



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2017 – 03:16 PM EDT

PDB ID : 4W2E
Title : Crystal structure of Elongation Factor 4 (EF4/LepA) bound to the *Thermus thermophilus* 70S ribosome
Authors : Gagnon, M.G.; Lin, J.; Steitz, T.A.
Deposited on : unknown
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

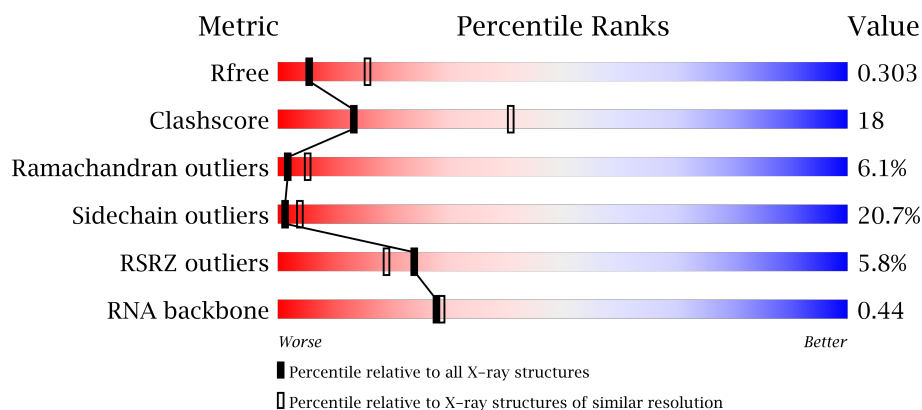
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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






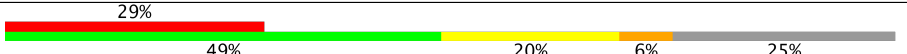

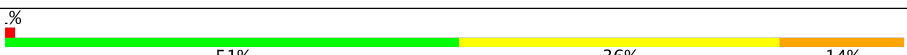

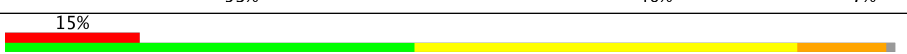


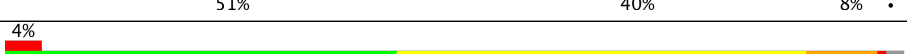
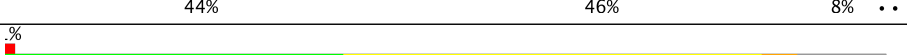
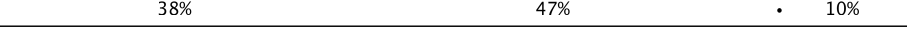




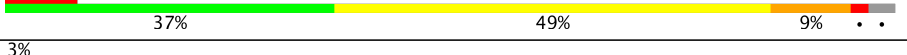
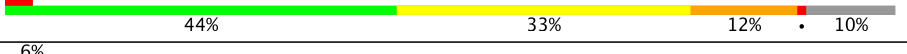

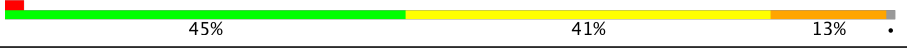
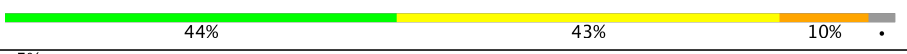

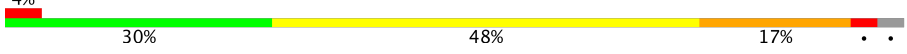

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	2915	<div> <div>3%</div> <div>34% 42% 20% . .</div> </div>
2	B	122	<div> <div>52% 39% 5% . .</div> </div>
3	D	276	<div> <div>0% 37% 49% 12% .</div> </div>
4	E	206	<div> <div>2%</div> <div>50% 38% 9% . .</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	205	
6	G	182	
7	H	180	
8	J	173	
9	K	147	
10	N	140	
11	O	122	
12	P	150	
13	Q	141	
14	R	118	
15	S	112	
16	T	146	
17	U	118	
18	V	101	
19	W	113	
20	X	96	
21	Y	110	
22	Z	206	
23	0	85	
24	1	98	
25	2	72	
26	3	60	
27	4	71	
28	5	60	
29	6	54	

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Mol	Chain	Length	Quality of chain
30	7	49	
31	8	65	
32	9	37	
33	x	76	
34	a	1521	
35	b	256	
36	c	239	
37	d	209	
38	e	162	
39	f	101	
40	g	156	
41	h	138	
42	i	128	
43	j	105	
44	k	129	
45	l	132	
46	m	126	
47	n	61	
48	o	89	
49	p	88	
50	q	105	
51	r	88	
52	s	93	
53	t	106	
54	u	27	

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Mol	Chain	Length	Quality of chain
55	w	76	
56	v	18	
57	y	679	

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
58	MG	6	101	-	-	-	X
58	MG	7	101	-	-	-	X
58	MG	7	102	-	-	-	X
58	MG	A	3002	-	-	-	X
58	MG	A	3004	-	-	-	X
58	MG	A	3005	-	-	-	X
58	MG	A	3006	-	-	-	X
58	MG	A	3008	-	-	-	X
58	MG	A	3011	-	-	-	X
58	MG	A	3021	-	-	-	X
58	MG	A	3022	-	-	-	X
58	MG	A	3023	-	-	-	X
58	MG	A	3027	-	-	-	X
58	MG	A	3032	-	-	-	X
58	MG	A	3033	-	-	-	X
58	MG	A	3034	-	-	-	X
58	MG	A	3039	-	-	-	X
58	MG	A	3041	-	-	-	X
58	MG	A	3045	-	-	-	X
58	MG	A	3047	-	-	-	X
58	MG	A	3048	-	-	-	X
58	MG	A	3056	-	-	-	X
58	MG	A	3059	-	-	-	X
58	MG	A	3072	-	-	-	X
58	MG	A	3079	-	-	-	X
58	MG	A	3080	-	-	-	X
58	MG	A	3086	-	-	-	X
58	MG	A	3093	-	-	-	X
58	MG	A	3095	-	-	-	X
58	MG	A	3107	-	-	-	X
58	MG	A	3109	-	-	-	X
58	MG	A	3114	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	A	3117	-	-	-	X
58	MG	A	3118	-	-	-	X
58	MG	A	3119	-	-	-	X
58	MG	A	3120	-	-	-	X
58	MG	A	3125	-	-	-	X
58	MG	A	3141	-	-	-	X
58	MG	A	3143	-	-	-	X
58	MG	A	3144	-	-	-	X
58	MG	A	3147	-	-	-	X
58	MG	A	3155	-	-	-	X
58	MG	A	3157	-	-	-	X
58	MG	A	3164	-	-	-	X
58	MG	A	3165	-	-	-	X
58	MG	A	3166	-	-	-	X
58	MG	A	3167	-	-	-	X
58	MG	A	3170	-	-	-	X
58	MG	A	3171	-	-	-	X
58	MG	A	3174	-	-	-	X
58	MG	A	3184	-	-	-	X
58	MG	A	3187	-	-	-	X
58	MG	A	3188	-	-	-	X
58	MG	A	3189	-	-	-	X
58	MG	A	3190	-	-	-	X
58	MG	A	3191	-	-	-	X
58	MG	A	3192	-	-	-	X
58	MG	A	3200	-	-	-	X
58	MG	A	3201	-	-	-	X
58	MG	A	3207	-	-	-	X
58	MG	A	3208	-	-	-	X
58	MG	A	3209	-	-	-	X
58	MG	A	3214	-	-	-	X
58	MG	A	3222	-	-	-	X
58	MG	A	3223	-	-	-	X
58	MG	A	3225	-	-	-	X
58	MG	A	3230	-	-	-	X
58	MG	A	3231	-	-	-	X
58	MG	A	3234	-	-	-	X
58	MG	A	3239	-	-	-	X
58	MG	A	3244	-	-	-	X
58	MG	A	3252	-	-	-	X
58	MG	A	3274	-	-	-	X
58	MG	A	3293	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	A	3295	-	-	-	X
58	MG	A	3297	-	-	-	X
58	MG	A	3311	-	-	-	X
58	MG	A	3313	-	-	-	X
58	MG	A	3316	-	-	-	X
58	MG	A	3319	-	-	-	X
58	MG	A	3324	-	-	-	X
58	MG	A	3341	-	-	-	X
58	MG	A	3352	-	-	-	X
58	MG	A	3363	-	-	-	X
58	MG	A	3380	-	-	-	X
58	MG	A	3382	-	-	-	X
58	MG	A	3396	-	-	-	X
58	MG	A	3399	-	-	-	X
58	MG	A	3410	-	-	-	X
58	MG	A	3414	-	-	-	X
58	MG	A	3417	-	-	-	X
58	MG	A	3420	-	-	-	X
58	MG	A	3423	-	-	-	X
58	MG	A	3437	-	-	-	X
58	MG	A	3446	-	-	-	X
58	MG	A	3455	-	-	-	X
58	MG	A	3476	-	-	-	X
58	MG	A	3486	-	-	-	X
58	MG	A	3487	-	-	-	X
58	MG	A	3490	-	-	-	X
58	MG	A	3493	-	-	-	X
58	MG	A	3498	-	-	-	X
58	MG	A	3500	-	-	-	X
58	MG	A	3501	-	-	-	X
58	MG	A	3513	-	-	-	X
58	MG	A	3516	-	-	-	X
58	MG	A	3520	-	-	-	X
58	MG	A	3523	-	-	-	X
58	MG	A	3529	-	-	-	X
58	MG	A	3530	-	-	-	X
58	MG	A	3540	-	-	-	X
58	MG	A	3541	-	-	-	X
58	MG	A	3557	-	-	-	X
58	MG	A	3564	-	-	-	X
58	MG	A	3568	-	-	-	X
58	MG	A	3601	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	A	3616	-	-	-	X
58	MG	B	210	-	-	-	X
58	MG	D	301	-	-	-	X
58	MG	D	303	-	-	-	X
58	MG	E	301	-	-	-	X
58	MG	F	302	-	-	-	X
58	MG	F	304	-	-	-	X
58	MG	N	201	-	-	-	X
58	MG	P	201	-	-	-	X
58	MG	Q	201	-	-	-	X
58	MG	Q	202	-	-	-	X
58	MG	Q	204	-	-	-	X
58	MG	R	201	-	-	-	X
58	MG	U	201	-	-	-	X
58	MG	V	202	-	-	-	X
58	MG	a	3306	-	-	-	X
58	MG	a	3309	-	-	-	X
58	MG	a	3313	-	-	-	X
58	MG	a	3318	-	-	-	X
58	MG	a	3323	-	-	-	X
58	MG	a	3330	-	-	-	X
58	MG	a	3331	-	-	-	X
58	MG	a	3351	-	-	-	X
58	MG	a	3355	-	-	-	X
58	MG	a	3368	-	-	-	X
58	MG	a	3376	-	-	-	X
58	MG	a	3378	-	-	-	X
58	MG	a	3382	-	-	-	X
58	MG	a	3395	-	-	-	X
58	MG	a	3397	-	-	-	X
58	MG	a	3401	-	-	-	X
58	MG	a	3406	-	-	-	X
58	MG	a	3422	-	-	-	X
58	MG	a	3435	-	-	-	X
58	MG	a	3439	-	-	-	X
58	MG	a	3447	-	-	-	X
58	MG	a	3466	-	-	-	X
58	MG	a	3471	-	-	-	X
58	MG	a	3487	-	-	-	X
58	MG	l	202	-	-	-	X
58	MG	n	101	-	-	-	X
58	MG	x	3002	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 152111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2873	Total	C	N	O	P	0	0	0
			61879	27541	11577	19890	2871			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			

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

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

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	130	Total	C	N	O	S	0	0	0
			641	381	130	130				

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	S	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	0	74	Total	C	N	O	S	0	0	0
			591	366	126	98	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	4	69	Total	C	N	O	S	0	0	0
			557	350	101	101	5			

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 33 is a RNA chain called E-site tRNA.

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

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	a	1496	Total	C	N	O	P	0	0	0
			32163	14314	5963	10390	1496			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	b	231	Total	C	N	O	S	0	0	0
			1850	1181	331	333	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	c	206	Total	C	N	O	S	0	0	0
			1550	974	302	273	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

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

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	f	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	g	155	Total	C	N	O	S	0	0	0
			1227	764	242	215	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	i	127	Total	C	N	O	0	0	0
			983	623	193	167			

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	j	96	Total	C	N	O	0	0	0
			698	434	134	130			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	l	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	m	119	Total	C	N	O	S	0	0	0
			924	570	192	160	2			

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

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

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	s	83	Total	C	N	O	S	0	0	0
			650	415	120	113	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	t	96	Total	C	N	O	S	0	0	0
			724	443	155	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	w	76	Total	C	N	O	P S	0	0	0
			1643	740	291	534	76 2			

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	v	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			

- Molecule 57 is a protein called 50S ribosomal protein L9, Elongation factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	y	644	Total	C	N	O	S	0	0	0
			4000	2438	760	799	3			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	P	2	Total	Mg	0	0
			2	2		
58	B	18	Total	Mg	0	0
			18	18		
58	6	1	Total	Mg	0	0
			1	1		
58	W	1	Total	Mg	0	0
			1	1		
58	N	1	Total	Mg	0	0
			1	1		
58	X	1	Total	Mg	0	0
			1	1		
58	y	2	Total	Mg	0	0
			2	2		
58	f	1	Total	Mg	0	0
			1	1		
58	E	4	Total	Mg	0	0
			4	4		
58	V	2	Total	Mg	0	0
			2	2		
58	w	6	Total	Mg	0	0
			6	6		
58	A	635	Total	Mg	0	0
			635	635		
58	n	1	Total	Mg	0	0
			1	1		
58	5	1	Total	Mg	0	0
			1	1		
58	x	3	Total	Mg	0	0
			3	3		
58	R	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	D	5	Total 5	Mg 5	0	0
58	e	1	Total 1	Mg 1	0	0
58	v	1	Total 1	Mg 1	0	0
58	Z	1	Total 1	Mg 1	0	0
58	a	187	Total 187	Mg 187	0	0
58	U	4	Total 4	Mg 4	0	0
58	9	1	Total 1	Mg 1	0	0
58	m	1	Total 1	Mg 1	0	0
58	0	3	Total 3	Mg 3	0	0
58	G	3	Total 3	Mg 3	0	0
58	Q	5	Total 5	Mg 5	0	0
58	7	3	Total 3	Mg 3	0	0
58	8	1	Total 1	Mg 1	0	0
58	O	1	Total 1	Mg 1	0	0
58	1	2	Total 2	Mg 2	0	0
58	F	5	Total 5	Mg 5	0	0

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

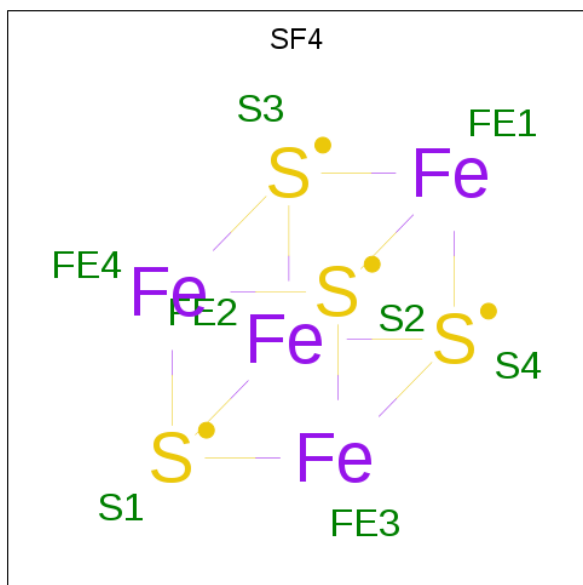
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y	1	Total 1	Zn 1	0	0
59	6	1	Total 1	Zn 1	0	0
59	4	1	Total 1	Zn 1	0	0

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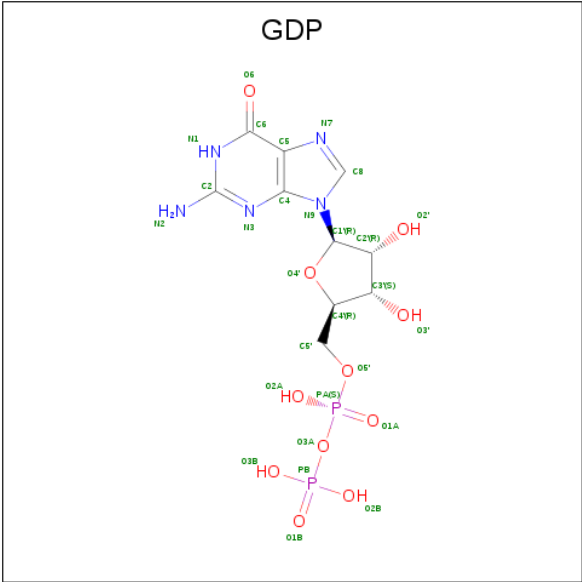
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	n	1	Total	Zn	0	0
			1	1		
59	5	1	Total	Zn	0	0
			1	1		
59	9	1	Total	Zn	0	0
			1	1		

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



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

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	A	710	Total	O	0	2
			710	710		
62	B	34	Total	O	0	0
			34	34		
62	D	4	Total	O	0	0
			4	4		
62	E	7	Total	O	0	0
			7	7		
62	F	5	Total	O	0	0
			5	5		
62	G	1	Total	O	0	0
			1	1		
62	H	1	Total	O	0	0
			1	1		
62	N	1	Total	O	0	0
			1	1		
62	O	3	Total	O	0	0
			3	3		
62	P	3	Total	O	0	0
			3	3		
62	Q	4	Total	O	0	0
			4	4		

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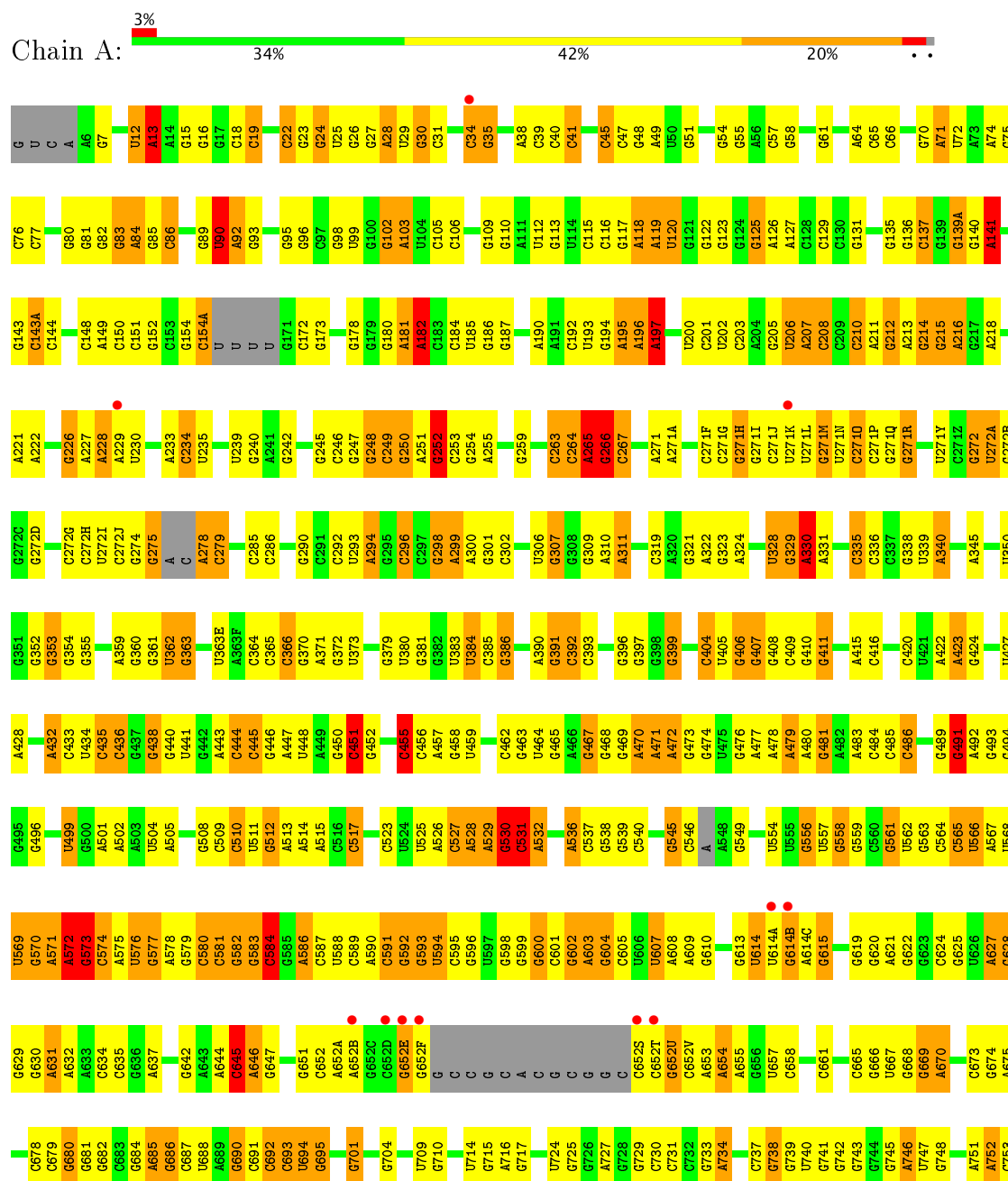
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	R	3	Total 3	O 3	0	0
62	U	2	Total 2	O 2	0	0
62	V	1	Total 1	O 1	0	0
62	W	2	Total 2	O 2	0	0
62	Y	1	Total 1	O 1	0	0
62	0	4	Total 4	O 4	0	0
62	1	2	Total 2	O 2	0	0
62	3	1	Total 1	O 1	0	0
62	5	1	Total 1	O 1	0	0
62	7	2	Total 2	O 2	0	0
62	8	4	Total 4	O 4	0	0
62	9	1	Total 1	O 1	0	0
62	x	1	Total 1	O 1	0	0
62	a	167	Total 167	O 167	0	0
62	l	1	Total 1	O 1	0	0
62	v	3	Total 3	O 3	0	0

3 Residue-property plots

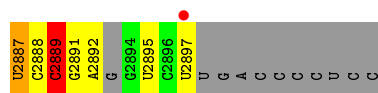
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 23S Ribosomal RNA



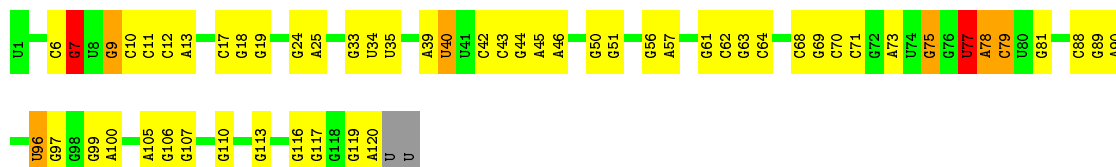






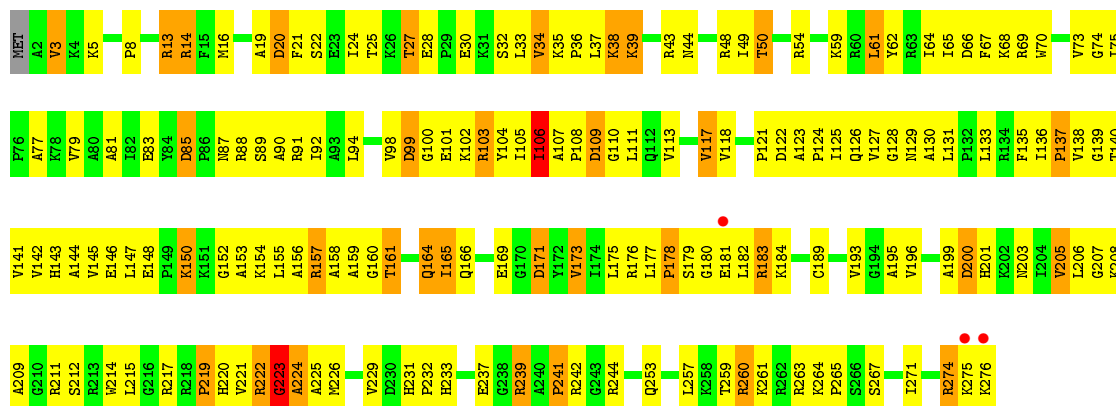
• Molecule 2: 5S Ribosomal RNA

Chain B: 52% 39% 5% ..



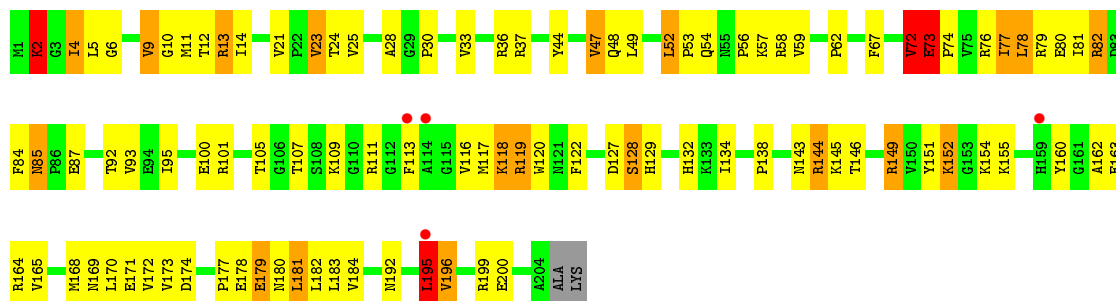
• Molecule 3: 50S ribosomal protein L2

Chain D: 37% 49% 12% ..



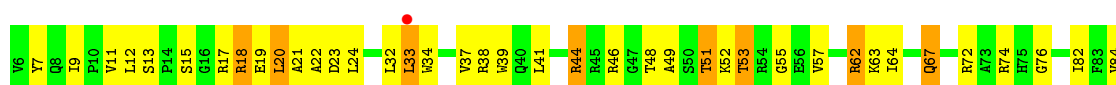
• Molecule 4: 50S ribosomal protein L3

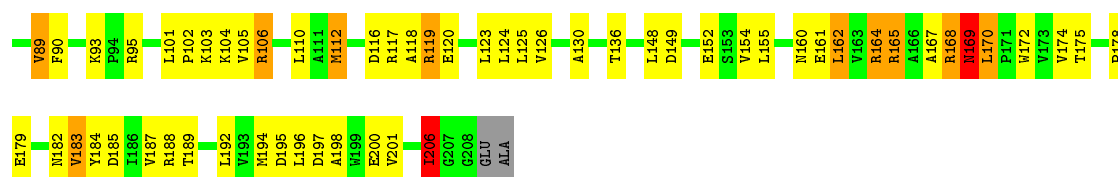
Chain E: 2% 50% 38% 9% ..



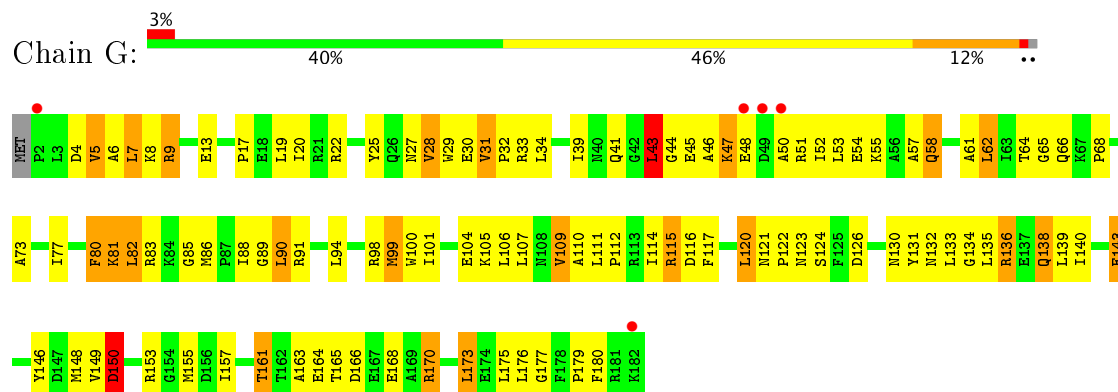
• Molecule 5: 50S ribosomal protein L4

Chain F: 52% 38% 9% ..

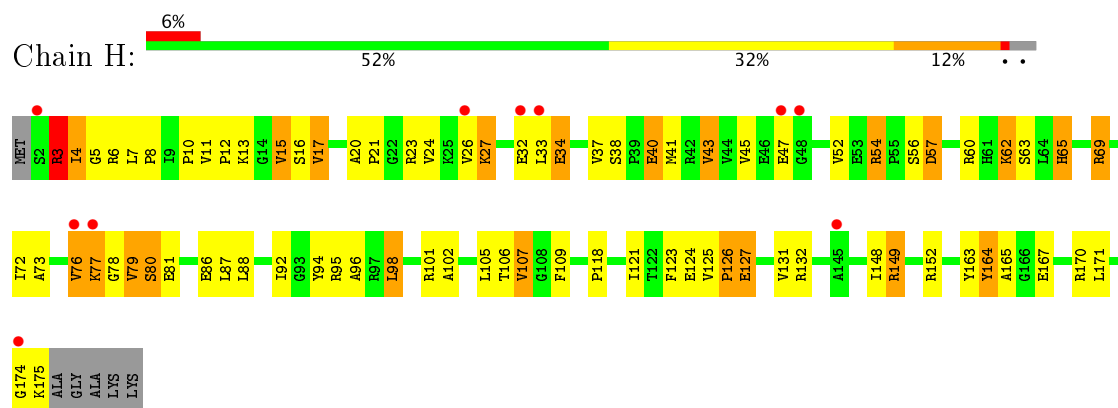




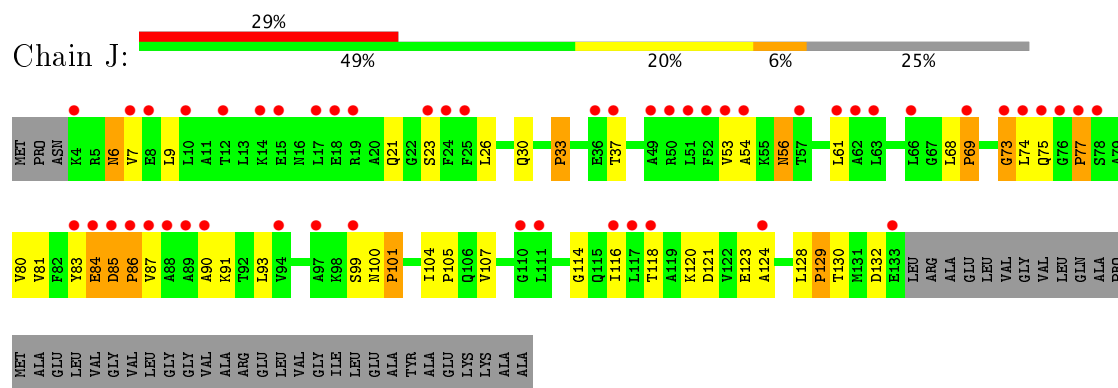
• Molecule 6: 50S ribosomal protein L5



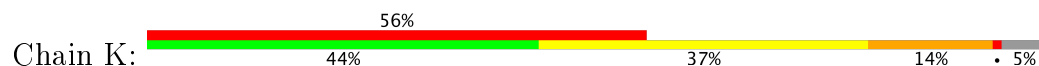
• Molecule 7: 50S ribosomal protein L6

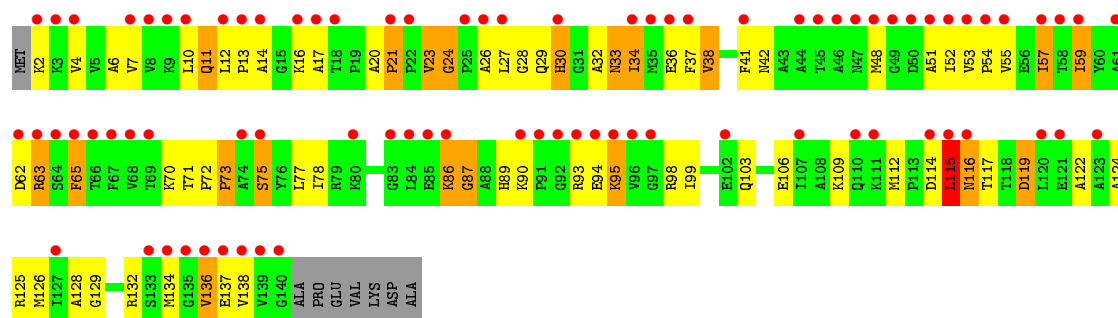


• Molecule 8: 50S ribosomal protein L10

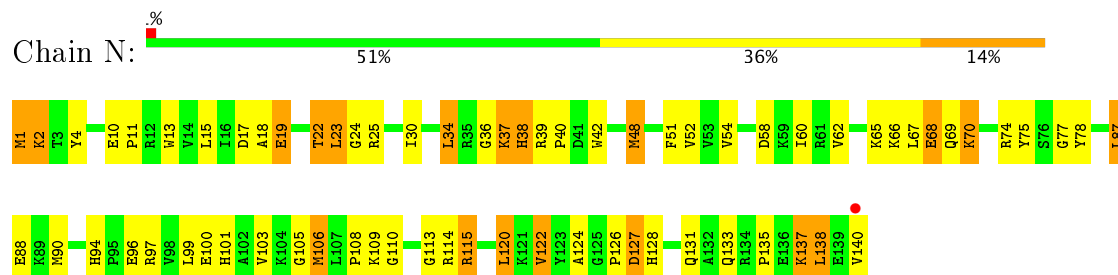


• Molecule 9: 50S ribosomal protein L11

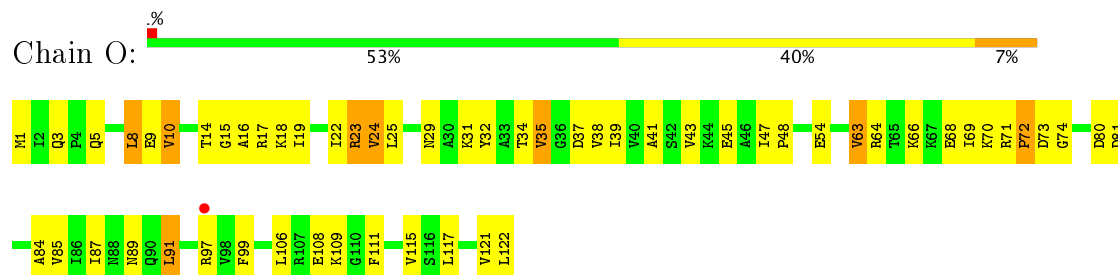




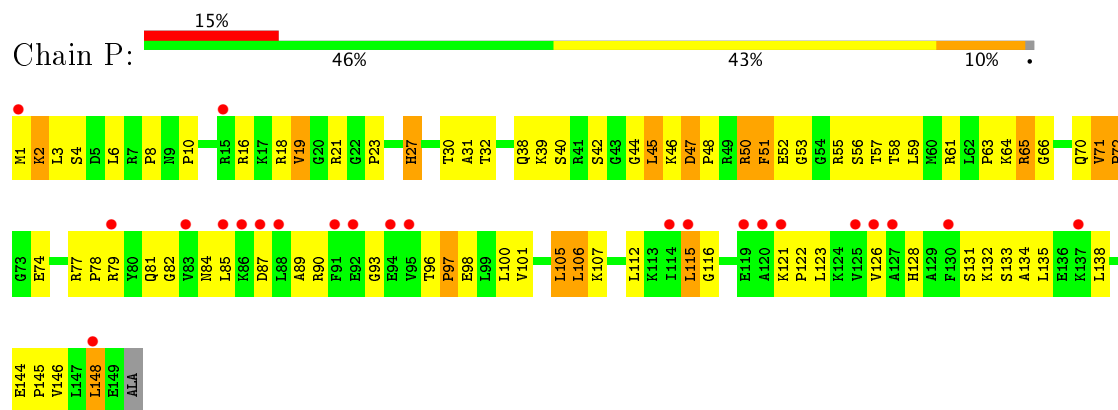
- Molecule 10: 50S ribosomal protein L13



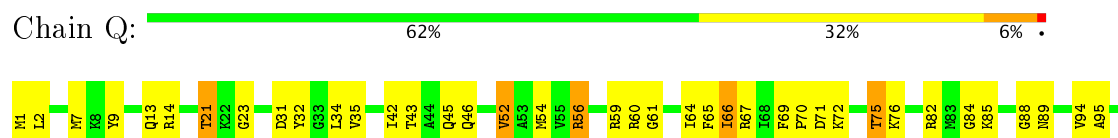
- Molecule 11: 50S ribosomal protein L14

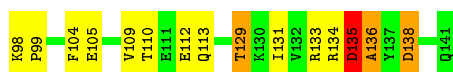


- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16

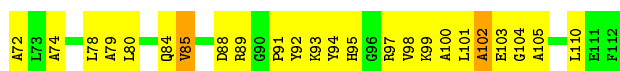
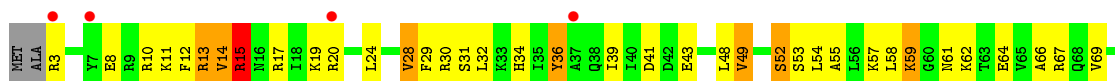
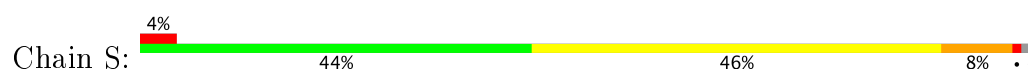




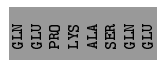
- Molecule 14: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L19

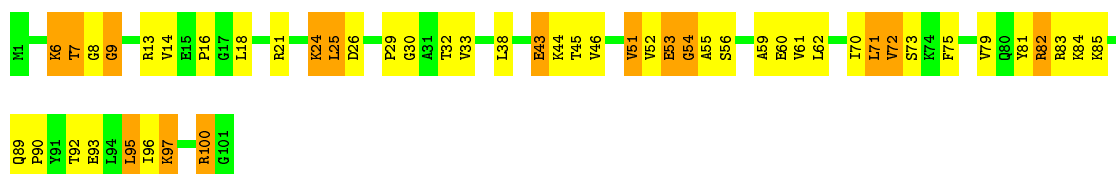


- Molecule 17: 50S ribosomal protein L20

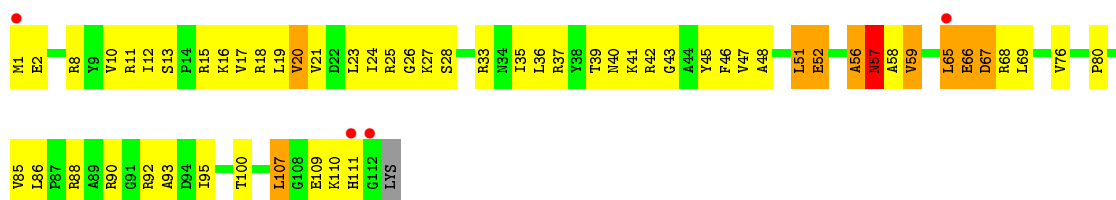


- Molecule 18: 50S ribosomal protein L21

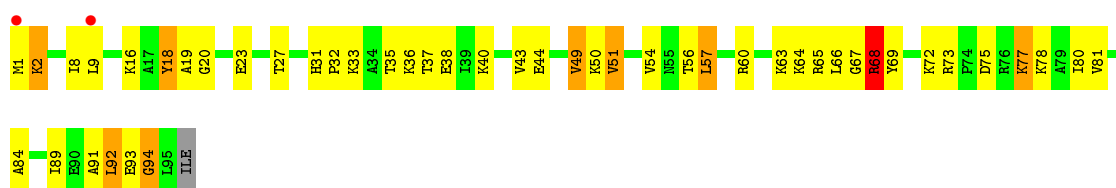




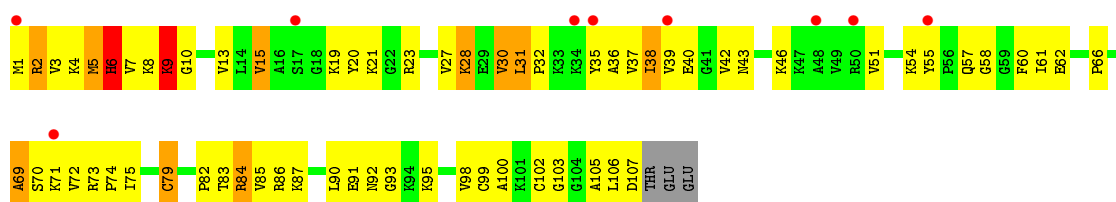
• Molecule 19: 50S ribosomal protein L22



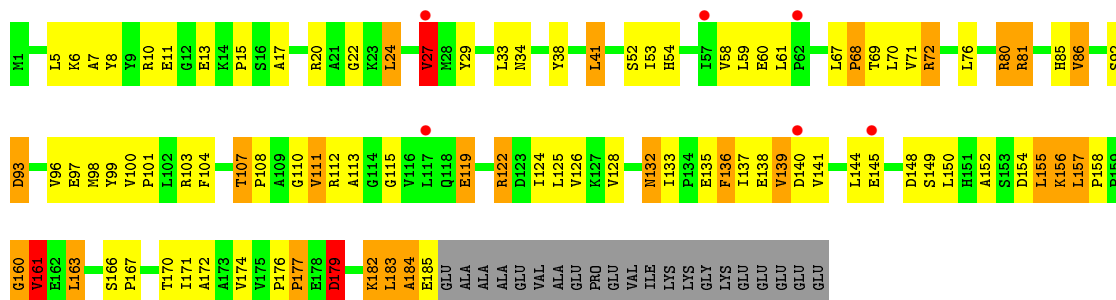
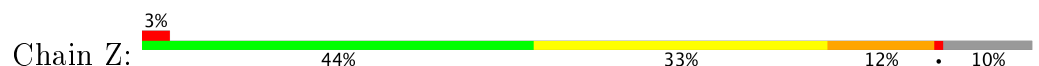
• Molecule 20: 50S ribosomal protein L23



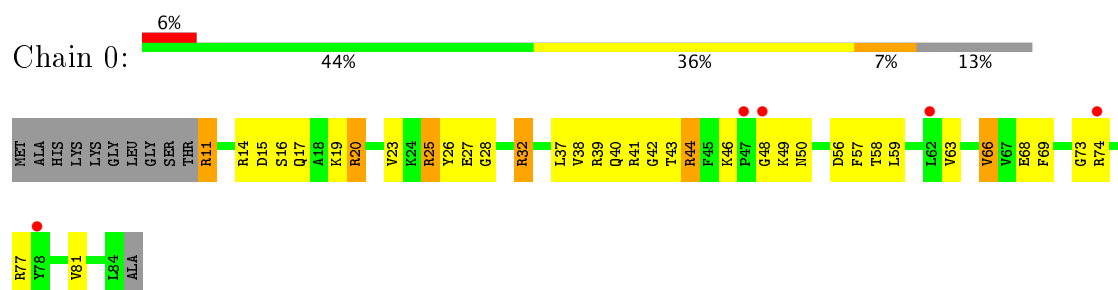
• Molecule 21: 50S ribosomal protein L24



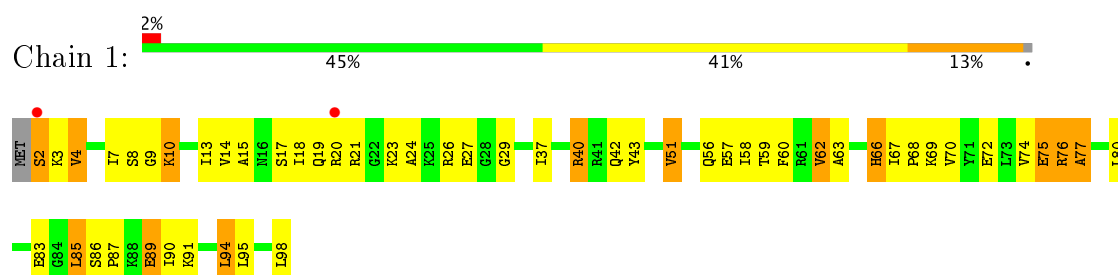
• Molecule 22: 50S ribosomal protein L25



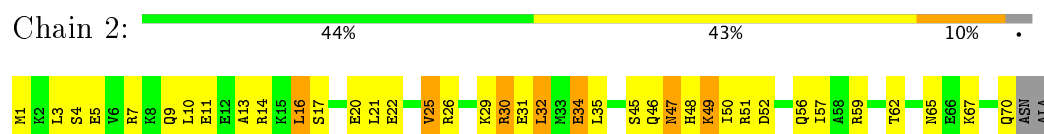
- Molecule 23: 50S ribosomal protein L27



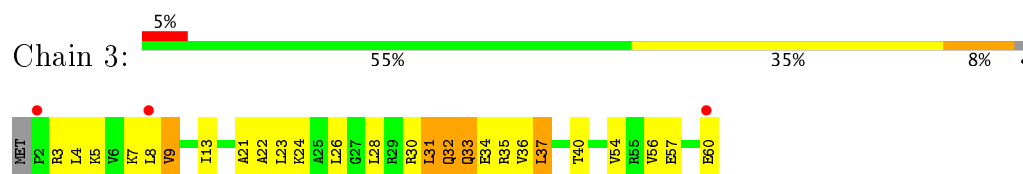
- Molecule 24: 50S ribosomal protein L28



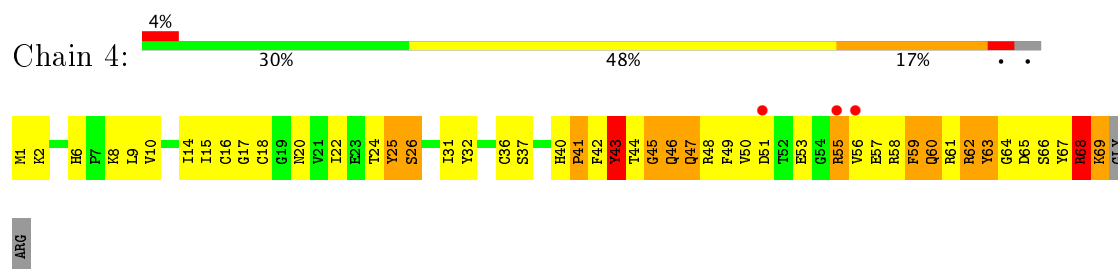
- Molecule 25: 50S ribosomal protein L29



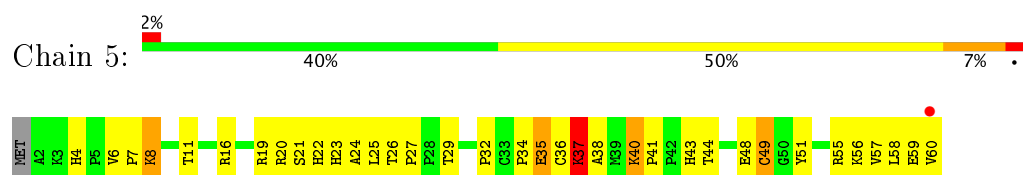
- Molecule 26: 50S ribosomal protein L30

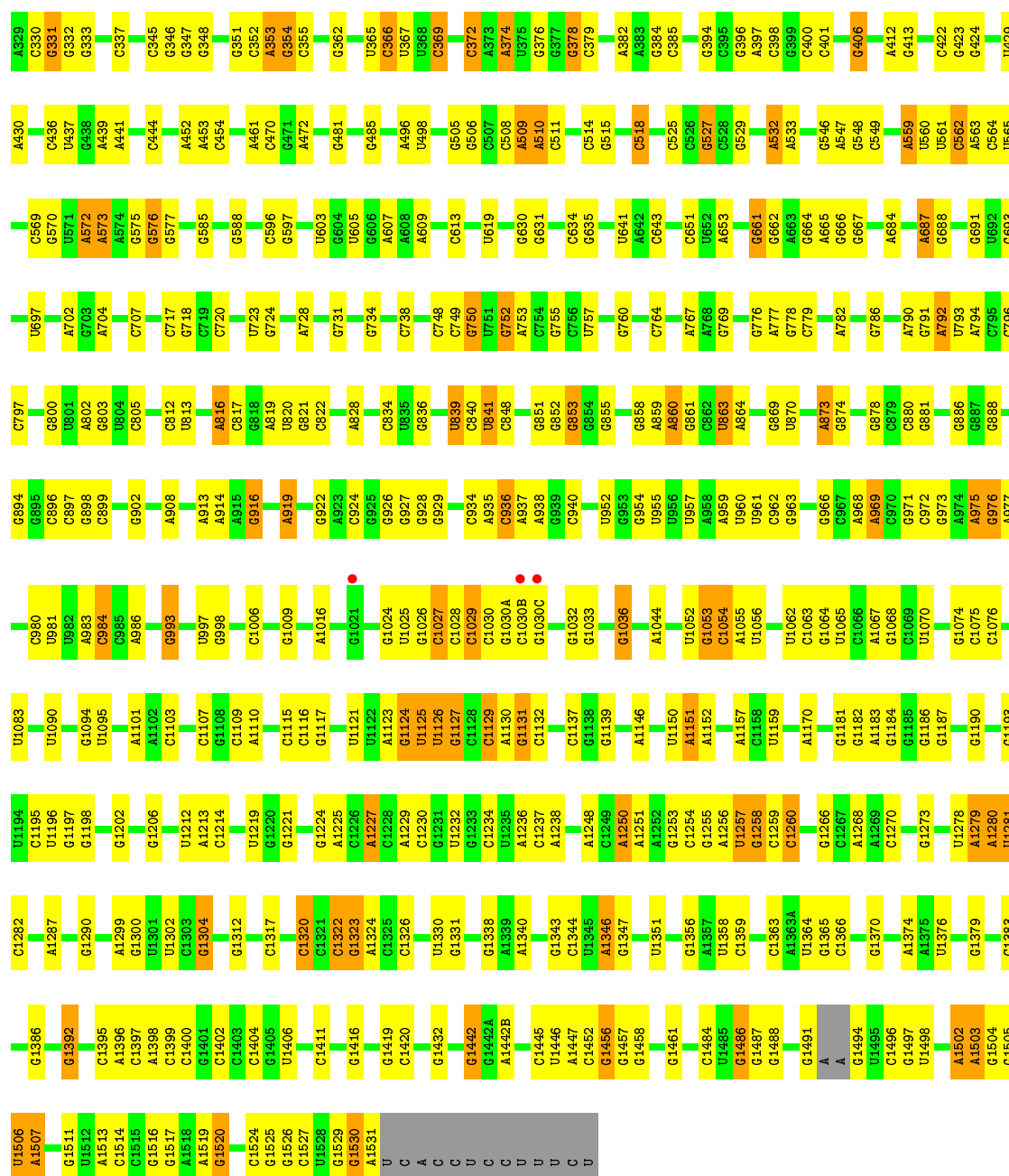


- Molecule 27: 50S ribosomal protein L31

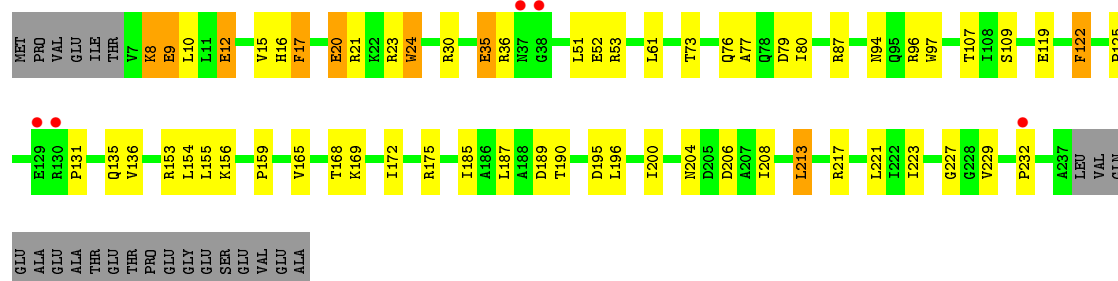


- Molecule 28: 50S ribosomal protein L32



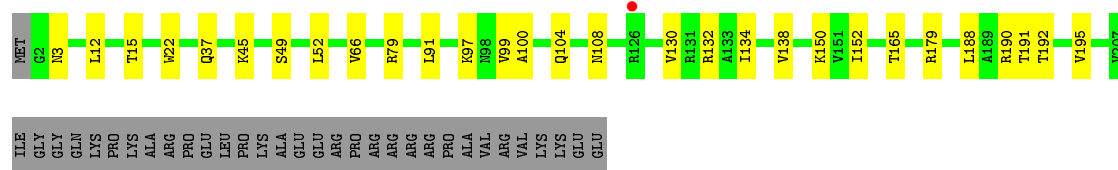


• Molecule 35: 30S ribosomal protein S2




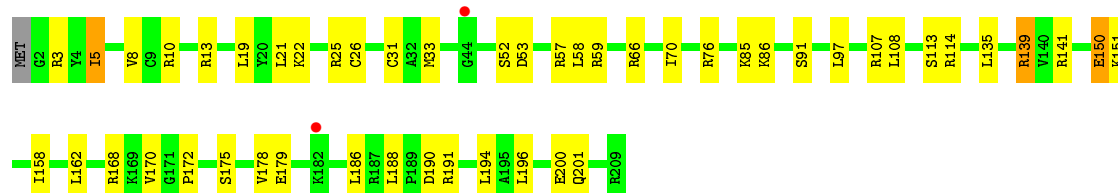
- Molecule 36: 30S ribosomal protein S3

Chain c: 



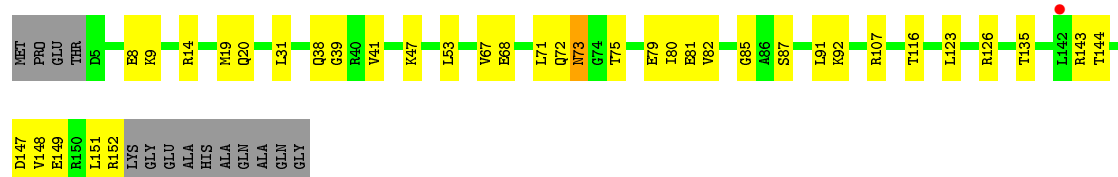
- Molecule 37: 30S ribosomal protein S4

Chain d: 



- Molecule 38: 30S ribosomal protein S5

Chain e: 




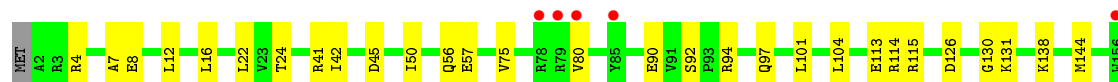
- Molecule 39: 30S ribosomal protein S6

Chain f: 




- Molecule 40: 30S ribosomal protein S7

Chain g: 



- Molecule 41: 30S ribosomal protein S8

Chain h: 



- Molecule 42: 30S ribosomal protein S9

Chain i: 81% 16% ..



- Molecule 43: 30S ribosomal protein S10

Chain j: 3% 68% 24% 9%



- Molecule 44: 30S ribosomal protein S11

Chain k: 2% 77% 12% 12%



- Molecule 45: 30S ribosomal protein S12

Chain l: % 77% 15% 8%



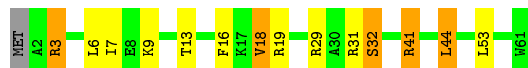
- Molecule 46: 30S ribosomal protein S13

Chain m: 2% 75% 16% 6%



- Molecule 47: 30S ribosomal protein S14 type Z

Chain n: 75% 15% 8%

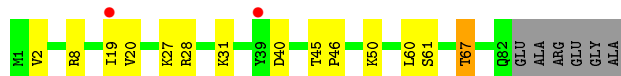
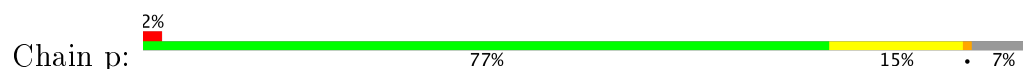


- Molecule 48: 30S ribosomal protein S15

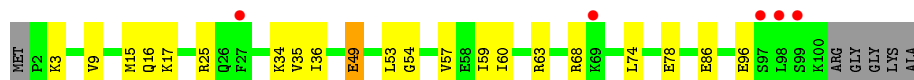
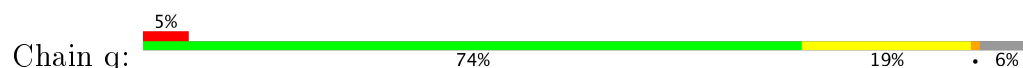
Chain o: 3% 85% 13%



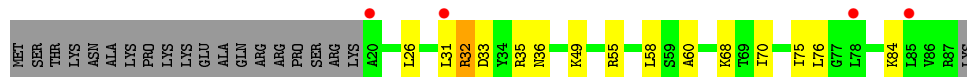
- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18



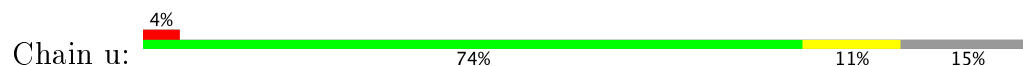
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20

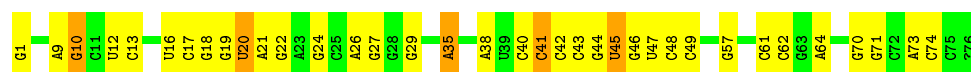


- Molecule 54: 30S ribosomal protein Thx

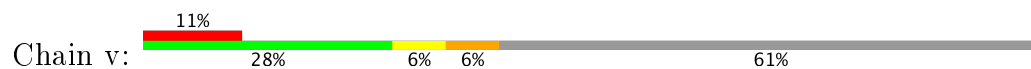


- Molecule 55: P-site tRNA

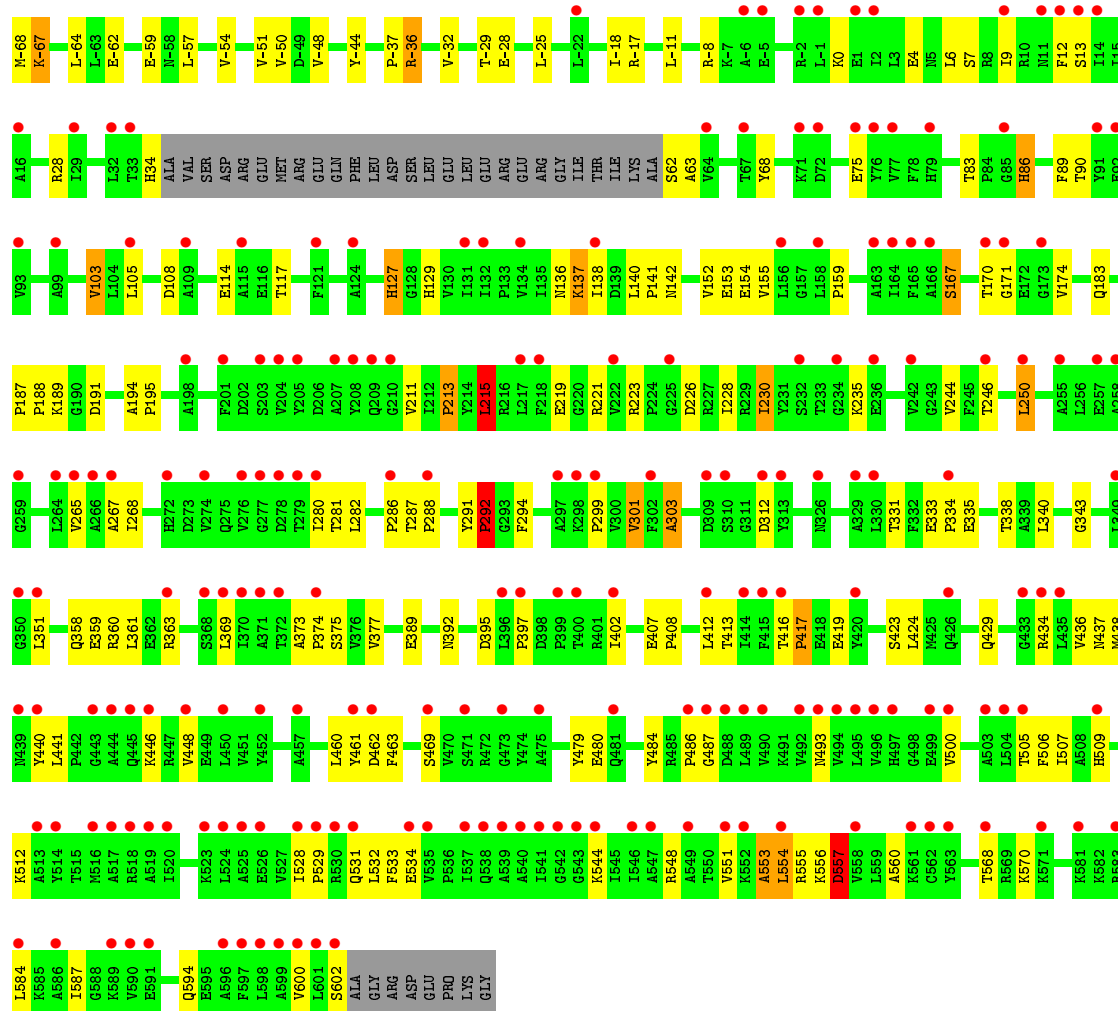




• Molecule 56: mRNA



• Molecule 57: 50S ribosomal protein L9, Elongation factor 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	239.29Å 272.85Å 431.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.90 49.76 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.76-2.90) 93.1 (49.76-2.89)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.238 , 0.304 0.239 , 0.303	Depositor DCC
R_{free} test set	29233 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	152111	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GDP, ZN, MIA, SF4, MG, F3O, 4SU, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.86	29/69298 (0.0%)	1.53	1145/108168 (1.1%)
2	B	0.61	0/2878	1.24	15/4490 (0.3%)
3	D	0.66	1/2186 (0.0%)	0.84	0/2944
4	E	0.64	0/1592	0.87	2/2149 (0.1%)
5	F	0.60	0/1619	0.80	2/2193 (0.1%)
6	G	0.45	0/1450	0.73	0/1959
7	H	0.47	0/1356	0.72	1/1834 (0.1%)
8	J	0.42	0/640	0.86	7/889 (0.8%)
9	K	0.30	0/1044	0.56	0/1416
10	N	0.58	0/1144	0.75	0/1543
11	O	0.75	0/943	0.88	1/1269 (0.1%)
12	P	0.53	0/1152	0.85	1/1533 (0.1%)
13	Q	0.62	0/1143	0.72	0/1527
14	R	0.51	0/982	0.74	0/1312
15	S	0.45	0/887	0.73	0/1180
16	T	0.62	0/1105	0.79	0/1477
17	U	0.63	0/977	0.78	1/1301 (0.1%)
18	V	0.56	0/782	0.78	0/1049
19	W	0.61	0/897	0.84	0/1205
20	X	0.56	0/764	0.76	0/1025
21	Y	0.54	0/819	0.78	1/1095 (0.1%)
22	Z	0.53	0/1483	0.71	0/2017
23	0	0.53	0/599	0.73	0/798
24	1	0.61	0/762	0.79	0/1014
25	2	0.50	0/590	0.70	0/781
26	3	0.57	0/474	0.81	1/635 (0.2%)
27	4	0.52	0/570	0.82	0/768
28	5	0.57	0/473	0.74	0/639
29	6	0.56	0/460	0.73	0/613
30	7	0.64	0/438	0.82	0/575
31	8	0.59	0/519	0.66	0/684
32	9	0.61	0/310	0.77	0/407

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	x	0.60	0/1602	1.35	18/2493 (0.7%)
34	a	0.87	14/36002 (0.0%)	1.53	589/56188 (1.0%)
35	b	0.54	0/1885	0.82	1/2547 (0.0%)
36	c	0.58	0/1574	0.71	0/2127
37	d	0.59	0/1685	0.81	2/2262 (0.1%)
38	e	0.69	0/1145	0.83	0/1543
39	f	0.47	0/819	0.69	1/1111 (0.1%)
40	g	0.55	0/1246	0.70	0/1674
41	h	0.58	0/1108	0.75	0/1494
42	i	0.56	0/1002	0.78	0/1346
43	j	0.54	0/711	0.77	0/968
44	k	0.53	0/844	0.69	0/1145
45	l	0.65	0/946	0.87	2/1274 (0.2%)
46	m	0.58	0/934	0.84	0/1256
47	n	0.66	0/501	0.91	3/664 (0.5%)
48	o	0.54	0/739	0.74	0/985
49	p	0.65	0/697	0.80	0/939
50	q	0.66	0/836	0.81	0/1117
51	r	0.49	0/560	0.66	0/746
52	s	0.62	0/665	0.84	0/897
53	t	0.51	0/726	0.79	0/961
54	u	0.51	0/203	0.76	0/266
55	w	0.88	2/1626 (0.1%)	1.58	40/2530 (1.6%)
56	v	0.82	0/165	1.41	3/254 (1.2%)
57	y	0.78	13/4067 (0.3%)	1.12	30/5503 (0.5%)
All	All	0.78	59/162624 (0.0%)	1.36	1866/242779 (0.8%)

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
3	D	0	1
8	J	0	1
42	i	0	1
46	m	0	2
52	s	0	1
53	t	0	1
57	y	0	23
All	All	0	30

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	1	G	OP3-P	-10.81	1.48	1.61
34	a	1125	U	P-O5'	7.89	1.67	1.59
1	A	945	A	N9-C4	-7.33	1.33	1.37
1	A	945	A	N3-C4	-7.19	1.30	1.34
1	A	2790	A	N9-C4	7.08	1.42	1.37
34	a	1125	U	O3'-P	6.66	1.69	1.61
34	a	1323	G	N7-C5	-6.48	1.35	1.39
1	A	2765	A	N9-C4	-6.40	1.34	1.37
1	A	2287	A	N9-C4	-6.38	1.34	1.37
55	w	45	U	N1-C2	6.25	1.44	1.38
3	D	237	GLU	CG-CD	6.19	1.61	1.51
34	a	975	A	N9-C4	-6.08	1.34	1.37
1	A	2058	A	N9-C4	-6.02	1.34	1.37
1	A	2566	A	N3-C4	-5.96	1.31	1.34
34	a	563	A	N9-C4	-5.68	1.34	1.37
34	a	767	A	N9-C4	5.67	1.41	1.37
1	A	265	A	N9-C4	-5.65	1.34	1.37
1	A	1021	A	C5-C6	-5.62	1.35	1.41
1	A	1571	A	N9-C4	-5.61	1.34	1.37
1	A	1021	A	N9-C4	-5.59	1.34	1.37
1	A	1667	G	N9-C8	-5.59	1.33	1.37
1	A	2765	A	N7-C5	-5.57	1.35	1.39
34	a	563	A	N3-C4	-5.57	1.31	1.34
34	a	1227	A	N9-C4	-5.56	1.34	1.37
34	a	1281	U	N1-C2	5.52	1.43	1.38
1	A	197	A	N9-C4	-5.50	1.34	1.37
57	y	141	PRO	N-CD	5.47	1.55	1.47
1	A	526	A	N9-C4	-5.46	1.34	1.37
1	A	1021	A	N7-C5	-5.45	1.35	1.39
1	A	1190	G	C6-N1	5.45	1.43	1.39
57	y	299	PRO	N-CD	5.45	1.55	1.47
34	a	1530	G	N9-C4	-5.42	1.33	1.38
34	a	983	A	N7-C5	-5.38	1.36	1.39
57	y	188	PRO	N-CD	5.38	1.55	1.47
1	A	973	A	N9-C4	-5.30	1.34	1.37
1	A	959	A	N9-C4	-5.29	1.34	1.37
57	y	195	PRO	N-CD	5.26	1.55	1.47
57	y	374	PRO	N-CD	5.24	1.55	1.47
57	y	397	PRO	N-CD	5.22	1.55	1.47
1	A	1674	G	N7-C5	-5.21	1.36	1.39
34	a	397	A	N7-C5	-5.20	1.36	1.39
1	A	820	A	N3-C4	-5.18	1.31	1.34
57	y	529	PRO	N-CD	5.18	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1142(A)	A	N9-C4	-5.17	1.34	1.37
57	y	288	PRO	N-CD	5.17	1.55	1.47
1	A	1322	A	N9-C4	-5.15	1.34	1.37
1	A	958	U	N1-C2	5.15	1.43	1.38
57	y	189	LYS	C-N	5.14	1.42	1.33
34	a	975	A	C5-C6	-5.14	1.36	1.41
57	y	334	PRO	N-CD	5.13	1.55	1.47
1	A	1919	A	C6-N1	-5.10	1.31	1.35
57	y	408	PRO	N-CD	5.09	1.54	1.47
34	a	1125	U	C4'-C3'	5.09	1.58	1.53
1	A	2506	U	C2-N3	5.08	1.41	1.37
57	y	292	PRO	N-CD	5.08	1.54	1.47
57	y	460	LEU	C-O	5.08	1.32	1.23
1	A	1828	G	N1-C2	-5.05	1.33	1.37
1	A	528	A	C5-C6	-5.04	1.36	1.41
1	A	2242	G	N9-C4	-5.03	1.33	1.38

