/1	0.71	0.73	90,90,90,90	0
87	MG	A1	3863	1/1	0.71	0.24	125,125,125,125	0
87	MG	A6	2273	1/1	0.71	0.22	90,90,90,90	0
87	MG	A2	2233	1/1	0.71	0.13	80,80,80,80	0
87	MG	A5	4229	1/1	0.71	0.38	81,81,81,81	0
87	MG	BP	211	1/1	0.71	0.73	123,123,123,123	0
87	MG	A2	2177	1/1	0.71	0.30	83,83,83,83	0
87	MG	CL	202	1/1	0.71	0.31	82,82,82,82	0
87	MG	CL	204	1/1	0.71	0.49	83,83,83,83	0
87	MG	A1	4425	1/1	0.71	0.21	106,106,106,106	0
87	MG	A2	2210	1/1	0.71	0.42	81,81,81,81	0
87	MG	A1	4143	1/1	0.71	0.24	70,70,70,70	0
87	MG	A1	3907	1/1	0.71	0.30	50,50,50,50	0
87	MG	A5	4538	1/1	0.71	0.37	67,67,67,67	0
87	MG	A1	3943	1/1	0.71	0.33	59,59,59,59	0
87	MG	A1	4071	1/1	0.71	0.20	71,71,71,71	0
87	MG	A2	2255	1/1	0.71	0.08	107,107,107,107	0
87	MG	A5	3854	1/1	0.71	0.31	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A1	3753	7/7	0.71	0.97	243,243,243,243	7
87	MG	A1	4105	1/1	0.72	0.27	84,84,84,84	0
87	MG	A6	2140	1/1	0.72	0.23	61,61,61,61	0
86	OHX	A2	2047	7/7	0.72	0.32	188,188,188,188	7
87	MG	A1	3817	1/1	0.72	0.39	63,63,63,63	0
87	MG	A6	2173	1/1	0.72	0.22	71,71,71,71	0
87	MG	A5	4565	1/1	0.72	0.16	87,87,87,87	0
87	MG	A5	4192	1/1	0.72	0.37	95,95,95,95	0
87	MG	A5	4194	1/1	0.72	0.40	88,88,88,88	0
86	OHX	A1	3786	7/7	0.72	0.31	184,184,184,184	7
87	MG	A5	4040	1/1	0.72	0.24	46,46,46,46	0
87	MG	A5	4335	1/1	0.72	0.36	94,94,94,94	0
87	MG	A2	2155	1/1	0.72	0.29	86,86,86,86	0
87	MG	A1	4269	1/1	0.72	0.74	87,87,87,87	0
87	MG	A6	2194	1/1	0.72	0.17	67,67,67,67	0
87	MG	A5	4076	1/1	0.72	0.30	64,64,64,64	0
87	MG	BV	205	1/1	0.72	0.81	68,68,68,68	0
87	MG	A6	2200	1/1	0.72	0.23	82,82,82,82	0
87	MG	DC	405	1/1	0.72	0.67	72,72,72,72	0
87	MG	A1	4385	1/1	0.72	0.86	65,65,65,65	0
87	MG	A1	4474	1/1	0.72	0.29	72,72,72,72	0
87	MG	A2	2172	1/1	0.72	0.22	69,69,69,69	0
87	MG	A6	2233	1/1	0.72	0.39	63,63,63,63	0
87	MG	A5	3852	1/1	0.72	0.23	49,49,49,49	0
87	MG	A5	4514	1/1	0.72	1.55	98,98,98,98	0
87	MG	A4	234	1/1	0.72	0.31	74,74,74,74	0
87	MG	A1	4317	1/1	0.72	0.28	92,92,92,92	0
86	OHX	A2	2028	7/7	0.72	0.38	180,180,180,180	7
87	MG	A1	4480	1/1	0.72	0.55	91,91,91,91	0
87	MG	Db	102	1/1	0.72	1.28	70,70,70,70	0
86	OHX	A1	3778	7/7	0.72	0.37	150,150,150,150	7
87	MG	A1	3891	1/1	0.72	0.22	58,58,58,58	0
87	MG	A5	4297	1/1	0.72	0.34	56,56,56,56	0
87	MG	A1	3925	1/1	0.72	0.21	40,40,40,40	0
86	OHX	A1	3815	7/7	0.72	0.53	183,183,183,183	7
88	ZN	Do	203	1/1	0.72	0.15	181,181,181,181	0
87	MG	A1	4161	1/1	0.73	0.29	73,73,73,73	0
87	MG	A5	4440	1/1	0.73	0.64	76,76,76,76	0
87	MG	A5	3923	1/1	0.73	0.28	68,68,68,68	0
86	OHX	A8	218	7/7	0.73	0.45	221,221,221,221	7
87	MG	A1	3405	1/1	0.73	0.18	71,71,71,71	0
87	MG	A1	4374	1/1	0.73	1.18	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4189	1/1	0.73	0.37	96,96,96,96	0
87	MG	A4	229	1/1	0.73	0.16	54,54,54,54	0
87	MG	A5	4024	1/1	0.73	0.37	42,42,42,42	0
87	MG	A1	3857	1/1	0.73	0.26	53,53,53,53	0
87	MG	A4	240	1/1	0.73	0.29	72,72,72,72	0
87	MG	A1	4226	1/1	0.73	0.83	63,63,63,63	0
87	MG	A6	2231	1/1	0.73	0.32	69,69,69,69	0
87	MG	A6	2288	1/1	0.73	0.50	106,106,106,106	0
87	MG	Ca	201	1/1	0.73	0.28	67,67,67,67	0
87	MG	DB	415	1/1	0.73	0.29	91,91,91,91	0
87	MG	A1	4264	1/1	0.73	0.23	65,65,65,65	0
87	MG	A6	2116	1/1	0.73	0.25	80,80,80,80	0
87	MG	A2	2203	1/1	0.73	0.33	68,68,68,68	0
87	MG	A1	4271	1/1	0.73	0.24	58,58,58,58	0
87	MG	A5	4089	1/1	0.73	0.20	81,81,81,81	0
87	MG	A5	4250	1/1	0.73	0.61	110,110,110,110	0
87	MG	A1	4037	1/1	0.73	0.17	83,83,83,83	0
87	MG	A5	4100	1/1	0.73	0.33	86,86,86,86	0
87	MG	A1	4042	1/1	0.73	0.33	68,68,68,68	0
87	MG	A1	4194	1/1	0.73	0.32	96,96,96,96	0
87	MG	A5	4126	1/1	0.73	0.27	100,100,100,100	0
87	MG	A1	3912	1/1	0.73	0.66	84,84,84,84	0
87	MG	A1	4444	1/1	0.73	1.27	81,81,81,81	0
87	MG	A1	3868	1/1	0.73	0.26	55,55,55,55	0
87	MG	A6	2258	1/1	0.73	0.22	71,71,71,71	0
86	OHX	A3	213	7/7	0.73	0.22	195,195,195,195	7
87	MG	A1	3876	1/1	0.73	0.38	68,68,68,68	0
87	MG	A5	4314	1/1	0.73	0.21	56,56,56,56	0
87	MG	Bj	106	1/1	0.74	0.34	75,75,75,75	0
87	MG	A5	4043	1/1	0.74	0.28	35,35,35,35	0
87	MG	A6	2196	1/1	0.74	0.57	83,83,83,83	0
87	MG	A2	2098	1/1	0.74	0.30	62,62,62,62	0
87	MG	A1	4440	1/1	0.74	0.61	55,55,55,55	0
87	MG	A6	2210	1/1	0.74	0.25	72,72,72,72	0
87	MG	A2	2101	1/1	0.74	0.12	59,59,59,59	0
87	MG	BA	306	1/1	0.74	0.43	74,74,74,74	0
87	MG	A7	222	1/1	0.74	0.38	94,94,94,94	0
87	MG	A5	3408	1/1	0.74	0.62	63,63,63,63	0
86	OHX	A6	2087	7/7	0.74	0.23	205,205,205,205	7
87	MG	A8	228	1/1	0.74	0.33	86,86,86,86	0
87	MG	A6	2106	1/1	0.74	0.34	64,64,64,64	0
87	MG	A5	3848	1/1	0.74	0.32	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	DA	301	1/1	0.74	0.23	86,86,86,86	0
87	MG	A2	2149	1/1	0.74	0.28	83,83,83,83	0
86	OHX	A5	3798	7/7	0.74	0.27	202,202,202,202	7
87	MG	A5	3859	1/1	0.74	0.23	50,50,50,50	0
86	OHX	A5	3811	7/7	0.74	0.30	214,214,214,214	7
87	MG	A1	4149	1/1	0.74	0.17	74,74,74,74	0
87	MG	A1	4189	1/1	0.74	0.21	59,59,59,59	0
87	MG	A1	4285	1/1	0.74	0.31	64,64,64,64	0
87	MG	A5	4381	1/1	0.74	0.24	96,96,96,96	0
87	MG	A6	2321	1/1	0.74	0.48	93,93,93,93	0
87	MG	A5	4385	1/1	0.74	0.30	74,74,74,74	0
87	MG	A1	4060	1/1	0.74	0.20	67,67,67,67	0
86	OHX	A6	2074	7/7	0.74	0.32	176,176,176,176	7
87	MG	A4	217	1/1	0.74	0.38	69,69,69,69	0
87	MG	BV	202	1/1	0.74	0.22	73,73,73,73	0
87	MG	A6	2179	1/1	0.74	0.20	47,47,47,47	0
87	MG	A1	4108	1/1	0.74	0.23	60,60,60,60	0
87	MG	A1	4427	1/1	0.74	0.26	77,77,77,77	0
87	MG	A6	2272	1/1	0.74	0.31	115,115,115,115	0
87	MG	A1	4362	1/1	0.74	0.19	85,85,85,85	0
87	MG	Bj	104	1/1	0.74	0.29	86,86,86,86	0
87	MG	A1	4459	1/1	0.75	0.39	88,88,88,88	0
87	MG	A1	4463	1/1	0.75	0.20	76,76,76,76	0
86	OHX	A1	3774	7/7	0.75	0.18	206,206,206,206	7
87	MG	BJ	201	1/1	0.75	0.18	81,81,81,81	0
87	MG	A1	4467	1/1	0.75	0.30	68,68,68,68	0
86	OHX	A6	2060	7/7	0.75	0.27	165,165,165,165	7
87	MG	BO	205	1/1	0.75	0.82	58,58,58,58	0
87	MG	A5	3988	1/1	0.75	0.35	51,51,51,51	0
87	MG	A1	4132	1/1	0.75	0.17	64,64,64,64	0
86	OHX	A5	3777	7/7	0.75	0.34	187,187,187,187	7
87	MG	A5	4231	1/1	0.75	0.17	105,105,105,105	0
87	MG	A5	4035	1/1	0.75	0.14	39,39,39,39	0
86	OHX	A2	2075	7/7	0.75	0.28	204,204,204,204	7
86	OHX	A2	2037	7/7	0.75	0.38	197,197,197,197	7
87	MG	A1	4276	1/1	0.75	0.26	95,95,95,95	0
87	MG	A2	2212	1/1	0.75	0.34	100,100,100,100	0
87	MG	A7	219	1/1	0.75	0.23	71,71,71,71	0
87	MG	A1	4219	1/1	0.75	0.16	85,85,85,85	0
87	MG	Ba	203	1/1	0.75	0.22	70,70,70,70	0
87	MG	A5	4423	1/1	0.75	0.33	82,82,82,82	0
87	MG	A2	2215	1/1	0.75	0.34	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4390	1/1	0.75	0.22	82,82,82,82	0
87	MG	A8	233	1/1	0.75	0.30	78,78,78,78	0
86	OHX	A5	3799	7/7	0.75	0.29	168,168,168,168	7
87	MG	A2	2197	1/1	0.75	0.25	80,80,80,80	0
87	MG	A2	2097	1/1	0.75	0.22	78,78,78,78	0
87	MG	A1	4082	1/1	0.75	0.20	73,73,73,73	0
87	MG	A5	4094	1/1	0.75	0.31	69,69,69,69	0
87	MG	A1	4085	1/1	0.75	0.18	35,35,35,35	0
87	MG	A3	220	1/1	0.75	0.46	83,83,83,83	0
87	MG	A1	4086	1/1	0.75	0.55	58,58,58,58	0
87	MG	A1	4236	1/1	0.75	0.34	73,73,73,73	0
87	MG	A1	4432	1/1	0.75	0.76	79,79,79,79	0
87	MG	A6	2119	1/1	0.75	0.26	70,70,70,70	0
87	MG	A5	3831	1/1	0.75	0.19	37,37,37,37	0
87	MG	A2	2247	1/1	0.75	0.23	86,86,86,86	0
87	MG	A4	226	1/1	0.75	0.34	70,70,70,70	0
87	MG	A1	4011	1/1	0.75	0.23	50,50,50,50	0
87	MG	A2	2159	1/1	0.75	0.26	88,88,88,88	0
87	MG	A1	4095	1/1	0.75	0.27	56,56,56,56	0
87	MG	Dd	201	1/1	0.75	0.31	77,77,77,77	0
87	MG	A2	2225	1/1	0.75	0.44	79,79,79,79	0
87	MG	A6	2156	1/1	0.75	0.36	62,62,62,62	0
87	MG	A1	4038	1/1	0.75	0.22	89,89,89,89	0
87	MG	A6	2166	1/1	0.75	0.26	64,64,64,64	0
87	MG	A1	4041	1/1	0.75	0.21	70,70,70,70	0
87	MG	A1	4193	1/1	0.75	0.35	72,72,72,72	0
87	MG	A3	222	1/1	0.76	0.17	66,66,66,66	0
87	MG	A5	4095	1/1	0.76	0.27	79,79,79,79	0
87	MG	A1	4148	1/1	0.76	0.21	94,94,94,94	0
87	MG	A5	3870	1/1	0.76	0.33	56,56,56,56	0
87	MG	A5	4108	1/1	0.76	0.30	74,74,74,74	0
87	MG	A5	4394	1/1	0.76	0.22	73,73,73,73	0
87	MG	A5	4111	1/1	0.76	0.25	65,65,65,65	0
87	MG	A1	4376	1/1	0.76	0.68	71,71,71,71	0
87	MG	A1	4310	1/1	0.76	1.21	67,67,67,67	0
87	MG	A5	4272	1/1	0.76	0.18	69,69,69,69	0
87	MG	A5	4273	1/1	0.76	1.30	75,75,75,75	0
87	MG	A5	4580	1/1	0.76	0.19	82,82,82,82	0
87	MG	A5	4279	1/1	0.76	1.08	63,63,63,63	0
87	MG	A2	2095	1/1	0.76	0.24	63,63,63,63	0
87	MG	A1	4316	1/1	0.76	0.70	65,65,65,65	0
87	MG	A1	4470	1/1	0.76	0.13	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	3990	1/1	0.76	0.43	54,54,54,54	0
87	MG	A1	4396	1/1	0.76	0.16	74,74,74,74	0
87	MG	A5	4451	1/1	0.76	0.31	80,80,80,80	0
87	MG	A8	229	1/1	0.76	0.21	95,95,95,95	0
87	MG	A2	2179	1/1	0.76	0.25	81,81,81,81	0
87	MG	A5	4153	1/1	0.76	0.24	83,83,83,83	0
86	OHX	A6	2090	7/7	0.76	0.47	212,212,212,212	7
87	MG	A2	2160	1/1	0.76	0.37	66,66,66,66	0
87	MG	A5	3951	1/1	0.76	0.27	40,40,40,40	0
87	MG	A1	4074	1/1	0.76	0.12	57,57,57,57	0
87	MG	A6	2280	1/1	0.76	0.39	79,79,79,79	0
87	MG	A1	4341	1/1	0.76	0.25	118,118,118,118	0
87	MG	A6	2105	1/1	0.76	0.22	78,78,78,78	0
87	MG	A6	2211	1/1	0.76	0.14	86,86,86,86	0
87	MG	A6	2285	1/1	0.76	0.26	74,74,74,74	0
87	MG	A1	4342	1/1	0.76	0.21	79,79,79,79	0
87	MG	A5	4196	1/1	0.76	0.10	66,66,66,66	0
87	MG	A1	4255	1/1	0.76	0.32	87,87,87,87	0
87	MG	A5	4059	1/1	0.76	0.32	71,71,71,71	0
87	MG	A1	3906	1/1	0.76	0.34	91,91,91,91	0
87	MG	A1	4144	1/1	0.76	0.82	82,82,82,82	0
87	MG	A1	4289	1/1	0.76	0.28	74,74,74,74	0
87	MG	A5	4355	1/1	0.76	0.19	66,66,66,66	0
87	MG	A5	3840	1/1	0.76	0.15	26,26,26,26	0
87	MG	A1	4260	1/1	0.76	0.23	75,75,75,75	0
87	MG	A5	3851	1/1	0.76	0.30	45,45,45,45	0
87	MG	A1	4261	1/1	0.76	0.31	79,79,79,79	0
86	OHX	A5	3665	7/7	0.76	0.23	184,184,184,184	7
87	MG	A1	4212	1/1	0.76	0.26	67,67,67,67	0
86	OHX	A5	3768	7/7	0.77	0.75	198,198,198,198	7
87	MG	A1	4257	1/1	0.77	0.15	88,88,88,88	0
87	MG	A1	4443	1/1	0.77	0.39	65,65,65,65	0
86	OHX	A5	3770	7/7	0.77	0.29	198,198,198,198	7
87	MG	A1	4324	1/1	0.77	0.20	79,79,79,79	0
87	MG	A6	2271	1/1	0.77	0.28	95,95,95,95	0
87	MG	A1	4014	1/1	0.77	0.40	56,56,56,56	0
87	MG	A5	4410	1/1	0.77	0.69	66,66,66,66	0
87	MG	A5	3907	1/1	0.77	0.35	75,75,75,75	0
87	MG	A5	3915	1/1	0.77	0.26	78,78,78,78	0
87	MG	A5	4579	1/1	0.77	0.71	57,57,57,57	0
87	MG	A5	3916	1/1	0.77	0.27	49,49,49,49	0
87	MG	A6	2336	1/1	0.77	0.43	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4326	1/1	0.77	1.26	80,80,80,80	0
87	MG	A1	4110	1/1	0.77	0.19	71,71,71,71	0
87	MG	AC	302	1/1	0.77	0.27	74,74,74,74	0
87	MG	A6	2118	1/1	0.77	0.32	57,57,57,57	0
87	MG	A5	4155	1/1	0.77	0.45	95,95,95,95	0
87	MG	A5	3955	1/1	0.77	0.32	62,62,62,62	0
87	MG	A1	3822	1/1	0.77	0.21	50,50,50,50	0
86	OHX	CP	202	7/7	0.77	0.63	221,221,221,221	7
87	MG	A5	4322	1/1	0.77	0.39	61,61,61,61	0
87	MG	A6	2218	1/1	0.77	0.23	53,53,53,53	0
87	MG	A1	4343	1/1	0.77	0.39	78,78,78,78	0
87	MG	A1	4408	1/1	0.77	0.79	81,81,81,81	0
87	MG	DB	414	1/1	0.77	1.34	76,76,76,76	0
87	MG	A5	4039	1/1	0.77	0.34	63,63,63,63	0
87	MG	A6	2232	1/1	0.77	0.29	77,77,77,77	0
87	MG	A1	4411	1/1	0.77	0.23	94,94,94,94	0
87	MG	A5	4045	1/1	0.77	0.29	63,63,63,63	0
87	MG	A1	4224	1/1	0.77	0.22	72,72,72,72	0
87	MG	A6	2138	1/1	0.77	0.36	94,94,94,94	0
86	OHX	A2	2087	7/7	0.77	0.19	196,196,196,196	7
87	MG	A5	4072	1/1	0.77	0.27	56,56,56,56	0
87	MG	A6	2306	1/1	0.77	0.16	103,103,103,103	0
87	MG	A2	2241	1/1	0.77	0.47	108,108,108,108	0
87	MG	A5	4220	1/1	0.77	0.37	82,82,82,82	0
87	MG	A2	2206	1/1	0.77	0.15	78,78,78,78	0
87	MG	A5	4079	1/1	0.77	0.24	67,67,67,67	0
87	MG	A4	235	1/1	0.77	0.14	119,119,119,119	0
87	MG	A1	4363	1/1	0.77	0.34	46,46,46,46	0
87	MG	A5	4541	1/1	0.77	0.52	107,107,107,107	0
87	MG	A6	2253	1/1	0.77	0.29	85,85,85,85	0
87	MG	A1	4278	1/1	0.77	0.24	67,67,67,67	0
87	MG	A5	4088	1/1	0.77	0.18	41,41,41,41	0
87	MG	A6	2323	1/1	0.77	0.26	77,77,77,77	0
87	MG	A5	4572	1/1	0.78	0.24	77,77,77,77	0
87	MG	A2	2115	1/1	0.78	0.32	78,78,78,78	0
87	MG	Be	201	1/1	0.78	0.60	88,88,88,88	0
87	MG	BE	201	1/1	0.78	0.27	55,55,55,55	0
87	MG	A1	4327	1/1	0.78	0.14	108,108,108,108	0
87	MG	A5	4477	1/1	0.78	0.48	66,66,66,66	0
87	MG	A5	3925	1/1	0.78	0.23	57,57,57,57	0
87	MG	A1	4329	1/1	0.78	0.65	85,85,85,85	0
87	MG	A5	4345	1/1	0.78	0.74	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	3995	1/1	0.78	0.28	63,63,63,63	0
87	MG	A2	2094	1/1	0.78	0.36	68,68,68,68	0
87	MG	A7	229	1/1	0.78	1.04	98,98,98,98	0
87	MG	BL	201	1/1	0.78	0.23	51,51,51,51	0
87	MG	A6	2101	1/1	0.78	0.31	51,51,51,51	0
87	MG	A1	3896	1/1	0.78	0.25	40,40,40,40	0
87	MG	A4	220	1/1	0.78	0.45	70,70,70,70	0
87	MG	A5	4021	1/1	0.78	0.31	35,35,35,35	0
87	MG	A2	2169	1/1	0.78	0.19	105,105,105,105	0
87	MG	A6	2261	1/1	0.78	0.24	76,76,76,76	0
87	MG	A6	2322	1/1	0.78	0.52	77,77,77,77	0
87	MG	A2	2133	1/1	0.78	0.17	72,72,72,72	0
87	MG	A4	231	1/1	0.78	0.30	45,45,45,45	0
87	MG	A1	4464	1/1	0.78	0.26	63,63,63,63	0
87	MG	A6	2121	1/1	0.78	0.37	64,64,64,64	0
87	MG	A5	4387	1/1	0.78	0.38	93,93,93,93	0
87	MG	A6	2126	1/1	0.78	0.22	78,78,78,78	0
87	MG	A1	4164	1/1	0.78	0.27	78,78,78,78	0
87	MG	A1	4321	1/1	0.78	0.16	88,88,88,88	0
87	MG	A2	2232	1/1	0.78	0.26	125,125,125,125	0
87	MG	A6	2227	1/1	0.78	0.28	67,67,67,67	0
87	MG	A1	4473	1/1	0.78	0.27	111,111,111,111	0
87	MG	A5	4409	1/1	0.78	0.45	59,59,59,59	0
87	MG	A5	3896	1/1	0.78	0.34	67,67,67,67	0
87	MG	A6	2338	1/1	0.78	0.50	80,80,80,80	0
87	MG	A5	4083	1/1	0.78	0.23	70,70,70,70	0
87	MG	Df	203	1/1	0.78	0.26	93,93,93,93	0
87	MG	A5	4202	1/1	0.78	0.41	45,45,45,45	0
87	MG	A5	3898	1/1	0.78	0.25	44,44,44,44	0
87	MG	A5	4206	1/1	0.78	0.19	110,110,110,110	0
87	MG	A4	249	1/1	0.78	0.29	75,75,75,75	0
86	OHX	A5	3765	7/7	0.78	0.21	201,201,201,201	7
87	MG	A5	3989	1/1	0.79	0.41	76,76,76,76	0
87	MG	A1	4129	1/1	0.79	0.24	75,75,75,75	0
87	MG	A5	4002	1/1	0.79	0.33	40,40,40,40	0
87	MG	A1	4072	1/1	0.79	0.26	73,73,73,73	0
87	MG	A6	2157	1/1	0.79	0.41	70,70,70,70	0
87	MG	A1	4419	1/1	0.79	0.49	79,79,79,79	0
87	MG	A1	3848	1/1	0.79	0.42	75,75,75,75	0
86	OHX	A5	3693	7/7	0.79	0.27	181,181,181,181	7
87	MG	BR	203	1/1	0.79	0.26	65,65,65,65	0
87	MG	A5	4544	1/1	0.79	0.38	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4334	1/1	0.79	0.38	104,104,104,104	0
86	OHX	A6	2086	7/7	0.79	0.78	215,215,215,215	7
87	MG	A5	4360	1/1	0.79	0.23	85,85,85,85	0
87	MG	A1	4339	1/1	0.79	0.65	97,97,97,97	0
86	OHX	A5	3816	7/7	0.79	0.27	195,195,195,195	7
87	MG	A5	4374	1/1	0.79	0.42	95,95,95,95	0
87	MG	Ba	201	1/1	0.79	0.36	66,66,66,66	0
87	MG	A5	4218	1/1	0.79	0.22	57,57,57,57	0
87	MG	A1	3974	1/1	0.79	0.25	35,35,35,35	0
87	MG	A1	3978	1/1	0.79	0.40	73,73,73,73	0
87	MG	A1	4248	1/1	0.79	0.71	78,78,78,78	0
87	MG	A5	4384	1/1	0.79	0.25	77,77,77,77	0
87	MG	A1	4356	1/1	0.79	0.26	65,65,65,65	0
87	MG	A3	232	1/1	0.79	0.24	95,95,95,95	0
86	OHX	A1	3765	7/7	0.79	0.35	173,173,173,173	7
86	OHX	A1	3745	7/7	0.79	0.29	178,178,178,178	7
87	MG	A5	4247	1/1	0.79	0.18	64,64,64,64	0
87	MG	A1	4360	1/1	0.79	0.53	88,88,88,88	0
87	MG	A1	4101	1/1	0.79	0.33	86,86,86,86	0
87	MG	A1	4453	1/1	0.79	1.13	114,114,114,114	0
87	MG	A5	3875	1/1	0.79	0.35	78,78,78,78	0
86	OHX	A6	2061	7/7	0.79	0.29	172,172,172,172	7
87	MG	A5	4258	1/1	0.79	0.32	70,70,70,70	0
87	MG	A8	201	1/1	0.79	0.17	92,92,92,92	0
87	MG	A5	3887	1/1	0.79	0.41	84,84,84,84	0
87	MG	A1	3888	1/1	0.79	0.30	67,67,67,67	0
87	MG	A5	4265	1/1	0.79	1.24	80,80,80,80	0
87	MG	A5	4424	1/1	0.79	0.47	86,86,86,86	0
87	MG	A5	4425	1/1	0.79	0.28	65,65,65,65	0
87	MG	A5	4432	1/1	0.79	0.41	95,95,95,95	0
87	MG	A6	2104	1/1	0.79	0.30	68,68,68,68	0
87	MG	A6	2238	1/1	0.79	0.19	73,73,73,73	0
86	OHX	A5	3785	7/7	0.79	0.35	126,126,126,126	7
87	MG	DC	404	1/1	0.79	0.34	70,70,70,70	0
87	MG	A1	4302	1/1	0.79	0.57	114,114,114,114	0
87	MG	A1	4259	1/1	0.79	0.24	102,102,102,102	0
86	OHX	A1	3796	7/7	0.79	0.29	174,174,174,174	7
87	MG	A5	4471	1/1	0.79	0.18	61,61,61,61	0
87	MG	A5	4130	1/1	0.79	0.28	49,49,49,49	0
87	MG	A5	4309	1/1	0.79	0.80	64,64,64,64	0
87	MG	A6	2329	1/1	0.79	1.14	138,138,138,138	0
86	OHX	A2	2051	7/7	0.79	0.52	209,209,209,209	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4263	1/1	0.79	1.37	71,71,71,71	0
87	MG	A1	4016	1/1	0.79	0.34	40,40,40,40	0
87	MG	A1	4118	1/1	0.79	0.18	74,74,74,74	0
87	MG	A1	4323	1/1	0.79	0.14	92,92,92,92	0
87	MG	A1	4178	1/1	0.79	0.17	70,70,70,70	0
87	MG	A1	4398	1/1	0.79	0.28	49,49,49,49	0
87	MG	A5	3960	1/1	0.79	0.24	49,49,49,49	0
87	MG	A1	4122	1/1	0.79	0.28	57,57,57,57	0
87	MG	A5	4169	1/1	0.79	0.20	90,90,90,90	0
87	MG	A5	4172	1/1	0.79	0.32	67,67,67,67	0
87	MG	A1	4407	1/1	0.79	0.66	113,113,113,113	0
87	MG	A5	4510	1/1	0.79	1.84	86,86,86,86	0
87	MG	A5	4181	1/1	0.80	0.29	80,80,80,80	0
87	MG	A5	4186	1/1	0.80	0.23	84,84,84,84	0
87	MG	A6	2189	1/1	0.80	0.32	42,42,42,42	0
87	MG	A1	3875	1/1	0.80	0.15	60,60,60,60	0
87	MG	A1	4508	1/1	0.80	0.39	58,58,58,58	0
86	OHX	A1	3726	7/7	0.80	0.22	178,178,178,178	7
87	MG	A6	2197	1/1	0.80	0.20	74,74,74,74	0
87	MG	A5	4435	1/1	0.80	0.18	87,87,87,87	0
86	OHX	A1	3793	7/7	0.80	0.29	232,232,232,232	7
87	MG	A1	4215	1/1	0.80	0.18	65,65,65,65	0
87	MG	A1	4133	1/1	0.80	0.25	91,91,91,91	0
86	OHX	A5	3810	7/7	0.80	0.55	199,199,199,199	7
86	OHX	A5	3780	7/7	0.80	0.43	211,211,211,211	7
87	MG	CG	304	1/1	0.80	0.30	72,72,72,72	0
87	MG	A6	2216	1/1	0.80	0.13	64,64,64,64	0
87	MG	A7	227	1/1	0.80	0.55	100,100,100,100	0
87	MG	A4	216	1/1	0.80	0.42	64,64,64,64	0
87	MG	A5	4091	1/1	0.80	0.12	54,54,54,54	0
87	MG	A5	4344	1/1	0.80	0.48	66,66,66,66	0
86	OHX	A6	2099	7/7	0.80	0.35	184,184,184,184	7
86	OHX	A1	3734	7/7	0.80	0.28	190,190,190,190	7
87	MG	A8	231	1/1	0.80	0.23	71,71,71,71	0
87	MG	Af	201	1/1	0.80	0.13	88,88,88,88	0
87	MG	CX	201	1/1	0.80	0.31	68,68,68,68	0
87	MG	A1	4145	1/1	0.80	0.22	54,54,54,54	0
87	MG	A5	4490	1/1	0.80	0.25	90,90,90,90	0
87	MG	A5	4235	1/1	0.80	0.23	75,75,75,75	0
86	OHX	A5	3818	7/7	0.80	0.62	226,226,226,226	7
87	MG	A1	4192	1/1	0.80	0.28	86,86,86,86	0
87	MG	A1	3908	1/1	0.80	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4370	1/1	0.80	0.21	59,59,59,59	0
87	MG	A5	4124	1/1	0.80	0.17	78,78,78,78	0
87	MG	DD	302	1/1	0.80	0.18	66,66,66,66	0
87	MG	A4	237	1/1	0.80	0.29	94,94,94,94	0
87	MG	A1	3909	1/1	0.80	0.44	67,67,67,67	0
87	MG	A1	4303	1/1	0.80	0.36	105,105,105,105	0
87	MG	A5	4134	1/1	0.80	0.22	84,84,84,84	0
87	MG	A5	3993	1/1	0.80	0.26	25,25,25,25	0
87	MG	A5	4000	1/1	0.80	0.44	53,53,53,53	0
87	MG	Ba	208	1/1	0.80	0.53	68,68,68,68	0
87	MG	A1	4073	1/1	0.80	0.13	57,57,57,57	0
87	MG	A5	4022	1/1	0.80	0.46	52,52,52,52	0
87	MG	DY	201	1/1	0.80	0.27	59,59,59,59	0
87	MG	A2	2185	1/1	0.80	0.14	72,72,72,72	0
87	MG	A6	2319	1/1	0.80	0.22	64,64,64,64	0
87	MG	A6	2320	1/1	0.80	1.56	117,117,117,117	0
87	MG	A1	3977	1/1	0.80	0.31	76,76,76,76	0
87	MG	A1	4462	1/1	0.80	0.42	71,71,71,71	0
87	MG	BD	302	1/1	0.80	0.22	79,79,79,79	0
87	MG	A5	4405	1/1	0.80	0.89	69,69,69,69	0
87	MG	A1	4503	1/1	0.80	1.26	77,77,77,77	0
87	MG	A1	4504	1/1	0.80	1.16	98,98,98,98	0
87	MG	BO	209	1/1	0.81	1.55	95,95,95,95	0
87	MG	A5	4378	1/1	0.81	1.17	75,75,75,75	0
87	MG	A5	4110	1/1	0.81	0.17	63,63,63,63	0
87	MG	CS	202	1/1	0.81	0.41	63,63,63,63	0
86	OHX	A2	2054	7/7	0.81	0.18	227,227,227,227	7
87	MG	A1	4423	1/1	0.81	0.57	85,85,85,85	0
86	OHX	A5	3734	7/7	0.81	0.31	208,208,208,208	7
86	OHX	A5	3748	7/7	0.81	0.27	183,183,183,183	7
87	MG	A5	3986	1/1	0.81	0.27	53,53,53,53	0
87	MG	BR	204	1/1	0.81	0.35	67,67,67,67	0
87	MG	A5	4558	1/1	0.81	0.44	63,63,63,63	0
87	MG	A5	4393	1/1	0.81	0.79	97,97,97,97	0
87	MG	A5	4262	1/1	0.81	0.23	60,60,60,60	0
86	OHX	A1	3732	7/7	0.81	0.26	166,166,166,166	7
87	MG	A1	3404	1/1	0.81	0.28	74,74,74,74	0
87	MG	A5	4136	1/1	0.81	0.28	46,46,46,46	0
87	MG	A6	2242	1/1	0.81	0.37	87,87,87,87	0
87	MG	A5	3995	1/1	0.81	0.39	53,53,53,53	0
87	MG	A5	4139	1/1	0.81	0.20	99,99,99,99	0
87	MG	A1	3882	1/1	0.81	0.31	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4151	1/1	0.81	0.14	64,64,64,64	0
87	MG	A6	2147	1/1	0.81	0.28	44,44,44,44	0
87	MG	A7	215	1/1	0.81	0.26	46,46,46,46	0
87	MG	A5	4294	1/1	0.81	0.21	62,62,62,62	0
87	MG	A5	4004	1/1	0.81	0.43	55,55,55,55	0
87	MG	A5	4156	1/1	0.81	0.28	65,65,65,65	0
87	MG	A5	4428	1/1	0.81	0.10	75,75,75,75	0
87	MG	A5	4431	1/1	0.81	0.38	118,118,118,118	0
87	MG	A5	3845	1/1	0.81	0.31	51,51,51,51	0
87	MG	A4	232	1/1	0.81	0.22	74,74,74,74	0
87	MG	A5	4023	1/1	0.81	0.39	44,44,44,44	0
87	MG	A6	2318	1/1	0.81	0.22	68,68,68,68	0
86	OHX	A6	2068	7/7	0.81	0.55	217,217,217,217	7
87	MG	A1	4247	1/1	0.81	0.24	74,74,74,74	0
87	MG	A5	3856	1/1	0.81	0.33	54,54,54,54	0
87	MG	A1	4112	1/1	0.81	0.21	58,58,58,58	0
87	MG	A6	2168	1/1	0.81	0.33	77,77,77,77	0
87	MG	A1	4490	1/1	0.81	0.28	77,77,77,77	0
87	MG	DB	412	1/1	0.81	0.48	70,70,70,70	0
87	MG	A1	4115	1/1	0.81	0.36	62,62,62,62	0
86	OHX	A6	2071	7/7	0.81	0.44	160,160,160,160	7
86	OHX	A6	2073	7/7	0.81	0.22	186,186,186,186	7
87	MG	A1	4167	1/1	0.81	1.06	66,66,66,66	0
87	MG	A5	4483	1/1	0.81	0.49	112,112,112,112	0
87	MG	A5	4336	1/1	0.81	0.46	77,77,77,77	0
87	MG	A5	3879	1/1	0.81	0.25	61,61,61,61	0
87	MG	A1	3826	1/1	0.81	0.19	51,51,51,51	0
87	MG	A2	2259	1/1	0.81	0.51	63,63,63,63	0
87	MG	A1	4399	1/1	0.81	0.54	85,85,85,85	0
87	MG	A5	3895	1/1	0.81	0.26	32,32,32,32	0
87	MG	A1	4177	1/1	0.81	0.90	76,76,76,76	0
87	MG	A5	4212	1/1	0.81	0.19	73,73,73,73	0
87	MG	A5	4496	1/1	0.81	0.23	77,77,77,77	0
86	OHX	A5	3778	7/7	0.81	0.20	153,153,153,153	7
87	MG	A5	4499	1/1	0.81	0.39	76,76,76,76	0
86	OHX	A6	2051	7/7	0.81	0.21	167,167,167,167	7
87	MG	Da	203	1/1	0.81	0.21	54,54,54,54	0
86	OHX	A5	3822	7/7	0.81	0.60	205,205,205,205	7
87	MG	A5	4219	1/1	0.81	0.33	74,74,74,74	0
87	MG	De	202	1/1	0.81	0.73	52,52,52,52	0
87	MG	CE	301	1/1	0.81	0.16	57,57,57,57	0
87	MG	A3	228	1/1	0.81	0.35	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	BL	203	1/1	0.81	0.21	61,61,61,61	0
86	OHX	A6	2052	7/7	0.81	0.14	211,211,211,211	7
87	MG	A1	3981	1/1	0.81	0.35	41,41,41,41	0
87	MG	A5	4533	1/1	0.81	0.19	83,83,83,83	0
87	MG	A1	4472	1/1	0.81	0.27	86,86,86,86	0
87	MG	Bj	108	1/1	0.82	1.98	66,66,66,66	0
86	OHX	A1	3772	7/7	0.82	0.27	171,171,171,171	7
87	MG	A5	4517	1/1	0.82	0.54	73,73,73,73	0
87	MG	A6	2302	1/1	0.82	0.17	108,108,108,108	0
87	MG	A5	4522	1/1	0.82	0.26	73,73,73,73	0
87	MG	A1	4012	1/1	0.82	0.38	41,41,41,41	0
87	MG	A2	2148	1/1	0.82	0.24	89,89,89,89	0
87	MG	A5	4363	1/1	0.82	0.29	83,83,83,83	0
87	MG	A6	2309	1/1	0.82	0.39	105,105,105,105	0
87	MG	A5	4365	1/1	0.82	0.28	80,80,80,80	0
87	MG	A1	4268	1/1	0.82	0.19	65,65,65,65	0
87	MG	A1	3850	1/1	0.82	0.36	64,64,64,64	0
86	OHX	A5	3800	7/7	0.82	0.27	203,203,203,203	7
87	MG	A6	2224	1/1	0.82	0.12	47,47,47,47	0
87	MG	A1	4154	1/1	0.82	0.20	91,91,91,91	0
87	MG	A1	4484	1/1	0.82	1.48	106,106,106,106	0
87	MG	A5	4228	1/1	0.82	0.35	82,82,82,82	0
87	MG	A1	3852	1/1	0.82	0.26	70,70,70,70	0
86	OHX	A2	2079	7/7	0.82	0.22	157,157,157,157	7
87	MG	A5	4383	1/1	0.82	0.29	69,69,69,69	0
87	MG	A5	3884	1/1	0.82	0.29	54,54,54,54	0
87	MG	A5	3885	1/1	0.82	0.18	58,58,58,58	0
86	OHX	A5	3769	7/7	0.82	0.28	169,169,169,169	7
86	OHX	A2	2069	7/7	0.82	0.46	191,191,191,191	7
87	MG	A5	4246	1/1	0.82	0.35	38,38,38,38	0
87	MG	A1	4430	1/1	0.82	0.35	67,67,67,67	0
86	OHX	A2	2072	7/7	0.82	0.38	207,207,207,207	7
87	MG	A5	4395	1/1	0.82	0.92	58,58,58,58	0
87	MG	A1	4498	1/1	0.82	0.23	60,60,60,60	0
86	OHX	A1	3599	7/7	0.82	0.27	196,196,196,196	7
87	MG	A5	3902	1/1	0.82	0.15	31,31,31,31	0
87	MG	A6	2330	1/1	0.82	0.35	80,80,80,80	0
87	MG	A1	4053	1/1	0.82	0.19	76,76,76,76	0
87	MG	A5	3914	1/1	0.82	0.42	69,69,69,69	0
87	MG	A7	224	1/1	0.82	0.15	69,69,69,69	0
87	MG	A1	3937	1/1	0.82	0.39	40,40,40,40	0
87	MG	A2	2239	1/1	0.82	0.18	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	AS	202	1/1	0.82	0.51	63,63,63,63	0
87	MG	A6	2146	1/1	0.82	0.25	49,49,49,49	0
87	MG	BP	208	1/1	0.82	0.16	52,52,52,52	0
87	MG	A5	3926	1/1	0.82	0.31	53,53,53,53	0
87	MG	A5	4427	1/1	0.82	0.47	102,102,102,102	0
87	MG	A5	4277	1/1	0.82	0.56	85,85,85,85	0
87	MG	A6	2154	1/1	0.82	0.36	56,56,56,56	0
87	MG	A1	4119	1/1	0.82	0.24	78,78,78,78	0
87	MG	A5	3941	1/1	0.82	0.27	51,51,51,51	0
87	MG	A5	4292	1/1	0.82	0.26	113,113,113,113	0
87	MG	DA	303	1/1	0.82	0.25	53,53,53,53	0
87	MG	DB	408	1/1	0.82	0.29	67,67,67,67	0
87	MG	A5	3944	1/1	0.82	0.20	36,36,36,36	0
87	MG	AX	201	1/1	0.82	0.14	70,70,70,70	0
87	MG	A1	4293	1/1	0.82	1.13	110,110,110,110	0
87	MG	A5	4149	1/1	0.82	0.25	63,63,63,63	0
87	MG	A1	4188	1/1	0.82	0.35	82,82,82,82	0
87	MG	A1	4452	1/1	0.82	2.08	112,112,112,112	0
87	MG	A1	4063	1/1	0.82	0.23	73,73,73,73	0
87	MG	A2	2240	1/1	0.82	0.53	97,97,97,97	0
87	MG	A1	4455	1/1	0.82	0.24	79,79,79,79	0
87	MG	DG	302	1/1	0.82	0.43	65,65,65,65	0
87	MG	A6	2181	1/1	0.82	0.31	77,77,77,77	0
87	MG	A5	4480	1/1	0.82	0.19	76,76,76,76	0
87	MG	A6	2277	1/1	0.82	0.26	79,79,79,79	0
87	MG	A2	2214	1/1	0.82	0.23	75,75,75,75	0
87	MG	CZ	201	1/1	0.82	0.21	74,74,74,74	0
87	MG	A5	4329	1/1	0.82	0.42	86,86,86,86	0
87	MG	DO	208	1/1	0.82	0.45	77,77,77,77	0
87	MG	A5	4174	1/1	0.82	0.18	75,75,75,75	0
86	OHX	A1	3664	7/7	0.82	0.15	207,207,207,207	7
87	MG	A1	4307	1/1	0.82	0.24	71,71,71,71	0
86	OHX	BP	201	7/7	0.82	0.41	115,115,115,115	7
87	MG	A5	3412	1/1	0.82	0.71	68,68,68,68	0
86	OHX	A5	3786	7/7	0.82	0.41	238,238,238,238	7
87	MG	A1	4200	1/1	0.82	0.26	71,71,71,71	0
86	OHX	DM	201	7/7	0.82	0.23	208,208,208,208	7
87	MG	A5	4498	1/1	0.82	0.27	90,90,90,90	0
87	MG	Dp	102	1/1	0.82	0.28	63,63,63,63	0
87	MG	A5	4038	1/1	0.82	0.20	42,42,42,42	0
86	OHX	BR	201	7/7	0.82	0.18	181,181,181,181	7
86	OHX	A1	3709	7/7	0.82	0.19	176,176,176,176	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4348	1/1	0.82	0.43	58,58,58,58	0
87	MG	A5	4198	1/1	0.82	0.22	58,58,58,58	0
87	MG	A6	2310	1/1	0.83	0.28	89,89,89,89	0
87	MG	A6	2205	1/1	0.83	0.26	72,72,72,72	0
87	MG	A6	2207	1/1	0.83	0.12	57,57,57,57	0
87	MG	A1	4134	1/1	0.83	0.27	69,69,69,69	0
87	MG	A1	4352	1/1	0.83	0.20	93,93,93,93	0
87	MG	A1	4354	1/1	0.83	0.21	61,61,61,61	0
87	MG	A6	2212	1/1	0.83	0.16	91,91,91,91	0
87	MG	A1	3839	1/1	0.83	0.29	64,64,64,64	0
87	MG	A5	3890	1/1	0.83	0.35	82,82,82,82	0
86	OHX	AC	301	7/7	0.83	0.86	213,213,213,213	7
87	MG	A2	2108	1/1	0.83	0.17	56,56,56,56	0
86	OHX	A1	3792	7/7	0.83	0.58	213,213,213,213	7
87	MG	A1	4458	1/1	0.83	0.77	92,92,92,92	0
87	MG	A5	4568	1/1	0.83	0.38	64,64,64,64	0
87	MG	Bm	201	1/1	0.83	0.62	68,68,68,68	0
87	MG	A4	230	1/1	0.83	0.30	71,71,71,71	0
87	MG	A2	2113	1/1	0.83	0.41	80,80,80,80	0
87	MG	A2	2249	1/1	0.83	0.19	85,85,85,85	0
87	MG	A4	233	1/1	0.83	0.20	57,57,57,57	0
86	OHX	A5	3688	7/7	0.83	0.17	212,212,212,212	7
87	MG	A1	3946	1/1	0.83	0.34	41,41,41,41	0
87	MG	A5	3922	1/1	0.83	0.20	54,54,54,54	0
86	OHX	A1	3759	7/7	0.83	0.50	149,149,149,149	7
87	MG	A1	4227	1/1	0.83	0.19	52,52,52,52	0
87	MG	A1	4468	1/1	0.83	1.20	79,79,79,79	0
87	MG	A5	3927	1/1	0.83	0.32	49,49,49,49	0
87	MG	A2	2132	1/1	0.83	0.10	77,77,77,77	0
87	MG	A1	4084	1/1	0.83	0.34	67,67,67,67	0
86	OHX	A5	3823	7/7	0.83	0.12	225,225,225,225	7
87	MG	A5	4434	1/1	0.83	0.37	72,72,72,72	0
86	OHX	A7	213	7/7	0.83	0.28	181,181,181,181	7
87	MG	A7	230	1/1	0.83	0.22	61,61,61,61	0
87	MG	A7	233	1/1	0.83	0.27	60,60,60,60	0
87	MG	A7	235	1/1	0.83	0.38	74,74,74,74	0
87	MG	BC	406	1/1	0.83	0.29	61,61,61,61	0
87	MG	A2	2137	1/1	0.83	0.21	97,97,97,97	0
87	MG	A5	3958	1/1	0.83	0.26	64,64,64,64	0
87	MG	A1	4159	1/1	0.83	0.26	84,84,84,84	0
86	OHX	A8	215	7/7	0.83	0.33	151,151,151,151	7
87	MG	A5	4452	1/1	0.83	0.84	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A8	217	7/7	0.83	0.33	169,169,169,169	7
87	MG	A2	2186	1/1	0.83	0.28	76,76,76,76	0
87	MG	A1	4403	1/1	0.83	0.17	71,71,71,71	0
87	MG	DB	404	1/1	0.83	0.29	68,68,68,68	0
86	OHX	A1	3728	7/7	0.83	0.16	203,203,203,203	7
86	OHX	A2	2074	7/7	0.83	0.26	191,191,191,191	7
87	MG	A1	3897	1/1	0.83	0.30	75,75,75,75	0
87	MG	A2	2230	1/1	0.83	0.15	94,94,94,94	0
87	MG	A1	3903	1/1	0.83	0.29	85,85,85,85	0
87	MG	A5	3410	1/1	0.83	0.27	61,61,61,61	0
87	MG	A1	4183	1/1	0.83	0.27	51,51,51,51	0
87	MG	BP	203	1/1	0.83	0.36	71,71,71,71	0
86	OHX	A5	3763	7/7	0.83	0.48	197,197,197,197	7
86	OHX	A1	3810	7/7	0.83	0.66	199,199,199,199	7
87	MG	A5	4028	1/1	0.83	0.41	47,47,47,47	0
86	OHX	A2	2084	7/7	0.83	0.18	183,183,183,183	7
87	MG	A5	4036	1/1	0.83	0.17	60,60,60,60	0
87	MG	A5	3841	1/1	0.83	0.33	44,44,44,44	0
87	MG	A2	2154	1/1	0.83	0.34	74,74,74,74	0
87	MG	DM	202	1/1	0.83	0.24	70,70,70,70	0
87	MG	A5	4205	1/1	0.83	0.28	79,79,79,79	0
87	MG	A5	4352	1/1	0.83	0.29	67,67,67,67	0
87	MG	A1	4116	1/1	0.83	0.39	65,65,65,65	0
87	MG	DP	204	1/1	0.83	0.29	78,78,78,78	0
87	MG	A5	3850	1/1	0.83	0.33	55,55,55,55	0
87	MG	A5	4210	1/1	0.83	0.26	79,79,79,79	0
87	MG	DV	204	1/1	0.83	1.04	83,83,83,83	0
87	MG	A5	4506	1/1	0.83	0.27	80,80,80,80	0
86	OHX	A1	3738	7/7	0.83	0.33	138,138,138,138	7
87	MG	A5	4053	1/1	0.83	0.35	65,65,65,65	0
87	MG	A6	2185	1/1	0.83	0.19	71,71,71,71	0
87	MG	A2	2200	1/1	0.83	0.16	88,88,88,88	0
87	MG	A1	3819	1/1	0.83	0.11	63,63,63,63	0
87	MG	A5	4371	1/1	0.83	0.23	90,90,90,90	0
87	MG	A1	4125	1/1	0.83	0.25	56,56,56,56	0
87	MG	A3	221	1/1	0.83	0.13	69,69,69,69	0