All (1866) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2096	U	O5'-P-OP1	-18.05	89.04	110.70
34	a	1281	U	N3-C2-O2	-14.81	111.83	122.20
1	A	1021	A	C2-N3-C4	-13.57	103.82	110.60
1	A	945	A	N1-C6-N6	13.26	126.56	118.60
1	A	1190	G	N1-C6-O6	13.08	127.75	119.90
1	A	945	A	C6-C5-N7	-12.08	123.84	132.30
1	A	1190	G	C5-C6-O6	-12.00	121.40	128.60
34	a	1281	U	N1-C2-N3	11.79	121.97	114.90
1	A	2200	C	C6-N1-C2	-11.61	115.66	120.30
34	a	1126	U	C5-C6-N1	11.60	128.50	122.70
1	A	1791	A	O5'-P-OP1	-11.36	95.48	105.70
1	A	945	A	C2-N3-C4	-11.33	104.94	110.60
1	A	814	C	O5'-P-OP2	-11.04	95.77	105.70
34	a	1127	G	N3-C4-N9	-10.99	119.40	126.00
1	A	1798	U	O5'-P-OP2	-10.83	95.95	105.70
34	a	1281	U	C6-N1-C2	-10.79	114.52	121.00
1	A	2059	A	N1-C6-N6	10.64	124.99	118.60
34	a	1129	C	C6-N1-C2	-10.45	116.12	120.30
34	a	1125	U	N3-C2-O2	10.12	129.29	122.20
34	a	1126	U	C2-N1-C1'	10.03	129.73	117.70
1	A	1021	A	N1-C6-N6	9.91	124.55	118.60
34	a	365	U	C5-C6-N1	-9.91	117.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	518	C	C5-C4-N4	9.90	127.13	120.20
34	a	975	A	N1-C6-N6	9.90	124.54	118.60
1	A	1776	G	O5'-P-OP2	-9.88	96.81	105.70
1	A	945	A	C5-N7-C8	-9.86	98.97	103.90
1	A	1021	A	C5-N7-C8	-9.82	98.99	103.90
1	A	2791	C	C6-N1-C2	-9.72	116.41	120.30
34	a	975	A	C5-N7-C8	-9.68	99.06	103.90
34	a	518	C	N3-C4-N4	-9.63	111.26	118.00
34	a	365	U	C2-N1-C1'	-9.61	106.17	117.70
1	A	2539	C	O5'-P-OP2	-9.56	97.09	105.70
1	A	2096	U	C5-C6-N1	9.52	127.46	122.70
34	a	518	C	C6-N1-C1'	9.49	132.18	120.80
34	a	1281	U	C5-C4-O4	9.45	131.57	125.90
34	a	1279	A	N7-C8-N9	9.43	118.51	113.80
1	A	945	A	C5-C6-N1	-9.42	112.99	117.70
1	A	1142(A)	A	C2-N3-C4	-9.39	105.91	110.60
1	A	2202	C	C6-N1-C2	-9.38	116.55	120.30
34	a	560	U	O5'-P-OP2	-9.31	97.32	105.70
34	a	792	A	O4'-C1'-N9	9.29	115.64	108.20
1	A	2610	C	C6-N1-C2	-9.19	116.62	120.30
1	A	632	A	C8-N9-C4	9.15	109.46	105.80
1	A	1977	A	C2-N3-C4	-9.14	106.03	110.60
34	a	518	C	C2-N1-C1'	-9.11	108.78	118.80
1	A	945	A	C4-C5-C6	9.09	121.55	117.00
34	a	1127	G	C8-N9-C1'	9.09	138.81	127.00
1	A	2059	A	C5-C6-N6	-9.07	116.44	123.70
34	a	527	G	C8-N9-C4	-9.04	102.78	106.40
1	A	774	A	O5'-P-OP2	-9.03	97.58	105.70
34	a	527	G	N9-C4-C5	9.03	109.01	105.40
34	a	253	U	O5'-P-OP1	-8.99	97.61	105.70
1	A	2501	C	O5'-P-OP2	-8.99	97.61	105.70
34	a	1129	C	O4'-C1'-N1	8.98	115.39	108.20
1	A	1021	A	N7-C8-N9	8.97	118.28	113.80
1	A	528	A	N7-C8-N9	8.96	118.28	113.80
1	A	528	A	C5-N7-C8	-8.96	99.42	103.90
1	A	1109	C	C2-N1-C1'	8.93	128.62	118.80
1	A	197	A	O5'-P-OP2	-8.91	97.68	105.70
34	a	975	A	C4-C5-N7	8.88	115.14	110.70
1	A	253	C	C6-N1-C2	8.88	123.85	120.30
1	A	383	U	O4'-C1'-N1	8.87	115.30	108.20
1	A	1109	C	C5-C6-N1	8.85	125.42	121.00
1	A	1967	C	O5'-P-OP2	-8.80	97.78	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	x	50	U	C5-C4-O4	8.77	131.16	125.90
34	a	1279	A	C8-N9-C4	-8.77	102.29	105.80
1	A	2506	U	C5-C6-N1	8.75	127.08	122.70
1	A	2496	C	N3-C2-O2	-8.74	115.78	121.90
1	A	1190	G	C4-C5-N7	8.68	114.27	110.80
1	A	1647	G	O5'-P-OP1	-8.67	97.89	105.70
1	A	1558	A	N1-C6-N6	8.65	123.79	118.60
1	A	2096	U	C2-N1-C1'	8.64	128.07	117.70
57	y	463	PHE	N-CA-C	8.64	134.32	111.00
1	A	1792	G	O5'-P-OP2	-8.63	97.93	105.70
34	a	1127	G	N9-C4-C5	8.62	108.85	105.40
34	a	1524	C	N3-C4-C5	8.58	125.33	121.90
34	a	1530	G	N3-C4-C5	8.58	132.89	128.60
1	A	1021	A	N1-C2-N3	8.56	133.58	129.30
34	a	1150	U	C5-C4-O4	8.56	131.04	125.90
1	A	2503	A	C2-N3-C4	8.55	114.88	110.60
1	A	1558	A	C2-N3-C4	-8.54	106.33	110.60
33	x	50	U	C2-N3-C4	8.54	132.12	127.00
34	a	266	G	C5-N7-C8	-8.53	100.03	104.30
55	w	73	A	O4'-C1'-N9	8.51	115.01	108.20
1	A	1983	C	N1-C2-O2	-8.50	113.80	118.90
1	A	1781	C	N1-C2-O2	8.46	123.98	118.90
1	A	2073	C	O5'-P-OP2	-8.46	98.09	105.70
1	A	973	A	C2-N3-C4	-8.45	106.37	110.60
1	A	2448	A	N1-C6-N6	8.45	123.67	118.60
34	a	1257	U	N1-C2-O2	8.45	128.71	122.80
1	A	330	A	C2-N3-C4	-8.44	106.38	110.60
1	A	1109	C	C6-N1-C2	-8.43	116.93	120.30
34	a	1116	C	C6-N1-C2	8.42	123.67	120.30
1	A	1153	C	C6-N1-C2	-8.41	116.93	120.30
34	a	1127	G	C4-N9-C1'	-8.38	115.61	126.50
1	A	1021	A	C6-C5-N7	-8.37	126.44	132.30
1	A	1350	C	O5'-P-OP1	-8.35	98.19	105.70
1	A	2554	U	C5-C4-O4	-8.31	120.91	125.90
1	A	1599	C	C6-N1-C2	-8.29	116.99	120.30
1	A	528	A	C2-N3-C4	-8.28	106.46	110.60
1	A	945	A	N1-C2-N3	8.27	133.43	129.30
55	w	45	U	N3-C2-O2	-8.26	116.42	122.20
34	a	575	G	C5-C6-O6	-8.26	123.65	128.60
34	a	1123	A	C5-C6-N6	8.26	130.30	123.70
1	A	1131	G	O5'-P-OP2	-8.24	98.28	105.70
1	A	1300	U	N3-C2-O2	-8.21	116.45	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1380	G	O5'-P-OP2	-8.20	98.32	105.70
1	A	746	A	O4'-C1'-N9	8.19	114.75	108.20
1	A	2242	G	N3-C4-C5	8.19	132.69	128.60
34	a	1530	G	N3-C4-N9	-8.19	121.09	126.00
33	x	68	C	N1-C2-O2	8.18	123.81	118.90
1	A	693	C	N3-C2-O2	-8.17	116.18	121.90
34	a	365	U	N1-C2-N3	8.17	119.80	114.90
34	a	436	C	C5-C6-N1	8.17	125.08	121.00
34	a	776	G	O5'-P-OP1	-8.16	98.36	105.70
1	A	782	A	C8-N9-C4	8.15	109.06	105.80
1	A	2275	C	O5'-P-OP2	-8.15	98.37	105.70
1	A	1021	A	C5-C6-N1	-8.13	113.63	117.70
34	a	333	G	C5-C6-O6	-8.13	123.72	128.60
1	A	2424	C	C6-N1-C2	-8.12	117.05	120.30
1	A	530	G	N1-C6-O6	-8.11	115.04	119.90
34	a	1322	C	O5'-P-OP2	-8.10	98.41	105.70
34	a	117	G	N9-C4-C5	-8.10	102.16	105.40
1	A	1981	A	N1-C6-N6	8.08	123.45	118.60
33	x	64	A	C6-N1-C2	8.08	123.45	118.60
1	A	2202	C	C5-C6-N1	8.07	125.03	121.00
1	A	528	A	C6-C5-N7	-8.05	126.67	132.30
1	A	240	G	C4-C5-N7	-8.05	107.58	110.80
34	a	91	C	N1-C2-O2	8.03	123.72	118.90
1	A	1952	A	N1-C6-N6	8.03	123.42	118.60
1	A	263	C	N1-C2-O2	7.99	123.69	118.90
34	a	266	G	P-O3'-C3'	7.96	129.26	119.70
34	a	10	A	N1-C6-N6	7.94	123.36	118.60
1	A	528	A	N1-C6-N6	7.93	123.36	118.60
34	a	1074	G	C5-C6-O6	-7.92	123.85	128.60
34	a	70	G	C5-C6-O6	-7.89	123.87	128.60
1	A	2239	G	O5'-P-OP2	-7.89	98.60	105.70
1	A	2774	C	C6-N1-C2	7.89	123.45	120.30
34	a	1126	U	C6-N1-C2	-7.87	116.28	121.00
34	a	365	U	C6-N1-C1'	7.87	132.21	121.20
1	A	512	G	O4'-C1'-N9	7.86	114.49	108.20
1	A	645	C	N1-C2-O2	7.84	123.61	118.90
1	A	2506	U	N3-C4-O4	7.84	124.89	119.40
1	A	1774	C	N3-C4-C5	-7.83	118.77	121.90
34	a	975	A	C6-C5-N7	-7.83	126.82	132.30
1	A	2766	G	C6-C5-N7	-7.83	125.70	130.40
1	A	945	A	C4-C5-N7	7.82	114.61	110.70
1	A	745	G	N1-C6-O6	-7.80	115.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1002	G	O5'-P-OP2	-7.79	98.69	105.70
1	A	2024	G	C8-N9-C4	-7.78	103.29	106.40
55	w	73	A	N7-C8-N9	7.77	117.69	113.80
34	a	976	G	N1-C6-O6	7.77	124.56	119.90
1	A	1021	A	C8-N9-C4	-7.76	102.69	105.80
34	a	1107	C	N1-C2-O2	-7.75	114.25	118.90
1	A	1108	U	C2-N1-C1'	7.74	126.99	117.70
1	A	528	A	C8-N9-C4	-7.74	102.70	105.80
34	a	820	U	N3-C2-O2	-7.73	116.79	122.20
1	A	1667	G	C8-N9-C4	7.73	109.49	106.40
34	a	1065	U	O5'-P-OP2	-7.73	98.74	105.70
1	A	12	U	N1-C2-O2	7.73	128.21	122.80
34	a	1392	G	C5-C6-O6	7.72	133.23	128.60
34	a	266	G	N7-C8-N9	7.72	116.96	113.10
1	A	2227	A	O5'-P-OP2	-7.71	98.76	105.70
1	A	2271	G	N3-C4-N9	7.69	130.62	126.00
1	A	2638	G	N3-C4-C5	-7.69	124.76	128.60
1	A	2394	C	C2-N1-C1'	7.68	127.25	118.80
1	A	364	C	C6-N1-C2	-7.68	117.23	120.30
1	A	530	G	C5-C6-O6	7.67	133.20	128.60
1	A	80	G	N1-C6-O6	7.65	124.49	119.90
1	A	678	C	N3-C4-C5	-7.65	118.84	121.90
1	A	581	C	C6-N1-C2	-7.63	117.25	120.30
1	A	1645	G	O5'-P-OP2	-7.63	98.84	105.70
1	A	1653	G	C4-N9-C1'	7.62	136.41	126.50
1	A	1189	A	O5'-P-OP2	-7.62	98.84	105.70
1	A	2499	C	N1-C2-O2	-7.62	114.33	118.90
1	A	2605	U	C6-N1-C2	-7.61	116.43	121.00
34	a	1524	C	C6-N1-C2	7.61	123.34	120.30
34	a	1257	U	N3-C2-O2	-7.60	116.88	122.20
34	a	241	C	C6-N1-C2	7.59	123.34	120.30
1	A	1272	A	O4'-C1'-N9	7.59	114.27	108.20
34	a	1511	G	C5-C6-O6	-7.58	124.05	128.60
34	a	333	G	N1-C6-O6	7.58	124.45	119.90
34	a	1076	C	C6-N1-C2	-7.58	117.27	120.30
1	A	1108	U	N1-C2-O2	7.58	128.10	122.80
33	x	56	C	N1-C2-O2	7.58	123.45	118.90
34	a	266	G	C4-C5-N7	7.57	113.83	110.80
34	a	1127	G	C6-C5-N7	7.57	134.94	130.40
1	A	566	U	C6-N1-C2	-7.56	116.46	121.00
1	A	392	C	N1-C2-O2	7.56	123.44	118.90
1	A	2391	G	O4'-C1'-N9	7.56	114.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2271	G	N9-C4-C5	-7.54	102.38	105.40
34	a	976	G	C5-C6-N1	-7.54	107.73	111.50
34	a	1123	A	N3-C4-N9	-7.54	121.37	127.40
34	a	1125	U	C6-N1-C2	7.51	125.51	121.00
1	A	2503	A	O5'-P-OP1	-7.51	98.94	105.70
1	A	13	A	C8-N9-C4	-7.50	102.80	105.80
1	A	1005	C	N1-C2-O2	7.50	123.40	118.90
34	a	797	C	N1-C2-O2	-7.50	114.40	118.90
1	A	591	C	C6-N1-C2	-7.50	117.30	120.30
1	A	1653	G	C6-C5-N7	-7.50	125.90	130.40
1	A	933	A	O4'-C1'-N9	7.50	114.20	108.20
1	A	2573	C	N3-C2-O2	7.49	127.14	121.90
1	A	2496	C	N1-C2-O2	7.49	123.39	118.90
1	A	1918	A	N1-C6-N6	-7.47	114.12	118.60
34	a	971	G	O4'-C1'-N9	7.47	114.18	108.20
1	A	746	A	C8-N9-C4	-7.47	102.81	105.80
1	A	1030	G	C5-C6-O6	-7.47	124.12	128.60
1	A	584	C	N3-C2-O2	-7.46	116.68	121.90
1	A	129	C	C6-N1-C2	7.46	123.28	120.30
1	A	531	C	N3-C2-O2	-7.46	116.68	121.90
1	A	1030	G	N9-C4-C5	-7.45	102.42	105.40
1	A	226	G	N1-C6-O6	-7.44	115.43	119.90
34	a	91	C	C2-N3-C4	7.44	123.62	119.90
34	a	1027	C	N1-C2-O2	7.42	123.35	118.90
1	A	141	A	N1-C6-N6	7.41	123.05	118.60
55	w	20	U	C2-N1-C1'	7.41	126.59	117.70
34	a	819	A	N1-C6-N6	7.40	123.04	118.60
1	A	1980	G	C8-N9-C4	7.40	109.36	106.40
1	A	2200	C	N3-C2-O2	-7.40	116.72	121.90
34	a	317	G	C6-C5-N7	-7.38	125.97	130.40
34	a	509	A	C8-N9-C4	-7.38	102.85	105.80
1	A	2605	U	N3-C2-O2	-7.38	117.03	122.20
1	A	486	C	C6-N1-C2	7.37	123.25	120.30
1	A	2200	C	C5-C6-N1	7.37	124.69	121.00
1	A	2820	A	N1-C6-N6	7.37	123.02	118.60
1	A	2620	C	O5'-P-OP2	-7.36	99.08	105.70
1	A	240	G	C5-C6-O6	7.36	133.01	128.60
1	A	819	A	N1-C6-N6	7.36	123.01	118.60
1	A	1681	G	N3-C4-C5	7.36	132.28	128.60
1	A	2428	G	P-O3'-C3'	7.35	128.52	119.70
34	a	1202	G	O5'-P-OP2	-7.35	99.08	105.70
33	x	64	A	C5-C6-N6	7.33	129.56	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1061	U	O4'-C1'-N1	7.32	114.06	108.20
34	a	1502	A	C6-C5-N7	-7.32	127.18	132.30
34	a	510	A	C5-C6-N6	7.32	129.55	123.70
1	A	1021	A	C4-C5-N7	7.31	114.36	110.70
1	A	985	C	C6-N1-C2	7.31	123.22	120.30
34	a	976	G	C4-C5-C6	7.31	123.18	118.80
34	a	1219	U	C2-N3-C4	-7.30	122.62	127.00
34	a	1486	G	C5-C6-O6	-7.29	124.22	128.60
1	A	1212	G	C8-N9-C4	7.29	109.32	106.40
1	A	1665	A	C8-N9-C4	7.29	108.72	105.80
1	A	438	G	N1-C6-O6	7.28	124.27	119.90
1	A	1002	G	O5'-P-OP1	7.28	119.44	110.70
1	A	531	C	N3-C4-C5	-7.28	118.99	121.90
34	a	1125	U	N1-C2-O2	-7.27	117.71	122.80
34	a	834	C	C6-N1-C2	7.27	123.21	120.30
1	A	2059	A	N9-C4-C5	-7.26	102.89	105.80
1	A	2443	C	C5-C6-N1	-7.26	117.37	121.00
1	A	2494	G	C5-C6-O6	-7.26	124.25	128.60
34	a	813	U	O5'-P-OP1	7.23	119.37	110.70
34	a	1123	A	C6-N1-C2	7.22	122.93	118.60
1	A	1406	U	O5'-P-OP1	-7.21	99.21	105.70
1	A	2088	G	N3-C4-N9	-7.19	121.68	126.00
34	a	1304	G	N1-C6-O6	7.19	124.21	119.90
34	a	1520	G	O5'-P-OP2	-7.19	99.23	105.70
1	A	1634	A	C8-N9-C4	7.18	108.67	105.80
34	a	955	U	C5-C4-O4	7.18	130.21	125.90
1	A	226	G	O4'-C1'-N9	7.18	113.94	108.20
1	A	1300	U	N1-C2-O2	7.17	127.82	122.80
34	a	366	C	N3-C2-O2	-7.17	116.88	121.90
34	a	1198	G	O5'-P-OP2	7.17	119.31	110.70
1	A	2572	A	N1-C6-N6	-7.17	114.30	118.60
34	a	916	G	C8-N9-C4	-7.17	103.53	106.40
34	a	385	C	C6-N1-C2	-7.17	117.43	120.30
34	a	515	G	N1-C6-O6	7.17	124.20	119.90
1	A	528	A	N1-C2-N3	7.17	132.88	129.30
1	A	2202	C	C2-N1-C1'	7.16	126.68	118.80
1	A	2275	C	C6-N1-C2	7.16	123.17	120.30
1	A	859	G	N3-C4-N9	-7.16	121.70	126.00
55	w	9	A	C8-N9-C4	7.16	108.67	105.80
34	a	266	G	C8-N9-C4	-7.15	103.54	106.40
34	a	1502	A	C2-N3-C4	-7.15	107.03	110.60
34	a	972	C	C6-N1-C2	-7.14	117.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1036	G	C4-N9-C1'	7.14	135.79	126.50
1	A	570	G	C4-C5-N7	-7.14	107.94	110.80
34	a	1511	G	N1-C6-O6	7.14	124.18	119.90
1	A	2439	A	O4'-C1'-N9	-7.13	102.50	108.20
55	w	73	A	C5-N7-C8	-7.12	100.34	103.90
1	A	1691	C	N1-C2-O2	-7.12	114.63	118.90
34	a	1331	G	O4'-C1'-N9	7.12	113.90	108.20
1	A	2834	G	N1-C6-O6	-7.12	115.63	119.90
1	A	1698	A	C6-C5-N7	-7.11	127.32	132.30
1	A	2766	G	N1-C6-O6	7.11	124.17	119.90
1	A	528	A	C4-C5-N7	7.11	114.25	110.70
1	A	1613	G	C4-C5-N7	-7.10	107.96	110.80
34	a	873	A	C2-N3-C4	7.09	114.15	110.60
34	a	510	A	N1-C6-N6	-7.09	114.34	118.60
1	A	915	C	N3-C2-O2	-7.09	116.94	121.90
1	A	2022	U	N1-C2-O2	-7.08	117.84	122.80
1	A	1800	C	N1-C2-O2	-7.08	114.65	118.90
1	A	399	G	N3-C4-C5	7.08	132.14	128.60
1	A	2582	G	C2-N3-C4	7.07	115.44	111.90
1	A	2617	C	C6-N1-C2	-7.07	117.47	120.30
1	A	2790	A	C2-N3-C4	7.06	114.13	110.60
1	A	2500	U	O5'-P-OP1	-7.06	99.34	105.70
34	a	529	G	N1-C6-O6	7.06	124.14	119.90
1	A	1300	U	C2-N1-C1'	7.06	126.17	117.70
1	A	340	A	O5'-P-OP1	-7.05	99.35	105.70
1	A	2516	G	N1-C6-O6	7.05	124.13	119.90
1	A	645	C	C2-N1-C1'	7.05	126.55	118.80
1	A	2197	U	N3-C2-O2	-7.04	117.27	122.20
34	a	374	A	N1-C6-N6	7.04	122.83	118.60
55	w	45	U	C6-N1-C2	-7.04	116.78	121.00
34	a	1324	A	C8-N9-C4	-7.03	102.99	105.80
1	A	1633	G	N1-C6-O6	7.03	124.12	119.90
1	A	933	A	C5-N7-C8	-7.03	100.39	103.90
1	A	1950	G	C5-C6-O6	7.02	132.81	128.60
1	A	2011	U	OP1-P-O3'	7.02	120.64	105.20
1	A	2287	A	C2-N3-C4	-7.02	107.09	110.60
1	A	2325	G	C8-N9-C4	-7.02	103.59	106.40
1	A	859	G	C4-N9-C1'	-7.01	117.38	126.50
1	A	30	G	N3-C4-N9	7.00	130.20	126.00
1	A	1501	C	C5-C6-N1	7.00	124.50	121.00
1	A	1614	A	O5'-P-OP1	-7.00	99.40	105.70
1	A	446	G	C8-N9-C4	-6.99	103.60	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	436	C	C2-N1-C1'	6.99	126.49	118.80
1	A	818	G	N1-C6-O6	6.99	124.09	119.90
1	A	2394	C	N1-C2-O2	6.99	123.09	118.90
1	A	2509	G	C5-C6-O6	-6.99	124.41	128.60
1	A	1796	U	C5-C4-O4	6.98	130.09	125.90
1	A	2605	U	C5-C6-N1	6.98	126.19	122.70
1	A	2765	A	C2-N3-C4	-6.98	107.11	110.60
1	A	2056	G	C4-C5-N7	6.97	113.59	110.80
1	A	1782	C	C6-N1-C2	-6.97	117.51	120.30
1	A	958	U	N3-C2-O2	-6.97	117.32	122.20
34	a	757	U	O5'-P-OP2	-6.96	99.43	105.70
1	A	2096	U	N1-C2-O2	6.96	127.67	122.80
1	A	945	A	O5'-P-OP2	-6.96	99.44	105.70
34	a	1124	G	N3-C4-C5	-6.96	125.12	128.60
34	a	1322	C	C6-N1-C2	6.96	123.08	120.30
34	a	366	C	N1-C2-O2	6.95	123.07	118.90
45	l	84	LEU	CA-CB-CG	6.94	131.27	115.30
1	A	693	C	C6-N1-C2	-6.94	117.52	120.30
1	A	2789	C	O4'-C1'-N1	6.94	113.75	108.20
34	a	888	G	O5'-P-OP2	-6.94	99.45	105.70
1	A	2229	C	N3-C2-O2	-6.94	117.04	121.90
1	A	584	C	C2-N1-C1'	6.93	126.42	118.80
34	a	728	A	N1-C6-N6	6.93	122.76	118.60
1	A	2624	G	N3-C4-N9	6.93	130.16	126.00
1	A	2766	G	C4-C5-N7	6.92	113.57	110.80
1	A	1204	A	C2-N3-C4	-6.91	107.14	110.60
1	A	2056	G	C6-C5-N7	-6.91	126.25	130.40
34	a	852	G	N1-C2-N2	-6.91	109.98	116.20
34	a	38	G	N1-C6-O6	6.90	124.04	119.90
1	A	945	A	C4-N9-C1'	6.90	138.71	126.30
34	a	959	A	C8-N9-C4	6.89	108.56	105.80
1	A	734	A	C8-N9-C4	6.88	108.55	105.80
1	A	2609	U	C5-C6-N1	-6.88	119.26	122.70
1	A	1776	G	C8-N9-C4	6.88	109.15	106.40
34	a	1502	A	C5-N7-C8	-6.88	100.46	103.90
1	A	1827	C	C6-N1-C2	-6.87	117.55	120.30
1	A	1966	A	O5'-P-OP1	-6.87	99.52	105.70
34	a	1494	G	N3-C4-C5	-6.86	125.17	128.60
1	A	1647	G	O5'-P-OP2	6.86	118.93	110.70
34	a	576	G	C6-C5-N7	-6.86	126.29	130.40
1	A	2767	C	N1-C2-O2	6.86	123.01	118.90
57	y	215	LEU	N-CA-C	-6.86	92.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	679	C	C5-C6-N1	-6.85	117.57	121.00
34	a	894	G	N1-C6-O6	6.85	124.01	119.90
55	w	62	C	N3-C4-C5	-6.84	119.16	121.90
34	a	573	A	O5'-P-OP2	-6.84	99.54	105.70
1	A	1698	A	N1-C6-N6	6.83	122.70	118.60
34	a	1331	G	N1-C6-O6	-6.83	115.80	119.90
1	A	945	A	C8-N9-C1'	-6.83	115.41	127.70
2	B	70	C	C6-N1-C2	-6.82	117.57	120.30
34	a	1290	G	N1-C6-O6	6.82	123.99	119.90
34	a	1503	A	O4'-C1'-N9	6.81	113.65	108.20
1	A	2229	C	O5'-P-OP2	-6.81	99.57	105.70
1	A	740	U	OP1-P-OP2	-6.81	109.39	119.60
1	A	933	A	N7-C8-N9	6.80	117.20	113.80
57	y	215	LEU	CB-CG-CD1	6.80	122.56	111.00
1	A	90	U	C5-C6-N1	6.80	126.10	122.70
1	A	1745	C	C5-C6-N1	6.79	124.40	121.00
1	A	561	G	C8-N9-C4	6.79	109.12	106.40
55	w	29	G	N1-C6-O6	6.79	123.97	119.90
1	A	1991	U	C5-C6-N1	-6.78	119.31	122.70
1	A	451	C	N3-C4-N4	6.78	122.75	118.00
1	A	1796	U	C2-N1-C1'	-6.78	109.56	117.70
1	A	2791	C	C2-N1-C1'	6.77	126.25	118.80
1	A	1191	G	N3-C4-C5	6.77	131.98	128.60
1	A	265	A	C2-N3-C4	-6.76	107.22	110.60
1	A	801	G	N1-C6-O6	-6.76	115.84	119.90
34	a	510	A	N9-C4-C5	6.76	108.50	105.80
1	A	1823	G	O5'-P-OP2	6.75	118.80	110.70
1	A	12	U	N3-C2-O2	-6.75	117.48	122.20
1	A	1253	A	OP1-P-OP2	6.75	129.72	119.60
34	a	929	G	N1-C6-O6	-6.74	115.85	119.90
1	A	2200	C	C2-N1-C1'	6.74	126.22	118.80
1	A	798	G	OP1-P-OP2	-6.74	109.49	119.60
1	A	945	A	N7-C8-N9	6.74	117.17	113.80
34	a	1126	U	C5-C4-O4	-6.74	121.86	125.90
1	A	1799	G	N1-C6-O6	-6.73	115.86	119.90
1	A	1927	A	C8-N9-C4	6.73	108.49	105.80
34	a	105	G	O5'-P-OP2	-6.73	99.64	105.70
8	J	77	PRO	N-CA-CB	6.73	111.37	103.30
1	A	1030	G	C8-N9-C4	6.72	109.09	106.40
1	A	1622	G	C5-C6-O6	-6.72	124.57	128.60
1	A	2566	A	N9-C4-C5	6.72	108.49	105.80
34	a	687	A	P-O3'-C3'	6.72	127.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	45	U	O4'-C1'-N1	6.72	113.58	108.20
1	A	1677	A	N1-C6-N6	-6.72	114.57	118.60
1	A	584	C	C6-N1-C2	-6.71	117.61	120.30
1	A	573	G	C5-C6-O6	-6.71	124.57	128.60
1	A	2582	G	C5-C6-N1	6.71	114.86	111.50
1	A	2073	C	N1-C2-O2	6.70	122.92	118.90
1	A	2712(A)	A	N9-C4-C5	6.70	108.48	105.80
34	a	365	U	C5-C4-O4	6.70	129.92	125.90
1	A	234	C	N1-C2-O2	6.70	122.92	118.90
1	A	1958	C	O5'-P-OP1	6.70	118.73	110.70
1	A	2199	A	OP2-P-O3'	6.69	119.92	105.20
34	a	963	G	C2-N3-C4	-6.68	108.56	111.90
34	a	975	A	C2-N3-C4	-6.68	107.26	110.60
34	a	1234	C	C6-N1-C2	-6.68	117.63	120.30
1	A	2040	C	N3-C2-O2	-6.68	117.22	121.90
1	A	1778	U	N3-C4-C5	6.67	118.60	114.60
34	a	1511	G	C6-C5-N7	-6.65	126.41	130.40
1	A	206	U	N3-C2-O2	-6.65	117.55	122.20
1	A	1300	U	P-O3'-C3'	6.65	127.68	119.70
1	A	773	U	C6-N1-C2	6.64	124.99	121.00
1	A	1694	C	N1-C2-O2	-6.64	114.92	118.90
1	A	1190	G	C5-N7-C8	-6.64	100.98	104.30
1	A	2034	U	C2-N1-C1'	6.64	125.67	117.70
55	w	1	G	C8-N9-C4	-6.63	103.75	106.40
1	A	986	C	C6-N1-C2	6.63	122.95	120.30
1	A	1790	C	N3-C2-O2	6.63	126.54	121.90
1	A	1698	A	N7-C8-N9	6.62	117.11	113.80
34	a	320	C	C6-N1-C2	6.62	122.95	120.30
34	a	91	C	N3-C4-C5	-6.62	119.25	121.90
34	a	839	U	C2-N1-C1'	6.61	125.64	117.70
34	a	812	C	N1-C2-O2	6.61	122.86	118.90
1	A	859	G	N3-C4-C5	6.60	131.90	128.60
34	a	822	C	N1-C2-O2	-6.60	114.94	118.90
1	A	1129	A	N1-C6-N6	-6.59	114.64	118.60
1	A	2646	C	C6-N1-C2	-6.59	117.66	120.30
1	A	1095	A	O4'-C1'-N9	6.59	113.47	108.20
55	w	20	U	N1-C2-O2	6.59	127.41	122.80
1	A	844	C	C6-N1-C2	6.59	122.93	120.30
1	A	2080	G	C5-C6-O6	-6.59	124.65	128.60
1	A	531	C	C4-C5-C6	6.58	120.69	117.40
34	a	515	G	C5-C6-O6	-6.57	124.66	128.60
1	A	1227	G	N1-C6-O6	6.57	123.84	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	A	N1-C2-N3	6.57	132.58	129.30
1	A	582	G	C8-N9-C4	-6.57	103.77	106.40
34	a	980	C	C5-C6-N1	6.57	124.28	121.00
34	a	1530	G	C4-N9-C1'	-6.56	117.97	126.50
34	a	1127	G	C4-C5-N7	-6.56	108.17	110.80
1	A	1634	A	N7-C8-N9	-6.55	110.52	113.80
34	a	1027	C	N3-C2-O2	-6.55	117.32	121.90
1	A	1313	U	C2-N1-C1'	6.55	125.56	117.70
1	A	673	C	N3-C4-N4	6.55	122.58	118.00
1	A	2506	U	O5'-P-OP2	6.55	118.56	110.70
1	A	1837	C	N1-C2-O2	-6.54	114.97	118.90
1	A	1721	G	C4-C5-N7	6.54	113.42	110.80
34	a	1129	C	P-O3'-C3'	6.54	127.55	119.70
34	a	813	U	OP1-P-OP2	-6.53	109.80	119.60
1	A	990	A	N1-C6-N6	6.53	122.52	118.60
1	A	392	C	N3-C2-O2	-6.53	117.33	121.90
34	a	1432	G	C8-N9-C4	-6.53	103.79	106.40
1	A	1038	C	C6-N1-C2	-6.53	117.69	120.30
1	A	116	C	O5'-P-OP2	-6.52	99.83	105.70
1	A	830	G	O5'-P-OP1	-6.52	99.83	105.70
1	A	1981	A	C5-C6-N6	-6.52	118.48	123.70
1	A	2499	C	C2-N3-C4	-6.52	116.64	119.90
33	x	4	C	C6-N1-C2	-6.52	117.69	120.30
34	a	1331	G	C8-N9-C4	-6.52	103.79	106.40
1	A	1791	A	OP2-P-O3'	6.52	119.54	105.20
34	a	916	G	C4-N9-C1'	6.52	134.97	126.50
1	A	733	G	C4-C5-N7	6.51	113.41	110.80
1	A	561	G	N7-C8-N9	-6.51	109.84	113.10
1	A	210	C	C5-C6-N1	-6.51	117.75	121.00
34	a	839	U	N1-C2-O2	6.51	127.35	122.80
34	a	1117	G	C8-N9-C4	6.50	109.00	106.40
1	A	1899	G	N1-C2-N2	-6.50	110.35	116.20
1	A	2463	C	C5-C6-N1	6.50	124.25	121.00
34	a	861	G	N3-C4-N9	6.50	129.90	126.00
34	a	975	A	C5-C6-N6	-6.49	118.50	123.70
1	A	1667	G	N7-C8-N9	-6.49	109.86	113.10
1	A	2200	C	N1-C2-O2	6.49	122.79	118.90
34	a	778	G	O5'-P-OP2	-6.49	99.86	105.70
34	a	1502	A	N1-C6-N6	6.48	122.49	118.60
1	A	679	C	C2-N3-C4	-6.48	116.66	119.90
1	A	1897	G	N9-C4-C5	-6.47	102.81	105.40
1	A	573	G	O5'-P-OP2	-6.47	99.87	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1653	G	C4-C5-C6	6.47	122.68	118.80
1	A	2766	G	C5-C6-O6	-6.47	124.72	128.60
34	a	769	G	N3-C4-N9	6.47	129.88	126.00
34	a	514	C	C6-N1-C2	6.47	122.89	120.30
34	a	1526	G	C6-C5-N7	-6.46	126.52	130.40
55	w	74	C	C6-N1-C2	-6.46	117.72	120.30
1	A	1030	G	N3-C4-N9	6.46	129.88	126.00
1	A	1775	U	C5-C6-N1	-6.46	119.47	122.70
1	A	452	G	N1-C6-O6	6.46	123.77	119.90
33	x	4	C	N3-C2-O2	-6.46	117.38	121.90
1	A	1190	G	C6-C5-N7	-6.45	126.53	130.40
1	A	1629	U	N1-C2-N3	6.45	118.77	114.90
1	A	866	A	C8-N9-C4	-6.45	103.22	105.80
1	A	1108	U	C6-N1-C1'	-6.45	112.17	121.20
1	A	2073	C	N3-C2-O2	-6.45	117.39	121.90
1	A	945	A	O4'-C1'-N9	6.45	113.36	108.20
1	A	1061	U	C2-N1-C1'	6.44	125.43	117.70
1	A	2286	A	N7-C8-N9	6.44	117.02	113.80
1	A	2448	A	N9-C4-C5	-6.44	103.22	105.80
34	a	1255	G	C8-N9-C4	6.44	108.98	106.40
1	A	2785	C	C6-N1-C2	-6.43	117.73	120.30
34	a	1248	A	C2-N3-C4	6.43	113.81	110.60
1	A	2286	A	C8-N9-C4	-6.43	103.23	105.80
1	A	2064	C	N3-C2-O2	6.42	126.39	121.90
1	A	798	G	C8-N9-C4	-6.42	103.83	106.40
1	A	2825	C	C5-C6-N1	-6.42	117.79	121.00
34	a	518	C	O4'-C1'-N1	6.42	113.33	108.20
1	A	561	G	N1-C6-O6	-6.42	116.05	119.90
1	A	182	A	C8-N9-C4	-6.42	103.23	105.80
34	a	1198	G	N3-C2-N2	-6.41	115.41	119.90
34	a	28	G	N1-C6-O6	6.41	123.75	119.90
1	A	364	C	C5-C6-N1	6.41	124.21	121.00
5	F	62	ARG	NE-CZ-NH1	-6.41	117.09	120.30
34	a	254	G	O5'-P-OP1	-6.41	99.93	105.70
57	y	416	THR	C-N-CD	6.41	141.86	128.40
1	A	958	U	C6-N1-C2	-6.40	117.16	121.00
1	A	265	A	N1-C6-N6	6.40	122.44	118.60
1	A	819	A	C4-C5-N7	6.40	113.90	110.70
1	A	2615	U	N3-C4-O4	-6.39	114.92	119.40
1	A	1758	G	C4-C5-C6	6.39	122.64	118.80
1	A	2197	U	N1-C2-O2	6.39	127.27	122.80
1	A	2052	G	C4-C5-N7	-6.39	108.25	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2789	C	C2-N1-C1'	-6.39	111.77	118.80
34	a	275	G	N3-C4-C5	-6.39	125.41	128.60
1	A	1109	C	N1-C2-O2	6.38	122.73	118.90
1	A	1962	C	C5-C6-N1	6.38	124.19	121.00
1	A	573	G	N1-C6-O6	6.38	123.73	119.90
1	A	275	G	C8-N9-C4	-6.37	103.85	106.40
1	A	1962	C	C6-N1-C2	-6.37	117.75	120.30
1	A	2751	G	C4-N9-C1'	6.37	134.78	126.50
34	a	1488	G	N1-C6-O6	6.37	123.72	119.90
1	A	1672	C	C6-N1-C2	-6.37	117.75	120.30
1	A	1629	U	C4-C5-C6	6.37	123.52	119.70
34	a	317	G	N3-C4-N9	6.36	129.82	126.00
34	a	337	C	C6-N1-C2	-6.36	117.76	120.30
34	a	981	U	N3-C2-O2	6.35	126.65	122.20
1	A	2250	G	C5-C6-N1	6.35	114.67	111.50
1	A	680	G	O5'-P-OP2	-6.35	99.99	105.70
55	w	26	A	N1-C6-N6	6.35	122.41	118.60
1	A	2049	G	C8-N9-C4	-6.34	103.86	106.40
34	a	619	U	C5-C4-O4	6.34	129.71	125.90
1	A	788	A	N9-C4-C5	-6.34	103.26	105.80
34	a	241	C	N3-C4-C5	6.34	124.44	121.90
34	a	1506	U	N1-C2-O2	-6.34	118.36	122.80
1	A	208	C	N1-C2-O2	-6.34	115.10	118.90
1	A	580	C	N1-C2-O2	-6.34	115.10	118.90
1	A	1300	U	C6-N1-C2	-6.34	117.20	121.00
1	A	2050	C	O5'-P-OP1	-6.34	100.00	105.70
1	A	577	G	C8-N9-C4	-6.34	103.87	106.40
8	J	86	PRO	N-CA-CB	6.33	110.89	103.30
1	A	1698	A	C2-N3-C4	-6.32	107.44	110.60
1	A	2048	G	N1-C6-O6	6.32	123.69	119.90
1	A	531	C	C6-N1-C2	-6.32	117.77	120.30
1	A	139(A)	G	N3-C4-C5	-6.32	125.44	128.60
1	A	2549	G	O5'-P-OP2	-6.31	100.02	105.70
1	A	1328	G	N1-C6-O6	6.31	123.69	119.90
34	a	78	G	N1-C6-O6	-6.31	116.12	119.90
1	A	1204	A	N1-C6-N6	6.30	122.38	118.60
1	A	1558	A	C4-C5-N7	6.30	113.85	110.70
1	A	1212	G	N7-C8-N9	-6.30	109.95	113.10
1	A	1153	C	N3-C4-C5	-6.30	119.38	121.90
1	A	2516	G	C5-C6-O6	-6.30	124.82	128.60
1	A	1322	A	C2-N3-C4	-6.30	107.45	110.60
1	A	2820	A	O5'-P-OP2	-6.29	100.03	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2723	C	C6-N1-C2	-6.29	117.78	120.30
34	a	1123	A	C5-C6-N1	-6.29	114.55	117.70
1	A	915	C	N1-C2-O2	6.29	122.67	118.90
34	a	1127	G	N3-C4-C5	6.29	131.74	128.60
1	A	1460	A	O4'-C1'-N9	6.28	113.23	108.20
1	A	803	U	N1-C2-N3	6.28	118.67	114.90
34	a	864	A	N1-C6-N6	6.28	122.37	118.60
1	A	961	C	N3-C4-N4	6.28	122.40	118.00
1	A	2559	C	C4-C5-C6	6.28	120.54	117.40
34	a	527	G	C4-C5-N7	-6.27	108.29	110.80
34	a	1132	C	C6-N1-C2	-6.27	117.79	120.30
1	A	2022	U	N3-C2-O2	6.27	126.59	122.20
1	A	2271	G	C8-N9-C1'	-6.27	118.85	127.00
34	a	1461	G	C4-N9-C1'	6.27	134.65	126.50
1	A	1621	U	O5'-P-OP2	-6.27	100.06	105.70
34	a	1063	C	C2-N1-C1'	-6.27	111.91	118.80
55	w	41	C	N3-C4-C5	6.27	124.41	121.90
1	A	239	U	C6-N1-C2	6.26	124.76	121.00
1	A	265	A	C5-C6-N1	-6.26	114.57	117.70
1	A	275	G	C4-N9-C1'	6.26	134.64	126.50
1	A	1998	G	O5'-P-OP1	-6.26	100.06	105.70
1	A	2820	A	C5-N7-C8	-6.26	100.77	103.90
1	A	246	C	N1-C2-O2	-6.25	115.15	118.90
1	A	275	G	N7-C8-N9	6.25	116.23	113.10
1	A	1957	C	OP2-P-O3'	6.25	118.96	105.20
1	A	2065	C	O5'-P-OP1	-6.25	100.07	105.70
1	A	2522	U	N3-C4-O4	6.25	123.78	119.40
34	a	115	G	C5-C6-O6	-6.25	124.85	128.60
1	A	2576	G	C4-N9-C1'	6.25	134.63	126.50
34	a	1505	G	C4-C5-N7	-6.25	108.30	110.80
34	a	880	C	C6-N1-C2	6.24	122.80	120.30
1	A	1619	G	N3-C2-N2	-6.24	115.53	119.90
34	a	365	U	C4-C5-C6	6.24	123.44	119.70
1	A	561	G	C6-C5-N7	6.24	134.14	130.40
34	a	119	A	N1-C6-N6	-6.23	114.86	118.60
33	x	64	A	C5-C6-N1	-6.23	114.58	117.70
34	a	314	C	N3-C2-O2	-6.23	117.54	121.90
1	A	459	U	C5-C4-O4	-6.23	122.16	125.90
34	a	1125	U	O5'-P-OP2	6.23	118.17	110.70
1	A	491	G	N3-C4-N9	-6.22	122.27	126.00
1	A	1645	G	N3-C4-N9	6.22	129.73	126.00
1	A	364	C	C2-N1-C1'	6.22	125.64	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	748	C	C6-N1-C2	-6.22	117.81	120.30
34	a	841	U	C5-C6-N1	6.21	125.81	122.70
1	A	1430	C	C6-N1-C2	-6.21	117.82	120.30
34	a	1279	A	C5-N7-C8	-6.21	100.80	103.90
1	A	272	G	N1-C6-O6	6.21	123.63	119.90
1	A	1813	G	C8-N9-C4	6.21	108.88	106.40
1	A	1256	G	C8-N9-C4	-6.21	103.92	106.40
1	A	1772	G	C2-N3-C4	-6.21	108.80	111.90
1	A	2056	G	N1-C6-O6	6.20	123.62	119.90
34	a	940	C	N1-C2-O2	-6.20	115.18	118.90
1	A	129	C	C5-C6-N1	-6.20	117.90	121.00
34	a	860	A	C2-N3-C4	-6.20	107.50	110.60
1	A	467	G	C2-N3-C4	-6.20	108.80	111.90
1	A	2638	G	C8-N9-C4	-6.20	103.92	106.40
1	A	774	A	N1-C2-N3	6.20	132.40	129.30
1	A	1214	A	N1-C6-N6	-6.20	114.88	118.60
34	a	957	U	N1-C2-O2	-6.20	118.46	122.80
34	a	117	G	C6-C5-N7	-6.19	126.68	130.40
34	a	117	G	N3-C4-N9	6.19	129.72	126.00
35	b	213	LEU	CA-CB-CG	6.19	129.54	115.30
1	A	2059	A	C6-C5-N7	-6.19	127.97	132.30
34	a	1206	G	N3-C2-N2	-6.19	115.57	119.90
34	a	1036	G	C8-N9-C1'	-6.19	118.95	127.00
34	a	1187	G	C8-N9-C4	-6.19	103.92	106.40
1	A	2774	C	N3-C4-C5	6.19	124.37	121.90
1	A	592	G	N1-C6-O6	6.18	123.61	119.90
34	a	1053	G	N7-C8-N9	-6.18	110.01	113.10
1	A	190	A	OP2-P-O3'	6.18	118.79	105.20
1	A	2742	C	N1-C2-O2	-6.18	115.19	118.90
34	a	1151	A	N1-C6-N6	-6.18	114.89	118.60
34	a	319	G	N1-C6-O6	-6.17	116.20	119.90
1	A	13	A	N9-C4-C5	6.17	108.27	105.80
1	A	2717	G	N1-C6-O6	6.17	123.60	119.90
8	J	69	PRO	N-CA-CB	6.17	110.70	103.30
34	a	117	G	C4-C5-N7	6.17	113.27	110.80
34	a	805	C	C5-C6-N1	6.17	124.08	121.00
8	J	101	PRO	N-CA-CB	6.16	110.69	103.30
1	A	1034	G	C5-C6-O6	-6.16	124.91	128.60
1	A	788	A	C8-N9-C4	6.15	108.26	105.80
34	a	1363	C	C6-N1-C1'	6.15	128.18	120.80
1	A	584	C	N1-C2-O2	6.15	122.59	118.90
1	A	1190	G	N9-C4-C5	-6.15	102.94	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1944	U	C4-C5-C6	6.15	123.39	119.70
1	A	2474	C	N1-C2-O2	6.14	122.58	118.90
1	A	452	G	C5-C6-O6	-6.14	124.92	128.60
1	A	963	U	N1-C2-N3	-6.14	111.22	114.90
1	A	778	G	C5-C6-O6	-6.14	124.92	128.60
1	A	1166	C	C6-N1-C2	-6.14	117.84	120.30
34	a	115	G	P-O3'-C3'	6.14	127.06	119.70
1	A	450	G	C5-C6-N1	-6.13	108.43	111.50
1	A	2394	C	C6-N1-C2	-6.13	117.85	120.30
34	a	819	A	C6-C5-N7	-6.13	128.01	132.30
1	A	685	A	O5'-P-OP2	-6.13	100.18	105.70
1	A	961	C	C6-N1-C2	-6.13	117.85	120.30
1	A	2466	C	C6-N1-C2	6.13	122.75	120.30
34	a	123	C	C6-N1-C2	6.13	122.75	120.30
1	A	1271	G	C5-C6-N1	-6.13	108.44	111.50
1	A	1698	A	O4'-C1'-N9	6.13	113.10	108.20
1	A	2434	A	O5'-P-OP2	-6.13	100.19	105.70
33	x	23	A	N1-C6-N6	-6.13	114.92	118.60
1	A	795	C	C6-N1-C2	-6.12	117.85	120.30
1	A	2509	G	N1-C6-O6	6.12	123.57	119.90
1	A	687	C	C6-N1-C2	-6.12	117.85	120.30
34	a	852	G	N3-C2-N2	6.12	124.18	119.90
1	A	1939	U	O5'-P-OP1	-6.12	100.19	105.70
1	A	2095	C	O3'-P-O5'	6.12	115.62	104.00
1	A	2779	U	O5'-P-OP2	-6.12	100.19	105.70
1	A	565	C	OP1-P-OP2	-6.12	110.43	119.60
34	a	1363	C	O4'-C1'-N1	6.12	113.09	108.20
34	a	959	A	N1-C6-N6	6.11	122.27	118.60
34	a	1351	U	N1-C2-O2	-6.11	118.52	122.80
34	a	1432	G	N3-C4-C5	-6.11	125.54	128.60
1	A	570	G	C5-C6-O6	6.11	132.27	128.60
1	A	1245	G	N1-C6-O6	-6.11	116.23	119.90
34	a	1123	A	N9-C4-C5	6.11	108.24	105.80
34	a	1237	C	N3-C4-C5	6.11	124.34	121.90
1	A	866	A	N7-C8-N9	6.10	116.85	113.80
1	A	1320	C	C5-C4-N4	-6.10	115.93	120.20
34	a	605	U	C5-C4-O4	6.09	129.56	125.90
34	a	1491	G	C8-N9-C4	-6.09	103.96	106.40
1	A	985	C	C5-C6-N1	-6.09	117.95	121.00
1	A	2394	C	N3-C2-O2	-6.09	117.64	121.90
1	A	2610	C	N3-C2-O2	-6.09	117.64	121.90
34	a	1126	U	N3-C4-O4	6.09	123.66	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1620	G	C5-C6-N1	-6.08	108.46	111.50
2	B	96	U	N3-C2-O2	-6.08	117.94	122.20
1	A	1970	A	N1-C6-N6	6.08	122.25	118.60
1	A	1999	C	C6-N1-C2	6.08	122.73	120.30
1	A	2570	G	C8-N9-C4	6.07	108.83	106.40
8	J	105	PRO	N-CA-CB	6.07	110.58	103.30
1	A	2712(A)	A	C8-N9-C4	-6.06	103.38	105.80
34	a	117	G	C5-C6-O6	-6.06	124.96	128.60
34	a	1054	C	N1-C2-O2	6.06	122.54	118.90
1	A	1191	G	N3-C4-N9	-6.06	122.36	126.00
34	a	855	G	N1-C6-O6	6.06	123.53	119.90
1	A	1667	G	C5-N7-C8	6.05	107.33	104.30
34	a	748	C	N1-C2-O2	6.05	122.53	118.90
1	A	1214	A	N9-C4-C5	6.05	108.22	105.80
1	A	2592	G	C6-C5-N7	-6.05	126.77	130.40
1	A	1046	A	O4'-C1'-N9	6.05	113.04	108.20
1	A	1424	G	N3-C4-N9	6.05	129.63	126.00
1	A	2820	A	N9-C4-C5	-6.05	103.38	105.80
34	a	515	G	C6-C5-N7	-6.05	126.77	130.40
1	A	1617	C	C2-N1-C1'	-6.05	112.15	118.80
1	A	1992	G	P-O3'-C3'	6.05	126.96	119.70
55	w	57	G	C8-N9-C4	-6.04	103.98	106.40
1	A	1424	G	C6-C5-N7	-6.04	126.78	130.40
1	A	2324	C	C6-N1-C2	6.04	122.71	120.30
1	A	391	G	N1-C6-O6	6.03	123.52	119.90
1	A	806	C	N3-C4-C5	6.03	124.31	121.90
1	A	2417	C	C6-N1-C2	6.03	122.71	120.30
57	y	282	LEU	N-CA-C	-6.03	94.71	111.00
1	A	2019	A	C8-N9-C4	-6.03	103.39	105.80
1	A	298	G	N1-C6-O6	6.03	123.52	119.90
1	A	1653	G	N3-C4-C5	-6.03	125.58	128.60
34	a	1124	G	C8-N9-C4	-6.03	103.99	106.40
1	A	2780	G	N3-C4-N9	6.03	129.62	126.00
1	A	941	A	C8-N9-C4	6.03	108.21	105.80
34	a	527	G	C5-C6-O6	6.03	132.22	128.60
1	A	240	G	N9-C4-C5	6.02	107.81	105.40
1	A	1958	C	N3-C4-N4	6.02	122.22	118.00
1	A	1306	C	N1-C2-O2	6.02	122.51	118.90
1	A	2460	U	C5-C6-N1	-6.02	119.69	122.70
34	a	575	G	N1-C6-O6	6.02	123.51	119.90
1	A	328	U	C6-N1-C2	-6.02	117.39	121.00
1	A	2810	A	C8-N9-C4	6.02	108.21	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1221	G	C4-C5-N7	-6.02	108.39	110.80
1	A	733	G	C5-N7-C8	-6.01	101.29	104.30
1	A	2093	G	N9-C4-C5	6.01	107.81	105.40
34	a	394	G	O5'-P-OP2	-6.01	100.29	105.70
11	O	8	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	2078	C	O5'-P-OP1	-6.01	100.29	105.70
1	A	2856	C	N3-C2-O2	-6.00	117.70	121.90
1	A	1343	G	C8-N9-C4	-6.00	104.00	106.40
34	a	562	C	N3-C4-C5	6.00	124.30	121.90
55	w	57	G	N3-C4-C5	-6.00	125.60	128.60
1	A	2071	A	N1-C6-N6	6.00	122.20	118.60
1	A	781	A	C5-C6-N1	6.00	120.70	117.70
1	A	991	C	C6-N1-C2	-6.00	117.90	120.30
34	a	314	C	N1-C2-O2	5.99	122.50	118.90
1	A	818	G	O5'-P-OP1	5.99	117.89	110.70
1	A	446	G	O5'-P-OP2	-5.99	100.31	105.70
57	y	291	TYR	C-N-CD	5.99	140.98	128.40
1	A	2064	C	N1-C2-O2	-5.99	115.31	118.90
34	a	1258	G	C5-C6-N1	5.99	114.49	111.50
34	a	1502	A	C4-C5-N7	5.99	113.69	110.70
1	A	1555	G	N1-C6-O6	5.99	123.49	119.90
1	A	961	C	C4-C5-C6	5.98	120.39	117.40
1	A	964	C	N3-C4-C5	5.98	124.29	121.90
1	A	2610	C	N3-C4-C5	-5.98	119.51	121.90
1	A	2820	A	C4-C5-N7	5.98	113.69	110.70
2	B	71	C	N1-C2-O2	5.98	122.49	118.90
1	A	1698	A	C5-N7-C8	-5.98	100.91	103.90
1	A	379	G	C8-N9-C4	-5.98	104.01	106.40
1	A	1936	A	O4'-C1'-N9	5.98	112.98	108.20
1	A	1202	C	N1-C2-O2	-5.97	115.31	118.90
1	A	2586	C	N1-C2-O2	-5.97	115.32	118.90
1	A	2576	G	C8-N9-C1'	-5.97	119.23	127.00
57	y	159	PRO	C-N-CA	-5.97	106.77	121.70
34	a	855	G	C6-C5-N7	-5.97	126.82	130.40
39	f	75	LEU	CA-CB-CG	5.97	129.02	115.30
1	A	1899	G	C4-N9-C1'	5.96	134.25	126.50
8	J	33	PRO	N-CA-CB	5.96	110.46	103.30
34	a	1036	G	N3-C4-N9	5.96	129.58	126.00
34	a	748	C	P-O3'-C3'	5.96	126.86	119.70
1	A	1021	A	O5'-P-OP1	-5.96	100.34	105.70
1	A	1919	A	C8-N9-C4	-5.96	103.42	105.80
34	a	1124	G	C4-C5-N7	-5.96	108.42	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1628	G	C6-C5-N7	-5.96	126.83	130.40
34	a	1068	G	C4-N9-C1'	5.96	134.24	126.50
55	w	29	G	C6-C5-N7	-5.96	126.83	130.40
57	y	191	ASP	C-N-CD	5.95	140.90	128.40
1	A	512	G	N1-C6-O6	-5.95	116.33	119.90
34	a	401	C	C6-N1-C2	-5.95	117.92	120.30
34	a	575	G	O5'-P-OP2	-5.95	100.35	105.70
1	A	570	G	N9-C4-C5	5.95	107.78	105.40
1	A	1285	G	OP2-P-O3'	5.95	118.28	105.20
1	A	1897	G	C8-N9-C4	5.95	108.78	106.40
1	A	1227	G	C2-N3-C4	-5.94	108.93	111.90
1	A	1758	G	C6-C5-N7	-5.94	126.84	130.40
1	A	1653	G	P-O3'-C3'	5.94	126.82	119.70
1	A	714	U	C5-C6-N1	-5.93	119.74	122.70
1	A	2789	C	C6-N1-C2	5.93	122.67	120.30
34	a	573	A	C8-N9-C4	-5.93	103.43	105.80
34	a	23	C	C6-N1-C2	-5.92	117.93	120.30
34	a	1076	C	N3-C2-O2	-5.92	117.75	121.90
34	a	855	G	C5-C6-O6	-5.92	125.05	128.60
1	A	1958	C	OP1-P-OP2	-5.91	110.73	119.60
34	a	1219	U	N1-C2-O2	-5.91	118.66	122.80
34	a	1227	A	C2-N3-C4	-5.91	107.64	110.60
1	A	252	G	C6-C5-N7	-5.91	126.85	130.40
1	A	1698	A	N1-C2-N3	5.91	132.25	129.30
34	a	1254	C	C6-N1-C2	5.91	122.66	120.30
1	A	692	C	N3-C2-O2	-5.91	117.76	121.90
1	A	2889	C	C2-N1-C1'	5.91	125.30	118.80
34	a	515	G	C4-C5-N7	5.91	113.16	110.80
1	A	2395	C	C6-N1-C2	-5.90	117.94	120.30
34	a	258	G	C8-N9-C1'	-5.90	119.33	127.00
34	a	805	C	C5-C4-N4	-5.90	116.07	120.20
34	a	91	C	N3-C2-O2	-5.90	117.77	121.90
1	A	526	A	N1-C6-N6	-5.90	115.06	118.60
34	a	301	G	N1-C6-O6	5.90	123.44	119.90
1	A	451	C	N3-C2-O2	5.89	126.03	121.90
1	A	1034	G	N1-C6-O6	5.89	123.44	119.90
33	x	15	G	N3-C2-N2	5.89	124.03	119.90
1	A	742	G	C8-N9-C4	5.89	108.76	106.40
34	a	1525	G	C5-N7-C8	-5.89	101.36	104.30
1	A	1772	G	N1-C6-O6	5.89	123.43	119.90
1	A	1896	G	N1-C6-O6	5.89	123.43	119.90
57	y	441	LEU	C-N-CD	5.89	140.76	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	A	N7-C8-N9	5.88	116.74	113.80
1	A	661	C	C6-N1-C2	5.88	122.65	120.30
1	A	701	G	C8-N9-C4	5.88	108.75	106.40
1	A	1653	G	C8-N9-C4	-5.88	104.05	106.40
34	a	258	G	C6-C5-N7	-5.88	126.87	130.40
34	a	717	C	N3-C2-O2	5.88	126.02	121.90
1	A	859	G	C8-N9-C1'	5.88	134.64	127.00
1	A	944	G	C6-C5-N7	-5.88	126.87	130.40
1	A	1992	G	O4'-C1'-N9	-5.88	103.50	108.20
34	a	1150	U	C2-N3-C4	5.88	130.53	127.00
1	A	1950	G	N1-C6-O6	-5.88	116.37	119.90
34	a	394	G	C5-C6-O6	5.88	132.12	128.60
34	a	1187	G	N9-C4-C5	5.88	107.75	105.40
1	A	1992	G	N3-C4-N9	5.87	129.52	126.00
1	A	139(A)	G	C8-N9-C4	-5.87	104.05	106.40
34	a	117	G	N1-C6-O6	5.87	123.42	119.90
34	a	1527	C	C4-C5-C6	-5.87	114.47	117.40
1	A	558	G	N1-C6-O6	5.86	123.42	119.90
1	A	1061	U	C5-C6-N1	5.86	125.63	122.70
1	A	2624	G	N3-C4-C5	-5.86	125.67	128.60
1	A	190	A	N1-C6-N6	-5.86	115.08	118.60
1	A	2242	G	N3-C4-N9	-5.86	122.48	126.00
34	a	954	G	C8-N9-C4	5.86	108.74	106.40
34	a	1356	G	C5-C6-O6	5.86	132.11	128.60
37	d	139	ARG	NE-CZ-NH1	5.86	123.23	120.30
34	a	1254	C	N3-C4-C5	5.85	124.24	121.90
1	A	645	C	C6-N1-C2	-5.85	117.96	120.30
1	A	1796	U	C5-C6-N1	-5.85	119.78	122.70
34	a	79	G	N1-C6-O6	-5.85	116.39	119.90
1	A	1404	C	C2-N1-C1'	5.85	125.23	118.80
2	B	7	G	C8-N9-C4	-5.85	104.06	106.40
1	A	2443	C	C2-N3-C4	-5.85	116.98	119.90
55	w	73	A	C8-N9-C4	-5.84	103.46	105.80
1	A	1328	G	C5-C6-O6	-5.84	125.10	128.60
1	A	1299	G	O5'-P-OP2	-5.84	100.44	105.70
57	y	303	ALA	N-CA-C	-5.84	95.23	111.00
1	A	1973	G	N9-C4-C5	5.84	107.73	105.40
1	A	2096	U	OP1-P-OP2	5.84	128.35	119.60
57	y	557	ASP	C-N-CA	5.84	136.29	121.70
1	A	2038	G	OP2-P-O3'	5.83	118.03	105.20
1	A	335	C	C5-C6-N1	5.83	123.92	121.00
1	A	2286	A	C2-N3-C4	-5.83	107.69	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2450	A	O5'-P-OP1	-5.83	100.45	105.70
34	a	333	G	C4-C5-N7	5.83	113.13	110.80
1	A	961	C	N3-C4-C5	-5.83	119.57	121.90
34	a	1280	A	N3-C4-C5	-5.83	122.72	126.80
1	A	2084	C	N3-C4-C5	5.82	124.23	121.90
1	A	2324	C	C5-C6-N1	-5.82	118.09	121.00
1	A	800	A	O5'-P-OP2	-5.82	100.46	105.70
1	A	1654	A	O5'-P-OP1	-5.82	100.46	105.70
1	A	797	C	O5'-P-OP2	-5.82	100.47	105.70
1	A	2566	A	N1-C6-N6	-5.82	115.11	118.60
57	y	407	GLU	C-N-CD	5.82	140.62	128.40
1	A	1239	G	C8-N9-C4	-5.81	104.08	106.40
34	a	509	A	N7-C8-N9	5.81	116.70	113.80
34	a	851	G	N1-C6-O6	5.81	123.39	119.90
1	A	2439	A	OP1-P-O3'	5.81	117.98	105.20
1	A	2559	C	C5-C6-N1	-5.81	118.10	121.00
1	A	2791	C	N3-C4-N4	5.81	122.06	118.00
1	A	195	A	C4-C5-N7	5.81	113.60	110.70
34	a	78	G	C5-C6-O6	5.80	132.08	128.60
34	a	1266	G	N3-C4-N9	-5.80	122.52	126.00
1	A	1921	G	N1-C6-O6	5.80	123.38	119.90
1	A	2789	C	C5-C6-N1	-5.80	118.10	121.00
1	A	1955	U	C5-C4-O4	5.80	129.38	125.90
34	a	1206	G	C5-C6-O6	-5.80	125.12	128.60
1	A	307	G	C8-N9-C4	-5.79	104.08	106.40
1	A	797	C	O5'-P-OP1	5.79	117.65	110.70
1	A	2179	C	N1-C2-O2	5.79	122.38	118.90
17	U	92	ARG	NE-CZ-NH1	-5.79	117.40	120.30
34	a	327	A	N1-C6-N6	5.79	122.08	118.60
34	a	330	C	OP1-P-O3'	5.79	117.95	105.20
34	a	1442	G	N1-C6-O6	5.79	123.38	119.90
1	A	1980	G	N9-C4-C5	-5.79	103.08	105.40
34	a	1124	G	N9-C4-C5	5.79	107.72	105.40
1	A	1343	G	C4-N9-C1'	5.79	134.03	126.50
1	A	531	C	N1-C2-O2	5.79	122.37	118.90
1	A	818	G	O5'-P-OP2	-5.78	100.49	105.70
1	A	1325	G	O4'-C1'-N9	5.78	112.83	108.20
33	x	56	C	N3-C2-O2	-5.78	117.85	121.90
34	a	258	G	C4-N9-C1'	5.78	134.02	126.50
34	a	406	G	N3-C4-N9	5.78	129.47	126.00
34	a	1123	A	N1-C6-N6	-5.78	115.13	118.60
1	A	808	G	C4-N9-C1'	5.78	134.01	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2448	A	C5-C6-N6	-5.78	119.08	123.70
1	A	2030	A	O4'-C1'-N9	5.78	112.82	108.20
34	a	976	G	C4-N9-C1'	5.77	134.00	126.50
1	A	1919	A	N1-C6-N6	-5.77	115.14	118.60
1	A	1979	C	C6-N1-C2	5.77	122.61	120.30
1	A	2174	C	C2-N3-C4	5.77	122.78	119.90
1	A	2335	A	O4'-C1'-N9	5.77	112.82	108.20
34	a	569	C	C6-N1-C2	5.77	122.61	120.30
1	A	945	A	N9-C4-C5	-5.77	103.49	105.80
1	A	2501	C	C5-C6-N1	-5.77	118.12	121.00
7	H	3	ARG	NE-CZ-NH1	5.76	123.18	120.30
34	a	1461	G	C6-C5-N7	-5.76	126.94	130.40
37	d	194	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	329	G	N3-C4-N9	5.76	129.46	126.00
34	a	362	G	N1-C6-O6	5.76	123.36	119.90
34	a	1237	C	C6-N1-C2	5.76	122.60	120.30
34	a	1343	G	N1-C2-N3	5.76	127.36	123.90
34	a	1420	C	N1-C2-O2	-5.76	115.44	118.90
57	y	553	ALA	N-CA-C	5.76	126.55	111.00
1	A	1653	G	C8-N9-C1'	-5.76	119.52	127.00
34	a	1036	G	N3-C4-C5	-5.76	125.72	128.60
33	x	68	C	C5-C6-N1	5.76	123.88	121.00
34	a	1402	C	C6-N1-C2	-5.75	118.00	120.30
1	A	868	U	C5-C6-N1	-5.75	119.82	122.70
1	A	1272	A	N1-C2-N3	5.75	132.18	129.30
1	A	1519	G	N3-C4-C5	-5.75	125.72	128.60
1	A	565	C	O5'-P-OP1	-5.75	100.53	105.70
1	A	572	A	N1-C6-N6	5.75	122.05	118.60
34	a	841	U	C6-N1-C2	-5.75	117.55	121.00
1	A	586	A	C2-N3-C4	-5.75	107.73	110.60
1	A	2458	G	N3-C2-N2	-5.74	115.88	119.90
1	A	2095	C	OP1-P-O3'	-5.74	92.57	105.20
4	E	47	VAL	CB-CA-C	-5.74	100.50	111.40
34	a	1392	G	C5-C6-N1	-5.74	108.63	111.50
55	w	40	C	N1-C2-O2	5.74	122.34	118.90
34	a	962	C	N1-C2-O2	-5.73	115.46	118.90
34	a	1359	C	N1-C2-O2	5.73	122.34	118.90
34	a	1290	G	C5-C6-O6	-5.73	125.16	128.60
34	a	1486	G	C4-N9-C1'	5.73	133.95	126.50
34	a	79	G	C5-C6-O6	5.73	132.03	128.60
34	a	1386	G	N3-C2-N2	-5.72	115.89	119.90
34	a	1530	G	C8-N9-C1'	5.72	134.44	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1758	G	C4-N9-C1'	5.72	133.94	126.50
1	A	1138	G	C5-C6-N1	5.72	114.36	111.50
1	A	973	A	N1-C2-N3	5.72	132.16	129.30
34	a	263	A	C5-C6-N1	5.72	120.56	117.70
1	A	2230	G	C5-C6-O6	5.72	132.03	128.60
34	a	1053	G	C8-N9-C4	5.72	108.69	106.40
1	A	1558	A	C5-N7-C8	-5.71	101.04	103.90
1	A	2243	U	O5'-P-OP1	5.71	117.55	110.70
34	a	37	U	N3-C4-O4	5.71	123.39	119.40
34	a	15	G	C4-C5-N7	5.71	113.08	110.80
34	a	936	C	C6-N1-C2	-5.71	118.02	120.30
34	a	717	C	N1-C2-O2	-5.71	115.48	118.90
34	a	1330	U	N3-C2-O2	-5.70	118.21	122.20
56	v	13	A	C8-N9-C4	-5.70	103.52	105.80
57	y	333	GLU	C-N-CD	5.70	140.37	128.40
1	A	1767	C	C6-N1-C2	-5.70	118.02	120.30
34	a	1227	A	C5-N7-C8	-5.70	101.05	103.90
1	A	330	A	C5-N7-C8	-5.69	101.05	103.90
1	A	781	A	C2-N3-C4	5.69	113.45	110.60
34	a	752	G	N1-C6-O6	-5.69	116.48	119.90
34	a	1456	G	N3-C4-C5	5.69	131.45	128.60
57	y	287	THR	C-N-CD	5.69	140.35	128.40
1	A	2556	C	N3-C4-N4	5.69	121.98	118.00
1	A	2611	U	C5-C4-O4	-5.69	122.48	125.90
34	a	1516	G	N3-C4-C5	5.69	131.44	128.60
34	a	1230	C	C5-C6-N1	5.69	123.84	121.00
1	A	1189	A	N1-C6-N6	5.69	122.01	118.60
1	A	1218	C	C6-N1-C2	-5.68	118.03	120.30
34	a	897	C	O5'-P-OP2	-5.68	100.58	105.70
1	A	2140	C	C5-C4-N4	5.68	124.18	120.20
34	a	232	G	N1-C6-O6	5.68	123.31	119.90
1	A	1902	C	N3-C2-O2	-5.68	117.92	121.90
1	A	2283	C	C6-N1-C2	-5.67	118.03	120.30
34	a	288	A	C4-C5-C6	5.67	119.84	117.00
1	A	80	G	C5-C6-O6	-5.67	125.20	128.60
1	A	581	C	C2-N1-C1'	5.67	125.04	118.80
1	A	1491	G	N1-C6-O6	-5.67	116.50	119.90
1	A	1369	G	C8-N9-C4	-5.67	104.13	106.40
1	A	1697	G	C5-C6-O6	-5.67	125.20	128.60
34	a	233	C	C6-N1-C2	-5.67	118.03	120.30
34	a	863	U	C2-N1-C1'	-5.67	110.89	117.70
1	A	979	G	N7-C8-N9	5.67	115.94	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1899	G	N3-C4-C5	-5.67	125.77	128.60
34	a	300	A	C8-N9-C4	-5.67	103.53	105.80
1	A	830	G	C5-C6-O6	5.67	132.00	128.60
34	a	91	C	C6-N1-C2	-5.67	118.03	120.30
1	A	1936	A	C8-N9-C4	-5.66	103.53	105.80
34	a	959	A	N9-C4-C5	-5.66	103.53	105.80
34	a	1229	A	OP1-P-O3'	5.66	117.66	105.20
1	A	1899	G	C8-N9-C1'	-5.66	119.64	127.00
1	A	1772	G	C6-C5-N7	-5.66	127.00	130.40
34	a	619	U	C6-N1-C1'	5.66	129.13	121.20
1	A	1972	A	O5'-P-OP1	-5.66	100.61	105.70
33	x	60	U	C2-N1-C1'	5.66	124.49	117.70
34	a	913	A	C4-C5-C6	5.66	119.83	117.00
34	a	406	G	C5-C6-O6	-5.66	125.21	128.60
34	a	1067	A	N1-C6-N6	-5.66	115.21	118.60
1	A	139(A)	G	N1-C6-O6	-5.66	116.51	119.90
1	A	399	G	C2-N3-C4	-5.65	109.07	111.90
1	A	1416	G	O4'-C1'-N9	5.65	112.72	108.20
1	A	2070	G	C5-C6-N1	5.65	114.33	111.50
1	A	1657	C	N3-C4-N4	-5.65	114.04	118.00
1	A	2612	C	C6-N1-C2	5.65	122.56	120.30
34	a	302	G	N1-C6-O6	-5.65	116.51	119.90
34	a	572	A	N1-C2-N3	-5.65	126.47	129.30
1	A	645	C	C5-C6-N1	5.65	123.83	121.00
1	A	141	A	C5-N7-C8	-5.65	101.08	103.90
34	a	1514	C	C4-C5-C6	5.65	120.22	117.40
1	A	1493	C	C6-N1-C2	-5.65	118.04	120.30
1	A	2503	A	N1-C2-N3	-5.65	126.48	129.30
1	A	263	C	C2-N1-C1'	5.64	125.01	118.80
1	A	2276	G	N3-C4-N9	5.64	129.38	126.00
1	A	803	U	C4-C5-C6	5.64	123.08	119.70
34	a	10	A	C5-C6-N6	-5.64	119.19	123.70
34	a	369	C	C6-N1-C2	-5.64	118.04	120.30
34	a	549	C	N1-C2-O2	-5.64	115.52	118.90
1	A	1214	A	C5-C6-N6	5.64	128.21	123.70
1	A	1572	A	N1-C6-N6	5.64	121.98	118.60
34	a	1324	A	N9-C4-C5	5.64	108.05	105.80
34	a	1326	C	N1-C2-O2	-5.64	115.52	118.90
1	A	272(A)	U	C5-C6-N1	5.63	125.52	122.70
1	A	2828	C	C5-C6-N1	-5.63	118.19	121.00
34	a	325	A	C8-N9-C4	5.63	108.05	105.80
1	A	576	U	C5-C6-N1	5.63	125.51	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	331	G	OP1-P-O3'	5.63	117.58	105.20
34	a	880	C	C5-C6-N1	-5.63	118.19	121.00
34	a	1029	C	P-O3'-C3'	5.63	126.45	119.70
12	P	44	GLY	N-CA-C	-5.63	99.04	113.10
1	A	570	G	C8-N9-C4	-5.62	104.15	106.40
1	A	2508	G	O5'-P-OP2	-5.62	100.64	105.70
34	a	117	G	C8-N9-C1'	-5.62	119.69	127.00
1	A	983	A	N1-C6-N6	5.62	121.97	118.60
1	A	1797	C	C6-N1-C2	5.62	122.55	120.30
1	A	961	C	OP1-P-OP2	5.62	128.03	119.60
1	A	2693	A	C8-N9-C4	-5.62	103.55	105.80
34	a	1402	C	N3-C4-C5	-5.62	119.65	121.90
1	A	737	C	C6-N1-C2	5.62	122.55	120.30
1	A	1052	C	C5-C6-N1	5.62	123.81	121.00
47	n	44	LEU	CA-CB-CG	5.62	128.22	115.30
8	J	129	PRO	N-CA-CB	5.62	110.04	103.30
34	a	1125	U	C2-N1-C1'	-5.62	110.96	117.70
1	A	2638	G	N3-C4-N9	5.62	129.37	126.00
34	a	975	A	N7-C8-N9	5.62	116.61	113.80
1	A	945	A	N9-C1'-C2'	5.62	121.30	114.00
1	A	1787	A	C4-N9-C1'	5.62	136.41	126.30
1	A	2519	U	C2-N3-C4	-5.62	123.63	127.00
34	a	1399	C	O5'-P-OP1	-5.61	100.65	105.70
1	A	527	C	N3-C2-O2	-5.61	117.97	121.90
34	a	803	G	C5-C6-O6	5.61	131.96	128.60
34	a	976	G	N3-C2-N2	-5.61	115.97	119.90
55	w	29	G	C5-C6-O6	-5.61	125.23	128.60
34	a	569	C	C5-C6-N1	-5.61	118.20	121.00
57	y	140	LEU	C-N-CD	5.61	140.17	128.40
1	A	695	G	N1-C6-O6	5.60	123.26	119.90
1	A	137	C	C6-N1-C2	-5.60	118.06	120.30
1	A	569	U	N3-C2-O2	-5.60	118.28	122.20
1	A	1913	A	N1-C6-N6	5.60	121.96	118.60
1	A	571	A	O5'-P-OP1	-5.60	100.66	105.70
34	a	406	G	C4-N9-C1'	5.60	133.78	126.50
1	A	963	U	C6-N1-C2	5.60	124.36	121.00
1	A	1955	U	N1-C2-N3	5.60	118.26	114.90
1	A	2432	A	C8-N9-C4	5.59	108.04	105.80
34	a	1526	G	N1-C6-O6	5.59	123.26	119.90
1	A	830	G	N1-C6-O6	-5.59	116.55	119.90
1	A	2638	G	C4-N9-C1'	5.59	133.77	126.50
1	A	2503	A	N3-C4-N9	5.59	131.87	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	C	O5'-P-OP2	-5.59	100.67	105.70
34	a	796	C	C6-N1-C2	5.59	122.53	120.30
1	A	335	C	C6-N1-C2	-5.58	118.07	120.30
34	a	44	G	N1-C6-O6	-5.58	116.55	119.90
34	a	353	A	OP2-P-O3'	5.58	117.49	105.20
1	A	2554	U	N3-C4-O4	5.58	123.31	119.40
1	A	742	G	N1-C6-O6	5.58	123.25	119.90
34	a	345	C	N3-C2-O2	-5.58	117.99	121.90
34	a	750	G	N3-C4-C5	-5.58	125.81	128.60
1	A	581	C	N3-C2-O2	-5.58	118.00	121.90
1	A	1006	C	C5-C6-N1	5.58	123.79	121.00
1	A	1571	A	N1-C6-N6	-5.58	115.25	118.60
1	A	1721	G	C5-C6-O6	-5.58	125.25	128.60
1	A	1973	G	N3-C2-N2	-5.58	116.00	119.90
55	w	73	A	C4-C5-N7	5.58	113.49	110.70
34	a	937	A	N1-C6-N6	-5.58	115.25	118.60
1	A	1617	C	N1-C2-O2	-5.58	115.56	118.90
1	A	1562	A	N1-C6-N6	5.57	121.94	118.60
1	A	1314	C	C2-N1-C1'	5.57	124.93	118.80
1	A	1617	C	C6-N1-C1'	5.57	127.49	120.80
34	a	1363	C	N1-C2-O2	-5.57	115.56	118.90
1	A	1191	G	C4-N9-C1'	-5.57	119.27	126.50
1	A	141	A	C6-C5-N7	-5.56	128.41	132.30
1	A	263	C	C6-N1-C1'	-5.56	114.12	120.80
34	a	258	G	N3-C4-N9	5.56	129.34	126.00
34	a	899	C	C6-N1-C2	5.56	122.53	120.30
1	A	574	C	C6-N1-C2	5.56	122.53	120.30
1	A	973	A	C5-C6-N1	-5.56	114.92	117.70
1	A	2027	G	O5'-P-OP2	-5.56	100.69	105.70
1	A	2496	C	C5-C6-N1	-5.56	118.22	121.00
1	A	2546	U	N3-C2-O2	-5.56	118.31	122.20
55	w	45	U	N3-C4-O4	-5.56	115.51	119.40
1	A	1992	G	C5-C6-N1	5.56	114.28	111.50
26	3	31	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	841	A	O5'-P-OP2	-5.56	100.70	105.70
1	A	2638	G	C6-C5-N7	-5.56	127.07	130.40
34	a	1396	A	N1-C2-N3	5.56	132.08	129.30
1	A	815	C	C2-N1-C1'	5.55	124.91	118.80
34	a	365	U	N1-C2-O2	-5.55	118.91	122.80
34	a	1344	C	C6-N1-C2	5.55	122.52	120.30
1	A	399	G	C8-N9-C4	5.55	108.62	106.40
34	a	973	G	C4-C5-N7	-5.55	108.58	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1320	C	C6-N1-C1'	-5.55	114.14	120.80
1	A	2419	U	O5'-P-OP2	-5.55	100.71	105.70
1	A	2820	A	C6-C5-N7	-5.55	128.42	132.30
1	A	805	G	C8-N9-C4	5.54	108.62	106.40
34	a	1129	C	N3-C2-O2	-5.54	118.02	121.90
34	a	559	A	O5'-P-OP2	-5.54	100.71	105.70
34	a	1206	G	N1-C6-O6	5.54	123.22	119.90
1	A	381	G	N1-C6-O6	5.54	123.22	119.90
1	A	501	A	N1-C6-N6	-5.54	115.28	118.60
34	a	111	G	C5-C6-O6	-5.54	125.28	128.60
34	a	816	A	C8-N9-C4	5.54	108.02	105.80
1	A	803	U	C5-C6-N1	-5.54	119.93	122.70
1	A	1628	G	N1-C6-O6	5.54	123.22	119.90
1	A	1992	G	N3-C4-C5	-5.54	125.83	128.60
1	A	1208	C	C5-C6-N1	5.54	123.77	121.00
1	A	2308	G	O4'-C1'-N9	-5.53	103.77	108.20
1	A	307	G	N7-C8-N9	5.53	115.87	113.10
1	A	2766	G	C4-N9-C1'	5.53	133.69	126.50
34	a	651	C	C6-N1-C2	-5.53	118.09	120.30
1	A	195	A	C5-N7-C8	-5.53	101.14	103.90
1	A	1681	G	N3-C4-N9	-5.53	122.68	126.00
1	A	2198	A	OP1-P-O3'	5.53	117.36	105.20
1	A	2550	G	C6-C5-N7	-5.53	127.08	130.40
1	A	2579	C	N1-C2-O2	-5.53	115.58	118.90
1	A	751	A	N1-C2-N3	-5.52	126.54	129.30
1	A	1277	G	C8-N9-C4	5.52	108.61	106.40
34	a	913	A	P-O3'-C3'	5.52	126.33	119.70
1	A	1252	G	C6-C5-N7	-5.52	127.09	130.40
1	A	2503	A	C5-C6-N6	-5.52	119.28	123.70
34	a	1366	C	N1-C2-O2	-5.52	115.59	118.90
1	A	1199	U	C5-C6-N1	-5.52	119.94	122.70
1	A	1620	G	N1-C6-O6	5.52	123.21	119.90
34	a	881	G	O5'-P-OP2	5.52	117.32	110.70
1	A	614	U	O4'-C1'-N1	5.51	112.61	108.20
34	a	1524	C	C2-N3-C4	-5.51	117.14	119.90
1	A	561	G	C5-C6-N1	5.51	114.25	111.50
1	A	2742	C	C6-N1-C2	5.51	122.50	120.30
57	y	155	VAL	CB-CA-C	-5.51	100.93	111.40
34	a	981	U	C5-C4-O4	-5.51	122.59	125.90
34	a	878	G	N1-C6-O6	5.51	123.20	119.90
34	a	1346	A	C8-N9-C4	5.51	108.00	105.80
1	A	857	C	N1-C2-O2	-5.51	115.60	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2040	C	N1-C2-O2	5.51	122.20	118.90
1	A	2235	G	C6-C5-N7	-5.50	127.10	130.40
55	w	12	U	C5-C6-N1	-5.50	119.95	122.70
1	A	2001	A	N1-C2-N3	5.50	132.05	129.30
1	A	2638	G	C4-C5-C6	5.50	122.10	118.80
34	a	1346	A	OP1-P-O3'	5.50	117.31	105.20
34	a	976	G	C8-N9-C1'	-5.50	119.85	127.00
57	y	187	PRO	C-N-CD	5.50	139.95	128.40
1	A	1598	C	C5-C4-N4	-5.50	116.35	120.20
34	a	271	C	C6-N1-C2	-5.50	118.10	120.30
1	A	2546	U	C5-C6-N1	-5.50	119.95	122.70
47	n	53	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	997	G	O5'-P-OP1	-5.49	100.76	105.70
34	a	25	C	C6-N1-C2	-5.49	118.10	120.30
1	A	1761	C	C6-N1-C2	5.49	122.50	120.30
55	w	24	G	C5-N7-C8	-5.49	101.55	104.30
1	A	364	C	N1-C2-O2	5.49	122.19	118.90
34	a	1486	G	N3-C4-C5	-5.49	125.86	128.60
34	a	481	G	C5-C6-O6	-5.49	125.31	128.60
1	A	1778	U	N3-C4-O4	-5.48	115.56	119.40
34	a	1230	C	C6-N1-C2	-5.48	118.11	120.30
1	A	979	G	N1-C6-O6	5.48	123.19	119.90
1	A	1202	C	N3-C2-O2	5.48	125.74	121.90
34	a	1502	A	N7-C8-N9	5.48	116.54	113.80
34	a	1248	A	C5-C6-N1	5.48	120.44	117.70
57	y	103	VAL	CB-CA-C	-5.48	101.00	111.40
1	A	948	G	N1-C6-O6	5.47	123.18	119.90
1	A	1702	G	N9-C4-C5	5.47	107.59	105.40
34	a	559	A	C2-N3-C4	5.47	113.34	110.60
34	a	1494	G	N3-C4-N9	5.47	129.28	126.00
1	A	693	C	N1-C2-O2	5.47	122.18	118.90
1	A	2239	G	N1-C6-O6	5.47	123.18	119.90
1	A	2612	C	N3-C4-C5	5.47	124.09	121.90
1	A	1950	G	N9-C4-C5	5.47	107.59	105.40
1	A	2262	U	O5'-P-OP1	-5.47	100.78	105.70
34	a	1221	G	C5-C6-O6	5.47	131.88	128.60
1	A	941	A	O5'-P-OP1	-5.47	100.78	105.70
1	A	1395	A	O4'-C1'-N9	5.47	112.58	108.20
33	x	50	U	N3-C4-C5	-5.46	111.32	114.60
34	a	400	C	N3-C4-C5	-5.46	119.71	121.90
34	a	1083	U	C2-N3-C4	5.46	130.28	127.00
1	A	266	G	C6-C5-N7	-5.46	127.12	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	374	PRO	CA-N-CD	-5.46	103.85	111.50
1	A	22	C	N1-C2-O2	5.46	122.17	118.90
34	a	1195	C	N1-C2-O2	-5.46	115.62	118.90
1	A	2047	U	N1-C2-N3	5.46	118.17	114.90
1	A	2767	C	C2-N1-C1'	5.46	124.80	118.80
34	a	369	C	C5-C6-N1	5.46	123.73	121.00
1	A	298	G	C4-C5-N7	5.46	112.98	110.80
1	A	2581	G	O4'-C1'-N9	5.46	112.56	108.20
1	A	2088	G	N9-C4-C5	5.45	107.58	105.40
34	a	70	G	N1-C6-O6	5.45	123.17	119.90
34	a	976	G	C6-C5-N7	-5.45	127.13	130.40
34	a	1461	G	C8-N9-C1'	-5.45	119.91	127.00
1	A	1938	A	C8-N9-C4	5.45	107.98	105.80
55	w	70	G	N1-C6-O6	5.45	123.17	119.90
55	w	73	A	C6-C5-N7	-5.45	128.49	132.30
1	A	796	C	OP1-P-OP2	5.45	127.77	119.60
34	a	225	C	C5-C6-N1	-5.45	118.28	121.00
34	a	1502	A	C5-C6-N1	-5.45	114.98	117.70
1	A	1142(A)	A	N3-C4-C5	5.44	130.61	126.80
34	a	295	C	C6-N1-C2	5.44	122.48	120.30
1	A	1950	G	C4-C5-N7	-5.44	108.62	110.80
34	a	508	C	N1-C2-O2	-5.44	115.64	118.90
34	a	529	G	C5-C6-O6	-5.44	125.34	128.60
34	a	975	A	N9-C4-C5	-5.44	103.62	105.80
1	A	1799	G	C4-C5-N7	-5.44	108.62	110.80
34	a	397	A	C4-C5-C6	5.44	119.72	117.00
34	a	61	G	N1-C6-O6	5.43	123.16	119.90
1	A	2584	U	C5-C4-O4	5.43	129.16	125.90
34	a	317	G	C5-C6-O6	-5.43	125.34	128.60
34	a	1496	C	N1-C2-O2	-5.43	115.64	118.90
34	a	1525	G	C4-C5-N7	5.43	112.97	110.80
1	A	2252	G	OP2-P-O3'	5.43	117.14	105.20
1	A	1108	U	P-O3'-C3'	5.43	126.21	119.70
1	A	90	U	N1-C2-O2	5.43	126.60	122.80
34	a	940	C	N3-C2-O2	5.43	125.70	121.90
1	A	1599	C	C5-C6-N1	5.42	123.71	121.00
34	a	929	G	C6-C5-N7	5.42	133.65	130.40
1	A	933	A	C6-C5-N7	-5.42	128.51	132.30
1	A	24	G	N1-C6-O6	5.42	123.15	119.90
1	A	1109	C	C6-N1-C1'	-5.42	114.30	120.80
1	A	1700	A	N1-C6-N6	5.42	121.85	118.60
33	x	23	A	C4-C5-C6	-5.42	114.29	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	x	68	C	N3-C2-O2	-5.42	118.11	121.90
34	a	986	A	C5-C6-N6	-5.42	119.37	123.70
1	A	48	G	N9-C4-C5	5.41	107.56	105.40
1	A	997	G	C8-N9-C4	5.41	108.56	106.40
1	A	1493	C	C2-N1-C1'	5.41	124.75	118.80
1	A	47	C	O5'-P-OP1	-5.41	100.83	105.70
1	A	436	C	N1-C2-O2	5.41	122.14	118.90
1	A	810	U	C5-C6-N1	-5.41	120.00	122.70
1	A	1138	G	N1-C6-O6	-5.41	116.65	119.90
34	a	819	A	C5-N7-C8	-5.41	101.20	103.90
1	A	1019	U	N3-C2-O2	-5.41	118.42	122.20
1	A	2059	A	C4-C5-N7	5.41	113.40	110.70
34	a	667	G	C8-N9-C4	-5.41	104.24	106.40
1	A	2502	G	O5'-P-OP2	-5.40	100.84	105.70
1	A	1842	G	C6-C5-N7	-5.40	127.16	130.40
34	a	1225	A	N1-C2-N3	-5.40	126.60	129.30
1	A	673	C	C5-C4-N4	-5.40	116.42	120.20
1	A	2178	C	C5-C4-N4	5.40	123.98	120.20
1	A	562	U	OP1-P-OP2	5.40	127.70	119.60
34	a	576	G	C4-N9-C1'	5.40	133.52	126.50
57	y	213	PRO	CA-N-CD	-5.40	103.94	111.50
34	a	194	C	C5-C4-N4	-5.40	116.42	120.20
1	A	661	C	N3-C2-O2	5.39	125.68	121.90
1	A	959	A	C6-N1-C2	5.39	121.84	118.60
1	A	1314	C	N1-C2-O2	5.39	122.14	118.90
34	a	436	C	C5-C4-N4	-5.39	116.42	120.20
1	A	1136	G	N1-C6-O6	5.39	123.14	119.90
34	a	1074	G	C8-N9-C4	5.39	108.56	106.40
34	a	365	U	O4'-C1'-N1	5.39	112.51	108.20
34	a	436	C	C6-N1-C2	-5.39	118.14	120.30
1	A	979	G	N1-C2-N3	5.39	127.13	123.90
1	A	2257	U	N3-C2-O2	5.39	125.97	122.20
1	A	1990	C	N3-C4-C5	-5.39	119.75	121.90
1	A	1702	G	C8-N9-C4	-5.38	104.25	106.40
1	A	1955	U	C5-C6-N1	-5.38	120.01	122.70
1	A	2573	C	N3-C4-N4	5.38	121.77	118.00
34	a	515	G	C5-N7-C8	-5.38	101.61	104.30
34	a	1221	G	C5-N7-C8	5.38	106.99	104.30
34	a	1266	G	C8-N9-C1'	5.38	134.00	127.00
55	w	10	G	C5-N7-C8	-5.38	101.61	104.30
57	y	246	THR	C-N-CD	5.38	139.70	128.40
1	A	2325	G	N1-C6-O6	-5.38	116.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2501	C	C6-N1-C2	5.38	122.45	120.30
1	A	818	G	C6-C5-N7	-5.38	127.17	130.40
1	A	2096	U	C6-N1-C2	-5.38	117.77	121.00
34	a	20	U	N3-C2-O2	5.38	125.97	122.20
34	a	924	C	C2-N3-C4	5.38	122.59	119.90
1	A	298	G	C5-N7-C8	-5.38	101.61	104.30
1	A	1794	U	O5'-P-OP1	-5.38	100.86	105.70
34	a	769	G	N3-C4-C5	-5.38	125.91	128.60
34	a	728	A	C6-C5-N7	-5.38	128.54	132.30
1	A	1204	A	O4'-C1'-N9	5.37	112.50	108.20
1	A	2096	U	N3-C2-O2	-5.37	118.44	122.20
34	a	1461	G	N3-C4-N9	5.37	129.22	126.00
1	A	1069	A	P-O3'-C3'	5.37	126.15	119.70
1	A	2587	A	OP2-P-O3'	5.37	117.02	105.20
1	A	2820	A	C2-N3-C4	-5.37	107.92	110.60
1	A	1210	A	C5-C6-N1	5.37	120.38	117.70
34	a	548	G	C5-C6-O6	-5.37	125.38	128.60
34	a	1281	U	N3-C4-O4	-5.37	115.64	119.40
1	A	2271	G	N1-C2-N2	-5.37	111.37	116.20
2	B	75	G	C8-N9-C4	-5.37	104.25	106.40
34	a	20	U	N1-C2-O2	-5.37	119.04	122.80
34	a	1491	G	N3-C4-C5	-5.37	125.92	128.60
1	A	489	G	C6-C5-N7	-5.37	127.18	130.40
1	A	1932	A	N1-C6-N6	5.37	121.82	118.60
1	A	2095	C	P-O3'-C3'	-5.37	113.26	119.70
34	a	894	G	C5-C6-O6	-5.37	125.38	128.60
55	w	70	G	N3-C2-N2	-5.37	116.14	119.90
2	B	96	U	C6-N1-C2	-5.36	117.78	121.00
1	A	2250	G	C8-N9-C4	5.36	108.54	106.40
1	A	22	C	N3-C2-O2	-5.36	118.15	121.90
1	A	255	A	C2-N3-C4	-5.36	107.92	110.60
1	A	1343	G	N7-C8-N9	5.36	115.78	113.10
1	A	1655	A	N1-C6-N6	5.36	121.81	118.60
1	A	206	U	N1-C2-N3	5.36	118.11	114.90
1	A	462	C	C6-N1-C2	5.36	122.44	120.30
1	A	819	A	C5-N7-C8	-5.36	101.22	103.90
1	A	2024	G	N7-C8-N9	5.36	115.78	113.10
1	A	2056	G	C5-C6-O6	-5.36	125.39	128.60
1	A	2454	G	C6-N1-C2	-5.36	121.89	125.10
34	a	219	C	N3-C2-O2	-5.35	118.15	121.90
1	A	340	A	C2-N3-C4	-5.35	107.93	110.60
1	A	752	A	P-O3'-C3'	5.35	126.12	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1190	G	N3-C2-N2	-5.35	116.16	119.90
34	a	852	G	N9-C4-C5	-5.35	103.26	105.40
1	A	2080	G	C4-C5-N7	5.35	112.94	110.80
1	A	602	G	C4-N9-C1'	5.35	133.45	126.50
1	A	1123	C	C4-C5-C6	5.35	120.07	117.40
1	A	2503	A	C5-C6-N1	5.35	120.37	117.70
1	A	1822	G	C8-N9-C4	5.34	108.54	106.40
34	a	886	G	C5-C6-O6	-5.34	125.39	128.60
1	A	1667	G	C8-N9-C1'	-5.34	120.06	127.00
1	A	2088	G	C8-N9-C1'	5.34	133.94	127.00
1	A	2341	G	C5-C6-O6	-5.34	125.39	128.60
34	a	748	C	N3-C2-O2	-5.34	118.16	121.90
57	y	159	PRO	O-C-N	-5.34	114.16	122.70
1	A	786	C	C6-N1-C2	5.34	122.44	120.30
1	A	1278	A	C2-N3-C4	-5.34	107.93	110.60
1	A	311	A	N1-C6-N6	5.34	121.80	118.60
1	A	1828	G	N1-C6-O6	-5.34	116.70	119.90
34	a	1186	G	C8-N9-C1'	5.34	133.94	127.00
1	A	83	G	O5'-P-OP1	-5.33	100.90	105.70
1	A	977	G	C5-N7-C8	5.33	106.97	104.30
1	A	1628	G	C4-N9-C1'	5.33	133.43	126.50
1	A	1669	A	C6-N1-C2	-5.33	115.40	118.60
1	A	2271	G	C4-C5-N7	5.33	112.93	110.80
1	A	933	A	C8-N9-C4	-5.33	103.67	105.80
1	A	2276	G	N9-C4-C5	-5.33	103.27	105.40
1	A	48	G	C5-C6-O6	5.33	131.80	128.60
1	A	1817	G	O5'-P-OP2	-5.33	100.90	105.70
1	A	2370	G	O5'-P-OP1	-5.33	100.90	105.70
34	a	913	A	N1-C2-N3	5.33	131.96	129.30
1	A	298	G	N7-C8-N9	5.33	115.76	113.10
1	A	782	A	N7-C8-N9	-5.33	111.14	113.80
1	A	1721	G	N9-C4-C5	-5.33	103.27	105.40
34	a	993	G	C4-N9-C1'	5.33	133.43	126.50
1	A	2507	C	C2-N1-C1'	5.33	124.66	118.80
1	A	2611	U	N3-C4-O4	5.33	123.13	119.40
1	A	2751	G	C8-N9-C1'	-5.33	120.08	127.00
34	a	1126	U	C6-N1-C1'	-5.33	113.74	121.20
1	A	986	C	C2-N1-C1'	-5.32	112.94	118.80
1	A	1558	A	C6-C5-N7	-5.32	128.57	132.30
34	a	619	U	C2-N1-C1'	-5.32	111.31	117.70
34	a	1514	C	C5-C6-N1	-5.32	118.34	121.00
1	A	1823	G	N9-C4-C5	-5.32	103.27	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	362	G	C6-C5-N7	-5.32	127.21	130.40
1	A	1199	U	O5'-P-OP2	-5.32	100.92	105.70
34	a	908	A	OP2-P-O3'	5.32	116.89	105.20
1	A	958	U	N1-C2-O2	5.31	126.52	122.80
1	A	2439	A	P-O3'-C3'	5.31	126.08	119.70
1	A	459	U	N3-C4-O4	5.31	123.12	119.40
34	a	527	G	N3-C4-N9	-5.31	122.81	126.00
1	A	2506	U	C5-C4-O4	-5.31	122.71	125.90
34	a	1505	G	C5-C6-O6	5.31	131.79	128.60
1	A	1656	C	C4-C5-C6	5.31	120.05	117.40
1	A	1954	G	C5-C6-O6	-5.31	125.42	128.60
57	y	343	GLY	O-C-N	-5.31	114.20	122.70
34	a	12	U	N1-C2-N3	5.31	118.08	114.90
34	a	317	G	N1-C6-O6	5.30	123.08	119.90
34	a	1198	G	N9-C4-C5	5.30	107.52	105.40
34	a	532	A	N1-C6-N6	5.30	121.78	118.60
34	a	869	G	N3-C4-N9	-5.30	122.82	126.00
1	A	927	G	C6-C5-N7	-5.30	127.22	130.40
1	A	1005	C	N3-C4-C5	5.30	124.02	121.90
1	A	1222	C	C6-N1-C2	-5.30	118.18	120.30
34	a	839	U	N3-C2-O2	-5.30	118.49	122.20
34	a	1395	C	C5-C4-N4	5.30	123.91	120.20
34	a	1432	G	N9-C4-C5	5.30	107.52	105.40
1	A	1204	A	C4-C5-N7	5.30	113.35	110.70
1	A	1502	C	C6-N1-C2	-5.30	118.18	120.30
1	A	1781	C	N3-C2-O2	-5.30	118.19	121.90
34	a	1260	C	N1-C2-O2	5.30	122.08	118.90
1	A	195	A	C4-C5-C6	-5.29	114.35	117.00
1	A	2051	A	N1-C6-N6	5.29	121.78	118.60
1	A	1198	U	OP1-P-OP2	5.29	127.54	119.60
1	A	2384	G	C8-N9-C4	-5.29	104.28	106.40
1	A	80	G	C6-C5-N7	-5.29	127.23	130.40
1	A	600	G	C5-C6-N1	-5.29	108.86	111.50
1	A	1035	U	C5-C4-O4	5.29	129.07	125.90
1	A	2253	G	N1-C6-O6	5.29	123.07	119.90
34	a	1224	G	N1-C6-O6	-5.29	116.73	119.90
1	A	1911	U	N3-C2-O2	-5.29	118.50	122.20
1	A	2811	G	C4-C5-N7	5.29	112.91	110.80
1	A	678	C	C6-N1-C2	-5.28	118.19	120.30
1	A	775	G	O5'-P-OP1	-5.28	100.94	105.70
34	a	275	G	N3-C4-N9	5.28	129.17	126.00
34	a	314	C	C6-N1-C2	-5.28	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	643	C	N1-C2-O2	-5.28	115.73	118.90
1	A	1395	A	N1-C6-N6	5.28	121.77	118.60
1	A	1306	C	N3-C2-O2	-5.28	118.20	121.90
34	a	750	G	C8-N9-C4	-5.28	104.29	106.40
34	a	767	A	N3-C4-C5	-5.28	123.10	126.80
34	a	1131	G	C4-N9-C1'	5.28	133.37	126.50
1	A	139(A)	G	C5-C6-N1	5.28	114.14	111.50
1	A	517	C	C6-N1-C2	-5.28	118.19	120.30
34	a	738	C	C5-C6-N1	5.28	123.64	121.00
1	A	1199	U	C2-N3-C4	-5.28	123.83	127.00
2	B	11	C	C6-N1-C2	5.28	122.41	120.30
57	y	136	ASN	N-CA-C	5.28	125.25	111.00
1	A	704	G	N1-C6-O6	-5.28	116.73	119.90
1	A	2780	G	N3-C2-N2	5.28	123.59	119.90
1	A	2642	G	OP1-P-OP2	-5.27	111.69	119.60
1	A	438	G	C5-C6-O6	-5.27	125.44	128.60
34	a	514	C	C2-N1-C1'	-5.27	113.00	118.80
34	a	333	G	N9-C4-C5	-5.27	103.29	105.40
1	A	1368	G	N1-C6-O6	-5.27	116.74	119.90
1	A	1378	A	C2-N3-C4	-5.27	107.97	110.60
1	A	2261	C	N1-C2-O2	-5.27	115.74	118.90
1	A	2049	G	O5'-P-OP2	-5.27	100.96	105.70
34	a	1257	U	C2-N1-C1'	5.27	124.02	117.70
34	a	1330	U	N1-C2-O2	5.27	126.49	122.80
1	A	2080	G	N3-C4-N9	5.27	129.16	126.00
34	a	311	C	C5-C6-N1	-5.27	118.37	121.00
34	a	1068	G	C8-N9-C1'	-5.27	120.15	127.00
1	A	602	G	C6-C5-N7	-5.26	127.24	130.40
34	a	301	G	C6-C5-N7	-5.26	127.24	130.40
34	a	1052	U	N1-C2-O2	5.26	126.49	122.80
34	a	1110	A	C8-N9-C4	-5.26	103.69	105.80
2	B	79	C	OP2-P-O3'	5.26	116.78	105.20
34	a	251	G	C5-C6-O6	-5.26	125.44	128.60
1	A	1965	C	C5-C4-N4	-5.26	116.52	120.20
1	A	2229	C	N1-C2-O2	5.26	122.06	118.90
34	a	253	U	N3-C2-O2	5.26	125.88	122.20
34	a	588	G	C8-N9-C4	-5.26	104.30	106.40
1	A	526	A	N9-C4-C5	5.26	107.90	105.80
1	A	790	C	N1-C2-O2	5.26	122.06	118.90
1	A	792	G	O4'-C1'-N9	-5.26	103.99	108.20
2	B	75	G	C6-C5-N7	-5.26	127.24	130.40
57	y	194	ALA	C-N-CD	5.26	139.45	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1662	C	OP2-P-O3'	5.26	116.77	105.20
1	A	2010	G	C8-N9-C4	-5.26	104.30	106.40
1	A	2120	G	C5-C6-O6	5.26	131.75	128.60
1	A	48	G	C5-C6-N1	-5.26	108.87	111.50
1	A	1899	G	N3-C4-N9	5.26	129.15	126.00
1	A	2516	G	N9-C4-C5	-5.26	103.30	105.40
1	A	234	C	C6-N1-C1'	-5.25	114.49	120.80
1	A	432	A	C8-N9-C4	-5.25	103.70	105.80
1	A	819	A	N9-C4-C5	-5.25	103.70	105.80
34	a	1496	C	N3-C2-O2	5.25	125.58	121.90
1	A	474	G	N3-C4-N9	5.25	129.15	126.00
1	A	979	G	C8-N9-C4	-5.25	104.30	106.40
34	a	569	C	C2-N3-C4	-5.25	117.27	119.90
1	A	808	G	C8-N9-C1'	-5.25	120.17	127.00
34	a	19	C	N3-C4-C5	-5.25	119.80	121.90
1	A	1696	G	C5-N7-C8	-5.25	101.67	104.30
1	A	1952	A	C6-C5-N7	-5.25	128.62	132.30
34	a	454	C	C6-N1-C2	-5.25	118.20	120.30
34	a	728	A	C5-C6-N6	-5.25	119.50	123.70
34	a	1358	U	C5-C6-N1	-5.25	120.08	122.70
1	A	806	C	O5'-P-OP2	-5.25	100.98	105.70
1	A	1781	C	C6-N1-C1'	-5.25	114.50	120.80
34	a	585	G	N1-C6-O6	5.25	123.05	119.90
1	A	2586	C	OP2-P-O3'	5.25	116.74	105.20
1	A	2704	C	C6-N1-C2	-5.25	118.20	120.30
34	a	267	C	N3-C4-C5	5.24	124.00	121.90
34	a	664	G	C4-C5-N7	-5.24	108.70	110.80
34	a	1198	G	C4-C5-N7	-5.24	108.70	110.80
55	w	20	U	N3-C2-O2	-5.24	118.53	122.20
1	A	2230	G	N1-C6-O6	-5.24	116.75	119.90
1	A	566	U	N3-C2-O2	-5.24	118.53	122.20
1	A	1787	A	C8-N9-C1'	-5.24	118.27	127.70
1	A	2308	G	C4-C5-N7	5.24	112.90	110.80
2	B	7	G	N7-C8-N9	5.24	115.72	113.10
55	w	74	C	N3-C4-C5	-5.24	119.80	121.90
1	A	690	G	C8-N9-C4	-5.24	104.31	106.40
34	a	684	A	C8-N9-C4	-5.24	103.70	105.80
34	a	969	A	N1-C6-N6	5.24	121.74	118.60
1	A	1300	U	C5-C6-N1	5.24	125.32	122.70
1	A	632	A	N7-C8-N9	-5.24	111.18	113.80
1	A	781	A	OP1-P-OP2	5.24	127.45	119.60
1	A	1553	A	O4'-C1'-N9	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1224	G	N9-C4-C5	5.24	107.49	105.40
1	A	678	C	N1-C2-O2	-5.23	115.76	118.90
1	A	1153	C	C5-C6-N1	5.23	123.62	121.00
1	A	1247	A	C8-N9-C4	5.23	107.89	105.80
1	A	2875	C	N1-C2-O2	-5.23	115.76	118.90
34	a	1075	C	OP1-P-O3'	5.23	116.71	105.20
1	A	239	U	N3-C4-C5	5.23	117.74	114.60
1	A	1022	G	C4-N9-C1'	-5.23	119.70	126.50
34	a	634	C	C6-N1-C2	-5.23	118.21	120.30
45	l	29	GLY	N-CA-C	-5.23	100.03	113.10
34	a	1109	C	C2-N1-C1'	5.23	124.55	118.80
57	y	417	PRO	CA-N-CD	-5.23	104.18	111.50
1	A	805	G	C8-N9-C1'	-5.23	120.20	127.00
1	A	1698	A	C4-C5-C6	5.23	119.61	117.00
1	A	1988	C	N1-C2-O2	5.23	122.04	118.90
1	A	2271	G	N3-C2-N2	5.22	123.56	119.90
1	A	2612	C	C2-N1-C1'	-5.22	113.05	118.80
34	a	1323	G	C6-C5-N7	-5.22	127.27	130.40
1	A	932	G	C4-C5-N7	-5.22	108.71	110.80
1	A	961	C	N1-C2-O2	-5.22	115.77	118.90
1	A	1629	U	N3-C4-C5	-5.22	111.47	114.60
2	B	77	U	OP1-P-O3'	5.22	116.69	105.20
34	a	406	G	C6-C5-N7	-5.22	127.27	130.40
34	a	852	G	C6-C5-N7	-5.22	127.27	130.40
1	A	141	A	N7-C8-N9	5.22	116.41	113.80
34	a	984	C	N1-C2-O2	5.22	122.03	118.90
34	a	1406	U	C5-C6-N1	-5.22	120.09	122.70
34	a	1227	A	N1-C6-N6	5.22	121.73	118.60
1	A	1357	U	N1-C2-O2	-5.22	119.15	122.80
1	A	206	U	C5-C4-O4	5.21	129.03	125.90
1	A	818	G	C5-C6-O6	-5.21	125.47	128.60
1	A	1251	C	C6-N1-C2	-5.21	118.21	120.30
1	A	2573	C	C5-C4-N4	-5.21	116.55	120.20
1	A	2592	G	N1-C6-O6	5.21	123.03	119.90
1	A	1787	A	O4'-C1'-N9	-5.21	104.03	108.20
1	A	1982	C	N3-C4-N4	5.21	121.65	118.00
1	A	470	A	O5'-P-OP1	-5.21	101.01	105.70
1	A	1699	G	O5'-P-OP2	-5.21	101.01	105.70
34	a	106	C	N1-C2-O2	-5.21	115.77	118.90
34	a	394	G	N1-C6-O6	-5.21	116.77	119.90
1	A	583	G	C8-N9-C4	-5.21	104.32	106.40
1	A	782	A	N9-C4-C5	-5.21	103.72	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	855	G	C4-C5-N7	5.21	112.88	110.80
55	w	26	A	N9-C4-C5	-5.21	103.72	105.80
1	A	526	A	C5-C6-N6	5.21	127.87	123.70
1	A	915	C	C6-N1-C2	-5.21	118.22	120.30
34	a	1363	C	C2-N1-C1'	-5.21	113.07	118.80
1	A	1191	G	C8-N9-C4	5.21	108.48	106.40
1	A	340	A	C5-C6-N1	-5.20	115.10	117.70
1	A	517	C	N3-C4-N4	5.20	121.64	118.00
1	A	808	G	N1-C6-O6	5.20	123.02	119.90
1	A	1813	G	N7-C8-N9	-5.20	110.50	113.10
34	a	1127	G	N3-C2-N2	-5.20	116.26	119.90
1	A	2873	A	O4'-C1'-N9	5.20	112.36	108.20
34	a	1506	U	N3-C2-O2	5.20	125.84	122.20
1	A	1958	C	C5-C4-N4	-5.20	116.56	120.20
34	a	1290	G	C6-C5-N7	-5.20	127.28	130.40
55	w	20	U	C6-N1-C1'	-5.20	113.92	121.20
34	a	1131	G	C4-C5-C6	5.20	121.92	118.80
1	A	103	A	N1-C6-N6	5.20	121.72	118.60
1	A	234	C	C2-N1-C1'	5.20	124.51	118.80
34	a	397	A	C6-C5-N7	-5.20	128.66	132.30
1	A	514	A	C5-C6-N1	-5.19	115.10	117.70
1	A	825	C	N3-C4-C5	-5.19	119.82	121.90
34	a	1281	U	C4-C5-C6	5.19	122.82	119.70
1	A	807	U	C5-C4-O4	-5.19	122.79	125.90
34	a	1232	U	N1-C2-O2	5.19	126.43	122.80
1	A	265	A	O4'-C1'-N9	5.19	112.35	108.20
1	A	531	C	C2-N1-C1'	5.19	124.50	118.80
1	A	2054	A	OP2-P-O3'	5.19	116.61	105.20
34	a	585	G	C6-C5-N7	-5.19	127.29	130.40
34	a	916	G	C5-C6-O6	5.19	131.71	128.60
57	y	292	PRO	CA-N-CD	-5.19	104.24	111.50
1	A	1007	C	N3-C4-N4	5.18	121.63	118.00
1	A	1161	C	N1-C2-O2	5.18	122.01	118.90
1	A	2627	G	C6-C5-N7	-5.18	127.29	130.40
34	a	782	A	N1-C6-N6	-5.18	115.49	118.60
1	A	734	A	C2-N3-C4	-5.18	108.01	110.60
1	A	1227	G	C6-C5-N7	-5.18	127.29	130.40
1	A	2571	C	C6-N1-C2	5.18	122.37	120.30
1	A	445	C	OP2-P-O3'	5.18	116.59	105.20
34	a	317	G	C4-C5-N7	5.18	112.87	110.80
2	B	71	C	C5-C6-N1	5.18	123.59	121.00
34	a	396	G	C8-N9-C4	-5.18	104.33	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	662	G	O4'-C1'-N9	5.18	112.34	108.20
34	a	1524	C	C5-C6-N1	-5.18	118.41	121.00
1	A	187	G	N1-C6-O6	5.17	123.00	119.90
1	A	1637	A	C8-N9-C4	5.17	107.87	105.80
55	w	24	G	N3-C4-N9	-5.17	122.89	126.00
1	A	944	G	C4-N9-C1'	5.17	133.22	126.50
1	A	1666	G	O5'-P-OP2	5.17	116.91	110.70
1	A	1136	G	C5-C6-O6	-5.17	125.50	128.60
1	A	2765	A	C6-C5-N7	-5.17	128.68	132.30
34	a	406	G	N3-C4-C5	-5.17	126.01	128.60
34	a	1356	G	C4-C5-N7	-5.17	108.73	110.80
34	a	1513	A	N9-C4-C5	5.17	107.87	105.80
34	a	916	G	N3-C4-C5	-5.17	126.02	128.60
1	A	727	A	N1-C6-N6	5.17	121.70	118.60
1	A	949	C	C6-N1-C2	-5.17	118.23	120.30
1	A	1339	G	C8-N9-C4	-5.17	104.33	106.40
34	a	1416	G	C2-N3-C4	-5.17	109.32	111.90
34	a	1486	G	N3-C4-N9	5.17	129.10	126.00
47	n	18	VAL	CB-CA-C	-5.17	101.58	111.40
1	A	572	A	C6-C5-N7	-5.17	128.68	132.30
1	A	2730	C	OP1-P-O3'	5.17	116.56	105.20
1	A	2574	G	N3-C4-N9	-5.16	122.90	126.00
1	A	2791	C	N3-C4-C5	-5.16	119.83	121.90
34	a	1115	C	C6-N1-C2	5.16	122.37	120.30
1	A	577	G	OP1-P-O3'	5.16	116.56	105.20
57	y	528	ILE	C-N-CD	5.16	139.24	128.40
1	A	1021	A	N3-C4-C5	5.16	130.41	126.80
1	A	1424	G	C8-N9-C1'	-5.16	120.30	127.00
1	A	2605	U	N1-C2-O2	5.16	126.41	122.80
55	w	43	C	C5-C6-N1	-5.16	118.42	121.00
56	v	18	C	N3-C2-O2	-5.16	118.29	121.90
1	A	467	G	N1-C6-O6	5.16	122.99	119.90
1	A	729	G	C6-C5-N7	-5.16	127.31	130.40
1	A	2690	C	N1-C2-O2	5.16	121.99	118.90
34	a	378	G	N1-C6-O6	5.16	122.99	119.90
34	a	436	C	N3-C4-N4	5.16	121.61	118.00
34	a	1214	C	N3-C4-C5	-5.16	119.84	121.90
1	A	2525	G	N3-C2-N2	5.15	123.51	119.90
1	A	115	C	OP2-P-O3'	5.15	116.53	105.20
1	A	1667	G	N3-C4-N9	5.15	129.09	126.00
1	A	2608	G	C8-N9-C4	5.15	108.46	106.40
1	A	2617	C	C4-C5-C6	5.15	119.98	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	A	C5-C6-N6	-5.15	119.58	123.70
1	A	857	C	C5-C6-N1	-5.15	118.42	121.00
1	A	1645	G	C5-C6-O6	-5.15	125.51	128.60
1	A	1751	C	N3-C4-N4	-5.15	114.39	118.00
1	A	1698	A	C8-N9-C4	-5.15	103.74	105.80
1	A	946	G	C5-C6-O6	-5.15	125.51	128.60
1	A	2634	G	OP2-P-O3'	5.15	116.53	105.20
1	A	265	A	C5-N7-C8	-5.15	101.33	103.90
34	a	800	G	N3-C4-C5	-5.15	126.03	128.60
1	A	586	A	OP2-P-O3'	5.14	116.52	105.20
1	A	2481	G	C5-C6-O6	-5.14	125.51	128.60
1	A	249	C	C2-N1-C1'	5.14	124.46	118.80
1	A	1665	A	N9-C4-C5	-5.14	103.74	105.80
1	A	1989	G	N1-C6-O6	5.14	122.98	119.90
34	a	297	G	N3-C4-N9	-5.14	122.92	126.00
34	a	720	C	N3-C4-C5	5.14	123.96	121.90
1	A	30	G	N9-C4-C5	-5.14	103.34	105.40
1	A	577	G	N7-C8-N9	5.14	115.67	113.10
1	A	977	G	C4-C5-N7	-5.14	108.75	110.80
1	A	1209	G	O5'-P-OP1	-5.14	101.08	105.70
1	A	1338	G	N3-C4-C5	-5.14	126.03	128.60
1	A	1813	G	C5-N7-C8	5.14	106.87	104.30
56	v	13	A	N9-C4-C5	5.14	107.86	105.80
5	F	169	ASN	N-CA-C	5.14	124.87	111.00
34	a	379	C	C2-N1-C1'	-5.14	113.15	118.80
34	a	1126	U	P-O3'-C3'	5.14	125.86	119.70
34	a	115	G	N1-C6-O6	5.14	122.98	119.90
34	a	317	G	N9-C4-C5	-5.14	103.34	105.40
34	a	820	U	N1-C2-O2	5.14	126.40	122.80
34	a	1227	A	C6-C5-N7	-5.14	128.70	132.30
1	A	207	A	C8-N9-C4	5.13	107.85	105.80
55	w	12	U	O5'-P-OP2	-5.13	101.08	105.70
1	A	1653	G	N3-C4-N9	5.13	129.08	126.00
34	a	691	G	C6-C5-N7	-5.13	127.32	130.40
34	a	1366	C	N3-C4-C5	-5.13	119.85	121.90
1	A	210	C	C2-N3-C4	-5.13	117.33	119.90
1	A	491	G	C4-N9-C1'	-5.13	119.83	126.50
1	A	499	U	N1-C2-N3	5.13	117.98	114.90
1	A	2018	G	N3-C4-N9	5.13	129.08	126.00
1	A	2073	C	N3-C4-N4	-5.13	114.41	118.00
34	a	1056	U	C2-N3-C4	5.13	130.08	127.00
1	A	581	C	OP1-P-OP2	-5.13	111.91	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2542	A	O5'-P-OP1	-5.13	101.09	105.70
1	A	2609	U	C6-N1-C2	5.13	124.08	121.00
1	A	2611	U	C2-N1-C1'	5.13	123.85	117.70
1	A	1700	A	C5-C6-N6	-5.12	119.60	123.70
1	A	1973	G	C4-C5-N7	-5.12	108.75	110.80
1	A	2059	A	C8-N9-C4	5.12	107.85	105.80
1	A	203	C	N3-C2-O2	5.12	125.48	121.90
34	a	1123	A	N3-C4-C5	5.12	130.38	126.80
1	A	1501	C	N3-C4-N4	5.12	121.58	118.00
1	A	18	C	C6-N1-C2	-5.12	118.25	120.30
1	A	857	C	C2-N1-C1'	-5.12	113.17	118.80
1	A	1128	A	N3-C4-C5	5.12	130.38	126.80
1	A	2025	C	C2-N1-C1'	5.12	124.43	118.80
34	a	225	C	C6-N1-C2	5.12	122.35	120.30
1	A	1499	C	C2-N1-C1'	-5.12	113.17	118.80
1	A	2048	G	C5-C6-O6	-5.12	125.53	128.60
1	A	2519	U	N1-C2-O2	-5.12	119.22	122.80
1	A	16	G	O5'-P-OP1	-5.11	101.10	105.70
1	A	2587	A	C2-N3-C4	5.11	113.16	110.60
34	a	613	C	C6-N1-C2	-5.11	118.25	120.30
1	A	143(A)	C	C6-N1-C2	-5.11	118.26	120.30
1	A	1142(A)	A	C5-C6-N1	-5.11	115.14	117.70
34	a	966	G	C5-C6-N1	5.11	114.06	111.50
1	A	918	A	O5'-P-OP1	-5.11	101.10	105.70
1	A	2597	G	N3-C4-C5	-5.11	126.05	128.60
1	A	328	U	C5-C6-N1	5.11	125.25	122.70
1	A	1796	U	C6-N1-C1'	5.11	128.35	121.20
1	A	2494	G	N1-C6-O6	5.11	122.96	119.90
34	a	12	U	C6-N1-C2	-5.11	117.94	121.00
34	a	354	G	N3-C4-C5	-5.11	126.05	128.60
1	A	1781	C	C2-N1-C1'	5.10	124.42	118.80
1	A	1051	G	N1-C6-O6	5.10	122.96	119.90
1	A	1204	A	C5-N7-C8	-5.10	101.35	103.90
1	A	1979	C	C5-C6-N1	-5.10	118.45	121.00
34	a	424	G	N1-C6-O6	-5.10	116.84	119.90
34	a	306	G	N1-C6-O6	-5.10	116.84	119.90
1	A	391	G	C5-C6-O6	-5.09	125.54	128.60
1	A	981	A	C2-N3-C4	-5.09	108.05	110.60
1	A	1006	C	O5'-P-OP1	-5.09	101.11	105.70
1	A	1776	G	O5'-P-OP1	5.09	116.81	110.70
1	A	2766	G	N7-C8-N9	5.09	115.65	113.10
34	a	1025	U	N1-C2-O2	5.09	126.37	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1254	C	C5-C6-N1	-5.09	118.45	121.00
1	A	1362	C	C6-N1-C2	-5.09	118.26	120.30
34	a	372	C	C5-C6-N1	5.09	123.55	121.00
34	a	1524	C	N3-C4-N4	-5.09	114.44	118.00
4	E	78	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	239	U	N1-C2-O2	5.09	126.36	122.80
1	A	491	G	C8-N9-C1'	5.09	133.62	127.00
1	A	805	G	N3-C4-N9	5.09	129.05	126.00
2	B	99	G	C4-N9-C1'	5.09	133.12	126.50
1	A	1924	C	C4-C5-C6	5.09	119.94	117.40
34	a	952	U	N3-C2-O2	5.09	125.76	122.20
1	A	688	U	N3-C4-C5	5.08	117.65	114.60
1	A	1142(A)	A	N3-C4-N9	-5.08	123.33	127.40
1	A	2249	U	N3-C4-O4	5.08	122.96	119.40
1	A	2790	A	N3-C4-N9	5.08	131.47	127.40
1	A	2185	C	C2-N3-C4	5.08	122.44	119.90
1	A	2556	C	C2-N1-C1'	5.08	124.39	118.80
34	a	60	A	OP1-P-O3'	5.08	116.38	105.20
34	a	576	G	C4-C5-C6	5.08	121.85	118.80
1	A	2188	C	N1-C2-O2	5.08	121.95	118.90
1	A	2376	A	N1-C6-N6	-5.08	115.55	118.60
1	A	2522	U	OP2-P-O3'	5.08	116.38	105.20
2	B	75	G	C4-N9-C1'	5.08	133.10	126.50
1	A	455	C	C5-C4-N4	-5.08	116.65	120.20
1	A	479	A	O4'-C1'-N9	5.08	112.26	108.20
1	A	645	C	N3-C2-O2	-5.08	118.35	121.90
1	A	745	G	C6-N1-C2	-5.08	122.06	125.10
1	A	1665	A	N7-C8-N9	-5.08	111.26	113.80
34	a	661	G	C8-N9-C4	-5.08	104.37	106.40
1	A	2096	U	C6-N1-C1'	-5.07	114.10	121.20
34	a	750	G	C4-N9-C1'	5.07	133.10	126.50
1	A	1780	A	O5'-P-OP2	-5.07	101.14	105.70
1	A	1996	C	C6-N1-C2	5.07	122.33	120.30
1	A	2597	G	C4-C5-N7	-5.07	108.77	110.80
1	A	526	A	C4-C5-N7	-5.07	108.17	110.70
1	A	1289	C	C6-N1-C2	5.07	122.33	120.30
33	x	9	A	N1-C6-N6	5.07	121.64	118.60
34	a	21	G	OP2-P-O3'	5.07	116.36	105.20
34	a	812	C	N3-C2-O2	-5.07	118.35	121.90
1	A	1257	C	C2-N1-C1'	5.07	124.38	118.80
1	A	991	C	C5-C6-N1	5.07	123.53	121.00
1	A	1673	U	C5-C4-O4	5.07	128.94	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2028	U	N3-C4-C5	-5.07	111.56	114.60
2	B	99	G	C8-N9-C1'	-5.07	120.41	127.00
34	a	283	C	O5'-P-OP1	-5.07	101.14	105.70
34	a	1374	A	C5-C6-N6	5.07	127.75	123.70
34	a	189(A)	C	O5'-P-OP2	-5.07	101.14	105.70
34	a	986	A	C6-N1-C2	-5.06	115.56	118.60
1	A	214	G	O4'-C1'-N9	5.06	112.25	108.20
1	A	1982	C	C5-C4-N4	-5.06	116.66	120.20
34	a	376	G	N1-C6-O6	5.06	122.94	119.90
55	w	27	G	C8-N9-C4	5.06	108.42	106.40
1	A	738	G	C8-N9-C4	-5.06	104.38	106.40
34	a	609	A	O5'-P-OP1	-5.06	101.15	105.70
34	a	1125	U	C5-C6-N1	-5.06	120.17	122.70
1	A	615	G	N1-C6-O6	5.06	122.93	119.90
34	a	18	C	N3-C2-O2	-5.06	118.36	121.90
34	a	1484	C	C6-N1-C2	-5.06	118.28	120.30
34	a	1494	G	C4-N9-C1'	5.06	133.07	126.50
1	A	2593	U	C5-C4-O4	-5.06	122.87	125.90
1	A	2000	G	OP1-P-OP2	5.05	127.18	119.60
34	a	1486	G	C6-C5-N7	-5.05	127.37	130.40
1	A	1774	C	C6-N1-C2	-5.05	118.28	120.30
34	a	858	G	C6-C5-N7	-5.05	127.37	130.40
1	A	594	U	C5-C6-N1	-5.05	120.17	122.70
1	A	950	G	O5'-P-OP2	-5.05	101.15	105.70
1	A	1790	C	C5-C4-N4	-5.05	116.66	120.20
34	a	1127	G	C5-C6-O6	5.05	131.63	128.60
1	A	1272	A	O5'-P-OP2	-5.05	101.16	105.70
34	a	1404	C	N3-C4-C5	5.05	123.92	121.90
1	A	263	C	N3-C2-O2	-5.05	118.37	121.90
1	A	2242	G	C2-N3-C4	-5.05	109.38	111.90
34	a	1027	C	C5-C4-N4	5.05	123.73	120.20
1	A	450	G	C4-C5-C6	5.04	121.83	118.80
1	A	824	A	O5'-P-OP1	-5.04	101.16	105.70
1	A	2088	G	N3-C2-N2	-5.04	116.37	119.90
1	A	2124	G	C5-C6-O6	5.04	131.63	128.60
1	A	19	C	C5-C6-N1	-5.04	118.48	121.00
1	A	445	C	O5'-P-OP2	-5.04	101.16	105.70
1	A	1745	C	C6-N1-C2	-5.04	118.28	120.30
1	A	1756	G	C8-N9-C4	-5.04	104.38	106.40
55	w	35	A	C2-N3-C4	-5.04	108.08	110.60
1	A	778	G	N3-C4-N9	5.04	129.02	126.00
1	A	2580	U	N3-C2-O2	-5.04	118.67	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	990	A	N7-C8-N9	5.04	116.32	113.80
1	A	2253	G	OP1-P-OP2	-5.04	112.04	119.60
1	A	2504	U	C5-C6-N1	-5.04	120.18	122.70
1	A	1372	U	C2-N1-C1'	5.04	123.74	117.70
1	A	2864	G	N1-C2-N2	-5.04	111.67	116.20
34	a	189(A)	C	N3-C4-C5	5.04	123.92	121.90
1	A	1996	C	N1-C2-O2	-5.03	115.88	118.90
34	a	585	G	N9-C4-C5	-5.03	103.39	105.40
1	A	1210	A	P-O3'-C3'	5.03	125.74	119.70
34	a	424	G	N9-C4-C5	5.03	107.41	105.40
1	A	2233	U	C5-C6-N1	-5.03	120.18	122.70
34	a	200	G	C5-C6-O6	5.03	131.62	128.60
34	a	805	C	C4-C5-C6	-5.03	114.89	117.40
57	y	230	ILE	CB-CA-C	-5.03	101.54	111.60
1	A	2645	G	O5'-P-OP2	-5.03	101.17	105.70
1	A	593	G	N1-C6-O6	5.03	122.92	119.90
1	A	1829	A	OP2-P-O3'	5.03	116.26	105.20
1	A	1934	C	C6-N1-C2	5.03	122.31	120.30
1	A	2502	G	N1-C6-O6	5.03	122.92	119.90
1	A	2609	U	N1-C2-O2	-5.03	119.28	122.80
34	a	603	U	N1-C2-O2	-5.03	119.28	122.80
34	a	863	U	O4'-C1'-N1	5.03	112.22	108.20
1	A	467	G	C6-C5-N7	-5.03	127.38	130.40
1	A	1353	A	N1-C6-N6	-5.03	115.58	118.60
34	a	1190	G	C5-C6-O6	-5.03	125.58	128.60
1	A	576	U	C5-C4-O4	-5.02	122.89	125.90
1	A	782	A	C5-C6-N6	-5.02	119.68	123.70
55	w	41	C	C2-N3-C4	-5.02	117.39	119.90
1	A	2271	G	C8-N9-C4	5.02	108.41	106.40
1	A	2285	C	C6-N1-C2	5.02	122.31	120.30
1	A	2773	C	N1-C2-O2	-5.02	115.89	118.90
34	a	570	G	OP2-P-O3'	5.02	116.25	105.20
55	w	42	C	C6-N1-C2	5.02	122.31	120.30
1	A	1368	G	C5-C6-N1	5.02	114.01	111.50
1	A	574	C	N1-C2-N3	-5.02	115.69	119.20
1	A	2864	G	C6-C5-N7	-5.02	127.39	130.40
1	A	2874	C	C6-N1-C2	5.02	122.31	120.30
1	A	1972	A	N1-C6-N6	-5.02	115.59	118.60
34	a	62	U	N1-C2-N3	5.02	117.91	114.90
34	a	279	A	N1-C6-N6	5.02	121.61	118.60
34	a	779	C	C5-C4-N4	5.02	123.71	120.20
34	a	1250	A	C8-N9-C4	-5.02	103.79	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1680	U	N1-C2-N3	5.02	117.91	114.90
34	a	791	G	O5'-P-OP2	5.02	116.72	110.70
34	a	1507	A	N3-C4-C5	-5.02	123.29	126.80
1	A	981	A	N1-C6-N6	5.01	121.61	118.60
1	A	2726	U	O5'-P-OP1	-5.01	101.19	105.70
21	Y	9	LYS	N-CA-C	-5.01	97.46	111.00
34	a	797	C	N3-C2-O2	5.01	125.41	121.90
34	a	919	A	C8-N9-C4	-5.01	103.79	105.80
34	a	1074	G	N9-C4-C5	-5.01	103.39	105.40
34	a	869	G	N3-C4-C5	5.01	131.11	128.60
1	A	441	U	C5-C6-N1	5.01	125.21	122.70
1	A	1310	G	N1-C2-N2	-5.01	111.69	116.20
1	A	2201	C	C6-N1-C2	-5.01	118.30	120.30
34	a	635	G	C6-C5-N7	-5.01	127.39	130.40
34	a	834	C	C5-C6-N1	-5.01	118.50	121.00
34	a	898	G	C5-C6-O6	-5.01	125.59	128.60
1	A	86	C	OP2-P-O3'	5.01	116.22	105.20
1	A	139(A)	G	N7-C8-N9	5.01	115.61	113.10
1	A	665	C	O5'-P-OP2	5.01	116.71	110.70
1	A	1137	G	N1-C6-O6	-5.01	116.89	119.90
1	A	1305	C	N3-C4-C5	5.01	123.90	121.90
34	a	724	G	C5-C6-O6	-5.01	125.59	128.60
1	A	1821	A	C8-N9-C4	5.01	107.80	105.80
1	A	1246	A	C8-N9-C4	5.01	107.80	105.80
1	A	1310	G	N3-C2-N2	5.01	123.40	119.90
1	A	2050	C	C5-C6-N1	-5.01	118.50	121.00
1	A	2040	C	C2-N1-C1'	5.00	124.31	118.80
1	A	918	A	N1-C6-N6	5.00	121.60	118.60
1	A	1653	G	N7-C8-N9	5.00	115.60	113.10
1	A	2606	C	C2-N3-C4	-5.00	117.40	119.90
34	a	111	G	N1-C2-N2	5.00	120.70	116.20
34	a	853	G	N3-C4-N9	5.00	129.00	126.00
34	a	924	C	C5-C4-N4	5.00	123.70	120.20
34	a	1320	C	C5-C6-N1	-5.00	118.50	121.00
1	A	330	A	N1-C6-N6	5.00	121.60	118.60
1	A	1052	C	N1-C2-O2	5.00	121.90	118.90
34	a	767	A	C4-C5-C6	5.00	119.50	117.00
34	a	1320	C	C6-N1-C2	5.00	122.30	120.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	223	GLY	Peptide
8	J	6	ASN	Peptide
42	i	45	ALA	Peptide
46	m	7	VAL	Peptide
46	m	8	GLU	Peptide
52	s	28	LYS	Peptide
53	t	10	LEU	Peptide
57	y	127	HIS	Peptide
57	y	137	LYS	Peptide
57	y	152	VAL	Peptide
57	y	171	GLY	Peptide
57	y	174	VAL	Peptide
57	y	226	ASP	Peptide
57	y	230	ILE	Peptide
57	y	235	LYS	Peptide
57	y	250	LEU	Peptide
57	y	268	ILE	Peptide
57	y	292	PRO	Peptide
57	y	294	PHE	Mainchain
57	y	301	VAL	Peptide
57	y	331	THR	Peptide
57	y	389	GLU	Peptide
57	y	395	ASP	Peptide
57	y	419	GLU	Peptide
57	y	480	GLU	Peptide
57	y	553	ALA	Peptide
57	y	554	LEU	Peptide
57	y	557	ASP	Peptide
57	y	6	LEU	Peptide
57	y	86	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61879	0	31203	1311	0
2	B	2573	0	1306	33	0
3	D	2136	0	2217	141	0
4	E	1559	0	1618	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1584	0	1625	73	0
6	G	1425	0	1443	67	0
7	H	1330	0	1407	56	0
8	J	641	0	309	12	0
9	K	1025	0	1066	56	0
10	N	1117	0	1184	55	0
11	O	933	0	996	37	0
12	P	1135	0	1212	70	0
13	Q	1122	0	1179	40	0
14	R	968	0	1033	39	0
15	S	877	0	938	39	0
16	T	1091	0	1151	53	0
17	U	959	0	1019	60	0
18	V	771	0	830	29	0
19	W	886	0	940	36	0
20	X	750	0	814	41	0
21	Y	806	0	881	35	0
22	Z	1451	0	1457	73	0
23	0	591	0	607	34	0
24	1	755	0	826	38	0
25	2	588	0	643	22	0
26	3	469	0	518	15	0
27	4	557	0	537	42	0
28	5	459	0	476	29	0
29	6	453	0	473	17	0
30	7	430	0	480	17	0
31	8	511	0	571	31	0
32	9	307	0	335	12	0
33	x	1581	0	805	0	0
34	a	32163	0	16234	0	0
35	b	1850	0	1871	0	0
36	c	1550	0	1539	0	0
37	d	1655	0	1673	0	0
38	e	1129	0	1185	0	0
39	f	806	0	793	0	0
40	g	1227	0	1232	0	0
41	h	1088	0	1126	0	0
42	i	983	0	986	0	0
43	j	698	0	637	0	0
44	k	829	0	825	0	0
45	l	930	0	980	0	0
46	m	924	0	960	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	n	492	0	528	0	0
48	o	728	0	760	0	0
49	p	681	0	697	0	0
50	q	823	0	891	0	0
51	r	555	0	618	0	0
52	s	650	0	655	0	0
53	t	724	0	787	0	0
54	u	199	0	208	0	0
55	w	1643	0	849	0	0
56	v	148	0	76	0	0
57	y	4000	0	3218	0	0
58	0	3	0	0	0	0
58	5	1	0	0	0	0
58	6	1	0	0	0	0
58	7	3	0	0	0	0
58	8	1	0	0	0	0
58	9	1	0	0	0	0
58	A	635	0	0	0	0
58	B	18	0	0	0	0
58	D	5	0	0	0	0
58	E	4	0	0	0	0
58	F	5	0	0	0	0
58	G	3	0	0	0	0
58	N	1	0	0	0	0
58	O	1	0	0	0	0
58	P	2	0	0	0	0
58	Q	5	0	0	0	0
58	R	3	0	0	0	0
58	U	4	0	0	0	0
58	V	2	0	0	0	0
58	W	1	0	0	0	0
58	X	1	0	0	0	0
58	Z	1	0	0	0	0
58	a	187	0	0	0	0
58	e	1	0	0	0	0
58	f	1	0	0	0	0
58	l	2	0	0	0	0
58	m	1	0	0	0	0
58	n	1	0	0	0	0
58	v	1	0	0	0	0
58	w	6	0	0	0	0
58	x	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	y	2	0	0	0	0
59	4	1	0	0	0	0
59	5	1	0	0	0	0
59	6	1	0	0	0	0
59	9	1	0	0	0	0
59	Y	1	0	0	0	0
59	n	1	0	0	0	0
60	d	8	0	0	0	0
61	y	28	0	12	0	0
62	0	4	0	0	0	0
62	1	2	0	0	0	0
62	3	1	0	0	0	0
62	5	1	0	0	0	0
62	7	2	0	0	0	0
62	8	4	0	0	0	0
62	9	1	0	0	0	0
62	A	710	0	0	110	0
62	B	34	0	0	2	0
62	D	4	0	0	1	0
62	E	7	0	0	1	0
62	F	5	0	0	0	0
62	G	1	0	0	0	0
62	H	1	0	0	0	0
62	N	1	0	0	0	0
62	O	3	0	0	0	0
62	P	3	0	0	0	0
62	Q	4	0	0	1	0
62	R	3	0	0	0	0
62	U	2	0	0	1	0
62	V	1	0	0	1	0
62	W	2	0	0	0	0
62	Y	1	0	0	0	0
62	a	167	0	0	0	0
62	l	1	0	0	0	0
62	v	3	0	0	0	0
62	x	1	0	0	0	0
All	All	152111	0	101439	2398	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (2398) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:G:H1	1:A:893:C:N4	1.56	1.02
1:A:1019:U:HO2'	1:A:1021:A:H2	1.08	0.99
1:A:2106:G:H1	1:A:2183:C:H42	0.98	0.96
12:P:100:LEU:HD12	12:P:112:LEU:HD11	1.48	0.96
1:A:143:G:H1'	20:X:37:THR:HG21	1.49	0.94
1:A:272(J):C:H42	1:A:363:G:H1	1.11	0.94
8:J:26:LEU:HA	8:J:84:GLU:HA	1.50	0.93
1:A:731:C:OP1	62:A:4180:HOH:O	1.86	0.92
1:A:2269:A:OP1	62:A:4197:HOH:O	1.88	0.89
1:A:1416:G:H1	1:A:1582:C:H42	1.21	0.89
7:H:43:VAL:HA	7:H:52:VAL:HG12	1.54	0.88
22:Z:52:SER:OG	22:Z:53:ILE:N	2.06	0.87
1:A:1143:A:OP1	10:N:25:ARG:NH2	2.07	0.87
1:A:818:G:OP2	62:A:4259:HOH:O	1.91	0.87
1:A:2121:G:H1	1:A:2177:C:H42	1.21	0.87
1:A:2106:G:H1	1:A:2183:C:N4	1.72	0.87
1:A:250:G:H2'	1:A:251:A:C8	2.10	0.86
1:A:1603:A:OP1	62:A:4195:HOH:O	1.91	0.86
1:A:335:C:H4'	21:Y:73:ARG:HD3	1.54	0.86
1:A:1784:A:OP2	62:A:4084:HOH:O	1.92	0.86
1:A:1170:G:H1	1:A:1179:C:H42	1.26	0.84
20:X:57:LEU:HD13	20:X:78:LYS:HB2	1.57	0.84
1:A:1036:G:H1	1:A:1119:C:H42	1.26	0.84
1:A:2705:A:OP2	62:A:4090:HOH:O	1.96	0.84
1:A:370:G:OP2	62:A:3759:HOH:O	1.94	0.84
27:4:59:PHE:HA	27:4:61:ARG:H	1.43	0.83
1:A:1639:U:OP1	62:A:3946:HOH:O	1.96	0.83
1:A:817:C:OP2	62:A:3879:HOH:O	1.95	0.83
3:D:171:ASP:OD1	3:D:171:ASP:N	2.12	0.82
22:Z:138:GLU:H	22:Z:156:LYS:HZ1	1.27	0.82
1:A:1364:G:OP1	24:1:2:SER:N	2.12	0.82
1:A:2006:C:OP1	62:A:3935:HOH:O	1.97	0.82
1:A:1604:C:OP2	62:A:4195:HOH:O	1.97	0.82
5:F:101:LEU:HD12	5:F:102:PRO:HD2	1.59	0.82
1:A:411:G:OP1	62:A:3865:HOH:O	1.98	0.81
1:A:999:U:OP2	62:A:4063:HOH:O	1.99	0.81
1:A:1268:A:OP1	62:A:3935:HOH:O	1.98	0.81
1:A:956:G:O6	62:A:4311:HOH:O	1.98	0.81
5:F:168:ARG:O	5:F:170:LEU:N	2.14	0.81
31:8:33:ASN:HA	31:8:36:LYS:HD2	1.61	0.81
12:P:39:LYS:HG3	12:P:45:LEU:HD12	1.63	0.81
23:0:23:VAL:HG23	23:0:38:VAL:HG22	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272(J):C:N4	1:A:363:G:H1	1.78	0.80
1:A:2292:C:OP1	15:S:17:ARG:NH2	2.15	0.80
1:A:847:U:O4	1:A:933:A:N6	2.15	0.80
1:A:1176:G:N2	1:A:1178:C:OP2	2.15	0.80
1:A:993:G:OP1	17:U:50:ARG:NH2	2.15	0.80
24:1:75:GLU:O	24:1:77:ALA:N	2.15	0.80
4:E:12:THR:HG22	4:E:13:ARG:H	1.47	0.79
5:F:11:VAL:HB	5:F:18:ARG:HB3	1.65	0.79
1:A:2125:G:H21	1:A:2173:A:H62	1.26	0.79
1:A:271(J):C:N3	1:A:271(M):G:O6	2.15	0.79
1:A:1059:G:N2	9:K:126:MET:O	2.16	0.79
1:A:523:C:O2	1:A:554:U:O2'	2.00	0.79
22:Z:144:LEU:HD21	22:Z:150:LEU:HD21	1.64	0.79
1:A:862:G:OP2	62:A:4253:HOH:O	1.99	0.79
1:A:800:A:OP1	62:A:4085:HOH:O	2.01	0.79
2:B:81:G:OP2	62:B:315:HOH:O	2.00	0.79
2:B:17:C:H42	2:B:68:C:H42	1.31	0.79
7:H:109:PHE:HE2	7:H:152:ARG:HH21	1.31	0.79
31:8:6:THR:HG22	31:8:63:PRO:HD2	1.64	0.78
1:A:759:G:O6	62:A:4237:HOH:O	1.97	0.78
7:H:3:ARG:HG3	7:H:3:ARG:HH11	1.48	0.78
1:A:2107:C:H42	1:A:2182:G:H1	1.31	0.78
1:A:883:G:N2	1:A:893:C:N3	2.31	0.78
1:A:943:U:OP2	62:A:4137:HOH:O	2.02	0.78
1:A:1009:A:OP2	10:N:37:LYS:NZ	2.16	0.78
1:A:576:U:OP1	62:A:4055:HOH:O	2.01	0.78
1:A:1378:A:O2'	1:A:1380:G:N7	2.16	0.78
20:X:54:VAL:HG22	20:X:81:VAL:HG12	1.66	0.78
22:Z:29:TYR:HB3	22:Z:34:ASN:HD22	1.49	0.78
1:A:693:C:H2'	1:A:694:U:H6	1.50	0.77
7:H:149:ARG:NH1	7:H:167:GLU:OE1	2.18	0.77
1:A:1766:U:H2'	1:A:1767:C:H6	1.49	0.77
1:A:862:G:OP2	62:A:4252:HOH:O	2.02	0.77
5:F:51:THR:O	5:F:93:LYS:NZ	2.15	0.77
1:A:2600:A:N6	62:A:3922:HOH:O	2.18	0.77
17:U:76:TYR:OH	17:U:92:ARG:NH1	2.18	0.76
22:Z:150:LEU:HB2	22:Z:172:ALA:HB3	1.67	0.76
1:A:1019:U:H3	1:A:1142(A):A:H62	1.29	0.76
4:E:72:VAL:HA	4:E:73:GLU:HG2	1.68	0.76
1:A:1190:G:N7	62:A:4068:HOH:O	2.16	0.76
19:W:18:ARG:NH1	19:W:76:VAL:O	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:A:H2	1:A:1241:A:H62	1.33	0.76
1:A:2052:G:H4'	4:E:143:ASN:O	1.85	0.76
1:A:1999:C:O2	1:A:2687:U:O2'	2.04	0.76
4:E:127:ASP:OD2	62:E:403:HOH:O	2.02	0.76
15:S:58:LEU:HB3	15:S:59:LYS:HB2	1.68	0.76
17:U:88:ILE:HD13	17:U:109:LEU:HD23	1.69	0.76
9:K:95:LYS:HG2	9:K:137:GLU:HB3	1.69	0.75
1:A:1315:C:OP2	62:A:4060:HOH:O	2.05	0.75
1:A:883:G:H1	1:A:893:C:H42	0.81	0.75
1:A:1639:U:OP2	62:A:3924:HOH:O	2.05	0.75
1:A:319:C:N4	1:A:323:G:O6	2.18	0.75
11:O:80:ASP:OD2	16:T:64:ARG:NH2	2.20	0.75
23:O:39:ARG:HD3	23:O:58:THR:HG23	1.68	0.75
18:V:7:THR:O	62:V:301:HOH:O	2.05	0.75
20:X:18:TYR:O	20:X:20:GLY:N	2.20	0.74
22:Z:124:ILE:HG12	22:Z:125:LEU:H	1.51	0.74
1:A:1566:A:OP1	3:D:211:ARG:NH1	2.21	0.74
1:A:2074:U:H2'	1:A:2075:U:C6	2.22	0.74
29:6:3:SER:OG	29:6:4:GLU:N	2.18	0.74
1:A:2630:G:HO2'	1:A:2892:A:HO2'	1.36	0.74
3:D:158:ALA:O	3:D:161:THR:OG1	2.03	0.74
1:A:1058:G:N2	9:K:126:MET:SD	2.61	0.74
10:N:120:LEU:HD22	10:N:122:VAL:HG22	1.68	0.74
3:D:141:VAL:HG12	3:D:164:GLN:HG3	1.70	0.74
7:H:3:ARG:NH1	7:H:4:ILE:H	1.86	0.74
1:A:567:A:OP1	62:A:3875:HOH:O	2.04	0.74
22:Z:144:LEU:HD22	22:Z:148:ASP:HB3	1.69	0.74
27:4:16:CYS:HB2	27:4:36:CYS:HB3	1.70	0.73
1:A:2581:G:OP2	62:A:4009:HOH:O	2.06	0.73
6:G:66:GLN:OE1	6:G:98:ARG:NE	2.16	0.73
1:A:2150:U:H2'	1:A:2151:G:H8	1.52	0.73
1:A:739:G:OP1	62:A:4079:HOH:O	2.06	0.73
3:D:85:ASP:OD2	3:D:88:ARG:NH1	2.22	0.73
23:O:56:ASP:OD2	23:O:58:THR:OG1	2.07	0.73
1:A:928:G:O6	62:A:3951:HOH:O	2.05	0.73
1:A:120:U:OP2	62:A:3725:HOH:O	2.05	0.73
14:R:38:VAL:HG23	14:R:39:PRO:HD3	1.70	0.73
9:K:13:PRO:HA	9:K:52:ILE:HA	1.69	0.73
1:A:1314:C:OP1	62:A:4060:HOH:O	2.06	0.73
1:A:2349:G:OP1	62:A:3754:HOH:O	2.05	0.73
1:A:2683:C:OP1	16:T:55:ASN:ND2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:14:ILE:HG13	4:E:21:VAL:HG13	1.70	0.72
1:A:1108:U:O2'	1:A:1109:C:O5'	2.07	0.72
1:A:2592:G:OP1	62:A:4104:HOH:O	2.07	0.72
17:U:69:CYS:HB3	17:U:74:LEU:HD13	1.71	0.72
1:A:1441:G:H5''	1:A:1442:G:H5'	5.57	0.72
1:A:1170:G:N2	1:A:1179:C:N3	2.32	0.72
4:E:77:ILE:HG21	4:E:195:LEU:HD21	1.71	0.72
1:A:2591:C:H2'	1:A:2592:G:H8	1.54	0.72
21:Y:30:VAL:HG13	21:Y:37:VAL:HG12	1.71	0.72
9:K:51:ALA:HB1	9:K:73:PRO:HD2	1.72	0.72
1:A:2429:G:OP2	62:A:4144:HOH:O	2.08	0.72
1:A:944:G:OP2	62:A:4138:HOH:O	2.07	0.72
13:Q:138:ASP:OD1	22:Z:81:ARG:NH1	2.23	0.72
1:A:2124:G:H1	1:A:2174:C:H42	1.36	0.72
5:F:20:LEU:HD22	5:F:21:ALA:H	1.54	0.72
21:Y:83:THR:OG1	21:Y:84:ARG:N	2.22	0.72
1:A:1153:C:OP2	62:A:4063:HOH:O	2.08	0.71
1:A:1434:A:H61	1:A:1558:A:H62	1.38	0.71
3:D:92:ILE:HG22	3:D:106:ILE:HA	1.72	0.71
12:P:81:GLN:HG2	12:P:106:LEU:HD22	1.72	0.71
1:A:1309:G:H4'	30:7:7:PRO:HG2	1.70	0.71
1:A:2793:G:H1	1:A:2803:C:H42	1.35	0.71
1:A:444:C:H4'	5:F:49:ALA:HB2	1.72	0.71
1:A:1169:G:H1	1:A:1180:C:H42	1.38	0.71
16:T:65:LYS:HE3	16:T:67:SER:HB2	1.73	0.71
12:P:89:ALA:HA	12:P:121:LYS:HD3	1.71	0.71
1:A:1982:C:OP2	62:A:4222:HOH:O	2.08	0.71
1:A:372:G:OP2	24:1:69:LYS:NZ	2.21	0.71
9:K:59:ILE:HD11	9:K:63:ARG:HA	1.73	0.71
1:A:2222:G:H2'	1:A:2223:G:H8	1.56	0.71
1:A:2357:U:OP1	23:0:20:ARG:NH1	2.24	0.71
1:A:574:C:OP1	62:A:3780:HOH:O	2.08	0.71
29:6:9:LEU:HA	29:6:54:ILE:HB	1.73	0.70
9:K:99:ILE:HG23	9:K:103:GLN:HB3	1.73	0.70
1:A:2028:U:O4	62:A:3898:HOH:O	2.07	0.70
1:A:1021:A:H3'	1:A:1021:A:C8	2.26	0.70
1:A:1557:C:OP2	1:A:1558:A:O2'	2.10	0.70
1:A:226:G:H21	1:A:228:A:H62	1.37	0.70
1:A:2816:C:O3'	14:R:99:LYS:NZ	2.25	0.70
1:A:1187:G:H5''	18:V:81:TYR:CE2	2.27	0.70
1:A:2577:A:OP1	62:A:4077:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:G:O2'	62:A:4174:HOH:O	2.09	0.70
1:A:1375:C:OP1	62:A:3779:HOH:O	2.09	0.70
2:B:75:G:H1'	22:Z:27:VAL:HG11	1.74	0.70
13:Q:138:ASP:OD2	13:Q:138:ASP:N	2.21	0.70
19:W:13:SER:HB3	19:W:16:LYS:HG3	1.73	0.70
5:F:17:ARG:HH12	5:F:19:GLU:HG3	1.57	0.70
11:O:87:ILE:HD12	11:O:91:LEU:HA	1.74	0.70
1:A:2591:C:H2'	1:A:2592:G:C8	2.27	0.70
1:A:2023:G:H5'	1:A:2617:C:H4'	1.73	0.70
1:A:72:U:OP1	62:A:4058:HOH:O	2.09	0.70
7:H:56:SER:OG	7:H:57:ASP:N	2.25	0.70
7:H:3:ARG:HH12	7:H:5:GLY:H	1.40	0.70
27:4:44:THR:O	27:4:46:GLN:N	2.24	0.69
1:A:1478:G:H2'	1:A:1479:G:H8	1.57	0.69
1:A:906:G:O2'	13:Q:67:ARG:NH2	2.21	0.69
21:Y:13:VAL:HG12	21:Y:74:PRO:HA	1.73	0.69
1:A:2478:A:OP2	32:9:2:LYS:NZ	2.20	0.69
1:A:2822:G:H2'	1:A:2823:A:H5''	1.75	0.69
1:A:588:U:OP2	62:A:3884:HOH:O	2.09	0.69
17:U:85:LYS:NZ	17:U:116:ALA:O	2.25	0.69
20:X:35:THR:HB	20:X:38:GLU:HG2	1.75	0.69
29:6:23:THR:OG1	29:6:24:GLU:N	2.17	0.69
6:G:9:ARG:NH1	6:G:13:GLU:OE1	2.23	0.69
1:A:801:G:OP2	62:A:3758:HOH:O	2.11	0.69
1:A:1828:G:OP1	62:A:4095:HOH:O	2.10	0.69
1:A:693:C:H2'	1:A:694:U:C6	2.27	0.69
1:A:1936:A:H61	1:A:1963:U:H3	1.41	0.69
1:A:690:G:O2'	1:A:780:G:OP1	2.10	0.69
1:A:1165:U:H2'	1:A:1166:C:C6	2.27	0.69
13:Q:109:VAL:HG13	13:Q:113:GLN:HB3	1.75	0.69
23:0:37:LEU:N	23:0:59:LEU:O	2.20	0.69
24:1:18:ILE:HG23	24:1:37:ILE:HG12	1.74	0.69
1:A:1395:A:OP1	62:A:4195:HOH:O	2.11	0.69
1:A:249:C:OP1	62:A:3871:HOH:O	2.11	0.69
1:A:833:U:O2	12:P:55:ARG:NH2	2.26	0.69
1:A:118:A:C8	1:A:119:A:C8	2.81	0.68
1:A:1345:C:OP2	62:A:3747:HOH:O	2.11	0.68
16:T:108:ARG:HA	16:T:111:ARG:HH11	1.57	0.68
1:A:1021:A:H8	1:A:1021:A:H3'	1.58	0.68
1:A:1968:G:OP1	62:A:4104:HOH:O	2.10	0.68
1:A:2417:C:OP1	12:P:65:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:8:31:HIS:O	31:8:36:LYS:NZ	2.26	0.68
16:T:100:TYR:HB3	16:T:103:ARG:NH1	2.07	0.68
1:A:2588:G:OP1	62:A:4047:HOH:O	2.11	0.68
1:A:445:C:OP2	62:A:3767:HOH:O	2.10	0.68
6:G:115:ARG:O	6:G:117:PHE:N	2.27	0.68
27:4:56:VAL:HG23	27:4:57:GLU:HG3	1.76	0.68
10:N:42:TRP:HD1	10:N:48:MET:HE1	1.58	0.68
4:E:13:ARG:HD3	16:T:58:ASN:HD21	1.59	0.68
1:A:1045:A:H5''	1:A:1047:G:H1'	1.76	0.68
1:A:1349:A:OP1	62:A:4203:HOH:O	2.11	0.68
1:A:748:G:O6	19:W:90:ARG:NH1	2.27	0.68
1:A:1833:U:H2'	1:A:1834:U:H6	1.59	0.68
3:D:233:HIS:O	62:D:402:HOH:O	2.12	0.68
21:Y:99:CYS:HB2	21:Y:106:LEU:HD21	1.76	0.68
4:E:54:GLN:HB2	4:E:76:ARG:HG2	1.75	0.67
1:A:2017:U:OP1	62:A:3783:HOH:O	2.12	0.67
1:A:734:A:OP2	62:A:4236:HOH:O	2.11	0.67
1:A:1269:A:OP2	62:A:3940:HOH:O	2.11	0.67
1:A:1332:G:OP2	62:A:4361:HOH:O	2.12	0.67
1:A:2035:G:OP1	62:A:4075:HOH:O	2.11	0.67
14:R:18:LEU:HD22	14:R:22:ARG:HG3	1.77	0.67
18:V:71:LEU:HD11	18:V:84:LYS:HE3	1.76	0.67
1:A:1792:G:H5''	3:D:205:VAL:HG22	1.75	0.67
1:A:2115:G:N1	1:A:2119:A:OP2	2.28	0.67
1:A:2405:G:OP2	62:A:3835:HOH:O	2.13	0.67
1:A:574:C:OP2	62:A:4128:HOH:O	2.12	0.67
26:3:35:ARG:HE	26:3:37:LEU:HD21	1.60	0.67
27:4:42:PHE:HB3	27:4:43:TYR:HB2	1.75	0.67
1:A:674:G:OP2	62:A:3960:HOH:O	2.13	0.67
20:X:31:HIS:CD2	20:X:33:LYS:H	2.13	0.67
1:A:1175:U:OP1	1:A:1177:A:N6	2.27	0.67
1:A:1403:C:H5''	1:A:1471:A:H1'	1.77	0.67
1:A:1435:G:O6	1:A:1557:C:N4	2.21	0.67
1:A:794:G:OP2	62:A:4106:HOH:O	2.12	0.67
3:D:142:VAL:HG23	3:D:193:VAL:HA	1.77	0.67
1:A:1060:U:H4'	1:A:1061:U:H5'	1.77	0.67
6:G:66:GLN:HA	27:4:6:HIS:ND1	2.10	0.67
17:U:53:ARG:HA	17:U:56:ASP:HB2	1.77	0.67
3:D:101:GLU:OE1	3:D:103:ARG:NH1	2.27	0.66
1:A:1219:G:OP2	17:U:19:LYS:NZ	2.20	0.66
26:3:31:LEU:HD13	26:3:32:GLN:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:A:H62	1:A:1141:U:H3	1.43	0.66
1:A:1590:U:H2'	1:A:1591:G:C8	2.30	0.66
1:A:651:G:OP1	31:8:19:SER:OG	2.09	0.66
3:D:123:ALA:HB3	3:D:131:LEU:HD11	1.77	0.66
19:W:35:ILE:O	19:W:37:ARG:N	2.27	0.66
22:Z:72:ARG:NH2	22:Z:97:GLU:O	2.28	0.66
1:A:271(J):C:O2	1:A:271(M):G:N1	2.28	0.66
1:A:1395:A:OP1	62:A:3948:HOH:O	2.12	0.66
1:A:2101:G:H1	1:A:2188:C:H42	1.42	0.66
1:A:2589:A:OP1	62:A:4046:HOH:O	2.13	0.66
18:V:25:LEU:HD22	18:V:26:ASP:H	1.60	0.66
1:A:1405:U:H2'	1:A:1406:U:C6	2.30	0.66
1:A:192:C:OP2	62:A:3735:HOH:O	2.13	0.66
9:K:10:LEU:HD11	9:K:27:LEU:HD11	1.77	0.66
1:A:2111:C:OP2	1:A:2145:C:N4	2.29	0.66
1:A:40:C:H42	1:A:438:G:H1	1.42	0.66
5:F:17:ARG:NH1	5:F:18:ARG:O	2.28	0.66
1:A:2140:C:N3	1:A:2151:G:O6	2.29	0.65
5:F:178:PRO:HB2	5:F:201:VAL:HG21	1.75	0.65
4:E:77:ILE:HD12	4:E:78:LEU:H	1.61	0.65
8:J:118:THR:N	8:J:121:ASP:O	2.29	0.65
1:A:2789:C:O2'	1:A:2790:A:O5'	2.13	0.65
1:A:322:A:H3'	5:F:169:ASN:HD21	1.61	0.65
3:D:133:LEU:HA	3:D:136:ILE:HD12	1.78	0.65
14:R:28:LEU:O	14:R:31:HIS:N	2.28	0.65
1:A:141:A:H8	1:A:1408:C:HO2'	1.41	0.65
1:A:2106:G:N2	1:A:2183:C:N3	2.40	0.65
1:A:1783:A:H5'	1:A:2608:G:H4'	1.77	0.65
3:D:43:ARG:NH2	3:D:49:ILE:HD11	2.10	0.65
9:K:6:ALA:HB3	9:K:59:ILE:H	1.62	0.65
20:X:50:LYS:HB3	20:X:84:ALA:HB2	1.77	0.65
1:A:975:C:O2'	62:A:4062:HOH:O	2.15	0.65
22:Z:183:LEU:O	22:Z:185:GLU:N	2.29	0.65
12:P:63:PRO:HG2	31:8:25:MET:HB2	1.79	0.65
1:A:1942:C:OP2	1:A:1943:U:O2'	2.12	0.65
30:7:9:ARG:HG3	30:7:46:VAL:HG23	1.79	0.65
31:8:29:LYS:HD3	31:8:44:LYS:HB2	1.79	0.65
1:A:180:G:N2	1:A:215:G:O6	2.30	0.65
1:A:2199:A:H5'	1:A:2200:C:OP2	1.96	0.65
3:D:274:ARG:HB2	3:D:275:LYS:HB2	1.79	0.65
14:R:104:ARG:HG3	14:R:111:LEU:HD11	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2036:C:OP1	62:A:4073:HOH:O	2.14	0.65
8:J:56:ASN:HA	8:J:83:TYR:HA	1.78	0.65
24:1:7:ILE:HG22	24:1:8:SER:HB3	1.78	0.65
31:8:52:LYS:HG3	31:8:53:PRO:HD3	1.78	0.65
1:A:1254:A:OP2	62:A:4170:HOH:O	2.14	0.65
1:A:2025:C:H2'	1:A:2026:C:C6	2.32	0.65
1:A:83:G:O2'	1:A:102:G:N2	2.30	0.65
1:A:1250:G:N7	12:P:18:ARG:NH2	2.45	0.64
1:A:2385:C:OP2	62:A:3801:HOH:O	2.14	0.64
1:A:34:C:H2'	1:A:35:G:H5'	1.77	0.64
1:A:876:C:H2'	1:A:877:U:O4'	1.97	0.64
1:A:1790:C:O2'	3:D:209:ALA:HB2	1.96	0.64
1:A:467:G:OP1	30:7:33:ARG:NH1	2.29	0.64
1:A:979:G:N7	62:A:4020:HOH:O	2.29	0.64
27:4:45:GLY:C	27:4:47:GLN:H	2.01	0.64
1:A:1107:G:H4'	8:J:81:VAL:HA	1.79	0.64
1:A:2206:G:H5'	1:A:2207:G:C5	2.33	0.64
26:3:8:LEU:HB2	26:3:28:LEU:HD22	1.79	0.64
28:5:36:CYS:HB3	28:5:49:CYS:HB3	1.79	0.64
1:A:1451:C:H42	1:A:1459:G:H1	1.46	0.64
1:A:981:A:H8	1:A:982:C:C5	2.15	0.64
1:A:1071:G:O2'	1:A:1089:G:OP2	2.14	0.64
5:F:17:ARG:HG2	5:F:18:ARG:H	1.62	0.64
1:A:2109:U:O4	1:A:2179:C:N4	2.31	0.64
22:Z:7:ALA:HB2	22:Z:59:LEU:HD22	1.79	0.64
1:A:1776:G:OP2	62:A:3743:HOH:O	2.15	0.64
1:A:2122:U:H2'	1:A:2123:G:H8	1.62	0.64
1:A:747:U:H2'	19:W:88:ARG:HH21	1.62	0.64
3:D:44:ASN:HB3	3:D:50:THR:HG21	1.79	0.64
5:F:161:GLU:O	5:F:165:ARG:HB2	1.98	0.64
6:G:115:ARG:H	6:G:136:ARG:HH21	1.46	0.64
1:A:1022:G:H22	1:A:1142(A):A:H2	1.46	0.64
3:D:121:PRO:HB3	3:D:135:PHE:CE1	2.33	0.64
6:G:150:ASP:OD2	6:G:150:ASP:N	2.31	0.64
6:G:22:ARG:HH21	6:G:175:LEU:HD11	1.63	0.64
1:A:1161:C:H4'	18:V:8:GLY:HA2	1.80	0.64
1:A:2121:G:H1	1:A:2177:C:N4	1.92	0.64
1:A:2637:U:H5''	4:E:82:ARG:HH21	1.63	0.64
21:Y:51:VAL:HG13	21:Y:57:GLN:H	1.62	0.64
1:A:1786:A:H1'	1:A:1938:A:N6	2.14	0.63
1:A:1951:U:O4	62:A:4134:HOH:O	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2125:G:N2	1:A:2173:A:H62	1.93	0.63
1:A:120:U:OP2	62:A:3726:HOH:O	2.15	0.63
20:X:92:LEU:C	20:X:94:GLY:H	2.02	0.63
22:Z:104:PHE:HA	22:Z:139:VAL:HG23	1.80	0.63
27:4:45:GLY:O	27:4:47:GLN:N	2.30	0.63
1:A:1166:C:O2'	62:A:4045:HOH:O	2.16	0.63
1:A:2114:A:N3	1:A:2167:U:N3	2.45	0.63
12:P:27:HIS:HB3	12:P:32:THR:HG23	1.81	0.63
1:A:2319:G:H22	15:S:3:ARG:HA	1.64	0.63
1:A:2428:G:O2'	62:A:4383:HOH:O	2.14	0.63
8:J:6:ASN:HA	8:J:9:LEU:H	1.63	0.63
1:A:125:G:H5''	30:7:19:ARG:HD3	1.79	0.63
16:T:84:GLN:HG2	16:T:85:LYS:HG2	1.79	0.63
19:W:21:VAL:HG22	19:W:47:VAL:HG21	1.80	0.63
1:A:2419:U:OP2	31:8:33:ASN:ND2	2.31	0.63
1:A:184:C:H2'	1:A:185:U:H6	1.64	0.63
1:A:2201:C:H2'	1:A:2202:C:H6	1.64	0.63
2:B:51:G:N7	15:S:62:LYS:NZ	2.44	0.63
17:U:62:ILE:HG23	17:U:76:TYR:CE1	2.34	0.63
6:G:83:ARG:O	6:G:86:MET:HG3	1.99	0.63
16:T:13:ARG:NH2	16:T:14:TYR:OH	2.31	0.63
27:4:24:THR:OG1	27:4:25:TYR:N	2.32	0.62
1:A:592:G:H2'	1:A:593:G:H8	2.94	0.62
4:E:56:PRO:HA	4:E:59:VAL:HG23	1.81	0.62
2:B:105:A:OP1	22:Z:72:ARG:NH1	2.31	0.62
1:A:1766:U:H2'	1:A:1767:C:C6	2.33	0.62
1:A:2369:A:H2'	1:A:2370:G:H8	1.64	0.62
3:D:155:LEU:HD23	3:D:177:LEU:HD22	1.81	0.62
1:A:2305:A:H5''	6:G:134:GLY:HA3	1.80	0.62
22:Z:110:GLY:HA3	22:Z:174:VAL:HG11	1.80	0.62
1:A:2740:A:H2'	1:A:2741:A:C8	2.33	0.62
1:A:1138:G:N2	10:N:106:MET:SD	2.67	0.62
3:D:264:LYS:HG3	3:D:265:PRO:HD2	1.80	0.62
6:G:173:LEU:HA	6:G:176:LEU:HD12	1.81	0.62
7:H:54:ARG:NE	7:H:56:SER:O	2.17	0.62
22:Z:126:VAL:HG11	22:Z:161:VAL:HG22	1.79	0.62
25:2:10:LEU:HD13	25:2:14:ARG:HH12	1.64	0.62
29:6:2:ALA:HA	29:6:6:ARG:HG2	1.82	0.62
1:A:1491:G:O4'	3:D:99:ASP:HB3	2.00	0.62
1:A:2051:A:H5'	1:A:2578:G:O4'	2.00	0.62
7:H:11:VAL:HG12	7:H:15:VAL:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:36:GLY:O	10:N:38:HIS:N	2.32	0.62
1:A:1048:A:OP2	1:A:1109:C:N4	2.33	0.62
32:9:17:ILE:HG22	32:9:24:TYR:HB2	1.81	0.62
1:A:2102:U:O2	1:A:2187:G:O6	2.18	0.62
1:A:2334:G:O6	23:0:74:ARG:NH2	2.33	0.62
1:A:422:A:H2'	1:A:423:A:C8	2.35	0.62
25:2:16:LEU:HD23	25:2:17:SER:H	1.64	0.62
29:6:47:THR:O	29:6:49:HIS:ND1	2.32	0.62
1:A:2482:G:H22	13:Q:52:VAL:HG11	1.65	0.62
6:G:161:THR:HG23	6:G:163:ALA:H	1.64	0.62
9:K:125:ARG:O	9:K:129:GLY:N	2.32	0.62
1:A:1412:A:H2'	1:A:1413:G:C8	2.34	0.62
3:D:8:PRO:HB3	3:D:14:ARG:HB2	1.82	0.62
10:N:96:GLU:OE2	10:N:96:GLU:N	2.23	0.62
11:O:115:VAL:HG12	11:O:121:VAL:HG21	1.81	0.62
1:A:2784:C:H2'	1:A:2785:C:H6	1.65	0.61
1:A:610:G:N2	1:A:619:G:H1'	2.14	0.61
6:G:27:ASN:O	6:G:29:TRP:N	2.31	0.61
1:A:1798:U:H5''	3:D:260:ARG:HB3	1.81	0.61
1:A:1187:G:H5''	18:V:81:TYR:HE2	1.64	0.61
1:A:2781:A:H5''	1:A:2782:G:H5'	1.82	0.61
25:2:47:ASN:ND2	25:2:47:ASN:H	1.96	0.61
29:6:13:CYS:SG	29:6:47:THR:HG21	2.40	0.61
1:A:1394:U:OP1	62:A:3947:HOH:O	2.16	0.61
14:R:22:ARG:HE	14:R:69:ASP:HA	1.65	0.61
15:S:69:VAL:HA	15:S:72:ALA:HB3	1.83	0.61
27:4:55:ARG:O	27:4:60:GLN:NE2	2.33	0.61
21:Y:102:CYS:SG	21:Y:103:GLY:N	2.74	0.61
1:A:1819:A:H4'	1:A:1820:U:H5''	1.82	0.61
1:A:1940:U:H4'	1:A:1941:C:H5'	1.82	0.61
1:A:910:A:H2'	1:A:911:A:C8	2.35	0.61
1:A:1135:C:H3'	1:A:1137:G:OP1	2.00	0.61
1:A:1165:U:H2'	1:A:1166:C:H6	1.66	0.61
26:3:8:LEU:HD12	26:3:31:LEU:HA	1.83	0.61
1:A:1259:G:H2'	1:A:1260:G:C8	2.35	0.61
1:A:2431:U:OP2	62:A:3867:HOH:O	2.16	0.61
1:A:271(J):C:N3	1:A:271(M):G:C6	2.68	0.61
18:V:62:LEU:HD11	18:V:95:LEU:HB2	1.83	0.61
27:4:61:ARG:HH21	27:4:63:TYR:HB2	1.64	0.61
1:A:2222:G:H2'	1:A:2223:G:C8	2.35	0.61
17:U:78:THR:O	17:U:81:HIS:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2793:G:N2	1:A:2803:C:N3	2.49	0.61
3:D:146:GLU:HB2	3:D:189:CYS:HB3	1.83	0.61
6:G:106:LEU:HA	6:G:110:ALA:HB3	1.81	0.61
14:R:44:LEU:HD11	14:R:79:LEU:HD13	13.35	0.61
6:G:25:TYR:OH	6:G:168:GLU:OE1	2.18	0.60
7:H:20:ALA:HB1	7:H:21:PRO:HD2	1.83	0.60
1:A:2331:G:H4'	23:0:43:THR:H	1.66	0.60
1:A:2394:C:OP2	31:8:30:ARG:NH1	2.33	0.60
16:T:100:TYR:HB3	16:T:103:ARG:HH12	1.65	0.60
1:A:2104:G:H1	1:A:2185:C:H42	1.49	0.60
1:A:226:G:N2	1:A:228:A:H62	1.97	0.60
1:A:2638:G:N2	1:A:2775:A:H2'	2.17	0.60
1:A:1651:G:H5'	14:R:39:PRO:HG2	1.83	0.60
24:1:85:LEU:HD23	24:1:90:ILE:HG12	1.82	0.60
1:A:2124:G:H1	1:A:2174:C:N4	1.99	0.60
1:A:2820:A:OP2	14:R:2:ARG:NH2	2.35	0.60
1:A:944:G:H5''	1:A:945:A:O5'	2.01	0.60
11:O:89:ASN:O	11:O:91:LEU:HD23	2.00	0.60
1:A:1341:U:O4	20:X:16:LYS:NZ	2.35	0.60
1:A:2419:U:O4	62:A:3927:HOH:O	2.17	0.60
10:N:58:ASP:HB3	10:N:124:ALA:HB1	1.82	0.60
20:X:92:LEU:O	20:X:94:GLY:N	2.32	0.60
22:Z:110:GLY:N	22:Z:144:LEU:O	2.35	0.60
4:E:154:LYS:HD3	4:E:155:LYS:H	1.67	0.60
22:Z:10:ARG:HD3	22:Z:38:TYR:HB3	1.83	0.60
27:4:66:SER:OG	27:4:67:TYR:N	2.34	0.60
1:A:285:C:H2'	1:A:286:C:H6	1.67	0.60
1:A:624:C:H2'	1:A:625:G:H8	2.40	0.60
19:W:1:MET:HG3	19:W:2:GLU:H	1.66	0.60
12:P:84:ASN:HA	12:P:115:LEU:O	2.02	0.60
20:X:35:THR:HG22	20:X:37:THR:H	1.66	0.60
1:A:1709:U:C2	1:A:1750:G:N2	2.70	0.60
3:D:67:PHE:HD2	3:D:153:ALA:HB3	1.66	0.60
6:G:6:ALA:HA	6:G:9:ARG:HB2	1.84	0.60
1:A:577:G:H2'	1:A:578:A:C8	2.37	0.60
4:E:23:VAL:HG21	4:E:183:LEU:HD23	1.84	0.60
1:A:1054:A:N6	1:A:1105:U:H3	2.01	0.59
1:A:184:C:H2'	1:A:185:U:C6	2.37	0.59
1:A:576:U:H2'	1:A:577:G:C8	2.36	0.59
1:A:620:G:H5'	1:A:620:G:N3	2.17	0.59
1:A:2793:G:H1	1:A:2803:C:N4	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2025:C:H2'	1:A:2026:C:H6	1.66	0.59
1:A:2107:C:N4	1:A:2182:G:H1	2.00	0.59
25:2:30:ARG:HH21	25:2:34:GLU:HG3	1.67	0.59
1:A:2577:A:H5''	1:A:2578:G:H5'	1.84	0.59
1:A:264:C:O2'	1:A:428:A:N1	2.36	0.59
1:A:31:C:OP1	62:A:4125:HOH:O	2.17	0.59
3:D:184:LYS:HG3	3:D:271:ILE:HD11	1.84	0.59
1:A:1246:A:OP1	5:F:38:ARG:NH1	2.36	0.59
1:A:1652:A:OP1	14:R:8:ARG:NH1	2.31	0.59
5:F:155:LEU:HB2	5:F:189:THR:HG21	1.85	0.59
7:H:80:SER:OG	7:H:81:GLU:N	2.35	0.59
19:W:56:ALA:O	19:W:58:ALA:N	2.35	0.59
22:Z:52:SER:HG	22:Z:53:ILE:H	1.47	0.59
26:3:21:ALA:O	26:3:24:LYS:N	2.34	0.59
6:G:5:VAL:HG13	27:4:25:TYR:HE1	1.68	0.59
1:A:1441:G:O2'	1:A:1628:G:OP1	2.21	0.59
1:A:2201:C:H2'	1:A:2202:C:C6	2.38	0.59
1:A:2287:A:O2'	1:A:2288:A:H5''	2.02	0.59
1:A:2287:A:H62	1:A:2344:U:H3	1.49	0.59
10:N:128:HIS:O	10:N:128:HIS:ND1	2.35	0.59
4:E:5:LEU:HD11	4:E:79:ARG:HB2	1.85	0.59
18:V:82:ARG:O	18:V:83:ARG:NH1	2.28	0.59
9:K:124:ALA:O	9:K:128:ALA:N	2.34	0.59
27:4:40:HIS:O	27:4:43:TYR:HB3	2.03	0.58
1:A:2879:C:OP2	62:A:4028:HOH:O	2.16	0.58
16:T:91:ARG:HB2	16:T:121:ILE:HG13	1.84	0.58
1:A:271:A:N3	1:A:365:C:O2'	2.33	0.58
7:H:170:ARG:O	7:H:171:LEU:HD23	2.03	0.58
11:O:63:VAL:HG21	11:O:85:VAL:HG23	1.85	0.58
16:T:35:LYS:HZ1	16:T:38:ASN:HA	1.68	0.58
16:T:55:ASN:H	16:T:59:THR:HG22	1.67	0.58
22:Z:128:VAL:HG22	22:Z:132:ASN:HD22	1.67	0.58
1:A:2074:U:OP1	62:A:3911:HOH:O	2.17	0.58
1:A:2144:U:H1'	1:A:2148:G:H22	1.68	0.58
7:H:7:LEU:HB3	7:H:69:ARG:NH1	2.18	0.58
11:O:10:VAL:HG21	11:O:16:ALA:HB3	1.84	0.58
1:A:1124:C:OP1	62:A:4392:HOH:O	2.17	0.58
1:A:2640:G:OP1	10:N:97:ARG:NH2	2.36	0.58
2:B:63:G:H2'	2:B:64:C:C6	2.39	0.58
4:E:49:LEU:HD23	4:E:81:ILE:HG12	1.86	0.58
1:A:1470:G:O6	62:A:3775:HOH:O	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:G:H1	1:A:922:U:H3	1.51	0.58
6:G:43:LEU:HB2	6:G:89:GLY:HA2	1.85	0.58
11:O:73:ASP:OD1	16:T:32:TYR:OH	2.22	0.58
1:A:1094:U:H2'	1:A:1095:A:H3'	1.85	0.58
1:A:1105:U:H2'	1:A:1106:G:C8	2.38	0.58
1:A:1174:A:H5''	1:A:1177:A:H61	1.69	0.58
1:A:493:G:H2'	1:A:494:G:O4'	2.03	0.58
1:A:577:G:O2'	1:A:1254:A:OP1	2.22	0.58
12:P:126:VAL:HG12	12:P:148:LEU:HD22	1.85	0.58
1:A:537:C:H2'	1:A:538:G:H8	1.68	0.58
5:F:117:ARG:NH2	5:F:189:THR:O	2.36	0.58
8:J:26:LEU:O	8:J:114:GLY:N	2.34	0.58
19:W:17:VAL:O	19:W:20:VAL:HG23	2.02	0.58
19:W:67:ASP:N	19:W:67:ASP:OD2	2.30	0.58
1:A:857:C:H4'	23:O:23:VAL:HG11	1.85	0.58
1:A:1370:C:HO2'	1:A:1811:G:HO2'	1.52	0.58
1:A:557:U:H2'	1:A:558:G:H8	1.69	0.58
1:A:590:A:H2'	1:A:591:C:C6	2.38	0.58
10:N:30:ILE:HG23	10:N:52:VAL:HG11	1.86	0.58
21:Y:35:TYR:CE2	21:Y:69:ALA:HB3	2.39	0.58
1:A:1721:G:H5'	1:A:1722:A:OP2	2.04	0.58
1:A:1876:A:H2'	1:A:1877:A:C8	2.39	0.58
1:A:2249:U:O4	62:A:3938:HOH:O	2.15	0.58
3:D:19:ALA:HB3	3:D:21:PHE:CE2	2.39	0.58
1:A:1466:G:O2'	1:A:1546:C:O2'	2.19	0.58
1:A:272(J):C:N3	1:A:363:G:N2	2.47	0.58
1:A:2888:C:H2'	1:A:2889:C:H6	1.69	0.58
1:A:29:U:H2'	1:A:30:G:C8	2.39	0.58
6:G:54:GLU:O	6:G:57:ALA:N	2.37	0.58
8:J:73:GLY:O	8:J:75:GLN:N	2.29	0.58
14:R:103:ARG:HH12	14:R:110:PRO:HD3	1.69	0.58
16:T:35:LYS:HZ3	16:T:37:GLY:HA2	1.68	0.58
1:A:528:A:C8	1:A:528:A:H3'	2.38	0.57
19:W:66:GLU:O	19:W:68:ARG:N	2.35	0.57
1:A:590:A:H2'	1:A:591:C:H6	1.69	0.57
3:D:211:ARG:HG3	3:D:214:TRP:CZ3	2.39	0.57
5:F:9:ILE:HG21	5:F:125:LEU:HD22	1.86	0.57
19:W:66:GLU:HA	19:W:69:LEU:HD12	1.86	0.57
20:X:50:LYS:O	20:X:84:ALA:N	2.34	0.57
26:3:8:LEU:HD21	26:3:23:LEU:HD21	1.87	0.57
1:A:1419:A:O2'	1:A:1421:G:N7	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:C:H2'	1:A:590:A:C8	2.39	0.57
3:D:73:VAL:O	3:D:75:ILE:N	2.34	0.57
15:S:15:ARG:O	15:S:19:LYS:HG2	2.03	0.57
1:A:1020:A:N6	1:A:1142:U:OP2	2.38	0.57
1:A:1431:U:H2'	1:A:1432:C:H6	1.70	0.57
1:A:2327:A:H2'	1:A:2328:A:C8	2.38	0.57
1:A:2287:A:N6	1:A:2344:U:H3	2.03	0.57
19:W:56:ALA:O	19:W:59:VAL:N	2.37	0.57
22:Z:6:LYS:HA	22:Z:60:GLU:HB2	1.86	0.57
1:A:1221(A):C:H2'	1:A:1222:C:H6	1.69	0.57
1:A:1639:U:O2'	1:A:1640:C:H5'	2.05	0.57
1:A:1673:U:OP1	62:A:3941:HOH:O	2.18	0.57
1:A:2096:U:H6	1:A:2096:U:OP1	1.88	0.57
1:A:2330:G:H4'	23:0:44:ARG:HH12	1.69	0.57
1:A:2790:A:H2'	1:A:2790:A:N3	2.19	0.57
1:A:796:C:H2'	1:A:797:C:C6	2.40	0.57
12:P:52:GLU:OE1	12:P:55:ARG:NH1	2.38	0.57
15:S:67:ARG:HG3	15:S:100:ALA:HB1	1.86	0.57
22:Z:126:VAL:HG22	22:Z:163:LEU:HA	1.87	0.57
1:A:1598:C:H5'	20:X:36:LYS:HB2	1.87	0.57
1:A:2319:G:N2	15:S:3:ARG:HA	2.20	0.57
5:F:33:LEU:O	5:F:37:VAL:HG23	2.05	0.57
6:G:120:LEU:HD22	6:G:131:TYR:OH	2.04	0.57
12:P:38:GLN:NE2	12:P:45:LEU:HD23	2.20	0.57
21:Y:38:ILE:HG23	21:Y:66:PRO:HA	1.87	0.57
1:A:38:A:H2'	1:A:39:C:C6	2.39	0.57
27:4:48:ARG:CZ	27:4:48:ARG:HA	2.34	0.57
1:A:2095:C:N4	1:A:2096:U:O4	2.38	0.57
5:F:37:VAL:O	5:F:41:LEU:HD12	2.03	0.57
1:A:1057:A:H62	1:A:1086:A:H2'	1.70	0.56
1:A:1810:A:H2'	1:A:1811:G:O4'	2.05	0.56
1:A:2749:A:OP2	1:A:2750:A:O2'	2.19	0.56
1:A:330:A:HO2'	1:A:331:A:H8	1.53	0.56
1:A:528:A:H8	1:A:528:A:H3'	1.70	0.56
1:A:743:G:N7	62:A:3980:HOH:O	2.33	0.56
1:A:984:A:H5''	1:A:985:C:H5	1.70	0.56
1:A:1800:C:OP1	3:D:260:ARG:NH2	2.38	0.56
1:A:2101:G:H1	1:A:2188:C:N4	2.03	0.56
1:A:479:A:N3	1:A:481:G:H5''	2.20	0.56
1:A:84:A:H5''	21:Y:8:LYS:HG2	1.87	0.56
31:8:26:LYS:HE3	31:8:48:PHE:CG	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2455:G:H2'	1:A:2456:C:C6	2.41	0.56
1:A:652:C:H2'	1:A:652(A):A:H5''	1.87	0.56
12:P:71:VAL:HG22	12:P:72:PRO:HA	1.87	0.56
1:A:1809:A:H2'	1:A:1810:A:C8	2.41	0.56
1:A:2857:G:N2	1:A:2860:A:OP2	2.37	0.56
1:A:66:C:C2	1:A:89:G:N2	2.74	0.56
4:E:56:PRO:C	4:E:58:ARG:H	2.09	0.56
9:K:28:GLY:C	9:K:30:HIS:H	2.07	0.56
1:A:564:C:H5'	13:Q:32:TYR:CE1	79.41	0.56
10:N:4:TYR:CD2	17:U:100:VAL:HG11	2.41	0.56
19:W:45:TYR:HD2	19:W:46:PHE:CD1	2.23	0.56
1:A:2469:A:H4'	13:Q:56:ARG:HG3	1.88	0.56
1:A:2794:C:N4	1:A:2802:G:H1	2.03	0.56
12:P:46:LYS:HD3	12:P:51:PHE:CE1	2.40	0.56
1:A:1794:U:H2'	1:A:1795:C:C6	2.41	0.56
1:A:2619:C:H2'	1:A:2620:C:H6	1.70	0.56
1:A:2360:A:H1'	12:P:61:ARG:HH12	1.71	0.56
16:T:106:SER:O	16:T:110:ILE:HG13	2.04	0.56
1:A:1339:G:H5''	20:X:16:LYS:HD2	1.87	0.56
1:A:83:G:H1	1:A:102:G:HO2'	1.51	0.56
1:A:1312:U:OP2	20:X:63:LYS:NZ	2.30	0.56
3:D:161:THR:HG22	3:D:178:PRO:HG3	1.87	0.56
14:R:29:LEU:HD12	14:R:83:ILE:HD13	1.87	0.56
1:A:2849:U:O4	16:T:23:ARG:NH2	2.39	0.56
17:U:108:GLU:O	17:U:112:ARG:HG2	2.05	0.56
22:Z:124:ILE:HD12	22:Z:155:LEU:HD21	1.87	0.56
28:5:20:ARG:O	28:5:22:HIS:N	2.38	0.56
1:A:1933:G:N2	1:A:1968:G:H1'	2.21	0.56
1:A:2230:G:H2'	1:A:2231:C:C6	2.41	0.56
1:A:2428:G:H4'	1:A:2429:G:O5'	2.06	0.56
1:A:910:A:C6	1:A:911:A:C6	2.93	0.56
3:D:211:ARG:HG3	3:D:214:TRP:CE3	2.40	0.56
1:A:564:C:H5'	13:Q:32:TYR:HE1	80.32	0.56
1:A:2115:G:H2'	1:A:2116:G:H5''	1.88	0.56
1:A:2343:C:H2'	1:A:2344:U:H6	1.71	0.56
3:D:124:PRO:HB2	3:D:126:GLN:HB2	1.87	0.56
6:G:7:LEU:HD12	6:G:104:GLU:HA	1.87	0.56
13:Q:133:ARG:O	13:Q:135:ASP:N	2.38	0.56
21:Y:15:VAL:HG21	21:Y:42:VAL:HG11	1.87	0.56
29:6:16:CYS:SG	29:6:18:ARG:NH1	2.78	0.56
1:A:1843:C:H5'	3:D:253:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2125:G:H21	1:A:2173:A:N6	1.99	0.56
1:A:2415:G:O3'	12:P:66:GLY:HA2	2.06	0.56
1:A:139(A):G:N2	20:X:44:GLU:OE1	2.33	0.56
1:A:2024:G:H2'	1:A:2025:C:H6	1.71	0.56
1:A:292:C:H2'	1:A:293:U:C6	2.40	0.56
3:D:182:LEU:O	3:D:271:ILE:N	2.36	0.56
1:A:2056:G:N2	28:5:4:HIS:O	2.37	0.55
1:A:2502:G:H5''	1:A:2503:A:C5'	2.36	0.55
6:G:62:LEU:HD23	6:G:143:GLU:HB2	1.87	0.55
7:H:96:ALA:HB2	7:H:105:LEU:HD13	1.86	0.55
1:A:1061:U:O2'	1:A:1063:G:OP2	2.24	0.55
1:A:2512:C:H4'	4:E:122:PHE:CE2	2.42	0.55
1:A:192:C:H2'	1:A:193:U:H5'	1.87	0.55
1:A:2248:C:H2'	1:A:2249:U:H5'	1.87	0.55
1:A:263:C:H2'	1:A:264:C:O4'	2.07	0.55
1:A:330:A:O2'	1:A:331:A:H8	1.88	0.55
1:A:539:G:H2'	1:A:540:C:C6	2.41	0.55
15:S:31:SER:OG	15:S:32:LEU:N	2.40	0.55
15:S:52:SER:O	15:S:55:ALA:N	2.39	0.55
1:A:2199:A:H5''	1:A:2200:C:H5	1.71	0.55
1:A:480:A:H2	1:A:499:U:O2	1.88	0.55
4:E:105:THR:O	4:E:196:VAL:HG23	2.06	0.55
16:T:35:LYS:NZ	16:T:37:GLY:HA2	2.21	0.55
1:A:2257:U:O2'	1:A:2258:C:H5'	2.07	0.55
1:A:604:G:H2'	1:A:605:C:H6	1.71	0.55
7:H:7:LEU:HB3	7:H:69:ARG:HH11	1.71	0.55
1:A:1062:G:H1	1:A:1076:C:H42	1.55	0.55
1:A:2286:A:H4'	1:A:2287:A:O5'	2.05	0.55
3:D:38:LYS:HE3	3:D:39:LYS:O	2.06	0.55
3:D:67:PHE:CD2	3:D:153:ALA:HB3	2.42	0.55
14:R:79:LEU:HD23	14:R:83:ILE:HB	1.88	0.55
22:Z:182:LYS:O	22:Z:184:ALA:N	2.40	0.55
1:A:1268:A:C2	1:A:2013:A:C4	2.95	0.55
18:V:30:GLY:H	18:V:61:VAL:HG23	1.71	0.55
1:A:372:G:H3'	24:1:66:HIS:CE1	2.41	0.55
27:4:61:ARG:NH2	27:4:63:TYR:HB2	2.22	0.55
1:A:2144:U:H1'	1:A:2148:G:N2	2.21	0.55
1:A:2224:G:H4'	1:A:2226:C:C2	2.42	0.55
1:A:2537:U:H2'	1:A:2538:C:H6	1.71	0.55
3:D:43:ARG:CZ	3:D:49:ILE:HD11	2.36	0.55
4:E:101:ARG:NH1	4:E:169:ASN:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:19:ILE:HG22	11:O:43:VAL:HA	1.88	0.55
27:4:41:PRO:HA	27:4:44:THR:OG1	2.07	0.55
1:A:2270:G:H2'	1:A:2271:G:C8	2.42	0.55
4:E:37:ARG:HD2	4:E:44:TYR:OH	2.06	0.55
1:A:2751:G:H4'	7:H:4:ILE:HD11	1.89	0.55
1:A:680:G:H2'	1:A:681:G:C8	2.42	0.55
11:O:25:LEU:HD12	11:O:38:VAL:HG12	1.87	0.55
1:A:2025:C:C2	1:A:2026:C:C5	2.95	0.54
1:A:2419:U:P	31:8:33:ASN:HD22	2.30	0.54
1:A:833:U:H2'	1:A:834:C:C6	2.64	0.54
11:O:17:ARG:HH11	11:O:17:ARG:HB3	4.59	0.54
5:F:33:LEU:HB3	12:P:6:LEU:HD21	1.89	0.54
1:A:2279:G:OP2	23:0:11:ARG:NH1	2.41	0.54
30:7:43:THR:HG23	30:7:44:PRO:HD2	1.89	0.54
1:A:139(A):G:H2'	1:A:140:G:C8	2.41	0.54
1:A:201:C:H2'	1:A:202:U:H5''	3.71	0.54
1:A:2203:U:O2'	1:A:2205:C:H5'	2.07	0.54
3:D:27:THR:OG1	3:D:28:GLU:N	2.41	0.54
16:T:35:LYS:HD3	16:T:37:GLY:H	1.71	0.54
17:U:102:GLU:HB3	17:U:105:VAL:HB	1.89	0.54
23:0:23:VAL:HG13	23:0:26:TYR:HE2	1.72	0.54
24:1:24:ALA:O	24:1:27:GLU:N	2.41	0.54
26:3:32:GLN:HE21	26:3:32:GLN:HA	1.71	0.54
1:A:2134:A:OP2	1:A:2156:G:N1	2.40	0.54
5:F:63:LYS:HA	5:F:76:GLY:O	2.08	0.54
6:G:32:PRO:HB3	6:G:163:ALA:HB2	1.89	0.54
11:O:63:VAL:HG13	11:O:106:LEU:HD11	1.90	0.54
31:8:31:HIS:CD2	31:8:32:LEU:HD22	2.43	0.54
1:A:1021:A:C3'	1:A:1021:A:C8	2.89	0.54
1:A:1063:G:O2'	9:K:87:GLY:HA3	2.06	0.54
1:A:1413:G:H2'	1:A:1414:G:H8	1.71	0.54
1:A:2100:G:N3	1:A:2190:G:N2	2.56	0.54
1:A:2554:U:H2'	1:A:2555:U:C6	2.42	0.54
1:A:2721:A:N7	62:A:3793:HOH:O	2.33	0.54
1:A:477:A:H2'	1:A:478:A:C8	2.42	0.54
3:D:34:VAL:HG12	3:D:62:TYR:O	2.07	0.54
15:S:39:ILE:HB	15:S:49:VAL:HG13	1.89	0.54
17:U:44:ASN:HD21	18:V:75:PHE:H	1.55	0.54
1:A:2867:G:OP2	16:T:119:LYS:NZ	2.40	0.54
1:A:692:C:O2'	3:D:38:LYS:HE2	2.07	0.54
3:D:30:GLU:HB3	3:D:33:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:41:LEU:HA	5:F:44:ARG:HG2	1.89	0.54
19:W:40:ASN:O	19:W:41:LYS:HD3	2.08	0.54
1:A:1028:A:N6	1:A:1125:G:H2'	2.22	0.54
1:A:1266:G:O5'	19:W:15:ARG:NH2	2.40	0.54
1:A:1291:C:H2'	1:A:1292:U:C6	2.42	0.54
1:A:353:G:H2'	1:A:354:G:H8	1.73	0.54
1:A:2312:U:H5'	6:G:88:ILE:HD11	1.88	0.54
1:A:2749:A:H1'	7:H:63:SER:OG	2.07	0.54
12:P:85:LEU:HG	12:P:116:GLY:HA2	1.88	0.54
20:X:89:ILE:HG22	20:X:92:LEU:H	1.73	0.54
27:4:68:ARG:NH2	27:4:69:LYS:O	2.41	0.54
1:A:2385:C:H2'	1:A:2386:C:H6	1.73	0.54
1:A:254:G:O6	31:8:5:LYS:HD3	2.08	0.54
1:A:264:C:O2	62:A:4211:HOH:O	2.16	0.54
1:A:2749:A:H4'	7:H:62:LYS:HG2	1.90	0.54
1:A:510:C:H2'	1:A:511:U:O4'	2.07	0.54
2:B:18:G:H2'	2:B:19:G:H8	1.72	0.54
3:D:121:PRO:HB3	3:D:135:PHE:HE1	1.73	0.54
15:S:28:VAL:HG21	15:S:98:VAL:HG13	1.89	0.54
18:V:56:SER:H	18:V:100:ARG:HB2	1.72	0.54
1:A:2716:U:O2'	1:A:2717:G:H5'	2.07	0.54
1:A:321:G:O2'	1:A:340:A:N3	2.41	0.54
1:A:715:G:H2'	1:A:716:A:O4'	2.07	0.54
1:A:998:C:OP2	17:U:92:ARG:NH2	2.41	0.54
16:T:16:ARG:NH2	16:T:83:ILE:O	2.30	0.54
22:Z:67:LEU:HD23	22:Z:68:PRO:HD2	1.90	0.54
1:A:1553:A:O2'	1:A:1554:A:H8	1.90	0.54
1:A:2096:U:H2'	1:A:2097:C:H6	1.73	0.54
1:A:2141:G:H2'	1:A:2142:C:O4'	2.08	0.54
24:1:60:PHE:HE1	24:1:91:LYS:HG3	1.73	0.54
3:D:125:ILE:HG13	3:D:137:PRO:HG2	1.90	0.54
3:D:77:ALA:HB3	3:D:117:VAL:HG23	1.88	0.54
6:G:126:ASP:OD2	6:G:130:ASN:HB2	2.06	0.54
1:A:1079:C:H4'	9:K:132:ARG:HH22	1.73	0.54
9:K:14:ALA:HA	9:K:41:PHE:HE2	1.72	0.54
27:4:68:ARG:HA	27:4:68:ARG:NE	2.23	0.53
1:A:1507:A:O2'	1:A:1508:A:O4'	2.27	0.53
1:A:2103:C:N3	1:A:2186:G:O6	2.41	0.53
1:A:484:C:H42	1:A:496:G:H1	1.55	0.53
1:A:531:C:OP1	1:A:561:G:N1	2.41	0.53
10:N:15:LEU:HD12	10:N:137:LYS:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:30:ILE:O	10:N:34:LEU:HB2	2.09	0.53
4:E:152:LYS:HG2	10:N:78:TYR:CZ	2.43	0.53
15:S:64:GLU:HA	15:S:67:ARG:HB2	1.89	0.53
1:A:1259:G:H2'	1:A:1260:G:H8	1.73	0.53
1:A:1803:A:O2'	3:D:259:THR:HG21	2.08	0.53
1:A:644:A:H4'	1:A:645:C:C5	2.43	0.53
2:B:17:C:N4	2:B:68:C:H42	2.01	0.53
3:D:89:SER:HB2	3:D:159:ALA:HB2	1.90	0.53
1:A:1422:G:H5'	11:O:48:PRO:HB3	100.88	0.53
24:1:18:ILE:HG12	24:1:37:ILE:HG23	1.90	0.53
25:2:9:GLN:HE22	25:2:56:GLN:HB3	1.74	0.53
1:A:491:G:H2'	1:A:492:A:C8	2.42	0.53
15:S:13:ARG:O	15:S:15:ARG:N	2.36	0.53
1:A:2521:C:O2'	1:A:2564:A:N3	2.41	0.53
1:A:271(A):A:H2	1:A:272(D):G:N3	2.07	0.53
1:A:924:C:H2'	1:A:925:C:C6	2.44	0.53
2:B:7:G:H4'	15:S:29:PHE:CD1	2.43	0.53
3:D:69:ARG:NH2	3:D:128:GLY:O	2.41	0.53
4:E:116:VAL:HG11	4:E:138:PRO:HB3	1.91	0.53
20:X:40:LYS:HG3	20:X:51:VAL:HG12	1.89	0.53
1:A:2101:G:N2	1:A:2188:C:N3	2.53	0.53
1:A:2787:C:H1'	4:E:62:PRO:HG3	1.91	0.53
1:A:7:G:H4'	10:N:13:TRP:CH2	2.43	0.53
13:Q:66:ILE:HG23	13:Q:104:PHE:HD2	1.74	0.53
21:Y:2:ARG:NH1	21:Y:4:LYS:HA	2.23	0.53
28:5:20:ARG:C	28:5:22:HIS:H	2.12	0.53
3:D:139:GLY:H	3:D:165:ILE:HB	1.73	0.53
24:1:85:LEU:H	24:1:85:LEU:HD13	1.74	0.53
32:9:32:HIS:O	32:9:34:GLN:HG3	2.09	0.53
1:A:1171:G:O6	1:A:1178:C:N3	2.41	0.53
1:A:1265:A:OP1	1:A:1265:A:H8	1.92	0.53
1:A:12:U:H2'	1:A:12:U:O2	2.09	0.53
1:A:1882:C:H2'	1:A:1883:G:O4'	2.09	0.53
1:A:464:U:H4'	30:7:5:TRP:CZ3	2.44	0.53
1:A:607:U:OP1	5:F:102:PRO:HA	2.09	0.53
1:A:828:U:O2'	1:A:829:A:H5'	2.08	0.53
6:G:77:ILE:HD12	6:G:82:LEU:HD11	1.91	0.53
13:Q:35:VAL:O	13:Q:129:THR:HG22	2.09	0.53
1:A:1364:G:OP2	24:1:3:LYS:HG3	2.08	0.53
4:E:92:THR:O	4:E:95:ILE:HG23	2.09	0.53
23:0:50:ASN:ND2	23:0:81:VAL:O	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:C:H42	1:A:1114:G:H22	1.57	0.53
1:A:390:A:H4'	1:A:391:G:H5'	1.91	0.53
3:D:65:ILE:HD11	3:D:92:ILE:HG21	1.91	0.53
13:Q:65:PHE:HB2	13:Q:105:GLU:HB2	1.91	0.53
14:R:12:ARG:HD2	14:R:20:LEU:HD22	1.91	0.53
22:Z:108:PRO:HB3	22:Z:144:LEU:HB2	1.91	0.53
1:A:1131:G:C4	10:N:75:TYR:HB2	2.44	0.52
1:A:2406:U:H2'	1:A:2406:U:OP2	2.09	0.52
1:A:278:A:O2'	1:A:279:C:OP1	2.25	0.52
1:A:86:C:H42	1:A:96:G:H1	1.57	0.52
15:S:66:ALA:HA	15:S:69:VAL:HG12	1.92	0.52
19:W:24:ILE:O	19:W:26:GLY:N	2.42	0.52
20:X:67:GLY:O	20:X:69:TYR:N	2.34	0.52
23:0:23:VAL:HG13	23:0:26:TYR:CE2	2.44	0.52
1:A:105:C:H2'	1:A:106:C:H6	1.74	0.52
1:A:2748:A:N3	7:H:63:SER:HB3	2.24	0.52
2:B:43:C:OP1	27:4:2:LYS:HB2	2.10	0.52
6:G:5:VAL:HG23	6:G:8:LYS:HB2	1.92	0.52
9:K:26:ALA:HA	9:K:29:GLN:CD	2.30	0.52
21:Y:31:LEU:HD12	21:Y:36:ALA:O	2.09	0.52
27:4:53:GLU:HG3	27:4:55:ARG:H	1.73	0.52
28:5:32:PRO:HB3	28:5:37:LYS:HE2	1.91	0.52
29:6:9:LEU:N	29:6:23:THR:O	2.34	0.52
1:A:1442:G:H2'	1:A:1443:G:H8	1.74	0.52
1:A:2345:G:N3	1:A:2381:C:H2'	2.23	0.52
1:A:539:G:H2'	1:A:540:C:H6	1.75	0.52
1:A:582:G:H2'	1:A:583:G:C8	2.45	0.52
4:E:128:SER:OG	4:E:129:HIS:N	2.41	0.52
5:F:117:ARG:HA	5:F:120:GLU:OE1	2.08	0.52
7:H:109:PHE:HE2	7:H:152:ARG:NH2	2.03	0.52
1:A:2279:G:O6	23:0:14:ARG:HD2	2.09	0.52
1:A:1105:U:H2'	1:A:1106:G:H8	1.75	0.52
1:A:1178:C:H2'	1:A:1179:C:H6	1.75	0.52
1:A:1301:A:O2'	1:A:1303:G:N7	2.40	0.52
1:A:141:A:H8	1:A:1408:C:O2'	1.91	0.52
1:A:2537:U:H2'	1:A:2538:C:C6	2.45	0.52
1:A:587:C:OP2	12:P:21:ARG:NH2	2.38	0.52
1:A:653:A:H2'	1:A:654:A:O4'	2.09	0.52
13:Q:34:LEU:HD11	13:Q:129:THR:HB	1.91	0.52
18:V:21:ARG:HA	18:V:93:GLU:HA	1.91	0.52
1:A:2529:G:O6	32:9:31:LYS:NZ	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:C:H3'	1:A:845:G:N2	2.24	0.52
1:A:588:U:H1'	5:F:90:PHE:CD1	2.44	0.52
11:O:17:ARG:HB2	11:O:45:GLU:HB3	1.91	0.52
15:S:58:LEU:CB	15:S:59:LYS:HB2	2.37	0.52
1:A:2284:C:OP1	29:6:3:SER:HB3	2.10	0.52
1:A:2285:C:OP2	29:6:6:ARG:NH1	2.42	0.52
1:A:1417:C:H2'	1:A:1418:G:O4'	2.10	0.52
1:A:271(G):C:C2'	1:A:271(H):G:H5'	2.39	0.52
3:D:147:LEU:HD13	3:D:155:LEU:HD11	1.92	0.52
19:W:45:TYR:HD2	19:W:46:PHE:HD1	1.58	0.52
1:A:1062:G:H2'	1:A:1063:G:C8	2.44	0.52
1:A:292:C:H2'	1:A:293:U:H6	1.74	0.52
1:A:829:A:N7	1:A:2248:C:H5'	2.25	0.52
3:D:108:PRO:HB3	3:D:143:HIS:CE1	2.45	0.52
6:G:39:ILE:HG23	6:G:157:ILE:HG12	1.91	0.52
7:H:24:VAL:HG11	7:H:72:ILE:HD11	1.92	0.52
7:H:76:VAL:O	7:H:78:GLY:N	2.43	0.52
9:K:65:PHE:HD2	9:K:65:PHE:H	1.58	0.52
26:3:9:VAL:HG12	26:3:32:GLN:HE22	1.75	0.52
1:A:1344:G:H5'	1:A:1384:A:N6	2.23	0.52
1:A:1776:G:H1	1:A:1788:C:H42	1.58	0.52
1:A:1932:A:H2'	1:A:1933:G:O4'	2.09	0.52
1:A:193:U:C2	1:A:194:G:C8	2.98	0.52
1:A:2136:C:O2'	1:A:2137:C:O4'	2.28	0.52
1:A:2287:A:N6	1:A:2344:U:N3	2.57	0.52
1:A:296:C:O3'	21:Y:95:LYS:NZ	2.35	0.52
1:A:307:G:H8	1:A:307:G:O5'	1.93	0.52
1:A:773:U:O2'	3:D:48:ARG:HD3	2.10	0.52
3:D:89:SER:HB2	3:D:159:ALA:CB	2.39	0.52
9:K:72:PRO:HG2	9:K:77:LEU:HD21	1.92	0.52
1:A:1680:U:C2'	1:A:1681:G:H5'	2.40	0.52
1:A:1911:U:H2'	1:A:1918:A:N1	2.25	0.52
1:A:600:G:H2'	1:A:601:C:C6	2.45	0.52
9:K:55:VAL:HG22	9:K:57:ILE:HG13	1.91	0.52
13:Q:56:ARG:HH11	13:Q:56:ARG:HB2	1.75	0.52
1:A:1379:A:H4'	1:A:1380:G:OP2	2.09	0.52
1:A:571:A:C8	1:A:2030:A:N6	2.78	0.52
1:A:2105:C:N3	1:A:2184:G:O6	2.43	0.52
1:A:2758:A:C2	1:A:2759:G:H1'	2.45	0.52
4:E:163:GLU:HG2	4:E:164:ARG:N	2.25	0.52
1:A:336:C:HO2'	21:Y:35:TYR:HH	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1820:U:O2	3:D:201:HIS:HB3	2.09	0.51
1:A:2385:C:H2'	1:A:2386:C:C6	2.45	0.51
1:A:307:G:H2'	1:A:309:G:N7	2.26	0.51
1:A:399:G:OP2	62:A:4204:HOH:O	2.19	0.51
1:A:557:U:H2'	1:A:558:G:C8	2.45	0.51
1:A:958:U:H4'	62:A:4311:HOH:O	2.10	0.51
11:O:15:GLY:HA2	11:O:47:ILE:HD11	1.92	0.51
13:Q:109:VAL:CG1	13:Q:113:GLN:HB3	2.39	0.51
16:T:29:ARG:NH1	16:T:87:ASP:OD2	2.43	0.51
19:W:35:ILE:C	19:W:37:ARG:H	2.13	0.51
21:Y:75:ILE:HD13	21:Y:82:PRO:HA	1.92	0.51
22:Z:11:GLU:N	22:Z:13:GLU:OE1	2.38	0.51
24:1:2:SER:HB2	24:1:43:TYR:HD2	1.74	0.51
1:A:1959:G:C6	1:A:1960:A:C5	2.98	0.51
1:A:2572:A:N7	4:E:144:ARG:HD2	2.24	0.51
7:H:118:PRO:HD2	7:H:121:ILE:HB	1.92	0.51
11:O:34:THR:OG1	11:O:35:VAL:N	2.42	0.51
1:A:1257:C:H2'	1:A:1258:C:C6	2.45	0.51
1:A:1794:U:H2'	1:A:1795:C:H6	1.75	0.51
1:A:1827:C:OP2	3:D:222:ARG:NH1	2.44	0.51
1:A:1933:G:H22	1:A:1968:G:H1'	1.76	0.51
1:A:2445:G:OP1	5:F:74:ARG:NH2	2.39	0.51
1:A:666:G:C5	1:A:667:U:C5	2.98	0.51
3:D:67:PHE:HB3	3:D:153:ALA:H	1.75	0.51
10:N:23:LEU:HA	10:N:60:ILE:HD11	1.93	0.51
22:Z:124:ILE:HG12	22:Z:125:LEU:N	2.22	0.51
1:A:1882:C:H5''	24:1:26:ARG:HH21	1.75	0.51
1:A:1095:A:H2'	1:A:1096:A:C8	2.45	0.51
1:A:1385:G:O6	1:A:1403:C:N4	2.43	0.51
1:A:1504:C:H2'	1:A:1505:C:C6	2.45	0.51
1:A:1918:A:O2'	1:A:1920:C:N4	2.43	0.51
1:A:338:G:H2'	1:A:339:U:H6	1.75	0.51
5:F:102:PRO:HB2	5:F:105:VAL:HG23	1.91	0.51
1:A:2303:G:N3	6:G:132:ASN:ND2	2.57	0.51
9:K:98:ARG:HA	9:K:136:VAL:HG23	1.91	0.51
1:A:954:G:H4'	13:Q:13:GLN:HE21	1.75	0.51
13:Q:75:THR:HG23	13:Q:88:GLY:HA3	1.92	0.51
17:U:49:HIS:HA	17:U:52:ARG:HB3	1.93	0.51
1:A:1051:G:N2	1:A:1108:U:O4	2.43	0.51
1:A:1119:C:H2'	1:A:1120:G:H8	3.59	0.51
1:A:143:G:H1'	20:X:37:THR:CG2	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:C:OP1	62:A:3734:HOH:O	2.19	0.51
1:A:1786:A:C4	1:A:1938:A:C6	2.99	0.51
1:A:2252:G:H2'	1:A:2253:G:H8	1.75	0.51
1:A:2627:G:N2	1:A:2777:G:OP2	2.43	0.51
1:A:2839:G:H5'	14:R:46:GLY:HA2	1.93	0.51
1:A:814:C:H2'	1:A:815:C:H6	1.75	0.51
3:D:16:MET:HE1	3:D:208:LYS:HG2	1.92	0.51
9:K:75:SER:OG	9:K:75:SER:O	2.27	0.51
12:P:38:GLN:HE21	12:P:45:LEU:HD23	1.74	0.51
1:A:1356:G:N2	1:A:1376:C:C2	2.78	0.51
1:A:2678:C:H2'	1:A:2679:A:C8	2.46	0.51
2:B:39:A:O2'	2:B:46:A:N1	2.42	0.51
4:E:49:LEU:CD2	4:E:81:ILE:HG12	2.41	0.51
5:F:164:ARG:HA	5:F:167:ALA:HB3	1.93	0.51
12:P:2:LYS:HE3	12:P:4:SER:OG	2.11	0.51
20:X:72:LYS:HG2	20:X:73:ARG:O	2.10	0.51
31:8:61:LEU:O	31:8:62:LEU:HD23	2.11	0.51
1:A:1047:G:OP1	1:A:1047:G:H4'	2.09	0.51
1:A:1778:U:H2'	1:A:1784:A:N6	2.26	0.51
1:A:2168:G:N2	1:A:2171:A:H62	2.08	0.51
1:A:2529:G:H5''	1:A:2530:A:H5''	1.93	0.51
3:D:83:GLU:HB2	3:D:92:ILE:CD1	2.40	0.51
3:D:92:ILE:HD13	3:D:104:TYR:CD2	2.45	0.51
7:H:87:LEU:HD13	7:H:148:ILE:HG21	1.93	0.51
13:Q:43:THR:O	13:Q:46:GLN:N	2.43	0.51
22:Z:104:PHE:CE2	22:Z:119:GLU:HB3	2.45	0.51
31:8:16:ILE:HD11	31:8:59:LYS:HG2	1.92	0.51
1:A:242:G:H5''	31:8:64:TYR:CE2	2.45	0.51
1:A:1021:A:O2'	1:A:1123:C:H5''	2.11	0.51
1:A:1499:C:H2'	1:A:1500:G:C8	2.45	0.51
1:A:2079:U:H3	1:A:2241:A:H61	1.58	0.51
1:A:2427:C:H5''	1:A:2428:G:OP1	2.11	0.51
1:A:2576:G:OP1	62:A:4077:HOH:O	2.19	0.51
1:A:582:G:C6	1:A:583:G:C6	2.98	0.51
1:A:642:G:H21	1:A:646:A:H2	1.58	0.51
3:D:43:ARG:HA	3:D:48:ARG:O	2.10	0.51
6:G:105:LYS:HE3	6:G:143:GLU:OE1	2.11	0.51
5:F:34:TRP:CH2	12:P:8:PRO:HB3	2.46	0.51
20:X:8:ILE:HD12	20:X:43:VAL:HG23	1.92	0.51
1:A:1478:G:N3	1:A:1479:G:C8	2.78	0.51
1:A:2436:G:C5	1:A:2437:U:C5	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:38:VAL:O	9:K:42:ASN:HB2	2.11	0.51
14:R:12:ARG:HB2	14:R:17:ARG:HB2	1.92	0.51
16:T:77:PRO:HB2	16:T:80:SER:HB2	1.93	0.51
1:A:1078:U:H5''	1:A:1079:C:OP1	2.11	0.51
1:A:2105:C:H2'	1:A:2106:G:O4'	2.11	0.51
27:4:48:ARG:NE	27:4:48:ARG:HA	2.25	0.50
1:A:1070:A:H5'	1:A:1072:C:OP2	2.11	0.50
1:A:1607:C:N4	1:A:1621:U:H2'	2.26	0.50
1:A:1633:G:O5'	1:A:1633:G:H8	1.94	0.50
1:A:848:G:H2'	1:A:849:A:C8	2.46	0.50
6:G:120:LEU:HB2	6:G:179:PRO:O	2.11	0.50
1:A:956:G:H8	13:Q:14:ARG:HH21	1.59	0.50
16:T:28:VAL:O	16:T:46:GLU:HA	2.12	0.50
19:W:68:ARG:O	19:W:110:LYS:N	2.41	0.50
26:3:5:LYS:HE3	26:3:34:GLU:OE1	2.11	0.50
1:A:1273:U:H4'	1:A:1275:A:OP2	2.11	0.50
1:A:1422:G:H1'	1:A:1495:A:H61	1.76	0.50
1:A:2032:G:O2'	4:E:145:LYS:HE3	2.11	0.50
1:A:359:A:H2'	1:A:360:G:H5'	1.93	0.50
3:D:274:ARG:HB2	3:D:275:LYS:CB	2.40	0.50
16:T:35:LYS:HD3	16:T:37:GLY:N	2.26	0.50
24:1:56:GLN:NE2	24:1:87:PRO:HD3	2.26	0.50
1:A:1845:G:H1	1:A:1895:C:H42	1.59	0.50
1:A:26:G:OP1	19:W:80:PRO:HB3	2.11	0.50
1:A:624:C:H2'	1:A:625:G:C8	3.22	0.50
5:F:184:TYR:O	5:F:188:ARG:HB2	2.12	0.50
7:H:69:ARG:HE	7:H:73:ALA:HB2	1.76	0.50
13:Q:84:GLY:O	13:Q:85:LYS:HB2	2.11	0.50
4:E:12:THR:HG21	16:T:11:GLU:HG2	1.93	0.50
17:U:106:PHE:HA	17:U:109:LEU:HD12	1.93	0.50
1:A:1036:G:H1	1:A:1119:C:N4	2.02	0.50
1:A:1167:U:H2'	1:A:1168:G:C8	2.46	0.50
1:A:1487:G:H2'	1:A:1488:G:H8	1.76	0.50
1:A:1974:C:C4	1:A:1975:G:N7	2.79	0.50
1:A:234:C:H2'	1:A:235:U:O4'	2.12	0.50
1:A:271(O):C:H2'	1:A:271(P):C:C6	2.45	0.50
1:A:2735:G:H2'	1:A:2736:G:H8	1.77	0.50
1:A:845:G:OP2	1:A:845:G:N2	2.32	0.50
11:O:71:ARG:O	11:O:74:GLY:N	2.43	0.50
28:5:40:LYS:NZ	28:5:41:PRO:O	2.28	0.50
29:6:13:CYS:HB2	29:6:49:HIS:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1177:A:H3'	1:A:1178:C:C6	2.47	0.50
1:A:117:G:H5''	1:A:118:A:OP2	2.12	0.50
1:A:2790:A:O2'	1:A:2791:C:H5	1.94	0.50
1:A:300:A:H1'	1:A:319:C:H1'	1.92	0.50
1:A:981:A:C8	1:A:982:C:C5	2.99	0.50
3:D:68:LYS:HD2	3:D:70:TRP:CZ2	2.46	0.50
1:A:1335:U:OP1	20:X:65:ARG:HD3	2.11	0.50
25:2:29:LYS:HG2	25:2:57:ILE:HD13	1.92	0.50