87	MG	A5	4531	1/1	0.83	0.26	65,65,65,65	0
86	OHX	A2	2065	7/7	0.83	0.34	166,166,166,166	7
86	OHX	A5	3772	7/7	0.83	0.58	137,137,137,137	7
88	ZN	Cf	501	1/1	0.83	0.16	152,152,152,152	0
87	MG	A2	2099	1/1	0.83	0.20	53,53,53,53	0
87	MG	A5	4508	1/1	0.84	0.17	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4159	1/1	0.84	0.26	64,64,64,64	0
86	OHX	A2	2060	7/7	0.84	0.35	168,168,168,168	7
87	MG	A5	4513	1/1	0.84	0.43	53,53,53,53	0
86	OHX	A2	2080	7/7	0.84	0.12	191,191,191,191	7
87	MG	A5	4340	1/1	0.84	0.80	61,61,61,61	0
87	MG	A5	4166	1/1	0.84	0.27	57,57,57,57	0
86	OHX	A2	2032	7/7	0.84	0.15	200,200,200,200	7
86	OHX	BB	402	7/7	0.84	0.23	173,173,173,173	7
86	OHX	A1	3788	7/7	0.84	0.59	232,232,232,232	7
87	MG	A5	4530	1/1	0.84	0.55	113,113,113,113	0
87	MG	A2	2250	1/1	0.84	0.06	97,97,97,97	0
87	MG	A2	2122	1/1	0.84	0.20	74,74,74,74	0
87	MG	A1	3854	1/1	0.84	0.21	57,57,57,57	0
87	MG	A5	4182	1/1	0.84	0.30	66,66,66,66	0
87	MG	CI	303	1/1	0.84	0.20	62,62,62,62	0
87	MG	A5	4354	1/1	0.84	0.72	60,60,60,60	0
87	MG	A1	4077	1/1	0.84	0.34	77,77,77,77	0
87	MG	Bo	204	1/1	0.84	0.15	76,76,76,76	0
87	MG	A5	4546	1/1	0.84	0.47	66,66,66,66	0
87	MG	A1	4080	1/1	0.84	0.17	60,60,60,60	0
87	MG	A4	228	1/1	0.84	0.26	70,70,70,70	0
87	MG	A1	4162	1/1	0.84	0.35	79,79,79,79	0
87	MG	A1	4331	1/1	0.84	0.30	62,62,62,62	0
87	MG	A1	3945	1/1	0.84	0.34	50,50,50,50	0
87	MG	A5	4199	1/1	0.84	0.43	70,70,70,70	0
86	OHX	A1	3697	7/7	0.84	0.27	182,182,182,182	7
87	MG	A1	4335	1/1	0.84	0.42	86,86,86,86	0
87	MG	A1	3953	1/1	0.84	0.36	43,43,43,43	0
87	MG	A1	3969	1/1	0.84	0.35	49,49,49,49	0
87	MG	A2	2130	1/1	0.84	0.14	56,56,56,56	0
87	MG	A5	4208	1/1	0.84	0.21	75,75,75,75	0
87	MG	A5	4380	1/1	0.84	0.71	89,89,89,89	0
87	MG	A6	2127	1/1	0.84	0.40	41,41,41,41	0
87	MG	A2	2217	1/1	0.84	0.50	117,117,117,117	0
87	MG	A2	2257	1/1	0.84	0.56	75,75,75,75	0
87	MG	A6	2264	1/1	0.84	0.16	62,62,62,62	0
87	MG	A5	3838	1/1	0.84	0.39	39,39,39,39	0
87	MG	A6	2265	1/1	0.84	0.17	73,73,73,73	0
87	MG	A7	217	1/1	0.84	0.36	55,55,55,55	0
87	MG	A1	3874	1/1	0.84	0.29	60,60,60,60	0
87	MG	A6	2270	1/1	0.84	0.43	90,90,90,90	0
87	MG	A5	4222	1/1	0.84	0.30	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4054	1/1	0.84	0.24	71,71,71,71	0
87	MG	A5	4225	1/1	0.84	0.32	66,66,66,66	0
86	OHX	A2	2083	7/7	0.84	0.57	185,185,185,185	7
87	MG	A1	3989	1/1	0.84	0.26	42,42,42,42	0
87	MG	A5	4401	1/1	0.84	0.18	64,64,64,64	0
87	MG	A5	4066	1/1	0.84	0.20	73,73,73,73	0
87	MG	A6	2135	1/1	0.84	0.23	58,58,58,58	0
87	MG	A6	2137	1/1	0.84	0.33	71,71,71,71	0
86	OHX	A6	2089	7/7	0.84	0.21	212,212,212,212	7
87	MG	A5	3853	1/1	0.84	0.27	67,67,67,67	0
87	MG	A5	4245	1/1	0.84	0.23	66,66,66,66	0
87	MG	A5	4077	1/1	0.84	0.37	55,55,55,55	0
86	OHX	A5	3776	7/7	0.84	0.24	184,184,184,184	7
87	MG	A1	3884	1/1	0.84	0.30	64,64,64,64	0
86	OHX	A2	2058	7/7	0.84	0.29	201,201,201,201	7
87	MG	A1	4001	1/1	0.84	0.31	50,50,50,50	0
87	MG	A1	4275	1/1	0.84	0.34	74,74,74,74	0
87	MG	A5	3867	1/1	0.84	0.21	27,27,27,27	0
87	MG	AI	303	1/1	0.84	0.56	73,73,73,73	0
86	OHX	A6	2050	7/7	0.84	0.16	206,206,206,206	7
87	MG	A2	2140	1/1	0.84	0.39	69,69,69,69	0
87	MG	A1	4015	1/1	0.84	0.36	63,63,63,63	0
86	OHX	A6	2097	7/7	0.84	0.25	181,181,181,181	7
87	MG	BN	305	1/1	0.84	1.37	56,56,56,56	0
87	MG	A6	2175	1/1	0.84	0.28	62,62,62,62	0
87	MG	A5	4449	1/1	0.84	1.43	122,122,122,122	0
87	MG	A6	2178	1/1	0.84	0.25	71,71,71,71	0
87	MG	BN	306	1/1	0.84	0.55	55,55,55,55	0
87	MG	A5	4453	1/1	0.84	0.57	66,66,66,66	0
87	MG	A5	4463	1/1	0.84	0.10	89,89,89,89	0
87	MG	A1	4375	1/1	0.84	0.32	51,51,51,51	0
87	MG	A1	4021	1/1	0.84	0.32	54,54,54,54	0
87	MG	A5	4473	1/1	0.84	0.83	94,94,94,94	0
87	MG	A2	2144	1/1	0.84	0.27	57,57,57,57	0
86	OHX	A5	3782	7/7	0.84	0.29	169,169,169,169	7
87	MG	A5	4293	1/1	0.84	0.33	76,76,76,76	0
87	MG	A1	4214	1/1	0.84	0.58	55,55,55,55	0
87	MG	A1	4391	1/1	0.84	0.85	89,89,89,89	0
86	OHX	DR	201	7/7	0.84	0.21	171,171,171,171	7
86	OHX	A1	3799	7/7	0.84	0.16	165,165,165,165	7
86	OHX	A1	3804	7/7	0.84	0.34	152,152,152,152	7
87	MG	A5	3911	1/1	0.84	0.15	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A5	3790	7/7	0.84	0.20	157,157,157,157	7
87	MG	A1	4401	1/1	0.84	0.26	69,69,69,69	0
87	MG	A6	2204	1/1	0.84	0.17	70,70,70,70	0
86	OHX	A5	3658	7/7	0.84	0.32	141,141,141,141	7
86	OHX	A6	2054	7/7	0.84	0.28	169,169,169,169	7
87	MG	A1	4142	1/1	0.84	0.35	68,68,68,68	0
86	OHX	A2	2085	7/7	0.84	0.44	200,200,200,200	7
87	MG	A5	4152	1/1	0.84	0.18	79,79,79,79	0
86	OHX	A2	2070	7/7	0.84	0.18	202,202,202,202	7
87	MG	A5	4332	1/1	0.84	0.10	73,73,73,73	0
87	MG	A1	4415	1/1	0.84	0.70	85,85,85,85	0
87	MG	A1	4309	1/1	0.84	0.51	99,99,99,99	0
87	MG	A1	3830	1/1	0.84	0.28	60,60,60,60	0
87	MG	A1	4424	1/1	0.85	0.31	50,50,50,50	0
87	MG	A5	4291	1/1	0.85	0.73	78,78,78,78	0
87	MG	A1	3869	1/1	0.85	0.26	69,69,69,69	0
87	MG	BL	202	1/1	0.85	0.35	78,78,78,78	0
87	MG	A5	3858	1/1	0.85	0.31	43,43,43,43	0
86	OHX	A6	2069	7/7	0.85	0.17	206,206,206,206	7
87	MG	A1	3871	1/1	0.85	0.30	48,48,48,48	0
87	MG	A5	4426	1/1	0.85	0.27	70,70,70,70	0
87	MG	A5	4311	1/1	0.85	0.24	78,78,78,78	0
87	MG	A1	4283	1/1	0.85	0.91	91,91,91,91	0
87	MG	A6	2235	1/1	0.85	0.25	77,77,77,77	0
87	MG	A6	2236	1/1	0.85	0.20	76,76,76,76	0
87	MG	A1	4347	1/1	0.85	0.35	86,86,86,86	0
87	MG	A5	4042	1/1	0.85	0.24	75,75,75,75	0
87	MG	A2	2199	1/1	0.85	0.16	72,72,72,72	0
86	OHX	BI	302	7/7	0.85	0.29	177,177,177,177	7
87	MG	A5	4049	1/1	0.85	0.29	70,70,70,70	0
87	MG	A1	4170	1/1	0.85	0.13	50,50,50,50	0
86	OHX	A1	3812	7/7	0.85	0.54	187,187,187,187	7
87	MG	A6	2141	1/1	0.85	0.41	78,78,78,78	0
87	MG	A1	4445	1/1	0.85	0.46	69,69,69,69	0
87	MG	A1	3818	1/1	0.85	0.19	63,63,63,63	0
86	OHX	A5	3781	7/7	0.85	0.14	199,199,199,199	7
87	MG	A1	3821	1/1	0.85	0.47	71,71,71,71	0
87	MG	A5	3891	1/1	0.85	0.24	50,50,50,50	0
86	OHX	A5	3750	7/7	0.85	0.22	199,199,199,199	7
86	OHX	A5	3762	7/7	0.85	0.41	153,153,153,153	7
86	OHX	A1	3736	7/7	0.85	0.23	174,174,174,174	7
87	MG	A1	3976	1/1	0.85	0.48	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A6	2077	7/7	0.85	0.17	197,197,197,197	7
87	MG	AB	302	1/1	0.85	0.13	63,63,63,63	0
87	MG	A1	3902	1/1	0.85	0.26	47,47,47,47	0
87	MG	A8	234	1/1	0.85	0.46	64,64,64,64	0
87	MG	A1	4253	1/1	0.85	0.26	110,110,110,110	0
87	MG	A5	4216	1/1	0.85	0.32	80,80,80,80	0
87	MG	A1	4382	1/1	0.85	0.25	81,81,81,81	0
87	MG	A6	2180	1/1	0.85	0.49	87,87,87,87	0
87	MG	DA	305	1/1	0.85	1.20	69,69,69,69	0
87	MG	A1	3984	1/1	0.85	0.35	51,51,51,51	0
87	MG	A5	3917	1/1	0.85	0.36	44,44,44,44	0
87	MG	A5	3918	1/1	0.85	0.27	79,79,79,79	0
87	MG	A5	4223	1/1	0.85	0.30	78,78,78,78	0
87	MG	A1	3841	1/1	0.85	0.20	47,47,47,47	0
87	MG	A1	3846	1/1	0.85	0.21	37,37,37,37	0
87	MG	A5	4226	1/1	0.85	0.35	76,76,76,76	0
87	MG	A1	4195	1/1	0.85	0.13	83,83,83,83	0
87	MG	A5	4104	1/1	0.85	0.24	52,52,52,52	0
86	OHX	CG	302	7/7	0.85	0.29	197,197,197,197	7
86	OHX	A6	2082	7/7	0.85	0.25	180,180,180,180	7
87	MG	A4	236	1/1	0.85	0.16	100,100,100,100	0
86	OHX	A1	3737	7/7	0.85	0.16	183,183,183,183	7
86	OHX	A1	3723	7/7	0.85	0.24	161,161,161,161	7
87	MG	A5	3934	1/1	0.85	0.23	61,61,61,61	0
86	OHX	Dg	201	7/7	0.85	0.37	153,153,153,153	7
87	MG	A5	3943	1/1	0.85	0.39	38,38,38,38	0
87	MG	A1	3915	1/1	0.85	0.23	32,32,32,32	0
87	MG	A5	4132	1/1	0.85	0.26	66,66,66,66	0
87	MG	A1	3917	1/1	0.85	0.19	31,31,31,31	0
87	MG	A5	4520	1/1	0.85	0.25	81,81,81,81	0
87	MG	DP	207	1/1	0.85	1.09	64,64,64,64	0
86	OHX	A5	3775	7/7	0.85	0.30	152,152,152,152	7
87	MG	A5	4527	1/1	0.85	0.22	78,78,78,78	0
87	MG	A1	4151	1/1	0.85	0.34	71,71,71,71	0
87	MG	A5	4257	1/1	0.85	0.29	70,70,70,70	0
87	MG	A6	2290	1/1	0.85	0.18	82,82,82,82	0
87	MG	A5	4389	1/1	0.85	0.82	66,66,66,66	0
87	MG	BB	404	1/1	0.85	0.28	57,57,57,57	0
86	OHX	A1	3729	7/7	0.85	0.37	167,167,167,167	7
87	MG	A2	2161	1/1	0.85	0.23	58,58,58,58	0
87	MG	A1	4336	1/1	0.85	0.20	80,80,80,80	0
87	MG	Df	205	1/1	0.85	0.43	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	3847	1/1	0.85	0.32	61,61,61,61	0
87	MG	A5	4270	1/1	0.85	0.26	57,57,57,57	0
86	OHX	A5	3813	7/7	0.85	0.22	191,191,191,191	7
87	MG	A5	3849	1/1	0.85	0.31	41,41,41,41	0
87	MG	A1	4034	1/1	0.85	0.18	46,46,46,46	0
87	MG	A1	4340	1/1	0.85	0.67	96,96,96,96	0
87	MG	A6	2220	1/1	0.85	0.13	91,91,91,91	0
87	MG	A6	2228	1/1	0.86	0.21	89,89,89,89	0
87	MG	BC	403	1/1	0.86	0.48	72,72,72,72	0
87	MG	A1	4405	1/1	0.86	0.40	61,61,61,61	0
87	MG	A5	4542	1/1	0.86	1.22	59,59,59,59	0
87	MG	A5	4085	1/1	0.86	0.28	79,79,79,79	0
86	OHX	A1	3783	7/7	0.86	0.21	152,152,152,152	7
86	OHX	A1	3768	7/7	0.86	0.37	137,137,137,137	7
87	MG	BF	4102	1/1	0.86	0.38	76,76,76,76	0
87	MG	A5	4233	1/1	0.86	0.19	91,91,91,91	0
87	MG	A1	4485	1/1	0.86	0.14	93,93,93,93	0
87	MG	A5	4090	1/1	0.86	0.34	45,45,45,45	0
87	MG	A1	4486	1/1	0.86	0.38	55,55,55,55	0
87	MG	A1	4410	1/1	0.86	0.45	69,69,69,69	0
87	MG	A1	4338	1/1	0.86	0.58	84,84,84,84	0
87	MG	A5	4097	1/1	0.86	0.24	37,37,37,37	0
86	OHX	CN	201	7/7	0.86	0.22	174,174,174,174	7
87	MG	A5	4563	1/1	0.86	0.35	89,89,89,89	0
86	OHX	A1	3690	7/7	0.86	0.24	178,178,178,178	7
87	MG	A1	4093	1/1	0.86	0.22	55,55,55,55	0
87	MG	A1	3825	1/1	0.86	0.16	47,47,47,47	0
87	MG	A5	4570	1/1	0.86	0.64	76,76,76,76	0
87	MG	A5	4255	1/1	0.86	0.25	72,72,72,72	0
86	OHX	A1	3809	7/7	0.86	0.15	192,192,192,192	7
87	MG	A6	2145	1/1	0.86	0.28	46,46,46,46	0
87	MG	A5	4114	1/1	0.86	0.19	38,38,38,38	0
87	MG	A5	4260	1/1	0.86	0.64	80,80,80,80	0
87	MG	A5	4261	1/1	0.86	0.24	71,71,71,71	0
87	MG	A1	4499	1/1	0.86	0.22	65,65,65,65	0
87	MG	A5	4118	1/1	0.86	0.26	57,57,57,57	0
86	OHX	A1	3604	7/7	0.86	0.21	254,254,254,254	7
87	MG	A7	218	1/1	0.86	0.42	43,43,43,43	0
86	OHX	A6	2094	7/7	0.86	0.19	180,180,180,180	7
87	MG	BO	206	1/1	0.86	0.70	69,69,69,69	0
87	MG	A1	4351	1/1	0.86	0.11	97,97,97,97	0
87	MG	A1	4296	1/1	0.86	0.36	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	CX	202	1/1	0.86	0.57	81,81,81,81	0
87	MG	A5	4276	1/1	0.86	0.23	60,60,60,60	0
87	MG	A1	4297	1/1	0.86	0.56	94,94,94,94	0
87	MG	A1	4197	1/1	0.86	0.16	74,74,74,74	0
87	MG	A5	3945	1/1	0.86	0.26	56,56,56,56	0
87	MG	A1	4250	1/1	0.86	0.30	56,56,56,56	0
87	MG	A6	2171	1/1	0.86	0.21	77,77,77,77	0
87	MG	A1	4300	1/1	0.86	0.27	76,76,76,76	0
87	MG	A8	223	1/1	0.86	0.34	50,50,50,50	0
86	OHX	A2	2050	7/7	0.86	0.19	181,181,181,181	7
87	MG	A3	223	1/1	0.86	0.19	75,75,75,75	0
87	MG	A5	3966	1/1	0.86	0.38	56,56,56,56	0
87	MG	A5	3971	1/1	0.86	0.36	53,53,53,53	0
86	OHX	A5	3794	7/7	0.86	0.20	179,179,179,179	7
87	MG	A5	4458	1/1	0.86	0.64	76,76,76,76	0
87	MG	A5	4459	1/1	0.86	1.14	84,84,84,84	0
87	MG	A5	4154	1/1	0.86	0.22	54,54,54,54	0
87	MG	A5	3827	1/1	0.86	0.39	67,67,67,67	0
87	MG	A1	3889	1/1	0.86	0.43	74,74,74,74	0
87	MG	A1	4306	1/1	0.86	0.13	68,68,68,68	0
86	OHX	A1	3681	7/7	0.86	0.18	146,146,146,146	7
87	MG	A5	3994	1/1	0.86	0.34	39,39,39,39	0
87	MG	A2	2198	1/1	0.86	0.27	80,80,80,80	0
87	MG	A5	3998	1/1	0.86	0.37	41,41,41,41	0
87	MG	A1	4158	1/1	0.86	0.28	87,87,87,87	0
87	MG	A1	4373	1/1	0.86	0.51	56,56,56,56	0
86	OHX	A5	3735	7/7	0.86	0.26	149,149,149,149	7
87	MG	A5	4011	1/1	0.86	0.29	54,54,54,54	0
87	MG	A6	2192	1/1	0.86	0.34	81,81,81,81	0
87	MG	A2	2110	1/1	0.86	0.32	57,57,57,57	0
86	OHX	A6	2098	7/7	0.86	0.30	144,144,144,144	7
87	MG	A2	2251	1/1	0.86	0.28	77,77,77,77	0
87	MG	A1	4383	1/1	0.86	0.11	62,62,62,62	0
87	MG	A6	2294	1/1	0.86	0.16	54,54,54,54	0
87	MG	A1	4384	1/1	0.86	0.32	61,61,61,61	0
87	MG	A6	2201	1/1	0.86	0.21	72,72,72,72	0
87	MG	A5	3857	1/1	0.86	0.30	53,53,53,53	0
87	MG	A6	2202	1/1	0.86	0.27	71,71,71,71	0
86	OHX	A5	3802	7/7	0.86	0.36	151,151,151,151	7
87	MG	A2	2114	1/1	0.86	0.41	84,84,84,84	0
87	MG	A1	4174	1/1	0.86	0.16	57,57,57,57	0
87	MG	A1	4223	1/1	0.86	0.31	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4050	1/1	0.86	0.20	39,39,39,39	0
87	MG	A1	4392	1/1	0.86	1.45	86,86,86,86	0
87	MG	A6	2314	1/1	0.86	1.38	112,112,112,112	0
87	MG	A1	4078	1/1	0.86	0.20	80,80,80,80	0
87	MG	Da	204	1/1	0.86	0.58	52,52,52,52	0
87	MG	A1	4079	1/1	0.86	0.26	75,75,75,75	0
87	MG	A5	4060	1/1	0.86	0.32	57,57,57,57	0
87	MG	A6	2213	1/1	0.86	0.11	65,65,65,65	0
86	OHX	A5	3808	7/7	0.86	0.37	182,182,182,182	7
87	MG	A1	4033	1/1	0.86	0.26	48,48,48,48	0
87	MG	A5	4073	1/1	0.86	0.36	66,66,66,66	0
87	MG	Dg	203	1/1	0.86	1.38	88,88,88,88	0
87	MG	A5	4524	1/1	0.86	0.17	85,85,85,85	0
87	MG	A5	4526	1/1	0.86	0.40	83,83,83,83	0
87	MG	A1	4229	1/1	0.86	0.17	89,89,89,89	0
87	MG	A1	4402	1/1	0.86	0.18	65,65,65,65	0
87	MG	A6	2111	1/1	0.86	0.12	51,51,51,51	0
87	MG	A1	3965	1/1	0.86	0.41	80,80,80,80	0
87	MG	A1	3968	1/1	0.86	0.20	68,68,68,68	0
87	MG	A1	4332	1/1	0.87	0.33	74,74,74,74	0
87	MG	A1	3950	1/1	0.87	0.21	48,48,48,48	0
87	MG	A1	4497	1/1	0.87	0.18	79,79,79,79	0
87	MG	A1	3952	1/1	0.87	0.32	89,89,89,89	0
87	MG	A1	4267	1/1	0.87	0.25	82,82,82,82	0
87	MG	A5	4536	1/1	0.87	0.31	73,73,73,73	0
86	OHX	A5	3647	7/7	0.87	0.11	204,204,204,204	7
87	MG	BQ	201	1/1	0.87	0.58	65,65,65,65	0
87	MG	A1	4199	1/1	0.87	0.32	74,74,74,74	0
87	MG	A1	4270	1/1	0.87	0.43	57,57,57,57	0
86	OHX	A1	3512	7/7	0.87	0.49	197,197,197,197	7
87	MG	A6	2186	1/1	0.87	0.72	104,104,104,104	0
87	MG	A1	3887	1/1	0.87	0.21	54,54,54,54	0
86	OHX	A1	3773	7/7	0.87	0.30	159,159,159,159	7
87	MG	A6	2190	1/1	0.87	0.10	74,74,74,74	0
86	OHX	A6	2013	7/7	0.87	0.24	180,180,180,180	7
87	MG	A6	2305	1/1	0.87	0.23	76,76,76,76	0
87	MG	A6	2193	1/1	0.87	0.16	75,75,75,75	0
86	OHX	A6	2023	7/7	0.87	0.23	177,177,177,177	7
87	MG	A5	3883	1/1	0.87	0.23	36,36,36,36	0
86	OHX	A5	3698	7/7	0.87	0.20	173,173,173,173	7
87	MG	A2	2129	1/1	0.87	0.30	59,59,59,59	0
87	MG	A3	227	1/1	0.87	0.64	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4433	1/1	0.87	0.76	67,67,67,67	0
87	MG	A5	4567	1/1	0.87	0.27	59,59,59,59	0
86	OHX	A5	3711	7/7	0.87	0.19	164,164,164,164	7
87	MG	Bd	201	1/1	0.87	0.48	106,106,106,106	0
87	MG	A1	4437	1/1	0.87	0.18	60,60,60,60	0
87	MG	Bg	201	1/1	0.87	0.17	63,63,63,63	0
87	MG	A5	4243	1/1	0.87	0.23	45,45,45,45	0
87	MG	A6	2206	1/1	0.87	0.20	63,63,63,63	0
87	MG	A1	4438	1/1	0.87	0.47	82,82,82,82	0
87	MG	A5	4577	1/1	0.87	0.52	76,76,76,76	0
87	MG	A5	3899	1/1	0.87	0.23	73,73,73,73	0
86	OHX	A1	3808	7/7	0.87	0.21	194,194,194,194	7
87	MG	A1	4353	1/1	0.87	0.21	77,77,77,77	0
86	OHX	A1	3564	7/7	0.87	0.23	136,136,136,136	7
87	MG	A1	4220	1/1	0.87	0.20	103,103,103,103	0
87	MG	A5	3912	1/1	0.87	0.43	77,77,77,77	0
87	MG	A5	4415	1/1	0.87	0.28	75,75,75,75	0
87	MG	A1	3837	1/1	0.87	0.27	68,68,68,68	0
87	MG	A2	2173	1/1	0.87	0.16	82,82,82,82	0
87	MG	A5	4422	1/1	0.87	0.51	52,52,52,52	0
87	MG	A5	4101	1/1	0.87	0.18	64,64,64,64	0
87	MG	A1	3840	1/1	0.87	0.36	59,59,59,59	0
86	OHX	DD	301	7/7	0.87	0.28	134,134,134,134	7
87	MG	A2	2178	1/1	0.87	0.24	73,73,73,73	0
86	OHX	A5	3789	7/7	0.87	0.28	165,165,165,165	7
87	MG	A1	4365	1/1	0.87	0.20	66,66,66,66	0
87	MG	A6	2225	1/1	0.87	0.23	59,59,59,59	0
87	MG	A7	239	1/1	0.87	0.27	71,71,71,71	0
86	OHX	A1	3700	7/7	0.87	0.35	185,185,185,185	7
87	MG	A8	221	1/1	0.87	0.16	33,33,33,33	0
86	OHX	A2	2061	7/7	0.87	0.31	142,142,142,142	7
87	MG	A1	3916	1/1	0.87	0.33	73,73,73,73	0
87	MG	A1	4460	1/1	0.87	0.20	67,67,67,67	0
87	MG	A5	4129	1/1	0.87	0.62	94,94,94,94	0
87	MG	A1	4372	1/1	0.87	0.23	71,71,71,71	0
87	MG	A1	4163	1/1	0.87	0.35	81,81,81,81	0
87	MG	A5	3938	1/1	0.87	0.30	45,45,45,45	0
87	MG	A1	4097	1/1	0.87	0.35	73,73,73,73	0
87	MG	A6	2122	1/1	0.87	0.28	55,55,55,55	0
87	MG	A1	4165	1/1	0.87	0.35	57,57,57,57	0
87	MG	A5	4455	1/1	0.87	0.67	60,60,60,60	0
86	OHX	A5	3752	7/7	0.87	0.28	127,127,127,127	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4169	1/1	0.87	0.33	80,80,80,80	0
87	MG	BB	403	1/1	0.87	0.21	53,53,53,53	0
87	MG	A1	4304	1/1	0.87	0.58	102,102,102,102	0
87	MG	A5	4300	1/1	0.87	0.60	51,51,51,51	0
87	MG	A5	4472	1/1	0.87	0.41	75,75,75,75	0
87	MG	A5	4307	1/1	0.87	0.09	78,78,78,78	0
87	MG	A5	4308	1/1	0.87	0.71	52,52,52,52	0
87	MG	A2	2142	1/1	0.87	0.38	65,65,65,65	0
87	MG	A5	3964	1/1	0.87	0.37	57,57,57,57	0
87	MG	DD	307	1/1	0.87	0.69	77,77,77,77	0
87	MG	A1	3853	1/1	0.87	0.11	43,43,43,43	0
86	OHX	A2	2062	7/7	0.87	0.20	196,196,196,196	7
87	MG	A6	2252	1/1	0.87	0.36	117,117,117,117	0
87	MG	A5	3974	1/1	0.87	0.42	40,40,40,40	0
87	MG	A6	2136	1/1	0.87	0.27	48,48,48,48	0
87	MG	A1	3855	1/1	0.87	0.19	40,40,40,40	0
86	OHX	A1	3616	7/7	0.87	0.25	117,117,117,117	7
87	MG	A5	4489	1/1	0.87	0.25	82,82,82,82	0
87	MG	A5	4161	1/1	0.87	0.21	51,51,51,51	0
87	MG	A2	2190	1/1	0.87	0.14	82,82,82,82	0
86	OHX	A1	3758	7/7	0.87	0.22	139,139,139,139	7
87	MG	A5	4326	1/1	0.87	0.25	75,75,75,75	0
87	MG	A5	4327	1/1	0.87	0.20	94,94,94,94	0
86	OHX	A2	2076	7/7	0.87	0.14	185,185,185,185	7
87	MG	A5	4168	1/1	0.87	0.26	74,74,74,74	0
87	MG	A1	3934	1/1	0.87	0.27	46,46,46,46	0
87	MG	DY	202	1/1	0.87	0.24	55,55,55,55	0
87	MG	A5	3829	1/1	0.87	0.18	35,35,35,35	0
86	OHX	A1	3666	7/7	0.87	0.23	142,142,142,142	7
87	MG	A5	3834	1/1	0.87	0.43	59,59,59,59	0
87	MG	A5	3835	1/1	0.87	0.31	49,49,49,49	0
86	OHX	A2	2019	7/7	0.87	0.17	174,174,174,174	7
87	MG	A5	4014	1/1	0.87	0.33	54,54,54,54	0
87	MG	A1	4050	1/1	0.87	0.28	63,63,63,63	0
87	MG	A5	4187	1/1	0.87	0.38	78,78,78,78	0
86	OHX	A5	3771	7/7	0.87	0.29	176,176,176,176	7
87	MG	A1	4488	1/1	0.87	0.29	73,73,73,73	0
87	MG	A6	2164	1/1	0.87	0.32	57,57,57,57	0
87	MG	A5	4027	1/1	0.87	0.41	53,53,53,53	0
87	MG	A1	4127	1/1	0.87	0.19	65,65,65,65	0
87	MG	A5	4033	1/1	0.87	0.12	31,31,31,31	0
86	OHX	A1	3770	7/7	0.87	0.21	179,179,179,179	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A5	3774	7/7	0.87	0.28	148,148,148,148	7
86	OHX	DP	201	7/7	0.88	0.34	155,155,155,155	7
87	MG	A5	3947	1/1	0.88	0.18	40,40,40,40	0
87	MG	A1	3831	1/1	0.88	0.36	56,56,56,56	0
87	MG	A1	4179	1/1	0.88	0.31	69,69,69,69	0
87	MG	BR	202	1/1	0.88	0.23	58,58,58,58	0
87	MG	A1	4180	1/1	0.88	0.81	79,79,79,79	0
87	MG	A5	3961	1/1	0.88	0.25	55,55,55,55	0
87	MG	A1	4181	1/1	0.88	0.35	61,61,61,61	0
87	MG	BR	205	1/1	0.88	0.75	99,99,99,99	0
87	MG	A1	3929	1/1	0.88	0.33	75,75,75,75	0
87	MG	A5	3968	1/1	0.88	0.19	50,50,50,50	0
87	MG	A5	4171	1/1	0.88	0.24	108,108,108,108	0
86	OHX	A6	2037	7/7	0.88	0.25	138,138,138,138	7
87	MG	A1	4491	1/1	0.88	0.85	80,80,80,80	0
87	MG	A5	3982	1/1	0.88	0.23	52,52,52,52	0
86	OHX	A6	2043	7/7	0.88	0.20	156,156,156,156	7
87	MG	A5	4534	1/1	0.88	1.30	72,72,72,72	0
87	MG	A5	4180	1/1	0.88	0.26	81,81,81,81	0
87	MG	A5	4537	1/1	0.88	0.12	83,83,83,83	0
87	MG	A6	2214	1/1	0.88	0.25	53,53,53,53	0
87	MG	A1	3838	1/1	0.88	0.25	67,67,67,67	0
86	OHX	A6	2047	7/7	0.88	0.23	156,156,156,156	7
87	MG	A1	4496	1/1	0.88	0.96	82,82,82,82	0
87	MG	A1	3942	1/1	0.88	0.33	38,38,38,38	0
87	MG	A5	4356	1/1	0.88	0.46	74,74,74,74	0
87	MG	A6	2221	1/1	0.88	0.50	69,69,69,69	0
86	OHX	A1	3708	7/7	0.88	0.18	158,158,158,158	7
87	MG	A5	4547	1/1	0.88	0.83	88,88,88,88	0
86	OHX	CI	301	7/7	0.88	0.17	172,172,172,172	7
87	MG	CY	204	1/1	0.88	0.14	56,56,56,56	0
87	MG	A1	4092	1/1	0.88	0.31	66,66,66,66	0
87	MG	A5	4369	1/1	0.88	0.81	69,69,69,69	0
87	MG	A1	3844	1/1	0.88	0.21	48,48,48,48	0
87	MG	A1	4292	1/1	0.88	0.23	67,67,67,67	0
86	OHX	A1	3655	7/7	0.88	0.23	150,150,150,150	7
86	OHX	A5	3779	7/7	0.88	0.40	167,167,167,167	7
87	MG	A2	2175	1/1	0.88	0.36	68,68,68,68	0
87	MG	A3	214	1/1	0.88	0.31	70,70,70,70	0
87	MG	A5	4026	1/1	0.88	0.40	53,53,53,53	0
87	MG	A1	3960	1/1	0.88	0.19	54,54,54,54	0
86	OHX	A1	3712	7/7	0.88	0.46	180,180,180,180	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A5	3405	7/7	0.88	0.31	118,118,118,118	7
87	MG	A5	3833	1/1	0.88	0.33	54,54,54,54	0
86	OHX	A5	3532	7/7	0.88	0.17	164,164,164,164	7
87	MG	A3	224	1/1	0.88	0.21	62,62,62,62	0
87	MG	A3	226	1/1	0.88	0.21	69,69,69,69	0
86	OHX	A2	2025	7/7	0.88	0.14	219,219,219,219	7
86	OHX	A6	2057	7/7	0.88	0.43	134,134,134,134	7
87	MG	A6	2247	1/1	0.88	0.52	88,88,88,88	0
86	OHX	A6	2058	7/7	0.88	0.24	196,196,196,196	7
87	MG	A6	2109	1/1	0.88	0.33	54,54,54,54	0
87	MG	A1	4113	1/1	0.88	0.33	70,70,70,70	0
86	OHX	A5	3685	7/7	0.88	0.26	141,141,141,141	7
87	MG	A6	2117	1/1	0.88	0.26	64,64,64,64	0
87	MG	A5	4227	1/1	0.88	0.20	46,46,46,46	0
86	OHX	A5	3791	7/7	0.88	0.23	175,175,175,175	7
87	MG	A5	4058	1/1	0.88	0.21	59,59,59,59	0
86	OHX	A1	3750	7/7	0.88	0.35	118,118,118,118	7
87	MG	A1	3986	1/1	0.88	0.37	41,41,41,41	0
86	OHX	A5	3793	7/7	0.88	0.22	158,158,158,158	7
87	MG	A5	4413	1/1	0.88	0.14	80,80,80,80	0
86	OHX	A2	2036	7/7	0.88	0.24	162,162,162,162	7
87	MG	A2	2124	1/1	0.88	0.24	79,79,79,79	0
87	MG	A7	234	1/1	0.88	0.31	90,90,90,90	0
86	OHX	A5	3796	7/7	0.88	0.26	176,176,176,176	7
86	OHX	A1	3755	7/7	0.88	0.33	135,135,135,135	7
86	OHX	A1	3756	7/7	0.88	0.24	158,158,158,158	7
87	MG	A1	3877	1/1	0.88	0.29	34,34,34,34	0
87	MG	A1	3879	1/1	0.88	0.44	89,89,89,89	0
86	OHX	A5	3719	7/7	0.88	0.24	180,180,180,180	7
87	MG	A1	4231	1/1	0.88	0.83	82,82,82,82	0
86	OHX	A5	3725	7/7	0.88	0.18	171,171,171,171	7
87	MG	A8	232	1/1	0.88	0.16	43,43,43,43	0
87	MG	A1	4442	1/1	0.88	0.48	91,91,91,91	0
87	MG	A5	4430	1/1	0.88	0.31	95,95,95,95	0
87	MG	A4	238	1/1	0.88	0.33	68,68,68,68	0
87	MG	A2	2136	1/1	0.88	0.15	70,70,70,70	0
87	MG	A4	241	1/1	0.88	0.73	60,60,60,60	0
86	OHX	A5	3733	7/7	0.88	0.21	162,162,162,162	7
87	MG	AE	301	1/1	0.88	0.76	88,88,88,88	0
87	MG	A6	2148	1/1	0.88	0.33	39,39,39,39	0
87	MG	A5	4443	1/1	0.88	0.24	64,64,64,64	0
87	MG	A2	2202	1/1	0.88	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4446	1/1	0.88	0.20	64,64,64,64	0
87	MG	A5	4093	1/1	0.88	0.30	64,64,64,64	0
87	MG	A1	4146	1/1	0.88	0.32	91,91,91,91	0
87	MG	A1	3892	1/1	0.88	0.28	75,75,75,75	0
87	MG	A6	2291	1/1	0.88	0.56	100,100,100,100	0
86	OHX	A2	2017	7/7	0.88	0.12	186,186,186,186	7
87	MG	A1	4245	1/1	0.88	0.21	73,73,73,73	0
87	MG	A5	4457	1/1	0.88	0.25	78,78,78,78	0
86	OHX	A4	211	7/7	0.88	0.33	108,108,108,108	7
86	OHX	A1	3789	7/7	0.88	0.32	189,189,189,189	7
86	OHX	A1	3790	7/7	0.88	0.18	164,164,164,164	7
87	MG	A1	3901	1/1	0.88	0.32	74,74,74,74	0
87	MG	A5	4468	1/1	0.88	0.79	73,73,73,73	0
87	MG	A1	4251	1/1	0.88	0.23	71,71,71,71	0
87	MG	AS	201	1/1	0.88	0.11	105,105,105,105	0
87	MG	A5	4288	1/1	0.88	0.78	49,49,49,49	0
86	OHX	A1	3791	7/7	0.88	0.18	149,149,149,149	7
86	OHX	A5	3753	7/7	0.88	0.12	207,207,207,207	7
86	OHX	A5	3758	7/7	0.88	0.20	167,167,167,167	7
86	OHX	A2	2039	7/7	0.88	0.36	157,157,157,157	7
87	MG	A5	4296	1/1	0.88	0.41	54,54,54,54	0
87	MG	DR	202	1/1	0.88	0.99	67,67,67,67	0
87	MG	A5	4125	1/1	0.88	0.14	67,67,67,67	0
87	MG	DV	202	1/1	0.88	0.40	35,35,35,35	0
86	OHX	A2	2057	7/7	0.88	0.17	173,173,173,173	7
87	MG	DW	201	1/1	0.88	1.32	85,85,85,85	0
87	MG	A5	4304	1/1	0.88	0.28	66,66,66,66	0
87	MG	A5	4306	1/1	0.88	0.38	72,72,72,72	0
86	OHX	A1	3794	7/7	0.88	0.29	150,150,150,150	7
87	MG	BN	303	1/1	0.88	0.94	72,72,72,72	0
87	MG	A5	3921	1/1	0.88	0.25	82,82,82,82	0
87	MG	A1	3406	1/1	0.88	0.18	67,67,67,67	0
87	MG	A2	2216	1/1	0.88	0.12	63,63,63,63	0
87	MG	A1	4361	1/1	0.88	1.09	126,126,126,126	0
86	OHX	A8	213	7/7	0.88	0.21	146,146,146,146	7
86	OHX	A5	3767	7/7	0.88	0.16	185,185,185,185	7
86	OHX	A1	3766	7/7	0.88	0.42	135,135,135,135	7
86	OHX	A2	2046	7/7	0.88	0.42	139,139,139,139	7
87	MG	A1	3824	1/1	0.88	0.30	65,65,65,65	0
87	MG	BP	206	1/1	0.88	0.19	86,86,86,86	0
86	OHX	A6	2025	7/7	0.88	0.14	161,161,161,161	7
87	MG	A5	4505	1/1	0.88	1.86	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A6	2198	1/1	0.88	0.17	49,49,49,49	0
86	OHX	A6	2026	7/7	0.88	0.16	176,176,176,176	7
87	MG	A1	4421	1/1	0.89	0.41	63,63,63,63	0
86	OHX	BA	301	7/7	0.89	0.47	217,217,217,217	7
87	MG	A1	4315	1/1	0.89	0.78	62,62,62,62	0
87	MG	A5	3991	1/1	0.89	0.28	46,46,46,46	0
87	MG	A5	4178	1/1	0.89	0.26	83,83,83,83	0
87	MG	A2	2088	1/1	0.89	0.33	59,59,59,59	0
87	MG	A6	2239	1/1	0.89	0.23	82,82,82,82	0
87	MG	A4	219	1/1	0.89	0.26	59,59,59,59	0
87	MG	A2	2223	1/1	0.89	1.95	156,156,156,156	0
87	MG	A4	221	1/1	0.89	0.28	43,43,43,43	0
86	OHX	A1	3741	7/7	0.89	0.26	151,151,151,151	7
86	OHX	A6	2067	7/7	0.89	0.24	136,136,136,136	7
87	MG	A1	4322	1/1	0.89	0.26	74,74,74,74	0
86	OHX	A5	3669	7/7	0.89	0.28	109,109,109,109	7
87	MG	A5	4357	1/1	0.89	0.64	75,75,75,75	0
86	OHX	A5	3671	7/7	0.89	0.21	171,171,171,171	7
87	MG	A5	4193	1/1	0.89	0.28	43,43,43,43	0
86	OHX	A5	3784	7/7	0.89	0.21	173,173,173,173	7
86	OHX	A1	3744	7/7	0.89	0.49	205,205,205,205	7
87	MG	A1	4043	1/1	0.89	0.37	62,62,62,62	0
87	MG	A5	4366	1/1	0.89	0.43	65,65,65,65	0
86	OHX	A2	2063	7/7	0.89	0.13	183,183,183,183	7
86	OHX	A5	3787	7/7	0.89	0.22	195,195,195,195	7
87	MG	A1	4240	1/1	0.89	0.23	59,59,59,59	0
87	MG	A1	4049	1/1	0.89	0.17	59,59,59,59	0
87	MG	A5	4553	1/1	0.89	1.10	73,73,73,73	0
87	MG	A1	3833	1/1	0.89	0.34	49,49,49,49	0
86	OHX	A1	3748	7/7	0.89	0.20	163,163,163,163	7
86	OHX	A1	3797	7/7	0.89	0.17	171,171,171,171	7
87	MG	A4	243	1/1	0.89	0.20	48,48,48,48	0
87	MG	A6	2266	1/1	0.89	0.61	106,106,106,106	0
86	OHX	A5	3707	7/7	0.89	0.47	135,135,135,135	7
86	OHX	A1	3687	7/7	0.89	0.35	182,182,182,182	7
87	MG	A5	4215	1/1	0.89	0.26	52,52,52,52	0
86	OHX	A6	2075	7/7	0.89	0.13	194,194,194,194	7
87	MG	A2	2183	1/1	0.89	0.22	49,49,49,49	0
87	MG	A5	4046	1/1	0.89	0.16	39,39,39,39	0
87	MG	A1	3842	1/1	0.89	0.40	77,77,77,77	0
86	OHX	Bj	103	7/7	0.89	0.44	138,138,138,138	7
87	MG	A1	4070	1/1	0.89	0.30	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4391	1/1	0.89	0.60	57,57,57,57	0
87	MG	A1	4254	1/1	0.89	0.26	72,72,72,72	0
86	OHX	A5	3727	7/7	0.89	0.19	167,167,167,167	7
87	MG	A5	3861	1/1	0.89	0.21	65,65,65,65	0
87	MG	A1	4348	1/1	0.89	0.16	73,73,73,73	0
86	OHX	A6	2078	7/7	0.89	0.15	185,185,185,185	7
87	MG	A5	4065	1/1	0.89	0.25	68,68,68,68	0
87	MG	A2	2246	1/1	0.89	0.12	100,100,100,100	0
87	MG	A6	2165	1/1	0.89	0.38	51,51,51,51	0
86	OHX	A6	1991	7/7	0.89	0.23	149,149,149,149	7
87	MG	A5	4407	1/1	0.89	0.12	95,95,95,95	0
87	MG	A2	2126	1/1	0.89	0.32	54,54,54,54	0
87	MG	A5	3878	1/1	0.89	0.25	56,56,56,56	0
87	MG	A5	4411	1/1	0.89	0.29	94,94,94,94	0
87	MG	A1	4171	1/1	0.89	0.18	79,79,79,79	0
86	OHX	A1	3803	7/7	0.89	0.17	196,196,196,196	7
86	OHX	A5	3741	7/7	0.89	0.14	185,185,185,185	7
87	MG	A2	2252	1/1	0.89	0.21	89,89,89,89	0
86	OHX	A6	2085	7/7	0.89	0.51	188,188,188,188	7
86	OHX	A2	2086	7/7	0.89	0.61	156,156,156,156	7
87	MG	A6	2297	1/1	0.89	0.86	68,68,68,68	0
87	MG	A7	236	1/1	0.89	0.39	102,102,102,102	0
87	MG	A1	3859	1/1	0.89	0.40	78,78,78,78	0
87	MG	A1	3861	1/1	0.89	0.25	34,34,34,34	0
87	MG	A1	3956	1/1	0.89	0.32	45,45,45,45	0
87	MG	A2	2134	1/1	0.89	0.17	74,74,74,74	0
87	MG	A6	2307	1/1	0.89	0.54	94,94,94,94	0
87	MG	A1	3864	1/1	0.89	0.20	46,46,46,46	0
87	MG	BO	208	1/1	0.89	0.23	75,75,75,75	0
87	MG	A5	4092	1/1	0.89	0.31	82,82,82,82	0
86	OHX	A1	3607	7/7	0.89	0.15	204,204,204,204	7
87	MG	A5	3905	1/1	0.89	0.27	75,75,75,75	0
86	OHX	A1	3782	7/7	0.89	0.25	186,186,186,186	7
87	MG	A1	3970	1/1	0.89	0.33	69,69,69,69	0
87	MG	A5	4098	1/1	0.89	0.14	55,55,55,55	0
87	MG	A5	4444	1/1	0.89	0.42	66,66,66,66	0
87	MG	A1	3972	1/1	0.89	0.42	45,45,45,45	0
87	MG	A1	4280	1/1	0.89	0.11	51,51,51,51	0
86	OHX	A2	2064	7/7	0.89	0.31	169,169,169,169	7
86	OHX	A5	3760	7/7	0.89	0.11	202,202,202,202	7
86	OHX	A6	2091	7/7	0.89	0.28	165,165,165,165	7
86	OHX	A6	2039	7/7	0.89	0.17	168,168,168,168	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4278	1/1	0.89	0.88	82,82,82,82	0
87	MG	A2	2204	1/1	0.89	1.48	109,109,109,109	0
86	OHX	A1	3784	7/7	0.89	0.23	169,169,169,169	7
87	MG	A1	4389	1/1	0.89	0.61	46,46,46,46	0
87	MG	A5	4116	1/1	0.89	0.36	56,56,56,56	0
87	MG	A5	4290	1/1	0.89	0.48	47,47,47,47	0
86	OHX	A6	2045	7/7	0.89	0.30	124,124,124,124	7
87	MG	A5	4467	1/1	0.89	0.14	70,70,70,70	0
87	MG	BT	202	1/1	0.89	0.65	89,89,89,89	0
86	OHX	A6	2046	7/7	0.89	0.19	204,204,204,204	7
87	MG	A1	3883	1/1	0.89	0.36	37,37,37,37	0
87	MG	A5	4295	1/1	0.89	0.19	61,61,61,61	0
87	MG	A1	4114	1/1	0.89	0.42	71,71,71,71	0
87	MG	A5	3928	1/1	0.89	0.32	90,90,90,90	0
87	MG	DO	206	1/1	0.89	0.73	55,55,55,55	0
87	MG	A1	4202	1/1	0.89	0.21	67,67,67,67	0
87	MG	A5	4302	1/1	0.89	0.19	72,72,72,72	0
87	MG	DP	203	1/1	0.89	0.38	37,37,37,37	0
87	MG	A1	4205	1/1	0.89	0.13	63,63,63,63	0
86	OHX	A1	3704	7/7	0.89	0.15	176,176,176,176	7
87	MG	A5	3937	1/1	0.89	0.34	69,69,69,69	0
86	OHX	CB	301	7/7	0.89	0.18	162,162,162,162	7
87	MG	DS	203	1/1	0.89	0.33	65,65,65,65	0
87	MG	DS	204	1/1	0.89	0.72	63,63,63,63	0
87	MG	A1	4117	1/1	0.89	0.27	80,80,80,80	0
87	MG	A5	3942	1/1	0.89	0.33	38,38,38,38	0
87	MG	A1	3993	1/1	0.89	0.29	52,52,52,52	0
87	MG	A3	219	1/1	0.89	0.35	40,40,40,40	0
87	MG	A5	4142	1/1	0.89	0.23	91,91,91,91	0
86	OHX	A1	3813	7/7	0.89	0.17	201,201,201,201	7
86	OHX	A2	2029	7/7	0.89	0.34	150,150,150,150	7
87	MG	Bj	105	1/1	0.89	0.87	64,64,64,64	0
87	MG	CI	302	1/1	0.89	0.27	63,63,63,63	0
86	OHX	A1	3762	7/7	0.89	0.32	144,144,144,144	7
86	OHX	A3	210	7/7	0.89	0.19	175,175,175,175	7
87	MG	CL	203	1/1	0.89	0.22	61,61,61,61	0
87	MG	A1	4305	1/1	0.89	0.30	65,65,65,65	0
87	MG	A1	4128	1/1	0.89	0.28	63,63,63,63	0
87	MG	CQ	201	1/1	0.89	0.14	75,75,75,75	0
87	MG	A1	4414	1/1	0.89	0.23	90,90,90,90	0