1:A:1139:G:H5'	10:N:23:LEU:HD21	1.92	0.50
3:D:161:THR:H	3:D:196:VAL:HB	1.76	0.50
1:A:2025:C:P	4:E:149:ARG:HH21	2.35	0.50
6:G:58:GLN:H	6:G:58:GLN:HE21	1.60	0.50
14:R:22:ARG:HD3	14:R:69:ASP:O	2.11	0.50
19:W:15:ARG:HH21	28:5:20:ARG:HE	1.58	0.50
24:1:17:SER:HB2	24:1:40:ARG:HG2	1.94	0.50
1:A:1970:A:OP2	62:A:3905:HOH:O	2.20	0.50
1:A:2139:C:H42	1:A:2152:G:H1	1.60	0.50
1:A:411:G:C5	12:P:72:PRO:HB3	2.45	0.50
1:A:447:A:C4	1:A:473:G:N7	2.80	0.50
1:A:84:A:N1	1:A:98:G:O2'	2.33	0.50
2:B:106:G:C2	2:B:107:G:C8	2.99	0.50
5:F:101:LEU:HD12	5:F:102:PRO:CD	2.36	0.50
16:T:35:LYS:NZ	16:T:38:ASN:HA	2.27	0.50
1:A:1614:A:N1	19:W:93:ALA:HB2	2.27	0.50
1:A:1339:G:N3	62:A:4281:HOH:O	2.34	0.50
1:A:1385:G:H1'	1:A:1386:C:C6	2.46	0.50
1:A:1652:A:C2'	1:A:1653:G:H5'	2.41	0.50
1:A:2697:G:C2	1:A:2711:A:C2	3.00	0.50
1:A:627:A:H4'	1:A:628:G:OP1	2.11	0.50
2:B:12:C:H2'	23:0:73:GLY:HA3	1.94	0.50
2:B:63:G:H2'	2:B:64:C:H6	1.75	0.50
3:D:261:LYS:HZ2	3:D:263:ARG:HB2	1.77	0.50
7:H:86:GLU:O	7:H:165:ALA:HB2	2.12	0.50
10:N:15:LEU:HB2	10:N:135:PRO:HB2	1.94	0.50
17:U:25:TRP:O	17:U:28:ARG:HB2	2.11	0.50
17:U:52:ARG:O	17:U:55:ARG:HG3	2.12	0.50
28:5:20:ARG:HA	28:5:23:HIS:CD2	2.46	0.50
1:A:1439:A:C2	1:A:1553:A:C5	3.00	0.50
1:A:570:G:H2'	1:A:2030:A:C6	2.47	0.50
2:B:40:U:C5	27:4:2:LYS:HG3	2.46	0.50
11:O:108:GLU:CD	11:O:108:GLU:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:8:VAL:HG23	17:U:11:ARG:HH21	1.76	0.50
1:A:1988:C:C2	1:A:1989:G:C8	3.00	0.49
1:A:2849:U:H4'	1:A:2868:A:C2	2.47	0.49
1:A:285:C:H2'	1:A:286:C:C6	2.46	0.49
1:A:532:A:OP1	1:A:561:G:N2	2.36	0.49
7:H:3:ARG:CG	7:H:3:ARG:HH11	2.22	0.49
9:K:48:MET:SD	9:K:72:PRO:HD3	2.52	0.49
12:P:101:VAL:HA	12:P:106:LEU:HB3	1.94	0.49
12:P:93:GLY:O	12:P:123:LEU:HD22	2.11	0.49
27:4:61:ARG:HH21	27:4:63:TYR:HD2	1.59	0.49
1:A:1495:A:H2'	1:A:1496:A:C8	2.46	0.49
1:A:2233:U:H2'	1:A:2234:G:C8	2.47	0.49
1:A:290:G:H1	1:A:350:U:H3	1.59	0.49
1:A:613:G:O2'	1:A:614(C):A:N1	2.40	0.49
5:F:46:ARG:HB3	5:F:48:THR:HG23	1.93	0.49
7:H:60:ARG:HH11	7:H:60:ARG:HB2	4.65	0.49
12:P:47:ASP:OD2	12:P:50:ARG:NH2	2.44	0.49
17:U:75:ASN:OD1	17:U:78:THR:N	2.39	0.49
1:A:2232:U:P	24:1:40:ARG:HH12	2.35	0.49
1:A:1055:G:H1	1:A:1104:C:H42	1.59	0.49
1:A:1278:A:OP1	14:R:36:THR:HG23	2.12	0.49
1:A:1424:G:H2'	1:A:1425:G:O4'	2.12	0.49
1:A:741:G:O2'	1:A:1676:A:OP1	2.28	0.49
1:A:1796:U:H2'	1:A:1797:C:C6	2.47	0.49
1:A:2369:A:H2'	1:A:2370:G:C8	2.47	0.49
1:A:2632:A:HO2'	1:A:2811:G:HO2'	1.58	0.49
1:A:361:G:C2'	1:A:362:U:H5'	2.42	0.49
1:A:380:U:H5'	24:1:18:ILE:HD12	1.93	0.49
1:A:90:U:O2'	1:A:92:A:O4'	2.31	0.49
3:D:146:GLU:HA	3:D:152:GLY:O	2.12	0.49
18:V:62:LEU:CD1	18:V:95:LEU:HB2	2.42	0.49
19:W:57:ASN:OD1	19:W:57:ASN:N	2.46	0.49
26:3:7:LYS:HE3	26:3:32:GLN:HE21	1.76	0.49
1:A:1056:G:H5''	1:A:1057:A:O4'	2.12	0.49
1:A:149:A:H2'	1:A:150:C:O4'	2.12	0.49
1:A:1792:G:H2'	1:A:1793:C:H6	1.76	0.49
1:A:2093:G:C6	1:A:2225:A:C8	3.00	0.49
1:A:910:A:N1	1:A:2277:G:H1'	2.27	0.49
4:E:4:ILE:HG12	4:E:28:ALA:HB1	1.93	0.49
10:N:67:LEU:HA	10:N:87:LEU:HD13	1.93	0.49
1:A:1253:A:N7	62:A:3862:HOH:O	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2319:G:H22	15:S:3:ARG:HD2	1.77	0.49
1:A:724:U:H2'	1:A:725:G:O4'	2.12	0.49
3:D:36:PRO:HA	3:D:61:LEU:HD12	1.95	0.49
4:E:30:PRO:HB3	4:E:92:THR:HG22	1.95	0.49
1:A:674:G:O2'	5:F:74:ARG:HD3	2.12	0.49
6:G:111:LEU:HB2	6:G:112:PRO:HD3	1.95	0.49
6:G:65:GLY:HA3	27:4:9:LEU:HD21	1.94	0.49
15:S:102:ALA:O	15:S:105:ALA:N	2.45	0.49
29:6:40:CYS:HB3	29:6:43:CYS:HB2	1.93	0.49
1:A:1164:G:C6	1:A:1165:U:C4	3.01	0.49
1:A:1504:C:H2'	1:A:1505:C:H6	1.77	0.49
1:A:1878:G:H2'	1:A:1879:C:C6	2.48	0.49
1:A:2518:A:H2'	1:A:2518:A:N3	2.27	0.49
1:A:272(I):U:H2'	1:A:272(J):C:H6	1.76	0.49
12:P:97:PRO:HD3	12:P:126:VAL:O	2.12	0.49
13:Q:110:THR:OG1	13:Q:113:GLN:HB2	2.12	0.49
62:A:4282:HOH:O	17:U:50:ARG:HB2	2.12	0.49
20:X:51:VAL:HG21	20:X:81:VAL:HB	1.95	0.49
20:X:67:GLY:C	20:X:69:TYR:H	2.16	0.49
1:A:2199:A:H3'	1:A:2200:C:H6	1.78	0.49
1:A:197:A:N6	1:A:2430:A:H2'	2.28	0.49
1:A:2502:G:H5''	1:A:2503:A:H5''	1.94	0.49
1:A:2556:C:H2'	1:A:2557:G:O4'	2.12	0.49
1:A:41:C:C2	1:A:438:G:N2	2.81	0.49
1:A:528:A:C8	1:A:528:A:C3'	2.96	0.49
1:A:1500:G:O2'	3:D:100:GLY:O	2.26	0.49
1:A:1820:U:O4	3:D:199:ALA:HB1	2.13	0.49
4:E:105:THR:OG1	4:E:199:ARG:NH2	2.45	0.49
5:F:13:SER:C	5:F:15:SER:H	2.16	0.49
8:J:116:ILE:O	8:J:123:GLU:N	2.44	0.49
15:S:34:HIS:CD2	15:S:54:LEU:HD13	2.48	0.49
1:A:1205:U:H4'	1:A:1206:G:OP2	2.12	0.49
1:A:2096:U:P	1:A:2096:U:O4'	2.70	0.49
1:A:2137:C:H2'	1:A:2138:C:H5''	1.94	0.49
1:A:2870:C:H2'	1:A:2871:C:O4'	2.13	0.49
1:A:98:G:C6	1:A:99:U:C4	9.72	0.49
4:E:9:VAL:HG13	4:E:25:VAL:HG12	1.95	0.49
1:A:322:A:C3'	5:F:169:ASN:HD21	2.24	0.49
12:P:128:HIS:CE1	12:P:148:LEU:HD21	2.48	0.49
14:R:13:HIS:CE1	14:R:16:HIS:HB2	2.48	0.49
24:1:15:ALA:O	24:1:40:ARG:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:U:H3	1:A:1142(A):A:N6	2.05	0.49
1:A:1515:G:H4'	1:A:1556:C:O2'	2.13	0.49
1:A:1780:A:OP1	62:A:4216:HOH:O	2.20	0.49
1:A:2377:A:H2'	1:A:2378:A:C8	2.47	0.49
1:A:2850:A:N7	1:A:2868:A:O2'	2.38	0.49
1:A:629:G:H2'	1:A:630:G:O4'	2.36	0.49
1:A:782:A:O2'	3:D:225:ALA:O	2.28	0.49
9:K:134:MET:HG3	9:K:136:VAL:HG12	1.94	0.49
16:T:30:VAL:HG22	16:T:86:ILE:HG12	1.95	0.49
17:U:24:TYR:HB2	17:U:29:SER:HB3	1.94	0.49
25:2:13:ALA:O	25:2:16:LEU:HB2	2.12	0.49
1:A:13:A:N1	1:A:525:U:H2'	2.28	0.49
1:A:1412:A:H2'	1:A:1413:G:H8	1.74	0.49
1:A:1553:A:O2'	1:A:1554:A:C8	2.65	0.49
1:A:1987:G:H2'	1:A:1988:C:H6	1.78	0.49
1:A:2423:U:H4'	1:A:2424:C:O5'	2.12	0.49
1:A:2767:C:C2	1:A:2768:C:C5	3.01	0.49
1:A:2885:C:O2'	28:5:34:PRO:HG3	2.13	0.49
4:E:12:THR:HG22	4:E:13:ARG:N	2.24	0.49
28:5:51:TYR:HE1	28:5:56:LYS:HE2	1.78	0.48
1:A:1174:A:H4'	1:A:1175:U:OP1	2.11	0.48
1:A:2055:C:OP1	28:5:8:LYS:NZ	2.31	0.48
1:A:2122:U:H2'	1:A:2123:G:C8	2.45	0.48
1:A:300:A:H1'	1:A:319:C:C1'	2.43	0.48
1:A:537:C:H2'	1:A:538:G:C8	2.47	0.48
1:A:570:G:H2'	1:A:2030:A:C5	2.49	0.48
1:A:586:A:H5'	5:F:89:VAL:HG21	1.94	0.48
4:E:47:VAL:O	4:E:80:GLU:HA	2.12	0.48
7:H:10:PRO:HB2	7:H:12:PRO:HD3	1.95	0.48
16:T:105:LEU:HB2	16:T:110:ILE:HG12	1.95	0.48
1:A:2876:G:H4'	16:T:2:ASN:ND2	2.28	0.48
17:U:40:PHE:CD2	18:V:75:PHE:CD2	3.01	0.48
24:1:2:SER:HB2	24:1:43:TYR:CD2	2.48	0.48
1:A:1207:C:H2'	1:A:1208:C:C6	2.48	0.48
1:A:1430:C:H2'	1:A:1431:U:C6	2.48	0.48
1:A:1518:U:H2'	1:A:1519:G:O4'	2.13	0.48
1:A:1530:C:H42	1:A:1539:G:H1	1.61	0.48
1:A:2040:C:H2'	1:A:2041:U:C6	2.48	0.48
1:A:66:C:O2	1:A:89:G:N2	2.46	0.48
62:A:4378:HOH:O	4:E:144:ARG:HD3	2.12	0.48
5:F:118:ALA:O	5:F:120:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:39:TRP:CE3	5:F:101:LEU:HD23	2.48	0.48
7:H:76:VAL:C	7:H:78:GLY:H	2.16	0.48
1:A:2293:C:H5''	15:S:89:ARG:HH21	1.77	0.48
22:Z:99:TYR:CZ	22:Z:125:LEU:HD13	2.48	0.48
23:O:42:GLY:O	23:O:57:PHE:CG	2.67	0.48
24:1:23:LYS:HB3	24:1:29:GLY:HA3	1.95	0.48
12:P:63:PRO:HB2	31:8:30:ARG:NH2	2.28	0.48
1:A:1062:G:H1	1:A:1076:C:N4	2.10	0.48
1:A:1120:G:H2'	1:A:1121:C:C6	2.48	0.48
1:A:2024:G:H2'	1:A:2025:C:C6	2.48	0.48
1:A:250:G:OP1	31:8:13:ARG:NH2	2.46	0.48
4:E:2:LYS:HA	4:E:84:PHE:CD2	2.48	0.48
16:T:56:GLY:O	16:T:59:THR:HG23	2.13	0.48
22:Z:138:GLU:H	22:Z:156:LYS:NZ	2.04	0.48
25:2:7:ARG:O	25:2:11:GLU:HG3	2.13	0.48
1:A:1025:G:C4	1:A:1135:C:H1'	2.48	0.48
1:A:299:A:N1	1:A:322:A:O2'	2.31	0.48
1:A:372:G:O2'	1:A:373:U:OP2	2.31	0.48
1:A:528:A:H2	1:A:2043:C:H4'	1.77	0.48
2:B:69:G:O6	62:B:331:HOH:O	2.19	0.48
4:E:120:TRP:CE3	4:E:155:LYS:HD3	2.48	0.48
5:F:123:LEU:HD12	5:F:124:LEU:H	1.78	0.48
6:G:80:PHE:N	6:G:80:PHE:CD1	2.80	0.48
7:H:27:LYS:HB3	7:H:27:LYS:HE2	1.62	0.48
9:K:119:ASP:HB3	9:K:122:ALA:H	1.77	0.48
13:Q:66:ILE:HG23	13:Q:104:PHE:CD2	2.49	0.48
18:V:24:LYS:HA	18:V:92:THR:OG1	2.12	0.48
20:X:31:HIS:O	20:X:77:LYS:HD3	2.13	0.48
20:X:92:LEU:C	20:X:94:GLY:N	2.67	0.48
24:1:58:ILE:HD11	24:1:87:PRO:HA	1.96	0.48
24:1:67:ILE:N	24:1:68:PRO:HD2	2.27	0.48
1:A:2025:C:H5'	4:E:149:ARG:NH2	2.28	0.48
1:A:2582:G:C2	1:A:2583:G:C8	3.00	0.48
4:E:120:TRP:CD1	4:E:155:LYS:HB3	2.48	0.48
6:G:61:ALA:HB2	6:G:68:PRO:HD3	1.96	0.48
21:Y:86:ARG:NH1	21:Y:100:ALA:HA	2.29	0.48
1:A:1548:C:H2'	1:A:1549:C:C6	2.47	0.48
1:A:1394:U:H4'	1:A:1603:A:H4'	1.96	0.48
1:A:182:A:N3	1:A:433:C:O2'	2.36	0.48
1:A:793:A:OP2	1:A:2072:G:H5'	2.14	0.48
1:A:301:G:H1'	1:A:302:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:C:H2'	1:A:645:C:O2	2.13	0.48
3:D:20:ASP:N	3:D:20:ASP:OD1	2.32	0.48
23:0:28:GLY:HA2	23:0:66:VAL:HG12	1.96	0.48
25:2:1:MET:HG3	25:2:5:GLU:HB2	1.95	0.48
1:A:1114:G:H2'	1:A:1115:G:C8	2.48	0.48
1:A:2819:G:H2'	1:A:2821:A:N7	2.28	0.48
3:D:200:ASP:OD2	3:D:203:ASN:ND2	2.47	0.48
14:R:87:TYR:OH	14:R:116:LEU:HB3	2.14	0.48
14:R:56:LYS:NZ	14:R:94:TYR:OH	2.47	0.48
1:A:536:A:H5'	17:U:53:ARG:HD3	1.95	0.48
18:V:52:VAL:O	18:V:54:GLY:N	2.40	0.48
21:Y:79:CYS:HB3	21:Y:102:CYS:HB3	1.95	0.48
1:A:1227:G:OP1	17:U:13:LYS:HE3	2.13	0.48
1:A:143(A):C:H2'	1:A:144:C:H6	1.78	0.48
1:A:1494:A:C2	1:A:1495:A:C4	3.01	0.48
1:A:1797:C:O3'	3:D:259:THR:HG22	2.13	0.48
1:A:1957:C:O2'	1:A:1985:G:H1'	2.13	0.48
1:A:2096:U:H2'	1:A:2097:C:C6	2.48	0.48
1:A:2420:C:P	31:8:33:ASN:H	2.35	0.48
1:A:2590:A:H5''	3:D:239:ARG:HE	1.79	0.48
1:A:686:G:N2	1:A:788:A:H61	2.12	0.48
2:B:61:G:C2	2:B:62:C:C2	3.01	0.48
2:B:68:C:H2'	2:B:69:G:H8	1.78	0.48
4:E:183:LEU:HD21	16:T:10:VAL:HG11	1.95	0.48
17:U:43:GLY:HA3	62:U:302:HOH:O	2.12	0.48
25:2:16:LEU:HD21	25:2:20:GLU:HB2	1.96	0.48
28:5:41:PRO:HG2	28:5:44:THR:HG21	1.95	0.48
31:8:53:PRO:O	31:8:57:ARG:HG3	2.14	0.48
1:A:1127:A:H2'	1:A:1128:A:H5''	1.95	0.48
1:A:1434:A:H2'	1:A:1435:G:C8	2.48	0.48
1:A:2018:G:H2'	1:A:2019:A:H8	1.78	0.48
1:A:275:G:C8	1:A:275:G:O5'	2.67	0.48
1:A:528:A:C2	1:A:2043:C:H4'	2.49	0.48
4:E:116:VAL:O	4:E:122:PHE:HB2	2.14	0.48
11:O:9:GLU:OE1	11:O:18:LYS:HE2	2.13	0.48
14:R:54:LEU:O	14:R:57:ARG:N	2.46	0.48
24:1:86:SER:O	24:1:90:ILE:HG13	2.14	0.48
27:4:14:ILE:HG12	27:4:31:ILE:HB	1.95	0.48
1:A:1823:G:OP1	3:D:54:ARG:NH1	2.38	0.48
1:A:186:G:H1	1:A:210:C:H42	1.62	0.48
1:A:2133:G:O2'	1:A:2156:G:O6	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:A:H5''	1:A:424:G:C5'	2.44	0.48
1:A:634:C:H2'	1:A:635:C:C6	2.48	0.48
3:D:24:ILE:HD11	3:D:91:ARG:HE	1.79	0.48
5:F:12:LEU:HB2	5:F:124:LEU:HD11	1.95	0.48
5:F:161:GLU:O	5:F:165:ARG:HD3	2.13	0.48
7:H:5:GLY:HA3	7:H:65:HIS:CD2	2.49	0.48
10:N:67:LEU:HB3	10:N:88:GLU:HG3	1.96	0.48
18:V:16:PRO:HA	18:V:96:ILE:HG22	1.96	0.48
24:1:62:VAL:HG13	24:1:63:ALA:O	2.14	0.47
1:A:1986:A:H2'	1:A:1987:G:H8	1.79	0.47
1:A:2097:C:H2'	1:A:2098:U:O4'	2.14	0.47
1:A:2529:G:H5''	1:A:2530:A:C5'	2.44	0.47
1:A:2615:U:C2	28:5:7:PRO:HA	2.49	0.47
1:A:468:G:H2'	1:A:469:G:O4'	2.14	0.47
2:B:6:C:H2'	2:B:7:G:H5''	1.96	0.47
4:E:177:PRO:O	4:E:180:ASN:N	2.46	0.47
1:A:252:G:P	12:P:50:ARG:HH12	2.37	0.47
17:U:57:PHE:O	17:U:60:LEU:N	2.46	0.47
1:A:1477:A:N6	1:A:1478:G:O6	2.47	0.47
1:A:1903:G:OP1	3:D:241:PRO:HB2	2.13	0.47
1:A:211:A:H2'	1:A:212:G:O4'	2.14	0.47
1:A:2639:A:H1'	1:A:2778:A:C2	2.50	0.47
1:A:2708:G:H2'	1:A:2709:G:H8	1.79	0.47
1:A:848:G:C4	1:A:933:A:H8	2.32	0.47
1:A:911:A:H5''	1:A:912:C:C5'	2.43	0.47
1:A:1695:G:H1'	3:D:8:PRO:O	2.14	0.47
12:P:38:GLN:HE21	12:P:45:LEU:HA	1.79	0.47
17:U:76:TYR:CZ	17:U:80:ILE:HG13	2.49	0.47
1:A:1116:C:H2'	1:A:1117:G:O4'	2.14	0.47
1:A:1388:G:H2'	1:A:1389:G:H8	1.79	0.47
1:A:1459:G:C6	1:A:1461:G:C5	3.02	0.47
1:A:2361:A:OP2	31:8:26:LYS:NZ	2.35	0.47
1:A:2590:A:O2'	1:A:2591:C:H5'	2.14	0.47
1:A:2729:G:H2'	1:A:2730:C:C6	2.49	0.47
1:A:2850:A:C2	1:A:2851:A:C4	3.02	0.47
1:A:604:G:H2'	1:A:605:C:C6	2.47	0.47
1:A:614:U:H5'	1:A:614(C):A:N6	2.29	0.47
1:A:950:G:C6	1:A:951:C:C4	3.02	0.47
3:D:223:GLY:O	3:D:225:ALA:N	2.47	0.47
3:D:242:ARG:O	3:D:244:ARG:HG2	2.15	0.47
3:D:70:TRP:CE2	3:D:150:LYS:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:100:GLU:O	4:E:172:VAL:HG23	2.14	0.47
4:E:111:ARG:HG3	4:E:160:TYR:CD1	2.49	0.47
5:F:89:VAL:HG12	5:F:90:PHE:N	2.29	0.47
8:J:54:ALA:HA	8:J:85:ASP:HA	1.95	0.47
19:W:65:LEU:HD12	19:W:65:LEU:H	1.80	0.47
22:Z:92:SER:OG	22:Z:93:ASP:N	2.44	0.47
25:2:32:LEU:HD23	25:2:32:LEU:HA	1.69	0.47
1:A:1208:C:C2	1:A:1209:G:C8	3.02	0.47
1:A:1422:G:C1'	1:A:1495:A:H61	2.27	0.47
1:A:2232:U:OP1	24:1:40:ARG:NH1	2.47	0.47
4:E:4:ILE:HG13	4:E:5:LEU:N	2.28	0.47
6:G:47:LYS:HD3	6:G:81:LYS:O	2.14	0.47
6:G:80:PHE:N	6:G:80:PHE:HD1	2.11	0.47
10:N:110:GLY:O	10:N:114:ARG:HG3	2.14	0.47
12:P:77:ARG:O	12:P:79:ARG:NE	2.48	0.47
15:S:10:ARG:HG2	15:S:91:PRO:HA	1.97	0.47
20:X:44:GLU:HG2	20:X:49:VAL:O	2.14	0.47
22:Z:22:GLY:O	22:Z:41:LEU:HB2	2.14	0.47
27:4:63:TYR:N	27:4:63:TYR:CD1	2.82	0.47
1:A:1792:G:H2'	1:A:1793:C:C6	2.50	0.47
1:A:1818:U:H2'	3:D:157:ARG:HG3	1.96	0.47
1:A:2736:G:C2	1:A:2737:G:C8	3.03	0.47
1:A:28:A:O2'	1:A:583:G:H5'	2.15	0.47
1:A:245:G:O2'	1:A:384:U:O2	2.23	0.47
5:F:103:LYS:O	5:F:106:ARG:HG2	2.14	0.47
5:F:182:ASN:ND2	5:F:185:ASP:OD2	2.45	0.47
6:G:133:LEU:HD21	6:G:157:ILE:HB	1.96	0.47
12:P:100:LEU:HA	12:P:100:LEU:HD23	1.60	0.47
12:P:31:ALA:O	12:P:32:THR:OG1	2.31	0.47
12:P:81:GLN:HG3	12:P:82:GLY:N	2.30	0.47
13:Q:32:TYR:CE2	13:Q:133:ARG:HG3	2.50	0.47
14:R:21:TYR:HB3	14:R:47:PHE:CD1	2.48	0.47
17:U:104:GLN:OE1	17:U:105:VAL:HG23	2.14	0.47
27:4:59:PHE:CA	27:4:61:ARG:H	2.20	0.47
29:6:40:CYS:O	29:6:44:ARG:N	2.47	0.47
32:9:14:CYS:HA	32:9:27:CYS:HB2	1.96	0.47
1:A:1416:G:H1	1:A:1582:C:N4	2.00	0.47
1:A:978:G:C2	1:A:986:C:C2	3.03	0.47
2:B:89:G:H2'	2:B:90:A:C8	2.50	0.47
5:F:155:LEU:HD12	5:F:174:VAL:HB	1.96	0.47
12:P:138:LEU:HD23	12:P:145:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:12:ARG:HB3	14:R:16:HIS:HB3	1.95	0.47
14:R:65:LEU:O	14:R:68:ARG:HG3	2.15	0.47
14:R:22:ARG:NE	14:R:69:ASP:HA	2.29	0.47
15:S:74:ALA:HA	15:S:110:LEU:HD11	1.96	0.47
15:S:11:LYS:HG2	15:S:91:PRO:HD3	1.97	0.47
17:U:88:ILE:HD13	17:U:109:LEU:CD2	2.41	0.47
1:A:126:A:C6	1:A:127:A:N1	2.83	0.47
1:A:1507:A:O2'	1:A:1508:A:O5'	2.22	0.47
1:A:2148:G:H2'	1:A:2149:G:H8	1.80	0.47
1:A:2648:C:H2'	1:A:2649:U:C6	2.50	0.47
1:A:945:A:N6	62:A:3805:HOH:O	2.47	0.47
24:1:3:LYS:HB3	24:1:4:VAL:HG13	1.97	0.47
1:A:1020:A:N1	1:A:1141:U:O2'	2.38	0.47
1:A:1361:G:H2'	1:A:1362:C:H6	1.79	0.47
1:A:2162:G:H2'	1:A:2163:C:C6	2.50	0.47
1:A:58:G:N2	1:A:70:G:C4	2.83	0.47
3:D:183:ARG:HB2	3:D:183:ARG:HE	1.39	0.47
3:D:16:MET:HE1	3:D:208:LYS:HE3	1.96	0.47
12:P:65:ARG:HD3	12:P:66:GLY:N	2.29	0.47
21:Y:5:MET:HE1	21:Y:32:PRO:HA	1.96	0.47
23:0:38:VAL:HG23	23:0:59:LEU:HB2	1.97	0.47
1:A:517:C:OP1	28:5:16:ARG:NH2	2.48	0.47
1:A:2815:C:O2	28:5:43:HIS:HE1	1.98	0.47
32:9:28:GLU:O	32:9:30:PRO:HD3	2.15	0.47
1:A:1239:G:H2'	1:A:1240:U:O4'	2.15	0.47
1:A:1478:G:O2'	1:A:1558:A:H2	1.98	0.47
1:A:1791:A:O2'	3:D:207:GLY:N	2.48	0.47
1:A:2028:U:H2'	1:A:2029:G:O4'	2.14	0.47
1:A:2334:G:C4	15:S:12:PHE:CD1	3.03	0.47
1:A:2512:C:H2'	1:A:2513:G:O4'	2.15	0.47
1:A:2660:A:H2'	1:A:2661:G:C8	2.50	0.47
1:A:2851:A:O5'	1:A:2851:A:H8	1.97	0.47
1:A:476:G:H4'	1:A:502:A:N1	2.29	0.47
19:W:20:VAL:HG21	19:W:43:GLY:HA3	1.96	0.47
22:Z:17:ALA:HA	22:Z:20:ARG:NH1	2.29	0.47
22:Z:5:LEU:HD22	22:Z:6:LYS:H	1.80	0.47
27:4:61:ARG:HG3	27:4:62:ARG:O	2.15	0.47
1:A:1798:U:H5'	3:D:259:THR:CG2	2.45	0.47
5:F:12:LEU:HB3	5:F:126:VAL:HG12	1.97	0.47
6:G:73:ALA:HB3	6:G:85:GLY:N	2.30	0.47
7:H:3:ARG:NE	7:H:3:ARG:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2840:C:H5''	14:R:53:HIS:CD2	2.50	0.47
31:8:52:LYS:HG3	31:8:53:PRO:CD	2.44	0.47
1:A:1176:G:H1'	1:A:1177:A:C5'	2.45	0.47
1:A:1221(A):C:H2'	1:A:1222:C:C6	2.48	0.47
1:A:1459:G:H2'	1:A:1461:G:O5'	2.15	0.47
1:A:1721:G:H3'	1:A:1722:A:H5''	1.97	0.47
1:A:652(F):G:H1	1:A:652(S):C:N4	2.13	0.47
1:A:848:G:N9	1:A:933:A:H8	2.13	0.47
3:D:35:LYS:HE3	3:D:35:LYS:HB2	1.69	0.47
4:E:101:ARG:CZ	4:E:171:GLU:HB2	2.45	0.47
5:F:7:TYR:OH	5:F:119:ARG:HD3	2.15	0.47
7:H:98:LEU:HD21	7:H:123:PHE:HB3	1.96	0.47
11:O:63:VAL:HG23	11:O:84:ALA:HA	1.95	0.47
20:X:57:LEU:N	20:X:57:LEU:HD12	2.30	0.47
25:2:10:LEU:HB3	25:2:14:ARG:NH1	2.30	0.46
1:A:1079:C:O5'	9:K:132:ARG:NH2	2.48	0.46
1:A:2582:G:N3	1:A:2582:G:H2'	2.29	0.46
1:A:625:G:N7	12:P:107:LYS:NZ	2.60	0.46
5:F:32:LEU:HD23	5:F:32:LEU:O	2.15	0.46
6:G:45:GLU:C	6:G:47:LYS:H	2.17	0.46
10:N:137:LYS:HD3	10:N:138:LEU:N	2.29	0.46
12:P:126:VAL:HG22	12:P:146:VAL:HB	1.97	0.46
17:U:44:ASN:N	17:U:44:ASN:OD1	2.46	0.46
22:Z:119:GLU:OE2	22:Z:122:ARG:NH1	2.48	0.46
1:A:1256:G:H1'	5:F:82:ILE:HD11	1.97	0.46
1:A:1381:G:C6	1:A:1382:G:C5	3.03	0.46
1:A:397:G:O2'	1:A:2230:G:N2	2.47	0.46
1:A:2335:A:C8	1:A:2337:G:C5	3.03	0.46
1:A:2343:C:H2'	1:A:2344:U:C6	2.49	0.46
1:A:472:A:H3'	1:A:473:G:H8	5.14	0.46
22:Z:160:GLY:N	22:Z:161:VAL:HB	2.30	0.46
22:Z:54:HIS:HB3	22:Z:101:PRO:HD3	1.96	0.46
1:A:82:G:N2	1:A:103:A:OP2	2.40	0.46
1:A:1055:G:H2'	1:A:1056:G:O4'	2.14	0.46
1:A:1428:C:C5	1:A:1569:A:H5''	2.51	0.46
1:A:181:A:C2	1:A:182:A:C4	3.03	0.46
1:A:1885:A:H2'	1:A:1886:C:O4'	2.16	0.46
1:A:2135:A:H61	1:A:2156:G:H1'	1.81	0.46
1:A:2107:C:N3	1:A:2182:G:N2	2.63	0.46
1:A:2405:G:O2'	1:A:2406:U:OP1	2.22	0.46
1:A:2661:G:C6	1:A:2662:A:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2680:C:OP2	4:E:111:ARG:NH2	2.47	0.46
2:B:78:A:C2	2:B:100:A:C4	3.04	0.46
7:H:87:LEU:N	7:H:131:VAL:O	2.48	0.46
14:R:63:ARG:HH21	14:R:77:ARG:HA	1.80	0.46
16:T:94:ALA:HB1	16:T:99:LEU:HD21	1.96	0.46
1:A:1052:C:O2'	1:A:1053:C:OP1	2.24	0.46
1:A:1264:G:C6	1:A:1265:A:N6	2.84	0.46
1:A:1292:U:H2'	1:A:1293:C:C6	2.50	0.46
1:A:1366:A:C4	1:A:1367:A:C8	3.03	0.46
1:A:1469:A:H2'	1:A:1470:G:O4'	2.16	0.46
1:A:1509(A):A:H2'	1:A:1509(B):A:O4'	2.15	0.46
1:A:1572:A:H5'	62:A:3776:HOH:O	2.16	0.46
1:A:1802:A:H8	1:A:1802:A:O5'	1.99	0.46
1:A:195:A:H5''	12:P:46:LYS:NZ	2.30	0.46
1:A:2114:A:H2'	1:A:2115:G:H5'	1.97	0.46
1:A:2230:G:H2'	1:A:2231:C:H6	1.78	0.46
1:A:2493:U:H2'	1:A:2494:G:O4'	2.15	0.46
1:A:265:A:H1'	1:A:266:G:O4'	2.16	0.46
5:F:165:ARG:H	5:F:167:ALA:H	1.62	0.46
10:N:68:GLU:O	10:N:70:LYS:N	2.47	0.46
10:N:75:TYR:CE2	10:N:77:GLY:HA2	2.50	0.46
13:Q:21:THR:OG1	13:Q:23:GLY:O	2.33	0.46
23:O:27:GLU:HG3	23:O:68:GLU:HA	1.98	0.46
1:A:2310:A:H2'	1:A:2311:A:H5''	1.98	0.46
1:A:2331:G:C6	1:A:2332:U:C4	3.04	0.46
1:A:2436:G:C6	1:A:2437:U:C4	3.03	0.46
1:A:2859:G:H2'	1:A:2860:A:C8	2.51	0.46
1:A:629:G:H3'	1:A:630:G:H5''	4.83	0.46
6:G:114:ILE:HG12	6:G:140:ILE:HD13	1.98	0.46
10:N:42:TRP:CE3	17:U:63:VAL:HG11	2.50	0.46
10:N:42:TRP:HD1	10:N:48:MET:CE	2.28	0.46
4:E:152:LYS:HG2	10:N:78:TYR:CE1	2.51	0.46
11:O:71:ARG:O	11:O:73:ASP:N	2.49	0.46
12:P:144:GLU:HA	12:P:145:PRO:HD3	1.78	0.46
12:P:84:ASN:HB2	12:P:87:ASP:OD2	2.16	0.46
1:A:2684:U:OP2	16:T:53:ARG:NH1	2.48	0.46
1:A:1315:C:H2'	1:A:1316:U:C6	2.51	0.46
1:A:1429:G:H2'	1:A:1430:C:C6	2.51	0.46
1:A:1442:G:H2'	1:A:1443:G:C8	2.50	0.46
1:A:1481:U:H2'	1:A:1482:G:C8	6.92	0.46
1:A:2554:U:H2'	1:A:2555:U:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:C:N4	1:A:438:G:H1	2.10	0.46
1:A:860:U:H1'	1:A:2268:A:H5'	1.97	0.46
1:A:875:G:H2'	1:A:876:C:O4'	2.16	0.46
2:B:78:A:H2'	2:B:79:C:O4'	2.15	0.46
20:X:32:PRO:HA	20:X:77:LYS:CD	2.46	0.46
22:Z:80:ARG:HH11	22:Z:80:ARG:HB2	1.80	0.46
1:A:248:G:H5''	1:A:386:G:N2	2.31	0.46
1:A:579:G:H2'	1:A:580:C:C6	2.51	0.46
6:G:89:GLY:C	6:G:90:LEU:HD23	2.36	0.46
11:O:97:ARG:HA	11:O:117:LEU:HD22	1.97	0.46
62:A:4383:HOH:O	12:P:56:SER:N	2.45	0.46
16:T:64:ARG:NH1	16:T:103:ARG:HA	2.31	0.46
17:U:19:LYS:HG2	17:U:22:LYS:HE3	1.98	0.46
17:U:92:ARG:HA	17:U:95:LEU:HB2	1.98	0.46
1:A:1371:G:HO2'	1:A:1372:U:H5	1.62	0.46
1:A:1491:G:N2	1:A:1500:G:H1'	2.31	0.46
1:A:2261:C:OP1	23:O:17:GLN:HB2	2.16	0.46
1:A:2267:A:H5''	1:A:2268:A:C5'	2.46	0.46
1:A:530:G:N3	1:A:530:G:O4'	2.47	0.46
14:R:104:ARG:HD2	14:R:107:ASP:OD1	2.16	0.46
1:A:105:C:O2'	21:Y:1:MET:HA	2.16	0.46
25:2:22:GLU:O	25:2:25:VAL:HG12	2.16	0.46
32:9:15:LYS:HB3	32:9:26:ILE:HD12	1.98	0.46
1:A:1742:G:H2'	1:A:1743:C:O4'	2.15	0.46
1:A:2048:G:C6	1:A:2049:G:C5	3.04	0.46
1:A:2590:A:H2'	1:A:2591:C:H6	1.80	0.46
1:A:272(I):U:H2'	1:A:272(J):C:C6	2.50	0.46
1:A:2815:C:O2'	28:5:43:HIS:ND1	2.46	0.46
1:A:568:U:H5'	1:A:945:A:N1	2.31	0.46
1:A:990:A:N6	1:A:1186:G:H1'	2.31	0.46
3:D:275:LYS:HD2	3:D:276:LYS:H	1.80	0.46
4:E:11:MET:HE2	4:E:24:THR:HB	1.98	0.46
13:Q:71:ASP:OD1	13:Q:71:ASP:N	2.49	0.46
16:T:48:ILE:O	16:T:64:ARG:N	2.43	0.46
16:T:2:ASN:HB3	16:T:5:ALA:HB3	1.98	0.46
20:X:63:LYS:O	20:X:64:LYS:HD3	2.16	0.46
22:Z:133:ILE:O	22:Z:135:GLU:HG3	2.15	0.46
1:A:458:G:C8	30:7:37:LYS:HG2	2.51	0.46
1:A:1090:U:C2	1:A:1102:C:H1'	2.51	0.46
1:A:2168:G:N1	1:A:2171:A:N7	2.64	0.46
1:A:2298:A:H2'	1:A:2299:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2771:C:H2'	1:A:2772:C:C6	2.51	0.46
1:A:2851:A:H2'	1:A:2852:G:O4'	2.16	0.46
1:A:306:U:H2'	1:A:307:G:O4'	2.15	0.46
1:A:435:C:O2'	1:A:436:C:H5'	2.89	0.46
3:D:109:ASP:N	3:D:195:ALA:O	2.37	0.46
1:A:1064:C:H5''	9:K:86:LYS:HB2	1.97	0.46
11:O:37:ASP:OD1	11:O:109:LYS:NZ	2.49	0.46
1:A:2562:U:H1'	11:O:23:ARG:HH11	1.79	0.46
11:O:39:ILE:HD12	11:O:41:ALA:HB2	1.98	0.46
13:Q:2:LEU:HD12	13:Q:2:LEU:H	1.80	0.46
19:W:48:ALA:O	19:W:52:GLU:HB2	2.16	0.46
26:3:36:VAL:C	26:3:37:LEU:HG	2.35	0.45
1:A:122:G:OP1	1:A:122:G:H8	5.15	0.45
1:A:1783:A:C2	1:A:2588:G:O4'	2.69	0.45
1:A:2199:A:H5''	1:A:2200:C:C5	2.51	0.45
1:A:2359:C:H2'	1:A:2360:A:C8	2.51	0.45
1:A:2677:G:H2'	1:A:2678:C:H6	1.81	0.45
1:A:271(G):C:H2'	1:A:271(H):G:H5'	1.98	0.45
1:A:2744:G:H1'	1:A:2761:G:N2	2.31	0.45
2:B:33:G:H2'	2:B:34:U:C6	2.51	0.45
9:K:34:ILE:H	9:K:34:ILE:HG12	1.55	0.45
14:R:72:ASP:OD1	14:R:75:LEU:HB2	2.16	0.45
15:S:30:ARG:HG2	15:S:31:SER:H	1.81	0.45
22:Z:29:TYR:CB	22:Z:34:ASN:HD22	2.24	0.45
1:A:1090:U:O2	1:A:1102:C:H1'	2.16	0.45
1:A:1193:G:H8	1:A:1193:G:H5''	4.34	0.45
1:A:1801:G:OP2	3:D:154:LYS:NZ	2.35	0.45
1:A:2123:G:N2	1:A:2176:A:H1'	2.32	0.45
1:A:2141:G:H22	1:A:2149:G:H22	1.64	0.45
1:A:607:U:H5	1:A:619:G:C5	2.34	0.45
1:A:631:A:N3	1:A:2415:G:O2'	2.38	0.45
1:A:903:C:H2'	1:A:904:C:C6	2.50	0.45
1:A:983:A:N3	1:A:983:A:H3'	5.24	0.45
3:D:154:LYS:C	3:D:155:LEU:HD12	2.36	0.45
9:K:37:PHE:O	9:K:41:PHE:HB3	2.15	0.45
22:Z:110:GLY:O	22:Z:113:ALA:HB3	2.15	0.45
23:0:27:GLU:HB2	23:0:69:PHE:HD1	1.81	0.45
1:A:2330:G:H4'	23:0:44:ARG:NH1	2.30	0.45
1:A:136:G:C2	1:A:137:C:C6	3.05	0.45
1:A:1477:A:C6	1:A:1478:G:C6	3.04	0.45
1:A:1499:C:H2'	1:A:1500:G:H8	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:A:H2'	1:A:208:C:O4'	2.17	0.45
1:A:2419:U:O2'	1:A:2420:C:H5'	2.16	0.45
1:A:2552:U:H2'	1:A:2554:U:OP2	2.17	0.45
3:D:133:LEU:HB3	3:D:173:VAL:HG11	1.97	0.45
3:D:68:LYS:HD2	3:D:70:TRP:CH2	2.51	0.45
4:E:119:ARG:HG2	4:E:160:TYR:CG	2.51	0.45
1:A:1079:C:H4'	9:K:132:ARG:NH2	2.31	0.45
22:Z:24:LEU:HD11	22:Z:86:VAL:CG2	2.46	0.45
22:Z:29:TYR:HB3	22:Z:34:ASN:ND2	2.24	0.45
1:A:1176:G:N3	1:A:1177:A:H5'	2.30	0.45
1:A:1386:C:H2'	1:A:1387:C:C6	2.52	0.45
1:A:1496:A:O5'	1:A:1496:A:H8	1.98	0.45
1:A:1845:G:H1	1:A:1895:C:N4	2.13	0.45
1:A:2469:A:H4'	13:Q:56:ARG:CG	2.46	0.45
1:A:247:G:C8	1:A:249:C:C6	3.04	0.45
1:A:2663:G:C6	1:A:2664:G:C4	3.04	0.45
1:A:467:G:P	30:7:33:ARG:HH12	2.40	0.45
1:A:85:G:H8	1:A:85:G:H5''	1.81	0.45
5:F:53:THR:HG23	5:F:55:GLY:H	1.81	0.45
9:K:20:ALA:HA	9:K:21:PRO:HD3	1.81	0.45
12:P:87:ASP:O	12:P:90:ARG:HG2	2.16	0.45
15:S:102:ALA:O	15:S:104:GLY:N	2.49	0.45
17:U:111:GLU:O	17:U:114:LYS:HB2	2.17	0.45
22:Z:8:TYR:HB2	22:Z:38:TYR:CE2	2.51	0.45
1:A:1266:G:OP2	28:5:19:ARG:HD2	2.16	0.45
30:7:8:ASN:HB3	30:7:11:LYS:HB3	1.98	0.45
1:A:2038:G:C6	1:A:2039:C:C4	3.04	0.45
1:A:2259:G:C2	1:A:2282:G:C6	3.05	0.45
1:A:432:A:H2'	1:A:433:C:C6	2.52	0.45
1:A:443:A:H1'	1:A:1201:C:O4'	2.15	0.45
1:A:484:C:N4	1:A:496:G:H1	2.14	0.45
1:A:556:G:C5	1:A:557:U:C4	3.04	0.45
3:D:13:ARG:HA	3:D:13:ARG:HD2	1.66	0.45
3:D:33:LEU:O	3:D:64:ILE:HG13	2.16	0.45
5:F:110:LEU:HD23	5:F:110:LEU:HA	1.76	0.45
6:G:43:LEU:HB3	6:G:44:GLY:H	1.61	0.45
14:R:60:LEU:O	14:R:63:ARG:N	2.49	0.45
25:2:46:GLN:HB3	25:2:48:HIS:CE1	2.51	0.45
1:A:1041:C:H42	1:A:1114:G:H1	1.63	0.45
1:A:1264:G:N7	1:A:1265:A:C5	2.84	0.45
1:A:1434:A:C2	1:A:1435:G:C5	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2189:U:H2'	1:A:2190:G:C8	2.52	0.45
1:A:588:U:H1'	5:F:90:PHE:CG	2.52	0.45
9:K:115:LEU:HB2	9:K:116:ASN:H	1.48	0.45
9:K:78:ILE:HG13	9:K:99:ILE:HG13	1.99	0.45
17:U:11:ARG:O	17:U:15:LYS:HB2	2.16	0.45
23:0:32:ARG:HE	23:0:32:ARG:HB3	1.53	0.45
1:A:1384:A:N3	1:A:1405:U:H1'	2.31	0.45
1:A:2303:G:O2'	6:G:132:ASN:HB2	2.17	0.45
1:A:2420:C:OP1	31:8:33:ASN:N	2.50	0.45
1:A:2675:A:H2'	1:A:2676:C:O4'	2.16	0.45
1:A:2630:G:O2'	1:A:2892:A:O2'	2.13	0.45
1:A:527:C:OP1	62:A:4072:HOH:O	2.21	0.45
1:A:595:C:H2'	1:A:596:G:O4'	2.17	0.45
1:A:652(E):G:C2	1:A:652(U):G:C2	3.05	0.45
1:A:816:C:O2'	62:A:4373:HOH:O	2.21	0.45
3:D:145:VAL:HB	3:D:155:LEU:HB2	1.98	0.45
10:N:75:TYR:CZ	10:N:77:GLY:HA2	2.52	0.45
15:S:93:LYS:O	15:S:95:HIS:N	2.49	0.45
17:U:28:ARG:HH11	17:U:38:THR:HG23	1.81	0.45
23:0:40:GLN:HE21	23:0:57:PHE:HB3	1.82	0.45
25:2:26:ARG:NH1	25:2:26:ARG:HB2	2.32	0.45
1:A:1164:G:C5	1:A:1165:U:C4	3.04	0.45
1:A:1968:G:H5''	62:A:4102:HOH:O	2.17	0.45
1:A:248:G:H5'	1:A:250:G:N7	2.31	0.45
1:A:652(F):G:H1	1:A:652(S):C:H42	1.65	0.45
1:A:831:G:N2	12:P:53:GLY:O	2.49	0.45
1:A:92:A:C8	1:A:93:G:C8	3.05	0.45
5:F:39:TRP:CD2	5:F:101:LEU:HD23	2.52	0.45
6:G:50:ALA:C	6:G:52:ILE:H	2.20	0.45
9:K:30:HIS:CD2	9:K:65:PHE:HB3	2.52	0.45
1:A:954:G:H4'	13:Q:13:GLN:NE2	2.30	0.45
15:S:92:TYR:HB2	15:S:98:VAL:HG21	1.98	0.45
1:A:2121:G:N2	1:A:2177:C:N3	2.58	0.45
1:A:2267:A:H5''	1:A:2268:A:H5'	1.99	0.45
1:A:245:G:O6	31:8:8:LYS:NZ	2.44	0.45
1:A:307:G:H21	1:A:330:A:N6	2.15	0.45
1:A:831:G:C6	1:A:832:G:C5	3.05	0.45
4:E:67:PHE:CD2	4:E:74:PRO:HA	2.51	0.45
9:K:109:LYS:HA	9:K:112:MET:SD	2.56	0.45
22:Z:100:VAL:HA	22:Z:101:PRO:HD3	1.85	0.45
22:Z:157:LEU:HD11	22:Z:163:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Z:24:LEU:HD11	22:Z:86:VAL:HG23	1.98	0.45
1:A:1182:A:H2'	1:A:1183:G:O4'	2.17	0.45
1:A:1583:A:O2'	1:A:1586:A:N6	2.50	0.45
1:A:1721:G:N3	1:A:1721:G:H5''	2.31	0.45
1:A:215:G:O3'	1:A:216:A:H4'	2.16	0.45
1:A:2257:U:H2'	1:A:2258:C:C6	2.51	0.45
1:A:2291:U:O2'	1:A:2374:C:O2	2.32	0.45
1:A:572:A:H3'	1:A:573:G:O4'	2.16	0.45
3:D:182:LEU:HB3	3:D:271:ILE:HB	1.98	0.45
3:D:92:ILE:HA	3:D:107:ALA:H	1.82	0.45
10:N:94:HIS:HB3	10:N:96:GLU:OE1	2.17	0.45
12:P:3:LEU:HD12	12:P:3:LEU:HA	1.62	0.45
18:V:32:THR:HG22	18:V:60:GLU:HB2	1.99	0.45
1:A:1047:G:H21	1:A:1111:A:N6	2.15	0.44
1:A:1204:A:H5'	1:A:1206:G:H1'	1.99	0.44
1:A:1250:G:OP2	12:P:21:ARG:NH1	2.50	0.44
1:A:1316:U:H2'	1:A:1317:A:C8	2.52	0.44
1:A:1403:C:H2'	1:A:1404:C:H6	1.82	0.44
1:A:1773:A:N7	1:A:1829:A:H1'	2.32	0.44
1:A:1773:A:C5	1:A:1829:A:H1'	2.51	0.44
1:A:1859:A:H2'	1:A:1860:G:O4'	2.17	0.44
1:A:1914:C:H2'	1:A:1915:U:C6	2.52	0.44
1:A:2014:A:C2	1:A:2015:A:N1	2.85	0.44
1:A:392:C:H5''	1:A:409:C:H5''	1.99	0.44
1:A:472:A:H5''	1:A:473:G:OP2	4.71	0.44
1:A:480:A:N3	1:A:480:A:H2'	2.32	0.44
1:A:602:G:N2	1:A:655:A:C8	2.73	0.44
2:B:39:A:O2'	2:B:40:U:H5'	2.16	0.44
9:K:30:HIS:HB3	9:K:32:ALA:HB2	1.99	0.44
9:K:90:LYS:HB2	9:K:93:ARG:NH2	2.32	0.44
10:N:103:VAL:O	10:N:106:MET:N	2.41	0.44
11:O:89:ASN:C	11:O:91:LEU:H	2.20	0.44
12:P:116:GLY:N	12:P:134:ALA:HB2	2.32	0.44
12:P:131:SER:O	12:P:133:SER:N	2.50	0.44
20:X:32:PRO:HA	20:X:77:LYS:HD3	1.99	0.44
13:Q:61:GLY:HA2	22:Z:177:PRO:HB2	1.98	0.44
22:Z:20:ARG:HB2	22:Z:20:ARG:CZ	2.46	0.44
1:A:1221(A):C:C2	1:A:1229:G:C2	3.06	0.44
1:A:1355:G:H8	1:A:1355:G:O5'	2.00	0.44
1:A:1975:G:C2	1:A:1976:U:C2	3.05	0.44
1:A:2018:G:H2'	1:A:2019:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2126:A:N6	1:A:2163:C:H4'	2.33	0.44
1:A:2195:C:H2'	1:A:2196:C:H6	1.82	0.44
1:A:271(Q):G:O2'	1:A:271(R):G:OP2	2.27	0.44
1:A:545:G:N2	1:A:546:C:H5	2.14	0.44
1:A:613:G:C6	1:A:614:U:N3	2.85	0.44
1:A:614(B):G:H5''	1:A:614(C):A:OP1	2.17	0.44
1:A:902:C:H2'	1:A:903:C:C6	2.52	0.44
1:A:978:G:C2	1:A:986:C:N3	2.86	0.44
6:G:17:PRO:HA	6:G:20:ILE:HD12	1.98	0.44
7:H:126:PRO:HB2	7:H:127:GLU:H	1.60	0.44
7:H:7:LEU:HA	7:H:8:PRO:HD2	1.70	0.44
1:A:1137:G:N2	10:N:105:GLY:O	2.50	0.44
21:Y:9:LYS:HA	21:Y:10:GLY:HA2	1.74	0.44
27:4:10:VAL:HG22	27:4:26:SER:O	2.18	0.44
29:6:36:LEU:HA	29:6:36:LEU:HD23	1.73	0.44
1:A:1094:U:H3'	1:A:1095:A:H5''	1.99	0.44
1:A:1395:A:H4'	1:A:1397:U:C5	2.52	0.44
1:A:1568:G:H4'	3:D:59:LYS:HB3	1.99	0.44
1:A:1572:A:H2'	1:A:1573:G:O4'	2.16	0.44
1:A:1592:C:H2'	1:A:1593:G:H8	1.82	0.44
1:A:2107:C:H2'	1:A:2108:C:O4'	2.18	0.44
1:A:2199:A:H3'	1:A:2200:C:C6	2.52	0.44
1:A:2478:A:H1'	1:A:2528:U:O2'	2.16	0.44
3:D:106:ILE:HG12	3:D:106:ILE:O	2.16	0.44
3:D:140:THR:O	3:D:165:ILE:HG12	2.18	0.44
3:D:166:GLN:HE22	3:D:176:ARG:NH2	2.15	0.44
3:D:177:LEU:HD11	3:D:183:ARG:HG2	2.00	0.44
3:D:220:HIS:CD2	3:D:220:HIS:C	2.89	0.44
4:E:177:PRO:O	4:E:179:GLU:N	2.50	0.44
5:F:178:PRO:HG2	5:F:179:GLU:OE1	2.17	0.44
5:F:183:VAL:O	5:F:187:VAL:HG23	2.17	0.44
5:F:53:THR:O	5:F:57:VAL:HG23	2.18	0.44
10:N:4:TYR:O	17:U:64:ARG:NH2	2.48	0.44
10:N:96:GLU:O	10:N:100:GLU:HG3	2.16	0.44
15:S:36:TYR:N	15:S:36:TYR:CD1	2.83	0.44
16:T:114:LEU:HA	16:T:114:LEU:HD23	1.80	0.44
1:A:578:A:O2'	17:U:33:ARG:NH2	2.51	0.44
21:Y:5:MET:HB3	21:Y:6:HIS:H	1.58	0.44
23:0:25:ARG:HD2	23:0:25:ARG:HA	1.72	0.44
1:A:118:A:N7	1:A:119:A:C8	2.85	0.44
1:A:172:C:H2'	1:A:173:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:165:ILE:HD13	3:D:175:LEU:HD21	2.00	0.44
4:E:199:ARG:HG3	4:E:200:GLU:O	2.17	0.44
8:J:130:THR:C	8:J:132:ASP:H	2.21	0.44
10:N:138:LEU:HD23	10:N:138:LEU:HA	1.78	0.44
10:N:42:TRP:HA	10:N:48:MET:SD	2.58	0.44
14:R:67:LEU:HD12	14:R:76:VAL:HG21	1.98	0.44
16:T:19:LEU:HD13	16:T:86:ILE:HD12	1.98	0.44
17:U:38:THR:O	17:U:41:ALA:HB3	2.17	0.44
22:Z:111:VAL:HG13	22:Z:115:GLY:O	2.17	0.44
24:1:72:GLU:O	24:1:75:GLU:HB2	2.17	0.44
25:2:17:SER:HB3	25:2:20:GLU:OE2	2.18	0.44
1:A:1275:A:H2	1:A:1295:C:O2	2.01	0.44
1:A:1359:A:H5'	1:A:1359:A:N3	2.32	0.44
1:A:1434:A:H61	1:A:1558:A:N6	2.10	0.44
1:A:1629:U:H2'	1:A:1630:G:C8	2.53	0.44
1:A:2222:G:C4	1:A:2223:G:C8	3.06	0.44
1:A:583:G:H2'	1:A:584:C:H6	1.82	0.44
1:A:603:A:H3'	12:P:90:ARG:NH2	2.32	0.44
1:A:895:U:H5''	1:A:895:U:H6	1.83	0.44
1:A:977:G:C5	1:A:987:G:C2	3.05	0.44
2:B:116:G:H2'	2:B:117:G:C8	2.53	0.44
3:D:145:VAL:HG12	3:D:146:GLU:O	2.18	0.44
4:E:107:THR:HA	4:E:163:GLU:O	2.18	0.44
1:A:1309:G:OP1	30:7:9:ARG:HB2	2.18	0.44
1:A:2054:A:C2	1:A:2616:C:C2	3.05	0.44
1:A:2339:G:H2'	1:A:2340:G:C8	2.53	0.44
1:A:1027:A:C2	1:A:2488:A:H5'	2.52	0.44
1:A:2574:G:H2'	1:A:2575:C:C6	2.53	0.44
1:A:2744:G:C2	1:A:2761:G:C4	3.06	0.44
1:A:456:C:C4	20:X:69:TYR:CE2	3.05	0.44
12:P:84:ASN:N	12:P:87:ASP:OD2	2.43	0.44
18:V:16:PRO:HB3	18:V:97:LYS:O	2.18	0.44
1:A:1442:G:H1	1:A:1549:C:H42	1.64	0.44
1:A:1833:U:H2'	1:A:1834:U:C6	2.47	0.44
1:A:2320:A:N3	1:A:2320:A:H2'	2.33	0.44
1:A:2471:C:H2'	1:A:2472:G:O4'	2.18	0.44
1:A:975:C:H4'	1:A:975:C:OP2	2.17	0.44
4:E:144:ARG:HB3	4:E:145:LYS:H	1.60	0.44
8:J:33:PRO:O	8:J:37:THR:N	2.50	0.44
12:P:3:LEU:HD12	12:P:6:LEU:HD12	1.99	0.44
1:A:1653:G:H3'	14:R:2:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:83:LEU:HD12	17:U:113:ALA:HB2	2.00	0.44
24:1:13:ILE:HG12	24:1:42:GLN:HB2	2.00	0.44
25:2:46:GLN:O	25:2:49:LYS:HB2	2.18	0.44
1:A:1289:C:H2'	1:A:1290:C:H6	1.83	0.44
1:A:1354:A:N7	1:A:1355:G:C4	2.86	0.44
1:A:2505:G:O6	1:A:2576:G:H2'	2.18	0.44
1:A:2810:A:N6	1:A:2891:G:O2'	2.43	0.44
1:A:330:A:H2	1:A:1210:A:H2'	1.83	0.44
1:A:598:G:H2'	1:A:599:G:O4'	2.17	0.44
1:A:701:G:H1	1:A:731:C:H42	1.65	0.44
6:G:41:GLN:HB3	6:G:43:LEU:HD22	1.99	0.44
7:H:54:ARG:HH21	7:H:57:ASP:HA	1.81	0.44
9:K:6:ALA:HB2	9:K:59:ILE:HG22	2.00	0.44
10:N:126:PRO:HG2	10:N:127:ASP:OD2	2.18	0.44
21:Y:79:CYS:CB	21:Y:102:CYS:HB3	2.48	0.44
22:Z:103:ARG:O	22:Z:138:GLU:HA	2.17	0.44
22:Z:157:LEU:HD22	22:Z:161:VAL:HG13	2.00	0.44
1:A:1344:G:H5'	1:A:1384:A:C6	2.53	0.44
1:A:2054:A:H2'	28:5:8:LYS:HE3	2.00	0.44
1:A:2098:U:H2'	1:A:2099:U:C6	2.53	0.44
1:A:2461:C:H42	1:A:2489:G:H1	1.66	0.44
1:A:2821:A:C2	1:A:2822:G:C4	3.06	0.44
1:A:427:U:OP1	3:D:13:ARG:NH2	85.34	0.44
1:A:634:C:H2'	1:A:635:C:H6	1.81	0.44
1:A:864:G:C6	1:A:865:C:N4	2.86	0.44
4:E:168:MET:O	4:E:170:LEU:N	2.50	0.44
5:F:149:ASP:OD2	5:F:149:ASP:N	2.48	0.44
6:G:121:ASN:HA	6:G:122:PRO:HD3	1.66	0.44
7:H:124:GLU:O	7:H:126:PRO:HD3	2.18	0.44
11:O:1:MET:HG2	11:O:32:TYR:CD2	2.52	0.44
13:Q:43:THR:HA	13:Q:94:VAL:HA	1.99	0.44
16:T:16:ARG:HD3	16:T:18:ASP:OD1	2.18	0.44
9:K:93:ARG:HG3	22:Z:112:ARG:O	2.18	0.44
27:4:16:CYS:SG	27:4:17:GLY:N	2.91	0.43
27:4:45:GLY:C	27:4:47:GLN:N	2.70	0.43
1:A:1398:C:H2'	1:A:1399:C:H6	1.82	0.43
1:A:2339:G:H2'	1:A:2340:G:H8	1.83	0.43
1:A:2519:U:C6	1:A:2542:A:N6	2.86	0.43
1:A:491:G:H2'	1:A:492:A:H8	1.83	0.43
1:A:517:C:O2'	19:W:18:ARG:NH2	2.50	0.43
1:A:76:C:N3	1:A:93:G:O6	25.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:C:H2'	1:A:903:C:H6	1.83	0.43
9:K:33:ASN:ND2	9:K:36:GLU:HB2	2.33	0.43
10:N:67:LEU:O	10:N:88:GLU:N	2.45	0.43
11:O:64:ARG:NH2	11:O:99:PHE:O	2.51	0.43
14:R:99:LYS:HA	14:R:112:ALA:HA	2.00	0.43
62:A:4282:HOH:O	17:U:51:LYS:HG2	2.18	0.43
23:O:15:ASP:OD1	23:O:16:SER:N	2.50	0.43
1:A:1187:G:OP2	62:A:3878:HOH:O	2.21	0.43
1:A:1257:C:OP1	5:F:72:ARG:NH2	2.51	0.43
1:A:1314:C:C2	1:A:1315:C:C5	3.07	0.43
1:A:1430:C:H2'	1:A:1431:U:H6	1.83	0.43
1:A:143:G:O2'	20:X:37:THR:HB	2.18	0.43
1:A:1450(A):C:N4	1:A:1451:C:H41	2.16	0.43
1:A:1487:G:H2'	1:A:1488:G:C8	2.53	0.43
1:A:2123:G:C4	1:A:2124:G:C8	3.05	0.43
1:A:2816:C:O2	1:A:2883:A:O2'	2.31	0.43
11:O:68:GLU:HG2	11:O:68:GLU:O	2.17	0.43
17:U:107:ALA:O	17:U:111:GLU:HG2	2.18	0.43
21:Y:28:LYS:HB3	21:Y:28:LYS:HE2	1.75	0.43
1:A:1119:C:H2'	1:A:1120:G:C8	4.35	0.43
1:A:2205:C:O2	1:A:2220:G:C2	2.71	0.43
1:A:2790:A:O2'	1:A:2791:C:C5	2.67	0.43
1:A:34:C:HO2'	1:A:35:G:P	2.40	0.43
1:A:57:C:H2'	1:A:58:G:O4'	2.18	0.43
1:A:590:A:OP1	5:F:95:ARG:NH1	2.51	0.43
1:A:681:G:H2'	1:A:682:G:O4'	2.18	0.43
1:A:847:U:H5'	62:A:3951:HOH:O	2.18	0.43
3:D:146:GLU:HG2	3:D:152:GLY:C	2.37	0.43
13:Q:1:MET:HB2	62:Q:4002:HOH:O	2.18	0.43
18:V:32:THR:HG22	18:V:60:GLU:HA	2.00	0.43
21:Y:92:ASN:N	21:Y:93:GLY:HA2	2.33	0.43
22:Z:179:ASP:HB3	22:Z:182:LYS:H	1.83	0.43
1:A:1102:C:H2'	1:A:1103:A:C8	2.53	0.43
1:A:213:A:H2'	1:A:214:G:O4'	2.18	0.43
1:A:24:G:C6	1:A:25:U:C4	3.07	0.43
1:A:2690:C:N4	1:A:2713:A:H1'	2.33	0.43
1:A:2887:U:H2'	1:A:2888:C:C6	2.53	0.43
1:A:804:A:H5''	1:A:805:G:OP1	2.19	0.43
6:G:170:ARG:HH21	6:G:180:PHE:CB	2.32	0.43
6:G:64:THR:HB	6:G:94:LEU:HD21	2.00	0.43
26:3:3:ARG:HB2	26:3:60:GLU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:G:H4'	1:A:126:A:OP2	2.19	0.43
1:A:150:C:H2'	1:A:151:C:C6	2.53	0.43
1:A:2347:C:H5	1:A:2382:G:C4	2.36	0.43
1:A:2604:U:H2'	1:A:2605:U:H6	1.83	0.43
1:A:586:A:OP2	62:A:3882:HOH:O	2.21	0.43
1:A:947:G:N2	1:A:971:C:C2	2.86	0.43
3:D:231:HIS:ND1	3:D:232:PRO:HD2	2.33	0.43
15:S:28:VAL:CG1	15:S:101:LEU:HD22	2.49	0.43
16:T:42:ILE:HA	16:T:42:ILE:HD13	1.78	0.43
18:V:72:VAL:HG13	18:V:85:LYS:HB3	1.99	0.43
21:Y:69:ALA:O	21:Y:71:LYS:N	2.51	0.43
22:Z:52:SER:HG	22:Z:53:ILE:N	2.11	0.43
1:A:1540:U:O4	1:A:1541:G:N1	2.51	0.43
1:A:2455:G:H2'	1:A:2456:C:H6	1.83	0.43
1:A:2745:C:H2'	1:A:2746:U:C6	2.54	0.43
1:A:515:A:H2'	62:A:4287:HOH:O	2.17	0.43
1:A:565:C:H2'	1:A:566:U:O4'	2.18	0.43
1:A:592:G:H2'	1:A:593:G:C8	3.67	0.43
2:B:17:C:H42	2:B:68:C:N4	2.09	0.43
3:D:126:GLN:HB3	3:D:129:ASN:ND2	2.34	0.43
3:D:137:PRO:O	3:D:140:THR:HG23	2.18	0.43
1:A:1843:C:H5'	3:D:253:GLN:HE22	1.82	0.43
7:H:86:GLU:HA	7:H:132:ARG:HA	2.01	0.43
12:P:100:LEU:O	12:P:105:LEU:HB2	2.17	0.43
12:P:45:LEU:HA	12:P:45:LEU:HD23	1.56	0.43
14:R:97:VAL:HG22	14:R:114:VAL:HG13	1.99	0.43
1:A:1216:G:P	17:U:12:ARG:HH21	2.42	0.43
20:X:89:ILE:HG22	20:X:92:LEU:N	2.34	0.43
22:Z:107:THR:HA	22:Z:108:PRO:HD3	1.87	0.43
27:4:15:ILE:HD12	27:4:32:TYR:CE1	2.54	0.43
28:5:51:TYR:CE1	28:5:56:LYS:HG2	2.53	0.43
31:8:40:GLU:O	31:8:44:LYS:HG3	2.19	0.43
31:8:4:MET:HE3	31:8:63:PRO:CG	2.49	0.43
1:A:1464:C:H2'	1:A:1465:G:C8	2.53	0.43
1:A:1766:U:C2	1:A:1767:C:C5	3.07	0.43
1:A:1815:A:OP2	3:D:54:ARG:NH2	2.50	0.43
1:A:1859:A:H3'	1:A:1860:G:H8	1.84	0.43
1:A:2364:C:H2'	1:A:2365:G:C8	2.53	0.43
1:A:2704:C:H2'	1:A:2705:A:O4'	2.19	0.43
1:A:354:G:H2'	1:A:355:G:H8	1.84	0.43
1:A:365:C:O5'	1:A:365:C:H6	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:232:PRO:HB3	3:D:244:ARG:CZ	2.49	0.43
4:E:152:LYS:HB2	4:E:152:LYS:HE3	1.90	0.43
4:E:36:ARG:NH1	4:E:85:ASN:ND2	2.67	0.43
5:F:17:ARG:NH1	5:F:19:GLU:HG3	2.29	0.43
5:F:198:ALA:O	5:F:201:VAL:HG22	2.19	0.43
5:F:20:LEU:HD22	5:F:21:ALA:N	2.28	0.43
1:A:249:C:HO2'	12:P:64:LYS:HZ2	1.56	0.43
13:Q:135:ASP:HB3	13:Q:136:ALA:H	1.42	0.43
13:Q:54:MET:HE3	13:Q:64:ILE:HD13	2.00	0.43
16:T:52:ILE:HG12	16:T:61:PHE:HB3	2.00	0.43
27:4:37:SER:HB2	27:4:43:TYR:CE1	2.53	0.43
29:6:10:LEU:HD12	29:6:54:ILE:HA	2.01	0.43
1:A:1107:G:H2'	1:A:1107:G:N3	2.33	0.43
1:A:2031:A:C6	1:A:2498:C:H1'	2.53	0.43
1:A:2628:C:H1'	1:A:2781:A:C4	2.54	0.43
1:A:298:G:OP1	21:Y:87:LYS:N	2.42	0.43
1:A:415:A:H2'	1:A:416:C:O4'	2.19	0.43
1:A:463:G:N1	1:A:467:G:C6	2.86	0.43
2:B:96:U:H2'	2:B:97:G:C8	2.54	0.43
11:O:71:ARG:HA	11:O:72:PRO:HD2	1.63	0.43
12:P:101:VAL:HG22	12:P:106:LEU:HD12	2.00	0.43
23:0:39:ARG:NH1	23:0:58:THR:OG1	2.51	0.43
29:6:21:TYR:CZ	29:6:38:LYS:HG2	2.53	0.43
32:9:17:ILE:HA	32:9:17:ILE:HD12	1.88	0.43
1:A:1286:A:C6	1:A:1329:U:C2	3.07	0.43
1:A:1540:U:H2'	1:A:1541:G:O4'	2.19	0.43
1:A:2739:U:O2'	1:A:2740:A:H5'	2.19	0.43
1:A:2747:G:N2	1:A:2748:A:H62	2.16	0.43
1:A:2817:G:C2	1:A:2818:G:H1'	2.53	0.43
1:A:300:A:H1'	1:A:319:C:O4'	2.19	0.43
1:A:455:C:H6	1:A:455:C:H2'	1.62	0.43
1:A:583:G:C4	1:A:584:C:C5	3.07	0.43
1:A:621:A:H5'	1:A:622:G:OP2	2.19	0.43
1:A:666:G:C5	1:A:667:U:H5	2.37	0.43
1:A:868:U:C4	1:A:869:G:N7	2.87	0.43
1:A:997:G:OP1	17:U:92:ARG:HG2	2.19	0.43
2:B:18:G:H2'	2:B:19:G:C8	2.52	0.43
3:D:143:HIS:HB2	3:D:156:ALA:O	2.19	0.43
6:G:115:ARG:H	6:G:115:ARG:HG2	2.23	0.43
6:G:136:ARG:HG3	6:G:136:ARG:H	1.69	0.43
7:H:26:VAL:HG12	7:H:79:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:38:VAL:HG12	9:K:42:ASN:HD22	1.83	0.43
12:P:27:HIS:HB3	12:P:32:THR:CG2	2.48	0.43
17:U:34:LYS:HD2	17:U:34:LYS:HA	1.51	0.43
23:O:49:LYS:O	23:O:50:ASN:HB2	2.19	0.43
1:A:858:U:OP2	23:O:77:ARG:NH2	2.52	0.43
1:A:1866:C:H2'	1:A:1876:A:O4'	2.19	0.43
1:A:2389:G:H5''	1:A:2390:U:O4'	2.19	0.43
1:A:2844:G:H2'	1:A:2845:G:O4'	2.18	0.43
1:A:2887:U:O2'	1:A:2888:C:H5'	2.18	0.43
1:A:353:G:H2'	1:A:354:G:C8	2.52	0.43
1:A:709:U:H2'	1:A:710:G:O4'	2.18	0.43
1:A:839:U:O2	1:A:839:U:H2'	2.76	0.43
1:A:2820:A:P	14:R:2:ARG:HH22	2.42	0.43
17:U:44:ASN:ND2	18:V:75:PHE:O	2.52	0.43
1:A:559:G:H22	17:U:49:HIS:CE1	2.37	0.43
22:Z:59:LEU:HD12	22:Z:69:THR:HG21	2.00	0.43
24:1:40:ARG:HG3	24:1:40:ARG:H	1.69	0.42
1:A:1207:C:H2'	1:A:1208:C:H6	1.84	0.42
1:A:1434:A:N6	1:A:1558:A:H62	2.13	0.42
1:A:1434:A:C5	1:A:1560:G:N2	2.87	0.42
1:A:1684:C:H2'	1:A:1685:C:C6	2.54	0.42
1:A:2115:G:H4'	1:A:2166:G:N2	2.34	0.42
1:A:2678:C:H2'	1:A:2679:A:H8	1.84	0.42
1:A:2864:G:H2'	1:A:2865:U:O4'	2.19	0.42
1:A:675:A:OP1	5:F:63:LYS:HD2	2.19	0.42
1:A:692:C:O2'	1:A:693:C:H5'	2.18	0.42
6:G:99:MET:HB2	6:G:99:MET:HE2	1.94	0.42
7:H:98:LEU:HD23	7:H:125:VAL:HG23	2.01	0.42
7:H:3:ARG:CZ	7:H:4:ILE:H	2.32	0.42
10:N:36:GLY:C	10:N:38:HIS:H	2.22	0.42
12:P:19:VAL:CG2	12:P:31:ALA:HB1	2.49	0.42
1:A:2820:A:C4	14:R:4:LEU:HD11	2.54	0.42
15:S:24:LEU:O	15:S:85:VAL:HG22	2.19	0.42
18:V:59:ALA:HB2	18:V:96:ILE:HD13	1.99	0.42
1:A:1413:G:H2'	1:A:1414:G:C8	2.52	0.42
1:A:1509(A):A:H3'	1:A:1509(B):A:H8	1.84	0.42
1:A:1652:A:H2'	1:A:1653:G:H5'	2.00	0.42
1:A:2358:G:H22	12:P:55:ARG:HH12	1.67	0.42
1:A:1637:A:H4'	1:A:2711:A:O2'	2.18	0.42
1:A:272:G:H1	1:A:404:C:H42	1.67	0.42
1:A:471:A:N1	20:X:68:ARG:NH1	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:A:C2	1:A:609:A:C4	3.07	0.42
6:G:126:ASP:HB2	6:G:130:ASN:O	2.19	0.42
6:G:73:ALA:HB3	6:G:85:GLY:H	1.84	0.42
7:H:94:TYR:CD1	7:H:107:VAL:HA	2.54	0.42
9:K:12:LEU:HD11	9:K:23:VAL:HG22	2.01	0.42
23:0:40:GLN:NE2	23:0:43:THR:HA	2.34	0.42
26:3:8:LEU:HD23	26:3:23:LEU:HD11	2.00	0.42
1:A:1281:G:H8	1:A:1281:G:H5''	1.83	0.42
1:A:1381:G:C5	1:A:1382:G:N7	2.87	0.42
1:A:1680:U:H2'	1:A:1681:G:H5'	2.01	0.42
1:A:1688:U:H1'	1:A:1701:A:C6	2.54	0.42
1:A:2104:G:H1	1:A:2185:C:N4	2.15	0.42
1:A:2773:C:H5''	4:E:164:ARG:HG2	2.01	0.42
1:A:392:C:H2'	1:A:393:C:C6	2.53	0.42
1:A:438:G:H2'	1:A:440:G:H8	1.84	0.42
1:A:569:U:C4	1:A:570:G:C6	3.07	0.42
1:A:657:U:H2'	1:A:658:C:C6	2.54	0.42
1:A:990:A:C6	1:A:1186:G:H1'	2.54	0.42
3:D:177:LEU:O	3:D:180:GLY:N	2.41	0.42
6:G:133:LEU:CD2	6:G:157:ILE:HB	2.50	0.42
1:A:1009:A:P	10:N:37:LYS:HZ1	2.36	0.42
12:P:101:VAL:HG22	12:P:106:LEU:HB3	2.01	0.42
19:W:107:LEU:HD12	19:W:107:LEU:HA	1.84	0.42
23:0:63:VAL:O	23:0:81:VAL:HG11	2.20	0.42
24:1:95:LEU:HD13	24:1:95:LEU:HA	1.89	0.42
27:4:1:MET:HG2	27:4:6:HIS:CD2	2.54	0.42
1:A:1003:G:N2	1:A:1038:C:C4	39.92	0.42
1:A:839:U:O2'	1:A:1191:G:N3	2.52	0.42
1:A:1208:C:C4	1:A:1209:G:N7	2.87	0.42
1:A:1241:A:C2	1:A:1242:A:C4	3.08	0.42
1:A:1426:G:H8	1:A:1426:G:O5'	2.02	0.42
1:A:1767:C:C2	1:A:1768:U:C6	3.08	0.42
1:A:2013:A:C2	1:A:2014:A:C4	3.07	0.42
1:A:410:G:N2	1:A:2407:G:C5	2.87	0.42
1:A:250:G:C6	1:A:251:A:C6	3.07	0.42
1:A:2684:U:H2'	1:A:2685:G:O4'	2.18	0.42
1:A:2758:A:H2'	1:A:2759:G:O4'	2.20	0.42
1:A:322:A:H1'	1:A:339:U:O2	2.19	0.42
1:A:528:A:O2'	1:A:529:A:H5'	2.20	0.42
1:A:646:A:H2'	1:A:647:G:O4'	2.20	0.42
1:A:922:U:H1'	23:0:26:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:13:ARG:HD3	16:T:58:ASN:ND2	2.31	0.42
7:H:7:LEU:HD23	7:H:69:ARG:HH12	1.84	0.42
9:K:17:ALA:HB3	9:K:38:VAL:HG13	2.01	0.42
10:N:42:TRP:O	17:U:64:ARG:NH1	2.52	0.42
18:V:29:PRO:HA	18:V:61:VAL:HG23	2.01	0.42
18:V:6:LYS:HD2	18:V:9:GLY:HA2	2.02	0.42
21:Y:3:VAL:HG21	21:Y:32:PRO:O	2.19	0.42
26:3:30:ARG:NH1	26:3:33:GLN:OE1	2.52	0.42
1:A:1023:U:OP2	62:A:4174:HOH:O	2.22	0.42
1:A:1064:C:H4'	9:K:89:HIS:HD2	1.85	0.42
1:A:1257:C:H2'	1:A:1258:C:H6	1.84	0.42
1:A:1320:C:O2'	1:A:1329:U:OP1	2.31	0.42
1:A:1401:G:C2	1:A:1402:C:H1'	3.68	0.42
1:A:1406:U:H2'	1:A:1407:C:H6	1.84	0.42
1:A:1682:G:H2'	1:A:1683:C:C6	2.55	0.42
1:A:196:A:C2	12:P:51:PHE:HZ	2.37	0.42
1:A:300:A:N3	1:A:319:C:H1'	2.34	0.42
1:A:71:A:H4'	1:A:72:U:H5''	2.02	0.42
1:A:764:A:H2	3:D:219:PRO:HG3	1.83	0.42
3:D:79:VAL:HG12	3:D:113:VAL:HA	2.02	0.42
21:Y:86:ARG:HH12	21:Y:100:ALA:HA	1.83	0.42
22:Z:13:GLU:O	22:Z:15:PRO:HD3	2.19	0.42
23:0:23:VAL:CG1	23:0:26:TYR:HE2	2.33	0.42
29:6:12:GLU:HB2	29:6:19:ARG:HD2	2.01	0.42
30:7:31:LEU:HD23	30:7:31:LEU:HA	1.64	0.42
1:A:1067:A:H8	1:A:1067:A:OP1	2.03	0.42
1:A:112:U:H2'	1:A:113:G:O4'	2.19	0.42
1:A:1144:G:O2'	1:A:1145:C:H5'	3.23	0.42
1:A:1422:G:O2'	1:A:1423:G:H5'	3.29	0.42
1:A:1754:C:H2'	1:A:1755:A:O4'	2.20	0.42
1:A:1816:G:H8	3:D:62:TYR:CZ	2.37	0.42
1:A:2135:A:N6	1:A:2156:G:H1'	2.35	0.42
1:A:2838:G:C6	1:A:2839:G:N7	2.88	0.42
1:A:406:G:H5''	1:A:407:G:OP2	2.19	0.42
1:A:797:C:C2	1:A:798:G:C8	3.08	0.42
1:A:879:G:H2'	1:A:880:G:O4'	2.19	0.42
3:D:66:ASP:HB2	3:D:103:ARG:HD2	2.00	0.42
4:E:6:GLY:O	4:E:195:LEU:HA	2.19	0.42
20:X:89:ILE:CG2	20:X:91:ALA:HB3	2.49	0.42
22:Z:145:GLU:O	22:Z:148:ASP:HB2	2.20	0.42
31:8:41:ILE:HA	31:8:41:ILE:HD12	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:C:H2'	1:A:1119:C:O4'	2.35	0.42
1:A:2305:A:H2'	1:A:2306:C:O4'	2.20	0.42
1:A:2513:G:H2'	1:A:2514:U:C6	2.55	0.42
1:A:259:G:N1	1:A:267:C:N3	29.58	0.42
1:A:768:G:C4	1:A:769:G:C8	3.08	0.42
1:A:776:G:H4'	1:A:777:A:O5'	2.20	0.42
2:B:50:G:H5''	15:S:61:ASN:HD22	1.85	0.42
2:B:77:U:C2'	2:B:78:A:H5'	2.50	0.42
4:E:132:HIS:O	4:E:134:ILE:HG23	2.20	0.42
1:A:1009:A:H5''	17:U:63:VAL:CG2	2.49	0.42
25:2:32:LEU:HD21	25:2:50:ILE:HG23	2.01	0.42
32:9:3:VAL:HA	32:9:35:ARG:O	2.19	0.42
1:A:1167:U:C2	1:A:1183:G:N2	2.88	0.42
1:A:154:G:C6	1:A:154(A):C:N4	2.88	0.42
1:A:1804:C:O5'	1:A:1804:C:H6	2.03	0.42
1:A:1930:G:O2'	1:A:1968:G:O6	2.28	0.42
1:A:2070:G:C2	1:A:2442:C:C2	3.08	0.42
1:A:2248:C:C2'	1:A:2249:U:H5'	2.50	0.42
1:A:2813:A:H2'	1:A:2814:C:O4'	2.19	0.42
1:A:451:C:H4'	5:F:52:LYS:HE2	2.01	0.42
1:A:669:G:O2'	1:A:670:A:H5'	2.19	0.42
3:D:206:LEU:HD23	3:D:211:ARG:NE	2.34	0.42
3:D:261:LYS:NZ	3:D:263:ARG:HB2	2.34	0.42
5:F:162:LEU:HD13	5:F:162:LEU:HA	1.83	0.42
7:H:40:GLU:H	7:H:40:GLU:HG3	1.67	0.42
10:N:22:THR:O	10:N:24:GLY:N	2.53	0.42
12:P:47:ASP:HA	12:P:48:PRO:HD2	1.76	0.42
1:A:871:U:H5''	13:Q:69:PHE:CZ	2.55	0.42
11:O:122:LEU:HD12	16:T:72:VAL:HG11	2.02	0.42
22:Z:144:LEU:HD11	22:Z:150:LEU:HD23	2.02	0.42
1:A:1136:G:N3	1:A:1136:G:H2'	2.34	0.42
1:A:1205:U:H2'	1:A:1206:G:C8	5.36	0.42
1:A:1264:G:OP1	28:5:19:ARG:NH2	2.50	0.42
1:A:1791:A:H3'	1:A:1792:G:H8	1.85	0.42
1:A:185:U:H4'	1:A:218:A:H4'	2.02	0.42
1:A:1996:C:H4'	1:A:1997:G:OP1	2.19	0.42
1:A:2304:G:H5'	1:A:2305:A:OP2	2.20	0.42
1:A:26:G:C6	1:A:27:G:N1	2.88	0.42
1:A:2727:G:O2'	11:O:70:LYS:HE3	2.20	0.42
1:A:581:C:OP1	17:U:33:ARG:HG2	2.20	0.42
1:A:784:A:C8	1:A:792:G:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:A:H2	1:A:889:C:H5''	1.85	0.42
3:D:206:LEU:HA	3:D:211:ARG:HH21	1.85	0.42
7:H:98:LEU:HD13	7:H:102:ALA:O	2.19	0.42
9:K:93:ARG:CZ	9:K:94:GLU:HB2	2.49	0.42
12:P:81:GLN:HG2	12:P:106:LEU:CD2	2.44	0.42
14:R:21:TYR:OH	14:R:43:GLU:HG2	2.20	0.42
1:A:2685:G:P	16:T:51:ARG:HH22	2.42	0.42
17:U:28:ARG:HG2	17:U:38:THR:OG1	2.20	0.42
18:V:43:GLU:HB2	18:V:44:LYS:H	1.69	0.42
19:W:85:VAL:HG13	19:W:93:ALA:HB1	2.02	0.42
24:1:89:GLU:H	24:1:89:GLU:HG2	1.50	0.42
27:4:59:PHE:N	27:4:60:GLN:HB3	2.35	0.42
28:5:23:HIS:CD2	28:5:23:HIS:N	2.88	0.42
30:7:12:ARG:HG2	30:7:46:VAL:HG11	2.01	0.42
1:A:1406:U:H2'	1:A:1407:C:C6	2.55	0.42
1:A:143(A):C:O2'	1:A:144:C:H5'	2.20	0.42
1:A:1464:C:H2'	1:A:1465:G:H8	1.85	0.42
1:A:2039:C:H2'	1:A:2040:C:H6	1.84	0.42
1:A:2061:G:C2	1:A:2063:C:C4	3.08	0.42
1:A:2680:C:O2'	1:A:2681:C:H5'	2.20	0.42
1:A:584:C:H2'	1:A:584:C:O2	2.19	0.42
1:A:872:A:C4	1:A:874:G:N7	7.40	0.42
3:D:92:ILE:HD13	3:D:104:TYR:CE2	2.55	0.42
3:D:224:ALA:H	3:D:233:HIS:HB3	1.84	0.42
4:E:119:ARG:HD2	4:E:120:TRP:CD1	2.55	0.42
6:G:27:ASN:C	6:G:29:TRP:H	2.20	0.42
9:K:24:GLY:O	9:K:28:GLY:N	2.53	0.42
9:K:30:HIS:CE1	9:K:59:ILE:HB	2.55	0.42
16:T:27:THR:O	16:T:89:VAL:HG22	2.20	0.42
17:U:13:LYS:HE2	17:U:13:LYS:HB3	1.90	0.42
1:A:72:U:OP2	20:X:1:MET:N	2.53	0.42
27:4:40:HIS:HA	27:4:41:PRO:HD3	1.92	0.41
19:W:15:ARG:NH2	28:5:20:ARG:HE	2.18	0.41
1:A:1491:G:C6	1:A:1500:G:C2	3.07	0.41
1:A:2044:C:C2	1:A:2625:G:N2	2.87	0.41
1:A:2421:G:H5'	1:A:2422:A:OP2	2.19	0.41
1:A:2503:A:H2'	1:A:2503:A:N3	2.35	0.41
1:A:2586:C:O5'	1:A:2586:C:H6	2.03	0.41
1:A:571:A:C8	1:A:2030:A:C6	3.08	0.41
1:A:839:U:O2'	1:A:840:C:OP1	5.23	0.41
4:E:2:LYS:HA	4:E:84:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:116:ASP:OD2	12:P:1:MET:HB3	2.20	0.41
1:A:1652:A:OP1	14:R:8:ARG:HD3	2.20	0.41
15:S:99:LYS:O	15:S:102:ALA:HB3	2.19	0.41
15:S:105:ALA:HB1	15:S:110:LEU:HD13	2.00	0.41
16:T:23:ARG:HG3	16:T:120:ARG:CZ	2.50	0.41
1:A:564:C:H1'	17:U:37:GLU:OE1	2.20	0.41
1:A:139(A):G:N1	20:X:44:GLU:OE1	2.50	0.41
22:Z:119:GLU:HG3	22:Z:119:GLU:H	1.51	0.41
24:1:51:VAL:HG12	24:1:58:ILE:O	2.20	0.41
27:4:63:TYR:N	27:4:64:GLY:HA2	2.34	0.41
31:8:58:ILE:O	31:8:61:LEU:HB2	2.20	0.41
1:A:1171:G:C3'	1:A:1173:G:H5'	2.50	0.41
1:A:1168:G:C2	1:A:1182:A:C2	3.08	0.41
1:A:1517:G:C6	1:A:1518:U:C4	3.08	0.41
1:A:1773:A:H2'	1:A:1774:C:O4'	2.20	0.41
1:A:1978:A:H2'	1:A:1979:C:O4'	2.19	0.41
1:A:1983:C:H4'	1:A:2606:C:H4'	2.03	0.41
1:A:2129:C:H2'	1:A:2130:U:O4'	2.20	0.41
1:A:2250:G:H8	1:A:2497:A:OP2	2.04	0.41
1:A:2270:G:H2'	1:A:2271:G:H8	1.83	0.41
1:A:2291:U:O2'	1:A:2374:C:H1'	2.20	0.41
1:A:2373:G:C6	1:A:2374:C:N4	2.88	0.41
1:A:2576:G:O2'	1:A:2579:C:OP2	2.24	0.41
1:A:2723:C:OP1	4:E:109:LYS:HD3	2.21	0.41
1:A:2889:C:H2'	1:A:2889:C:O2	2.21	0.41
1:A:28:A:H1'	1:A:513:A:C2	2.55	0.41
1:A:338:G:C4	1:A:339:U:C6	3.07	0.41
1:A:65:C:H2'	1:A:66:C:C6	2.55	0.41
1:A:686:G:H5''	30:7:11:LYS:HE2	2.01	0.41
3:D:152:GLY:O	3:D:154:LYS:HG2	2.20	0.41
3:D:223:GLY:O	3:D:226:MET:N	2.48	0.41
4:E:117:MET:O	4:E:118:LYS:HB3	2.19	0.41
4:E:10:GLY:HA2	4:E:192:ASN:OD1	2.20	0.41
7:H:164:TYR:HA	7:H:164:TYR:HD2	1.73	0.41
15:S:69:VAL:HG13	15:S:101:LEU:HD12	2.02	0.41
17:U:81:HIS:CD2	17:U:84:LYS:HD3	2.55	0.41
22:Z:136:PHE:HA	22:Z:136:PHE:HD2	1.72	0.41
22:Z:176:PRO:HA	22:Z:177:PRO:HD3	1.82	0.41
24:1:70:VAL:O	24:1:74:VAL:HG23	2.20	0.41
27:4:69:LYS:HB3	27:4:69:LYS:HE2	1.86	0.41
19:W:23:LEU:HD11	28:5:27:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:51:TYR:HA	28:5:55:ARG:O	2.19	0.41
28:5:58:LEU:O	28:5:60:VAL:N	2.53	0.41
1:A:1144:G:C6	1:A:1145:C:N4	2.88	0.41
1:A:1352:U:O2'	1:A:1353:A:H5'	2.20	0.41
1:A:1500:G:N2	3:D:99:ASP:O	2.51	0.41
1:A:2023:G:H4'	1:A:2617:C:O3'	2.20	0.41
1:A:2309:A:N6	1:A:2310:A:C6	2.88	0.41
1:A:2373:G:C6	1:A:2374:C:C4	3.08	0.41
1:A:2883:A:H5''	1:A:2884:U:H5'	2.02	0.41
1:A:438:G:H2'	1:A:440:G:C8	2.54	0.41
1:A:565:C:C4	1:A:566:U:C5	3.07	0.41
1:A:675:A:H4'	5:F:67:GLN:OE1	2.20	0.41
6:G:22:ARG:NH2	6:G:175:LEU:HD11	2.32	0.41
7:H:101:ARG:NH2	7:H:121:ILE:O	2.53	0.41
8:J:85:ASP:O	8:J:87:VAL:N	2.54	0.41
10:N:18:ALA:O	10:N:19:GLU:HB2	2.20	0.41
1:A:2406:U:N3	12:P:72:PRO:HD2	2.35	0.41
13:Q:54:MET:HB2	13:Q:54:MET:HE3	1.91	0.41
15:S:61:ASN:OD1	15:S:64:GLU:HG3	2.20	0.41
19:W:15:ARG:HH21	28:5:20:ARG:NE	2.18	0.41
1:A:84:A:C5'	21:Y:8:LYS:HG2	2.49	0.41
22:Z:156:LYS:HD2	22:Z:157:LEU:H	1.85	0.41
22:Z:137:ILE:HG23	22:Z:156:LYS:HE3	2.01	0.41
22:Z:150:LEU:O	22:Z:171:ILE:HG12	2.20	0.41
1:A:1676:A:H2'	1:A:1677:A:O4'	2.19	0.41
1:A:2206:G:H5'	1:A:2207:G:N7	2.35	0.41
1:A:2506:U:C6	1:A:2507:C:H5	2.39	0.41
1:A:2531:A:H2	1:A:2658:C:O2	2.03	0.41
1:A:2861:G:C2	1:A:2862:G:C8	3.08	0.41
1:A:392:C:H2'	1:A:393:C:H6	1.85	0.41
1:A:483:A:H2'	1:A:484:C:O4'	2.21	0.41
1:A:827:U:H5'	1:A:828:U:O5'	2.19	0.41
6:G:138:GLN:HB2	6:G:155:MET:HE3	2.03	0.41
6:G:25:TYR:CE2	6:G:31:VAL:HA	2.55	0.41
10:N:100:GLU:HG2	10:N:122:VAL:HG21	2.03	0.41
10:N:115:ARG:HG3	10:N:115:ARG:O	2.21	0.41
11:O:43:VAL:HG12	11:O:54:GLU:HA	2.03	0.41
16:T:7:ILE:HA	16:T:7:ILE:HD13	1.88	0.41
18:V:51:VAL:HB	18:V:53:GLU:H	1.84	0.41
22:Z:98:MET:HB2	22:Z:98:MET:HE3	1.89	0.41
1:A:1144:G:H2'	1:A:1145:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:A:N3	1:A:178:G:H1'	2.35	0.41
1:A:1355:G:C6	1:A:1356:G:C5	3.08	0.41
1:A:1478:G:H2'	1:A:1479:G:C8	2.46	0.41
1:A:1439:A:N3	1:A:1553:A:C6	2.89	0.41
1:A:2072:G:C5	1:A:2073:C:C5	3.08	0.41
1:A:2099:U:H2'	1:A:2100:G:C8	2.55	0.41
1:A:2224:G:H4'	1:A:2226:C:O2	2.21	0.41
1:A:2812:G:N2	1:A:2889:C:C2	2.88	0.41
1:A:293:U:H5''	1:A:294:A:OP2	2.21	0.41
3:D:176:ARG:HA	3:D:181:GLU:O	2.21	0.41
3:D:179:SER:O	3:D:275:LYS:HB2	2.21	0.41
3:D:99:ASP:N	3:D:99:ASP:OD2	2.54	0.41
4:E:37:ARG:HD2	4:E:44:TYR:CZ	2.56	0.41
2:B:57:A:H1'	6:G:29:TRP:HB2	2.02	0.41
6:G:45:GLU:HG2	6:G:45:GLU:H	1.71	0.41
7:H:38:SER:OG	7:H:40:GLU:HG3	2.20	0.41
9:K:32:ALA:O	9:K:34:ILE:N	2.53	0.41
9:K:13:PRO:HG3	9:K:52:ILE:HG12	2.02	0.41
16:T:19:LEU:HA	16:T:19:LEU:HD23	1.78	0.41
17:U:97:ASP:O	17:U:101:ARG:HG3	2.21	0.41
21:Y:6:HIS:CD2	21:Y:7:VAL:HG23	2.56	0.41
1:A:77:C:OP1	25:2:59:ARG:HD3	2.21	0.41
1:A:250:G:P	31:8:13:ARG:HH21	2.43	0.41
1:A:1097:U:H2'	1:A:1098:A:H5'	2.03	0.41
1:A:77:C:H42	1:A:109:G:H1	1.67	0.41
1:A:1452:A:O2'	1:A:1453:U:H2'	2.19	0.41
1:A:247:G:C8	1:A:249:C:C5	3.08	0.41
1:A:301:G:C4	1:A:302:C:C5	3.09	0.41
1:A:370:G:H4'	1:A:371:A:OP2	2.20	0.41
1:A:894:C:H2'	1:A:895:U:O4'	2.20	0.41
3:D:161:THR:O	3:D:196:VAL:HG23	2.20	0.41
5:F:185:ASP:OD1	5:F:188:ARG:NH1	2.41	0.41
5:F:32:LEU:HB3	5:F:112:MET:HE1	2.03	0.41
9:K:12:LEU:HA	9:K:13:PRO:HD3	1.76	0.41
1:A:1006:C:H1'	10:N:106:MET:HB3	2.01	0.41
20:X:89:ILE:HG23	20:X:91:ALA:HB3	2.02	0.41
22:Z:53:ILE:HG22	22:Z:71:VAL:HB	2.02	0.41
1:A:1139:G:OP1	10:N:101:HIS:ND1	2.43	0.41
1:A:1149:G:H2'	1:A:1150:C:C6	2.56	0.41
1:A:1215:G:C6	1:A:1216:G:N7	3.60	0.41
1:A:1289:C:H2'	1:A:1290:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1668:A:H4'	1:A:1669:A:O5'	2.20	0.41
1:A:1838:C:C5	1:A:1899:G:C2	3.09	0.41
1:A:2243:U:H2'	1:A:2244:U:C6	2.55	0.41
1:A:2491:U:H6	1:A:2491:U:H5''	1.86	0.41
1:A:34:C:H2'	1:A:35:G:C5'	2.46	0.41
1:A:464:U:H2'	1:A:465:G:O4'	2.20	0.41
1:A:904:C:H2'	1:A:905:U:H6	1.85	0.41
6:G:50:ALA:O	6:G:53:LEU:HD23	2.21	0.41
7:H:94:TYR:CG	7:H:107:VAL:HG12	2.55	0.41
5:F:34:TRP:HA	12:P:6:LEU:HD22	2.03	0.41
17:U:61:TRP:O	17:U:64:ARG:N	2.54	0.41
22:Z:150:LEU:HA	22:Z:150:LEU:HD13	1.77	0.41
24:1:40:ARG:HE	24:1:40:ARG:HB2	1.30	0.41
25:2:31:GLU:O	25:2:35:LEU:HG	2.21	0.41
26:3:26:LEU:HB2	26:3:28:LEU:HD12	2.03	0.41
1:A:1063:G:O5'	1:A:1063:G:H8	2.04	0.41
1:A:1062:G:N2	1:A:1076:C:N3	2.66	0.41
1:A:151:C:H2'	1:A:152:G:C8	2.56	0.41
1:A:1707:G:H2'	1:A:1708:C:C6	2.56	0.41
1:A:234:C:H2'	1:A:235:U:C6	2.56	0.41
1:A:2367:G:H2'	1:A:2368:C:H6	1.86	0.41
1:A:2747:G:O6	1:A:2755:C:H5''	2.20	0.41
1:A:2869:G:H2'	1:A:2870:C:O4'	2.20	0.41
1:A:436:C:H6	1:A:436:C:H2'	3.73	0.41
1:A:833:U:H2'	1:A:834:C:H6	2.01	0.41
1:A:1813:G:N3	3:D:50:THR:OG1	2.53	0.41
4:E:52:LEU:HA	4:E:53:PRO:HD2	1.78	0.41
6:G:107:LEU:O	27:4:43:TYR:OH	2.39	0.41
7:H:76:VAL:HG12	7:H:77:LYS:N	2.36	0.41
9:K:112:MET:C	9:K:114:ASP:H	2.23	0.41
10:N:10:GLU:OE2	10:N:11:PRO:HD2	2.19	0.41
13:Q:70:PRO:HA	13:Q:95:ALA:HB2	2.02	0.41
17:U:36:ARG:HD2	17:U:40:PHE:CZ	2.55	0.41
25:2:16:LEU:CD2	25:2:20:GLU:HB2	2.51	0.41
28:5:36:CYS:SG	28:5:38:ALA:HB3	2.61	0.41
28:5:40:LYS:HE2	28:5:40:LYS:HB2	1.80	0.41
30:7:11:LYS:O	30:7:15:THR:OG1	2.24	0.41
31:8:23:VAL:HG11	31:8:47:LYS:HD3	2.02	0.41
31:8:30:ARG:HD3	31:8:30:ARG:HA	1.70	0.41
1:A:1130:U:O2	4:E:149:ARG:NH2	2.53	0.41
1:A:19:C:O2	1:A:916:G:N2	85.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2074:U:H2'	1:A:2075:U:H6	1.82	0.41
1:A:2343:C:O2'	1:A:2373:G:H4'	2.21	0.41
1:A:2418:A:H2'	1:A:2419:U:C6	2.55	0.41
1:A:2794:C:C2	1:A:2802:G:N2	2.82	0.41
1:A:609:A:OP1	12:P:18:ARG:NH2	33.19	0.41
1:A:881:G:H2'	1:A:882:G:O4'	2.21	0.41
2:B:88:C:H2'	2:B:89:G:O4'	2.19	0.41
3:D:164:GLN:HE21	3:D:164:GLN:HB3	1.66	0.41
6:G:47:LYS:CG	6:G:48:GLU:H	2.33	0.41
7:H:3:ARG:NH1	7:H:5:GLY:H	2.14	0.41
10:N:62:VAL:CG1	10:N:66:LYS:HD2	2.51	0.41
11:O:25:LEU:HB2	11:O:38:VAL:O	2.21	0.41
21:Y:46:LYS:HD3	21:Y:60:PHE:CD2	2.55	0.41
24:1:74:VAL:HB	24:1:75:GLU:OE2	2.21	0.41
25:2:21:LEU:HD23	25:2:21:LEU:HA	1.67	0.41
27:4:40:HIS:O	27:4:42:PHE:N	2.53	0.41
1:A:2485:G:H5''	13:Q:46:GLN:HE21	1.86	0.41
1:A:2536:G:C6	1:A:2537:U:C4	3.09	0.41
1:A:2782:G:N2	1:A:2783:G:H1'	2.36	0.41
1:A:686:G:H1'	30:7:6:GLN:O	2.21	0.41
1:A:691:C:H2'	1:A:692:C:H6	1.85	0.41
1:A:911:A:H2'	13:Q:9:TYR:OH	2.21	0.41
5:F:206:ILE:HG12	5:F:206:ILE:H	1.56	0.41
5:F:21:ALA:O	5:F:23:ASP:N	2.52	0.41
11:O:111:PHE:O	11:O:115:VAL:HG23	2.21	0.41
11:O:23:ARG:HG3	11:O:24:VAL:N	2.36	0.41
13:Q:98:LYS:HA	13:Q:99:PRO:HD3	1.96	0.41
15:S:78:LEU:C	15:S:80:LEU:H	2.24	0.41
24:1:90:ILE:O	24:1:94:LEU:HD12	2.21	0.41
1:A:2478:A:OP1	32:9:31:LYS:HD3	2.21	0.41
1:A:1265:A:C8	1:A:1267:U:C2	3.09	0.41
1:A:1270:C:H4'	1:A:1325:G:N7	2.36	0.41
1:A:1496:A:O2'	1:A:1497:U:O2	2.38	0.41
1:A:185:U:H2'	1:A:186:G:C8	2.56	0.41
1:A:1952:A:N3	11:O:22:ILE:HD12	2.36	0.41
1:A:2061:G:N3	1:A:2063:C:C5	2.89	0.41
1:A:66:C:C2	1:A:89:G:C2	3.09	0.41
1:A:947:G:N3	1:A:984:A:H2	2.18	0.41
2:B:9:G:C5	2:B:113:G:C6	3.09	0.41
3:D:130:ALA:C	3:D:131:LEU:HD12	2.41	0.41
3:D:43:ARG:HG3	3:D:49:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:33:LEU:HB3	7:H:34:GLU:H	1.67	0.41
1:A:1754:C:OP2	16:T:113:LYS:HE3	2.21	0.41
18:V:89:GLN:HA	18:V:90:PRO:HD3	1.88	0.41
21:Y:28:LYS:HD2	21:Y:40:GLU:HA	2.03	0.41
22:Z:152:ALA:HB1	22:Z:163:LEU:HD21	2.03	0.41
23:O:11:ARG:O	23:O:14:ARG:NH2	2.47	0.40
32:9:29:ASN:HA	32:9:30:PRO:HD3	1.90	0.40
1:A:1434:A:O2'	1:A:1435:G:H5'	2.21	0.40
1:A:2140:C:O2	1:A:2151:G:N1	2.36	0.40
1:A:2199:A:N3	1:A:2199:A:H2'	2.35	0.40
1:A:2206:G:HO2'	1:A:2207:G:P	2.44	0.40
1:A:2338:G:N2	1:A:2339:G:C4	2.88	0.40
1:A:2486:G:H2'	1:A:2487:G:O4'	2.21	0.40
3:D:81:ALA:HA	3:D:113:VAL:CG1	2.51	0.40
1:A:2638:G:P	4:E:82:ARG:HH22	2.44	0.40
6:G:99:MET:HG3	6:G:100:TRP:N	2.36	0.40
7:H:24:VAL:HG13	7:H:37:VAL:HG21	2.04	0.40
9:K:53:VAL:HA	9:K:54:PRO:HD3	1.92	0.40
12:P:84:ASN:HB3	12:P:85:LEU:H	1.63	0.40
15:S:62:LYS:HG3	15:S:97:ARG:HD2	2.03	0.40
16:T:29:ARG:HB3	16:T:87:ASP:HB2	2.04	0.40
17:U:76:TYR:HH	17:U:92:ARG:NH1	2.14	0.40
19:W:12:ILE:HG13	19:W:42:ARG:NH1	2.37	0.40
19:W:68:ARG:HB3	19:W:109:GLU:HG2	2.02	0.40
21:Y:19:LYS:HD3	21:Y:20:TYR:CE1	2.56	0.40
20:X:60:ARG:HH12	30:7:47:ARG:HH22	1.69	0.40
1:A:1141:U:H4'	1:A:1142(A):A:O4'	2.21	0.40
1:A:1142(A):A:C4	1:A:1144:G:C8	3.09	0.40
1:A:1548:C:H2'	1:A:1549:C:H6	1.87	0.40
1:A:1288:U:O2'	1:A:1647:G:N2	2.54	0.40
1:A:1798:U:H5'	3:D:259:THR:HG22	2.03	0.40
1:A:2058:A:C6	1:A:2059:A:N6	2.89	0.40
1:A:2079:U:H3	1:A:2241:A:N6	2.19	0.40
1:A:2133:G:C2	1:A:2157:G:C5	3.09	0.40
1:A:2099:U:H1'	1:A:2191:G:H22	1.86	0.40
1:A:2277:G:C6	1:A:2278:A:N7	2.90	0.40
1:A:2752:C:H2'	1:A:2753:A:O4'	2.21	0.40
1:A:485:C:H2'	1:A:486:C:C6	2.56	0.40
3:D:175:LEU:HA	3:D:175:LEU:HD23	1.57	0.40
3:D:206:LEU:HD22	3:D:211:ARG:HB3	2.03	0.40
5:F:154:VAL:N	5:F:172:TRP:O	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:121:ILE:HD13	7:H:121:ILE:HA	1.99	0.40
9:K:103:GLN:HA	9:K:106:GLU:HG2	2.03	0.40
1:A:1138:G:H1'	10:N:105:GLY:O	2.21	0.40
10:N:36:GLY:HA3	10:N:48:MET:CE	2.50	0.40
13:Q:34:LEU:HD12	13:Q:34:LEU:HA	1.81	0.40
4:E:181:LEU:HD11	16:T:6:LEU:HD23	2.02	0.40
21:Y:39:VAL:HB	21:Y:42:VAL:HG21	2.03	0.40
22:Z:166:SER:HA	22:Z:167:PRO:HD3	1.95	0.40
27:4:46:GLN:C	27:4:48:ARG:H	2.23	0.40
28:5:20:ARG:C	28:5:22:HIS:N	2.74	0.40
30:7:43:THR:HA	30:7:44:PRO:HD3	1.99	0.40
1:A:1388:G:H1	1:A:1399:C:H42	1.69	0.40
1:A:1434:A:H2'	1:A:1435:G:H8	1.87	0.40
1:A:1826:G:OP2	3:D:222:ARG:HB3	2.21	0.40
1:A:2057:A:O2'	1:A:2058:A:H5'	2.21	0.40
1:A:2126:A:H4'	1:A:2127:G:O5'	2.20	0.40
1:A:2135:A:N7	1:A:2136:C:N4	2.69	0.40
1:A:137:C:H42	1:A:226:G:H1	89.78	0.40
1:A:2370:G:C6	1:A:2371:G:C6	3.09	0.40
1:A:556:G:C6	1:A:557:U:C4	3.10	0.40
9:K:115:LEU:O	9:K:116:ASN:ND2	2.41	0.40
9:K:70:LYS:HB3	9:K:71:THR:H	1.61	0.40
10:N:1:MET:HG3	10:N:1:MET:H1	1.76	0.40
10:N:54:VAL:HB	10:N:122:VAL:HG13	2.04	0.40
11:O:64:ARG:NH1	11:O:81:ASP:OD2	2.54	0.40
12:P:115:LEU:HA	12:P:131:SER:OG	2.21	0.40
16:T:19:LEU:HA	16:T:20:PRO:HD2	1.67	0.40
24:1:76:ARG:H	24:1:76:ARG:HG3	1.72	0.40
1:A:1051:G:C6	1:A:1052:C:C4	3.10	0.40
1:A:1173:G:H2'	1:A:1173:G:OP2	2.22	0.40
1:A:1234:U:H2'	1:A:1235:G:O4'	2.22	0.40
1:A:1410:G:N2	1:A:1491:G:C4	46.23	0.40
1:A:1689:A:H62	1:A:1698:A:H2	1.68	0.40
1:A:1987:G:N3	1:A:1988:C:C6	2.90	0.40
1:A:2697:G:H2'	1:A:2698:U:O4'	2.21	0.40
1:A:2774:C:H2'	1:A:2775:A:O4'	2.22	0.40
1:A:365:C:H2'	1:A:366:C:O4'	2.21	0.40
1:A:906:G:H5''	1:A:907:U:OP2	2.20	0.40
1:A:926:A:H2'	1:A:927:G:H8	1.87	0.40
3:D:160:GLY:HA3	3:D:199:ALA:HA	2.03	0.40
6:G:31:VAL:HA	6:G:32:PRO:HD2	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:54:ARG:NH1	16:T:54:ARG:HG2	2.36	0.40
17:U:8:VAL:CG2	17:U:11:ARG:HH21	2.34	0.40
18:V:25:LEU:HD22	18:V:26:ASP:N	2.30	0.40
19:W:95:ILE:HG23	19:W:95:ILE:HD12	1.87	0.40
32:9:2:LYS:HE2	32:9:31:LYS:O	2.22	0.40
1:A:1022:G:C6	1:A:1141:U:C5	3.09	0.40
1:A:1421:G:O2'	1:A:1494:A:N6	2.54	0.40
1:A:1451:C:N4	1:A:1459:G:H1	2.15	0.40
1:A:1673:U:N3	1:A:1675:C:O4'	2.53	0.40
1:A:1792:G:C4	1:A:1793:C:C5	3.10	0.40
1:A:2083:G:H8	1:A:2083:G:O5'	2.03	0.40
1:A:45:C:H5''	1:A:215:G:H8	1.87	0.40
1:A:2631:G:O2'	1:A:2810:A:N1	2.50	0.40
1:A:27:G:N2	1:A:512:G:H1'	2.36	0.40
1:A:862:G:H2'	1:A:863:A:O4'	2.21	0.40
4:E:117:MET:O	4:E:119:ARG:N	2.50	0.40
9:K:21:PRO:HA	9:K:23:VAL:N	2.37	0.40
10:N:108:PRO:O	10:N:113:GLY:HA3	2.22	0.40
22:Z:144:LEU:HD11	22:Z:150:LEU:CD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	273/276 (99%)	233 (85%)	26 (10%)	14 (5%)	2	8
4	E	202/206 (98%)	165 (82%)	27 (13%)	10 (5%)	2	8
5	F	201/205 (98%)	152 (76%)	37 (18%)	12 (6%)	2	5
6	G	179/182 (98%)	143 (80%)	25 (14%)	11 (6%)	2	5
7	H	172/180 (96%)	128 (74%)	34 (20%)	10 (6%)	2	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	128/173 (74%)	69 (54%)	31 (24%)	28 (22%)	0	0
9	K	137/147 (93%)	94 (69%)	33 (24%)	10 (7%)	1	3
10	N	138/140 (99%)	106 (77%)	24 (17%)	8 (6%)	2	6
11	O	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	4	18
12	P	147/150 (98%)	108 (74%)	29 (20%)	10 (7%)	1	4
13	Q	139/141 (99%)	122 (88%)	12 (9%)	5 (4%)	4	17
14	R	116/118 (98%)	92 (79%)	21 (18%)	3 (3%)	6	24
15	S	108/112 (96%)	77 (71%)	20 (18%)	11 (10%)	1	1
16	T	129/146 (88%)	113 (88%)	15 (12%)	1 (1%)	22	57
17	U	114/118 (97%)	92 (81%)	16 (14%)	6 (5%)	2	7
18	V	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	1	2
19	W	110/113 (97%)	86 (78%)	14 (13%)	10 (9%)	1	2
20	X	93/96 (97%)	73 (78%)	12 (13%)	8 (9%)	1	2
21	Y	105/110 (96%)	82 (78%)	12 (11%)	11 (10%)	0	1
22	Z	183/206 (89%)	145 (79%)	24 (13%)	14 (8%)	1	3
23	0	72/85 (85%)	65 (90%)	6 (8%)	1 (1%)	13	41
24	1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	4
25	2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	12	39
26	3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	4	17
27	4	67/71 (94%)	42 (63%)	14 (21%)	11 (16%)	0	0
28	5	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	1	2
29	6	51/54 (94%)	43 (84%)	6 (12%)	2 (4%)	3	14
30	7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	8	30
31	8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
32	9	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	5	21
35	b	229/256 (90%)	167 (73%)	41 (18%)	21 (9%)	1	2
36	c	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	3	14
37	d	206/209 (99%)	163 (79%)	33 (16%)	10 (5%)	2	9
38	e	146/162 (90%)	108 (74%)	30 (20%)	8 (6%)	2	7
39	f	98/101 (97%)	70 (71%)	20 (20%)	8 (8%)	1	2
40	g	153/156 (98%)	123 (80%)	26 (17%)	4 (3%)	6	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	h	135/138 (98%)	115 (85%)	18 (13%)	2 (2%)	12	39
42	i	125/128 (98%)	98 (78%)	17 (14%)	10 (8%)	1	2
43	j	94/105 (90%)	73 (78%)	12 (13%)	9 (10%)	1	1
44	k	112/129 (87%)	88 (79%)	20 (18%)	4 (4%)	4	17
45	l	120/132 (91%)	106 (88%)	9 (8%)	5 (4%)	3	12
46	m	117/126 (93%)	91 (78%)	16 (14%)	10 (8%)	1	2
47	n	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	8
48	o	86/89 (97%)	69 (80%)	15 (17%)	2 (2%)	7	27
49	p	80/88 (91%)	61 (76%)	17 (21%)	2 (2%)	6	25
50	q	97/105 (92%)	78 (80%)	13 (13%)	6 (6%)	2	5
51	r	66/88 (75%)	57 (86%)	6 (9%)	3 (4%)	3	11
52	s	81/93 (87%)	64 (79%)	9 (11%)	8 (10%)	1	1
53	t	94/106 (89%)	74 (79%)	10 (11%)	10 (11%)	0	1
54	u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
57	y	640/679 (94%)	534 (83%)	67 (10%)	39 (6%)	2	5
All	All	6466/6910 (94%)	5145 (80%)	924 (14%)	397 (6%)	2	5