86	OHX	A2	2041	7/7	0.89	0.15	184,184,184,184	7
86	OHX	DQ	201	7/7	0.89	0.26	147,147,147,147	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4165	1/1	0.89	0.13	73,73,73,73	0
87	MG	A5	3976	1/1	0.89	0.23	43,43,43,43	0
87	MG	A5	3977	1/1	0.89	0.36	69,69,69,69	0
86	OHX	A2	2004	7/7	0.89	0.19	164,164,164,164	7
87	MG	A5	3873	1/1	0.90	0.34	60,60,60,60	0
87	MG	A2	2248	1/1	0.90	0.26	69,69,69,69	0
87	MG	A5	4055	1/1	0.90	0.22	81,81,81,81	0
86	OHX	A1	3722	7/7	0.90	0.22	150,150,150,150	7
87	MG	A5	4367	1/1	0.90	0.59	74,74,74,74	0
87	MG	BL	204	1/1	0.90	0.84	72,72,72,72	0
86	OHX	A5	3721	7/7	0.90	0.20	167,167,167,167	7
87	MG	A5	3882	1/1	0.90	0.06	74,74,74,74	0
87	MG	A5	4063	1/1	0.90	0.23	52,52,52,52	0
86	OHX	A6	2042	7/7	0.90	0.20	169,169,169,169	7
87	MG	A1	3860	1/1	0.90	0.24	59,59,59,59	0
87	MG	A1	4090	1/1	0.90	0.30	78,78,78,78	0
87	MG	A5	4069	1/1	0.90	0.20	88,88,88,88	0
87	MG	A5	4221	1/1	0.90	0.61	88,88,88,88	0
86	OHX	A1	3749	7/7	0.90	0.14	177,177,177,177	7
86	OHX	A5	3728	7/7	0.90	0.40	131,131,131,131	7
86	OHX	A1	3670	7/7	0.90	0.19	152,152,152,152	7
86	OHX	A2	1988	7/7	0.90	0.18	189,189,189,189	7
86	OHX	A1	3787	7/7	0.90	0.20	173,173,173,173	7
86	OHX	A3	212	7/7	0.90	0.35	159,159,159,159	7
87	MG	BP	205	1/1	0.90	0.24	53,53,53,53	0
86	OHX	A5	3744	7/7	0.90	0.26	140,140,140,140	7
86	OHX	A5	3801	7/7	0.90	0.28	156,156,156,156	7
87	MG	A1	3980	1/1	0.90	0.31	38,38,38,38	0
87	MG	BP	209	1/1	0.90	0.26	59,59,59,59	0
86	OHX	A1	3727	7/7	0.90	0.29	146,146,146,146	7
86	OHX	A2	2021	7/7	0.90	0.27	158,158,158,158	7
87	MG	A1	4295	1/1	0.90	0.19	62,62,62,62	0
86	OHX	A5	3751	7/7	0.90	0.22	148,148,148,148	7
87	MG	A1	3878	1/1	0.90	0.28	45,45,45,45	0
86	OHX	A6	2053	7/7	0.90	0.20	123,123,123,123	7
86	OHX	A4	215	7/7	0.90	0.20	175,175,175,175	7
87	MG	A5	4404	1/1	0.90	0.83	54,54,54,54	0
87	MG	BS	201	1/1	0.90	0.46	64,64,64,64	0
87	MG	A1	4210	1/1	0.90	0.62	44,44,44,44	0
87	MG	A1	4506	1/1	0.90	0.22	77,77,77,77	0
86	OHX	A1	3689	7/7	0.90	0.28	99,99,99,99	7
87	MG	AL	202	1/1	0.90	0.97	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A1	3730	7/7	0.90	0.19	135,135,135,135	7
87	MG	A1	4406	1/1	0.90	0.60	69,69,69,69	0
87	MG	Ba	202	1/1	0.90	0.54	63,63,63,63	0
87	MG	A5	4259	1/1	0.90	0.27	56,56,56,56	0
87	MG	A2	2138	1/1	0.90	0.13	56,56,56,56	0
87	MG	A1	4216	1/1	0.90	0.21	93,93,93,93	0
86	OHX	A2	2053	7/7	0.90	0.23	173,173,173,173	7
87	MG	A1	4123	1/1	0.90	0.31	77,77,77,77	0
87	MG	A5	4113	1/1	0.90	0.17	39,39,39,39	0
87	MG	CF	301	1/1	0.90	0.44	87,87,87,87	0
87	MG	A1	4008	1/1	0.90	0.34	36,36,36,36	0
87	MG	A7	231	1/1	0.90	0.25	87,87,87,87	0
86	OHX	A1	3691	7/7	0.90	0.28	175,175,175,175	7
86	OHX	A5	3821	7/7	0.90	0.18	223,223,223,223	7
86	OHX	A6	2063	7/7	0.90	0.21	176,176,176,176	7
87	MG	Ad	103	1/1	0.90	0.14	67,67,67,67	0
86	OHX	A5	3766	7/7	0.90	0.13	173,173,173,173	7
87	MG	A2	2213	1/1	0.90	0.21	107,107,107,107	0
87	MG	A5	4127	1/1	0.90	0.30	68,68,68,68	0
87	MG	A1	4320	1/1	0.90	0.25	59,59,59,59	0
87	MG	A8	224	1/1	0.90	0.20	67,67,67,67	0
87	MG	A8	226	1/1	0.90	0.22	62,62,62,62	0
87	MG	A1	4026	1/1	0.90	0.38	42,42,42,42	0
87	MG	A5	4286	1/1	0.90	0.31	58,58,58,58	0
87	MG	A5	3953	1/1	0.90	0.47	69,69,69,69	0
87	MG	A1	4136	1/1	0.90	0.24	53,53,53,53	0
87	MG	A5	3957	1/1	0.90	0.44	43,43,43,43	0
86	OHX	A7	212	7/7	0.90	0.51	165,165,165,165	7
86	OHX	A2	2073	7/7	0.90	0.25	147,147,147,147	7
86	OHX	A2	1998	7/7	0.90	0.26	135,135,135,135	7
86	OHX	A5	3585	7/7	0.90	0.21	163,163,163,163	7
86	OHX	A5	3591	7/7	0.90	0.23	209,209,209,209	7
86	OHX	A5	3623	7/7	0.90	0.21	156,156,156,156	7
87	MG	A5	4143	1/1	0.90	0.16	70,70,70,70	0
87	MG	DB	407	1/1	0.90	0.79	72,72,72,72	0
86	OHX	DB	402	7/7	0.90	0.19	145,145,145,145	7
87	MG	A5	4147	1/1	0.90	0.14	63,63,63,63	0
86	OHX	A1	3639	7/7	0.90	0.19	145,145,145,145	7
87	MG	A2	2157	1/1	0.90	0.28	82,82,82,82	0
86	OHX	A5	3656	7/7	0.90	0.20	169,169,169,169	7
87	MG	A5	4470	1/1	0.90	0.15	76,76,76,76	0
86	OHX	A1	3771	7/7	0.90	0.26	174,174,174,174	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	3411	1/1	0.90	0.22	82,82,82,82	0
86	OHX	A1	3739	7/7	0.90	0.20	185,185,185,185	7
87	MG	A2	2228	1/1	0.90	0.13	85,85,85,85	0
87	MG	A1	3835	1/1	0.90	0.18	41,41,41,41	0
87	MG	A5	3990	1/1	0.90	0.44	68,68,68,68	0
87	MG	A5	4160	1/1	0.90	0.15	53,53,53,53	0
86	OHX	AP	201	7/7	0.90	0.16	196,196,196,196	7
86	OHX	A2	2066	7/7	0.90	0.32	164,164,164,164	7
87	MG	A5	4163	1/1	0.90	0.22	58,58,58,58	0
86	OHX	A5	3683	7/7	0.90	0.24	119,119,119,119	7
87	MG	A1	3924	1/1	0.90	0.30	57,57,57,57	0
87	MG	DO	203	1/1	0.90	0.27	58,58,58,58	0
87	MG	A5	4487	1/1	0.90	1.23	76,76,76,76	0
87	MG	A1	4065	1/1	0.90	0.24	47,47,47,47	0
87	MG	A5	3837	1/1	0.90	0.33	58,58,58,58	0
87	MG	A1	4067	1/1	0.90	0.15	66,66,66,66	0
87	MG	A4	246	1/1	0.90	0.88	91,91,91,91	0
87	MG	A4	247	1/1	0.90	0.68	56,56,56,56	0
87	MG	A5	4008	1/1	0.90	0.36	42,42,42,42	0
86	OHX	A1	3776	7/7	0.90	0.34	123,123,123,123	7
87	MG	DS	202	1/1	0.90	0.19	75,75,75,75	0
86	OHX	A1	3554	7/7	0.90	0.20	159,159,159,159	7
87	MG	BA	303	1/1	0.90	0.25	30,30,30,30	0
87	MG	BA	304	1/1	0.90	0.20	62,62,62,62	0
87	MG	A2	2093	1/1	0.90	0.25	47,47,47,47	0
87	MG	A1	3931	1/1	0.90	0.26	40,40,40,40	0
86	OHX	A6	2079	7/7	0.90	0.17	161,161,161,161	7
87	MG	A5	4343	1/1	0.90	0.55	56,56,56,56	0
87	MG	A6	2143	1/1	0.90	0.35	45,45,45,45	0
86	OHX	A5	3783	7/7	0.90	0.25	154,154,154,154	7
87	MG	A5	4346	1/1	0.90	0.23	89,89,89,89	0
87	MG	A2	2096	1/1	0.90	0.29	76,76,76,76	0
87	MG	A5	4512	1/1	0.90	0.29	56,56,56,56	0
87	MG	A1	4173	1/1	0.90	0.14	45,45,45,45	0
87	MG	A1	4076	1/1	0.90	0.29	64,64,64,64	0
87	MG	A5	4350	1/1	0.90	0.95	58,58,58,58	0
87	MG	A6	2151	1/1	0.90	0.47	64,64,64,64	0
87	MG	BF	4101	1/1	0.90	0.24	64,64,64,64	0
87	MG	Dn	101	1/1	0.90	0.40	84,84,84,84	0
86	OHX	A6	2081	7/7	0.90	0.12	201,201,201,201	7
86	OHX	A6	2031	6/7	0.90	0.12	195,195,195,195	6
86	OHX	A1	3746	7/7	0.90	0.30	142,142,142,142	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A6	2163	1/1	0.90	0.34	58,58,58,58	0
86	OHX	A5	3712	7/7	0.90	0.25	149,149,149,149	7
87	MG	A2	2103	1/1	0.90	0.35	58,58,58,58	0
87	MG	A2	2105	1/1	0.90	0.28	55,55,55,55	0
87	MG	A5	3949	1/1	0.91	0.25	37,37,37,37	0
87	MG	A1	4358	1/1	0.91	0.41	86,86,86,86	0
86	OHX	A1	3752	7/7	0.91	0.10	207,207,207,207	7
87	MG	A5	3954	1/1	0.91	0.37	46,46,46,46	0
87	MG	A1	4157	1/1	0.91	0.29	87,87,87,87	0
87	MG	A2	2128	1/1	0.91	0.38	62,62,62,62	0
86	OHX	A5	3797	7/7	0.91	0.23	130,130,130,130	7
87	MG	A5	3959	1/1	0.91	0.40	61,61,61,61	0
87	MG	A5	4519	1/1	0.91	0.10	63,63,63,63	0
87	MG	A1	3913	1/1	0.91	0.32	86,86,86,86	0
87	MG	A1	4056	1/1	0.91	0.23	61,61,61,61	0
86	OHX	A2	2048	7/7	0.91	0.15	155,155,155,155	7
86	OHX	A6	2093	7/7	0.91	0.20	149,149,149,149	7
86	OHX	A6	2048	7/7	0.91	0.24	169,169,169,169	7
86	OHX	A1	3688	7/7	0.91	0.13	181,181,181,181	7
87	MG	BP	212	1/1	0.91	0.28	93,93,93,93	0
86	OHX	A2	2044	7/7	0.91	0.16	162,162,162,162	7
86	OHX	A5	3805	7/7	0.91	0.15	172,172,172,172	7
87	MG	A1	4494	1/1	0.91	0.35	87,87,87,87	0
86	OHX	A5	3736	7/7	0.91	0.30	143,143,143,143	7
87	MG	A1	3829	1/1	0.91	0.37	55,55,55,55	0
86	OHX	A2	2045	7/7	0.91	0.14	164,164,164,164	7
87	MG	A1	3923	1/1	0.91	0.24	44,44,44,44	0
86	OHX	A5	3742	7/7	0.91	0.31	143,143,143,143	7
87	MG	A1	3832	1/1	0.91	0.19	65,65,65,65	0
87	MG	A1	3927	1/1	0.91	0.20	31,31,31,31	0
86	OHX	A1	3660	7/7	0.91	0.27	137,137,137,137	7
86	OHX	A5	3746	7/7	0.91	0.23	151,151,151,151	7
87	MG	A5	4183	1/1	0.91	0.15	76,76,76,76	0
87	MG	A5	4184	1/1	0.91	0.29	55,55,55,55	0
87	MG	A6	2219	1/1	0.91	0.20	50,50,50,50	0
87	MG	BY	201	1/1	0.91	0.24	56,56,56,56	0
87	MG	A1	4505	1/1	0.91	0.89	145,145,145,145	0
86	OHX	A5	3747	7/7	0.91	0.20	160,160,160,160	7
86	OHX	A4	213	7/7	0.91	0.14	164,164,164,164	7
87	MG	Ba	204	1/1	0.91	0.69	74,74,74,74	0
86	OHX	A6	2056	7/7	0.91	0.12	178,178,178,178	7
87	MG	A5	4013	1/1	0.91	0.35	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A1	3731	7/7	0.91	0.23	119,119,119,119	7
87	MG	A5	4197	1/1	0.91	0.39	84,84,84,84	0
87	MG	A5	4564	1/1	0.91	0.31	79,79,79,79	0
87	MG	A5	4373	1/1	0.91	0.41	74,74,74,74	0
87	MG	A3	218	1/1	0.91	0.30	46,46,46,46	0
87	MG	A5	3830	1/1	0.91	0.19	39,39,39,39	0
86	OHX	A2	1960	7/7	0.91	0.14	173,173,173,173	7
86	OHX	A2	2081	7/7	0.91	0.16	199,199,199,199	7
86	OHX	A5	3754	7/7	0.91	0.23	147,147,147,147	7
87	MG	A2	2153	1/1	0.91	0.21	72,72,72,72	0
87	MG	A1	4191	1/1	0.91	0.17	58,58,58,58	0
86	OHX	A5	3756	7/7	0.91	0.26	158,158,158,158	7
87	MG	A3	225	1/1	0.91	0.34	61,61,61,61	0
86	OHX	A8	212	7/7	0.91	0.19	172,172,172,172	7
87	MG	Bj	110	1/1	0.91	0.76	94,94,94,94	0
87	MG	A5	4386	1/1	0.91	0.23	65,65,65,65	0
86	OHX	A5	3403	7/7	0.91	0.19	171,171,171,171	7
86	OHX	A1	3702	7/7	0.91	0.18	141,141,141,141	7
86	OHX	A5	3406	7/7	0.91	0.13	170,170,170,170	7
86	OHX	A5	3407	7/7	0.91	0.14	196,196,196,196	7
87	MG	A1	3963	1/1	0.91	0.22	56,56,56,56	0
87	MG	A1	4096	1/1	0.91	0.23	80,80,80,80	0
86	OHX	A8	220	7/7	0.91	0.23	111,111,111,111	7
86	OHX	A5	3764	7/7	0.91	0.26	120,120,120,120	7
87	MG	A5	4396	1/1	0.91	0.23	71,71,71,71	0
87	MG	A5	4051	1/1	0.91	0.15	77,77,77,77	0
87	MG	A4	218	1/1	0.91	0.33	59,59,59,59	0
87	MG	A1	4416	1/1	0.91	1.11	57,57,57,57	0
87	MG	A1	4418	1/1	0.91	0.48	48,48,48,48	0
87	MG	A2	2165	1/1	0.91	0.27	78,78,78,78	0
87	MG	A6	2112	1/1	0.91	0.33	64,64,64,64	0
87	MG	A5	4406	1/1	0.91	0.65	75,75,75,75	0
87	MG	A6	2115	1/1	0.91	0.37	47,47,47,47	0
87	MG	A5	4408	1/1	0.91	0.40	65,65,65,65	0
86	OHX	A1	3795	7/7	0.91	0.43	195,195,195,195	7
87	MG	A1	3858	1/1	0.91	0.33	64,64,64,64	0
87	MG	A1	4106	1/1	0.91	0.33	69,69,69,69	0
87	MG	A1	4308	1/1	0.91	0.75	59,59,59,59	0
87	MG	A1	3973	1/1	0.91	0.34	37,37,37,37	0
87	MG	A5	4238	1/1	0.91	0.50	44,44,44,44	0
87	MG	A5	4239	1/1	0.91	0.31	44,44,44,44	0
86	OHX	DJ	201	7/7	0.91	0.14	185,185,185,185	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4426	1/1	0.91	0.87	82,82,82,82	0
86	OHX	A6	2066	7/7	0.91	0.24	119,119,119,119	7
87	MG	A5	3877	1/1	0.91	0.32	60,60,60,60	0
86	OHX	A2	2024	7/7	0.91	0.24	174,174,174,174	7
86	OHX	A1	3707	7/7	0.91	0.20	135,135,135,135	7
87	MG	A8	238	1/1	0.91	0.32	93,93,93,93	0
87	MG	A6	2131	1/1	0.91	0.30	46,46,46,46	0
87	MG	A1	3979	1/1	0.91	0.41	52,52,52,52	0
87	MG	A2	2171	1/1	0.91	0.29	89,89,89,89	0
86	OHX	A1	3798	7/7	0.91	0.71	226,226,226,226	7
87	MG	A1	3983	1/1	0.91	0.13	65,65,65,65	0
86	OHX	A1	3674	7/7	0.91	0.19	159,159,159,159	7
87	MG	A1	4439	1/1	0.91	0.38	88,88,88,88	0
86	OHX	A1	3800	7/7	0.91	0.21	188,188,188,188	7
86	OHX	A5	3662	7/7	0.91	0.24	148,148,148,148	7
87	MG	A5	3892	1/1	0.91	0.20	45,45,45,45	0
87	MG	A6	2289	1/1	0.91	0.24	96,96,96,96	0
87	MG	A1	4225	1/1	0.91	0.27	67,67,67,67	0
87	MG	A6	2142	1/1	0.91	0.34	46,46,46,46	0
86	OHX	A6	2008	7/7	0.91	0.17	176,176,176,176	7
86	OHX	A1	3677	7/7	0.91	0.27	115,115,115,115	7
87	MG	DF	301	1/1	0.91	0.19	75,75,75,75	0
87	MG	A5	4266	1/1	0.91	0.28	72,72,72,72	0
87	MG	DF	304	1/1	0.91	0.61	57,57,57,57	0
87	MG	A5	3900	1/1	0.91	0.24	63,63,63,63	0
87	MG	A6	2295	1/1	0.91	0.15	79,79,79,79	0
86	OHX	A1	3711	7/7	0.91	0.17	155,155,155,155	7
87	MG	A5	4456	1/1	0.91	0.31	79,79,79,79	0
86	OHX	A5	3673	7/7	0.91	0.23	144,144,144,144	7
86	OHX	A5	3674	7/7	0.91	0.26	100,100,100,100	7
87	MG	A5	3910	1/1	0.91	0.32	57,57,57,57	0
87	MG	DN	301	1/1	0.91	0.24	77,77,77,77	0
87	MG	A5	4102	1/1	0.91	0.40	71,71,71,71	0
87	MG	DO	205	1/1	0.91	0.51	52,52,52,52	0
87	MG	A5	4103	1/1	0.91	0.33	74,74,74,74	0
87	MG	A6	2149	1/1	0.91	0.38	49,49,49,49	0
87	MG	A6	2303	1/1	0.91	0.33	60,60,60,60	0
87	MG	DO	209	1/1	0.91	0.79	62,62,62,62	0
87	MG	A5	4469	1/1	0.91	0.17	70,70,70,70	0
87	MG	A5	4109	1/1	0.91	0.29	88,88,88,88	0
87	MG	A5	3913	1/1	0.91	0.12	68,68,68,68	0
86	OHX	A5	3680	7/7	0.91	0.30	134,134,134,134	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A1	3678	7/7	0.91	0.16	186,186,186,186	7
87	MG	BC	402	1/1	0.91	0.28	54,54,54,54	0
86	OHX	A1	3806	7/7	0.91	0.25	198,198,198,198	7
87	MG	BC	405	1/1	0.91	0.56	49,49,49,49	0
86	OHX	A1	3807	7/7	0.91	0.17	167,167,167,167	7
87	MG	BC	407	1/1	0.91	0.57	58,58,58,58	0
86	OHX	A1	3721	7/7	0.91	0.17	153,153,153,153	7
86	OHX	A5	3696	7/7	0.91	0.18	167,167,167,167	7
86	OHX	AN	201	7/7	0.91	0.16	192,192,192,192	7
87	MG	A1	3890	1/1	0.91	0.34	61,61,61,61	0
87	MG	Da	201	1/1	0.91	0.28	54,54,54,54	0
87	MG	Da	202	1/1	0.91	0.49	84,84,84,84	0
87	MG	A5	4305	1/1	0.91	0.74	88,88,88,88	0
86	OHX	A5	3700	7/7	0.91	0.39	146,146,146,146	7
86	OHX	A5	3704	7/7	0.91	0.21	141,141,141,141	7
87	MG	A1	4030	1/1	0.91	0.19	37,37,37,37	0
86	OHX	A6	2041	7/7	0.91	0.26	145,145,145,145	7
87	MG	A1	4345	1/1	0.91	0.18	73,73,73,73	0
86	OHX	A5	3709	7/7	0.91	0.13	171,171,171,171	7
86	OHX	A1	3781	7/7	0.91	0.28	122,122,122,122	7
87	MG	A5	3939	1/1	0.91	0.39	42,42,42,42	0
87	MG	Dj	101	1/1	0.91	0.25	38,38,38,38	0
87	MG	Dj	102	1/1	0.91	1.24	74,74,74,74	0
87	MG	A2	2116	1/1	0.91	0.36	59,59,59,59	0
87	MG	A2	2120	1/1	0.91	0.35	73,73,73,73	0
86	OHX	A1	3684	7/7	0.91	0.15	143,143,143,143	7
86	OHX	A6	2088	7/7	0.91	0.23	160,160,160,160	7
86	OHX	A1	3724	7/7	0.91	0.24	144,144,144,144	7
87	MG	A2	2205	1/1	0.91	0.13	83,83,83,83	0
87	MG	A5	4148	1/1	0.91	0.26	75,75,75,75	0
87	MG	A5	4325	1/1	0.91	0.99	57,57,57,57	0
87	MG	A5	4321	1/1	0.92	0.22	77,77,77,77	0
86	OHX	A1	3705	7/7	0.92	0.14	164,164,164,164	7
87	MG	BQ	204	1/1	0.92	1.35	99,99,99,99	0
87	MG	A5	4144	1/1	0.92	0.71	75,75,75,75	0
87	MG	A1	3944	1/1	0.92	0.45	45,45,45,45	0
87	MG	A6	2339	1/1	0.92	0.20	64,64,64,64	0
87	MG	A1	4272	1/1	0.92	0.24	53,53,53,53	0
87	MG	A1	4377	1/1	0.92	0.76	54,54,54,54	0
87	MG	A2	2090	1/1	0.92	0.28	53,53,53,53	0
87	MG	A5	4521	1/1	0.92	0.71	68,68,68,68	0
87	MG	A1	4075	1/1	0.92	0.24	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A6	2084	7/7	0.92	0.15	196,196,196,196	7
87	MG	A1	3947	1/1	0.92	0.42	42,42,42,42	0
86	OHX	A2	1947	7/7	0.92	0.17	157,157,157,157	7
86	OHX	A5	3689	7/7	0.92	0.20	134,134,134,134	7
86	OHX	A1	3777	7/7	0.92	0.26	137,137,137,137	7
87	MG	A5	4158	1/1	0.92	0.27	62,62,62,62	0
86	OHX	A1	3740	7/7	0.92	0.30	107,107,107,107	7
86	OHX	A1	3811	7/7	0.92	0.32	183,183,183,183	7
87	MG	A1	4394	1/1	0.92	0.79	58,58,58,58	0
86	OHX	A6	2044	7/7	0.92	0.14	178,178,178,178	7
86	OHX	A1	3548	7/7	0.92	0.20	136,136,136,136	7
86	OHX	A1	3780	7/7	0.92	0.26	136,136,136,136	7
87	MG	A2	2180	1/1	0.92	0.12	101,101,101,101	0
87	MG	A5	3979	1/1	0.92	0.44	61,61,61,61	0
87	MG	A5	3980	1/1	0.92	0.35	58,58,58,58	0
86	OHX	A1	3742	7/7	0.92	0.31	140,140,140,140	7
87	MG	A5	3985	1/1	0.92	0.45	51,51,51,51	0
87	MG	A1	3971	1/1	0.92	0.34	35,35,35,35	0
86	OHX	A5	3710	7/7	0.92	0.18	132,132,132,132	7
87	MG	A6	2223	1/1	0.92	0.20	75,75,75,75	0
86	OHX	A5	3788	7/7	0.92	0.29	141,141,141,141	7
87	MG	Ch	301	1/1	0.92	0.18	44,44,44,44	0
87	MG	A2	2184	1/1	0.92	0.25	109,109,109,109	0
87	MG	A5	4555	1/1	0.92	0.68	63,63,63,63	0
87	MG	A5	3409	1/1	0.92	0.30	45,45,45,45	0
87	MG	A1	4294	1/1	0.92	0.21	78,78,78,78	0
86	OHX	A2	2059	7/7	0.92	0.11	183,183,183,183	7
87	MG	A1	4196	1/1	0.92	0.22	71,71,71,71	0
87	MG	A1	4409	1/1	0.92	1.01	58,58,58,58	0
86	OHX	A6	2049	7/7	0.92	0.14	175,175,175,175	7
87	MG	A5	4003	1/1	0.92	0.36	46,46,46,46	0
87	MG	A1	4099	1/1	0.92	0.26	71,71,71,71	0
87	MG	A5	4190	1/1	0.92	0.71	58,58,58,58	0
87	MG	A1	4412	1/1	0.92	0.32	104,104,104,104	0
87	MG	A1	4100	1/1	0.92	0.14	34,34,34,34	0
86	OHX	A3	209	7/7	0.92	0.16	180,180,180,180	7
86	OHX	A1	3676	7/7	0.92	0.22	148,148,148,148	7
87	MG	A6	2241	1/1	0.92	0.81	112,112,112,112	0
87	MG	A5	4574	1/1	0.92	0.34	74,74,74,74	0
87	MG	A5	3836	1/1	0.92	0.34	66,66,66,66	0
87	MG	A2	2189	1/1	0.92	0.21	55,55,55,55	0
87	MG	A1	4203	1/1	0.92	0.29	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A5	3724	7/7	0.92	0.26	124,124,124,124	7
87	MG	A1	3982	1/1	0.92	0.41	43,43,43,43	0
86	OHX	A2	2012	7/7	0.92	0.15	180,180,180,180	7
87	MG	A6	2108	1/1	0.92	0.27	52,52,52,52	0
87	MG	A5	4034	1/1	0.92	0.16	46,46,46,46	0
86	OHX	A1	3716	7/7	0.92	0.26	113,113,113,113	7
87	MG	A1	4211	1/1	0.92	0.34	102,102,102,102	0
87	MG	A1	3985	1/1	0.92	0.42	51,51,51,51	0
86	OHX	A1	3719	7/7	0.92	0.18	154,154,154,154	7
87	MG	A7	223	1/1	0.92	0.23	69,69,69,69	0
87	MG	A5	4213	1/1	0.92	0.44	52,52,52,52	0
87	MG	A1	4311	1/1	0.92	0.23	92,92,92,92	0
86	OHX	A5	3731	7/7	0.92	0.13	138,138,138,138	7
86	OHX	A5	3732	7/7	0.92	0.29	209,209,209,209	7
87	MG	A5	4044	1/1	0.92	0.22	35,35,35,35	0
86	OHX	A1	3569	7/7	0.92	0.17	144,144,144,144	7
87	MG	AL	203	1/1	0.92	0.63	80,80,80,80	0
87	MG	A5	4048	1/1	0.92	0.11	34,34,34,34	0
87	MG	A1	4218	1/1	0.92	0.18	69,69,69,69	0
87	MG	A6	2124	1/1	0.92	0.29	55,55,55,55	0
87	MG	A4	239	1/1	0.92	0.89	70,70,70,70	0
87	MG	A5	4403	1/1	0.92	0.40	81,81,81,81	0
86	OHX	CJ	201	7/7	0.92	0.28	105,105,105,105	7
86	OHX	A1	3751	7/7	0.92	0.14	189,189,189,189	7
87	MG	A6	2269	1/1	0.92	0.52	60,60,60,60	0
86	OHX	A1	3574	7/7	0.92	0.25	189,189,189,189	7
87	MG	A5	3868	1/1	0.92	0.21	44,44,44,44	0
87	MG	A6	2130	1/1	0.92	0.38	74,74,74,74	0
86	OHX	A1	3683	7/7	0.92	0.20	159,159,159,159	7
87	MG	A5	4062	1/1	0.92	0.28	37,37,37,37	0
86	OHX	A1	3754	7/7	0.92	0.24	159,159,159,159	7
87	MG	A5	4064	1/1	0.92	0.17	30,30,30,30	0
86	OHX	A2	2015	7/7	0.92	0.20	138,138,138,138	7
87	MG	A1	4126	1/1	0.92	0.26	84,84,84,84	0
87	MG	A5	3876	1/1	0.92	0.22	66,66,66,66	0
86	OHX	A6	2065	7/7	0.92	0.19	156,156,156,156	7
87	MG	A5	4071	1/1	0.92	0.23	79,79,79,79	0
86	OHX	A1	3686	7/7	0.92	0.13	204,204,204,204	7
86	OHX	A5	3551	7/7	0.92	0.17	142,142,142,142	7
87	MG	A1	4449	1/1	0.92	0.14	98,98,98,98	0
86	OHX	A2	1983	7/7	0.92	0.14	166,166,166,166	7
86	OHX	A2	2018	7/7	0.92	0.15	176,176,176,176	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	DB	409	1/1	0.92	0.62	56,56,56,56	0
87	MG	DB	411	1/1	0.92	1.23	61,61,61,61	0
87	MG	A1	4022	1/1	0.92	0.28	40,40,40,40	0
86	OHX	A5	3605	7/7	0.92	0.27	112,112,112,112	7
87	MG	A1	4027	1/1	0.92	0.44	65,65,65,65	0
87	MG	BC	404	1/1	0.92	1.23	67,67,67,67	0
87	MG	DC	403	1/1	0.92	0.41	65,65,65,65	0
87	MG	A1	4235	1/1	0.92	0.27	62,62,62,62	0
87	MG	A1	4457	1/1	0.92	0.21	97,97,97,97	0
86	OHX	A5	3621	7/7	0.92	0.23	123,123,123,123	7
87	MG	A5	3894	1/1	0.92	0.39	67,67,67,67	0
87	MG	DD	304	1/1	0.92	0.22	71,71,71,71	0
86	OHX	A2	2001	7/7	0.92	0.19	140,140,140,140	7
87	MG	A6	2152	1/1	0.92	0.44	64,64,64,64	0
87	MG	DF	302	1/1	0.92	0.59	48,48,48,48	0
86	OHX	A5	3633	7/7	0.92	0.26	126,126,126,126	7
86	OHX	A5	3637	7/7	0.92	0.17	178,178,178,178	7
86	OHX	A5	3642	7/7	0.92	0.21	118,118,118,118	7
87	MG	A6	2301	1/1	0.92	0.54	116,116,116,116	0
87	MG	A5	3901	1/1	0.92	0.28	85,85,85,85	0
87	MG	A5	4269	1/1	0.92	0.25	66,66,66,66	0
86	OHX	A5	3644	7/7	0.92	0.29	135,135,135,135	7
87	MG	A5	4096	1/1	0.92	0.33	72,72,72,72	0
87	MG	A5	3903	1/1	0.92	0.24	34,34,34,34	0
87	MG	A5	4274	1/1	0.92	0.09	51,51,51,51	0
87	MG	A1	4243	1/1	0.92	0.51	61,61,61,61	0
87	MG	A5	4461	1/1	0.92	0.26	62,62,62,62	0
86	OHX	A6	1977	7/7	0.92	0.19	128,128,128,128	7
87	MG	A2	2218	1/1	0.92	0.25	63,63,63,63	0
87	MG	A5	3909	1/1	0.92	0.42	70,70,70,70	0
87	MG	A5	4282	1/1	0.92	0.40	52,52,52,52	0
86	OHX	A8	216	7/7	0.92	0.12	198,198,198,198	7
87	MG	A1	4471	1/1	0.92	0.17	88,88,88,88	0
87	MG	A2	2151	1/1	0.92	0.15	49,49,49,49	0
87	MG	A5	4287	1/1	0.92	0.31	101,101,101,101	0
87	MG	A5	4107	1/1	0.92	0.14	66,66,66,66	0
86	OHX	A1	3623	7/7	0.92	0.22	147,147,147,147	7
87	MG	A6	2172	1/1	0.92	0.31	66,66,66,66	0
87	MG	A6	2313	1/1	0.92	1.07	78,78,78,78	0
87	MG	DT	201	1/1	0.92	0.53	63,63,63,63	0
86	OHX	A2	2055	7/7	0.92	0.28	116,116,116,116	7
87	MG	A1	4476	1/1	0.92	0.44	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	3834	1/1	0.92	0.10	44,44,44,44	0
86	OHX	A1	3645	7/7	0.92	0.27	102,102,102,102	7
87	MG	A5	4484	1/1	0.92	0.94	89,89,89,89	0
87	MG	A1	4054	1/1	0.92	0.38	65,65,65,65	0
87	MG	A5	4298	1/1	0.92	0.12	106,106,106,106	0
87	MG	A1	4055	1/1	0.92	0.21	58,58,58,58	0
86	OHX	A1	3733	7/7	0.92	0.33	125,125,125,125	7
86	OHX	A6	2024	7/7	0.92	0.15	156,156,156,156	7
86	OHX	DG	301	7/7	0.92	0.50	226,226,226,226	7
86	OHX	A2	2034	7/7	0.92	0.16	173,173,173,173	7
87	MG	A2	2229	1/1	0.92	0.10	60,60,60,60	0
87	MG	A6	2325	1/1	0.92	0.64	106,106,106,106	0
87	MG	Df	202	1/1	0.92	0.34	81,81,81,81	0
87	MG	A5	4494	1/1	0.92	0.40	111,111,111,111	0
86	OHX	A6	2080	7/7	0.92	0.30	167,167,167,167	7
87	MG	Dg	202	1/1	0.92	0.15	50,50,50,50	0
87	MG	A5	4310	1/1	0.92	0.57	69,69,69,69	0
86	OHX	A2	2068	7/7	0.92	0.38	177,177,177,177	7
87	MG	A6	2191	1/1	0.92	0.34	84,84,84,84	0
87	MG	Dm	201	1/1	0.92	0.27	75,75,75,75	0
87	MG	A1	3933	1/1	0.92	0.47	53,53,53,53	0
87	MG	Dp	101	1/1	0.92	0.17	54,54,54,54	0
87	MG	A5	4500	1/1	0.92	0.23	82,82,82,82	0
87	MG	A6	2331	1/1	0.92	0.15	79,79,79,79	0
87	MG	A5	4316	1/1	0.92	0.45	57,57,57,57	0
86	OHX	A5	3675	7/7	0.92	0.22	132,132,132,132	7
87	MG	A2	2162	1/1	0.92	0.44	84,84,84,84	0
86	OHX	A5	3676	7/7	0.92	0.17	155,155,155,155	7
86	OHX	A1	3407	7/7	0.92	0.29	138,138,138,138	7
87	MG	A5	4516	1/1	0.93	0.92	74,74,74,74	0
86	OHX	A1	3785	7/7	0.93	0.42	183,183,183,183	7
87	MG	A5	4328	1/1	0.93	0.66	72,72,72,72	0
87	MG	A1	3899	1/1	0.93	0.22	57,57,57,57	0
87	MG	A2	2192	1/1	0.93	0.31	66,66,66,66	0
87	MG	A5	3970	1/1	0.93	0.50	60,60,60,60	0
86	OHX	A6	2009	7/7	0.93	0.20	136,136,136,136	7
87	MG	A5	3973	1/1	0.93	0.37	38,38,38,38	0
86	OHX	A5	3518	7/7	0.93	0.18	159,159,159,159	7
87	MG	A1	4371	1/1	0.93	0.61	63,63,63,63	0
87	MG	A1	4032	1/1	0.93	0.18	46,46,46,46	0
87	MG	A1	3904	1/1	0.93	0.28	43,43,43,43	0
87	MG	A5	4339	1/1	0.93	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	BV	204	1/1	0.93	0.37	40,40,40,40	0
86	OHX	A2	2030	7/7	0.93	0.37	155,155,155,155	7
86	OHX	A5	3730	7/7	0.93	0.22	97,97,97,97	7
87	MG	A1	4036	1/1	0.93	0.30	71,71,71,71	0
87	MG	A5	3987	1/1	0.93	0.41	59,59,59,59	0
87	MG	A2	2118	1/1	0.93	0.32	47,47,47,47	0
86	OHX	A6	2017	7/7	0.93	0.21	132,132,132,132	7
87	MG	A1	4040	1/1	0.93	0.11	40,40,40,40	0
87	MG	A1	4265	1/1	0.93	0.33	74,74,74,74	0
87	MG	A1	3911	1/1	0.93	0.18	58,58,58,58	0
87	MG	A5	4175	1/1	0.93	0.21	114,114,114,114	0
87	MG	A1	4386	1/1	0.93	0.70	78,78,78,78	0
86	OHX	A6	2018	7/7	0.93	0.20	153,153,153,153	7
86	OHX	A6	2070	7/7	0.93	0.17	139,139,139,139	7
87	MG	A5	3996	1/1	0.93	0.48	46,46,46,46	0
87	MG	A5	3997	1/1	0.93	0.46	43,43,43,43	0
87	MG	A3	215	1/1	0.93	0.32	77,77,77,77	0
87	MG	A1	4044	1/1	0.93	0.27	44,44,44,44	0
87	MG	A5	3832	1/1	0.93	0.10	35,35,35,35	0
87	MG	A5	4361	1/1	0.93	0.23	92,92,92,92	0
87	MG	A1	4045	1/1	0.93	0.17	55,55,55,55	0
87	MG	A1	4046	1/1	0.93	0.41	50,50,50,50	0
87	MG	A5	4007	1/1	0.93	0.37	47,47,47,47	0
87	MG	A6	2237	1/1	0.93	0.18	96,96,96,96	0
86	OHX	A6	2022	7/7	0.93	0.14	145,145,145,145	7
87	MG	A5	4368	1/1	0.93	0.28	75,75,75,75	0
87	MG	A2	2125	1/1	0.93	0.47	61,61,61,61	0
87	MG	Bj	109	1/1	0.93	0.26	122,122,122,122	0
87	MG	A5	4019	1/1	0.93	0.48	48,48,48,48	0
86	OHX	A5	3612	7/7	0.93	0.19	147,147,147,147	7
87	MG	A5	4195	1/1	0.93	0.31	72,72,72,72	0
86	OHX	A5	3804	7/7	0.93	0.16	162,162,162,162	7
87	MG	A5	4573	1/1	0.93	0.74	56,56,56,56	0
87	MG	A1	4052	1/1	0.93	0.26	71,71,71,71	0
86	OHX	A5	3615	7/7	0.93	0.19	147,147,147,147	7
86	OHX	A5	3806	7/7	0.93	0.23	120,120,120,120	7
87	MG	A5	4200	1/1	0.93	0.53	70,70,70,70	0
87	MG	A1	3823	1/1	0.93	0.29	60,60,60,60	0
86	OHX	A1	3641	7/7	0.93	0.24	137,137,137,137	7
86	OHX	A5	3622	7/7	0.93	0.18	136,136,136,136	7
86	OHX	A1	3685	7/7	0.93	0.15	150,150,150,150	7
86	OHX	A5	3745	7/7	0.93	0.24	131,131,131,131	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A5	3815	7/7	0.93	0.26	221,221,221,221	7
87	MG	A5	4037	1/1	0.93	0.36	67,67,67,67	0
87	MG	A7	220	1/1	0.93	0.22	61,61,61,61	0
86	OHX	A5	3624	7/7	0.93	0.27	82,82,82,82	7
87	MG	A5	3855	1/1	0.93	0.40	55,55,55,55	0
86	OHX	A1	3763	7/7	0.93	0.36	157,157,157,157	7
87	MG	A5	4041	1/1	0.93	0.23	47,47,47,47	0
87	MG	A7	225	1/1	0.93	0.36	45,45,45,45	0
87	MG	A1	4066	1/1	0.93	0.25	53,53,53,53	0
86	OHX	A2	2003	7/7	0.93	0.23	147,147,147,147	7
86	OHX	A6	2028	7/7	0.93	0.26	136,136,136,136	7
86	OHX	A1	3720	7/7	0.93	0.20	139,139,139,139	7
87	MG	A4	227	1/1	0.93	0.10	53,53,53,53	0
86	OHX	A5	3646	7/7	0.93	0.20	135,135,135,135	7
87	MG	A7	232	1/1	0.93	0.20	91,91,91,91	0
87	MG	A5	3864	1/1	0.93	0.35	63,63,63,63	0
87	MG	A2	2143	1/1	0.93	0.23	82,82,82,82	0
86	OHX	A6	2032	7/7	0.93	0.16	143,143,143,143	7
86	OHX	A7	210	7/7	0.93	0.24	114,114,114,114	7
87	MG	A7	238	1/1	0.93	0.46	95,95,95,95	0
87	MG	A2	2146	1/1	0.93	0.27	71,71,71,71	0
87	MG	A6	2125	1/1	0.93	0.21	47,47,47,47	0
86	OHX	A5	3648	7/7	0.93	0.25	111,111,111,111	7
87	MG	A8	222	1/1	0.93	0.36	47,47,47,47	0
87	MG	A5	4057	1/1	0.93	0.41	82,82,82,82	0
86	OHX	A5	3650	7/7	0.93	0.22	133,133,133,133	7
87	MG	A8	225	1/1	0.93	0.29	58,58,58,58	0
87	MG	A6	2274	1/1	0.93	0.14	95,95,95,95	0
86	OHX	A8	211	7/7	0.93	0.23	135,135,135,135	7
87	MG	A5	4232	1/1	0.93	0.80	53,53,53,53	0
87	MG	A5	4061	1/1	0.93	0.23	83,83,83,83	0
87	MG	A1	3845	1/1	0.93	0.16	70,70,70,70	0
86	OHX	A5	3651	7/7	0.93	0.28	137,137,137,137	7
86	OHX	A6	2034	7/7	0.93	0.20	137,137,137,137	7
87	MG	A5	4240	1/1	0.93	0.96	77,77,77,77	0
87	MG	A1	4429	1/1	0.93	0.32	54,54,54,54	0
86	OHX	A5	3657	7/7	0.93	0.28	83,83,83,83	7
86	OHX	A6	2036	7/7	0.93	0.24	122,122,122,122	7
86	OHX	A2	1997	7/7	0.93	0.28	121,121,121,121	7
87	MG	A1	3957	1/1	0.93	0.45	50,50,50,50	0
87	MG	DB	403	1/1	0.93	0.40	36,36,36,36	0
87	MG	A1	3958	1/1	0.93	0.30	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4249	1/1	0.93	0.41	40,40,40,40	0
87	MG	A5	3889	1/1	0.93	0.40	86,86,86,86	0
87	MG	A5	4074	1/1	0.93	0.17	51,51,51,51	0
86	OHX	A1	3769	7/7	0.93	0.19	142,142,142,142	7
87	MG	A6	2139	1/1	0.93	0.34	72,72,72,72	0
87	MG	A1	4204	1/1	0.93	0.22	59,59,59,59	0
87	MG	A5	4439	1/1	0.93	0.17	56,56,56,56	0
87	MG	A1	3961	1/1	0.93	0.33	33,33,33,33	0
86	OHX	A8	219	7/7	0.93	0.22	166,166,166,166	7
87	MG	A5	4442	1/1	0.93	0.49	76,76,76,76	0
87	MG	A1	4441	1/1	0.93	0.81	61,61,61,61	0
87	MG	A5	4082	1/1	0.93	0.31	46,46,46,46	0
87	MG	A1	3964	1/1	0.93	0.39	50,50,50,50	0
87	MG	DD	303	1/1	0.93	0.62	67,67,67,67	0
87	MG	BA	305	1/1	0.93	0.49	61,61,61,61	0
86	OHX	A2	2258	7/7	0.93	0.17	162,162,162,162	7
87	MG	A5	4448	1/1	0.93	0.66	64,64,64,64	0
86	OHX	A1	3743	7/7	0.93	0.37	148,148,148,148	7
87	MG	A5	4450	1/1	0.93	0.27	73,73,73,73	0
86	OHX	DC	402	7/7	0.93	0.27	145,145,145,145	7
87	MG	BB	405	1/1	0.93	0.62	51,51,51,51	0
86	OHX	A5	3672	7/7	0.93	0.24	142,142,142,142	7
87	MG	A5	4454	1/1	0.93	0.57	68,68,68,68	0
87	MG	A6	2153	1/1	0.93	0.39	54,54,54,54	0
86	OHX	A1	3662	7/7	0.93	0.30	119,119,119,119	7
87	MG	A6	2155	1/1	0.93	0.31	41,41,41,41	0
87	MG	A2	2164	1/1	0.93	0.16	74,74,74,74	0
86	OHX	DI	302	7/7	0.93	0.25	160,160,160,160	7
86	OHX	A2	2071	7/7	0.93	0.27	162,162,162,162	7
87	MG	A5	4462	1/1	0.93	0.64	83,83,83,83	0
87	MG	A6	2311	1/1	0.93	0.59	76,76,76,76	0
87	MG	A6	2161	1/1	0.93	0.40	55,55,55,55	0
86	OHX	A1	3725	7/7	0.93	0.21	191,191,191,191	7
87	MG	A1	4328	1/1	0.93	1.25	76,76,76,76	0
86	OHX	A2	2027	7/7	0.93	0.16	166,166,166,166	7
86	OHX	A5	3773	7/7	0.93	0.19	141,141,141,141	7
87	MG	DP	205	1/1	0.93	0.20	56,56,56,56	0
87	MG	A5	4284	1/1	0.93	0.18	69,69,69,69	0
87	MG	DP	208	1/1	0.93	0.29	42,42,42,42	0
86	OHX	BD	301	7/7	0.93	0.25	138,138,138,138	7
86	OHX	A2	1954	7/7	0.93	0.23	162,162,162,162	7
86	OHX	A2	2038	7/7	0.93	0.18	195,195,195,195	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A1	3675	7/7	0.93	0.14	169,169,169,169	7
86	OHX	A1	3609	7/7	0.93	0.22	122,122,122,122	7
87	MG	A5	3924	1/1	0.93	0.35	39,39,39,39	0
87	MG	DT	202	1/1	0.93	1.35	89,89,89,89	0
87	MG	A2	2176	1/1	0.93	0.35	64,64,64,64	0
87	MG	A6	2176	1/1	0.93	0.47	67,67,67,67	0
86	OHX	A2	1946	7/7	0.93	0.17	156,156,156,156	7
86	OHX	A1	3619	7/7	0.93	0.30	128,128,128,128	7
87	MG	A1	4466	1/1	0.93	0.17	80,80,80,80	0
87	MG	A1	3881	1/1	0.93	0.23	39,39,39,39	0
86	OHX	A6	1970	7/7	0.93	0.15	160,160,160,160	7
87	MG	A5	4119	1/1	0.93	0.27	65,65,65,65	0
86	OHX	A1	3680	7/7	0.93	0.25	127,127,127,127	7
87	MG	A1	4120	1/1	0.93	0.17	26,26,26,26	0
86	OHX	A6	1984	7/7	0.93	0.14	174,174,174,174	7
87	MG	A1	4234	1/1	0.93	0.35	82,82,82,82	0
86	OHX	A6	1988	7/7	0.93	0.22	138,138,138,138	7
87	MG	BO	207	1/1	0.93	0.66	56,56,56,56	0
86	OHX	A1	3524	7/7	0.93	0.20	139,139,139,139	7
86	OHX	CP	201	7/7	0.93	0.14	177,177,177,177	7
86	OHX	A6	1999	7/7	0.93	0.21	140,140,140,140	7
87	MG	A5	3948	1/1	0.93	0.29	28,28,28,28	0
87	MG	A1	4006	1/1	0.93	0.36	42,42,42,42	0
86	OHX	Cg	401	7/7	0.93	0.14	182,182,182,182	7
87	MG	A1	4010	1/1	0.93	0.40	61,61,61,61	0
87	MG	Dl	101	1/1	0.93	0.47	112,112,112,112	0
87	MG	A1	4482	1/1	0.93	0.16	129,129,129,129	0
87	MG	A2	2104	1/1	0.93	0.28	63,63,63,63	0
87	MG	Do	202	1/1	0.93	0.44	50,50,50,50	0
87	MG	A5	3956	1/1	0.93	0.30	39,39,39,39	0
87	MG	A1	3893	1/1	0.93	0.19	26,26,26,26	0
86	OHX	A5	3716	7/7	0.93	0.42	115,115,115,115	7
86	OHX	A6	2062	7/7	0.93	0.24	163,163,163,163	7
86	OHX	A6	2003	7/7	0.93	0.20	177,177,177,177	7
87	MG	A1	4139	1/1	0.93	0.18	56,56,56,56	0
87	MG	A5	3963	1/1	0.93	0.37	44,44,44,44	0
87	MG	A1	4019	1/1	0.93	0.42	42,42,42,42	0
86	OHX	A2	2006	7/7	0.94	0.15	162,162,162,162	7
86	OHX	A6	2064	7/7	0.94	0.12	164,164,164,164	7
87	MG	A6	2208	1/1	0.94	0.11	56,56,56,56	0
86	OHX	A5	3653	7/7	0.94	0.25	130,130,130,130	7
87	MG	A1	4102	1/1	0.94	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4068	1/1	0.94	0.23	72,72,72,72	0
87	MG	A1	3936	1/1	0.94	0.33	34,34,34,34	0
87	MG	A5	4070	1/1	0.94	0.33	56,56,56,56	0
86	OHX	A1	3608	7/7	0.94	0.19	160,160,160,160	7
87	MG	A1	3938	1/1	0.94	0.29	48,48,48,48	0
86	OHX	BP	202	7/7	0.94	0.14	139,139,139,139	7
87	MG	A1	4107	1/1	0.94	0.18	74,74,74,74	0
87	MG	A5	4507	1/1	0.94	0.93	92,92,92,92	0
86	OHX	A2	2035	7/7	0.94	0.26	120,120,120,120	7
87	MG	A5	4289	1/1	0.94	0.42	112,112,112,112	0
87	MG	BN	302	1/1	0.94	0.28	44,44,44,44	0
86	OHX	A5	3659	7/7	0.94	0.26	106,106,106,106	7
86	OHX	A5	3661	7/7	0.94	0.17	134,134,134,134	7
87	MG	A2	2150	1/1	0.94	0.15	102,102,102,102	0
86	OHX	A1	3615	7/7	0.94	0.20	139,139,139,139	7
86	OHX	A5	3663	7/7	0.94	0.25	136,136,136,136	7
87	MG	A1	3948	1/1	0.94	0.40	55,55,55,55	0
87	MG	A1	4266	1/1	0.94	0.18	70,70,70,70	0
87	MG	A6	2226	1/1	0.94	0.22	68,68,68,68	0
86	OHX	A6	1962	7/7	0.94	0.18	126,126,126,126	7
87	MG	A1	3951	1/1	0.94	0.43	46,46,46,46	0
87	MG	A5	4303	1/1	0.94	0.60	57,57,57,57	0
86	OHX	A5	3666	7/7	0.94	0.28	127,127,127,127	7
87	MG	A5	4525	1/1	0.94	0.70	66,66,66,66	0
87	MG	Aa	201	1/1	0.94	0.58	82,82,82,82	0
86	OHX	A5	3667	7/7	0.94	0.34	100,100,100,100	7
86	OHX	A5	3668	7/7	0.94	0.20	163,163,163,163	7
86	OHX	AI	301	7/7	0.94	0.13	156,156,156,156	7
87	MG	A1	4124	1/1	0.94	0.23	53,53,53,53	0
86	OHX	A1	3618	7/7	0.94	0.13	158,158,158,158	7
86	OHX	A6	2072	7/7	0.94	0.32	133,133,133,133	7
87	MG	A5	4535	1/1	0.94	0.17	68,68,68,68	0
87	MG	A5	3886	1/1	0.94	0.28	43,43,43,43	0
86	OHX	A6	1978	7/7	0.94	0.18	146,146,146,146	7
86	OHX	A6	1982	7/7	0.94	0.20	123,123,123,123	7
86	OHX	A2	1931	7/7	0.94	0.19	143,143,143,143	7
87	MG	A1	4446	1/1	0.94	0.19	62,62,62,62	0
87	MG	A1	4131	1/1	0.94	0.15	75,75,75,75	0
86	OHX	A2	2049	7/7	0.94	0.16	140,140,140,140	7
86	OHX	A5	3678	7/7	0.94	0.23	111,111,111,111	7
86	OHX	A5	3679	7/7	0.94	0.15	174,174,174,174	7
86	OHX	A6	1989	7/7	0.94	0.19	122,122,122,122	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4287	1/1	0.94	0.27	61,61,61,61	0
86	OHX	A6	1990	7/7	0.94	0.17	177,177,177,177	7
86	OHX	A1	3627	7/7	0.94	0.18	130,130,130,130	7
87	MG	A1	4138	1/1	0.94	0.30	62,62,62,62	0
87	MG	A5	4112	1/1	0.94	0.23	65,65,65,65	0
87	MG	BV	203	1/1	0.94	0.27	63,63,63,63	0
86	OHX	A5	3686	7/7	0.94	0.19	121,121,121,121	7
87	MG	A1	3975	1/1	0.94	0.32	67,67,67,67	0
87	MG	A5	4331	1/1	0.94	0.19	104,104,104,104	0
86	OHX	A6	1994	7/7	0.94	0.19	133,133,133,133	7
86	OHX	A6	1996	7/7	0.94	0.16	148,148,148,148	7
87	MG	A6	2263	1/1	0.94	0.20	89,89,89,89	0
87	MG	A5	3908	1/1	0.94	0.28	37,37,37,37	0
87	MG	A5	4122	1/1	0.94	0.31	52,52,52,52	0
87	MG	A5	4123	1/1	0.94	0.12	39,39,39,39	0
86	OHX	A5	3690	7/7	0.94	0.21	130,130,130,130	7
86	OHX	A5	3691	7/7	0.94	0.18	155,155,155,155	7
86	OHX	A1	3692	7/7	0.94	0.21	124,124,124,124	7
86	OHX	A5	3694	7/7	0.94	0.23	127,127,127,127	7
87	MG	Ba	206	1/1	0.94	0.28	61,61,61,61	0
86	OHX	A5	3695	7/7	0.94	0.20	158,158,158,158	7
86	OHX	A1	3695	7/7	0.94	0.13	163,163,163,163	7
86	OHX	A1	3696	7/7	0.94	0.25	143,143,143,143	7
86	OHX	A1	3747	7/7	0.94	0.34	118,118,118,118	7
86	OHX	A5	3702	7/7	0.94	0.24	121,121,121,121	7
86	OHX	A5	3703	7/7	0.94	0.21	123,123,123,123	7
86	OHX	A6	2010	7/7	0.94	0.13	181,181,181,181	7
86	OHX	A5	3705	7/7	0.94	0.17	152,152,152,152	7
86	OHX	A8	206	7/7	0.94	0.19	136,136,136,136	7
87	MG	A7	216	1/1	0.94	0.37	78,78,78,78	0
87	MG	A5	4140	1/1	0.94	0.16	56,56,56,56	0
86	OHX	A5	3706	7/7	0.94	0.18	139,139,139,139	7
86	OHX	A1	3628	7/7	0.94	0.18	154,154,154,154	7
87	MG	A1	4160	1/1	0.94	0.24	70,70,70,70	0
87	MG	A5	4145	1/1	0.94	0.18	57,57,57,57	0
86	OHX	A5	3708	7/7	0.94	0.17	141,141,141,141	7
87	MG	A1	3999	1/1	0.94	0.34	37,37,37,37	0
86	OHX	A6	2015	7/7	0.94	0.22	159,159,159,159	7
87	MG	A1	4003	1/1	0.94	0.46	48,48,48,48	0
86	OHX	A1	3699	7/7	0.94	0.25	107,107,107,107	7
87	MG	A5	3935	1/1	0.94	0.29	51,51,51,51	0
87	MG	A5	3936	1/1	0.94	0.42	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A1	3629	7/7	0.94	0.18	128,128,128,128	7
87	MG	A6	2102	1/1	0.94	0.22	63,63,63,63	0
87	MG	A1	4168	1/1	0.94	0.16	44,44,44,44	0
86	OHX	A6	2021	7/7	0.94	0.21	131,131,131,131	7
86	OHX	A5	3713	7/7	0.94	0.23	122,122,122,122	7
86	OHX	A5	3715	7/7	0.94	0.23	100,100,100,100	7
86	OHX	A1	3701	7/7	0.94	0.38	112,112,112,112	7
87	MG	A6	2298	1/1	0.94	0.09	77,77,77,77	0
87	MG	A1	3856	1/1	0.94	0.28	38,38,38,38	0
87	MG	A6	2300	1/1	0.94	0.55	56,56,56,56	0
86	OHX	A5	3717	7/7	0.94	0.50	108,108,108,108	7
87	MG	A5	3950	1/1	0.94	0.43	38,38,38,38	0
87	MG	A1	4018	1/1	0.94	0.42	38,38,38,38	0
87	MG	A6	2114	1/1	0.94	0.36	61,61,61,61	0
87	MG	A6	2304	1/1	0.94	0.10	81,81,81,81	0
86	OHX	A5	3718	7/7	0.94	0.14	157,157,157,157	7
86	OHX	A1	3635	7/7	0.94	0.29	84,84,84,84	7
87	MG	A8	227	1/1	0.94	0.19	65,65,65,65	0
86	OHX	DH	201	7/7	0.94	0.14	142,142,142,142	7
87	MG	A1	4025	1/1	0.94	0.45	39,39,39,39	0
87	MG	A8	230	1/1	0.94	0.55	68,68,68,68	0
86	OHX	DI	301	7/7	0.94	0.20	118,118,118,118	7
87	MG	A5	4388	1/1	0.94	0.46	47,47,47,47	0
87	MG	A1	3862	1/1	0.94	0.23	76,76,76,76	0
86	OHX	A6	2096	7/7	0.94	0.19	156,156,156,156	7
87	MG	A6	2123	1/1	0.94	0.35	51,51,51,51	0
87	MG	A1	4031	1/1	0.94	0.22	32,32,32,32	0
87	MG	A1	4185	1/1	0.94	0.24	65,65,65,65	0
87	MG	A8	239	1/1	0.94	0.12	93,93,93,93	0
86	OHX	A5	3723	7/7	0.94	0.18	180,180,180,180	7
87	MG	A5	3967	1/1	0.94	0.36	57,57,57,57	0
87	MG	A5	4185	1/1	0.94	0.76	49,49,49,49	0
86	OHX	A1	3802	7/7	0.94	0.40	146,146,146,146	7
87	MG	A5	4398	1/1	0.94	0.20	54,54,54,54	0
87	MG	DB	405	1/1	0.94	0.80	62,62,62,62	0
86	OHX	A1	3636	7/7	0.94	0.16	148,148,148,148	7
86	OHX	A5	3726	7/7	0.94	0.16	135,135,135,135	7
86	OHX	A1	3403	7/7	0.94	0.14	169,169,169,169	7
86	OHX	A6	2100	7/7	0.94	0.32	206,206,206,206	7
86	OHX	A5	3729	7/7	0.94	0.19	165,165,165,165	7
87	MG	A3	216	1/1	0.94	0.16	67,67,67,67	0
87	MG	A1	4039	1/1	0.94	0.37	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4346	1/1	0.94	0.32	53,53,53,53	0
87	MG	A5	3981	1/1	0.94	0.42	79,79,79,79	0
86	OHX	A2	2078	7/7	0.94	0.27	169,169,169,169	7
86	OHX	A6	2029	7/7	0.94	0.23	141,141,141,141	7
86	OHX	A6	2030	7/7	0.94	0.11	170,170,170,170	7
87	MG	DC	407	1/1	0.94	0.73	75,75,75,75	0
87	MG	A5	4412	1/1	0.94	0.33	104,104,104,104	0
86	OHX	A1	3453	7/7	0.94	0.31	134,134,134,134	0
86	OHX	A1	3651	7/7	0.94	0.19	131,131,131,131	7
87	MG	A5	4201	1/1	0.94	0.16	49,49,49,49	0
87	MG	DD	308	1/1	0.94	1.18	70,70,70,70	0
86	OHX	A1	3652	7/7	0.94	0.26	115,115,115,115	7
87	MG	A1	4355	1/1	0.94	0.25	53,53,53,53	0
87	MG	A5	4204	1/1	0.94	0.12	56,56,56,56	0
86	OHX	A6	2035	7/7	0.94	0.20	129,129,129,129	7
86	OHX	A1	3761	7/7	0.94	0.11	173,173,173,173	7
87	MG	A1	3885	1/1	0.94	0.27	61,61,61,61	0
86	OHX	A2	2014	7/7	0.94	0.25	166,166,166,166	7
87	MG	A2	2220	1/1	0.94	0.15	111,111,111,111	0
86	OHX	A1	3714	7/7	0.94	0.23	118,118,118,118	7
87	MG	DL	201	1/1	0.94	1.06	94,94,94,94	0
87	MG	A2	2100	1/1	0.94	0.25	67,67,67,67	0
87	MG	A1	4208	1/1	0.94	0.63	58,58,58,58	0
87	MG	A5	3999	1/1	0.94	0.25	32,32,32,32	0
87	MG	A5	4433	1/1	0.94	0.14	83,83,83,83	0
86	OHX	A1	3657	7/7	0.94	0.15	166,166,166,166	7
86	OHX	A2	1987	7/7	0.94	0.20	147,147,147,147	7
87	MG	A1	4366	1/1	0.94	0.28	86,86,86,86	0
86	OHX	A2	2002	7/7	0.94	0.11	169,169,169,169	7
86	OHX	A5	3521	7/7	0.94	0.21	150,150,150,150	7
87	MG	DP	202	1/1	0.94	0.20	56,56,56,56	0
87	MG	A1	3895	1/1	0.94	0.22	92,92,92,92	0
87	MG	A2	2107	1/1	0.94	0.45	66,66,66,66	0
86	OHX	A1	3549	7/7	0.94	0.25	139,139,139,139	7
86	OHX	A5	3541	7/7	0.94	0.23	113,113,113,113	7
87	MG	A5	4015	1/1	0.94	0.41	45,45,45,45	0
87	MG	A5	4017	1/1	0.94	0.43	62,62,62,62	0
87	MG	A5	4018	1/1	0.94	0.41	40,40,40,40	0
86	OHX	A2	2040	7/7	0.94	0.12	171,171,171,171	7
87	MG	A2	2112	1/1	0.94	0.38	95,95,95,95	0
86	OHX	A5	3557	7/7	0.94	0.16	154,154,154,154	7
86	OHX	A5	3572	7/7	0.94	0.19	145,145,145,145	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4381	1/1	0.94	0.66	65,65,65,65	0
87	MG	A2	2234	1/1	0.94	0.26	94,94,94,94	0
86	OHX	A5	3755	7/7	0.94	0.17	174,174,174,174	7
87	MG	A6	2174	1/1	0.94	0.18	50,50,50,50	0
87	MG	A5	4031	1/1	0.94	0.45	39,39,39,39	0
86	OHX	A1	3667	7/7	0.94	0.29	92,92,92,92	7
87	MG	A2	2117	1/1	0.94	0.37	80,80,80,80	0
86	OHX	A3	211	7/7	0.94	0.23	137,137,137,137	7
86	OHX	A1	3668	7/7	0.94	0.18	151,151,151,151	7
87	MG	A1	4388	1/1	0.94	0.51	78,78,78,78	0
86	OHX	A5	3761	7/7	0.94	0.16	146,146,146,146	7
86	OHX	A5	3609	7/7	0.94	0.14	153,153,153,153	7
86	OHX	A5	3611	7/7	0.94	0.25	115,115,115,115	7
86	OHX	A2	1966	7/7	0.94	0.23	101,101,101,101	7
87	MG	A1	4393	1/1	0.94	0.72	78,78,78,78	0
86	OHX	A4	209	7/7	0.94	0.15	153,153,153,153	7
87	MG	A6	2188	1/1	0.94	0.21	38,38,38,38	0
86	OHX	A1	3566	7/7	0.94	0.19	122,122,122,122	7
86	OHX	A4	212	7/7	0.94	0.26	118,118,118,118	7
87	MG	A1	4397	1/1	0.94	0.20	80,80,80,80	0
86	OHX	A2	2056	7/7	0.94	0.23	130,130,130,130	7
86	OHX	A2	2043	7/7	0.94	0.12	192,192,192,192	7
86	OHX	A5	3630	7/7	0.94	0.21	128,128,128,128	7
87	MG	A5	4052	1/1	0.94	0.21	46,46,46,46	0
86	OHX	A6	2055	7/7	0.94	0.29	131,131,131,131	7
86	OHX	A5	3634	7/7	0.94	0.17	130,130,130,130	7
86	OHX	A1	3586	7/7	0.94	0.18	117,117,117,117	7
86	OHX	BB	401	7/7	0.94	0.19	111,111,111,111	7
86	OHX	A2	1979	7/7	0.94	0.21	121,121,121,121	7
86	OHX	A1	3679	7/7	0.94	0.27	114,114,114,114	7
86	OHX	A2	2020	7/7	0.94	0.20	118,118,118,118	7
87	MG	A6	2203	1/1	0.94	0.39	63,63,63,63	0
87	MG	A1	3930	1/1	0.94	0.34	38,38,38,38	0
86	OHX	A1	3606	7/7	0.94	0.17	132,132,132,132	7
87	MG	A5	4523	1/1	0.95	0.30	65,65,65,65	0
86	OHX	A2	2011	7/7	0.95	0.16	154,154,154,154	7
86	OHX	A5	3560	7/7	0.95	0.23	106,106,106,106	7
87	MG	A6	2183	1/1	0.95	0.26	64,64,64,64	0
87	MG	A5	4150	1/1	0.95	0.61	68,68,68,68	0
86	OHX	A5	3571	7/7	0.95	0.19	143,143,143,143	7
86	OHX	A1	3713	7/7	0.95	0.24	101,101,101,101	7
87	MG	A1	4051	1/1	0.95	0.36	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A5	3583	7/7	0.95	0.17	137,137,137,137	7
86	OHX	A5	3714	7/7	0.95	0.21	126,126,126,126	7
87	MG	A5	3978	1/1	0.95	0.28	29,29,29,29	0
86	OHX	A5	3584	7/7	0.95	0.22	119,119,119,119	7
86	OHX	A5	3820	7/7	0.95	0.39	80,80,80,80	7
86	OHX	A6	2059	7/7	0.95	0.15	153,153,153,153	7
86	OHX	A6	1986	7/7	0.95	0.14	165,165,165,165	7
87	MG	A1	4186	1/1	0.95	0.19	75,75,75,75	0
86	OHX	A5	3593	7/7	0.95	0.15	134,134,134,134	7
87	MG	BN	307	1/1	0.95	0.80	58,58,58,58	0
86	OHX	A7	207	7/7	0.95	0.17	145,145,145,145	7
87	MG	A1	3926	1/1	0.95	0.29	55,55,55,55	0
87	MG	A1	4062	1/1	0.95	0.32	72,72,72,72	0
87	MG	A5	4167	1/1	0.95	0.24	71,71,71,71	0
86	OHX	A7	209	7/7	0.95	0.20	115,115,115,115	7
87	MG	A5	4550	1/1	0.95	1.13	83,83,83,83	0
86	OHX	A5	3594	7/7	0.95	0.18	131,131,131,131	7
86	OHX	A7	211	7/7	0.95	0.21	117,117,117,117	7
86	OHX	A5	3595	7/7	0.95	0.19	125,125,125,125	7
87	MG	A5	4173	1/1	0.95	0.30	67,67,67,67	0
86	OHX	A5	3722	7/7	0.95	0.14	164,164,164,164	7
87	MG	A5	4358	1/1	0.95	0.59	54,54,54,54	0
86	OHX	A5	3602	7/7	0.95	0.24	109,109,109,109	7
86	OHX	A2	1982	7/7	0.95	0.19	125,125,125,125	7
86	OHX	A5	3607	7/7	0.95	0.23	142,142,142,142	7
87	MG	A5	4362	1/1	0.95	0.34	60,60,60,60	0
86	OHX	A1	3673	7/7	0.95	0.22	154,154,154,154	7
87	MG	BP	210	1/1	0.95	0.57	46,46,46,46	0
87	MG	A5	4001	1/1	0.95	0.40	48,48,48,48	0
86	OHX	A1	3760	7/7	0.95	0.18	136,136,136,136	7
86	OHX	A1	3519	7/7	0.95	0.17	137,137,137,137	7
87	MG	A1	4469	1/1	0.95	0.44	66,66,66,66	0
87	MG	A5	4006	1/1	0.95	0.38	40,40,40,40	0
86	OHX	A5	3614	7/7	0.95	0.22	120,120,120,120	7
87	MG	A1	3941	1/1	0.95	0.35	52,52,52,52	0
86	OHX	A1	3520	7/7	0.95	0.18	129,129,129,129	7
86	OHX	A5	3620	7/7	0.95	0.20	113,113,113,113	7
87	MG	A6	2217	1/1	0.95	0.75	87,87,87,87	0
86	OHX	A2	2000	7/7	0.95	0.20	140,140,140,140	7
87	MG	A5	4376	1/1	0.95	0.87	67,67,67,67	0
87	MG	A5	4016	1/1	0.95	0.30	42,42,42,42	0
86	OHX	DA	302	7/7	0.95	0.32	157,157,157,157	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A6	1998	7/7	0.95	0.14	147,147,147,147	7
87	MG	A1	4209	1/1	0.95	0.17	76,76,76,76	0
87	MG	A5	4020	1/1	0.95	0.43	33,33,33,33	0
87	MG	A1	4083	1/1	0.95	0.19	44,44,44,44	0
86	OHX	DC	401	7/7	0.95	0.16	148,148,148,148	7
86	OHX	A1	3539	7/7	0.95	0.21	103,103,103,103	7
87	MG	A5	3843	1/1	0.95	0.25	50,50,50,50	0
87	MG	A5	4025	1/1	0.95	0.32	38,38,38,38	0
86	OHX	A1	3542	7/7	0.95	0.19	159,159,159,159	7
86	OHX	A5	3626	7/7	0.95	0.18	147,147,147,147	7
86	OHX	A5	3740	7/7	0.95	0.21	155,155,155,155	7
87	MG	A5	4029	1/1	0.95	0.40	44,44,44,44	0
87	MG	A5	4030	1/1	0.95	0.45	39,39,39,39	0
86	OHX	A5	3628	7/7	0.95	0.18	129,129,129,129	7
87	MG	A1	3954	1/1	0.95	0.24	45,45,45,45	0
86	OHX	A5	3629	7/7	0.95	0.25	100,100,100,100	7
86	OHX	A5	3743	7/7	0.95	0.24	167,167,167,167	7
87	MG	A6	2234	1/1	0.95	0.17	92,92,92,92	0
86	OHX	A6	2004	7/7	0.95	0.19	105,105,105,105	7
86	OHX	A6	2005	7/7	0.95	0.18	145,145,145,145	7
86	OHX	A6	2007	7/7	0.95	0.12	164,164,164,164	7
87	MG	A5	4400	1/1	0.95	0.30	86,86,86,86	0
87	MG	A7	237	1/1	0.95	0.43	69,69,69,69	0
87	MG	A1	4098	1/1	0.95	0.19	54,54,54,54	0
86	OHX	A1	3767	7/7	0.95	0.19	158,158,158,158	7
86	OHX	A5	3638	7/7	0.95	0.18	135,135,135,135	7
86	OHX	A5	3749	7/7	0.95	0.13	178,178,178,178	7
87	MG	Be	202	1/1	0.95	0.44	67,67,67,67	0
87	MG	Bf	202	1/1	0.95	0.51	69,69,69,69	0
87	MG	A1	3967	1/1	0.95	0.42	40,40,40,40	0
87	MG	A5	3865	1/1	0.95	0.28	37,37,37,37	0
86	OHX	A5	3639	7/7	0.95	0.16	157,157,157,157	7
86	OHX	A2	1956	7/7	0.95	0.18	128,128,128,128	7
87	MG	A5	3869	1/1	0.95	0.37	58,58,58,58	0
86	OHX	A5	3643	7/7	0.95	0.14	150,150,150,150	7
86	OHX	A1	3624	7/7	0.95	0.26	137,137,137,137	7
86	OHX	A5	3645	7/7	0.95	0.20	141,141,141,141	7
87	MG	A6	2251	1/1	0.95	0.55	73,73,73,73	0
87	MG	A5	4416	1/1	0.95	0.54	48,48,48,48	0
87	MG	A5	4417	1/1	0.95	0.66	50,50,50,50	0
87	MG	A5	3874	1/1	0.95	0.31	32,32,32,32	0
86	OHX	A2	2016	7/7	0.95	0.15	156,156,156,156	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A6	2014	7/7	0.95	0.16	144,144,144,144	7
87	MG	A1	4367	1/1	0.95	0.18	69,69,69,69	0
87	MG	A5	4236	1/1	0.95	0.14	19,19,19,19	0
87	MG	A5	4237	1/1	0.95	0.21	51,51,51,51	0
86	OHX	A1	3682	7/7	0.95	0.13	145,145,145,145	7
87	MG	A6	2256	1/1	0.95	0.19	73,73,73,73	0
87	MG	A1	4111	1/1	0.95	0.26	65,65,65,65	0
87	MG	A5	4429	1/1	0.95	0.17	58,58,58,58	0
87	MG	DB	406	1/1	0.95	0.63	47,47,47,47	0
86	OHX	A1	3550	7/7	0.95	0.18	130,130,130,130	7
87	MG	A6	2260	1/1	0.95	0.24	62,62,62,62	0
86	OHX	A3	207	7/7	0.95	0.15	167,167,167,167	7
86	OHX	A2	2031	7/7	0.95	0.13	140,140,140,140	7
86	OHX	A1	3633	7/7	0.95	0.22	101,101,101,101	7
87	MG	A3	217	1/1	0.95	0.41	56,56,56,56	0
87	MG	A5	4436	1/1	0.95	0.76	90,90,90,90	0
86	OHX	A1	3634	7/7	0.95	0.15	133,133,133,133	7
86	OHX	A1	3557	7/7	0.95	0.18	121,121,121,121	7
86	OHX	A1	3558	7/7	0.95	0.17	139,139,139,139	7
86	OHX	A1	3638	7/7	0.95	0.16	141,141,141,141	7
87	MG	A1	4380	1/1	0.95	0.21	95,95,95,95	0
86	OHX	A2	1968	7/7	0.95	0.18	134,134,134,134	7
86	OHX	A2	1965	7/7	0.95	0.20	138,138,138,138	7
86	OHX	A2	1995	7/7	0.95	0.13	171,171,171,171	7
86	OHX	A4	214	7/7	0.95	0.15	167,167,167,167	7
86	OHX	A6	2092	7/7	0.95	0.38	182,182,182,182	7
86	OHX	A1	3694	7/7	0.95	0.21	131,131,131,131	7
86	OHX	A6	2033	7/7	0.95	0.31	133,133,133,133	7
86	OHX	A5	3670	7/7	0.95	0.22	109,109,109,109	7
87	MG	A6	2279	1/1	0.95	0.23	81,81,81,81	0
87	MG	A6	2120	1/1	0.95	0.38	51,51,51,51	0
87	MG	A1	3872	1/1	0.95	0.28	37,37,37,37	0
87	MG	A1	4130	1/1	0.95	0.28	69,69,69,69	0
86	OHX	A1	3646	7/7	0.95	0.21	110,110,110,110	7
87	MG	A1	3997	1/1	0.95	0.35	40,40,40,40	0
86	OHX	A1	3573	7/7	0.95	0.18	120,120,120,120	7
87	MG	A5	4271	1/1	0.95	0.82	68,68,68,68	0
86	OHX	A2	1980	7/7	0.95	0.15	152,152,152,152	7
87	MG	A2	2121	1/1	0.95	0.37	61,61,61,61	0
87	MG	A1	4262	1/1	0.95	0.21	70,70,70,70	0
87	MG	A5	4275	1/1	0.95	0.43	63,63,63,63	0
87	MG	A5	4466	1/1	0.95	0.23	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A4	222	1/1	0.95	0.37	43,43,43,43	0
87	MG	A4	224	1/1	0.95	0.18	30,30,30,30	0
87	MG	A4	225	1/1	0.95	0.38	65,65,65,65	0
87	MG	A1	4004	1/1	0.95	0.42	57,57,57,57	0
86	OHX	BC	401	7/7	0.95	0.21	130,130,130,130	7
86	OHX	A6	2038	7/7	0.95	0.18	169,169,169,169	7
87	MG	A1	4009	1/1	0.95	0.44	51,51,51,51	0
86	OHX	A2	2009	7/7	0.95	0.11	144,144,144,144	7
86	OHX	A6	2040	7/7	0.95	0.24	87,87,87,87	7
86	OHX	CG	301	7/7	0.95	0.13	147,147,147,147	7
87	MG	A2	2127	1/1	0.95	0.33	49,49,49,49	0
86	OHX	A1	3590	7/7	0.95	0.14	135,135,135,135	7
86	OHX	A5	3681	7/7	0.95	0.31	112,112,112,112	7
87	MG	A1	4017	1/1	0.95	0.40	48,48,48,48	0
86	OHX	A1	3658	7/7	0.95	0.19	118,118,118,118	7
87	MG	A2	2131	1/1	0.95	0.19	65,65,65,65	0
87	MG	A5	3932	1/1	0.95	0.31	34,34,34,34	0
86	OHX	A5	3684	7/7	0.95	0.20	122,122,122,122	7
86	OHX	A1	3659	7/7	0.95	0.16	156,156,156,156	7
87	MG	A1	4152	1/1	0.95	0.19	34,34,34,34	0
86	OHX	CL	201	7/7	0.95	0.17	134,134,134,134	7
86	OHX	Ag	401	7/7	0.95	0.14	167,167,167,167	7
86	OHX	A1	3661	7/7	0.95	0.23	118,118,118,118	7
86	OHX	A1	3706	7/7	0.95	0.16	135,135,135,135	7
86	OHX	CS	201	7/7	0.95	0.18	129,129,129,129	7
86	OHX	A1	3600	7/7	0.95	0.22	100,100,100,100	7
87	MG	A1	4286	1/1	0.95	0.84	57,57,57,57	0
86	OHX	A6	1947	7/7	0.95	0.17	134,134,134,134	7
86	OHX	A5	3404	7/7	0.95	0.24	111,111,111,111	7
86	OHX	A6	1955	7/7	0.95	0.15	153,153,153,153	7
87	MG	A6	2162	1/1	0.95	0.49	63,63,63,63	0
87	MG	A5	4128	1/1	0.95	0.16	66,66,66,66	0
86	OHX	A6	1961	7/7	0.95	0.24	132,132,132,132	7
87	MG	A5	4313	1/1	0.95	0.47	66,66,66,66	0
86	OHX	A1	3601	7/7	0.95	0.15	184,184,184,184	7
87	MG	A1	4428	1/1	0.95	0.80	58,58,58,58	0
86	OHX	A5	3488	7/7	0.95	0.18	125,125,125,125	0
87	MG	A6	2167	1/1	0.95	0.30	46,46,46,46	0
87	MG	BB	406	1/1	0.95	0.64	59,59,59,59	0
86	OHX	A2	2022	7/7	0.95	0.17	138,138,138,138	7
86	OHX	A5	3803	7/7	0.95	0.23	107,107,107,107	7
86	OHX	A1	3710	7/7	0.95	0.18	122,122,122,122	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A2	2010	7/7	0.95	0.22	119,119,119,119	7
87	MG	A1	4434	1/1	0.95	1.00	55,55,55,55	0
87	MG	Dp	103	1/1	0.95	0.33	72,72,72,72	0
87	MG	A5	4141	1/1	0.95	0.11	66,66,66,66	0
87	MG	A1	4435	1/1	0.95	0.20	105,105,105,105	0
87	MG	A1	3910	1/1	0.95	0.33	58,58,58,58	0
86	OHX	A6	1979	7/7	0.95	0.18	116,116,116,116	7
86	OHX	A5	3547	7/7	0.95	0.24	104,104,104,104	7
86	OHX	A6	1981	7/7	0.95	0.21	110,110,110,110	7
87	MG	A1	3939	1/1	0.96	0.32	32,32,32,32	0
86	OHX	A2	2023	7/7	0.96	0.14	136,136,136,136	7
87	MG	A1	4091	1/1	0.96	0.29	65,65,65,65	0
86	OHX	A2	2005	7/7	0.96	0.15	134,134,134,134	7
87	MG	A6	2144	1/1	0.96	0.36	51,51,51,51	0
86	OHX	A5	3664	7/7	0.96	0.29	106,106,106,106	7
87	MG	A1	4094	1/1	0.96	0.21	34,34,34,34	0
86	OHX	A2	2067	7/7	0.96	0.25	108,108,108,108	7
86	OHX	A2	1986	7/7	0.96	0.17	124,124,124,124	7
87	MG	A5	4532	1/1	0.96	0.44	95,95,95,95	0
86	OHX	A2	2026	7/7	0.96	0.14	140,140,140,140	7
86	OHX	A1	3577	7/7	0.96	0.16	122,122,122,122	7
86	OHX	A1	3579	7/7	0.96	0.23	97,97,97,97	7
86	OHX	A6	2012	7/7	0.96	0.14	149,149,149,149	7
87	MG	A1	3949	1/1	0.96	0.32	43,43,43,43	0
87	MG	Ad	104	1/1	0.96	0.23	65,65,65,65	0
87	MG	A5	4539	1/1	0.96	0.76	77,77,77,77	0
87	MG	A5	4342	1/1	0.96	0.21	50,50,50,50	0
86	OHX	A1	3801	7/7	0.96	0.32	125,125,125,125	7
86	OHX	A1	3665	7/7	0.96	0.24	104,104,104,104	7
86	OHX	A1	3580	7/7	0.96	0.17	149,149,149,149	7
86	OHX	A6	2016	7/7	0.96	0.16	124,124,124,124	7
87	MG	A1	3955	1/1	0.96	0.39	42,42,42,42	0
86	OHX	A1	3582	7/7	0.96	0.23	92,92,92,92	7
86	OHX	A1	3583	7/7	0.96	0.17	147,147,147,147	7
87	MG	A5	4548	1/1	0.96	0.63	74,74,74,74	0
86	OHX	A6	2019	7/7	0.96	0.18	127,127,127,127	7
86	OHX	A1	3669	7/7	0.96	0.15	130,130,130,130	7
87	MG	A5	4551	1/1	0.96	0.24	62,62,62,62	0
86	OHX	A1	3585	7/7	0.96	0.16	122,122,122,122	7
86	OHX	A2	2008	7/7	0.96	0.17	135,135,135,135	7
86	OHX	A5	3682	7/7	0.96	0.17	110,110,110,110	7
87	MG	A6	2170	1/1	0.96	0.21	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	A1	4413	1/1	0.96	0.24	106,106,106,106	0
87	MG	CB	302	1/1	0.96	0.16	93,93,93,93	0
86	OHX	A1	3587	7/7	0.96	0.14	147,147,147,147	7
86	OHX	A1	3589	7/7	0.96	0.24	97,97,97,97	7
86	OHX	Ad	101	7/7	0.96	0.17	130,130,130,130	7
87	MG	CG	303	1/1	0.96	0.30	54,54,54,54	0
86	OHX	CY	202	7/7	0.96	0.15	130,130,130,130	7
86	OHX	A5	3687	7/7	0.96	0.21	109,109,109,109	7
86	OHX	A5	3814	7/7	0.96	0.19	114,114,114,114	7
86	OHX	A1	3592	7/7	0.96	0.20	108,108,108,108	7
86	OHX	A5	3402	7/7	0.96	0.19	116,116,116,116	7
86	OHX	A1	3593	7/7	0.96	0.18	113,113,113,113	7
86	OHX	A1	3596	7/7	0.96	0.20	120,120,120,120	7
87	MG	A2	2174	1/1	0.96	0.21	53,53,53,53	0
86	OHX	A5	3692	7/7	0.96	0.15	170,170,170,170	7
86	OHX	A2	1932	7/7	0.96	0.18	117,117,117,117	7
86	OHX	A3	206	7/7	0.96	0.14	140,140,140,140	7
86	OHX	A1	3402	7/7	0.96	0.20	130,130,130,130	7
86	OHX	A5	3472	7/7	0.96	0.23	105,105,105,105	0
86	OHX	A5	3697	7/7	0.96	0.14	167,167,167,167	7
86	OHX	A3	208	7/7	0.96	0.19	126,126,126,126	7
86	OHX	A5	3493	7/7	0.96	0.20	102,102,102,102	7
86	OHX	A5	3513	7/7	0.96	0.19	115,115,115,115	7
86	OHX	A2	1934	7/7	0.96	0.18	123,123,123,123	7
86	OHX	A1	3602	7/7	0.96	0.22	99,99,99,99	7
87	MG	A5	4005	1/1	0.96	0.36	31,31,31,31	0
87	MG	Ch	302	1/1	0.96	0.18	53,53,53,53	0
87	MG	BL	205	1/1	0.96	0.59	62,62,62,62	0
87	MG	A1	3988	1/1	0.96	0.34	67,67,67,67	0
87	MG	A5	4010	1/1	0.96	0.43	50,50,50,50	0
86	OHX	A2	1989	7/7	0.96	0.17	131,131,131,131	7
87	MG	A1	4140	1/1	0.96	0.32	56,56,56,56	0
86	OHX	A5	3538	7/7	0.96	0.19	104,104,104,104	7
87	MG	A5	3825	1/1	0.96	0.16	29,29,29,29	0
86	OHX	A5	3540	7/7	0.96	0.19	119,119,119,119	7
87	MG	A1	3992	1/1	0.96	0.31	41,41,41,41	0
87	MG	A5	3828	1/1	0.96	0.10	34,34,34,34	0
86	OHX	A2	2052	7/7	0.96	0.24	117,117,117,117	7
87	MG	BO	203	1/1	0.96	0.77	74,74,74,74	0
87	MG	BO	204	1/1	0.96	0.37	53,53,53,53	0
86	OHX	A8	214	7/7	0.96	0.16	125,125,125,125	7
86	OHX	A5	3544	7/7	0.96	0.21	97,97,97,97	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A5	4209	1/1	0.96	0.40	53,53,53,53	0
86	OHX	A1	3506	7/7	0.96	0.19	103,103,103,103	7
86	OHX	A2	1992	7/7	0.96	0.15	123,123,123,123	7
86	OHX	A1	3518	7/7	0.96	0.17	140,140,140,140	7
86	OHX	A1	3757	7/7	0.96	0.27	73,73,73,73	7
87	MG	BP	204	1/1	0.96	0.34	51,51,51,51	0
86	OHX	A5	3566	7/7	0.96	0.23	99,99,99,99	7
86	OHX	A5	3568	7/7	0.96	0.20	103,103,103,103	7
87	MG	A1	4007	1/1	0.96	0.22	29,29,29,29	0
86	OHX	A1	3610	7/7	0.96	0.20	121,121,121,121	7
86	OHX	A2	2013	7/7	0.96	0.19	116,116,116,116	7
87	MG	A5	3846	1/1	0.96	0.17	37,37,37,37	0
87	MG	A1	3865	1/1	0.96	0.10	31,31,31,31	0
87	MG	A1	3866	1/1	0.96	0.11	87,87,87,87	0
87	MG	A1	3867	1/1	0.96	0.31	61,61,61,61	0
86	OHX	A5	3577	7/7	0.96	0.18	128,128,128,128	7
86	OHX	A2	1937	7/7	0.96	0.20	122,122,122,122	7
87	MG	BQ	203	1/1	0.96	0.87	63,63,63,63	0
87	MG	A1	4461	1/1	0.96	0.12	86,86,86,86	0
86	OHX	A5	3720	7/7	0.96	0.17	101,101,101,101	7
86	OHX	A2	1969	7/7	0.96	0.15	144,144,144,144	7
86	OHX	A1	3536	7/7	0.96	0.16	136,136,136,136	7
87	MG	A5	4421	1/1	0.96	0.60	55,55,55,55	0
86	OHX	A5	3588	7/7	0.96	0.23	106,106,106,106	7
87	MG	A6	2229	1/1	0.96	0.23	65,65,65,65	0
87	MG	A6	2230	1/1	0.96	0.13	86,86,86,86	0
87	MG	DA	304	1/1	0.96	0.74	69,69,69,69	0
87	MG	A1	4020	1/1	0.96	0.34	52,52,52,52	0
87	MG	A1	4312	1/1	0.96	0.70	60,60,60,60	0
87	MG	A1	4166	1/1	0.96	0.32	74,74,74,74	0
87	MG	A5	3863	1/1	0.96	0.28	51,51,51,51	0
86	OHX	A5	3589	7/7	0.96	0.20	93,93,93,93	7
86	OHX	A1	3620	7/7	0.96	0.16	139,139,139,139	7
87	MG	A5	3866	1/1	0.96	0.30	51,51,51,51	0
87	MG	A1	4023	1/1	0.96	0.42	42,42,42,42	0
87	MG	A1	4024	1/1	0.96	0.40	40,40,40,40	0
86	OHX	A1	3764	7/7	0.96	0.15	159,159,159,159	7
86	OHX	A1	3621	7/7	0.96	0.18	119,119,119,119	7
87	MG	BY	202	1/1	0.96	0.44	85,85,85,85	0
87	MG	A5	4438	1/1	0.96	0.43	58,58,58,58	0
87	MG	A5	4248	1/1	0.96	0.23	99,99,99,99	0
86	OHX	A2	1973	7/7	0.96	0.18	136,136,136,136	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	4029	1/1	0.96	0.18	29,29,29,29	0
87	MG	A1	3880	1/1	0.96	0.31	42,42,42,42	0
86	OHX	DV	201	7/7	0.96	0.16	126,126,126,126	7
86	OHX	A1	3541	7/7	0.96	0.23	109,109,109,109	7
86	OHX	A5	3603	7/7	0.96	0.25	107,107,107,107	7
86	OHX	A5	3604	7/7	0.96	0.20	113,113,113,113	7
87	MG	DD	305	1/1	0.96	0.21	74,74,74,74	0
86	OHX	A2	1999	7/7	0.96	0.13	168,168,168,168	7
87	MG	A1	3886	1/1	0.96	0.35	72,72,72,72	0
87	MG	A5	3881	1/1	0.96	0.29	60,60,60,60	0
86	OHX	A1	3544	7/7	0.96	0.20	96,96,96,96	7
86	OHX	A5	3608	7/7	0.96	0.15	125,125,125,125	7
86	OHX	A1	3546	7/7	0.96	0.19	106,106,106,106	7
86	OHX	A5	3610	7/7	0.96	0.14	161,161,161,161	7
86	OHX	A1	3630	7/7	0.96	0.16	119,119,119,119	7
86	OHX	Bj	101	7/7	0.96	0.18	100,100,100,100	7
86	OHX	A5	3613	7/7	0.96	0.17	137,137,137,137	7
86	OHX	A1	3632	7/7	0.96	0.10	170,170,170,170	7
87	MG	A5	4268	1/1	0.96	0.40	96,96,96,96	0
87	MG	A5	4080	1/1	0.96	0.35	71,71,71,71	0
86	OHX	A6	1939	7/7	0.96	0.17	134,134,134,134	0
86	OHX	A5	3618	7/7	0.96	0.24	101,101,101,101	7
86	OHX	A1	3547	7/7	0.96	0.19	99,99,99,99	7
87	MG	DO	204	1/1	0.96	0.63	57,57,57,57	0
87	MG	A5	3893	1/1	0.96	0.30	73,73,73,73	0
86	OHX	A2	1943	7/7	0.96	0.22	123,123,123,123	7
86	OHX	A2	1959	7/7	0.96	0.15	147,147,147,147	7
87	MG	A2	2106	1/1	0.96	0.36	57,57,57,57	0
86	OHX	A2	1945	7/7	0.96	0.14	140,140,140,140	7
86	OHX	A6	1963	7/7	0.96	0.18	103,103,103,103	7
86	OHX	A6	1967	7/7	0.96	0.17	112,112,112,112	7
87	MG	A5	4280	1/1	0.96	0.84	49,49,49,49	0
87	MG	A1	4350	1/1	0.96	0.93	76,76,76,76	0
87	MG	DP	206	1/1	0.96	0.88	55,55,55,55	0
87	MG	A5	4474	1/1	0.96	0.73	44,44,44,44	0
86	OHX	A5	3627	7/7	0.96	0.24	80,80,80,80	7
86	OHX	A1	3552	7/7	0.96	0.20	115,115,115,115	7
86	OHX	A6	1973	7/7	0.96	0.20	87,87,87,87	7
87	MG	DS	201	1/1	0.96	0.21	61,61,61,61	0
86	OHX	A6	1974	7/7	0.96	0.19	116,116,116,116	7
87	MG	A6	2107	1/1	0.96	0.41	52,52,52,52	0
86	OHX	A5	3631	7/7	0.96	0.24	89,89,89,89	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A6	1976	7/7	0.96	0.28	105,105,105,105	7
86	OHX	A2	1961	7/7	0.96	0.15	150,150,150,150	7
86	OHX	A5	3635	7/7	0.96	0.14	147,147,147,147	7
87	MG	A6	2113	1/1	0.96	0.26	48,48,48,48	0
86	OHX	A1	3640	7/7	0.96	0.16	153,153,153,153	7
87	MG	A2	2244	1/1	0.96	0.14	99,99,99,99	0
87	MG	A6	2283	1/1	0.96	0.21	75,75,75,75	0
87	MG	A5	4105	1/1	0.96	0.28	68,68,68,68	0
86	OHX	A2	2042	7/7	0.96	0.13	155,155,155,155	7
86	OHX	A6	1980	7/7	0.96	0.22	133,133,133,133	7
87	MG	A6	2286	1/1	0.96	0.29	75,75,75,75	0
86	OHX	A5	3640	7/7	0.96	0.15	147,147,147,147	7
87	MG	A5	3919	1/1	0.96	0.24	66,66,66,66	0
86	OHX	A5	3641	7/7	0.96	0.18	127,127,127,127	7
86	OHX	A1	3643	7/7	0.96	0.16	153,153,153,153	7
86	OHX	A1	3715	7/7	0.96	0.18	120,120,120,120	7
86	OHX	A2	1984	7/7	0.96	0.18	108,108,108,108	7
86	OHX	A1	3717	7/7	0.96	0.19	141,141,141,141	7
86	OHX	A1	3560	7/7	0.96	0.18	116,116,116,116	7
86	OHX	A1	3647	7/7	0.96	0.16	129,129,129,129	7
87	MG	A5	4120	1/1	0.96	0.39	49,49,49,49	0
86	OHX	A1	3649	7/7	0.96	0.16	167,167,167,167	7
86	OHX	A5	3649	7/7	0.96	0.20	129,129,129,129	7
87	MG	Dj	103	1/1	0.96	1.50	65,65,65,65	0
86	OHX	A1	3650	7/7	0.96	0.31	120,120,120,120	7
87	MG	A5	3930	1/1	0.96	0.18	29,29,29,29	0
86	OHX	A1	3561	7/7	0.96	0.20	110,110,110,110	7
86	OHX	A1	3562	7/7	0.96	0.17	143,143,143,143	7
87	MG	A1	4081	1/1	0.96	0.14	56,56,56,56	0
86	OHX	A5	3654	7/7	0.96	0.17	116,116,116,116	7
86	OHX	A5	3655	7/7	0.96	0.27	124,124,124,124	7
86	OHX	A6	1997	7/7	0.96	0.19	125,125,125,125	7
88	ZN	Aa	202	1/1	0.96	0.11	92,92,92,92	0
86	OHX	A1	3563	7/7	0.96	0.17	131,131,131,131	7
86	OHX	A1	3656	7/7	0.96	0.19	114,114,114,114	7
87	MG	A4	223	1/1	0.96	0.43	44,44,44,44	0
86	OHX	A6	2000	7/7	0.96	0.19	128,128,128,128	7
86	OHX	A6	2001	7/7	0.96	0.17	149,149,149,149	7
86	OHX	A7	203	7/7	0.97	0.22	105,105,105,105	7
86	OHX	A6	1954	7/7	0.97	0.13	141,141,141,141	7
86	OHX	A5	3652	7/7	0.97	0.17	150,150,150,150	7
86	OHX	A1	3530	7/7	0.97	0.17	125,125,125,125	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A6	1958	7/7	0.97	0.16	133,133,133,133	7
87	MG	A5	4047	1/1	0.97	0.25	57,57,57,57	0
86	OHX	A6	1959	7/7	0.97	0.21	107,107,107,107	7
87	MG	A1	4330	1/1	0.97	0.16	82,82,82,82	0
86	OHX	A1	3531	7/7	0.97	0.15	140,140,140,140	7
86	OHX	A8	204	7/7	0.97	0.20	101,101,101,101	7
86	OHX	A1	3532	7/7	0.97	0.20	87,87,87,87	7
86	OHX	A8	209	7/7	0.97	0.18	130,130,130,130	7
86	OHX	A8	210	7/7	0.97	0.17	133,133,133,133	7
87	MG	A5	4504	1/1	0.97	0.45	84,84,84,84	0
86	OHX	A1	3534	7/7	0.97	0.19	106,106,106,106	7
86	OHX	A6	1964	7/7	0.97	0.18	132,132,132,132	7
87	MG	A6	2177	1/1	0.97	0.23	79,79,79,79	0
86	OHX	A5	3660	7/7	0.97	0.22	108,108,108,108	7
86	OHX	A6	1965	7/7	0.97	0.15	123,123,123,123	7
87	MG	A5	4281	1/1	0.97	0.49	56,56,56,56	0
87	MG	A1	3962	1/1	0.97	0.41	61,61,61,61	0
87	MG	A5	3842	1/1	0.97	0.08	34,34,34,34	0