All (397) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	14	ARG
3	D	224	ALA
4	E	195	LEU
5	F	89	VAL
5	F	130	ALA
5	F	136	THR
5	F	168	ARG
5	F	169	ASN
6	G	28	VAL
6	G	47	LYS
6	G	115	ARG
6	G	150	ASP
7	H	80	SER
8	J	7	VAL
8	J	53	VAL
8	J	56	ASN
8	J	74	LEU

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Mol	Chain	Res	Type
8	J	77	PRO
8	J	80	VAL
8	J	93	LEU
8	J	99	SER
8	J	100	ASN
8	J	107	VAL
8	J	128	LEU
9	K	7	VAL
9	K	115	LEU
10	N	23	LEU
10	N	37	LYS
10	N	69	GLN
11	O	72	PRO
12	P	45	LEU
13	Q	59	ARG
13	Q	134	ARG
13	Q	135	ASP
16	T	55	ASN
17	U	86	ALA
19	W	25	ARG
19	W	36	LEU
19	W	57	ASN
20	X	18	TYR
20	X	19	ALA
20	X	77	LYS
21	Y	5	MET
21	Y	6	HIS
22	Z	161	VAL
22	Z	177	PRO
22	Z	179	ASP
22	Z	182	LYS
22	Z	184	ALA
24	1	76	ARG
24	1	77	ALA
26	3	13	ILE
27	4	51	ASP
30	7	46	VAL
35	b	9	GLU
35	b	12	GLU
35	b	17	PHE
35	b	23	ARG
35	b	77	ALA