86	OHX	A6	1966	7/7	0.97	0.20	92,92,92,92	7
87	MG	A5	3844	1/1	0.97	0.18	59,59,59,59	0
86	OHX	A2	1976	7/7	0.97	0.15	139,139,139,139	7
86	OHX	A6	1968	7/7	0.97	0.16	101,101,101,101	7
87	MG	A1	3966	1/1	0.97	0.46	60,60,60,60	0
86	OHX	A1	3612	7/7	0.97	0.15	146,146,146,146	7
86	OHX	A6	1972	7/7	0.97	0.20	109,109,109,109	7
86	OHX	A1	3613	7/7	0.97	0.23	98,98,98,98	7
86	OHX	A1	3614	7/7	0.97	0.19	112,112,112,112	7
87	MG	A1	4349	1/1	0.97	0.37	119,119,119,119	0
86	OHX	A1	3693	7/7	0.97	0.20	100,100,100,100	7
86	OHX	A1	3538	7/7	0.97	0.20	105,105,105,105	7
86	OHX	A2	1977	7/7	0.97	0.12	174,174,174,174	7
86	OHX	A1	3617	7/7	0.97	0.14	144,144,144,144	7
87	MG	A5	4528	1/1	0.97	0.28	97,97,97,97	0
86	OHX	A1	3540	7/7	0.97	0.14	141,141,141,141	7
87	MG	A5	4299	1/1	0.97	0.30	80,80,80,80	0
86	OHX	A1	3698	7/7	0.97	0.17	105,105,105,105	7
87	MG	A5	4301	1/1	0.97	0.06	71,71,71,71	0
86	OHX	A2	1939	7/7	0.97	0.15	144,144,144,144	7
86	OHX	A2	2007	7/7	0.97	0.21	146,146,146,146	7
86	OHX	A6	1985	7/7	0.97	0.18	114,114,114,114	7
86	OHX	A1	3543	7/7	0.97	0.15	137,137,137,137	7
87	MG	A4	244	1/1	0.97	0.20	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A6	1987	7/7	0.97	0.18	113,113,113,113	7
86	OHX	A2	1955	7/7	0.97	0.17	123,123,123,123	7
86	OHX	A1	3703	7/7	0.97	0.20	93,93,93,93	7
87	MG	A4	248	1/1	0.97	0.34	114,114,114,114	0
87	MG	A1	4172	1/1	0.97	0.22	54,54,54,54	0
86	OHX	A2	1940	7/7	0.97	0.18	100,100,100,100	7
86	OHX	A1	3625	7/7	0.97	0.21	92,92,92,92	7
86	OHX	A6	1992	7/7	0.97	0.14	125,125,125,125	7
87	MG	A2	2089	1/1	0.97	0.32	49,49,49,49	0
86	OHX	A6	1993	7/7	0.97	0.17	129,129,129,129	7
86	OHX	A1	3626	7/7	0.97	0.15	162,162,162,162	7
86	OHX	A6	1995	7/7	0.97	0.12	143,143,143,143	7
86	OHX	A2	1958	7/7	0.97	0.16	139,139,139,139	7
86	OHX	A2	1921	7/7	0.97	0.19	113,113,113,113	7
86	OHX	A5	3401	7/7	0.97	0.19	102,102,102,102	0
86	OHX	A2	1985	7/7	0.97	0.14	144,144,144,144	7
86	OHX	A2	1944	7/7	0.97	0.17	109,109,109,109	7
87	MG	A1	3996	1/1	0.97	0.46	48,48,48,48	0
86	OHX	A1	3631	7/7	0.97	0.14	141,141,141,141	7
87	MG	A1	4378	1/1	0.97	0.62	51,51,51,51	0
86	OHX	A2	1928	7/7	0.97	0.17	126,126,126,126	7
87	MG	A5	4559	1/1	0.97	0.27	74,74,74,74	0
86	OHX	A6	2002	7/7	0.97	0.21	96,96,96,96	7
87	MG	A1	4002	1/1	0.97	0.33	37,37,37,37	0
87	MG	A5	4106	1/1	0.97	0.25	41,41,41,41	0
86	OHX	AL	201	7/7	0.97	0.17	119,119,119,119	7
86	OHX	A5	3441	7/7	0.97	0.24	96,96,96,96	0
87	MG	A1	4005	1/1	0.97	0.36	42,42,42,42	0
87	MG	BI	306	1/1	0.97	0.18	32,32,32,32	0
86	OHX	A5	3699	7/7	0.97	0.29	107,107,107,107	7
87	MG	BI	308	1/1	0.97	0.16	57,57,57,57	0
86	OHX	A1	3555	7/7	0.97	0.17	125,125,125,125	7
86	OHX	A1	3556	7/7	0.97	0.18	128,128,128,128	7
86	OHX	A6	2006	7/7	0.97	0.20	87,87,87,87	7
86	OHX	A5	3502	7/7	0.97	0.18	141,141,141,141	0
87	MG	A5	4117	1/1	0.97	0.09	49,49,49,49	0
87	MG	A2	2109	1/1	0.97	0.34	56,56,56,56	0
86	OHX	A5	3510	7/7	0.97	0.21	90,90,90,90	7
87	MG	A1	4013	1/1	0.97	0.29	47,47,47,47	0
86	OHX	A2	1962	7/7	0.97	0.16	136,136,136,136	7
86	OHX	A5	3515	7/7	0.97	0.16	121,121,121,121	7
86	OHX	A1	3637	7/7	0.97	0.12	146,146,146,146	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	A1	3828	1/1	0.97	0.28	43,43,43,43	0
87	MG	A5	3904	1/1	0.97	0.19	60,60,60,60	0
86	OHX	A2	1963	7/7	0.97	0.14	129,129,129,129	7
86	OHX	A5	3522	7/7	0.97	0.17	123,123,123,123	7
87	MG	A1	4400	1/1	0.97	0.14	70,70,70,70	0
86	OHX	A5	3528	7/7	0.97	0.16	163,163,163,163	0
86	OHX	A5	3529	7/7	0.97	0.20	93,93,93,93	7
86	OHX	A1	3559	7/7	0.97	0.17	116,116,116,116	7
86	OHX	A5	3533	7/7	0.97	0.16	118,118,118,118	7
87	MG	A5	4133	1/1	0.97	0.31	54,54,54,54	0
86	OHX	A5	3536	7/7	0.97	0.20	97,97,97,97	7
86	OHX	A6	2011	7/7	0.97	0.19	120,120,120,120	7
86	OHX	A2	1990	7/7	0.97	0.17	105,105,105,105	7
86	OHX	A2	1935	7/7	0.97	0.18	120,120,120,120	7
87	MG	A1	4028	1/1	0.97	0.41	28,28,28,28	0
86	OHX	A5	3542	7/7	0.97	0.23	103,103,103,103	7
86	OHX	A5	3543	7/7	0.97	0.21	109,109,109,109	7
86	OHX	A1	3642	7/7	0.97	0.11	139,139,139,139	7
86	OHX	A5	3546	7/7	0.97	0.16	132,132,132,132	7
87	MG	A1	3843	1/1	0.97	0.30	46,46,46,46	0
86	OHX	A1	3401	7/7	0.97	0.16	121,121,121,121	7
86	OHX	A5	3548	7/7	0.97	0.18	134,134,134,134	7
86	OHX	A5	3549	7/7	0.97	0.20	107,107,107,107	7
86	OHX	A5	3550	7/7	0.97	0.21	119,119,119,119	7
86	OHX	A1	3644	7/7	0.97	0.15	139,139,139,139	7
87	MG	A1	3849	1/1	0.97	0.38	56,56,56,56	0
86	OHX	A5	3555	7/7	0.97	0.14	152,152,152,152	0
87	MG	A6	2268	1/1	0.97	0.28	68,68,68,68	0
86	OHX	A5	3556	7/7	0.97	0.19	111,111,111,111	7
87	MG	A5	3931	1/1	0.97	0.33	35,35,35,35	0
86	OHX	A2	1993	7/7	0.97	0.11	159,159,159,159	7
86	OHX	A2	1994	7/7	0.97	0.16	118,118,118,118	7
86	OHX	A5	3561	7/7	0.97	0.17	121,121,121,121	7
86	OHX	A5	3562	7/7	0.97	0.20	104,104,104,104	7
86	OHX	A5	3563	7/7	0.97	0.19	98,98,98,98	7
86	OHX	A5	3564	7/7	0.97	0.13	143,143,143,143	7
86	OHX	A5	3565	7/7	0.97	0.19	105,105,105,105	7
86	OHX	A5	3738	7/7	0.97	0.20	101,101,101,101	7
87	MG	A1	4237	1/1	0.97	0.19	46,46,46,46	0
86	OHX	A5	3739	7/7	0.97	0.23	105,105,105,105	7
86	OHX	A2	1915	7/7	0.97	0.17	109,109,109,109	7
86	OHX	A5	3567	7/7	0.97	0.20	106,106,106,106	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A6	2020	7/7	0.97	0.20	88,88,88,88	7
87	MG	A5	3946	1/1	0.97	0.41	41,41,41,41	0
86	OHX	A1	3648	7/7	0.97	0.15	102,102,102,102	7
86	OHX	A1	3447	7/7	0.97	0.21	98,98,98,98	0
86	OHX	A5	3574	7/7	0.97	0.17	154,154,154,154	7
86	OHX	A5	3575	7/7	0.97	0.23	81,81,81,81	7
87	MG	A1	4246	1/1	0.97	0.27	80,80,80,80	0
87	MG	A5	3952	1/1	0.97	0.42	43,43,43,43	0
86	OHX	A5	3576	7/7	0.97	0.22	124,124,124,124	7
86	OHX	A1	3570	7/7	0.97	0.18	100,100,100,100	7
86	OHX	A5	3579	7/7	0.97	0.18	105,105,105,105	7
86	OHX	A5	3580	7/7	0.97	0.16	121,121,121,121	7
87	MG	DB	410	1/1	0.97	0.52	54,54,54,54	0
86	OHX	A5	3581	7/7	0.97	0.15	148,148,148,148	7
86	OHX	A1	3572	7/7	0.97	0.18	114,114,114,114	7
86	OHX	A2	1967	7/7	0.97	0.16	120,120,120,120	7
86	OHX	A1	3654	7/7	0.97	0.12	149,149,149,149	7
86	OHX	A5	3586	7/7	0.97	0.19	112,112,112,112	7
87	MG	A5	3962	1/1	0.97	0.36	41,41,41,41	0
86	OHX	A5	3587	7/7	0.97	0.22	96,96,96,96	7
86	OHX	A5	3757	7/7	0.97	0.10	192,192,192,192	7
86	OHX	A6	2027	7/7	0.97	0.12	189,189,189,189	7
86	OHX	A1	3735	7/7	0.97	0.24	83,83,83,83	7
86	OHX	A5	3590	7/7	0.97	0.21	114,114,114,114	7
87	MG	A1	4456	1/1	0.97	0.39	76,76,76,76	0
87	MG	A5	3969	1/1	0.97	0.41	37,37,37,37	0
86	OHX	A1	3816	7/7	0.97	0.10	150,150,150,150	7
86	OHX	A3	201	7/7	0.97	0.19	109,109,109,109	0
87	MG	A5	3972	1/1	0.97	0.29	55,55,55,55	0
87	MG	A5	4418	1/1	0.97	0.22	91,91,91,91	0
86	OHX	A3	205	7/7	0.97	0.17	113,113,113,113	7
86	OHX	A1	3472	7/7	0.97	0.18	109,109,109,109	7
87	MG	A5	3975	1/1	0.97	0.44	41,41,41,41	0
86	OHX	A5	3596	7/7	0.97	0.25	84,84,84,84	7
86	OHX	A5	3597	7/7	0.97	0.19	95,95,95,95	7
86	OHX	A5	3598	7/7	0.97	0.13	143,143,143,143	7
86	OHX	A5	3599	7/7	0.97	0.17	120,120,120,120	7
86	OHX	A5	3600	7/7	0.97	0.12	133,133,133,133	7
86	OHX	A1	3575	7/7	0.97	0.15	120,120,120,120	7
86	OHX	A1	3476	7/7	0.97	0.20	129,129,129,129	0
86	OHX	A1	3578	7/7	0.97	0.20	112,112,112,112	7
86	OHX	A1	3479	7/7	0.97	0.19	117,117,117,117	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	DO	202	1/1	0.97	0.64	61,61,61,61	0
87	MG	A6	2110	1/1	0.97	0.26	65,65,65,65	0
86	OHX	A5	3606	7/7	0.97	0.18	130,130,130,130	7
86	OHX	A1	3484	7/7	0.97	0.19	126,126,126,126	0
86	OHX	A1	3490	7/7	0.97	0.19	126,126,126,126	0
86	OHX	A1	3493	7/7	0.97	0.16	148,148,148,148	0
86	OHX	A4	206	7/7	0.97	0.17	104,104,104,104	7
87	MG	A5	4437	1/1	0.97	0.28	86,86,86,86	0
87	MG	A1	4475	1/1	0.97	0.78	64,64,64,64	0
87	MG	A1	4279	1/1	0.97	0.74	54,54,54,54	0
86	OHX	A4	207	7/7	0.97	0.17	129,129,129,129	7
86	OHX	A4	208	7/7	0.97	0.22	90,90,90,90	7
87	MG	A6	2327	1/1	0.97	0.14	108,108,108,108	0
86	OHX	A1	3663	7/7	0.97	0.30	126,126,126,126	7
86	OHX	A4	210	7/7	0.97	0.11	131,131,131,131	7
86	OHX	A1	3494	7/7	0.97	0.17	133,133,133,133	0
86	OHX	A5	3616	7/7	0.97	0.21	102,102,102,102	7
86	OHX	A5	3617	7/7	0.97	0.12	154,154,154,154	7
86	OHX	A1	3497	7/7	0.97	0.27	100,100,100,100	7
86	OHX	A5	3619	7/7	0.97	0.20	119,119,119,119	7
86	OHX	A1	3501	7/7	0.97	0.19	94,94,94,94	7
87	MG	A2	2195	1/1	0.97	0.24	90,90,90,90	0
86	OHX	A1	3588	7/7	0.97	0.20	104,104,104,104	7
86	OHX	A1	3503	7/7	0.97	0.17	111,111,111,111	7
86	OHX	A1	3504	7/7	0.97	0.20	105,105,105,105	7
87	MG	DV	203	1/1	0.97	0.24	65,65,65,65	0
86	OHX	A2	1949	7/7	0.97	0.15	135,135,135,135	7
86	OHX	A5	3625	7/7	0.97	0.17	117,117,117,117	7
86	OHX	A1	3672	7/7	0.97	0.23	99,99,99,99	7
86	OHX	A1	3511	7/7	0.97	0.17	154,154,154,154	0
86	OHX	A1	3594	7/7	0.97	0.13	144,144,144,144	7
87	MG	A5	4460	1/1	0.97	0.71	74,74,74,74	0
86	OHX	A1	3595	7/7	0.97	0.22	120,120,120,120	7
86	OHX	A2	1952	7/7	0.97	0.14	127,127,127,127	7
86	OHX	A1	3597	7/7	0.97	0.18	123,123,123,123	7
86	OHX	A5	3632	7/7	0.97	0.20	106,106,106,106	7
87	MG	A5	4465	1/1	0.97	0.40	62,62,62,62	0
86	OHX	A1	3598	7/7	0.97	0.15	139,139,139,139	7
87	MG	A5	4242	1/1	0.97	0.56	65,65,65,65	0
86	OHX	A2	1970	7/7	0.97	0.14	138,138,138,138	7
87	MG	Df	204	1/1	0.97	0.54	61,61,61,61	0
86	OHX	A2	1953	7/7	0.97	0.20	120,120,120,120	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A5	3636	7/7	0.97	0.15	111,111,111,111	7
86	OHX	A2	1974	7/7	0.97	0.12	170,170,170,170	7
86	OHX	Bj	102	7/7	0.97	0.21	102,102,102,102	7
86	OHX	A2	1975	7/7	0.97	0.14	141,141,141,141	7
86	OHX	A5	3812	7/7	0.97	0.13	135,135,135,135	7
87	MG	A5	4475	1/1	0.97	0.79	127,127,127,127	0
86	OHX	A6	1927	7/7	0.97	0.17	129,129,129,129	0
86	OHX	A6	1929	7/7	0.97	0.17	128,128,128,128	0
87	MG	A5	4252	1/1	0.97	0.23	68,68,68,68	0
86	OHX	A6	1933	7/7	0.97	0.20	104,104,104,104	7
86	OHX	A6	1934	7/7	0.97	0.21	105,105,105,105	7
86	OHX	A6	1936	7/7	0.97	0.20	100,100,100,100	7
86	OHX	A1	3527	7/7	0.97	0.22	94,94,94,94	7
86	OHX	A6	1940	7/7	0.97	0.15	129,129,129,129	7
86	OHX	A6	1941	7/7	0.97	0.17	112,112,112,112	7
88	ZN	Ad	105	1/1	0.97	0.18	83,83,83,83	0
88	ZN	Bm	202	1/1	0.97	0.18	56,56,56,56	0
86	OHX	A6	1942	7/7	0.97	0.19	114,114,114,114	7
87	MG	A6	2159	1/1	0.97	0.23	33,33,33,33	0
88	ZN	Cd	103	1/1	0.97	0.17	71,71,71,71	0
86	OHX	A1	3605	7/7	0.97	0.13	166,166,166,166	7
86	OHX	A6	1951	7/7	0.97	0.17	115,115,115,115	7
88	ZN	Dp	104	1/1	0.97	0.15	79,79,79,79	0
86	OHX	A5	3578	7/7	0.98	0.11	159,159,159,159	7
86	OHX	A6	1943	7/7	0.98	0.18	106,106,106,106	7
87	MG	A1	3905	1/1	0.98	0.16	19,19,19,19	0
87	MG	A1	4318	1/1	0.98	0.43	66,66,66,66	0
87	MG	A5	4509	1/1	0.98	0.92	134,134,134,134	0
86	OHX	A6	1944	7/7	0.98	0.15	115,115,115,115	7
86	OHX	A2	1927	7/7	0.98	0.17	115,115,115,115	7
86	OHX	A5	3759	7/7	0.98	0.20	80,80,80,80	7
86	OHX	A5	3582	7/7	0.98	0.20	95,95,95,95	7
86	OHX	A6	1948	7/7	0.98	0.17	114,114,114,114	7
86	OHX	A6	1949	7/7	0.98	0.17	102,102,102,102	7
86	OHX	A6	1950	7/7	0.98	0.14	140,140,140,140	0
86	OHX	A1	3454	7/7	0.98	0.18	106,106,106,106	7
86	OHX	A6	1952	7/7	0.98	0.15	123,123,123,123	7
87	MG	A1	4121	1/1	0.98	0.12	74,74,74,74	0
86	OHX	A6	1953	7/7	0.98	0.12	136,136,136,136	7
86	OHX	A1	3622	7/7	0.98	0.21	112,112,112,112	7
86	OHX	A1	3458	7/7	0.98	0.17	111,111,111,111	7
86	OHX	A6	1956	7/7	0.98	0.16	130,130,130,130	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A5	3592	7/7	0.98	0.20	102,102,102,102	7
86	OHX	A6	1957	7/7	0.98	0.14	144,144,144,144	7
86	OHX	A1	3545	7/7	0.98	0.19	78,78,78,78	7
86	OHX	A1	3459	7/7	0.98	0.21	86,86,86,86	7
86	OHX	A6	1960	7/7	0.98	0.15	120,120,120,120	7
86	OHX	A1	3460	7/7	0.98	0.18	111,111,111,111	0
87	MG	A6	2199	1/1	0.98	0.28	62,62,62,62	0
86	OHX	A1	3462	7/7	0.98	0.20	91,91,91,91	7
86	OHX	A1	3463	7/7	0.98	0.15	110,110,110,110	7
86	OHX	A1	3469	7/7	0.98	0.18	122,122,122,122	0
86	OHX	A5	3601	7/7	0.98	0.18	96,96,96,96	7
86	OHX	A1	3551	7/7	0.98	0.18	100,100,100,100	7
86	OHX	A6	2076	7/7	0.98	0.24	90,90,90,90	7
86	OHX	A1	3470	7/7	0.98	0.18	96,96,96,96	7
86	OHX	A1	3553	7/7	0.98	0.23	110,110,110,110	7
86	OHX	A1	3471	7/7	0.98	0.17	107,107,107,107	7
86	OHX	A6	1969	7/7	0.98	0.21	90,90,90,90	7
86	OHX	A2	1991	7/7	0.98	0.14	113,113,113,113	7
86	OHX	A6	1971	7/7	0.98	0.14	108,108,108,108	7
86	OHX	A1	3473	7/7	0.98	0.21	85,85,85,85	7
86	OHX	A1	3475	7/7	0.98	0.20	98,98,98,98	7
86	OHX	A2	1908	7/7	0.98	0.20	115,115,115,115	0
86	OHX	A6	1975	7/7	0.98	0.17	106,106,106,106	7
86	OHX	A1	3477	7/7	0.98	0.21	83,83,83,83	7
86	OHX	A1	3718	7/7	0.98	0.19	94,94,94,94	7
86	OHX	A1	3478	7/7	0.98	0.17	112,112,112,112	7
86	OHX	A5	3795	7/7	0.98	0.27	117,117,117,117	7
86	OHX	A2	1930	7/7	0.98	0.16	120,120,120,120	7
86	OHX	A1	3482	7/7	0.98	0.17	106,106,106,106	7
86	OHX	A1	3483	7/7	0.98	0.20	103,103,103,103	7
86	OHX	A2	1909	7/7	0.98	0.19	93,93,93,93	7
86	OHX	A6	1983	7/7	0.98	0.17	133,133,133,133	7
86	OHX	A1	3565	7/7	0.98	0.14	127,127,127,127	7
86	OHX	A1	3487	7/7	0.98	0.21	94,94,94,94	7
86	OHX	A1	3568	7/7	0.98	0.14	133,133,133,133	7
86	OHX	A1	3489	7/7	0.98	0.20	90,90,90,90	7
86	OHX	A2	1948	7/7	0.98	0.17	108,108,108,108	7
86	OHX	A1	3571	7/7	0.98	0.16	119,119,119,119	7
86	OHX	A2	1996	7/7	0.98	0.20	113,113,113,113	7
86	OHX	A5	3809	7/7	0.98	0.23	91,91,91,91	7
87	MG	A1	3959	1/1	0.98	0.43	43,43,43,43	0
87	MG	A5	4566	1/1	0.98	0.46	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A2	1911	7/7	0.98	0.21	124,124,124,124	0
86	OHX	A2	1971	7/7	0.98	0.14	110,110,110,110	7
86	OHX	A1	3653	7/7	0.98	0.12	153,153,153,153	7
86	OHX	A1	3498	7/7	0.98	0.23	89,89,89,89	7
86	OHX	A1	3576	7/7	0.98	0.18	83,83,83,83	7
86	OHX	A1	3500	7/7	0.98	0.18	87,87,87,87	7
86	OHX	A3	202	7/7	0.98	0.16	103,103,103,103	7
86	OHX	A3	203	7/7	0.98	0.16	118,118,118,118	7
86	OHX	A2	1972	7/7	0.98	0.17	138,138,138,138	7
86	OHX	CY	201	7/7	0.98	0.17	121,121,121,121	7
86	OHX	A1	3502	7/7	0.98	0.19	78,78,78,78	7
87	MG	A5	4578	1/1	0.98	0.26	74,74,74,74	0
86	OHX	Cd	101	7/7	0.98	0.18	135,135,135,135	7
86	OHX	A2	1950	7/7	0.98	0.13	122,122,122,122	7
86	OHX	A1	3581	7/7	0.98	0.23	73,73,73,73	7
87	MG	A7	214	1/1	0.98	0.47	55,55,55,55	0
86	OHX	A7	202	7/7	0.98	0.21	81,81,81,81	7
86	OHX	A2	1951	7/7	0.98	0.13	126,126,126,126	7
86	OHX	A7	206	7/7	0.98	0.17	115,115,115,115	7
86	OHX	A1	3505	7/7	0.98	0.17	124,124,124,124	7
86	OHX	A7	208	7/7	0.98	0.18	105,105,105,105	7
86	OHX	A1	3584	7/7	0.98	0.20	88,88,88,88	7
86	OHX	A2	1933	7/7	0.98	0.17	109,109,109,109	7
86	OHX	A1	3508	7/7	0.98	0.19	93,93,93,93	7
87	MG	A6	2257	1/1	0.98	0.26	65,65,65,65	0
86	OHX	A4	203	7/7	0.98	0.19	93,93,93,93	7
86	OHX	A4	204	7/7	0.98	0.17	122,122,122,122	7
86	OHX	A8	203	7/7	0.98	0.15	111,111,111,111	7
86	OHX	A5	3446	7/7	0.98	0.20	82,82,82,82	0
86	OHX	A8	205	7/7	0.98	0.14	107,107,107,107	7
86	OHX	A5	3447	7/7	0.98	0.22	107,107,107,107	0
86	OHX	A8	207	7/7	0.98	0.16	126,126,126,126	7
86	OHX	A8	208	7/7	0.98	0.19	115,115,115,115	7
86	OHX	A5	3455	7/7	0.98	0.20	100,100,100,100	0
86	OHX	A5	3456	7/7	0.98	0.18	85,85,85,85	7
86	OHX	A5	3459	7/7	0.98	0.20	100,100,100,100	0
86	OHX	A5	3462	7/7	0.98	0.19	102,102,102,102	0
86	OHX	A5	3463	7/7	0.98	0.22	130,130,130,130	0
86	OHX	A5	3464	7/7	0.98	0.17	98,98,98,98	7
86	OHX	A5	3465	7/7	0.98	0.20	91,91,91,91	7
87	MG	A5	3940	1/1	0.98	0.41	39,39,39,39	0
86	OHX	A5	3467	7/7	0.98	0.20	104,104,104,104	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	A1	3998	1/1	0.98	0.24	28,28,28,28	0
86	OHX	A4	205	7/7	0.98	0.16	122,122,122,122	7
87	MG	A1	4000	1/1	0.98	0.19	18,18,18,18	0
86	OHX	A5	3476	7/7	0.98	0.17	103,103,103,103	7
86	OHX	A5	3477	7/7	0.98	0.16	108,108,108,108	7
86	OHX	A5	3480	7/7	0.98	0.17	101,101,101,101	7
86	OHX	A5	3481	7/7	0.98	0.18	92,92,92,92	7
86	OHX	DB	401	7/7	0.98	0.20	98,98,98,98	7
86	OHX	A5	3482	7/7	0.98	0.22	85,85,85,85	7
86	OHX	A5	3483	7/7	0.98	0.18	103,103,103,103	7
87	MG	A5	4170	1/1	0.98	0.55	69,69,69,69	0
86	OHX	A5	3487	7/7	0.98	0.18	94,94,94,94	7
86	OHX	A1	3509	7/7	0.98	0.18	98,98,98,98	7
86	OHX	A5	3489	7/7	0.98	0.20	88,88,88,88	7
86	OHX	A5	3490	7/7	0.98	0.16	113,113,113,113	7
87	MG	A8	236	1/1	0.98	0.19	75,75,75,75	0
86	OHX	A5	3491	7/7	0.98	0.18	106,106,106,106	7
87	MG	A5	4176	1/1	0.98	0.19	89,89,89,89	0
86	OHX	A1	3510	7/7	0.98	0.22	92,92,92,92	7
86	OHX	A5	3494	7/7	0.98	0.18	97,97,97,97	7
86	OHX	A5	3495	7/7	0.98	0.20	92,92,92,92	7
87	MG	A6	2292	1/1	0.98	0.24	75,75,75,75	0
86	OHX	DO	201	7/7	0.98	0.20	93,93,93,93	7
86	OHX	A5	3496	7/7	0.98	0.20	73,73,73,73	7
86	OHX	A5	3498	7/7	0.98	0.21	89,89,89,89	7
86	OHX	A5	3677	7/7	0.98	0.18	113,113,113,113	7
86	OHX	A5	3499	7/7	0.98	0.20	84,84,84,84	7
86	OHX	De	201	7/7	0.98	0.21	91,91,91,91	7
86	OHX	Df	201	7/7	0.98	0.18	99,99,99,99	7
86	OHX	A5	3500	7/7	0.98	0.18	88,88,88,88	7
86	OHX	Dh	201	7/7	0.98	0.17	129,129,129,129	7
87	MG	A1	3820	1/1	0.98	0.28	47,47,47,47	0
86	OHX	Dj	104	7/7	0.98	0.18	105,105,105,105	7
86	OHX	Do	201	7/7	0.98	0.22	89,89,89,89	7
86	OHX	A5	3501	7/7	0.98	0.17	106,106,106,106	7
86	OHX	A2	1912	7/7	0.98	0.19	115,115,115,115	0
86	OHX	A5	3503	7/7	0.98	0.20	97,97,97,97	7
86	OHX	A5	3504	7/7	0.98	0.18	101,101,101,101	7
87	MG	A1	3827	1/1	0.98	0.28	47,47,47,47	0
86	OHX	A5	3505	7/7	0.98	0.16	94,94,94,94	7
86	OHX	A5	3506	7/7	0.98	0.19	102,102,102,102	7
86	OHX	A5	3507	7/7	0.98	0.20	75,75,75,75	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A5	3508	7/7	0.98	0.17	119,119,119,119	7
86	OHX	A5	3509	7/7	0.98	0.19	97,97,97,97	7
87	MG	A5	3983	1/1	0.98	0.41	47,47,47,47	0
87	MG	DD	306	1/1	0.98	0.42	77,77,77,77	0
87	MG	A5	3984	1/1	0.98	0.47	56,56,56,56	0
86	OHX	A2	1903	7/7	0.98	0.22	94,94,94,94	0
86	OHX	A5	3512	7/7	0.98	0.16	111,111,111,111	7
86	OHX	A1	3513	7/7	0.98	0.18	101,101,101,101	7
86	OHX	A5	3514	7/7	0.98	0.22	90,90,90,90	7
86	OHX	A1	3671	7/7	0.98	0.23	96,96,96,96	7
86	OHX	A5	3516	7/7	0.98	0.20	89,89,89,89	7
86	OHX	A5	3517	7/7	0.98	0.22	80,80,80,80	7
86	OHX	A1	3514	7/7	0.98	0.20	99,99,99,99	7
86	OHX	A5	3519	7/7	0.98	0.23	78,78,78,78	7
86	OHX	A5	3520	7/7	0.98	0.20	113,113,113,113	7
86	OHX	A1	3515	7/7	0.98	0.17	115,115,115,115	7
86	OHX	A1	3516	7/7	0.98	0.19	86,86,86,86	7
86	OHX	A5	3701	7/7	0.98	0.23	57,57,57,57	7
86	OHX	A5	3524	7/7	0.98	0.20	92,92,92,92	7
86	OHX	A5	3525	7/7	0.98	0.18	112,112,112,112	7
86	OHX	A5	3526	7/7	0.98	0.19	85,85,85,85	7
86	OHX	A5	3527	7/7	0.98	0.20	105,105,105,105	7
86	OHX	A2	1978	7/7	0.98	0.18	108,108,108,108	7
86	OHX	A2	2033	7/7	0.98	0.20	97,97,97,97	7
86	OHX	A5	3531	7/7	0.98	0.19	106,106,106,106	7
86	OHX	A2	1936	7/7	0.98	0.21	112,112,112,112	7
87	MG	A2	2119	1/1	0.98	0.26	67,67,67,67	0
86	OHX	A1	3521	7/7	0.98	0.23	84,84,84,84	7
86	OHX	A5	3534	7/7	0.98	0.20	92,92,92,92	7
87	MG	A5	4009	1/1	0.98	0.38	45,45,45,45	0
86	OHX	A1	3523	7/7	0.98	0.17	111,111,111,111	7
87	MG	A1	4064	1/1	0.98	0.29	69,69,69,69	0
87	MG	A5	4012	1/1	0.98	0.42	43,43,43,43	0
86	OHX	A5	3537	7/7	0.98	0.15	115,115,115,115	7
87	MG	A5	4234	1/1	0.98	0.11	67,67,67,67	0
86	OHX	A2	1916	7/7	0.98	0.17	110,110,110,110	7
86	OHX	A5	3539	7/7	0.98	0.19	125,125,125,125	7
86	OHX	BI	301	7/7	0.98	0.20	94,94,94,94	7
86	OHX	A1	3525	7/7	0.98	0.21	101,101,101,101	7
86	OHX	A1	3603	7/7	0.98	0.17	136,136,136,136	7
86	OHX	A2	1981	7/7	0.98	0.14	132,132,132,132	7
86	OHX	BN	301	7/7	0.98	0.19	116,116,116,116	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A5	3545	7/7	0.98	0.17	133,133,133,133	7
86	OHX	A1	3528	7/7	0.98	0.21	81,81,81,81	7
86	OHX	A1	3529	7/7	0.98	0.23	77,77,77,77	7
86	OHX	A2	1957	7/7	0.98	0.18	101,101,101,101	7
86	OHX	Bf	201	7/7	0.98	0.21	85,85,85,85	7
86	OHX	A2	1938	7/7	0.98	0.15	111,111,111,111	7
86	OHX	A2	1917	7/7	0.98	0.16	111,111,111,111	7
86	OHX	A5	3552	7/7	0.98	0.16	138,138,138,138	7
86	OHX	A5	3553	7/7	0.98	0.24	75,75,75,75	7
86	OHX	A5	3554	7/7	0.98	0.20	130,130,130,130	7
86	OHX	A1	3533	7/7	0.98	0.20	104,104,104,104	7
87	MG	A5	4032	1/1	0.98	0.46	41,41,41,41	0
86	OHX	Bo	201	7/7	0.98	0.19	97,97,97,97	7
86	OHX	A6	1909	7/7	0.98	0.19	84,84,84,84	0
87	MG	A1	4500	1/1	0.98	0.26	106,106,106,106	0
87	MG	A6	2150	1/1	0.98	0.41	48,48,48,48	0
86	OHX	A5	3558	7/7	0.98	0.21	85,85,85,85	7
86	OHX	A5	3559	7/7	0.98	0.15	109,109,109,109	7
87	MG	A5	4481	1/1	0.98	0.68	60,60,60,60	0
86	OHX	A6	1919	7/7	0.98	0.17	104,104,104,104	7
86	OHX	A5	3737	7/7	0.98	0.21	75,75,75,75	7
86	OHX	A6	1922	7/7	0.98	0.16	108,108,108,108	0
86	OHX	A6	1925	7/7	0.98	0.16	112,112,112,112	7
86	OHX	A1	3611	7/7	0.98	0.17	96,96,96,96	7
86	OHX	A2	1918	7/7	0.98	0.18	99,99,99,99	7
86	OHX	A6	1930	7/7	0.98	0.17	120,120,120,120	7
87	MG	A6	2160	1/1	0.98	0.44	45,45,45,45	0
86	OHX	A6	1932	7/7	0.98	0.16	109,109,109,109	7
86	OHX	A1	3535	7/7	0.98	0.21	102,102,102,102	7
86	OHX	A2	1941	7/7	0.98	0.17	117,117,117,117	7
86	OHX	A5	3569	7/7	0.98	0.17	110,110,110,110	7
86	OHX	A5	3570	7/7	0.98	0.24	97,97,97,97	7
86	OHX	A6	1935	7/7	0.98	0.17	102,102,102,102	7
86	OHX	A1	3537	7/7	0.98	0.17	119,119,119,119	7
86	OHX	A5	3573	7/7	0.98	0.18	107,107,107,107	7
88	ZN	Af	202	1/1	0.98	0.12	113,113,113,113	0
86	OHX	A2	1942	7/7	0.98	0.17	113,113,113,113	7
86	OHX	A2	1907	7/7	0.98	0.20	104,104,104,104	7
88	ZN	Bp	501	1/1	0.98	0.13	68,68,68,68	0
87	MG	A2	2163	1/1	0.98	0.18	80,80,80,80	0
87	MG	A5	4501	1/1	0.98	0.87	56,56,56,56	0
87	MG	A1	3900	1/1	0.98	0.16	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A1	3442	7/7	0.98	0.19	95,95,95,95	0
86	OHX	A2	1964	7/7	0.98	0.18	135,135,135,135	7
86	OHX	A5	3416	7/7	0.99	0.24	68,68,68,68	0
86	OHX	A5	3417	7/7	0.99	0.26	72,72,72,72	0
86	OHX	A5	3418	7/7	0.99	0.26	77,77,77,77	0
87	MG	A5	3824	1/1	0.99	0.28	37,37,37,37	0
86	OHX	A5	3419	7/7	0.99	0.24	79,79,79,79	0
86	OHX	A5	3420	7/7	0.99	0.23	74,74,74,74	0
86	OHX	A5	3421	7/7	0.99	0.23	81,81,81,81	0
87	MG	A5	4560	1/1	0.99	0.38	108,108,108,108	0
86	OHX	A5	3422	7/7	0.99	0.22	75,75,75,75	0
86	OHX	A5	3423	7/7	0.99	0.23	68,68,68,68	0
86	OHX	A5	3424	7/7	0.99	0.25	86,86,86,86	0
86	OHX	A5	3425	7/7	0.99	0.22	72,72,72,72	0
86	OHX	A5	3426	7/7	0.99	0.19	67,67,67,67	0
86	OHX	A5	3427	7/7	0.99	0.22	79,79,79,79	0
86	OHX	A5	3428	7/7	0.99	0.23	88,88,88,88	0
86	OHX	A5	3429	7/7	0.99	0.23	84,84,84,84	0
86	OHX	A5	3431	7/7	0.99	0.20	83,83,83,83	0
86	OHX	A5	3432	7/7	0.99	0.20	73,73,73,73	0
86	OHX	A5	3433	7/7	0.99	0.20	81,81,81,81	0
86	OHX	A5	3434	7/7	0.99	0.19	85,85,85,85	0
86	OHX	A5	3435	7/7	0.99	0.17	70,70,70,70	0
86	OHX	A5	3436	7/7	0.99	0.19	82,82,82,82	0
86	OHX	A5	3437	7/7	0.99	0.19	83,83,83,83	0
86	OHX	A5	3438	7/7	0.99	0.23	91,91,91,91	0
86	OHX	A5	3439	7/7	0.99	0.19	81,81,81,81	0
86	OHX	A6	1906	7/7	0.99	0.19	85,85,85,85	0
86	OHX	A5	3442	7/7	0.99	0.18	85,85,85,85	0
86	OHX	A5	3443	7/7	0.99	0.18	75,75,75,75	7
86	OHX	A5	3444	7/7	0.99	0.18	74,74,74,74	7
87	MG	A1	3873	1/1	0.99	0.38	62,62,62,62	0
86	OHX	A5	3445	7/7	0.99	0.19	73,73,73,73	0
86	OHX	A6	1907	7/7	0.99	0.22	91,91,91,91	0
86	OHX	A6	1908	7/7	0.99	0.22	101,101,101,101	0
86	OHX	A5	3448	7/7	0.99	0.19	93,93,93,93	0
86	OHX	A5	3449	7/7	0.99	0.19	85,85,85,85	7
86	OHX	A5	3451	7/7	0.99	0.18	81,81,81,81	7
86	OHX	A5	3452	7/7	0.99	0.21	86,86,86,86	7
86	OHX	A5	3453	7/7	0.99	0.18	102,102,102,102	0
87	MG	A1	4417	1/1	0.99	0.34	94,94,94,94	0
86	OHX	A5	3454	7/7	0.99	0.18	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A1	3495	7/7	0.99	0.18	101,101,101,101	7
87	MG	A1	4061	1/1	0.99	0.26	35,35,35,35	0
86	OHX	A6	1910	7/7	0.99	0.17	84,84,84,84	0
86	OHX	A5	3457	7/7	0.99	0.17	86,86,86,86	7
86	OHX	A5	3458	7/7	0.99	0.19	91,91,91,91	0
86	OHX	A6	1911	7/7	0.99	0.21	100,100,100,100	0
86	OHX	A5	3460	7/7	0.99	0.19	80,80,80,80	7
86	OHX	A5	3461	7/7	0.99	0.21	82,82,82,82	7
86	OHX	A6	1912	7/7	0.99	0.18	96,96,96,96	0
86	OHX	A6	1913	7/7	0.99	0.17	91,91,91,91	0
86	OHX	A6	1914	7/7	0.99	0.17	111,111,111,111	0
86	OHX	A6	1915	7/7	0.99	0.19	87,87,87,87	7
86	OHX	A5	3466	7/7	0.99	0.20	120,120,120,120	0
86	OHX	A6	1916	7/7	0.99	0.21	87,87,87,87	7
86	OHX	A5	3468	7/7	0.99	0.20	75,75,75,75	7
86	OHX	A5	3469	7/7	0.99	0.17	107,107,107,107	7
86	OHX	A5	3470	7/7	0.99	0.15	118,118,118,118	0
86	OHX	A5	3471	7/7	0.99	0.17	90,90,90,90	7
86	OHX	A6	1917	7/7	0.99	0.19	100,100,100,100	7
86	OHX	A5	3807	7/7	0.99	0.21	107,107,107,107	7
86	OHX	A5	3473	7/7	0.99	0.20	82,82,82,82	7
86	OHX	A5	3474	7/7	0.99	0.20	81,81,81,81	7
86	OHX	A5	3475	7/7	0.99	0.18	95,95,95,95	7
86	OHX	A6	1918	7/7	0.99	0.18	100,100,100,100	0
86	OHX	A1	3567	7/7	0.99	0.19	88,88,88,88	7
87	MG	A6	2248	1/1	0.99	0.15	75,75,75,75	0
86	OHX	A5	3478	7/7	0.99	0.21	76,76,76,76	7
86	OHX	A5	3479	7/7	0.99	0.17	110,110,110,110	0
86	OHX	A6	1920	7/7	0.99	0.19	87,87,87,87	7
86	OHX	A6	1921	7/7	0.99	0.19	92,92,92,92	7
86	OHX	A1	3496	7/7	0.99	0.20	97,97,97,97	7
86	OHX	A6	1923	7/7	0.99	0.18	76,76,76,76	7
86	OHX	A5	3484	7/7	0.99	0.17	99,99,99,99	7
86	OHX	A5	3485	7/7	0.99	0.18	85,85,85,85	7
86	OHX	A5	3486	7/7	0.99	0.17	75,75,75,75	7
86	OHX	A6	1924	7/7	0.99	0.17	83,83,83,83	7
86	OHX	A1	3426	7/7	0.99	0.22	73,73,73,73	0
86	OHX	A7	201	7/7	0.99	0.20	107,107,107,107	0
86	OHX	A6	1926	7/7	0.99	0.19	82,82,82,82	7
86	OHX	A1	3428	7/7	0.99	0.20	87,87,87,87	0
86	OHX	A7	204	7/7	0.99	0.21	75,75,75,75	7
86	OHX	A7	205	7/7	0.99	0.19	106,106,106,106	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	A6	1928	7/7	0.99	0.20	73,73,73,73	7
86	OHX	A5	3492	7/7	0.99	0.21	89,89,89,89	7
86	OHX	A1	3499	7/7	0.99	0.19	83,83,83,83	7
86	OHX	A1	3429	7/7	0.99	0.20	87,87,87,87	0
86	OHX	A6	1931	7/7	0.99	0.18	84,84,84,84	7
86	OHX	A1	3432	7/7	0.99	0.20	90,90,90,90	0
86	OHX	A5	3497	7/7	0.99	0.17	81,81,81,81	7
86	OHX	A1	3433	7/7	0.99	0.19	85,85,85,85	0
86	OHX	A8	202	7/7	0.99	0.23	77,77,77,77	0
86	OHX	A1	3435	7/7	0.99	0.18	85,85,85,85	0
86	OHX	A1	3437	7/7	0.99	0.21	74,74,74,74	7
86	OHX	A1	3438	7/7	0.99	0.19	91,91,91,91	7
87	MG	A1	3935	1/1	0.99	0.44	59,59,59,59	0
86	OHX	A6	1937	7/7	0.99	0.18	96,96,96,96	7
86	OHX	A6	1938	7/7	0.99	0.20	96,96,96,96	7
86	OHX	A1	3439	7/7	0.99	0.19	81,81,81,81	7
86	OHX	A1	3507	7/7	0.99	0.19	75,75,75,75	7
86	OHX	A1	3440	7/7	0.99	0.17	86,86,86,86	0
86	OHX	A1	3441	7/7	0.99	0.18	93,93,93,93	0
86	OHX	A2	1920	7/7	0.99	0.16	115,115,115,115	7
86	OHX	A1	3443	7/7	0.99	0.19	76,76,76,76	0
86	OHX	A6	1945	7/7	0.99	0.13	148,148,148,148	0
86	OHX	A5	3511	7/7	0.99	0.15	142,142,142,142	0
86	OHX	A6	1946	7/7	0.99	0.17	105,105,105,105	7
86	OHX	A1	3444	7/7	0.99	0.18	84,84,84,84	0
87	MG	A2	2235	1/1	0.99	0.20	80,80,80,80	0
86	OHX	A1	3445	7/7	0.99	0.17	81,81,81,81	0
86	OHX	A1	3446	7/7	0.99	0.20	79,79,79,79	7
86	OHX	A2	1902	7/7	0.99	0.20	102,102,102,102	0
86	OHX	A1	3448	7/7	0.99	0.18	85,85,85,85	7
86	OHX	A1	3517	7/7	0.99	0.15	99,99,99,99	7
86	OHX	A1	3449	7/7	0.99	0.19	99,99,99,99	0
86	OHX	A1	3591	7/7	0.99	0.18	95,95,95,95	7
86	OHX	A1	3450	7/7	0.99	0.19	95,95,95,95	0
86	OHX	A1	3451	7/7	0.99	0.17	105,105,105,105	0
87	MG	A1	4314	1/1	0.99	0.21	78,78,78,78	0
86	OHX	A5	3523	7/7	0.99	0.21	79,79,79,79	7
86	OHX	A1	3452	7/7	0.99	0.17	81,81,81,81	7
86	OHX	A1	3522	7/7	0.99	0.25	79,79,79,79	7
86	OHX	A2	1922	7/7	0.99	0.17	99,99,99,99	7
86	OHX	A2	1923	7/7	0.99	0.16	110,110,110,110	7
86	OHX	A1	3455	7/7	0.99	0.17	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A1	3526	7/7	0.99	0.17	126,126,126,126	7
86	OHX	A5	3530	7/7	0.99	0.17	105,105,105,105	7
86	OHX	A3	204	7/7	0.99	0.16	125,125,125,125	7
86	OHX	A1	3456	7/7	0.99	0.18	100,100,100,100	7
86	OHX	A1	3457	7/7	0.99	0.18	97,97,97,97	7
86	OHX	Db	101	7/7	0.99	0.20	86,86,86,86	0
86	OHX	A2	1924	7/7	0.99	0.17	111,111,111,111	7
86	OHX	A5	3535	7/7	0.99	0.19	77,77,77,77	7
86	OHX	A2	1925	7/7	0.99	0.12	138,138,138,138	0
86	OHX	A2	1926	7/7	0.99	0.14	112,112,112,112	7
86	OHX	A1	3461	7/7	0.99	0.17	104,104,104,104	0
86	OHX	A2	1913	7/7	0.99	0.18	129,129,129,129	0
86	OHX	A2	1914	7/7	0.99	0.17	92,92,92,92	7
86	OHX	A1	3464	7/7	0.99	0.19	88,88,88,88	7
86	OHX	A4	201	7/7	0.99	0.25	77,77,77,77	0
86	OHX	A4	202	7/7	0.99	0.22	80,80,80,80	0
86	OHX	A1	3465	7/7	0.99	0.18	94,94,94,94	7
86	OHX	A1	3466	7/7	0.99	0.18	90,90,90,90	7
86	OHX	A1	3467	7/7	0.99	0.18	91,91,91,91	7
86	OHX	A1	3468	7/7	0.99	0.20	74,74,74,74	7
86	OHX	A2	1929	7/7	0.99	0.19	90,90,90,90	7
86	OHX	A2	1901	7/7	0.99	0.22	95,95,95,95	0
86	OHX	A2	1904	7/7	0.99	0.17	99,99,99,99	0
86	OHX	A2	1910	7/7	0.99	0.18	104,104,104,104	0
86	OHX	A2	1906	7/7	0.99	0.18	98,98,98,98	0
86	OHX	A1	3474	7/7	0.99	0.18	92,92,92,92	7
87	MG	A2	2102	1/1	0.99	0.33	60,60,60,60	0
86	OHX	A2	1919	7/7	0.99	0.17	106,106,106,106	7
86	OHX	A1	3408	7/7	0.99	0.26	66,66,66,66	0
86	OHX	A1	3412	7/7	0.99	0.25	76,76,76,76	0
86	OHX	A1	3414	7/7	0.99	0.24	77,77,77,77	0
86	OHX	A1	3416	7/7	0.99	0.21	73,73,73,73	0
86	OHX	A1	3480	7/7	0.99	0.21	96,96,96,96	7
86	OHX	A1	3481	7/7	0.99	0.18	97,97,97,97	7
86	OHX	A1	3417	7/7	0.99	0.24	82,82,82,82	0
86	OHX	A1	3418	7/7	0.99	0.20	81,81,81,81	0
86	OHX	A1	3419	7/7	0.99	0.20	76,76,76,76	0
86	OHX	A1	3775	7/7	0.99	0.24	69,69,69,69	7
86	OHX	A1	3485	7/7	0.99	0.16	113,113,113,113	7
86	OHX	A1	3486	7/7	0.99	0.15	92,92,92,92	7
86	OHX	BO	201	7/7	0.99	0.18	97,97,97,97	7
86	OHX	A1	3421	7/7	0.99	0.21	80,80,80,80	0

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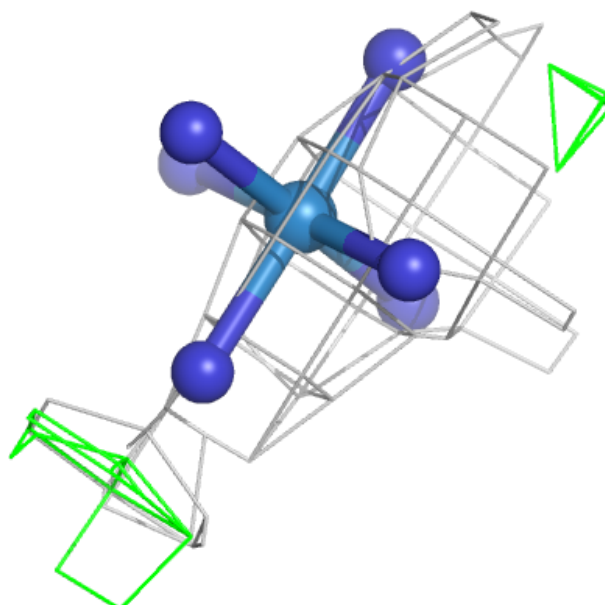
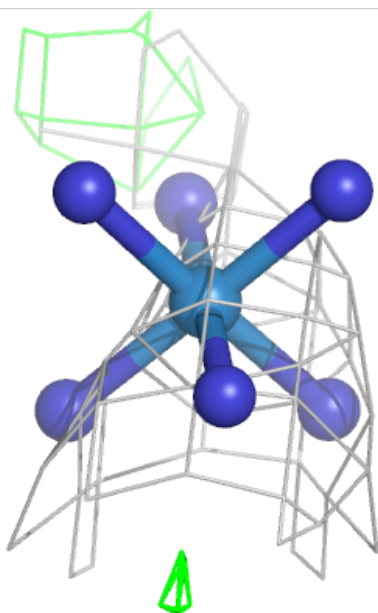
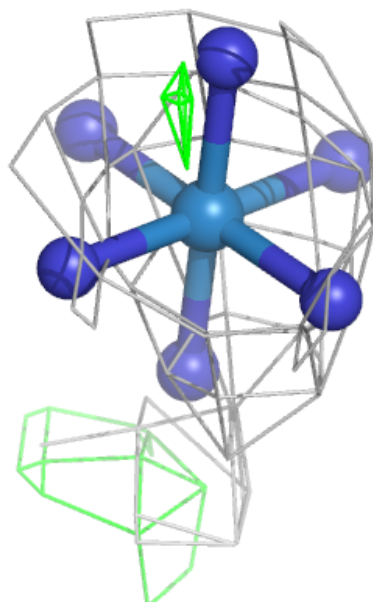
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	A1	3488	7/7	0.99	0.18	109,109,109,109	7
86	OHX	A1	3422	7/7	0.99	0.20	78,78,78,78	0
86	OHX	BT	201	7/7	0.99	0.21	78,78,78,78	0
86	OHX	Bb	101	7/7	0.99	0.20	77,77,77,77	0
86	OHX	A1	3423	7/7	0.99	0.18	75,75,75,75	0
86	OHX	A1	3491	7/7	0.99	0.19	90,90,90,90	7
86	OHX	A1	3492	7/7	0.99	0.16	98,98,98,98	7
86	OHX	A1	3424	7/7	0.99	0.18	81,81,81,81	0
86	OHX	A1	3425	7/7	0.99	0.20	85,85,85,85	0
86	OHX	A6	1901	7/7	0.99	0.24	78,78,78,78	0
88	ZN	Bj	111	1/1	0.99	0.17	44,44,44,44	0
86	OHX	A6	1902	7/7	0.99	0.25	90,90,90,90	0
86	OHX	A6	1903	7/7	0.99	0.22	84,84,84,84	0
86	OHX	A6	1904	7/7	0.99	0.23	88,88,88,88	0
88	ZN	Ca	202	1/1	0.99	0.12	73,73,73,73	0
86	OHX	A6	1905	7/7	0.99	0.20	88,88,88,88	0
86	OHX	A5	3413	7/7	0.99	0.30	71,71,71,71	0
86	OHX	A5	3414	7/7	0.99	0.27	69,69,69,69	0
88	ZN	Dj	105	1/1	0.99	0.17	48,48,48,48	0
87	MG	A1	4379	1/1	0.99	0.21	70,70,70,70	0
86	OHX	A5	3415	7/7	0.99	0.24	67,67,67,67	0
86	OHX	A1	3415	7/7	1.00	0.19	68,68,68,68	0
86	OHX	A1	3410	7/7	1.00	0.25	68,68,68,68	0
86	OHX	A1	3434	7/7	1.00	0.17	72,72,72,72	7
86	OHX	A1	3411	7/7	1.00	0.24	71,71,71,71	0
86	OHX	A1	3436	7/7	1.00	0.18	69,69,69,69	7
86	OHX	A5	3450	7/7	1.00	0.18	76,76,76,76	7
86	OHX	A2	1905	7/7	1.00	0.19	88,88,88,88	0
86	OHX	A1	3413	7/7	1.00	0.26	75,75,75,75	0
86	OHX	A1	3427	7/7	1.00	0.19	86,86,86,86	0
86	OHX	A1	3420	7/7	1.00	0.19	69,69,69,69	0
86	OHX	A5	3440	7/7	1.00	0.21	63,63,63,63	7
86	OHX	A1	3409	7/7	1.00	0.26	70,70,70,70	0
86	OHX	A1	3430	7/7	1.00	0.20	93,93,93,93	0
88	ZN	Dm	202	1/1	1.00	0.19	41,41,41,41	0
86	OHX	A1	3431	7/7	1.00	0.18	89,89,89,89	0
86	OHX	A5	3430	7/7	1.00	0.18	80,80,80,80	0