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Mol	Chain	Res	Type
35	b	165	VAL
37	d	150	GLU
37	d	179	GLU
37	d	200	GLU
38	e	72	GLN
39	f	36	ARG
41	h	51	VAL
42	i	95	LYS
42	i	105	ASP
42	i	118	LYS
43	j	34	VAL
43	j	87	THR
44	k	122	LYS
46	m	7	VAL
46	m	8	GLU
47	n	3	ARG
47	n	41	ARG
48	o	19	PRO
49	p	67	THR
50	q	17	LYS
50	q	34	LYS
50	q	49	GLU
50	q	53	LEU
52	s	27	GLU
53	t	9	ASN
53	t	10	LEU
53	t	11	SER
53	t	46	GLU
53	t	47	GLY
53	t	100	ILE
57	y	-67	LYS
57	y	-59	GLU
57	y	9	ILE
57	y	63	ALA
57	y	89	PHE
57	y	138	ILE
57	y	153	GLU
57	y	213	PRO
57	y	244	VAL
57	y	280	ILE
57	y	281	THR
57	y	373	ALA

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Mol	Chain	Res	Type
57	y	402	ILE
57	y	437	ASN
57	y	438	MET
57	y	487	GLY
57	y	555	ARG
57	y	600	VAL
3	D	3	VAL
3	D	90	ALA
3	D	110	GLY
3	D	127	VAL
3	D	241	PRO
4	E	2	LYS
4	E	151	TYR
5	F	119	ARG
5	F	160	ASN
6	G	116	ASP
7	H	76	VAL
7	H	77	LYS
7	H	92	ILE
7	H	126	PRO
8	J	21	GLN
8	J	73	GLY
8	J	101	PRO
8	J	104	ILE
8	J	120	LYS
9	K	33	ASN
10	N	19	GLU
11	O	5	GLN
12	P	23	PRO
12	P	42	SER
12	P	132	LYS
13	Q	136	ALA
15	S	13	ARG
15	S	14	VAL
15	S	57	LYS
15	S	88	ASP
15	S	102	ALA
15	S	103	GLU
17	U	79	PHE
18	V	24	LYS
18	V	54	GLY
18	V	55	ALA

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Mol	Chain	Res	Type
19	W	67	ASP
20	X	66	LEU
20	X	68	ARG
20	X	93	GLU
21	Y	70	SER
21	Y	105	ALA
22	Z	154	ASP
22	Z	183	LEU
24	1	10	LYS
27	4	18	CYS
27	4	45	GLY
27	4	60	GLN
27	4	62	ARG
27	4	68	ARG
28	5	21	SER
28	5	35	GLU
29	6	33	LYS
35	b	8	LYS
35	b	24	TRP
35	b	131	PRO
35	b	204	ASN
35	b	227	GLY
35	b	232	PRO
36	c	22	TRP
36	c	130	VAL
37	d	5	ILE
37	d	10	ARG
37	d	151	LYS
38	e	68	GLU
38	e	85	GLY
38	e	148	VAL
38	e	149	GLU
39	f	70	ASP
40	g	7	ALA
41	h	54	ASP
42	i	42	ARG
42	i	54	ASP
42	i	88	TYR
42	i	126	SER
42	i	127	LYS
43	j	27	ALA
43	j	36	GLY

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Mol	Chain	Res	Type
43	j	77	PRO
43	j	82	ILE
44	k	103	LEU
45	l	14	GLY
46	m	68	GLY
46	m	85	GLY
49	p	46	PRO
50	q	3	LYS
50	q	54	GLY
51	r	36	ASN
52	s	14	HIS
52	s	30	LEU
52	s	71	LEU
53	t	65	LYS
53	t	99	LEU
57	y	13	SER
57	y	167	SER
57	y	215	LEU
57	y	286	PRO
57	y	301	VAL
57	y	446	LYS
57	y	486	PRO
3	D	219	PRO
4	E	52	LEU
4	E	162	ALA
5	F	165	ARG
5	F	206	ILE
6	G	43	LEU
6	G	46	ALA
6	G	55	LYS
7	H	34	GLU
7	H	65	HIS
7	H	174	GLY
8	J	23	SER
8	J	30	GLN
8	J	61	LEU
8	J	69	PRO
8	J	91	LYS
9	K	11	GLN
9	K	73	PRO
9	K	87	GLY
10	N	22	THR

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Mol	Chain	Res	Type
13	Q	60	ARG
14	R	45	ARG
14	R	93	GLY
15	S	59	LYS
15	S	79	ALA
17	U	54	LYS
17	U	98	LEU
18	V	45	THR
18	V	97	LYS
19	W	27	LYS
19	W	56	ALA
19	W	66	GLU
22	Z	93	ASP
22	Z	155	LEU
22	Z	158	PRO
27	4	55	ARG
29	6	34	LEU
35	b	20	GLU
35	b	36	ARG
35	b	76	GLN
36	c	79	ARG
37	d	26	CYS
37	d	172	PRO
37	d	191	ARG
39	f	5	GLU
39	f	62	TRP
39	f	64	GLN
39	f	71	ARG
42	i	70	LYS
42	i	99	LEU
45	l	121	GLY
45	l	125	PRO
46	m	3	ARG
46	m	49	THR
47	n	32	SER
51	r	32	ARG
57	y	86	HIS
57	y	90	THR
57	y	267	ALA
4	E	72	VAL
5	F	67	GLN
5	F	194	MET

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Mol	Chain	Res	Type
8	J	84	GLU
9	K	16	LYS
11	O	29	ASN
12	P	97	PRO
12	P	122	PRO
15	S	84	GLN
15	S	94	TYR
17	U	87	GLY
18	V	43	GLU
20	X	2	LYS
21	Y	2	ARG
21	Y	54	LYS
22	Z	160	GLY
26	3	22	ALA
27	4	43	TYR
27	4	46	GLN
28	5	24	ALA
28	5	37	LYS
35	b	30	ARG
35	b	35	GLU
35	b	122	PHE
35	b	153	ARG
36	c	99	VAL
36	c	100	ALA
38	e	9	LYS
38	e	73	ASN
39	f	51	PRO
40	g	80	VAL
43	j	78	ASN
45	l	19	ARG
46	m	40	ASN
52	s	29	ARG
53	t	66	ALA
57	y	-17	ARG
57	y	417	PRO
57	y	560	ALA
3	D	223	GLY
4	E	57	LYS
4	E	73	GLU
4	E	128	SER
5	F	22	ALA
6	G	109	VAL

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Mol	Chain	Res	Type
6	G	177	GLY
8	J	85	ASP
8	J	90	ALA
8	J	124	ALA
10	N	2	LYS
10	N	40	PRO
10	N	65	LYS
12	P	10	PRO
12	P	78	PRO
14	R	28	LEU
15	S	15	ARG
18	V	100	ARG
19	W	28	SER
19	W	51	LEU
19	W	59	VAL
21	Y	58	GLY
21	Y	69	ALA
22	Z	157	LEU
23	0	48	GLY
24	1	9	GLY
24	1	83	GLU
25	2	67	LYS
27	4	47	GLN
28	5	59	GLU
32	9	36	GLN
36	c	3	ASN
36	c	66	VAL
37	d	175	SER
39	f	96	PRO
40	g	50	ILE
43	j	83	GLU
44	k	100	ALA
46	m	67	GLU
46	m	101	GLN
48	o	79	ARG
52	s	12	ASP
57	y	-36	ARG
57	y	137	LYS
57	y	303	ALA
57	y	500	VAL
57	y	594	GLN
3	D	144	ALA

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Mol	Chain	Res	Type
4	E	178	GLU
8	J	86	PRO
9	K	24	GLY
11	O	35	VAL
24	l	51	VAL
27	4	41	PRO
38	e	39	GLY
43	j	37	PRO
51	r	60	ALA
52	s	76	PRO
57	y	448	VAL
6	G	149	VAL
9	K	23	VAL
12	P	47	ASP
21	Y	15	VAL
21	Y	27	VAL
36	c	108	ASN
57	y	-37	PRO
3	D	106	ILE
3	D	137	PRO
3	D	178	PRO
7	H	17	VAL
17	U	8	VAL
18	V	9	GLY
22	Z	27	VAL
44	k	105	VAL
46	m	38	GLY
20	X	94	GLY
21	Y	72	VAL
53	t	102	GLY
57	y	-48	VAL
7	H	4	ILE
8	J	68	LEU
8	J	129	PRO
9	K	21	PRO
18	V	79	VAL
35	b	159	PRO
45	l	24	VAL
52	s	42	PRO
3	D	74	GLY
22	Z	68	PRO
40	g	130	GLY

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Mol	Chain	Res	Type
12	P	72	PRO
35	b	125	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	215/218 (99%)	163 (76%)	52 (24%)	1	2
4	E	164/166 (99%)	134 (82%)	30 (18%)	2	6
5	F	160/162 (99%)	133 (83%)	27 (17%)	2	7
6	G	143/156 (92%)	103 (72%)	40 (28%)	0	1
7	H	144/148 (97%)	115 (80%)	29 (20%)	1	4
9	K	104/111 (94%)	84 (81%)	20 (19%)	1	5
10	N	118/119 (99%)	93 (79%)	25 (21%)	1	4
11	O	100/100 (100%)	89 (89%)	11 (11%)	7	22
12	P	115/116 (99%)	93 (81%)	22 (19%)	2	5
13	Q	111/111 (100%)	93 (84%)	18 (16%)	3	8
14	R	101/101 (100%)	83 (82%)	18 (18%)	2	6
15	S	87/88 (99%)	74 (85%)	13 (15%)	3	10
16	T	115/127 (91%)	95 (83%)	20 (17%)	2	7
17	U	93/94 (99%)	72 (77%)	21 (23%)	1	3
18	V	80/82 (98%)	63 (79%)	17 (21%)	1	3
19	W	90/92 (98%)	74 (82%)	16 (18%)	2	6
20	X	77/78 (99%)	65 (84%)	12 (16%)	3	9
21	Y	85/91 (93%)	66 (78%)	19 (22%)	1	3
22	Z	156/179 (87%)	127 (81%)	29 (19%)	2	5
23	0	59/67 (88%)	50 (85%)	9 (15%)	3	10
24	1	80/83 (96%)	62 (78%)	18 (22%)	1	3
25	2	65/67 (97%)	50 (77%)	15 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	3	51/52 (98%)	42 (82%)	9 (18%)	2	6
27	4	60/63 (95%)	46 (77%)	14 (23%)	1	2
28	5	51/52 (98%)	39 (76%)	12 (24%)	1	2
29	6	51/52 (98%)	38 (74%)	13 (26%)	0	2
30	7	42/42 (100%)	33 (79%)	9 (21%)	1	3
31	8	53/55 (96%)	44 (83%)	9 (17%)	2	7
32	9	34/34 (100%)	30 (88%)	4 (12%)	6	18
35	b	193/220 (88%)	144 (75%)	49 (25%)	0	2
36	c	142/188 (76%)	121 (85%)	21 (15%)	3	11
37	d	169/181 (93%)	129 (76%)	40 (24%)	1	2
38	e	113/123 (92%)	83 (74%)	30 (26%)	0	2
39	f	83/90 (92%)	62 (75%)	21 (25%)	0	2
40	g	118/127 (93%)	93 (79%)	25 (21%)	1	4
41	h	114/119 (96%)	91 (80%)	23 (20%)	1	4
42	i	90/99 (91%)	76 (84%)	14 (16%)	3	9
43	j	65/92 (71%)	49 (75%)	16 (25%)	1	2
44	k	82/99 (83%)	71 (87%)	11 (13%)	4	13
45	l	97/109 (89%)	82 (84%)	15 (16%)	3	9
46	m	89/101 (88%)	73 (82%)	16 (18%)	2	6
47	n	49/50 (98%)	36 (74%)	13 (26%)	0	2
48	o	78/80 (98%)	68 (87%)	10 (13%)	5	15
49	p	69/74 (93%)	56 (81%)	13 (19%)	2	5
50	q	94/97 (97%)	78 (83%)	16 (17%)	2	7
51	r	59/77 (77%)	46 (78%)	13 (22%)	1	3
52	s	68/80 (85%)	50 (74%)	18 (26%)	0	2
53	t	69/82 (84%)	58 (84%)	11 (16%)	3	8
54	u	18/22 (82%)	15 (83%)	3 (17%)	2	7
57	y	289/560 (52%)	193 (67%)	96 (33%)	0	0
All	All	4952/5576 (89%)	3927 (79%)	1025 (21%)	1	4

All (1025) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	3	VAL
3	D	5	LYS
3	D	13	ARG
3	D	20	ASP
3	D	22	SER
3	D	25	THR
3	D	27	THR
3	D	32	SER
3	D	34	VAL
3	D	37	LEU
3	D	38	LYS
3	D	39	LYS
3	D	50	THR
3	D	61	LEU
3	D	85	ASP
3	D	87	ASN
3	D	94	LEU
3	D	98	VAL
3	D	99	ASP
3	D	102	LYS
3	D	103	ARG
3	D	105	ILE
3	D	106	ILE
3	D	109	ASP
3	D	111	LEU
3	D	117	VAL
3	D	118	VAL
3	D	122	ASP
3	D	138	VAL
3	D	148	GLU
3	D	150	LYS
3	D	157	ARG
3	D	161	THR
3	D	164	GLN
3	D	165	ILE
3	D	169	GLU
3	D	171	ASP
3	D	173	VAL
3	D	183	ARG
3	D	200	ASP
3	D	205	VAL
3	D	212	SER
3	D	215	LEU

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Mol	Chain	Res	Type
3	D	217	ARG
3	D	221	VAL
3	D	222	ARG
3	D	229	VAL
3	D	239	ARG
3	D	257	LEU
3	D	260	ARG
3	D	267	SER
3	D	274	ARG
4	E	2	LYS
4	E	4	ILE
4	E	9	VAL
4	E	13	ARG
4	E	23	VAL
4	E	33	VAL
4	E	48	GLN
4	E	72	VAL
4	E	73	GLU
4	E	77	ILE
4	E	82	ARG
4	E	85	ASN
4	E	87	GLU
4	E	93	VAL
4	E	113	PHE
4	E	118	LYS
4	E	119	ARG
4	E	144	ARG
4	E	146	THR
4	E	149	ARG
4	E	152	LYS
4	E	165	VAL
4	E	173	VAL
4	E	174	ASP
4	E	179	GLU
4	E	181	LEU
4	E	182	LEU
4	E	184	VAL
4	E	195	LEU
4	E	196	VAL
5	F	18	ARG
5	F	20	LEU
5	F	24	LEU

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Mol	Chain	Res	Type
5	F	33	LEU
5	F	44	ARG
5	F	51	THR
5	F	53	THR
5	F	62	ARG
5	F	64	ILE
5	F	84	VAL
5	F	104	LYS
5	F	106	ARG
5	F	112	MET
5	F	148	LEU
5	F	152	GLU
5	F	162	LEU
5	F	164	ARG
5	F	169	ASN
5	F	170	LEU
5	F	175	THR
5	F	183	VAL
5	F	192	LEU
5	F	195	ASP
5	F	196	LEU
5	F	197	ASP
5	F	200	GLU
5	F	206	ILE
6	G	4	ASP
6	G	5	VAL
6	G	7	LEU
6	G	9	ARG
6	G	19	LEU
6	G	28	VAL
6	G	30	GLU
6	G	31	VAL
6	G	33	ARG
6	G	34	LEU
6	G	43	LEU
6	G	51	ARG
6	G	58	GLN
6	G	62	LEU
6	G	80	PHE
6	G	81	LYS
6	G	82	LEU
6	G	90	LEU

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Mol	Chain	Res	Type
6	G	91	ARG
6	G	99	MET
6	G	101	ILE
6	G	109	VAL
6	G	120	LEU
6	G	123	ASN
6	G	124	SER
6	G	135	LEU
6	G	136	ARG
6	G	138	GLN
6	G	139	LEU
6	G	143	GLU
6	G	146	TYR
6	G	148	MET
6	G	150	ASP
6	G	153	ARG
6	G	161	THR
6	G	164	GLU
6	G	165	THR
6	G	166	ASP
6	G	170	ARG
6	G	173	LEU
7	H	3	ARG
7	H	6	ARG
7	H	13	LYS
7	H	15	VAL
7	H	16	SER
7	H	17	VAL
7	H	23	ARG
7	H	27	LYS
7	H	32	GLU
7	H	40	GLU
7	H	41	MET
7	H	43	VAL
7	H	45	VAL
7	H	47	GLU
7	H	54	ARG
7	H	57	ASP
7	H	62	LYS
7	H	69	ARG
7	H	79	VAL
7	H	88	LEU

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Mol	Chain	Res	Type
7	H	95	ARG
7	H	98	LEU
7	H	106	THR
7	H	107	VAL
7	H	127	GLU
7	H	149	ARG
7	H	163	TYR
7	H	164	TYR
7	H	175	LYS
9	K	2	LYS
9	K	4	VAL
9	K	11	GLN
9	K	30	HIS
9	K	34	ILE
9	K	38	VAL
9	K	57	ILE
9	K	59	ILE
9	K	62	ASP
9	K	63	ARG
9	K	65	PHE
9	K	75	SER
9	K	86	LYS
9	K	95	LYS
9	K	115	LEU
9	K	116	ASN
9	K	117	THR
9	K	119	ASP
9	K	136	VAL
9	K	138	VAL
10	N	1	MET
10	N	2	LYS
10	N	17	ASP
10	N	34	LEU
10	N	38	HIS
10	N	39	ARG
10	N	48	MET
10	N	51	PHE
10	N	68	GLU
10	N	70	LYS
10	N	74	ARG
10	N	87	LEU
10	N	90	MET

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Mol	Chain	Res	Type
10	N	99	LEU
10	N	106	MET
10	N	109	LYS
10	N	115	ARG
10	N	120	LEU
10	N	122	VAL
10	N	127	ASP
10	N	131	GLN
10	N	133	GLN
10	N	137	LYS
10	N	138	LEU
10	N	140	VAL
11	O	3	GLN
11	O	8	LEU
11	O	10	VAL
11	O	14	THR
11	O	23	ARG
11	O	24	VAL
11	O	31	LYS
11	O	63	VAL
11	O	66	LYS
11	O	69	ILE
11	O	91	LEU
12	P	2	LYS
12	P	16	ARG
12	P	19	VAL
12	P	27	HIS
12	P	30	THR
12	P	40	SER
12	P	50	ARG
12	P	51	PHE
12	P	57	THR
12	P	58	THR
12	P	59	LEU
12	P	65	ARG
12	P	70	GLN
12	P	71	VAL
12	P	74	GLU
12	P	96	THR
12	P	98	GLU
12	P	105	LEU
12	P	106	LEU

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Mol	Chain	Res	Type
12	P	115	LEU
12	P	135	LEU
12	P	148	LEU
13	Q	7	MET
13	Q	21	THR
13	Q	31	ASP
13	Q	42	ILE
13	Q	45	GLN
13	Q	52	VAL
13	Q	56	ARG
13	Q	66	ILE
13	Q	72	LYS
13	Q	75	THR
13	Q	76	LYS
13	Q	82	ARG
13	Q	89	ASN
13	Q	112	GLU
13	Q	129	THR
13	Q	131	ILE
13	Q	135	ASP
13	Q	138	ASP
14	R	15	SER
14	R	18	LEU
14	R	28	LEU
14	R	30	THR
14	R	36	THR
14	R	38	VAL
14	R	44	LEU
14	R	60	LEU
14	R	65	LEU
14	R	67	LEU
14	R	71	GLN
14	R	77	ARG
14	R	79	LEU
14	R	91	GLN
14	R	100	LEU
14	R	113	LEU
14	R	114	VAL
14	R	118	GLU
15	S	8	GLU
15	S	14	VAL
15	S	15	ARG

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Mol	Chain	Res	Type
15	S	20	ARG
15	S	28	VAL
15	S	36	TYR
15	S	41	ASP
15	S	43	GLU
15	S	48	LEU
15	S	49	VAL
15	S	52	SER
15	S	53	SER
15	S	85	VAL
16	T	9	LEU
16	T	17	THR
16	T	18	ASP
16	T	23	ARG
16	T	31	SER
16	T	34	VAL
16	T	40	THR
16	T	44	ASP
16	T	49	VAL
16	T	53	ARG
16	T	54	ARG
16	T	57	PHE
16	T	59	THR
16	T	75	ILE
16	T	78	LEU
16	T	93	ARG
16	T	96	ARG
16	T	118	ARG
16	T	123	GLN
16	T	124	ASP
17	U	8	VAL
17	U	11	ARG
17	U	18	LEU
17	U	19	LYS
17	U	20	LEU
17	U	33	ARG
17	U	34	LYS
17	U	36	ARG
17	U	55	ARG
17	U	56	ASP
17	U	63	VAL
17	U	64	ARG

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Mol	Chain	Res	Type
17	U	71	GLN
17	U	74	LEU
17	U	78	THR
17	U	85	LYS
17	U	92	ARG
17	U	95	LEU
17	U	101	ARG
17	U	104	GLN
17	U	112	ARG
18	V	6	LYS
18	V	7	THR
18	V	13	ARG
18	V	14	VAL
18	V	18	LEU
18	V	25	LEU
18	V	33	VAL
18	V	38	LEU
18	V	46	VAL
18	V	51	VAL
18	V	53	GLU
18	V	70	ILE
18	V	71	LEU
18	V	72	VAL
18	V	73	SER
18	V	82	ARG
18	V	95	LEU
19	W	8	ARG
19	W	10	VAL
19	W	11	ARG
19	W	19	LEU
19	W	20	VAL
19	W	33	ARG
19	W	39	THR
19	W	51	LEU
19	W	52	GLU
19	W	57	ASN
19	W	65	LEU
19	W	86	LEU
19	W	92	ARG
19	W	100	THR
19	W	107	LEU
19	W	111	HIS

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Mol	Chain	Res	Type
20	X	2	LYS
20	X	9	LEU
20	X	23	GLU
20	X	27	THR
20	X	49	VAL
20	X	51	VAL
20	X	56	THR
20	X	57	LEU
20	X	68	ARG
20	X	75	ASP
20	X	80	ILE
20	X	92	LEU
21	Y	6	HIS
21	Y	9	LYS
21	Y	21	LYS
21	Y	23	ARG
21	Y	28	LYS
21	Y	30	VAL
21	Y	31	LEU
21	Y	38	ILE
21	Y	43	ASN
21	Y	55	TYR
21	Y	61	ILE
21	Y	62	GLU
21	Y	79	CYS
21	Y	84	ARG
21	Y	85	VAL
21	Y	90	LEU
21	Y	91	GLU
21	Y	98	VAL
21	Y	107	ASP
22	Z	24	LEU
22	Z	27	VAL
22	Z	33	LEU
22	Z	41	LEU
22	Z	58	VAL
22	Z	61	LEU
22	Z	70	LEU
22	Z	72	ARG
22	Z	76	LEU
22	Z	80	ARG
22	Z	81	ARG

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Mol	Chain	Res	Type
22	Z	85	HIS
22	Z	86	VAL
22	Z	96	VAL
22	Z	107	THR
22	Z	111	VAL
22	Z	119	GLU
22	Z	122	ARG
22	Z	132	ASN
22	Z	136	PHE
22	Z	139	VAL
22	Z	140	ASP
22	Z	141	VAL
22	Z	149	SER
22	Z	156	LYS
22	Z	161	VAL
22	Z	163	LEU
22	Z	170	THR
22	Z	179	ASP
23	0	11	ARG
23	0	19	LYS
23	0	20	ARG
23	0	25	ARG
23	0	32	ARG
23	0	41	ARG
23	0	44	ARG
23	0	46	LYS
23	0	66	VAL
24	1	2	SER
24	1	4	VAL
24	1	10	LYS
24	1	14	VAL
24	1	19	GLN
24	1	20	ARG
24	1	21	ARG
24	1	40	ARG
24	1	57	GLU
24	1	59	THR
24	1	62	VAL
24	1	66	HIS
24	1	75	GLU
24	1	80	LEU
24	1	85	LEU

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Mol	Chain	Res	Type
24	1	89	GLU
24	1	94	LEU
24	1	98	LEU
25	2	3	LEU
25	2	4	SER
25	2	16	LEU
25	2	25	VAL
25	2	30	ARG
25	2	32	LEU
25	2	34	GLU
25	2	45	SER
25	2	47	ASN
25	2	49	LYS
25	2	51	ARG
25	2	52	ASP
25	2	62	THR
25	2	65	ASN
25	2	70	GLN
26	3	4	LEU
26	3	9	VAL
26	3	32	GLN
26	3	33	GLN
26	3	37	LEU
26	3	40	THR
26	3	54	VAL
26	3	56	VAL
26	3	57	GLU
27	4	8	LYS
27	4	20	ASN
27	4	22	ILE
27	4	25	TYR
27	4	26	SER
27	4	43	TYR
27	4	49	PHE
27	4	50	VAL
27	4	58	ARG
27	4	59	PHE
27	4	63	TYR
27	4	65	ASP
27	4	68	ARG
27	4	69	LYS
28	5	6	VAL

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Mol	Chain	Res	Type
28	5	8	LYS
28	5	11	THR
28	5	25	LEU
28	5	26	THR
28	5	29	THR
28	5	35	GLU
28	5	37	LYS
28	5	40	LYS
28	5	48	GLU
28	5	49	CYS
28	5	57	VAL
29	6	3	SER
29	6	4	GLU
29	6	6	ARG
29	6	13	CYS
29	6	19	ARG
29	6	23	THR
29	6	27	LYS
29	6	28	ARG
29	6	34	LEU
29	6	36	LEU
29	6	38	LYS
29	6	46	HIS
29	6	52	VAL
30	7	1	MET
30	7	10	ARG
30	7	14	LYS
30	7	23	ARG
30	7	24	THR
30	7	41	ARG
30	7	42	LEU
30	7	46	VAL
30	7	49	ARG
31	8	14	VAL
31	8	23	VAL
31	8	31	HIS
31	8	32	LEU
31	8	34	TRP
31	8	41	ILE
31	8	42	ARG
31	8	52	LYS
31	8	56	GLU

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Mol	Chain	Res	Type
32	9	4	ARG
32	9	9	ARG
32	9	22	ARG
32	9	26	ILE
35	b	8	LYS
35	b	9	GLU
35	b	10	LEU
35	b	12	GLU
35	b	15	VAL
35	b	16	HIS
35	b	17	PHE
35	b	20	GLU
35	b	21	ARG
35	b	24	TRP
35	b	35	GLU
35	b	51	LEU
35	b	52	GLU
35	b	53	ARG
35	b	61	LEU
35	b	73	THR
35	b	79	ASP
35	b	80	ILE
35	b	87	ARG
35	b	94	ASN
35	b	96	ARG
35	b	97	TRP
35	b	107	THR
35	b	109	SER
35	b	119	GLU
35	b	122	PHE
35	b	135	GLN
35	b	136	VAL
35	b	154	LEU
35	b	155	LEU
35	b	156	LYS
35	b	168	THR
35	b	169	LYS
35	b	172	ILE
35	b	175	ARG
35	b	185	ILE
35	b	187	LEU
35	b	189	ASP