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

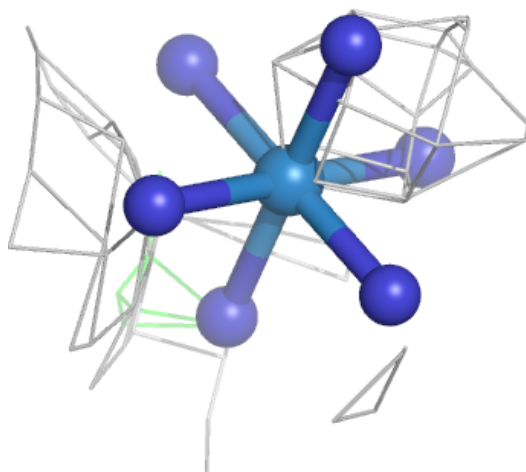
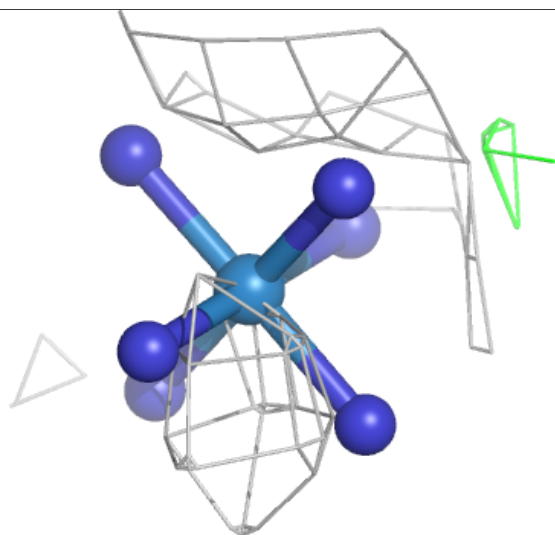
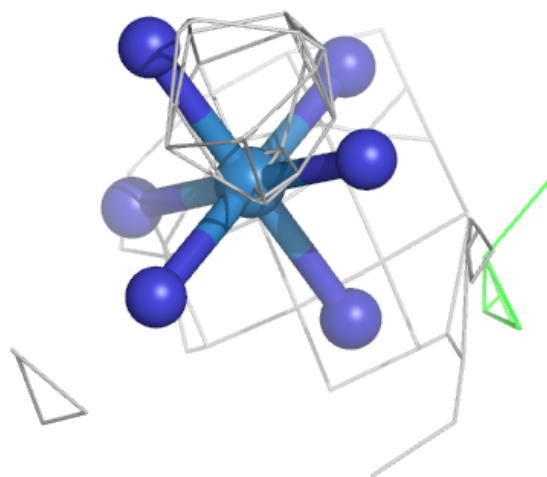
Electron density around OHX A6 2095:

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



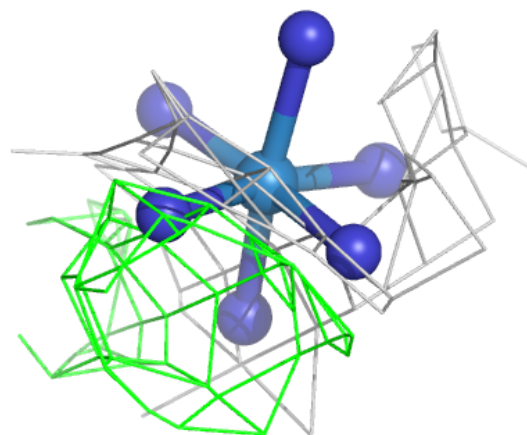
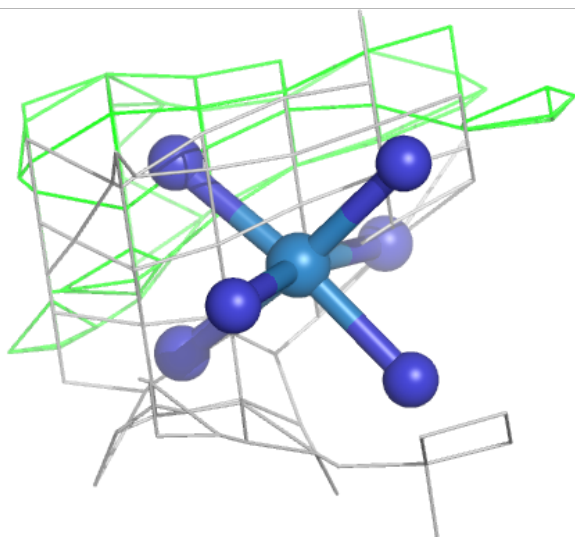
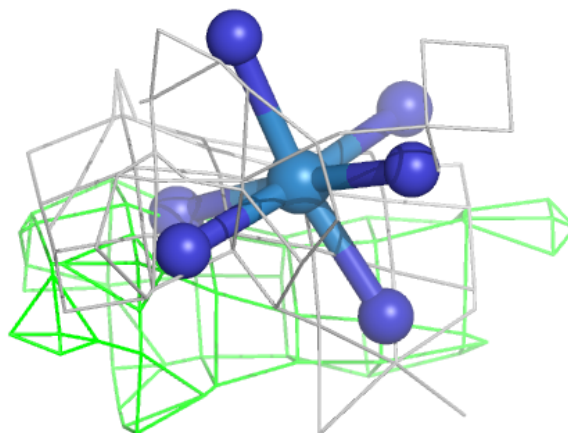
Electron density around OHX A6 2083:

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



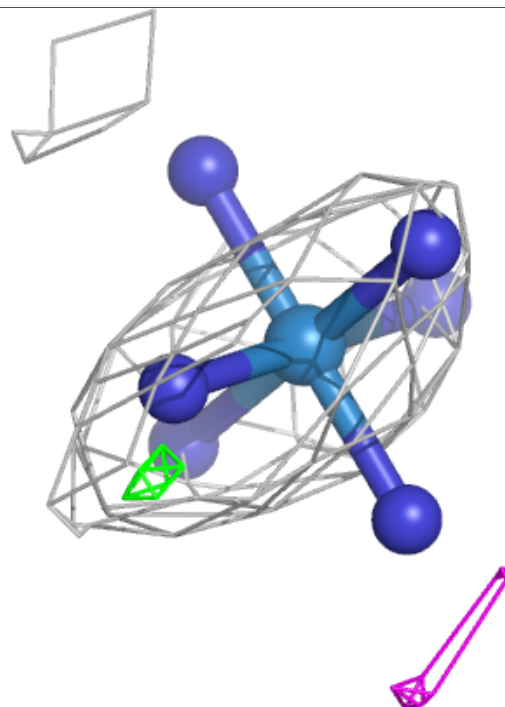
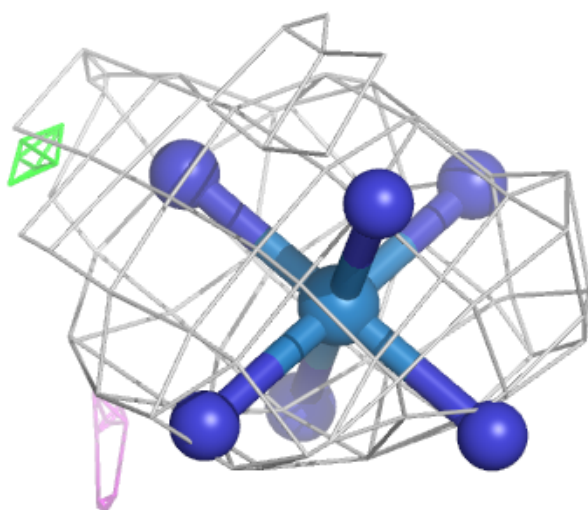
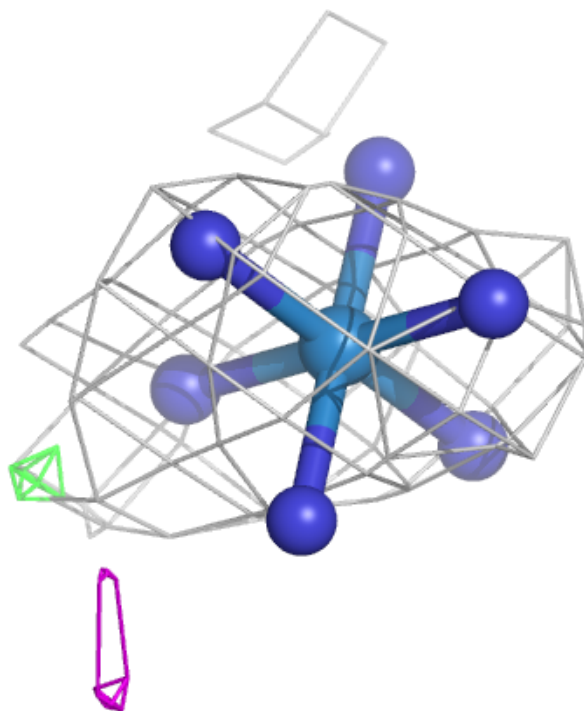
Electron density around OHX BI 303:

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



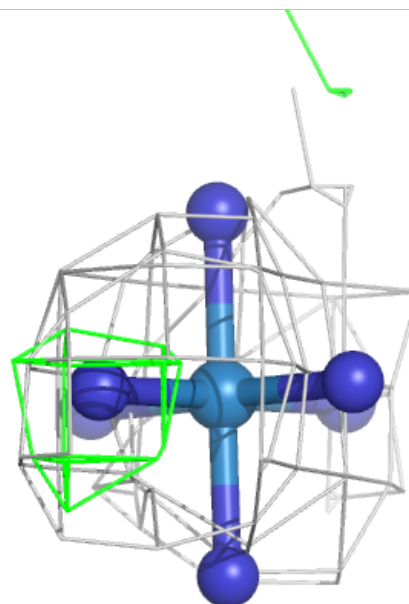
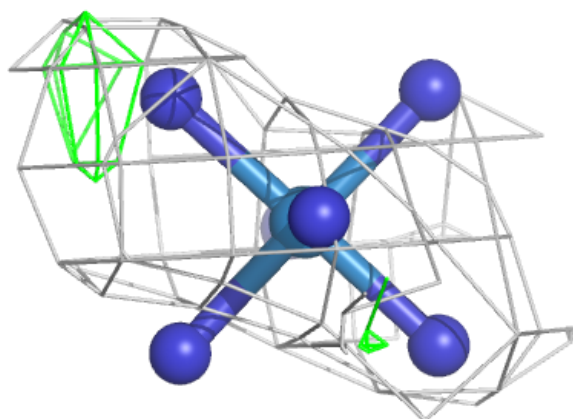
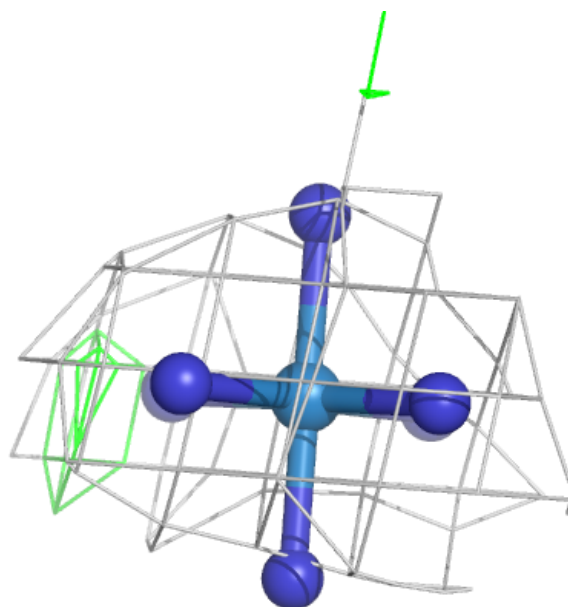
Electron density around OHX A1 3779:

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



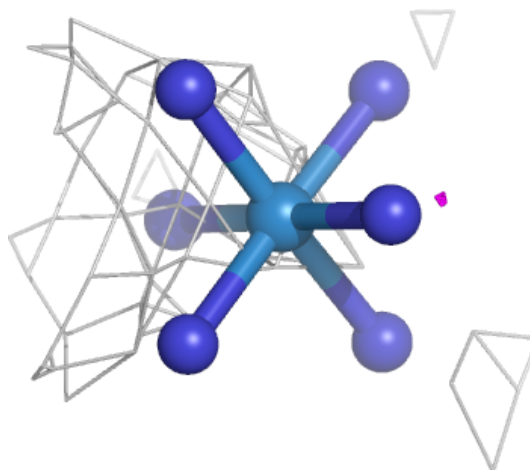
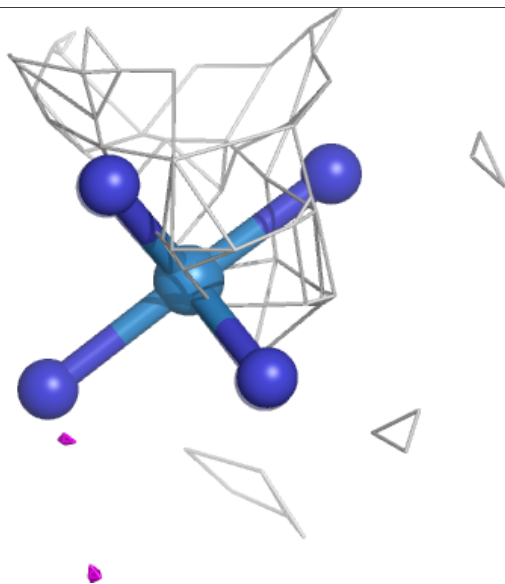
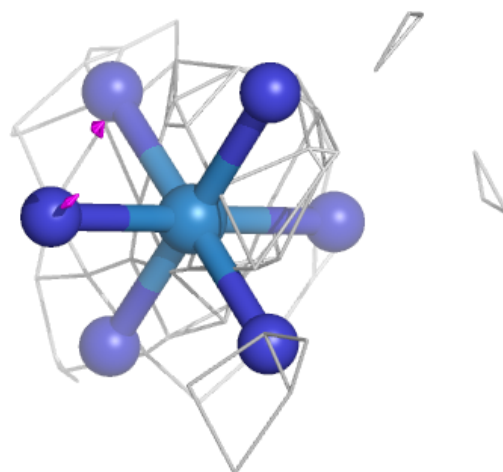
Electron density around OHX A5 3792:

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



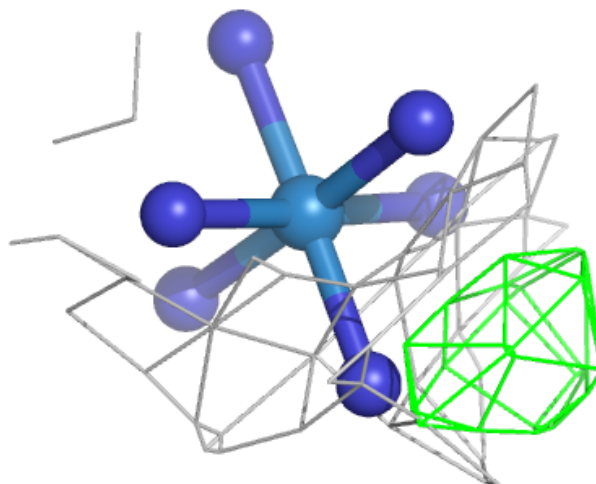
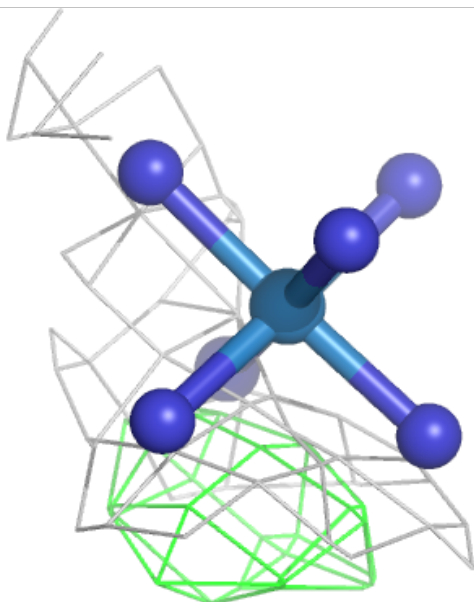
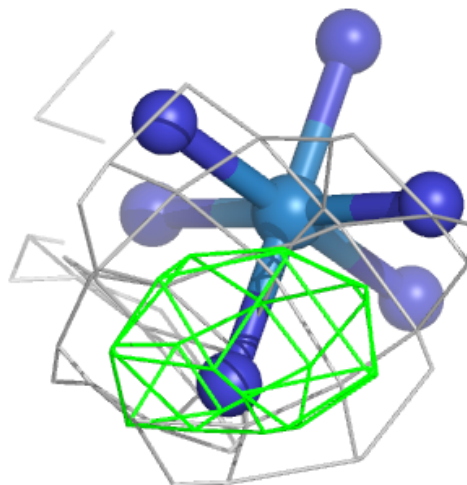
Electron density around OHX A1 3814:

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



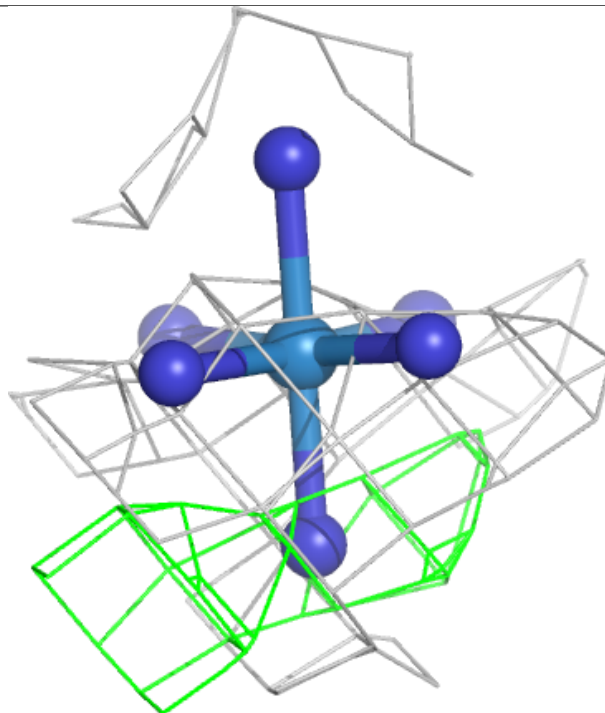
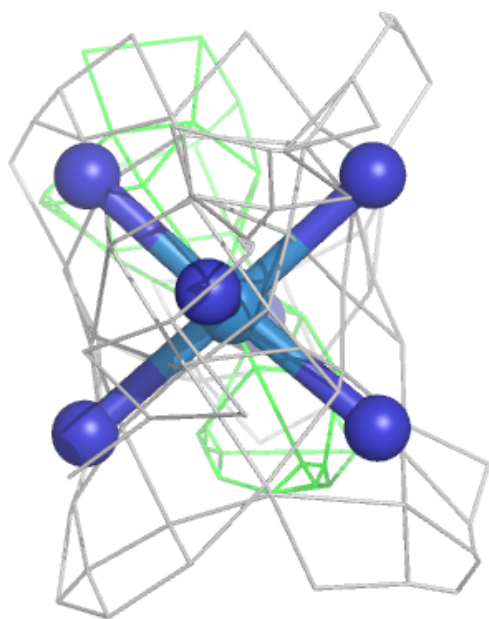
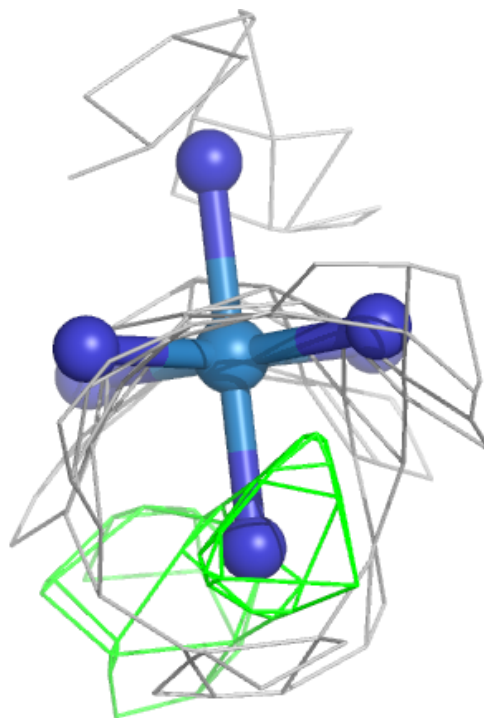
Electron density around OHX A5 3819:

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



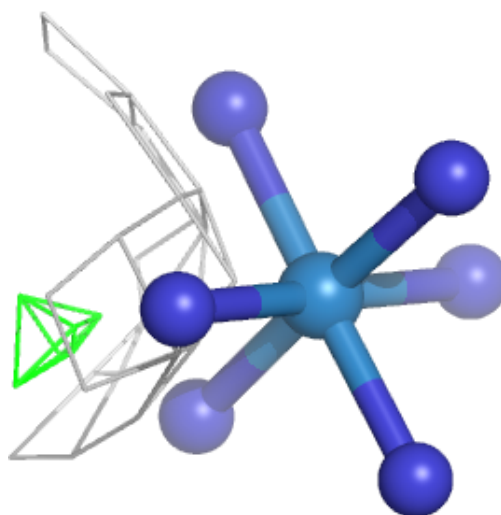
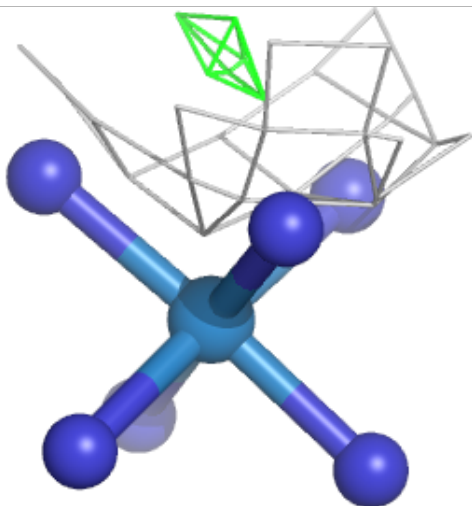
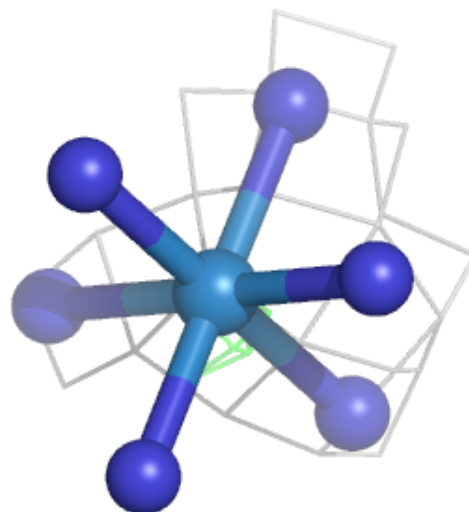
Electron density around OHX A1 3805:

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



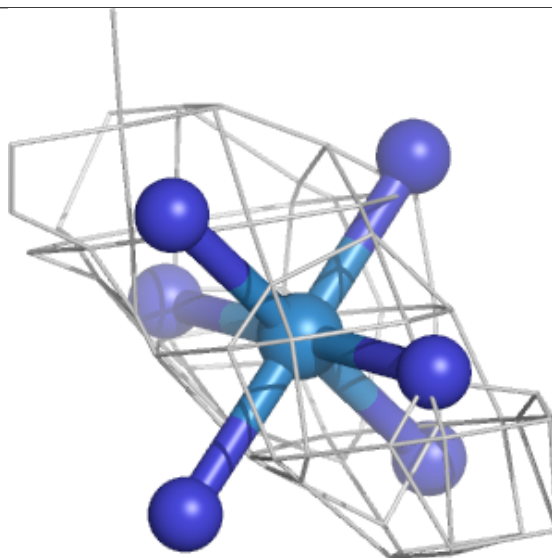
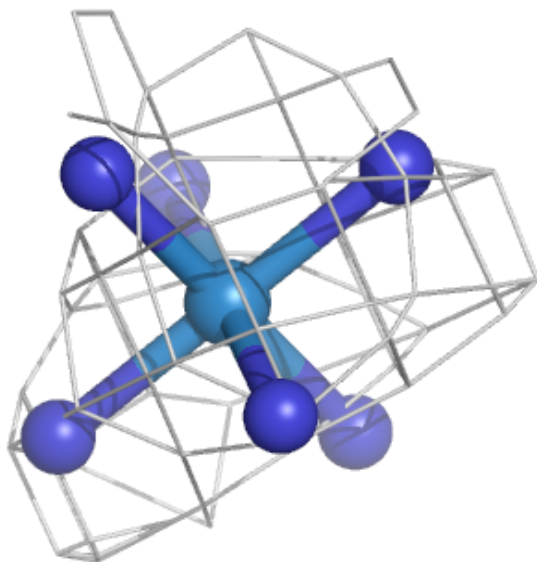
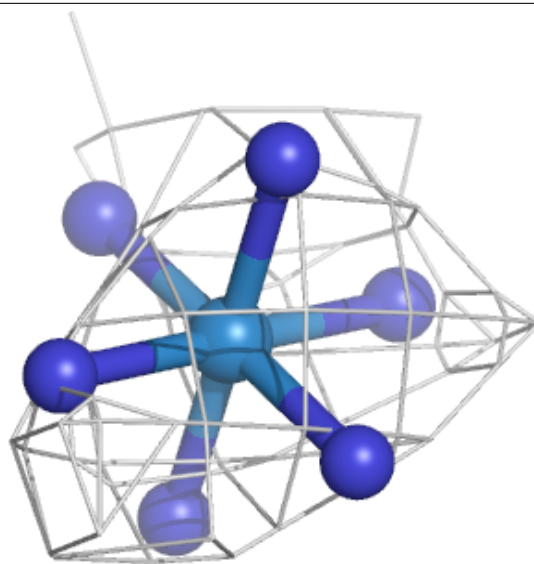
Electron density around OHX A1 3753:

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



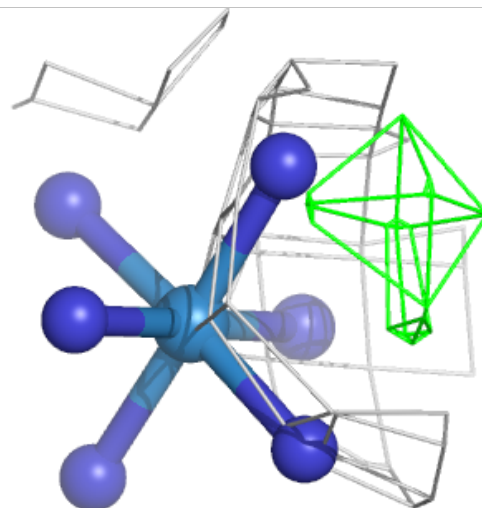
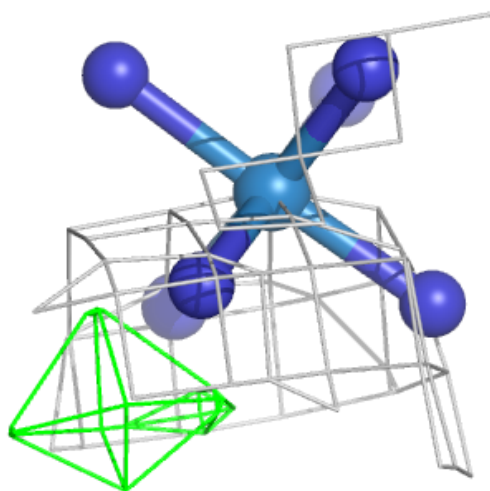
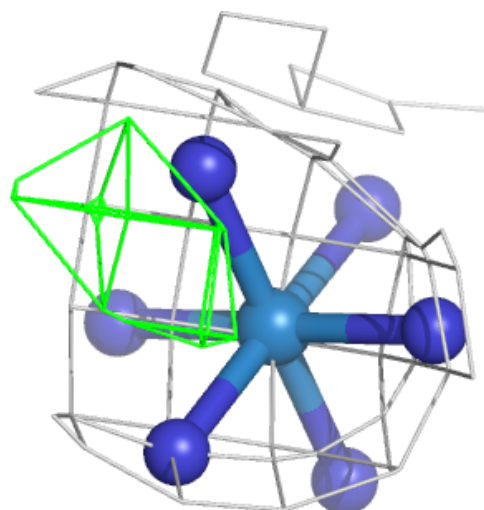
Electron density around OHX A1 3815:

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



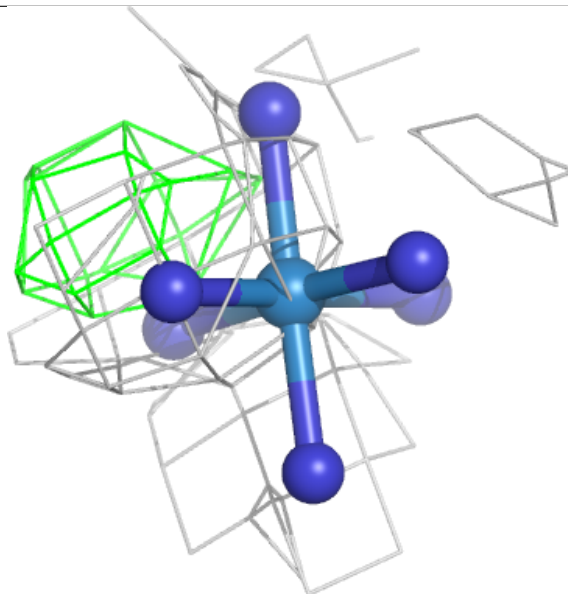
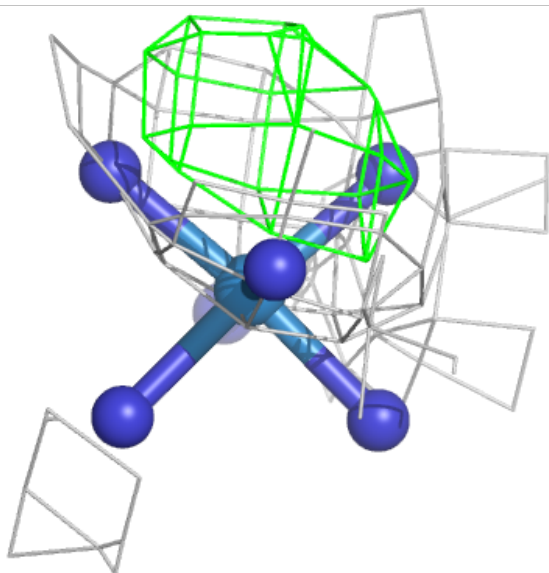
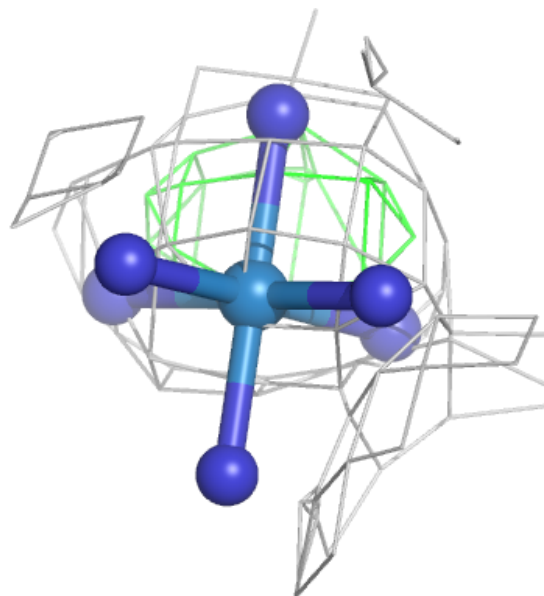
Electron density around OHX A8 218:

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



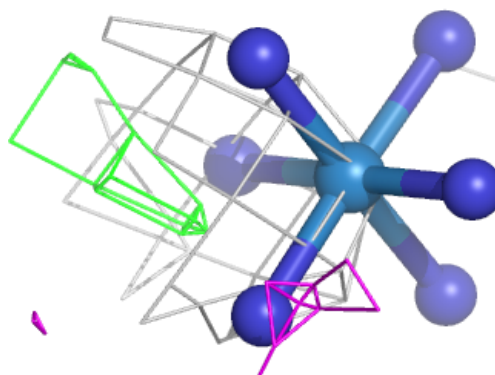
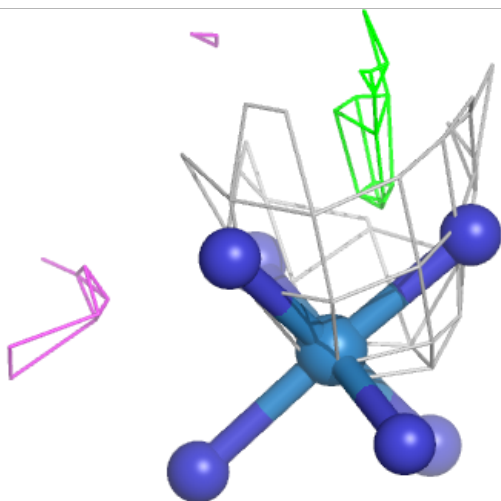
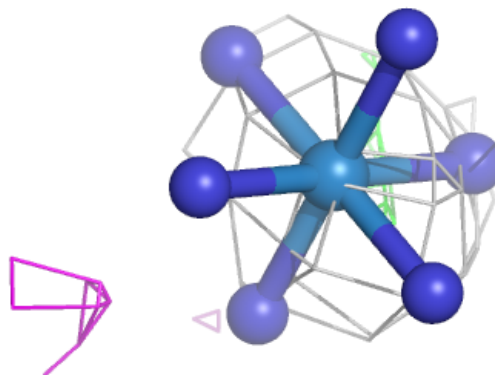
Electron density around OHX A6 2090:

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



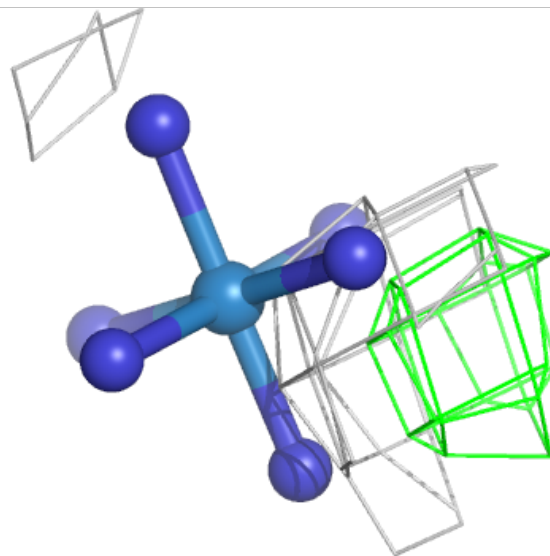
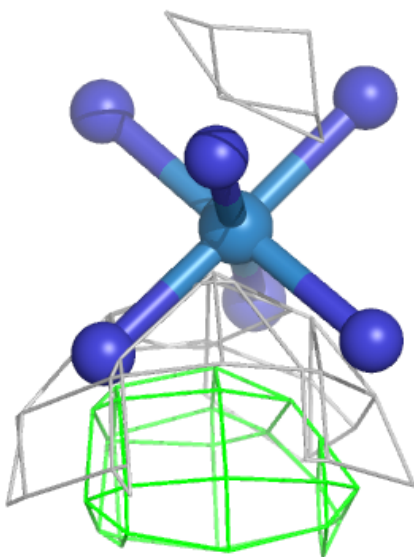
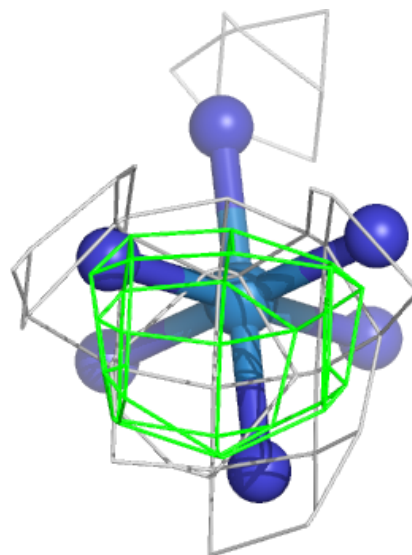
Electron density around OHX A5 3768:

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



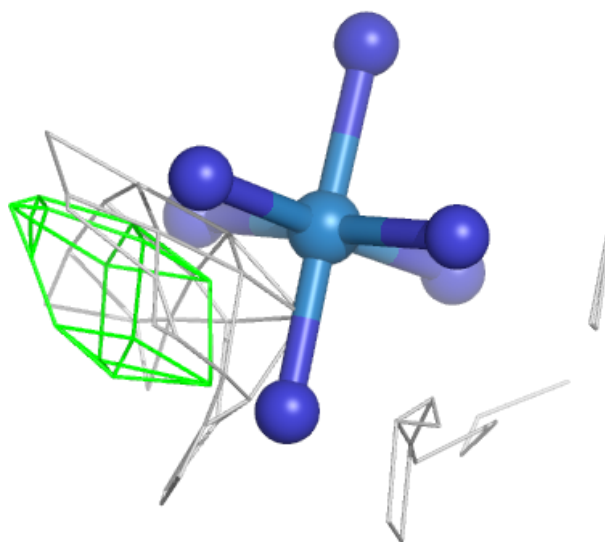
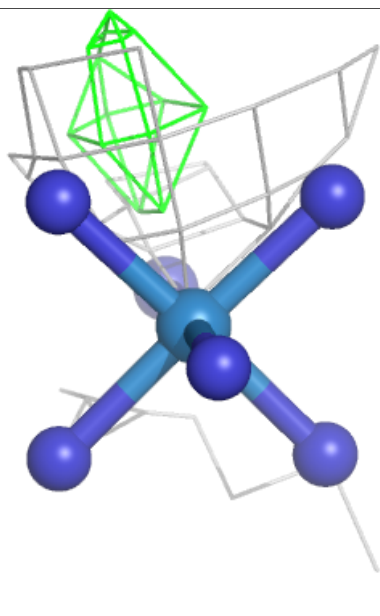
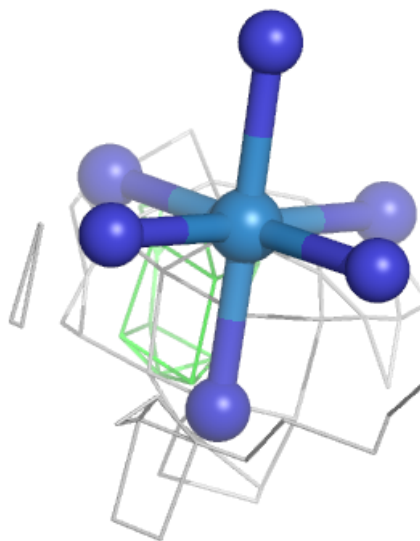
Electron density around OHX CP 202:

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



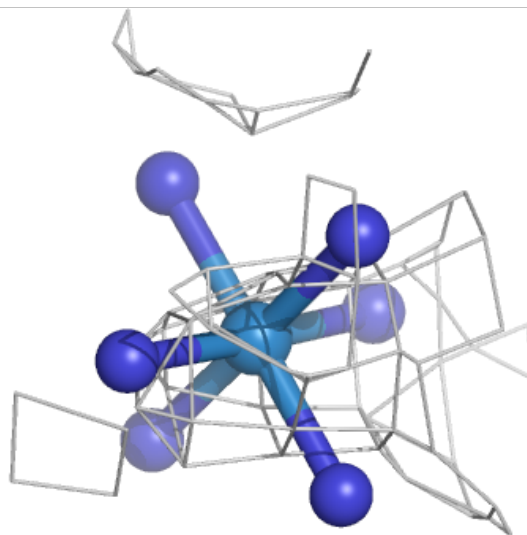
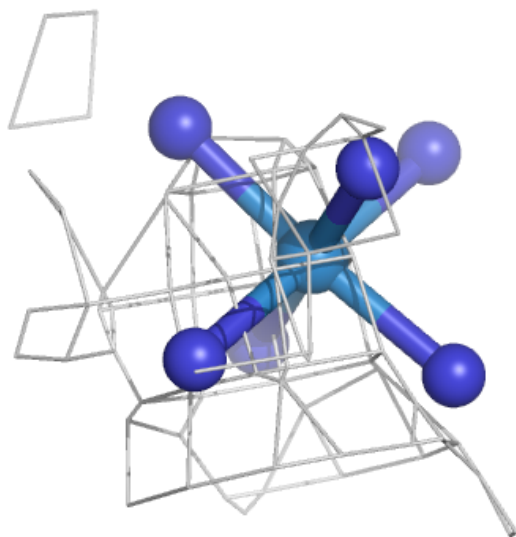
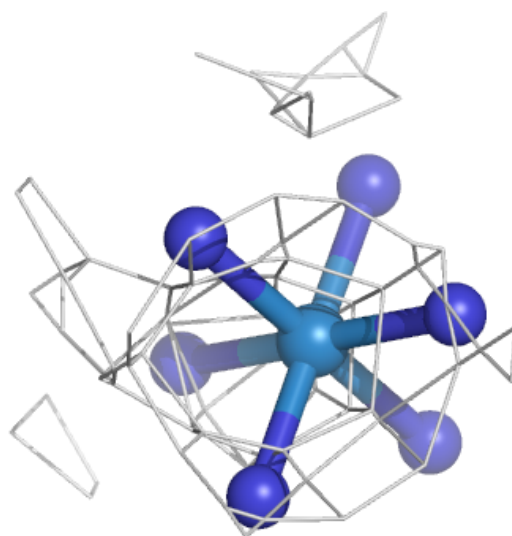
Electron density around OHX A6 2086:

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



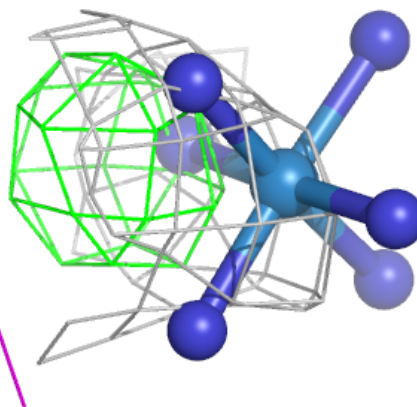
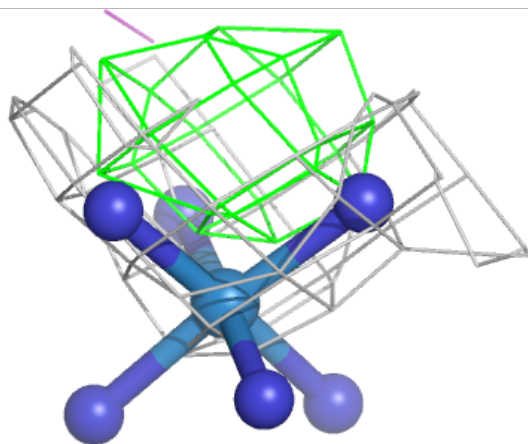
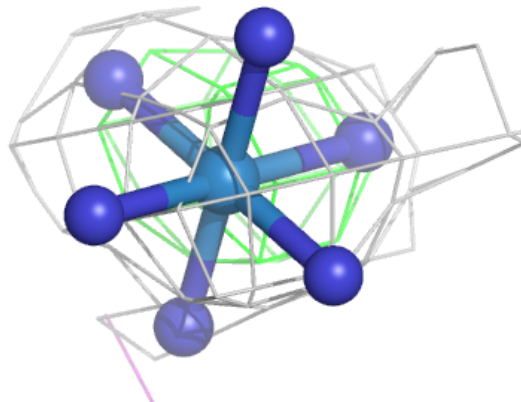
Electron density around OHX A2 2051:

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



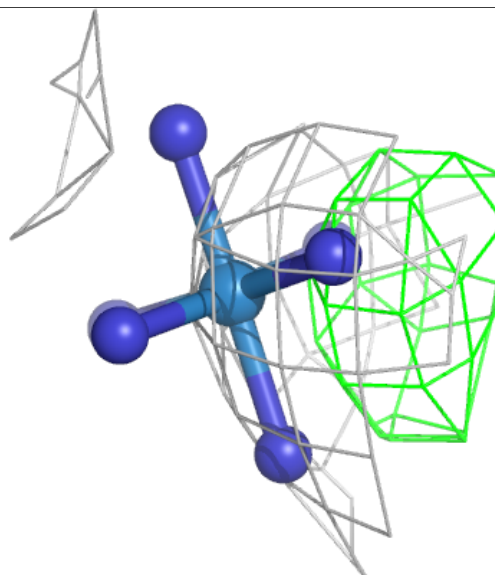
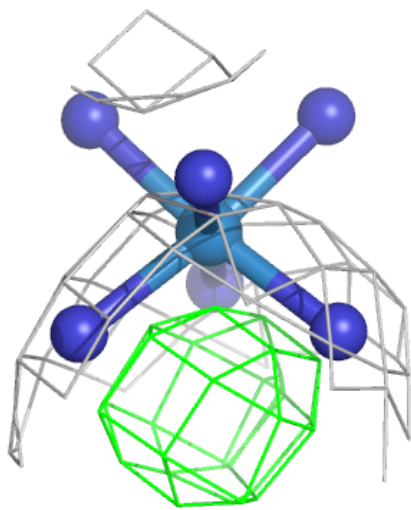
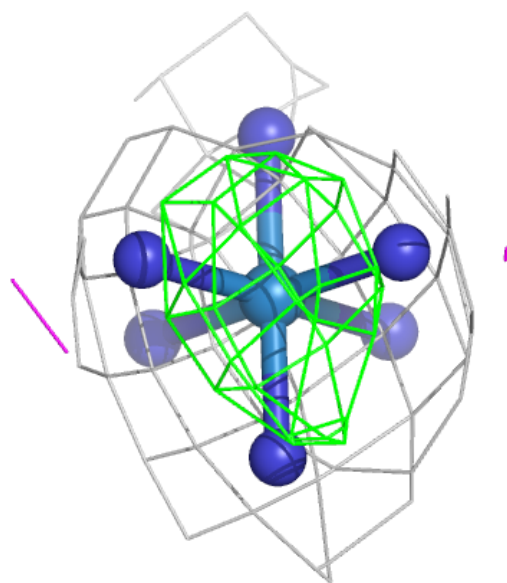
Electron density around OHX A5 3810:

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



Electron density around OHX A5 3780:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.