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Mol	Chain	Res	Type
35	b	190	THR
35	b	195	ASP
35	b	196	LEU
35	b	200	ILE
35	b	206	ASP
35	b	208	ILE
35	b	213	LEU
35	b	217	ARG
35	b	221	LEU
35	b	223	ILE
35	b	229	VAL
36	c	12	LEU
36	c	15	THR
36	c	37	GLN
36	c	45	LYS
36	c	49	SER
36	c	52	LEU
36	c	91	LEU
36	c	97	LYS
36	c	104	GLN
36	c	132	ARG
36	c	134	ILE
36	c	138	VAL
36	c	150	LYS
36	c	152	ILE
36	c	165	THR
36	c	179	ARG
36	c	188	LEU
36	c	190	ARG
36	c	191	THR
36	c	192	THR
36	c	195	VAL
37	d	3	ARG
37	d	5	ILE
37	d	8	VAL
37	d	13	ARG
37	d	19	LEU
37	d	21	LEU
37	d	22	LYS
37	d	25	ARG
37	d	31	CYS
37	d	33	MET

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Mol	Chain	Res	Type
37	d	52	SER
37	d	53	ASP
37	d	57	ARG
37	d	58	LEU
37	d	59	ARG
37	d	66	ARG
37	d	70	ILE
37	d	76	ARG
37	d	85	LYS
37	d	86	LYS
37	d	91	SER
37	d	97	LEU
37	d	107	ARG
37	d	108	LEU
37	d	113	SER
37	d	114	ARG
37	d	135	LEU
37	d	139	ARG
37	d	141	ARG
37	d	150	GLU
37	d	158	ILE
37	d	162	LEU
37	d	168	ARG
37	d	170	VAL
37	d	178	VAL
37	d	186	LEU
37	d	188	LEU
37	d	190	ASP
37	d	196	LEU
37	d	201	GLN
38	e	8	GLU
38	e	14	ARG
38	e	19	MET
38	e	20	GLN
38	e	31	LEU
38	e	38	GLN
38	e	41	VAL
38	e	47	LYS
38	e	53	LEU
38	e	67	VAL
38	e	71	LEU
38	e	73	ASN

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Mol	Chain	Res	Type
38	e	75	THR
38	e	79	GLU
38	e	80	ILE
38	e	81	GLU
38	e	82	VAL
38	e	87	SER
38	e	91	LEU
38	e	92	LYS
38	e	107	ARG
38	e	116	THR
38	e	123	LEU
38	e	126	ARG
38	e	135	THR
38	e	143	ARG
38	e	144	THR
38	e	147	ASP
38	e	151	LEU
38	e	152	ARG
39	f	9	VAL
39	f	10	LEU
39	f	15	ASP
39	f	16	GLN
39	f	25	ILE
39	f	31	GLU
39	f	36	ARG
39	f	43	LEU
39	f	54	LYS
39	f	64	GLN
39	f	65	VAL
39	f	69	GLU
39	f	72	VAL
39	f	73	ASN
39	f	74	ASP
39	f	75	LEU
39	f	79	LEU
39	f	82	ARG
39	f	86	ARG
39	f	98	LEU
39	f	100	ASN
40	g	4	ARG
40	g	8	GLU
40	g	12	LEU

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Mol	Chain	Res	Type
40	g	16	LEU
40	g	22	LEU
40	g	24	THR
40	g	41	ARG
40	g	42	ILE
40	g	45	ASP
40	g	56	GLN
40	g	57	GLU
40	g	75	VAL
40	g	90	GLU
40	g	92	SER
40	g	94	ARG
40	g	97	GLN
40	g	101	LEU
40	g	104	LEU
40	g	113	GLU
40	g	114	ARG
40	g	115	ARG
40	g	126	ASP
40	g	131	LYS
40	g	138	LYS
40	g	144	MET
41	h	2	LEU
41	h	3	THR
41	h	6	ILE
41	h	10	LEU
41	h	19	VAL
41	h	54	ASP
41	h	56	LYS
41	h	60	ARG
41	h	63	LEU
41	h	68	ARG
41	h	75	ARG
41	h	78	GLN
41	h	84	ARG
41	h	87	SER
41	h	88	LYS
41	h	91	ARG
41	h	100	ILE
41	h	104	ARG
41	h	111	ILE
41	h	112	LEU

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Mol	Chain	Res	Type
41	h	120	THR
41	h	122	ARG
41	h	137	VAL
42	i	23	ASN
42	i	25	LYS
42	i	27	THR
42	i	41	VAL
42	i	54	ASP
42	i	56	LEU
42	i	59	PHE
42	i	66	ARG
42	i	83	ARG
42	i	89	ASN
42	i	97	LYS
42	i	99	LEU
42	i	120	ARG
42	i	128	ARG
43	j	8	LEU
43	j	13	HIS
43	j	16	LEU
43	j	19	SER
43	j	21	GLN
43	j	35	SER
43	j	44	VAL
43	j	46	ARG
43	j	67	THR
43	j	70	ARG
43	j	71	LEU
43	j	89	ASP
43	j	92	THR
43	j	96	ILE
43	j	98	ILE
43	j	100	THR
44	k	16	SER
44	k	51	LYS
44	k	62	GLN
44	k	82	VAL
44	k	109	VAL
44	k	110	ASP
44	k	114	VAL
44	k	116	HIS
44	k	119	CYS

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Mol	Chain	Res	Type
44	k	125	PHE
44	k	126	ARG
45	l	27	LEU
45	l	33	ARG
45	l	41	ARG
45	l	44	THR
45	l	52	LEU
45	l	54	LYS
45	l	55	VAL
45	l	57	LYS
45	l	66	VAL
45	l	67	THR
45	l	84	LEU
45	l	86	ARG
45	l	89	ARG
45	l	97	ARG
45	l	100	ILE
46	m	3	ARG
46	m	11	ARG
46	m	15	VAL
46	m	19	LEU
46	m	48	LEU
46	m	49	THR
46	m	54	VAL
46	m	56	LEU
46	m	59	TYR
46	m	73	GLU
46	m	78	ILE
46	m	80	ARG
46	m	86	CYS
46	m	114	ARG
46	m	115	LYS
46	m	120	LYS
47	n	3	ARG
47	n	6	LEU
47	n	7	ILE
47	n	9	LYS
47	n	13	THR
47	n	16	PHE
47	n	18	VAL
47	n	19	ARG
47	n	29	ARG

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Mol	Chain	Res	Type
47	n	31	ARG
47	n	32	SER
47	n	41	ARG
47	n	44	LEU
48	o	17	ARG
48	o	26	GLU
48	o	38	ARG
48	o	39	LEU
48	o	66	LEU
48	o	71	GLN
48	o	77	ARG
48	o	82	ILE
48	o	83	GLU
48	o	87	ILE
49	p	2	VAL
49	p	8	ARG
49	p	19	ILE
49	p	20	VAL
49	p	27	LYS
49	p	28	ARG
49	p	31	LYS
49	p	40	ASP
49	p	45	THR
49	p	50	LYS
49	p	60	LEU
49	p	61	SER
49	p	67	THR
50	q	9	VAL
50	q	15	MET
50	q	16	GLN
50	q	25	ARG
50	q	35	VAL
50	q	36	ILE
50	q	49	GLU
50	q	57	VAL
50	q	59	ILE
50	q	60	ILE
50	q	63	ARG
50	q	68	ARG
50	q	74	LEU
50	q	78	GLU
50	q	86	GLU

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Mol	Chain	Res	Type
50	q	96	GLU
51	r	26	LEU
51	r	31	LEU
51	r	32	ARG
51	r	33	ASP
51	r	35	ARG
51	r	49	LYS
51	r	55	ARG
51	r	58	LEU
51	r	68	LYS
51	r	70	ILE
51	r	75	ILE
51	r	76	LEU
51	r	84	LYS
52	s	4	SER
52	s	6	LYS
52	s	12	ASP
52	s	14	HIS
52	s	22	LEU
52	s	27	GLU
52	s	28	LYS
52	s	31	ILE
52	s	32	LYS
52	s	37	ARG
52	s	38	SER
52	s	39	THR
52	s	41	VAL
52	s	48	THR
52	s	63	THR
52	s	65	ASN
52	s	76	PRO
52	s	78	ARG
53	t	8	ARG
53	t	19	SER
53	t	22	ARG
53	t	50	GLU
53	t	56	MET
53	t	62	LEU
53	t	80	ARG
53	t	83	ARG
53	t	84	LEU
53	t	92	LEU

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Mol	Chain	Res	Type
53	t	93	GLU
54	u	9	ARG
54	u	18	TYR
54	u	24	ARG
57	y	-68	MET
57	y	-67	LYS
57	y	-64	LEU
57	y	-62	GLU
57	y	-57	LEU
57	y	-54	VAL
57	y	-51	VAL
57	y	-50	VAL
57	y	-44	TYR
57	y	-36	ARG
57	y	-32	VAL
57	y	-29	THR
57	y	-28	GLU
57	y	-25	LEU
57	y	-18	ILE
57	y	-11	LEU
57	y	-8	ARG
57	y	0	LYS
57	y	4	GLU
57	y	7	SER
57	y	12	PHE
57	y	28	ARG
57	y	34	HIS
57	y	62	SER
57	y	68	TYR
57	y	75	GLU
57	y	83	THR
57	y	103	VAL
57	y	105	LEU
57	y	108	ASP
57	y	114	GLU
57	y	117	THR
57	y	127	HIS
57	y	129	HIS
57	y	142	ASN
57	y	154	GLU
57	y	167	SER
57	y	170	THR

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Mol	Chain	Res	Type
57	y	183	GLN
57	y	211	VAL
57	y	215	LEU
57	y	219	GLU
57	y	221	ARG
57	y	223	ARG
57	y	228	ILE
57	y	250	LEU
57	y	265	VAL
57	y	292	PRO
57	y	312	ASP
57	y	335	GLU
57	y	338	THR
57	y	340	LEU
57	y	351	LEU
57	y	358	GLN
57	y	359	GLU
57	y	360	ARG
57	y	361	LEU
57	y	363	ARG
57	y	369	LEU
57	y	375	SER
57	y	377	VAL
57	y	392	ASN
57	y	412	LEU
57	y	413	THR
57	y	423	SER
57	y	424	LEU
57	y	429	GLN
57	y	434	ARG
57	y	436	VAL
57	y	440	TYR
57	y	461	TYR
57	y	462	ASP
57	y	469	SER
57	y	479	TYR
57	y	484	TYR
57	y	493	ASN
57	y	505	THR
57	y	506	PHE
57	y	507	ILE
57	y	509	HIS

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Mol	Chain	Res	Type
57	y	512	LYS
57	y	531	GLN
57	y	532	LEU
57	y	533	PHE
57	y	534	GLU
57	y	544	LYS
57	y	548	ARG
57	y	551	VAL
57	y	554	LEU
57	y	556	LYS
57	y	557	ASP
57	y	568	THR
57	y	570	LYS
57	y	584	LEU
57	y	587	ILE
57	y	602	SER

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

Mol	Chain	Res	Type
3	D	164	GLN
3	D	166	GLN
3	D	220	HIS
3	D	253	GLN
4	E	85	ASN
5	F	69	HIS
5	F	169	ASN
6	G	41	GLN
6	G	58	GLN
6	G	123	ASN
9	K	29	GLN
9	K	42	ASN
9	K	89	HIS
10	N	8	GLN
11	O	29	ASN
12	P	128	HIS
13	Q	13	GLN
13	Q	57	HIS
14	R	50	HIS
14	R	91	GLN
15	S	34	HIS
16	T	58	ASN

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Mol	Chain	Res	Type
17	U	72	HIS
18	V	80	GLN
20	X	31	HIS
20	X	82	GLN
21	Y	6	HIS
22	Z	34	ASN
22	Z	50	GLN
22	Z	65	GLN
22	Z	73	GLN
22	Z	132	ASN
23	0	17	GLN
24	1	56	GLN
25	2	9	GLN
25	2	46	GLN
25	2	47	ASN
25	2	65	ASN
26	3	32	GLN
27	4	20	ASN
29	6	29	ASN
31	8	35	GLN
32	9	36	GLN
35	b	19	HIS
35	b	45	GLN
35	b	94	ASN
36	c	37	GLN
36	c	102	ASN
36	c	104	GLN
36	c	136	GLN
36	c	162	GLN
36	c	176	HIS
36	c	181	ASN
37	d	42	GLN
37	d	123	HIS
37	d	125	HIS
38	e	38	GLN
38	e	73	ASN
38	e	141	GLN
39	f	73	ASN
39	f	94	GLN
39	f	100	ASN
40	g	28	ASN
40	g	68	ASN

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Mol	Chain	Res	Type
40	g	86	GLN
41	h	82	HIS
42	i	89	ASN
42	i	124	GLN
43	j	56	HIS
44	k	38	ASN
45	l	99	HIS
46	m	12	ASN
46	m	92	HIS
48	o	28	GLN
48	o	71	GLN
49	p	76	GLN
50	q	26	GLN
52	s	14	HIS
52	s	47	HIS
52	s	56	GLN
52	s	65	ASN
52	s	83	HIS
53	t	16	HIS
53	t	75	ASN
57	y	127	HIS
57	y	142	ASN
57	y	183	GLN
57	y	426	GLN
57	y	493	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2865/2915 (98%)	639 (22%)	38 (1%)
2	B	119/122 (97%)	18 (15%)	0
33	x	71/76 (93%)	37 (52%)	0
34	a	1493/1521 (98%)	311 (20%)	0
55	w	73/76 (96%)	21 (28%)	0
56	v	6/18 (33%)	1 (16%)	0
All	All	4627/4728 (97%)	1027 (22%)	38 (0%)

All (1027) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A

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Mol	Chain	Res	Type
1	A	15	G
1	A	22	C
1	A	23	G
1	A	28	A
1	A	35	G
1	A	41	C
1	A	45	C
1	A	49	A
1	A	51	G
1	A	54	G
1	A	55	G
1	A	61	G
1	A	64	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	81	G
1	A	84	A
1	A	90	U
1	A	92	A
1	A	95	G
1	A	102	G
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	123	G
1	A	125	G
1	A	131	G
1	A	135	G
1	A	141	A
1	A	148	C
1	A	154(A)	C
1	A	181	A
1	A	182	A
1	A	196	A
1	A	197	A
1	A	200	U
1	A	205	G
1	A	206	U
1	A	212	G
1	A	215	G

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Mol	Chain	Res	Type
1	A	216	A
1	A	221	A
1	A	222	A
1	A	227	A
1	A	228	A
1	A	229	A
1	A	230	U
1	A	233	A
1	A	248	G
1	A	250	G
1	A	252	G
1	A	264	C
1	A	265	A
1	A	266	G
1	A	267	C
1	A	271(F)	C
1	A	271(H)	G
1	A	271(I)	G
1	A	271(K)	U
1	A	271(L)	U
1	A	271(M)	G
1	A	271(N)	U
1	A	271(O)	C
1	A	271(R)	G
1	A	271(Y)	U
1	A	272(A)	U
1	A	272(B)	G
1	A	272(G)	C
1	A	272(H)	C
1	A	274	G
1	A	279	C
1	A	294	A
1	A	296	C
1	A	299	A
1	A	310	A
1	A	311	A
1	A	324	A
1	A	329	G
1	A	330	A
1	A	345	A
1	A	352	G
1	A	353	G

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Mol	Chain	Res	Type
1	A	362	U
1	A	363	G
1	A	363(E)	U
1	A	366	C
1	A	384	U
1	A	385	C
1	A	386	G
1	A	396	G
1	A	404	C
1	A	405	U
1	A	406	G
1	A	407	G
1	A	408	G
1	A	411	G
1	A	420	C
1	A	423	A
1	A	434	U
1	A	435	C
1	A	444	C
1	A	448	U
1	A	451	C
1	A	455	C
1	A	457	A
1	A	470	A
1	A	471	A
1	A	472	A
1	A	481	G
1	A	491	G
1	A	504	U
1	A	505	A
1	A	508	G
1	A	509	C
1	A	530	G
1	A	531	C
1	A	532	A
1	A	536	A
1	A	545	G
1	A	549	G
1	A	556	G
1	A	563	G
1	A	572	A
1	A	573	G

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Mol	Chain	Res	Type
1	A	575	A
1	A	584	C
1	A	594	U
1	A	603	A
1	A	604	G
1	A	607	U
1	A	614(A)	U
1	A	614(B)	G
1	A	615	G
1	A	627	A
1	A	628	G
1	A	631	A
1	A	637	A
1	A	645	C
1	A	646	A
1	A	652(B)	A
1	A	652(E)	G
1	A	652(T)	C
1	A	652(U)	G
1	A	652(V)	C
1	A	654	A
1	A	668	G
1	A	669	G
1	A	670	A
1	A	684	G
1	A	686	G
1	A	694	U
1	A	695	G
1	A	717	G
1	A	730	C
1	A	738	G
1	A	752	A
1	A	753	C
1	A	764	A
1	A	775	G
1	A	776	G
1	A	782	A
1	A	783	A
1	A	784	A
1	A	785	G
1	A	792	G
1	A	794	G

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Mol	Chain	Res	Type
1	A	800	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	829	A
1	A	830	G
1	A	832	G
1	A	842	G
1	A	859	G
1	A	860	U
1	A	866	A
1	A	870	A
1	A	875	G
1	A	881	G
1	A	886	C
1	A	887	A
1	A	888	C
1	A	889	C
1	A	890	A
1	A	895	U
1	A	896	A
1	A	897	C
1	A	906	G
1	A	907	U
1	A	910	A
1	A	911	A
1	A	917	A
1	A	931	G
1	A	932	G
1	A	936	C
1	A	941	A
1	A	945	A
1	A	946	G
1	A	953	A
1	A	957	A
1	A	959	A
1	A	961	C
1	A	974	G
1	A	975	C
1	A	975(A)	G

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Mol	Chain	Res	Type
1	A	976	C
1	A	982	C
1	A	983	A
1	A	996	A
1	A	1005	C
1	A	1008	C
1	A	1012	U
1	A	1013	C
1	A	1015	G
1	A	1017	G
1	A	1022	G
1	A	1025	G
1	A	1027	A
1	A	1033	U
1	A	1034	G
1	A	1036	G
1	A	1038	C
1	A	1041	C
1	A	1042	G
1	A	1045	A
1	A	1046	A
1	A	1047	G
1	A	1052	C
1	A	1053	C
1	A	1054	A
1	A	1055	G
1	A	1058	G
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1067	A
1	A	1070	A
1	A	1073	A
1	A	1076	C
1	A	1079	C
1	A	1083	U
1	A	1084	A
1	A	1085	A
1	A	1088	A
1	A	1089	G
1	A	1095	A

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Mol	Chain	Res	Type
1	A	1109	C
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1115	G
1	A	1119	C
1	A	1124	C
1	A	1127	A
1	A	1128	A
1	A	1129	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1137	G
1	A	1142(A)	A
1	A	1143	A
1	A	1149	G
1	A	1152	C
1	A	1155	A
1	A	1156	A
1	A	1157	G
1	A	1171	G
1	A	1173	G
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1177	A
1	A	1206	G
1	A	1210	A
1	A	1211	U
1	A	1219	G
1	A	1220	A
1	A	1224	C
1	A	1230	C
1	A	1236	G
1	A	1244	G
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1273	U

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Mol	Chain	Res	Type
1	A	1275	A
1	A	1300	U
1	A	1301	A
1	A	1308	A
1	A	1313	U
1	A	1320	C
1	A	1321	A
1	A	1329	U
1	A	1332	G
1	A	1342	A
1	A	1347	G
1	A	1359	A
1	A	1360	A
1	A	1363	C
1	A	1365	A
1	A	1369	G
1	A	1373	A
1	A	1378	A
1	A	1380	G
1	A	1384	A
1	A	1385	G
1	A	1386	C
1	A	1398	C
1	A	1413	G
1	A	1416	G
1	A	1417	C
1	A	1420	U
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1436	G
1	A	1437	C
1	A	1445	A
1	A	1450	G
1	A	1451	C
1	A	1455	G
1	A	1459	G
1	A	1460	A
1	A	1461	G
1	A	1467	C
1	A	1471	A
1	A	1481	U

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Mol	Chain	Res	Type
1	A	1482	G
1	A	1490	A
1	A	1492	G
1	A	1493	C
1	A	1507	A
1	A	1508	A
1	A	1509	C
1	A	1509(A)	A
1	A	1511	C
1	A	1523	U
1	A	1526	G
1	A	1542	A
1	A	1543	C
1	A	1547	C
1	A	1553	A
1	A	1554	A
1	A	1558	A
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1581	G
1	A	1582	C
1	A	1584	C
1	A	1586	A
1	A	1588	C
1	A	1595	G
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1613	G
1	A	1617	C
1	A	1631(A)	A
1	A	1644	C
1	A	1648	C
1	A	1649	G
1	A	1651	G
1	A	1654	A
1	A	1674	G
1	A	1695	G
1	A	1696	G
1	A	1700	A
1	A	1702	G

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Mol	Chain	Res	Type
1	A	1705	G
1	A	1721	G
1	A	1722	A
1	A	1740	G
1	A	1745(A)	C
1	A	1746	G
1	A	1747	G
1	A	1756	G
1	A	1758	G
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1781	C
1	A	1791	A
1	A	1800	C
1	A	1802	A
1	A	1812	A
1	A	1816	G
1	A	1817	G
1	A	1820	U
1	A	1821	A
1	A	1828	G
1	A	1829	A
1	A	1838	C
1	A	1847	A
1	A	1877	A
1	A	1878	G
1	A	1889	A
1	A	1895	C
1	A	1900	A
1	A	1903	G
1	A	1906	G
1	A	1913	A
1	A	1914	C
1	A	1920	C
1	A	1921	G
1	A	1929	G
1	A	1930	G
1	A	1934	C
1	A	1937	A
1	A	1938	A

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Mol	Chain	Res	Type
1	A	1939	U
1	A	1941	C
1	A	1943	U
1	A	1955	U
1	A	1958	C
1	A	1960	A
1	A	1963	U
1	A	1964	G
1	A	1967	C
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1983	C
1	A	1992	G
1	A	1993	U
1	A	1996	C
1	A	1997	G
1	A	2020	A
1	A	2021	C
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2034	U
1	A	2035	G
1	A	2043	C
1	A	2049	G
1	A	2050	C
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C
1	A	2069	G
1	A	2070	G
1	A	2077	A
1	A	2087	G
1	A	2091	U
1	A	2096	U
1	A	2098	U
1	A	2105	C

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Mol	Chain	Res	Type
1	A	2110	G
1	A	2111	C
1	A	2113	U
1	A	2115	G
1	A	2116	G
1	A	2119	A
1	A	2127	G
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2135	A
1	A	2136	C
1	A	2137	C
1	A	2138	C
1	A	2141	G
1	A	2142	C
1	A	2146	C
1	A	2157	G
1	A	2158	A
1	A	2159	G
1	A	2161	C
1	A	2166	G
1	A	2167	U
1	A	2168	G
1	A	2169	A
1	A	2172	U
1	A	2178	C
1	A	2182	G
1	A	2184	G
1	A	2186	G
1	A	2187	G
1	A	2188	C
1	A	2189	U
1	A	2198	A
1	A	2199	A
1	A	2200	C
1	A	2201	C
1	A	2203	U
1	A	2206	G
1	A	2207	G
1	A	2208	A
1	A	2223	G

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Mol	Chain	Res	Type
1	A	2225	A
1	A	2226	C
1	A	2235	G
1	A	2238	G
1	A	2239	G
1	A	2243	U
1	A	2246	G
1	A	2251	G
1	A	2265	U
1	A	2268	A
1	A	2271	G
1	A	2273	A
1	A	2275	C
1	A	2279	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2305	A
1	A	2307	G
1	A	2308	G
1	A	2311	A
1	A	2319	G
1	A	2320	A
1	A	2321	G
1	A	2322	A
1	A	2325	G
1	A	2334	G
1	A	2336	A
1	A	2338	G
1	A	2343	C
1	A	2345	G
1	A	2347	C
1	A	2350	C
1	A	2374	C
1	A	2383	G
1	A	2385	C
1	A	2406	U
1	A	2408	U
1	A	2410	G
1	A	2414	G
1	A	2422	A
1	A	2424	C

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Mol	Chain	Res	Type
1	A	2425	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2434	A
1	A	2439	A
1	A	2441	C
1	A	2447	G
1	A	2448	A
1	A	2460	U
1	A	2469	A
1	A	2471	C
1	A	2474	C
1	A	2476	A
1	A	2478	A
1	A	2482	G
1	A	2491	U
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2505	G
1	A	2507	C
1	A	2511	U
1	A	2518	A
1	A	2519	U
1	A	2520	C
1	A	2528	U
1	A	2529	G
1	A	2535	G
1	A	2545	G
1	A	2554	U
1	A	2564	A
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2574	G
1	A	2581	G
1	A	2582	G
1	A	2586	C
1	A	2602	A
1	A	2605	U
1	A	2609	U

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Mol	Chain	Res	Type
1	A	2611	U
1	A	2612	C
1	A	2621	A
1	A	2629	A
1	A	2630	G
1	A	2639	A
1	A	2645	G
1	A	2654	A
1	A	2660	A
1	A	2663	G
1	A	2669	G
1	A	2679	A
1	A	2686	G
1	A	2689	U
1	A	2691	C
1	A	2702	U
1	A	2703	C
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U
1	A	2733	A
1	A	2744	G
1	A	2751	G
1	A	2755	C
1	A	2757	A
1	A	2758	A
1	A	2764	A
1	A	2765	A
1	A	2766	G
1	A	2778	A
1	A	2780	G
1	A	2784	C
1	A	2790	A
1	A	2791	C
1	A	2792	G
1	A	2802	G
1	A	2811	G
1	A	2818	G
1	A	2820	A
1	A	2821	A
1	A	2831	G

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Mol	Chain	Res	Type
1	A	2833	G
1	A	2835	A
1	A	2872	G
1	A	2880	C
1	A	2887	U
1	A	2889	C
1	A	2895	U
1	A	2897	U
2	B	7	G
2	B	9	G
2	B	10	C
2	B	13	A
2	B	24	G
2	B	25	A
2	B	35	U
2	B	40	U
2	B	42	C
2	B	44	G
2	B	45	A
2	B	56	G
2	B	73	A
2	B	77	U
2	B	78	A
2	B	110	G
2	B	119	G
2	B	120	A
33	x	2	C
33	x	4	C
33	x	5	G
33	x	7	A
33	x	9	A
33	x	10	G
33	x	11	C
33	x	14	A
33	x	19	G
33	x	20	U
33	x	21	A
33	x	23	A
33	x	25	C
33	x	26	A
33	x	32	PSU
33	x	34	G

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Mol	Chain	Res	Type
33	x	39	PSU
33	x	41	C
33	x	42	C
33	x	44	G
33	x	45	U
33	x	46	7MG
33	x	47	U
33	x	48	C
33	x	49	C
33	x	54	5MU
33	x	56	C
33	x	57	G
33	x	58	A
33	x	59	U
33	x	60	U
33	x	61	C
33	x	62	C
33	x	67	C
33	x	68	C
33	x	69	G
33	x	73	A
34	a	7	G
34	a	9	G
34	a	15	G
34	a	22	G
34	a	31	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	50	A
34	a	51	A
34	a	61	G
34	a	73	G
34	a	77	G
34	a	78	G
34	a	79	G
34	a	92	C
34	a	96	U
34	a	97	G
34	a	101	A
34	a	110	C

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Mol	Chain	Res	Type
34	a	116	A
34	a	120	A
34	a	121	C
34	a	131	C
34	a	133	U
34	a	144	G
34	a	151	A
34	a	159	G
34	a	163	C
34	a	167	G
34	a	171	A
34	a	182	U
34	a	189(G)	G
34	a	194	C
34	a	197	A
34	a	202	U
34	a	203	U
34	a	204	U
34	a	216	G
34	a	232	G
34	a	236	G
34	a	247	G
34	a	251	G
34	a	253	U
34	a	266	G
34	a	267	C
34	a	280	C
34	a	289	G
34	a	291	C
34	a	305	G
34	a	306	G
34	a	317	G
34	a	321	A
34	a	325	A
34	a	328	C
34	a	331	G
34	a	332	G
34	a	346	G
34	a	347	G
34	a	348	G
34	a	351	G
34	a	352	C

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Mol	Chain	Res	Type
34	a	353	A
34	a	354	G
34	a	355	C
34	a	366	C
34	a	367	U
34	a	369	C
34	a	372	C
34	a	374	A
34	a	378	G
34	a	382	A
34	a	384	G
34	a	398	C
34	a	406	G
34	a	412	A
34	a	413	G
34	a	422	C
34	a	423	G
34	a	429	U
34	a	430	A
34	a	437	U
34	a	439	A
34	a	441	A
34	a	444	C
34	a	452	A
34	a	453	A
34	a	461	A
34	a	470	C
34	a	472	A
34	a	485	G
34	a	496	A
34	a	498	U
34	a	505	G
34	a	506	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	518	C
34	a	525	C
34	a	527	G
34	a	532	A
34	a	533	A
34	a	546	G

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Mol	Chain	Res	Type
34	a	547	A
34	a	559	A
34	a	561	U
34	a	562	C
34	a	564	C
34	a	565	U
34	a	572	A
34	a	573	A
34	a	576	G
34	a	577	G
34	a	596	C
34	a	597	G
34	a	607	A
34	a	630	G
34	a	631	G
34	a	641	U
34	a	653	A
34	a	661	G
34	a	665	A
34	a	666	G
34	a	687	A
34	a	688	G
34	a	693	G
34	a	697	U
34	a	702	A
34	a	704	A
34	a	707	C
34	a	718	G
34	a	723	U
34	a	731	G
34	a	734	G
34	a	749	C
34	a	750	G
34	a	752	G
34	a	753	A
34	a	755	G
34	a	760	G
34	a	764	C
34	a	777	A
34	a	786	G
34	a	790	A
34	a	792	A

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Mol	Chain	Res	Type
34	a	793	U
34	a	794	A
34	a	802	A
34	a	816	A
34	a	817	C
34	a	821	G
34	a	828	A
34	a	836	G
34	a	839	U
34	a	840	C
34	a	841	U
34	a	848	C
34	a	853	G
34	a	859	A
34	a	860	A
34	a	863	U
34	a	870	U
34	a	873	A
34	a	874	G
34	a	896	C
34	a	902	G
34	a	914	A
34	a	916	G
34	a	919	A
34	a	922	G
34	a	926	G
34	a	927	G
34	a	928	G
34	a	934	C
34	a	935	A
34	a	936	C
34	a	938	A
34	a	960	U
34	a	961	U
34	a	968	A
34	a	969	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	984	C
34	a	993	G
34	a	997	U

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Mol	Chain	Res	Type
34	a	998	G
34	a	1006	C
34	a	1009	G
34	a	1016	A
34	a	1024	G
34	a	1026	G
34	a	1027	C
34	a	1028	C
34	a	1029	C
34	a	1030	C
34	a	1030(A)	G
34	a	1030(B)	C
34	a	1030(C)	G
34	a	1032	G
34	a	1033	G
34	a	1036	G
34	a	1044	A
34	a	1053	G
34	a	1054	C
34	a	1055	A
34	a	1062	U
34	a	1064	G
34	a	1070	U
34	a	1090	U
34	a	1094	G
34	a	1095	U
34	a	1101	A
34	a	1103	C
34	a	1121	U
34	a	1124	G
34	a	1125	U
34	a	1126	U
34	a	1127	G
34	a	1129	C
34	a	1130	A
34	a	1131	G
34	a	1137	C
34	a	1139	G
34	a	1146	A
34	a	1151	A
34	a	1152	A
34	a	1157	A

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Mol	Chain	Res	Type
34	a	1159	U
34	a	1170	A
34	a	1181	G
34	a	1182	G
34	a	1183	A
34	a	1184	G
34	a	1193	G
34	a	1196	U
34	a	1197	G
34	a	1212	U
34	a	1213	A
34	a	1227	A
34	a	1236	A
34	a	1238	A
34	a	1250	A
34	a	1251	A
34	a	1253	G
34	a	1256	A
34	a	1257	U
34	a	1258	G
34	a	1259	C
34	a	1260	C
34	a	1268	A
34	a	1270	C
34	a	1273	G
34	a	1278	U
34	a	1279	A
34	a	1280	A
34	a	1281	U
34	a	1282	C
34	a	1287	A
34	a	1299	A
34	a	1300	G
34	a	1302	U
34	a	1304	G
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1322	C
34	a	1323	G
34	a	1338	G
34	a	1340	A

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Mol	Chain	Res	Type
34	a	1346	A
34	a	1347	G
34	a	1364	U
34	a	1365	G
34	a	1370	G
34	a	1376	U
34	a	1379	G
34	a	1383	C
34	a	1392	G
34	a	1397	C
34	a	1398	A
34	a	1400	C
34	a	1411	C
34	a	1419	G
34	a	1442	G
34	a	1442(B)	A
34	a	1445	C
34	a	1446	U
34	a	1447	A
34	a	1452	C
34	a	1456	G
34	a	1457	G
34	a	1458	G
34	a	1486	G
34	a	1487	G
34	a	1497	G
34	a	1498	U
34	a	1502	A
34	a	1503	A
34	a	1504	G
34	a	1506	U
34	a	1507	A
34	a	1517	G
34	a	1519	A
34	a	1520	G
34	a	1529	G
34	a	1530	G
34	a	1531	A
55	w	10	G
55	w	13	C
55	w	16	U
55	w	17	C

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Mol	Chain	Res	Type
55	w	18	G
55	w	19	G
55	w	20	U
55	w	21	A
55	w	22	G
55	w	35	A
55	w	38	A
55	w	41	C
55	w	44	G
55	w	45	U
55	w	46	7MG
55	w	47	U
55	w	48	C
55	w	49	C
55	w	61	C
55	w	64	A
55	w	71	G
56	v	18	C

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	34	C
1	A	90	U
1	A	196	A
1	A	266	G
1	A	278	A
1	A	328	U
1	A	529	A
1	A	685	A
1	A	746	A
1	A	752	A
1	A	774	A
1	A	895	U
1	A	1033	U
1	A	1052	C
1	A	1069	A
1	A	1078	U
1	A	1108	U
1	A	1145	C
1	A	1174	A
1	A	1176	G

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Mol	Chain	Res	Type
1	A	1210	A
1	A	1300	U
1	A	1379	A
1	A	1529	G
1	A	1608	A
1	A	1617	C
1	A	1653	G
1	A	1992	G
1	A	2110	G
1	A	2132	U
1	A	2183	C
1	A	2187	G
1	A	2318	G
1	A	2428	G
1	A	2439	A
1	A	2611	U
1	A	2756	U
1	A	2873	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	PSU	w	32	55	16,21,22	1.36	1 (6%)	20,30,33	3.70	6 (30%)
55	MIA	w	37	55	23,31,32	2.31	4 (17%)	25,44,47	3.39	5 (20%)
55	PSU	w	39	55	16,21,22	1.26	1 (6%)	20,30,33	3.22	5 (25%)
55	7MG	w	46	55	20,26,27	1.69	2 (10%)	22,39,42	2.55	5 (22%)
55	5MU	w	54	55	14,22,23	0.77	1 (7%)	16,32,35	2.33	2 (12%)
55	PSU	w	55	55	16,21,22	1.47	3 (18%)	20,30,33	3.24	6 (30%)
55	F3O	w	76	55,58	30,36,37	1.06	1 (3%)	33,51,54	1.94	5 (15%)
55	4SU	w	8	55	14,21,22	1.25	2 (14%)	15,30,33	1.51	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PSU	x	32	33	16,21,22	1.19	1 (6%)	20,30,33	3.55	7 (35%)
33	MIA	x	37	33	18,24,32	1.24	2 (11%)	17,35,47	1.77	2 (11%)
33	PSU	x	39	33	16,21,22	1.32	1 (6%)	20,30,33	3.62	7 (35%)
33	7MG	x	46	33	20,26,27	1.54	3 (15%)	22,39,42	3.24	8 (36%)
33	5MU	x	54	33	14,22,23	0.83	1 (7%)	16,32,35	2.47	3 (18%)
33	PSU	x	55	33	16,21,22	1.44	1 (6%)	20,30,33	3.54	6 (30%)
33	4SU	x	8	33	14,21,22	1.31	1 (7%)	15,30,33	1.37	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	w	32	55	-	0/7/25/26	0/2/2/2
55	MIA	w	37	55	-	0/11/33/34	0/3/3/3
55	PSU	w	39	55	-	0/7/25/26	0/2/2/2
55	7MG	w	46	55	-	0/7/37/38	0/3/3/3
55	5MU	w	54	55	-	0/3/25/26	0/2/2/2
55	PSU	w	55	55	-	0/7/25/26	0/2/2/2
55	F3O	w	76	55,58	-	0/15/37/38	0/4/4/4
55	4SU	w	8	55	-	0/3/25/26	0/2/2/2
33	PSU	x	32	33	-	0/7/25/26	0/2/2/2
33	MIA	x	37	33	-	0/3/25/34	0/3/3/3
33	PSU	x	39	33	-	0/7/25/26	0/2/2/2
33	7MG	x	46	33	-	0/7/37/38	0/3/3/3
33	5MU	x	54	33	-	0/3/25/26	0/2/2/2
33	PSU	x	55	33	-	0/7/25/26	0/2/2/2
33	4SU	x	8	33	-	0/3/25/26	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	37	MIA	C2-S10	-9.28	1.67	1.75
33	x	55	PSU	C5-C1'	-4.67	1.48	1.52
55	w	55	PSU	C5-C1'	-4.10	1.48	1.52
33	x	8	4SU	C4-S4	-3.90	1.60	1.67
33	x	39	PSU	C5-C1'	-3.89	1.48	1.52
55	w	32	PSU	C5-C1'	-3.82	1.48	1.52
55	w	8	4SU	C4-S4	-3.48	1.60	1.67
33	x	32	PSU	C5-C1'	-3.14	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	39	PSU	C5-C1'	-3.07	1.49	1.52
55	w	55	PSU	C2-N3	-2.49	1.33	1.38
55	w	8	4SU	O5'-C5'	-2.17	1.41	1.44
33	x	54	5MU	O5'-C5'	-2.06	1.41	1.44
55	w	55	PSU	O5'-C5'	-2.05	1.41	1.44
55	w	54	5MU	C2-N3	-2.02	1.34	1.38
33	x	46	7MG	C4-N3	2.04	1.36	1.34
55	w	37	MIA	C6-N1	2.45	1.36	1.33
55	w	37	MIA	C2-N1	2.66	1.38	1.34
33	x	37	MIA	C2-N3	2.66	1.36	1.32
55	w	46	7MG	C5-C4	2.73	1.46	1.39
33	x	46	7MG	C5-C4	3.16	1.47	1.39
55	w	37	MIA	C5-C4	3.40	1.48	1.40
55	w	76	F3O	O3'-C	3.42	1.42	1.34
33	x	37	MIA	C5-C4	3.49	1.48	1.40
33	x	46	7MG	C6-C5	4.85	1.47	1.41
55	w	46	7MG	C6-C5	6.29	1.48	1.41

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	37	MIA	C11-S10-C2	-15.34	90.96	102.29
55	w	32	PSU	N1-C2-N3	-10.55	120.81	128.40
33	x	39	PSU	N1-C2-N3	-9.77	121.37	128.40
33	x	32	PSU	N1-C2-N3	-9.63	121.47	128.40
33	x	55	PSU	C5-C4-N3	-9.43	117.69	125.43
33	x	55	PSU	N1-C2-N3	-8.74	122.11	128.40
55	w	55	PSU	N1-C2-N3	-8.23	122.48	128.40
55	w	39	PSU	N1-C2-N3	-8.15	122.53	128.40
55	w	39	PSU	C5-C4-N3	-8.04	118.83	125.43
33	x	39	PSU	C5-C4-N3	-7.98	118.88	125.43
33	x	32	PSU	C5-C4-N3	-7.95	118.90	125.43
55	w	76	F3O	N3-C2-N1	-7.88	121.99	128.86
55	w	32	PSU	C5-C4-N3	-7.45	119.32	125.43
55	w	55	PSU	C5-C4-N3	-7.28	119.45	125.43
33	x	46	7MG	C5-C4-N3	-6.15	116.21	126.47
33	x	54	5MU	C5-C4-N3	-6.08	118.54	125.24
33	x	37	MIA	N3-C2-N1	-6.02	123.62	128.86
55	w	54	5MU	C5-C4-N3	-5.74	118.91	125.24
55	w	46	7MG	C5-C4-N3	-4.53	118.90	126.47
55	w	55	PSU	C5-C6-N1	-4.45	118.63	124.39
33	x	46	7MG	C5-C6-N1	-4.41	116.45	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	32	PSU	C5-C6-N1	-4.35	118.75	124.39
55	w	46	7MG	C5-C6-N1	-4.26	116.68	123.37
33	x	55	PSU	C5-C6-N1	-4.13	119.04	124.39
33	x	39	PSU	C5-C6-N1	-4.10	119.08	124.39
33	x	32	PSU	C5-C6-N1	-3.99	119.22	124.39
55	w	37	MIA	C5-C6-N1	-3.85	116.79	120.64
55	w	32	PSU	C5-C1'-C2'	-3.60	109.33	115.55
55	w	55	PSU	C5-C1'-C2'	-3.44	109.62	115.55
55	w	76	F3O	C1'-N9-C4	-3.42	120.72	126.64
55	w	8	4SU	C5-C4-N3	-3.14	119.77	123.73
33	x	37	MIA	C4-C5-N7	-2.98	106.53	109.41
33	x	8	4SU	C5-C4-N3	-2.90	120.06	123.73
55	w	37	MIA	C4-C5-N7	-2.88	106.63	109.41
33	x	46	7MG	C5-C4-N9	-2.69	102.39	106.31
55	w	76	F3O	O3'-C-O	-2.60	118.81	123.90
33	x	39	PSU	C5-C1'-C2'	-2.46	111.30	115.55
55	w	39	PSU	C5-C6-N1	-2.43	121.25	124.39
55	w	76	F3O	C3'-O3'-C	-2.26	114.05	117.85
33	x	54	5MU	C5-C6-N1	-2.20	119.77	122.15
33	x	32	PSU	C5-C1'-C2'	-2.07	111.97	115.55
33	x	39	PSU	O4'-C1'-C5	2.06	113.12	109.93
33	x	46	7MG	N2-C2-N3	2.07	120.55	117.24
33	x	55	PSU	O4'-C1'-C2'	2.19	107.97	104.45
33	x	46	7MG	C4-N9-C1'	2.21	131.92	126.58
55	w	46	7MG	C2-N3-C4	2.31	120.42	113.95
33	x	46	7MG	C2-N3-C4	2.37	120.61	113.95
55	w	37	MIA	C2-N1-C6	2.42	120.60	113.47
33	x	32	PSU	O4'-C1'-C5	2.67	114.07	109.93
55	w	39	PSU	C6-N1-C2	3.49	120.94	115.36
55	w	37	MIA	N6-C6-N1	3.73	123.21	118.54
33	x	8	4SU	C2-N3-C4	3.75	120.64	115.11
55	w	76	F3O	O3'-C-CA	3.90	121.26	111.56
33	x	55	PSU	C6-N1-C2	4.05	121.85	115.36
55	w	8	4SU	C2-N3-C4	4.29	121.43	115.11
33	x	39	PSU	C6-N1-C2	4.32	122.27	115.36
55	w	55	PSU	C6-N1-C2	4.32	122.27	115.36
33	x	46	7MG	C6-N1-C2	4.37	122.35	116.06
55	w	46	7MG	C6-N1-C2	4.45	122.46	116.06
33	x	32	PSU	C6-N1-C2	4.52	122.59	115.36
55	w	32	PSU	C6-N1-C2	4.79	123.03	115.36
55	w	55	PSU	C4-N3-C2	5.36	119.85	115.16
55	w	39	PSU	C4-N3-C2	6.06	120.46	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	32	PSU	C4-N3-C2	6.35	120.71	115.16
33	x	32	PSU	C4-N3-C2	6.42	120.77	115.16
33	x	55	PSU	C4-N3-C2	6.42	120.77	115.16
55	w	54	5MU	C4-N3-C2	6.78	121.09	115.16
33	x	39	PSU	C4-N3-C2	6.80	121.11	115.16
33	x	54	5MU	C4-N3-C2	6.85	121.15	115.16
55	w	46	7MG	N3-C4-N9	8.17	137.42	126.98
33	x	46	7MG	N3-C4-N9	11.28	141.39	126.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 914 ligands modelled in this entry, 912 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	SF4	d	501	37	0,12,12	0.00	-	0,24,24	0.00	-
61	GDP	y	703	58	25,30,30	1.29	2 (8%)	26,47,47	2.00	7 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	d	501	37	-	0/0/48/48	0/6/5/5
61	GDP	y	703	58	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	y	703	GDP	C5-C4	3.27	1.47	1.40
61	y	703	GDP	C6-C5	4.31	1.49	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	y	703	GDP	C5-C6-N1	-3.75	118.15	123.48
61	y	703	GDP	C4-C5-N7	-3.64	105.90	109.41
61	y	703	GDP	N3-C2-N1	-2.73	123.47	127.46
61	y	703	GDP	C6-C5-C4	-2.33	118.52	120.84
61	y	703	GDP	C4'-O4'-C1'	2.28	112.19	109.77
61	y	703	GDP	C6-N1-C2	3.69	121.37	116.06
61	y	703	GDP	C2-N3-C4	5.80	121.93	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	2873/2915 (98%)	-0.06	101 (3%) 44 38	35, 61, 175, 394	0
2	B	120/122 (98%)	-0.11	0 100 100	65, 93, 121, 133	0
3	D	275/276 (99%)	-0.01	3 (1%) 80 79	35, 56, 75, 108	0
4	E	204/206 (99%)	-0.14	4 (1%) 65 62	34, 57, 77, 101	0
5	F	203/205 (99%)	0.03	1 (0%) 90 90	38, 70, 108, 135	0
6	G	181/182 (99%)	-0.05	5 (2%) 53 48	68, 84, 106, 128	0
7	H	174/180 (96%)	0.41	10 (5%) 24 19	62, 96, 131, 154	0
8	J	130/173 (75%)	2.09	51 (39%) 0 0	129, 161, 183, 197	0
9	K	139/147 (94%)	2.83	82 (58%) 0 0	192, 218, 229, 234	0
10	N	140/140 (100%)	-0.01	1 (0%) 87 86	47, 64, 93, 110	0
11	O	122/122 (100%)	-0.00	1 (0%) 86 85	37, 52, 68, 75	0
12	P	149/150 (99%)	0.68	23 (15%) 2 1	42, 81, 109, 116	0
13	Q	141/141 (100%)	-0.00	0 100 100	44, 64, 80, 97	0
14	R	118/118 (100%)	0.33	2 (1%) 70 68	46, 66, 86, 102	0
15	S	110/112 (98%)	0.27	4 (3%) 43 37	75, 90, 102, 113	0
16	T	131/146 (89%)	-0.05	1 (0%) 86 85	49, 61, 94, 113	0
17	U	116/118 (98%)	-0.10	0 100 100	42, 56, 75, 83	0
18	V	101/101 (100%)	0.04	0 100 100	41, 73, 93, 104	0
19	W	112/113 (99%)	0.27	4 (3%) 43 37	46, 62, 89, 128	0
20	X	95/96 (98%)	0.18	2 (2%) 64 60	56, 74, 95, 116	0
21	Y	107/110 (97%)	0.64	9 (8%) 12 8	66, 79, 116, 137	0
22	Z	185/206 (89%)	0.28	6 (3%) 48 42	68, 90, 114, 135	0
23	0	74/85 (87%)	0.50	5 (6%) 18 13	50, 67, 85, 105	0
24	1	97/98 (98%)	0.36	2 (2%) 64 60	48, 68, 104, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	70/72 (97%)	0.15	0 100 100	69, 86, 100, 109	0
26	3	59/60 (98%)	0.41	3 (5%) 29 24	52, 68, 101, 116	0
27	4	69/71 (97%)	0.14	3 (4%) 36 31	80, 107, 150, 158	0
28	5	59/60 (98%)	-0.25	1 (1%) 70 68	41, 63, 81, 100	0
29	6	53/54 (98%)	0.05	0 100 100	62, 71, 85, 87	0
30	7	49/49 (100%)	0.08	2 (4%) 38 32	40, 49, 73, 96	0
31	8	64/65 (98%)	0.10	0 100 100	51, 59, 65, 86	0
32	9	37/37 (100%)	0.76	3 (8%) 13 9	52, 63, 78, 88	0
33	x	67/76 (88%)	5.05	66 (98%) 0 0	94, 267, 283, 306	0
34	a	1496/1521 (98%)	-0.26	4 (0%) 93 93	37, 60, 119, 295	0
35	b	231/256 (90%)	-0.11	5 (2%) 62 59	53, 84, 134, 165	0
36	c	206/239 (86%)	-0.37	1 (0%) 90 90	50, 65, 88, 99	0
37	d	208/209 (99%)	0.03	2 (0%) 82 81	52, 68, 95, 109	0
38	e	148/162 (91%)	-0.25	1 (0%) 87 86	40, 55, 72, 107	0
39	f	100/101 (99%)	0.23	2 (2%) 65 62	74, 106, 138, 146	0
40	g	155/156 (99%)	0.00	5 (3%) 48 42	54, 73, 124, 156	0
41	h	137/138 (99%)	0.04	0 100 100	47, 59, 72, 90	0
42	i	127/128 (99%)	0.06	0 100 100	45, 70, 91, 102	0
43	j	96/105 (91%)	-0.01	3 (3%) 49 43	42, 70, 119, 133	0
44	k	114/129 (88%)	0.05	2 (1%) 69 66	49, 77, 96, 104	0
45	l	122/132 (92%)	-0.17	1 (0%) 86 85	39, 53, 68, 80	0
46	m	119/126 (94%)	-0.03	2 (1%) 70 68	43, 72, 99, 111	0
47	n	60/61 (98%)	-0.27	0 100 100	42, 51, 66, 69	0
48	o	88/89 (98%)	0.20	3 (3%) 46 39	57, 74, 98, 107	0
49	p	82/88 (93%)	0.19	2 (2%) 59 55	45, 57, 69, 85	0
50	q	99/105 (94%)	0.12	5 (5%) 29 24	50, 62, 80, 93	0
51	r	68/88 (77%)	0.52	4 (5%) 23 18	67, 85, 107, 116	0
52	s	83/93 (89%)	-0.20	0 100 100	45, 57, 76, 89	0
53	t	96/106 (90%)	0.17	2 (2%) 64 60	51, 65, 88, 96	0
54	u	23/27 (85%)	0.43	1 (4%) 36 31	54, 62, 69, 79	0
55	w	68/76 (89%)	-0.31	0 100 100	43, 75, 96, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	v	7/18 (38%)	1.39	2 (28%) 1 0	49, 50, 130, 149	0
57	y	644/679 (94%)	1.55	204 (31%) 0 0	69, 151, 188, 213	0
All	All	11201/11638 (96%)	0.17	646 (5%) 24 19	34, 68, 168, 394	0

All (646) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	J	51	LEU	22.8
9	K	52	ILE	16.7
1	A	2178	C	16.4
1	A	2145	C	13.5
1	A	2165	G	13.0
1	A	1509	C	12.4
1	A	2179	C	10.7
33	x	34	G	10.7
1	A	2114	A	10.6
33	x	30	G	10.3
1	A	2182	G	10.2
8	J	53	VAL	10.2
57	y	13	SER	10.1
9	K	48	MET	9.9
1	A	2146	C	9.7
57	y	599	ALA	9.7
8	J	50	ARG	9.7
9	K	10	LEU	9.4
57	y	310	SER	9.4
33	x	35	A	9.1
1	A	2169	A	9.0
1	A	2164	C	9.0
8	J	89	ALA	9.0
1	A	2104	G	9.0
1	A	2159	G	8.8
8	J	7	VAL	8.7
33	x	31	A	8.7
1	A	2116	G	8.7
1	A	2166	G	8.7
57	y	209	GLN	8.5
33	x	56	C	8.4
33	x	36	A	8.3
57	y	600	VAL	8.3
9	K	51	ALA	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	2177	C	8.1
33	x	26	A	8.0
9	K	9	LYS	8.0
33	x	61	C	7.9
1	A	2105	C	7.8
33	x	33	U	7.8
9	K	8	VAL	7.8
33	x	64	A	7.8
9	K	47	ASN	7.7
57	y	539	ALA	7.6
9	K	95	LYS	7.4
9	K	13	PRO	7.3
1	A	2152	G	7.3
57	y	299	PRO	7.1
1	A	2181	G	7.0
57	y	217	LEU	7.0
1	A	2170	A	6.9
57	y	543	GLY	6.9
9	K	22	PRO	6.8
33	x	5	G	6.7
57	y	264	LEU	6.7
1	A	2107	C	6.7
57	y	554	LEU	6.6
19	W	112	GLY	6.6
1	A	2154	G	6.6
8	J	49	ALA	6.6
1	A	2125	G	6.6
9	K	96	VAL	6.5
1	A	2155	G	6.5
40	g	79	ARG	6.5
33	x	11	C	6.4
1	A	2173	A	6.3
1	A	2112	G	6.3
1	A	2151	G	6.3
57	y	266	ALA	6.3
57	y	517	ALA	6.3
1	A	2121	G	6.3
9	K	12	LEU	6.2
33	x	1	G	6.2
3	D	276	LYS	6.1
33	x	44	G	6.1
57	y	462	ASP	6.1

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Mol	Chain	Res	Type	RSRZ
57	y	542	GLY	6.1
33	x	20	U	6.1
33	x	13	C	6.1
33	x	3	C	6.1
1	A	2106	G	6.1
1	A	2133	G	6.1
57	y	156	LEU	6.0
9	K	16	LYS	6.0
9	K	2	LYS	5.9
57	y	92	GLU	5.9
1	A	2120	G	5.9
33	x	53	G	5.9
57	y	371	ALA	5.9
57	y	138	ILE	5.9
33	x	28	G	5.9
57	y	77	VAL	5.9
33	x	19	G	5.9
33	x	29	G	5.9
57	y	309	ASP	5.9
1	A	614(B)	G	5.9
1	A	2141	G	5.9
8	J	88	ALA	5.8
33	x	62	C	5.8
1	A	2176	A	5.8
57	y	416	THR	5.8
1	A	2138	C	5.8
57	y	225	GLY	5.7
9	K	107	ILE	5.7
40	g	156	TRP	5.6
57	y	513	ALA	5.6
1	A	2126	A	5.5
9	K	123	ALA	5.5
33	x	57	G	5.5
33	x	63	G	5.5
1	A	2123	G	5.5
9	K	57	ILE	5.5
10	N	140	VAL	5.5
57	y	16	ALA	5.4
33	x	65	G	5.4
57	y	205	TYR	5.4
8	J	54	ALA	5.4
57	y	529	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
57	y	525	ALA	5.3
57	y	435	LEU	5.3
57	y	414	ILE	5.3
57	y	329	ALA	5.3
1	A	2137	C	5.3
33	x	43	C	5.3
57	y	208	TYR	5.3
1	A	2142	C	5.3
33	x	60	U	5.3
33	x	52	G	5.2
1	A	2143	C	5.2
57	y	204	VAL	5.2
33	x	76	A	5.2
9	K	54	PRO	5.2
57	y	370	ILE	5.1
9	K	93	ARG	5.1
9	K	62	ASP	5.1
9	K	45	THR	5.1
9	K	66	THR	5.1
1	A	2167	U	5.1
33	x	2	C	5.1
8	J	90	ALA	5.1
33	x	70	G	5.0
1	A	2122	U	5.0
8	J	37	THR	5.0
8	J	62	ALA	5.0
33	x	47	U	5.0
8	J	116	ILE	5.0
57	y	313	TYR	5.0
33	x	10	G	5.0
57	y	397	PRO	4.9
1	A	2109	U	4.9
57	y	590	VAL	4.9
57	y	494	VAL	4.9
9	K	120	LEU	4.9
33	x	71	G	4.9
12	P	95	VAL	4.9
9	K	92	GLY	4.8
57	y	265	VAL	4.8
1	A	2128	C	4.8
9	K	41	PHE	4.8
57	y	368	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	2161	C	4.8
9	K	97	GLY	4.8
57	y	222	VAL	4.8
1	A	2162	G	4.7
33	x	18	G	4.7
1	A	2127	G	4.7
33	x	6	G	4.7
8	J	83	TYR	4.7
9	K	7	VAL	4.7
33	x	67	C	4.7
57	y	504	LEU	4.7
9	K	3	LYS	4.7
57	y	547	ALA	4.7
1	A	2117	A	4.7
1	A	2160	G	4.7
9	K	61	ALA	4.6
57	y	538	GLN	4.6
33	x	22	G	4.6
1	A	2144	U	4.6
57	y	218	PHE	4.6
9	K	68	VAL	4.6
57	y	596	ALA	4.6
33	x	12	U	4.6
57	y	369	LEU	4.6
56	v	12	A	4.5
57	y	601	LEU	4.5
57	y	302	PHE	4.5
24	l	2	SER	4.5
12	P	114	ILE	4.4
57	y	272	HIS	4.4
50	q	98	LEU	4.4
1	A	2134	A	4.4
57	y	496	VAL	4.4
12	P	85	LEU	4.4
57	y	64	VAL	4.4
57	y	492	VAL	4.3
9	K	110	GLN	4.3
1	A	2174	C	4.3
33	x	48	C	4.3
57	y	32	LEU	4.3
1	A	2131	G	4.3
33	x	27	G	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	2113	U	4.3
33	x	58	A	4.3
33	x	45	U	4.3
12	P	88	LEU	4.3
9	K	67	PHE	4.3
1	A	2190	G	4.3
48	o	20	GLY	4.2
33	x	38	A	4.2
57	y	493	ASN	4.2
8	J	23	SER	4.2
33	x	4	C	4.2
57	y	330	LEU	4.2
57	y	602	SER	4.2
9	K	134	MET	4.2
57	y	79	HIS	4.2
57	y	568	THR	4.2
9	K	44	ALA	4.1
57	y	29	ILE	4.1
6	G	2	PRO	4.1
8	J	8	GLU	4.1
57	y	374	PRO	4.1
1	A	2139	C	4.0
33	x	68	C	4.0
9	K	35	MET	4.0
33	x	23	A	4.0
8	J	94	VAL	4.0
57	y	91	TYR	4.0
57	y	541	ILE	4.0
33	x	69	G	4.0
8	J	118	THR	3.9
9	K	127	ILE	3.9
1	A	2153	G	3.9
57	y	433	GLY	3.9
1	A	2119	A	3.9
57	y	497	HIS	3.9
57	y	563	TYR	3.9
57	y	583	ARG	3.9
1	A	2140	C	3.9
57	y	516	MET	3.9
57	y	471	SER	3.9
8	J	61	LEU	3.8
43	j	85	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	2148	G	3.8
9	K	80	LYS	3.8
57	y	530	ARG	3.8
8	J	85	ASP	3.8
7	H	26	VAL	3.8
9	K	94	GLU	3.8
1	A	1175	U	3.8
1	A	2136	C	3.8
33	x	14	A	3.8
33	x	21	A	3.8
57	y	312	ASP	3.7
57	y	544	LYS	3.7
3	D	275	LYS	3.7
8	J	52	PHE	3.7
33	x	51	U	3.7
57	y	198	ALA	3.7
1	A	2175	C	3.7
57	y	520	ILE	3.7
9	K	18	THR	3.7
30	7	46	VAL	3.7
9	K	14	ALA	3.7
57	y	452	TYR	3.6
57	y	-5	GLU	3.6
9	K	17	ALA	3.6
33	x	25	C	3.6
57	y	489	LEU	3.6
57	y	279	THR	3.6
1	A	2163	C	3.6
57	y	242	VAL	3.6
57	y	495	LEU	3.6
9	K	65	PHE	3.6
9	K	49	GLY	3.6
53	t	101	GLY	3.6
9	K	25	PRO	3.6
8	J	4	LYS	3.6
33	x	15	G	3.6
57	y	503	ALA	3.5
57	y	33	THR	3.5
57	y	445	GLN	3.5
34	a	204	U	3.5
57	y	581	LYS	3.5
1	A	652(F)	G	3.5

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Mol	Chain	Res	Type	RSRZ
9	K	37	PHE	3.5
1	A	2168	G	3.4
57	y	286	PRO	3.4
57	y	448	VAL	3.4
57	y	552	LYS	3.4
57	y	526	GLU	3.4
1	A	271(K)	U	3.4
57	y	207	ALA	3.4
32	9	37	GLY	3.4
33	x	73	A	3.4
7	H	2	SER	3.4
40	g	80	VAL	3.4
57	y	350	GLY	3.4
57	y	487	GLY	3.3
33	x	72	C	3.3
1	A	1420	U	3.3
57	y	9	ILE	3.3
1	A	2147	G	3.3
1	A	2793	G	3.3
57	y	400	THR	3.3
57	y	444	ALA	3.3
21	Y	1	MET	3.3
8	J	14	LYS	3.3
22	Z	57	ILE	3.3
1	A	1046	A	3.3
57	y	561	LYS	3.3
9	K	21	PRO	3.3
1	A	2102	U	3.2
57	y	11	ASN	3.2
9	K	83	GLY	3.2
12	P	121	LYS	3.2
57	y	349	LEU	3.2
57	y	280	ILE	3.2
1	A	2101	G	3.2
20	X	1	MET	3.2
57	y	399	PRO	3.2
7	H	47	GLU	3.2
57	y	531	GLN	3.2
9	K	63	ARG	3.2
9	K	138	VAL	3.2
57	y	163	ALA	3.2
8	J	97	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
57	y	274	VAL	3.2
57	y	440	TYR	3.2
8	J	63	LEU	3.2
8	J	24	PHE	3.2
1	A	2156	G	3.2
57	y	93	VAL	3.2
57	y	-1	LEU	3.1
8	J	75	GLN	3.1
57	y	524	LEU	3.1
9	K	85	GLU	3.1
37	d	182	LYS	3.1
57	y	236	GLU	3.1
26	3	2	PRO	3.1
1	A	2135	A	3.1
57	y	457	ALA	3.1
57	y	131	ILE	3.1
19	W	65	LEU	3.1
1	A	2110	G	3.1
8	J	78	SER	3.0
57	y	446	LYS	3.0
8	J	17	LEU	3.0
39	f	97	PHE	3.0
57	y	132	ILE	3.0
12	P	83	VAL	3.0
9	K	27	LEU	3.0
57	y	551	VAL	3.0
57	y	72	ASP	3.0
57	y	-2	ARG	3.0
33	x	40	C	3.0
9	K	58	THR	3.0
57	y	537	ILE	3.0
57	y	558	VAL	3.0
15	S	37	ALA	2.9
57	y	166	ALA	2.9
57	y	586	ALA	2.9
50	q	99	SER	2.9
21	Y	39	VAL	2.9
27	4	55	ARG	2.9
57	y	523	LYS	2.9
57	y	75	GLU	2.9
1	A	652(S)	C	2.9
1	A	652(B)	A	2.9

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Mol	Chain	Res	Type	RSRZ
57	y	99	ALA	2.9
9	K	140	GLY	2.9
57	y	67	THR	2.9
57	y	473	GLY	2.9
15	S	20	ARG	2.9
57	y	250	LEU	2.9
1	A	2118	U	2.9
57	y	1	GLU	2.9
57	y	486	PRO	2.9
46	m	120	LYS	2.9
57	y	461	TYR	2.9
9	K	91	PRO	2.9
19	W	111	HIS	2.9
57	y	12	PHE	2.9
9	K	59	ILE	2.8
9	K	115	LEU	2.8
57	y	499	GLU	2.8
12	P	127	ALA	2.8
57	y	267	ALA	2.8
1	A	2189	U	2.8
33	x	50	U	2.8
12	P	126	VAL	2.8
33	x	74	C	2.8
57	y	597	PHE	2.8
57	y	426	GLN	2.8
9	K	55	VAL	2.8
39	f	98	LEU	2.8
1	A	652(D)	C	2.8
1	A	2132	U	2.7
57	y	164	ILE	2.7
1	A	2115	G	2.7
12	P	87	ASP	2.7
57	y	519	ALA	2.7
1	A	2129	C	2.7
6	G	48	GLU	2.7
57	y	540	ALA	2.7
8	J	84	GLU	2.7
34	a	1030(B)	C	2.7
56	v	13	A	2.7
9	K	64	SER	2.7
16	T	115	ARG	2.7
9	K	121	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
21	Y	35	TYR	2.7
1	A	2124	G	2.7
57	y	535	VAL	2.7
9	K	86	LYS	2.7
1	A	2103	C	2.7
57	y	518	ARG	2.7
57	y	396	LEU	2.7
9	K	137	GLU	2.7
49	p	39	TYR	2.7
57	y	598	LEU	2.7
34	a	1030(C)	G	2.7
12	P	86	LYS	2.7
57	y	85	GLY	2.7
57	y	173	GLY	2.7
57	y	415	PHE	2.7
57	y	591	GLU	2.7
1	A	652(T)	C	2.7
9	K	74	ALA	2.7
12	P	120	ALA	2.7
57	y	-6	ALA	2.7
9	K	133	SER	2.6
14	R	118	GLU	2.6
9	K	114	ASP	2.6
28	5	60	VAL	2.6
8	J	19	ARG	2.6
1	A	614(A)	U	2.6
1	A	2180	U	2.6
51	r	31	LEU	2.6
1	A	2183	C	2.6
9	K	50	ASP	2.6
57	y	514	TYR	2.6
8	J	77	PRO	2.6
35	b	129	GLU	2.6
12	P	130	PHE	2.6
1	A	34	C	2.6
43	j	73	ASP	2.6
57	y	134	VAL	2.6
8	J	124	ALA	2.6
57	y	288	PRO	2.6
12	P	137	LYS	2.6
57	y	14	ILE	2.6
9	K	30	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
57	y	105	LEU	2.6
12	P	92	GLU	2.6
9	K	84	LEU	2.5
57	y	534	GLU	2.5
6	G	49	ASP	2.5
22	Z	140	ASP	2.5
57	y	546	ILE	2.5
51	r	85	LEU	2.5
9	K	90	LYS	2.5
27	4	51	ASP	2.5
7	H	77	LYS	2.5
35	b	38	GLY	2.5
9	K	53	VAL	2.5
33	x	41	C	2.5
9	K	135	GLY	2.5
57	y	203	SER	2.5
57	y	363	ARG	2.5
33	x	49	C	2.5
7	H	33	LEU	2.5
57	y	450	LEU	2.5
12	P	1	MET	2.5
33	x	59	U	2.5
1	A	2157	G	2.5
23	0	62	LEU	2.5
8	J	10	LEU	2.5
8	J	111	LEU	2.5
57	y	500	VAL	2.5
8	J	110	GLY	2.5
50	q	69	LYS	2.5
57	y	562	CYS	2.5
1	A	1176	G	2.5
57	y	278	ASP	2.4
8	J	76	GLY	2.4
33	x	7	A	2.4
57	y	488	ASP	2.4
21	Y	48	ALA	2.4
8	J	18	GLU	2.4
9	K	34	ILE	2.4
1	A	2185	C	2.4
1	A	2897	U	2.4
23	0	48	GLY	2.4
57	y	475	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
51	r	78	LEU	2.4
21	Y	55	TYR	2.4
57	y	298	LYS	2.4
57	y	589	LYS	2.4
8	J	74	LEU	2.4
7	H	48	GLY	2.4
8	J	87	VAL	2.4
33	x	9	A	2.4
12	P	91	PHE	2.4
15	S	3	ARG	2.4
57	y	276	VAL	2.4
9	K	46	ALA	2.4
1	A	2108	C	2.4
22	Z	117	LEU	2.4
26	3	8	LEU	2.4
33	x	42	C	2.4
37	d	44	GLY	2.3
1	A	652(E)	G	2.3
34	a	1021	G	2.3
9	K	136	VAL	2.3
57	y	505	THR	2.3
5	F	33	LEU	2.3
38	e	142	LEU	2.3
57	y	326	ASN	2.3
1	A	2150	U	2.3
57	y	334	PRO	2.3
8	J	133	GLU	2.3
9	K	75	SER	2.3
35	b	37	ASN	2.3
8	J	25	PHE	2.3
57	y	171	GLY	2.3
57	y	509	HIS	2.3
23	0	78	TYR	2.3
57	y	109	ALA	2.3
57	y	549	ALA	2.3
30	7	49	ARG	2.3
1	A	2184	G	2.3
1	A	2172	U	2.3
23	0	47	PRO	2.3
57	y	257	GLU	2.3
57	y	124	ALA	2.3
57	y	158	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
57	y	434	ARG	2.3
57	y	439	ASN	2.3
57	y	481	GLN	2.3
8	J	69	PRO	2.3
9	K	69	THR	2.3
9	K	102	GLU	2.3
26	3	60	GLU	2.3
57	y	115	ALA	2.3
57	y	528	ILE	2.3
21	Y	34	LYS	2.3
40	g	78	ARG	2.3
46	m	48	LEU	2.3
50	q	27	PHE	2.3
57	y	165	PHE	2.3
8	J	57	THR	2.2
1	A	229	A	2.2
21	Y	50	ARG	2.2
4	E	114	ALA	2.2
44	k	19	ALA	2.2
57	y	210	GLY	2.2
54	u	18	TYR	2.2
7	H	174	GLY	2.2
12	P	148	LEU	2.2
4	E	195	LEU	2.2
57	y	170	THR	2.2
57	y	443	GLY	2.2
8	J	36	GLU	2.2
12	P	94	GLU	2.2
35	b	232	PRO	2.2
23	0	74	ARG	2.2
24	1	20	ARG	2.2
33	x	24	G	2.2
57	y	571	LYS	2.2
8	J	15	GLU	2.2
22	Z	62	PRO	2.2
27	4	56	VAL	2.2
9	K	111	LYS	2.2
20	X	9	LEU	2.2
21	Y	17	SER	2.2
44	k	109	VAL	2.2
57	y	420	TYR	2.2
57	y	259	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
8	J	99	SER	2.2
57	y	469	SER	2.2
35	b	130	ARG	2.2
57	y	71	LYS	2.2
8	J	117	LEU	2.2
49	p	19	ILE	2.2
57	y	297	ALA	2.2
7	H	32	GLU	2.2
12	P	15	ARG	2.2
32	9	23	VAL	2.2
57	y	277	GLY	2.1
57	y	121	PHE	2.1
4	E	159	HIS	2.1
57	y	234	GLY	2.1
57	y	351	LEU	2.1
1	A	2188	C	2.1
8	J	86	PRO	2.1
43	j	86	MET	2.1
45	l	18	VAL	2.1
57	y	490	VAL	2.1
15	S	7	TYR	2.1
3	D	181	GLU	2.1
57	y	258	ALA	2.1
9	K	4	VAL	2.1
9	K	139	VAL	2.1
22	Z	27	VAL	2.1
48	o	89	GLY	2.1
57	y	201	PHE	2.1
57	y	412	LEU	2.1
6	G	50	ALA	2.1
12	P	119	GLU	2.1
57	y	402	ILE	2.1
8	J	73	GLY	2.1
12	P	125	VAL	2.1
21	Y	71	LYS	2.1
53	t	100	ILE	2.1
57	y	-22	LEU	2.1
57	y	255	ALA	2.1
14	R	97	VAL	2.1
36	c	126	ARG	2.1
4	E	113	PHE	2.1
8	J	12	THR	2.1

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Mol	Chain	Res	Type	RSRZ
19	W	1	MET	2.1
6	G	182	LYS	2.1
32	9	15	LYS	2.1
9	K	26	ALA	2.1
51	r	20	ALA	2.1
12	P	79	ARG	2.1
22	Z	145	GLU	2.1
48	o	34	LEU	2.0
57	y	2	ILE	2.0
33	x	66	U	2.0
11	O	97	ARG	2.0
7	H	145	ALA	2.0
57	y	76	TYR	2.0
57	y	372	THR	2.0
7	H	76	VAL	2.0
57	y	232	SER	2.0
9	K	116	ASN	2.0
9	K	36	GLU	2.0
50	q	97	SER	2.0
40	g	85	TYR	2.0
57	y	246	THR	2.0
8	J	66	LEU	2.0
12	P	115	LEU	2.0
57	y	584	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	4SU	w	8	20/21	0.95	0.14	-	56,58,64,64	0
33	MIA	x	37	22/30	0.51	0.78	-	204,221,237,241	0
33	PSU	x	55	20/21	0.32	0.84	-	274,285,289,293	0
55	5MU	w	54	21/22	0.96	0.14	-	67,77,82,84	0
33	5MU	x	54	21/22	0.20	0.66	-	275,282,283,285	0
33	PSU	x	32	20/21	0.41	0.64	-	188,202,216,216	0
55	PSU	w	32	20/21	0.97	0.12	-	40,46,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	PSU	w	39	20/21	0.96	0.14	-	41,50,55,56	0
55	MIA	w	37	29/30	0.95	0.17	-	46,55,61,64	0
55	PSU	w	55	20/21	0.93	0.16	-	75,83,85,86	0
55	F3O	w	76	33/34	0.92	0.26	-	50,60,79,81	0
33	4SU	x	8	20/21	0.33	0.42	-	263,275,277,277	0
33	PSU	x	39	20/21	0.73	0.33	-	175,193,200,201	0
33	7MG	x	46	24/25	0.35	0.36	-	275,282,285,287	0
55	7MG	w	46	24/25	0.92	0.18	-	59,76,103,118	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3114	1/1	0.84	1.01	81.38	57,57,57,57	0
58	MG	A	3165	1/1	0.68	1.02	66.51	60,60,60,60	0
58	MG	A	3117	1/1	0.83	1.11	66.27	50,50,50,50	0
58	MG	A	3120	1/1	0.82	0.76	28.68	52,52,52,52	0
58	MG	a	3306	1/1	0.87	0.69	28.63	55,55,55,55	0
58	MG	a	3309	1/1	0.96	0.80	28.16	37,37,37,37	0
58	MG	A	3118	1/1	0.89	0.88	27.84	52,52,52,52	0
58	MG	7	102	1/1	0.83	1.36	27.62	66,66,66,66	0
58	MG	a	3397	1/1	0.97	0.39	25.06	27,27,27,27	0
58	MG	a	3323	1/1	0.62	0.51	23.90	69,69,69,69	0
58	MG	A	3072	1/1	0.87	0.32	23.23	43,43,43,43	0
58	MG	A	3274	1/1	0.95	0.47	22.68	45,45,45,45	0
58	MG	E	301	1/1	0.90	0.81	19.90	56,56,56,56	0
58	MG	D	303	1/1	0.89	0.92	19.54	49,49,49,49	0
58	MG	A	3032	1/1	0.79	0.32	19.47	50,50,50,50	0
58	MG	A	3039	1/1	0.85	0.84	18.59	59,59,59,59	0
58	MG	A	3093	1/1	0.66	0.31	18.50	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3500	1/1	0.96	0.29	18.31	40,40,40,40	0
58	MG	A	3056	1/1	0.58	0.42	18.18	68,68,68,68	0
58	MG	A	3191	1/1	0.98	0.36	17.61	33,33,33,33	0
58	MG	A	3107	1/1	0.91	1.42	17.34	75,75,75,75	0
58	MG	a	3447	1/1	0.98	0.41	16.48	36,36,36,36	0
58	MG	A	3231	1/1	0.76	0.39	16.36	48,48,48,48	0
58	MG	a	3401	1/1	0.93	0.38	16.12	44,44,44,44	0
58	MG	A	3316	1/1	0.94	0.31	15.98	47,47,47,47	0
58	MG	A	3095	1/1	0.78	0.40	15.30	63,63,63,63	0
58	MG	A	3023	1/1	0.89	0.31	15.20	48,48,48,48	0
58	MG	A	3234	1/1	0.96	0.36	14.55	48,48,48,48	0
58	MG	7	101	1/1	0.95	0.70	13.26	48,48,48,48	0
58	MG	A	3059	1/1	0.80	0.33	13.11	66,66,66,66	0
58	MG	A	3144	1/1	0.97	0.32	12.86	38,38,38,38	0
58	MG	A	3208	1/1	0.95	0.27	12.65	40,40,40,40	0
58	MG	A	3616	1/1	0.89	0.31	12.23	59,59,59,59	0
58	MG	V	202	1/1	0.88	0.75	12.19	51,51,51,51	0
58	MG	A	3446	1/1	0.94	0.29	12.02	39,39,39,39	0
58	MG	A	3557	1/1	0.96	0.33	11.95	60,60,60,60	0
58	MG	A	3011	1/1	0.59	0.46	11.78	79,79,79,79	0
58	MG	Q	202	1/1	0.90	0.95	11.56	51,51,51,51	0
58	MG	A	3541	1/1	0.96	0.26	11.54	56,56,56,56	0
58	MG	A	3005	1/1	0.89	0.37	11.44	40,40,40,40	0
58	MG	A	3174	1/1	0.81	0.32	11.36	59,59,59,59	0
58	MG	A	3423	1/1	0.89	0.22	11.35	59,59,59,59	0
58	MG	A	3414	1/1	0.91	0.28	11.25	31,31,31,31	0
58	MG	A	3187	1/1	0.96	0.44	11.04	47,47,47,47	0
58	MG	F	302	1/1	0.92	0.81	11.04	52,52,52,52	0
58	MG	A	3006	1/1	0.92	0.59	10.70	57,57,57,57	0
58	MG	A	3189	1/1	0.95	0.31	10.68	37,37,37,37	0
58	MG	A	3192	1/1	0.99	0.28	10.63	39,39,39,39	0
58	MG	A	3167	1/1	0.93	0.55	10.50	65,65,65,65	0
58	MG	A	3190	1/1	0.96	0.30	10.40	38,38,38,38	0
58	MG	A	3396	1/1	0.97	0.25	10.16	38,38,38,38	0
58	MG	A	3399	1/1	0.98	0.28	9.82	29,29,29,29	0
58	MG	A	3252	1/1	0.89	0.27	9.79	58,58,58,58	0
58	MG	A	3487	1/1	0.92	0.22	9.79	60,60,60,60	0
58	MG	P	201	1/1	0.79	0.54	9.54	54,54,54,54	0
58	MG	A	3529	1/1	0.94	0.24	9.50	56,56,56,56	0
58	MG	A	3184	1/1	0.98	0.39	9.46	40,40,40,40	0
58	MG	a	3330	1/1	0.89	0.55	9.00	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3493	1/1	0.90	0.37	8.73	33,33,33,33	0
58	MG	A	3080	1/1	0.93	0.30	8.46	54,54,54,54	0
58	MG	A	3501	1/1	0.96	0.25	8.41	46,46,46,46	0
58	MG	x	3002	1/1	0.78	1.22	8.37	101,101,101,101	0
58	MG	A	3297	1/1	0.79	0.24	8.34	67,67,67,67	0
58	MG	Q	204	1/1	0.91	0.63	8.34	56,56,56,56	0
58	MG	B	210	1/1	0.76	0.22	8.33	68,68,68,68	0
58	MG	A	3155	1/1	0.96	0.27	8.17	44,44,44,44	0
58	MG	A	3513	1/1	0.99	0.29	8.07	41,41,41,41	0
58	MG	A	3476	1/1	0.94	0.30	8.01	50,50,50,50	0
58	MG	A	3417	1/1	0.96	0.20	7.96	30,30,30,30	0
58	MG	A	3341	1/1	0.93	0.33	7.93	57,57,57,57	0
58	MG	A	3520	1/1	0.86	0.21	7.90	80,80,80,80	0
58	MG	A	3239	1/1	0.85	0.32	7.58	56,56,56,56	0
58	MG	A	3141	1/1	0.86	0.23	7.52	55,55,55,55	0
58	MG	A	3109	1/1	0.87	0.26	7.45	52,52,52,52	0
58	MG	a	3331	1/1	0.93	0.24	7.38	55,55,55,55	0
58	MG	a	3406	1/1	0.99	0.21	7.34	52,52,52,52	0
58	MG	A	3170	1/1	0.98	0.23	7.29	43,43,43,43	0
58	MG	A	3352	1/1	0.82	0.31	7.25	47,47,47,47	0
58	MG	Q	201	1/1	0.94	0.51	7.07	51,51,51,51	0
58	MG	A	3041	1/1	0.94	0.24	7.06	42,42,42,42	0
58	MG	a	3395	1/1	0.98	0.30	6.91	32,32,32,32	0
58	MG	A	3079	1/1	0.90	0.45	6.86	63,63,63,63	0
58	MG	a	3422	1/1	0.94	0.32	6.80	50,50,50,50	0
58	MG	A	3188	1/1	0.98	0.32	6.79	44,44,44,44	0
58	MG	a	3471	1/1	0.97	0.27	6.69	49,49,49,49	0
58	MG	A	3295	1/1	0.94	0.27	6.63	30,30,30,30	0
58	MG	A	3568	1/1	0.81	0.20	6.39	83,83,83,83	0
58	MG	A	3293	1/1	0.80	0.33	6.34	51,51,51,51	0
58	MG	A	3319	1/1	0.70	0.23	6.05	31,31,31,31	0
58	MG	A	3143	1/1	0.90	0.26	6.05	60,60,60,60	0
58	MG	A	3008	1/1	0.89	0.99	6.01	80,80,80,80	0
58	MG	A	3125	1/1	0.94	0.29	5.98	31,31,31,31	0
58	MG	A	3225	1/1	0.97	0.25	5.94	36,36,36,36	0
58	MG	A	3119	1/1	0.87	0.26	5.49	50,50,50,50	0
58	MG	A	3311	1/1	0.94	0.28	5.44	52,52,52,52	0
58	MG	N	201	1/1	0.76	0.40	5.41	57,57,57,57	0
58	MG	a	3487	1/1	0.98	0.32	5.39	35,35,35,35	0
58	MG	a	3368	1/1	0.87	0.23	5.34	44,44,44,44	0
58	MG	n	101	1/1	0.98	0.25	5.32	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	D	301	1/1	0.97	0.29	5.26	41,41,41,41	0
58	MG	A	3230	1/1	0.97	0.24	5.21	46,46,46,46	0
58	MG	A	3002	1/1	0.69	0.34	5.11	50,50,50,50	0
58	MG	6	101	1/1	0.80	0.32	5.08	64,64,64,64	0
58	MG	A	3363	1/1	0.94	0.18	5.04	30,30,30,30	0
58	MG	A	3045	1/1	0.85	0.21	4.98	68,68,68,68	0
58	MG	A	3455	1/1	0.95	0.22	4.92	73,73,73,73	0
58	MG	A	3516	1/1	0.88	0.21	4.84	55,55,55,55	0
58	MG	A	3420	1/1	0.96	0.20	4.83	31,31,31,31	0
58	MG	A	3022	1/1	0.93	0.28	4.73	33,33,33,33	0
58	MG	a	3439	1/1	0.97	0.21	4.63	48,48,48,48	0
58	MG	a	3378	1/1	0.96	0.24	4.62	39,39,39,39	0
58	MG	A	3564	1/1	0.79	0.21	4.51	75,75,75,75	0
58	MG	a	3355	1/1	0.97	0.20	4.38	39,39,39,39	0
58	MG	R	201	1/1	0.84	0.56	4.26	67,67,67,67	0
58	MG	a	3313	1/1	0.89	0.19	4.17	61,61,61,61	0
58	MG	a	3318	1/1	0.98	0.24	4.10	41,41,41,41	0
58	MG	a	3466	1/1	0.94	0.18	4.09	60,60,60,60	0
58	MG	A	3222	1/1	0.95	0.21	4.01	33,33,33,33	0
58	MG	A	3004	1/1	0.92	0.21	3.94	55,55,55,55	0
58	MG	l	202	1/1	0.95	0.33	3.93	61,61,61,61	0
58	MG	a	3435	1/1	0.93	0.19	3.91	57,57,57,57	0
58	MG	A	3157	1/1	0.34	0.24	3.84	118,118,118,118	0
58	MG	A	3530	1/1	0.99	0.25	3.82	38,38,38,38	0
58	MG	A	3601	1/1	0.85	0.19	3.80	45,45,45,45	0
58	MG	a	3376	1/1	0.91	0.20	3.65	46,46,46,46	0
58	MG	A	3490	1/1	0.87	0.25	3.58	47,47,47,47	0
58	MG	A	3200	1/1	0.95	0.18	3.42	44,44,44,44	0
58	MG	A	3209	1/1	0.79	0.18	3.38	71,71,71,71	0
58	MG	A	3086	1/1	0.88	0.19	3.30	50,50,50,50	0
58	MG	A	3540	1/1	0.96	0.22	3.15	55,55,55,55	0
58	MG	A	3164	1/1	0.95	0.19	3.03	51,51,51,51	0
58	MG	A	3171	1/1	0.82	0.18	3.00	37,37,37,37	0
58	MG	A	3027	1/1	0.93	0.25	2.97	44,44,44,44	0
58	MG	A	3437	1/1	0.97	0.20	2.91	28,28,28,28	0
58	MG	A	3380	1/1	0.94	0.19	2.90	52,52,52,52	0
58	MG	A	3207	1/1	0.90	0.17	2.83	40,40,40,40	0
58	MG	A	3047	1/1	0.94	0.19	2.79	39,39,39,39	0
58	MG	A	3382	1/1	0.94	0.24	2.78	36,36,36,36	0
58	MG	A	3021	1/1	0.98	0.18	2.72	34,34,34,34	0
58	MG	A	3147	1/1	0.94	0.23	2.72	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3048	1/1	0.91	0.20	2.64	43,43,43,43	0
58	MG	A	3523	1/1	0.98	0.23	2.63	36,36,36,36	0
58	MG	A	3214	1/1	0.92	0.41	2.58	52,52,52,52	0
58	MG	U	201	1/1	0.93	0.40	2.58	72,72,72,72	0
58	MG	F	304	1/1	0.91	0.27	2.56	60,60,60,60	0
58	MG	A	3033	1/1	0.94	0.19	2.47	39,39,39,39	0
58	MG	a	3351	1/1	0.94	0.19	2.42	36,36,36,36	0
58	MG	A	3244	1/1	0.85	0.20	2.42	59,59,59,59	0
58	MG	a	3382	1/1	0.97	0.22	2.34	31,31,31,31	0
58	MG	A	3034	1/1	0.83	0.20	2.29	71,71,71,71	0
58	MG	A	3498	1/1	0.86	0.18	2.29	76,76,76,76	0
58	MG	A	3223	1/1	0.88	0.31	2.28	61,61,61,61	0
58	MG	A	3166	1/1	0.96	0.30	2.25	57,57,57,57	0
58	MG	A	3486	1/1	0.94	0.23	2.23	40,40,40,40	0
58	MG	A	3313	1/1	0.93	0.17	2.13	44,44,44,44	0
58	MG	A	3410	1/1	0.75	0.20	2.07	51,51,51,51	0
58	MG	A	3324	1/1	0.96	0.22	2.02	43,43,43,43	0
58	MG	A	3201	1/1	0.92	0.20	2.00	63,63,63,63	0
58	MG	A	3067	1/1	0.81	0.16	1.93	70,70,70,70	0
58	MG	A	3442	1/1	0.93	0.17	1.88	56,56,56,56	0
58	MG	A	3485	1/1	0.97	0.22	1.86	38,38,38,38	0
58	MG	D	302	1/1	0.59	0.28	1.81	74,74,74,74	0
58	MG	A	3552	1/1	0.94	0.18	1.78	64,64,64,64	0
58	MG	A	3233	1/1	0.98	0.17	1.74	53,53,53,53	0
58	MG	A	3394	1/1	0.95	0.19	1.67	30,30,30,30	0
58	MG	A	3606	1/1	0.87	0.18	1.65	55,55,55,55	0
58	MG	A	3103	1/1	0.89	0.29	1.60	56,56,56,56	0
58	MG	A	3378	1/1	0.99	0.19	1.49	31,31,31,31	0
58	MG	A	3404	1/1	0.93	0.20	1.42	57,57,57,57	0
58	MG	A	3049	1/1	0.97	0.19	1.41	41,41,41,41	0
58	MG	A	3173	1/1	0.89	0.18	1.39	57,57,57,57	0
58	MG	A	3340	1/1	0.97	0.23	1.36	65,65,65,65	0
58	MG	A	3544	1/1	0.87	0.17	1.30	55,55,55,55	0
58	MG	G	202	1/1	0.69	0.24	1.29	67,67,67,67	0
58	MG	A	3007	1/1	0.93	0.27	1.24	46,46,46,46	0
58	MG	A	3509	1/1	0.97	0.24	1.24	51,51,51,51	0
58	MG	A	3323	1/1	0.91	0.15	1.18	42,42,42,42	0
58	MG	y	701	1/1	0.84	0.26	1.13	68,68,68,68	0
58	MG	A	3594	1/1	0.92	0.19	1.13	37,37,37,37	0
58	MG	A	3536	1/1	0.96	0.21	1.08	39,39,39,39	0
58	MG	A	3154	1/1	0.93	0.18	1.07	60,60,60,60	0
58	MG	A	3009	1/1	0.85	0.30	1.05	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	a	3414	1/1	0.95	0.20	1.02	50,50,50,50	0
58	MG	A	3364	1/1	0.97	0.16	1.00	61,61,61,61	0
58	MG	A	3077	1/1	0.96	0.13	0.95	48,48,48,48	0
58	MG	A	3215	1/1	0.88	0.18	0.95	66,66,66,66	0
58	MG	a	3486	1/1	0.91	0.19	0.95	38,38,38,38	0
58	MG	A	3046	1/1	0.90	0.17	0.95	55,55,55,55	0
58	MG	A	3384	1/1	0.95	0.23	0.94	51,51,51,51	0
58	MG	a	3415	1/1	0.97	0.20	0.89	62,62,62,62	0
58	MG	A	3450	1/1	0.95	0.16	0.82	57,57,57,57	0
58	MG	A	3358	1/1	0.96	0.18	0.82	63,63,63,63	0
58	MG	A	3397	1/1	0.89	0.16	0.72	36,36,36,36	0
58	MG	a	3438	1/1	0.99	0.16	0.69	34,34,34,34	0
58	MG	A	3545	1/1	0.94	0.23	0.69	64,64,64,64	0
58	MG	A	3163	1/1	0.96	0.15	0.64	34,34,34,34	0
58	MG	A	3128	1/1	0.96	0.19	0.63	45,45,45,45	0
58	MG	A	3494	1/1	0.97	0.17	0.56	42,42,42,42	0
58	MG	A	3480	1/1	0.98	0.15	0.48	35,35,35,35	0
58	MG	A	3362	1/1	0.97	0.17	0.47	50,50,50,50	0
58	MG	A	3196	1/1	0.93	0.18	0.44	44,44,44,44	0
58	MG	a	3440	1/1	0.78	0.14	0.42	69,69,69,69	0
58	MG	a	3467	1/1	0.94	0.14	0.30	62,62,62,62	0
58	MG	A	3565	1/1	0.82	0.14	0.28	67,67,67,67	0
58	MG	A	3015	1/1	0.98	0.20	0.25	43,43,43,43	0
58	MG	A	3598	1/1	0.82	0.13	0.20	74,74,74,74	0
58	MG	Q	205	1/1	0.90	0.17	0.13	55,55,55,55	0
58	MG	A	3251	1/1	0.91	0.14	0.13	35,35,35,35	0
58	MG	E	304	1/1	0.89	0.21	0.13	55,55,55,55	0
58	MG	A	3123	1/1	0.95	0.16	0.08	51,51,51,51	0
58	MG	a	3420	1/1	0.92	0.17	0.05	62,62,62,62	0
58	MG	a	3343	1/1	0.98	0.16	0.04	29,29,29,29	0
58	MG	a	3403	1/1	0.85	0.15	0.03	61,61,61,61	0
58	MG	A	3626	1/1	0.97	0.13	0.01	51,51,51,51	0
58	MG	a	3456	1/1	0.95	0.18	-0.02	59,59,59,59	0
58	MG	A	3537	1/1	0.98	0.18	-0.13	32,32,32,32	0
58	MG	A	3097	1/1	0.87	0.13	-0.17	60,60,60,60	0
58	MG	A	3342	1/1	0.94	0.16	-0.17	61,61,61,61	0
58	MG	A	3301	1/1	0.93	0.17	-0.17	57,57,57,57	0
60	SF4	d	501	8/8	0.99	0.16	-0.28	48,60,64,65	0
58	MG	A	3100	1/1	0.97	0.13	-0.29	45,45,45,45	0
58	MG	A	3024	1/1	0.92	0.14	-0.35	63,63,63,63	0
58	MG	A	3043	1/1	0.91	0.16	-0.40	59,59,59,59	0
58	MG	E	302	1/1	0.94	0.13	-0.44	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3140	1/1	0.93	0.16	-0.47	57,57,57,57	0
59	ZN	n	102	1/1	0.98	0.14	-0.50	61,61,61,61	0
58	MG	B	204	1/1	0.94	0.15	-0.52	85,85,85,85	0
58	MG	A	3289	1/1	0.94	0.14	-0.64	43,43,43,43	0
58	MG	A	3403	1/1	0.91	0.15	-0.65	40,40,40,40	0
58	MG	a	3327	1/1	0.85	0.12	-0.67	62,62,62,62	0
58	MG	A	3070	1/1	0.96	0.11	-0.70	57,57,57,57	0
58	MG	A	3473	1/1	0.96	0.15	-0.70	46,46,46,46	0
58	MG	A	3159	1/1	0.92	0.13	-0.72	78,78,78,78	0
58	MG	a	3346	1/1	0.89	0.14	-0.77	50,50,50,50	0
58	MG	A	3428	1/1	0.93	0.15	-0.81	36,36,36,36	0
61	GDP	y	703	28/28	0.93	0.15	-0.82	91,120,142,146	0
58	MG	A	3199	1/1	0.90	0.15	-0.91	42,42,42,42	0
59	ZN	5	102	1/1	0.94	0.08	-1.02	70,70,70,70	0
58	MG	a	3384	1/1	0.94	0.14	-1.02	49,49,49,49	0
58	MG	A	3508	1/1	0.93	0.13	-1.04	46,46,46,46	0
58	MG	A	3331	1/1	0.94	0.12	-1.06	54,54,54,54	0
58	MG	a	3418	1/1	0.89	0.11	-1.07	67,67,67,67	0
58	MG	a	3357	1/1	0.90	0.12	-1.20	48,48,48,48	0
59	ZN	Y	501	1/1	0.97	0.08	-1.20	92,92,92,92	0
58	MG	B	213	1/1	0.66	0.11	-1.22	81,81,81,81	0
58	MG	A	3388	1/1	0.85	0.15	-1.27	47,47,47,47	0
58	MG	a	3385	1/1	0.89	0.12	-1.28	33,33,33,33	0
58	MG	A	3462	1/1	0.94	0.12	-1.35	53,53,53,53	0
58	MG	a	3307	1/1	0.97	0.14	-1.35	35,35,35,35	0
58	MG	a	3409	1/1	0.88	0.10	-1.44	74,74,74,74	0
59	ZN	6	102	1/1	0.97	0.09	-1.48	70,70,70,70	0
59	ZN	9	102	1/1	0.97	0.10	-1.52	72,72,72,72	0
58	MG	A	3395	1/1	0.99	0.12	-1.58	31,31,31,31	0
58	MG	A	3430	1/1	0.88	0.14	-1.63	44,44,44,44	0
58	MG	A	3468	1/1	0.96	0.13	-1.64	48,48,48,48	0
58	MG	a	3387	1/1	0.94	0.08	-1.68	55,55,55,55	0
58	MG	A	3609	1/1	0.97	0.13	-1.68	39,39,39,39	0
58	MG	a	3451	1/1	0.86	0.13	-1.72	49,49,49,49	0
58	MG	A	3321	1/1	0.96	0.09	-1.90	41,41,41,41	0
58	MG	A	3181	1/1	0.82	0.10	-2.25	35,35,35,35	0
58	MG	A	3375	1/1	0.81	0.12	-2.28	55,55,55,55	0
58	MG	A	3219	1/1	0.96	0.11	-2.41	61,61,61,61	0
58	MG	a	3389	1/1	0.95	0.11	-2.49	38,38,38,38	0
58	MG	A	3017	1/1	0.99	0.11	-2.49	63,63,63,63	0
58	MG	a	3429	1/1	0.93	0.15	-2.50	49,49,49,49	0
58	MG	A	3433	1/1	0.89	0.08	-2.80	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3514	1/1	0.85	0.14	-2.96	34,34,34,34	0
58	MG	A	3407	1/1	0.92	0.10	-2.98	38,38,38,38	0
59	ZN	4	501	1/1	0.95	0.06	-3.10	117,117,117,117	0
58	MG	A	3553	1/1	0.96	0.08	-3.56	40,40,40,40	0
58	MG	a	3433	1/1	0.91	0.12	-3.56	32,32,32,32	0
58	MG	A	3176	1/1	0.98	0.10	-3.62	35,35,35,35	0
58	MG	A	3583	1/1	0.97	0.10	-3.64	55,55,55,55	0
58	MG	A	3026	1/1	0.94	0.09	-3.84	55,55,55,55	0
58	MG	a	3396	1/1	0.86	0.11	-3.88	42,42,42,42	0
58	MG	a	3312	1/1	0.98	0.07	-4.06	26,26,26,26	0
58	MG	A	3083	1/1	0.95	0.07	-4.37	37,37,37,37	0
58	MG	a	3443	1/1	0.97	0.06	-4.42	46,46,46,46	0
58	MG	A	3205	1/1	0.95	0.12	-5.64	43,43,43,43	0
58	MG	A	3374	1/1	0.89	0.15	-	58,58,58,58	0
58	MG	A	3229	1/1	0.96	0.14	-	46,46,46,46	0
58	MG	B	207	1/1	0.82	0.26	-	103,103,103,103	0
58	MG	A	3250	1/1	0.89	0.22	-	58,58,58,58	0
58	MG	A	3133	1/1	0.95	0.50	-	44,44,44,44	0
58	MG	A	3560	1/1	0.67	0.26	-	79,79,79,79	0
58	MG	A	3126	1/1	0.88	0.21	-	60,60,60,60	0
58	MG	a	3448	1/1	0.97	0.07	-	42,42,42,42	0
58	MG	A	3559	1/1	0.95	0.23	-	46,46,46,46	0
58	MG	A	3198	1/1	0.89	0.21	-	55,55,55,55	0
58	MG	A	3591	1/1	0.92	0.13	-	66,66,66,66	0
58	MG	A	3127	1/1	0.98	0.14	-	73,73,73,73	0
58	MG	a	3400	1/1	0.86	0.30	-	61,61,61,61	0
58	MG	A	3454	1/1	0.93	0.49	-	51,51,51,51	0
58	MG	A	3438	1/1	0.96	0.12	-	53,53,53,53	0
58	MG	A	3092	1/1	0.87	0.38	-	67,67,67,67	0
58	MG	A	3116	1/1	0.95	0.34	-	50,50,50,50	0
58	MG	a	3402	1/1	0.99	0.19	-	43,43,43,43	0
58	MG	A	3634	1/1	0.95	0.14	-	56,56,56,56	0
58	MG	a	3390	1/1	0.44	0.44	-	45,45,45,45	0
58	MG	A	3172	1/1	0.93	0.32	-	31,31,31,31	0
58	MG	A	3593	1/1	0.97	0.30	-	41,41,41,41	0
58	MG	A	3412	1/1	0.96	0.22	-	45,45,45,45	0
58	MG	a	3310	1/1	0.90	0.10	-	52,52,52,52	0
58	MG	A	3294	1/1	0.80	0.37	-	44,44,44,44	0
58	MG	A	3546	1/1	0.91	0.32	-	53,53,53,53	0
58	MG	U	204	1/1	0.97	0.13	-	37,37,37,37	0
58	MG	A	3139	1/1	0.90	0.58	-	62,62,62,62	0
58	MG	A	3445	1/1	0.96	0.08	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3610	1/1	0.93	0.23	-	61,61,61,61	0
58	MG	A	3195	1/1	0.98	0.23	-	41,41,41,41	0
58	MG	A	3282	1/1	0.57	0.44	-	66,66,66,66	0
58	MG	A	3270	1/1	0.80	0.24	-	61,61,61,61	0
58	MG	A	3303	1/1	0.95	0.07	-	55,55,55,55	0
58	MG	A	3355	1/1	0.88	0.13	-	84,84,84,84	0
58	MG	y	702	1/1	0.98	0.18	-	75,75,75,75	0
58	MG	A	3193	1/1	0.99	0.22	-	38,38,38,38	0
58	MG	9	101	1/1	0.93	0.30	-	57,57,57,57	0
58	MG	A	3134	1/1	0.88	0.46	-	67,67,67,67	0
58	MG	A	3499	1/1	0.96	0.10	-	60,60,60,60	0
58	MG	A	3344	1/1	0.95	0.06	-	53,53,53,53	0
58	MG	e	201	1/1	0.92	0.15	-	69,69,69,69	0
58	MG	a	3303	1/1	0.89	0.17	-	58,58,58,58	0
58	MG	a	3423	1/1	0.87	0.40	-	66,66,66,66	0
58	MG	A	3206	1/1	0.95	0.14	-	65,65,65,65	0
58	MG	A	3308	1/1	0.90	0.13	-	56,56,56,56	0
58	MG	A	3351	1/1	0.95	0.20	-	38,38,38,38	0
58	MG	A	3602	1/1	0.88	0.11	-	73,73,73,73	0
58	MG	A	3302	1/1	0.94	0.33	-	59,59,59,59	0
58	MG	a	3475	1/1	0.96	0.37	-	38,38,38,38	0
58	MG	A	3503	1/1	0.96	0.21	-	41,41,41,41	0
58	MG	A	3203	1/1	0.93	0.19	-	53,53,53,53	0
58	MG	A	3020	1/1	0.90	0.15	-	50,50,50,50	0
58	MG	a	3374	1/1	0.97	0.40	-	30,30,30,30	0
58	MG	a	3394	1/1	0.99	0.19	-	32,32,32,32	0
58	MG	A	3030	1/1	0.88	0.36	-	64,64,64,64	0
58	MG	a	3338	1/1	0.96	0.17	-	66,66,66,66	0
58	MG	A	3317	1/1	0.96	0.20	-	31,31,31,31	0
58	MG	A	3506	1/1	0.93	0.14	-	49,49,49,49	0
58	MG	A	3347	1/1	0.87	0.18	-	75,75,75,75	0
58	MG	a	3334	1/1	0.89	0.35	-	43,43,43,43	0
58	MG	A	3479	1/1	0.90	0.18	-	43,43,43,43	0
58	MG	A	3278	1/1	0.87	0.45	-	64,64,64,64	0
58	MG	w	106	1/1	0.95	0.18	-	45,45,45,45	0
58	MG	a	3446	1/1	0.94	0.18	-	68,68,68,68	0
58	MG	A	3469	1/1	0.92	0.13	-	54,54,54,54	0
58	MG	A	3607	1/1	0.80	0.17	-	90,90,90,90	0
58	MG	A	3246	1/1	0.84	0.24	-	49,49,49,49	0
58	MG	a	3358	1/1	0.87	0.35	-	70,70,70,70	0
58	MG	a	3308	1/1	0.91	0.21	-	41,41,41,41	0
58	MG	A	3475	1/1	0.95	0.07	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3492	1/1	0.96	0.10	-	62,62,62,62	0
58	MG	8	101	1/1	0.93	0.11	-	66,66,66,66	0
58	MG	A	3162	1/1	0.82	0.17	-	71,71,71,71	0
58	MG	a	3319	1/1	0.92	0.39	-	39,39,39,39	0
58	MG	A	3158	1/1	0.93	0.50	-	97,97,97,97	0
58	MG	v	101	1/1	0.84	0.51	-	89,89,89,89	0
58	MG	A	3018	1/1	0.85	0.23	-	49,49,49,49	0
58	MG	A	3633	1/1	0.97	0.31	-	64,64,64,64	0
58	MG	a	3477	1/1	0.94	0.13	-	68,68,68,68	0
58	MG	a	3454	1/1	0.91	0.24	-	39,39,39,39	0
58	MG	A	3052	1/1	0.79	0.38	-	59,59,59,59	0
58	MG	a	3349	1/1	0.93	0.38	-	47,47,47,47	0
58	MG	A	3400	1/1	0.97	0.09	-	35,35,35,35	0
58	MG	a	3391	1/1	0.69	0.15	-	72,72,72,72	0
58	MG	A	3447	1/1	0.97	0.22	-	67,67,67,67	0
58	MG	A	3150	1/1	0.90	0.14	-	74,74,74,74	0
58	MG	A	3221	1/1	0.93	0.48	-	58,58,58,58	0
58	MG	A	3054	1/1	0.71	0.27	-	71,71,71,71	0
58	MG	a	3360	1/1	0.86	0.35	-	40,40,40,40	0
58	MG	A	3526	1/1	0.97	0.11	-	41,41,41,41	0
58	MG	R	203	1/1	0.96	0.24	-	44,44,44,44	0
58	MG	V	201	1/1	0.81	0.14	-	53,53,53,53	0
58	MG	a	3393	1/1	0.83	0.52	-	69,69,69,69	0
58	MG	a	3311	1/1	0.95	0.20	-	51,51,51,51	0
58	MG	A	3019	1/1	0.92	0.27	-	49,49,49,49	0
58	MG	a	3302	1/1	0.94	0.26	-	58,58,58,58	0
58	MG	a	3381	1/1	0.97	0.18	-	55,55,55,55	0
58	MG	A	3010	1/1	0.89	0.20	-	41,41,41,41	0
58	MG	A	3413	1/1	0.98	0.25	-	51,51,51,51	0
58	MG	A	3515	1/1	0.91	0.29	-	48,48,48,48	0
58	MG	A	3149	1/1	0.94	0.18	-	53,53,53,53	0
58	MG	A	3550	1/1	0.95	0.13	-	58,58,58,58	0
58	MG	A	3481	1/1	0.82	0.32	-	65,65,65,65	0
58	MG	A	3071	1/1	0.96	0.21	-	41,41,41,41	0
58	MG	a	3459	1/1	0.90	0.26	-	91,91,91,91	0
58	MG	A	3087	1/1	0.76	0.29	-	58,58,58,58	0
58	MG	w	102	1/1	0.99	0.31	-	49,49,49,49	0
58	MG	A	3102	1/1	0.84	0.13	-	59,59,59,59	0
58	MG	a	3405	1/1	0.91	0.18	-	70,70,70,70	0
58	MG	A	3074	1/1	0.90	0.16	-	42,42,42,42	0
58	MG	A	3161	1/1	0.64	0.44	-	67,67,67,67	0
58	MG	A	3555	1/1	0.89	0.17	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	a	3428	1/1	0.85	0.26	-	46,46,46,46	0
58	MG	a	3416	1/1	0.95	0.25	-	61,61,61,61	0
58	MG	A	3614	1/1	0.85	0.16	-	75,75,75,75	0
58	MG	A	3459	1/1	0.97	0.18	-	36,36,36,36	0
58	MG	R	202	1/1	0.94	0.28	-	53,53,53,53	0
58	MG	a	3412	1/1	0.97	0.11	-	48,48,48,48	0
58	MG	A	3580	1/1	0.91	0.23	-	67,67,67,67	0
58	MG	A	3240	1/1	0.80	0.23	-	79,79,79,79	0
58	MG	A	3415	1/1	0.92	0.27	-	42,42,42,42	0
58	MG	A	3393	1/1	0.93	0.32	-	57,57,57,57	0
58	MG	A	3217	1/1	0.92	0.38	-	50,50,50,50	0
58	MG	A	3551	1/1	0.87	0.20	-	63,63,63,63	0
58	MG	A	3470	1/1	0.97	0.18	-	43,43,43,43	0
58	MG	A	3532	1/1	0.86	0.42	-	66,66,66,66	0
58	MG	A	3366	1/1	0.89	0.11	-	58,58,58,58	0
58	MG	A	3474	1/1	0.95	0.12	-	51,51,51,51	0
58	MG	5	101	1/1	0.86	0.58	-	69,69,69,69	0
58	MG	a	3342	1/1	0.94	0.46	-	50,50,50,50	0
58	MG	A	3632	1/1	0.96	0.26	-	63,63,63,63	0
58	MG	A	3271	1/1	0.93	0.16	-	57,57,57,57	0
58	MG	a	3339	1/1	0.91	0.24	-	50,50,50,50	0
58	MG	A	3359	1/1	0.95	0.13	-	45,45,45,45	0
58	MG	A	3365	1/1	0.92	0.13	-	51,51,51,51	0
58	MG	x	3003	1/1	0.54	1.35	-	215,215,215,215	0
58	MG	A	3272	1/1	0.87	0.35	-	62,62,62,62	0
58	MG	a	3399	1/1	0.96	0.18	-	36,36,36,36	0
58	MG	A	3590	1/1	0.92	0.13	-	59,59,59,59	0
58	MG	A	3050	1/1	0.89	0.12	-	39,39,39,39	0
58	MG	a	3452	1/1	0.96	0.10	-	52,52,52,52	0
58	MG	A	3623	1/1	0.95	0.20	-	52,52,52,52	0
58	MG	a	3350	1/1	0.89	0.12	-	73,73,73,73	0
58	MG	A	3456	1/1	0.93	0.29	-	47,47,47,47	0
58	MG	a	3457	1/1	0.93	0.33	-	41,41,41,41	0
58	MG	A	3402	1/1	0.94	0.09	-	50,50,50,50	0
58	MG	A	3441	1/1	0.93	0.14	-	73,73,73,73	0
58	MG	A	3261	1/1	0.91	0.23	-	61,61,61,61	0
58	MG	F	301	1/1	0.90	0.30	-	71,71,71,71	0
58	MG	A	3135	1/1	0.85	0.45	-	54,54,54,54	0
58	MG	A	3082	1/1	0.93	0.62	-	53,53,53,53	0
58	MG	A	3275	1/1	0.86	0.16	-	63,63,63,63	0
58	MG	A	3372	1/1	0.97	0.17	-	59,59,59,59	0
58	MG	A	3248	1/1	0.92	0.61	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3058	1/1	0.76	0.51	-	57,57,57,57	0
58	MG	A	3581	1/1	0.92	0.14	-	55,55,55,55	0
58	MG	A	3467	1/1	0.89	0.35	-	52,52,52,52	0
58	MG	A	3573	1/1	0.83	0.22	-	70,70,70,70	0
58	MG	A	3263	1/1	0.78	0.33	-	55,55,55,55	0
58	MG	A	3346	1/1	0.89	0.23	-	68,68,68,68	0
58	MG	a	3335	1/1	0.89	0.37	-	37,37,37,37	0
58	MG	a	3427	1/1	0.94	0.26	-	50,50,50,50	0
58	MG	a	3419	1/1	0.86	0.23	-	72,72,72,72	0
58	MG	A	3512	1/1	0.90	0.15	-	51,51,51,51	0
58	MG	A	3183	1/1	0.98	0.19	-	54,54,54,54	0
58	MG	A	3279	1/1	0.94	0.14	-	55,55,55,55	0
58	MG	A	3348	1/1	0.95	0.19	-	71,71,71,71	0
58	MG	A	3078	1/1	0.90	0.35	-	47,47,47,47	0
58	MG	A	3185	1/1	0.82	0.35	-	63,63,63,63	0
58	MG	B	201	1/1	0.95	0.33	-	51,51,51,51	0
58	MG	x	3001	1/1	0.51	0.28	-	237,237,237,237	0
58	MG	A	3101	1/1	0.80	0.32	-	74,74,74,74	0
58	MG	B	215	1/1	0.61	0.13	-	114,114,114,114	0
58	MG	A	3060	1/1	0.89	0.26	-	81,81,81,81	0
58	MG	A	3304	1/1	0.90	0.18	-	39,39,39,39	0
58	MG	A	3548	1/1	0.96	0.14	-	40,40,40,40	0
58	MG	a	3372	1/1	0.94	0.30	-	47,47,47,47	0
58	MG	A	3349	1/1	0.96	0.27	-	39,39,39,39	0
58	MG	a	3324	1/1	0.90	0.47	-	40,40,40,40	0
58	MG	A	3029	1/1	0.83	0.19	-	52,52,52,52	0
58	MG	A	3549	1/1	0.85	0.46	-	75,75,75,75	0
58	MG	A	3106	1/1	0.90	0.40	-	57,57,57,57	0
58	MG	A	3025	1/1	0.77	0.20	-	60,60,60,60	0
58	MG	A	3452	1/1	0.91	0.27	-	53,53,53,53	0
58	MG	A	3111	1/1	0.93	0.51	-	61,61,61,61	0
58	MG	A	3408	1/1	0.72	0.12	-	98,98,98,98	0
58	MG	a	3449	1/1	0.97	0.21	-	50,50,50,50	0
58	MG	a	3345	1/1	0.94	0.22	-	47,47,47,47	0
58	MG	a	3383	1/1	0.90	0.21	-	56,56,56,56	0
58	MG	A	3620	1/1	0.95	0.32	-	49,49,49,49	0
58	MG	A	3411	1/1	0.91	0.24	-	47,47,47,47	0
58	MG	a	3437	1/1	0.94	0.15	-	54,54,54,54	0
58	MG	w	104	1/1	0.96	0.09	-	38,38,38,38	0
58	MG	a	3347	1/1	0.96	0.23	-	41,41,41,41	0
58	MG	A	3595	1/1	0.93	0.15	-	63,63,63,63	0
58	MG	A	3322	1/1	0.90	0.24	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3367	1/1	0.90	0.48	-	51,51,51,51	0
58	MG	B	212	1/1	0.95	0.17	-	75,75,75,75	0
58	MG	a	3314	1/1	0.89	0.19	-	60,60,60,60	0
58	MG	A	3376	1/1	0.84	0.12	-	67,67,67,67	0
58	MG	A	3298	1/1	0.86	0.17	-	58,58,58,58	0
58	MG	a	3369	1/1	0.75	0.24	-	60,60,60,60	0
58	MG	a	3305	1/1	0.99	0.20	-	46,46,46,46	0
58	MG	A	3619	1/1	0.76	0.28	-	78,78,78,78	0
58	MG	A	3306	1/1	0.97	0.18	-	50,50,50,50	0
58	MG	A	3260	1/1	0.89	0.11	-	68,68,68,68	0
58	MG	B	211	1/1	0.90	0.34	-	61,61,61,61	0
58	MG	A	3392	1/1	0.93	0.22	-	47,47,47,47	0
58	MG	A	3227	1/1	0.92	0.44	-	43,43,43,43	0
58	MG	A	3124	1/1	0.83	0.14	-	54,54,54,54	0
58	MG	a	3470	1/1	0.93	0.15	-	56,56,56,56	0
58	MG	a	3353	1/1	0.92	0.15	-	48,48,48,48	0
58	MG	A	3131	1/1	0.90	0.29	-	53,53,53,53	0
58	MG	a	3473	1/1	0.97	0.45	-	43,43,43,43	0
58	MG	A	3216	1/1	0.65	0.36	-	62,62,62,62	0
58	MG	A	3605	1/1	0.90	0.24	-	70,70,70,70	0
58	MG	a	3417	1/1	0.96	0.31	-	37,37,37,37	0
58	MG	A	3290	1/1	0.91	0.23	-	49,49,49,49	0
58	MG	a	3336	1/1	0.90	0.29	-	62,62,62,62	0
58	MG	A	3121	1/1	0.84	0.18	-	62,62,62,62	0
58	MG	a	3329	1/1	0.84	0.16	-	46,46,46,46	0
58	MG	A	3236	1/1	0.81	0.55	-	67,67,67,67	0
58	MG	A	3044	1/1	0.73	0.37	-	72,72,72,72	0
58	MG	A	3110	1/1	0.86	0.28	-	42,42,42,42	0
58	MG	A	3335	1/1	0.89	0.10	-	56,56,56,56	0
58	MG	A	3089	1/1	0.88	0.19	-	47,47,47,47	0
58	MG	A	3571	1/1	0.91	0.37	-	89,89,89,89	0
58	MG	A	3531	1/1	0.94	0.07	-	91,91,91,91	0
58	MG	A	3281	1/1	0.89	0.14	-	57,57,57,57	0
58	MG	A	3612	1/1	0.97	0.05	-	53,53,53,53	0
58	MG	A	3085	1/1	0.85	0.34	-	52,52,52,52	0
58	MG	A	3314	1/1	0.95	0.23	-	54,54,54,54	0
58	MG	A	3505	1/1	0.92	0.18	-	68,68,68,68	0
58	MG	A	3156	1/1	0.96	0.08	-	86,86,86,86	0
58	MG	0	103	1/1	0.93	0.19	-	61,61,61,61	0
58	MG	A	3371	1/1	0.94	0.11	-	53,53,53,53	0
58	MG	A	3057	1/1	0.82	0.25	-	56,56,56,56	0
58	MG	A	3320	1/1	0.97	0.12	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	B	209	1/1	0.64	0.27	-	70,70,70,70	0
58	MG	a	3408	1/1	0.93	0.12	-	55,55,55,55	0
58	MG	0	102	1/1	0.85	0.10	-	61,61,61,61	0
58	MG	a	3434	1/1	0.85	0.24	-	54,54,54,54	0
58	MG	A	3224	1/1	0.89	0.44	-	51,51,51,51	0
58	MG	a	3301	1/1	0.92	0.23	-	49,49,49,49	0
58	MG	7	103	1/1	0.86	0.26	-	57,57,57,57	0
58	MG	a	3377	1/1	0.83	0.22	-	85,85,85,85	0
58	MG	A	3235	1/1	0.90	0.14	-	48,48,48,48	0
58	MG	l	201	1/1	0.90	0.47	-	61,61,61,61	0
58	MG	B	218	1/1	0.95	0.23	-	74,74,74,74	0
58	MG	A	3576	1/1	0.83	0.34	-	89,89,89,89	0
58	MG	A	3547	1/1	0.97	0.20	-	60,60,60,60	0
58	MG	A	3611	1/1	0.89	0.20	-	52,52,52,52	0
58	MG	a	3352	1/1	0.79	0.25	-	59,59,59,59	0
58	MG	A	3377	1/1	0.98	0.16	-	44,44,44,44	0
58	MG	A	3073	1/1	0.80	0.45	-	56,56,56,56	0
58	MG	Q	203	1/1	0.86	0.21	-	45,45,45,45	0
58	MG	A	3247	1/1	0.82	0.42	-	66,66,66,66	0
58	MG	U	202	1/1	0.94	0.37	-	62,62,62,62	0
58	MG	A	3339	1/1	0.80	0.17	-	68,68,68,68	0
58	MG	A	3152	1/1	0.74	0.44	-	68,68,68,68	0
58	MG	A	3031	1/1	0.91	0.17	-	70,70,70,70	0
58	MG	A	3204	1/1	0.93	0.24	-	43,43,43,43	0
58	MG	A	3115	1/1	0.96	0.12	-	48,48,48,48	0
58	MG	A	3332	1/1	0.98	0.20	-	39,39,39,39	0
58	MG	A	3112	1/1	0.83	0.36	-	66,66,66,66	0
58	MG	A	3325	1/1	0.93	0.28	-	52,52,52,52	0
58	MG	A	3495	1/1	0.98	0.25	-	40,40,40,40	0
58	MG	A	3461	1/1	0.86	0.50	-	59,59,59,59	0
58	MG	a	3442	1/1	0.93	0.08	-	45,45,45,45	0
58	MG	a	3365	1/1	0.95	0.73	-	45,45,45,45	0
58	MG	A	3588	1/1	0.98	0.17	-	40,40,40,40	0
58	MG	A	3266	1/1	0.91	0.38	-	61,61,61,61	0
58	MG	a	3304	1/1	0.94	0.09	-	55,55,55,55	0
58	MG	A	3567	1/1	0.92	0.17	-	47,47,47,47	0
58	MG	A	3066	1/1	0.78	0.19	-	56,56,56,56	0
58	MG	a	3375	1/1	0.96	0.56	-	41,41,41,41	0
58	MG	A	3562	1/1	0.88	0.19	-	59,59,59,59	0
58	MG	a	3481	1/1	0.93	0.27	-	46,46,46,46	0
58	MG	A	3586	1/1	0.86	0.28	-	55,55,55,55	0
58	MG	A	3525	1/1	0.89	0.15	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3558	1/1	0.94	0.14	-	73,73,73,73	0
58	MG	A	3603	1/1	0.75	0.34	-	82,82,82,82	0
58	MG	A	3466	1/1	0.93	0.08	-	67,67,67,67	0
58	MG	A	3630	1/1	0.97	0.18	-	43,43,43,43	0
58	MG	A	3449	1/1	0.93	0.23	-	51,51,51,51	0
58	MG	m	201	1/1	0.95	0.20	-	35,35,35,35	0
58	MG	A	3334	1/1	0.67	0.13	-	84,84,84,84	0
58	MG	A	3256	1/1	0.98	0.14	-	55,55,55,55	0
58	MG	A	3434	1/1	0.84	0.22	-	56,56,56,56	0
58	MG	A	3343	1/1	0.90	0.13	-	69,69,69,69	0
58	MG	A	3069	1/1	0.91	0.23	-	46,46,46,46	0
58	MG	a	3379	1/1	0.98	0.21	-	30,30,30,30	0
58	MG	a	3348	1/1	0.82	0.50	-	53,53,53,53	0
58	MG	A	3472	1/1	0.94	0.17	-	53,53,53,53	0
58	MG	A	3277	1/1	0.90	0.53	-	71,71,71,71	0
58	MG	A	3604	1/1	0.95	0.35	-	64,64,64,64	0
58	MG	A	3238	1/1	0.98	0.26	-	45,45,45,45	0
58	MG	A	3130	1/1	0.93	0.46	-	43,43,43,43	0
58	MG	a	3476	1/1	0.94	0.09	-	50,50,50,50	0
58	MG	A	3286	1/1	0.88	0.16	-	62,62,62,62	0
58	MG	A	3137	1/1	0.93	0.46	-	59,59,59,59	0
58	MG	A	3618	1/1	0.95	0.29	-	45,45,45,45	0
58	MG	A	3091	1/1	0.93	0.21	-	63,63,63,63	0
58	MG	A	3182	1/1	0.79	0.30	-	53,53,53,53	0
58	MG	A	3463	1/1	0.90	0.25	-	46,46,46,46	0
58	MG	A	3197	1/1	0.87	0.28	-	40,40,40,40	0
58	MG	A	3312	1/1	0.91	0.23	-	59,59,59,59	0
58	MG	A	3444	1/1	0.92	0.34	-	48,48,48,48	0
58	MG	A	3001	1/1	0.85	0.33	-	70,70,70,70	0
58	MG	A	3051	1/1	0.90	0.24	-	43,43,43,43	0
58	MG	a	3364	1/1	0.92	0.43	-	56,56,56,56	0
58	MG	Z	301	1/1	0.88	0.18	-	66,66,66,66	0
58	MG	A	3213	1/1	0.70	0.45	-	67,67,67,67	0
58	MG	A	3253	1/1	0.63	0.29	-	66,66,66,66	0
58	MG	A	3084	1/1	0.71	0.21	-	57,57,57,57	0
58	MG	A	3108	1/1	0.77	0.35	-	54,54,54,54	0
58	MG	A	3291	1/1	0.90	0.12	-	60,60,60,60	0
58	MG	w	101	1/1	0.87	0.75	-	60,60,60,60	0
58	MG	A	3012	1/1	0.96	0.15	-	37,37,37,37	0
58	MG	A	3326	1/1	0.88	0.17	-	69,69,69,69	0
58	MG	A	3427	1/1	0.95	0.16	-	62,62,62,62	0
58	MG	A	3569	1/1	0.82	0.45	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3596	1/1	0.83	0.20	-	45,45,45,45	0
58	MG	B	216	1/1	0.63	0.12	-	86,86,86,86	0
58	MG	A	3418	1/1	0.98	0.37	-	32,32,32,32	0
58	MG	A	3076	1/1	0.92	0.19	-	41,41,41,41	0
58	MG	a	3337	1/1	0.95	0.26	-	50,50,50,50	0
58	MG	A	3220	1/1	0.77	0.21	-	49,49,49,49	0
58	MG	A	3517	1/1	0.90	0.25	-	51,51,51,51	0
58	MG	A	3287	1/1	0.81	0.25	-	54,54,54,54	0
58	MG	A	3534	1/1	0.96	0.36	-	45,45,45,45	0
58	MG	D	305	1/1	0.82	0.18	-	37,37,37,37	0
58	MG	A	3578	1/1	0.91	0.23	-	64,64,64,64	0
58	MG	A	3307	1/1	0.96	0.20	-	45,45,45,45	0
58	MG	a	3468	1/1	0.88	0.18	-	69,69,69,69	0
58	MG	A	3390	1/1	0.95	0.24	-	46,46,46,46	0
58	MG	A	3406	1/1	0.91	0.14	-	56,56,56,56	0
58	MG	A	3042	1/1	0.87	0.16	-	92,92,92,92	0
58	MG	A	3296	1/1	0.97	0.36	-	52,52,52,52	0
58	MG	A	3431	1/1	0.90	0.35	-	69,69,69,69	0
58	MG	A	3460	1/1	0.98	0.19	-	44,44,44,44	0
58	MG	a	3411	1/1	0.93	0.16	-	53,53,53,53	0
58	MG	a	3483	1/1	0.99	0.17	-	39,39,39,39	0
58	MG	a	3321	1/1	0.88	0.18	-	48,48,48,48	0
58	MG	X	101	1/1	0.90	0.23	-	72,72,72,72	0
58	MG	A	3528	1/1	0.98	0.09	-	51,51,51,51	0
58	MG	A	3257	1/1	0.96	0.18	-	50,50,50,50	0
58	MG	A	3186	1/1	0.89	0.16	-	90,90,90,90	0
58	MG	A	3245	1/1	0.81	0.28	-	56,56,56,56	0
58	MG	A	3268	1/1	0.88	0.26	-	58,58,58,58	0
58	MG	A	3488	1/1	0.97	0.31	-	50,50,50,50	0
58	MG	A	3533	1/1	0.90	0.18	-	47,47,47,47	0
58	MG	A	3360	1/1	0.83	0.21	-	60,60,60,60	0
58	MG	a	3367	1/1	0.96	0.25	-	30,30,30,30	0
58	MG	a	3410	1/1	0.87	0.37	-	45,45,45,45	0
58	MG	A	3309	1/1	0.87	0.26	-	52,52,52,52	0
58	MG	A	3276	1/1	0.85	0.07	-	73,73,73,73	0
58	MG	A	3180	1/1	0.95	0.64	-	44,44,44,44	0
58	MG	a	3450	1/1	0.85	0.08	-	55,55,55,55	0
58	MG	A	3361	1/1	0.92	0.12	-	84,84,84,84	0
58	MG	A	3451	1/1	0.85	0.18	-	82,82,82,82	0
58	MG	a	3315	1/1	0.89	0.22	-	60,60,60,60	0
58	MG	A	3457	1/1	0.97	0.20	-	41,41,41,41	0
58	MG	A	3584	1/1	0.93	0.24	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	a	3370	1/1	0.91	0.18	-	66,66,66,66	0
58	MG	A	3061	1/1	0.91	0.22	-	54,54,54,54	0
58	MG	a	3326	1/1	0.92	0.21	-	48,48,48,48	0
58	MG	A	3369	1/1	0.97	0.17	-	54,54,54,54	0
58	MG	A	3338	1/1	0.97	0.28	-	30,30,30,30	0
58	MG	A	3265	1/1	0.60	0.18	-	61,61,61,61	0
58	MG	A	3280	1/1	0.95	0.28	-	32,32,32,32	0
58	MG	A	3328	1/1	0.84	0.20	-	62,62,62,62	0
58	MG	A	3613	1/1	0.93	0.17	-	52,52,52,52	0
58	MG	a	3380	1/1	0.90	0.22	-	57,57,57,57	0
58	MG	a	3366	1/1	0.89	0.23	-	38,38,38,38	0
58	MG	A	3175	1/1	0.83	0.38	-	46,46,46,46	0
58	MG	a	3432	1/1	0.96	0.09	-	46,46,46,46	0
58	MG	A	3249	1/1	0.98	0.11	-	31,31,31,31	0
58	MG	a	3472	1/1	0.76	0.17	-	61,61,61,61	0
58	MG	B	214	1/1	0.61	1.51	-	83,83,83,83	0
58	MG	A	3090	1/1	0.96	0.38	-	38,38,38,38	0
58	MG	A	3283	1/1	0.97	0.12	-	55,55,55,55	0
58	MG	a	3340	1/1	0.88	0.45	-	81,81,81,81	0
58	MG	A	3136	1/1	0.92	0.40	-	49,49,49,49	0
58	MG	a	3404	1/1	0.96	0.44	-	38,38,38,38	0
58	MG	A	3210	1/1	0.94	0.21	-	56,56,56,56	0
58	MG	A	3629	1/1	0.94	0.20	-	70,70,70,70	0
58	MG	A	3243	1/1	0.84	0.55	-	58,58,58,58	0
58	MG	A	3178	1/1	0.97	0.23	-	31,31,31,31	0
58	MG	A	3241	1/1	0.94	0.15	-	42,42,42,42	0
58	MG	A	3299	1/1	0.91	0.19	-	64,64,64,64	0
58	MG	A	3065	1/1	0.94	0.25	-	74,74,74,74	0
58	MG	A	3510	1/1	0.96	0.16	-	60,60,60,60	0
58	MG	A	3285	1/1	0.88	0.25	-	50,50,50,50	0
58	MG	A	3202	1/1	0.94	0.37	-	50,50,50,50	0
58	MG	B	203	1/1	0.96	0.07	-	56,56,56,56	0
58	MG	a	3317	1/1	0.97	0.31	-	26,26,26,26	0
58	MG	A	3096	1/1	0.94	0.23	-	58,58,58,58	0
58	MG	B	202	1/1	0.98	0.27	-	66,66,66,66	0
58	MG	A	3484	1/1	0.93	0.14	-	50,50,50,50	0
58	MG	A	3527	1/1	0.96	0.20	-	63,63,63,63	0
58	MG	A	3511	1/1	0.91	0.17	-	99,99,99,99	0
58	MG	a	3421	1/1	0.88	0.11	-	61,61,61,61	0
58	MG	A	3489	1/1	0.94	0.12	-	55,55,55,55	0
58	MG	a	3436	1/1	0.80	0.26	-	66,66,66,66	0
58	MG	A	3003	1/1	0.82	0.30	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3566	1/1	0.96	0.11	-	40,40,40,40	0
58	MG	A	3345	1/1	0.92	0.20	-	44,44,44,44	0
58	MG	A	3518	1/1	0.98	0.04	-	65,65,65,65	0
58	MG	A	3036	1/1	0.92	0.11	-	74,74,74,74	0
58	MG	A	3267	1/1	0.96	0.27	-	59,59,59,59	0
58	MG	A	3579	1/1	0.97	0.19	-	53,53,53,53	0
58	MG	A	3062	1/1	0.90	0.26	-	42,42,42,42	0
58	MG	A	3585	1/1	0.89	0.18	-	47,47,47,47	0
58	MG	A	3416	1/1	0.98	0.21	-	41,41,41,41	0
58	MG	a	3431	1/1	0.93	0.10	-	41,41,41,41	0
58	MG	A	3477	1/1	0.95	0.14	-	65,65,65,65	0
58	MG	a	3485	1/1	0.94	0.25	-	51,51,51,51	0
58	MG	A	3608	1/1	0.29	0.47	-	108,108,108,108	0
58	MG	A	3194	1/1	0.98	0.34	-	34,34,34,34	0
58	MG	A	3439	1/1	0.93	0.18	-	58,58,58,58	0
58	MG	A	3098	1/1	0.96	0.15	-	48,48,48,48	0
58	MG	A	3383	1/1	0.85	0.24	-	55,55,55,55	0
58	MG	A	3242	1/1	0.90	0.11	-	63,63,63,63	0
58	MG	A	3543	1/1	0.88	0.14	-	71,71,71,71	0
58	MG	A	3507	1/1	0.89	0.17	-	46,46,46,46	0
58	MG	A	3621	1/1	0.93	0.30	-	59,59,59,59	0
58	MG	a	3458	1/1	0.86	0.26	-	62,62,62,62	0
58	MG	a	3325	1/1	0.91	0.82	-	55,55,55,55	0
58	MG	a	3386	1/1	0.95	0.47	-	41,41,41,41	0
58	MG	A	3627	1/1	0.92	0.14	-	91,91,91,91	0
58	MG	E	303	1/1	0.92	0.19	-	41,41,41,41	0
58	MG	A	3563	1/1	0.83	0.19	-	73,73,73,73	0
58	MG	A	3356	1/1	0.92	0.24	-	57,57,57,57	0
58	MG	A	3168	1/1	0.91	0.41	-	48,48,48,48	0
58	MG	a	3453	1/1	0.97	0.07	-	41,41,41,41	0
58	MG	A	3016	1/1	0.93	0.14	-	49,49,49,49	0
58	MG	B	217	1/1	0.81	0.27	-	67,67,67,67	0
58	MG	A	3401	1/1	0.94	0.11	-	37,37,37,37	0
58	MG	A	3577	1/1	0.67	0.20	-	72,72,72,72	0
58	MG	A	3292	1/1	0.96	0.23	-	54,54,54,54	0
58	MG	a	3388	1/1	0.73	0.23	-	59,59,59,59	0
58	MG	f	201	1/1	0.83	0.25	-	92,92,92,92	0
58	MG	0	101	1/1	0.62	0.39	-	73,73,73,73	0
58	MG	A	3421	1/1	0.98	0.18	-	40,40,40,40	0
58	MG	A	3145	1/1	0.88	0.09	-	48,48,48,48	0
58	MG	a	3341	1/1	0.87	0.27	-	60,60,60,60	0
58	MG	a	3424	1/1	0.92	0.11	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3635	1/1	0.81	0.62	-	69,69,69,69	0
58	MG	a	3461	1/1	0.93	0.14	-	44,44,44,44	0
58	MG	A	3063	1/1	0.90	0.16	-	62,62,62,62	0
58	MG	A	3288	1/1	0.82	0.33	-	60,60,60,60	0
58	MG	a	3344	1/1	0.96	0.12	-	51,51,51,51	0
58	MG	A	3038	1/1	0.99	0.15	-	55,55,55,55	0
58	MG	a	3361	1/1	0.89	0.15	-	73,73,73,73	0
58	MG	A	3337	1/1	0.97	0.27	-	44,44,44,44	0
58	MG	a	3322	1/1	0.97	0.10	-	50,50,50,50	0
58	MG	A	3575	1/1	0.91	0.09	-	70,70,70,70	0
58	MG	A	3624	1/1	0.89	0.15	-	52,52,52,52	0
58	MG	A	3398	1/1	0.92	0.26	-	43,43,43,43	0
58	MG	A	3177	1/1	0.92	0.17	-	65,65,65,65	0
58	MG	A	3628	1/1	0.94	0.16	-	87,87,87,87	0
58	MG	F	303	1/1	0.93	0.11	-	36,36,36,36	0
58	MG	A	3478	1/1	0.88	0.11	-	65,65,65,65	0
58	MG	A	3353	1/1	0.86	0.17	-	79,79,79,79	0
58	MG	A	3122	1/1	0.83	0.19	-	35,35,35,35	0
58	MG	A	3254	1/1	0.74	0.37	-	67,67,67,67	0
58	MG	A	3497	1/1	0.92	0.25	-	50,50,50,50	0
58	MG	O	201	1/1	0.97	0.10	-	38,38,38,38	0
58	MG	A	3255	1/1	0.81	0.32	-	57,57,57,57	0
58	MG	A	3129	1/1	0.87	0.24	-	48,48,48,48	0
58	MG	a	3316	1/1	0.74	0.25	-	54,54,54,54	0
58	MG	A	3385	1/1	0.96	0.19	-	57,57,57,57	0
58	MG	a	3328	1/1	0.86	0.25	-	60,60,60,60	0
58	MG	a	3463	1/1	0.94	0.21	-	45,45,45,45	0
58	MG	A	3491	1/1	0.91	0.26	-	72,72,72,72	0
58	MG	A	3142	1/1	0.90	0.10	-	84,84,84,84	0
58	MG	B	206	1/1	0.82	0.17	-	75,75,75,75	0
58	MG	A	3453	1/1	0.95	0.16	-	44,44,44,44	0
58	MG	A	3064	1/1	0.89	0.37	-	50,50,50,50	0
58	MG	A	3284	1/1	0.76	0.28	-	67,67,67,67	0
58	MG	A	3422	1/1	0.96	0.18	-	52,52,52,52	0
58	MG	A	3535	1/1	0.97	0.21	-	49,49,49,49	0
58	MG	A	3381	1/1	0.96	0.24	-	43,43,43,43	0
58	MG	w	105	1/1	0.94	0.24	-	29,29,29,29	0
58	MG	A	3258	1/1	0.94	0.21	-	43,43,43,43	0
58	MG	a	3332	1/1	0.84	0.16	-	45,45,45,45	0
58	MG	A	3425	1/1	0.92	0.23	-	62,62,62,62	0
58	MG	A	3146	1/1	0.92	0.27	-	56,56,56,56	0
58	MG	A	3212	1/1	0.87	0.15	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3496	1/1	0.96	0.18	-	47,47,47,47	0
58	MG	a	3373	1/1	0.86	0.24	-	63,63,63,63	0
58	MG	A	3471	1/1	0.92	0.33	-	56,56,56,56	0
58	MG	A	3300	1/1	0.95	0.17	-	60,60,60,60	0
58	MG	a	3371	1/1	0.81	0.25	-	65,65,65,65	0
58	MG	A	3521	1/1	0.99	0.22	-	60,60,60,60	0
58	MG	A	3379	1/1	0.94	0.25	-	50,50,50,50	0
58	MG	a	3455	1/1	0.70	0.10	-	67,67,67,67	0
58	MG	A	3436	1/1	0.85	0.17	-	87,87,87,87	0
58	MG	A	3075	1/1	0.76	0.17	-	67,67,67,67	0
58	MG	A	3597	1/1	0.96	0.27	-	65,65,65,65	0
58	MG	A	3055	1/1	0.97	0.12	-	45,45,45,45	0
58	MG	A	3357	1/1	0.82	0.24	-	69,69,69,69	0
58	MG	A	3035	1/1	0.95	0.09	-	47,47,47,47	0
58	MG	D	304	1/1	0.91	0.36	-	74,74,74,74	0
58	MG	A	3625	1/1	0.92	0.19	-	84,84,84,84	0
58	MG	A	3305	1/1	0.81	0.28	-	70,70,70,70	0
58	MG	A	3429	1/1	0.98	0.25	-	30,30,30,30	0
58	MG	A	3409	1/1	0.97	0.25	-	60,60,60,60	0
58	MG	A	3600	1/1	0.86	0.25	-	64,64,64,64	0
58	MG	A	3539	1/1	0.96	0.13	-	52,52,52,52	0
58	MG	a	3398	1/1	0.97	0.39	-	27,27,27,27	0
58	MG	A	3315	1/1	0.94	0.26	-	56,56,56,56	0
58	MG	A	3572	1/1	0.68	0.38	-	70,70,70,70	0
58	MG	A	3104	1/1	0.87	0.21	-	64,64,64,64	0
58	MG	A	3519	1/1	0.97	0.30	-	30,30,30,30	0
58	MG	A	3556	1/1	0.96	0.16	-	55,55,55,55	0
58	MG	a	3359	1/1	0.88	0.14	-	65,65,65,65	0
58	MG	a	3462	1/1	0.92	0.13	-	74,74,74,74	0
58	MG	A	3617	1/1	0.81	0.19	-	65,65,65,65	0
58	MG	B	205	1/1	0.96	0.22	-	81,81,81,81	0
58	MG	A	3435	1/1	0.38	0.39	-	95,95,95,95	0
58	MG	A	3088	1/1	0.96	0.15	-	63,63,63,63	0
58	MG	a	3464	1/1	0.95	0.07	-	44,44,44,44	0
58	MG	A	3432	1/1	0.92	0.19	-	58,58,58,58	0
58	MG	A	3336	1/1	0.92	0.22	-	36,36,36,36	0
58	MG	a	3474	1/1	0.88	0.16	-	64,64,64,64	0
58	MG	A	3482	1/1	0.93	0.09	-	67,67,67,67	0
58	MG	A	3014	1/1	0.87	0.14	-	39,39,39,39	0
58	MG	A	3631	1/1	0.91	0.24	-	87,87,87,87	0
58	MG	a	3356	1/1	0.93	0.22	-	49,49,49,49	0
58	MG	A	3387	1/1	0.96	0.17	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
58	MG	A	3237	1/1	0.88	0.16	-	51,51,51,51	0
58	MG	a	3469	1/1	0.95	0.38	-	42,42,42,42	0
58	MG	A	3465	1/1	0.89	0.15	-	68,68,68,68	0
58	MG	a	3479	1/1	0.97	0.18	-	47,47,47,47	0
58	MG	A	3148	1/1	0.86	0.38	-	60,60,60,60	0
58	MG	A	3053	1/1	0.89	0.45	-	61,61,61,61	0
58	MG	a	3460	1/1	0.97	0.14	-	52,52,52,52	0
58	MG	a	3354	1/1	0.94	0.13	-	51,51,51,51	0
58	MG	G	201	1/1	0.89	0.16	-	71,71,71,71	0
58	MG	A	3599	1/1	0.96	0.21	-	57,57,57,57	0
58	MG	a	3425	1/1	0.84	0.25	-	47,47,47,47	0
58	MG	A	3424	1/1	0.97	0.27	-	57,57,57,57	0
58	MG	B	208	1/1	0.73	0.11	-	74,74,74,74	0
58	MG	A	3262	1/1	0.91	0.08	-	63,63,63,63	0
58	MG	A	3592	1/1	0.98	0.08	-	67,67,67,67	0
58	MG	A	3113	1/1	0.76	0.31	-	63,63,63,63	0
58	MG	A	3504	1/1	0.92	0.37	-	38,38,38,38	0
58	MG	P	202	1/1	0.85	0.27	-	86,86,86,86	0
58	MG	A	3615	1/1	0.85	0.23	-	50,50,50,50	0
58	MG	A	3179	1/1	0.98	0.18	-	43,43,43,43	0
58	MG	a	3484	1/1	0.83	0.23	-	67,67,67,67	0
58	MG	A	3589	1/1	0.85	0.24	-	46,46,46,46	0
58	MG	A	3169	1/1	0.97	0.29	-	57,57,57,57	0
58	MG	a	3465	1/1	0.98	0.07	-	57,57,57,57	0
58	MG	A	3426	1/1	0.83	0.28	-	55,55,55,55	0
58	MG	A	3464	1/1	0.89	0.25	-	49,49,49,49	0
58	MG	A	3354	1/1	0.66	0.24	-	101,101,101,101	0
58	MG	A	3561	1/1	0.96	0.14	-	54,54,54,54	0
58	MG	A	3502	1/1	0.88	0.25	-	56,56,56,56	0
58	MG	a	3482	1/1	0.97	0.14	-	37,37,37,37	0
58	MG	A	3333	1/1	0.94	0.08	-	62,62,62,62	0
58	MG	w	103	1/1	0.94	0.18	-	38,38,38,38	0
58	MG	A	3524	1/1	0.94	0.11	-	53,53,53,53	0
58	MG	A	3160	1/1	0.66	0.48	-	61,61,61,61	0
58	MG	a	3445	1/1	0.93	0.20	-	66,66,66,66	0
58	MG	A	3582	1/1	0.95	0.15	-	63,63,63,63	0
58	MG	A	3226	1/1	0.72	0.43	-	68,68,68,68	0
58	MG	A	3132	1/1	0.70	0.77	-	48,48,48,48	0
58	MG	A	3228	1/1	0.95	0.19	-	62,62,62,62	0
58	MG	a	3320	1/1	0.94	0.14	-	39,39,39,39	0
58	MG	A	3105	1/1	0.94	0.12	-	35,35,35,35	0
58	MG	A	3522	1/1	0.96	0.17	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3264	1/1	0.88	0.33	-	65,65,65,65	0
58	MG	A	3542	1/1	0.93	0.65	-	60,60,60,60	0
58	MG	a	3426	1/1	0.85	0.13	-	69,69,69,69	0
58	MG	a	3480	1/1	0.78	0.27	-	77,77,77,77	0
58	MG	A	3318	1/1	0.96	0.32	-	60,60,60,60	0
58	MG	G	203	1/1	0.94	0.09	-	69,69,69,69	0
58	MG	A	3037	1/1	0.90	0.27	-	61,61,61,61	0
58	MG	A	3273	1/1	0.81	0.42	-	77,77,77,77	0
58	MG	A	3232	1/1	0.92	0.30	-	36,36,36,36	0
58	MG	A	3218	1/1	0.95	0.45	-	32,32,32,32	0
58	MG	a	3413	1/1	0.88	0.14	-	54,54,54,54	0
58	MG	A	3099	1/1	0.92	0.20	-	34,34,34,34	0
58	MG	A	3538	1/1	0.97	0.17	-	40,40,40,40	0
58	MG	A	3389	1/1	0.97	0.25	-	30,30,30,30	0
58	MG	a	3363	1/1	0.94	0.24	-	43,43,43,43	0
58	MG	A	3040	1/1	0.80	0.27	-	58,58,58,58	0
58	MG	A	3094	1/1	0.99	0.27	-	31,31,31,31	0
58	MG	a	3441	1/1	0.94	0.19	-	62,62,62,62	0
58	MG	A	3587	1/1	0.96	0.25	-	48,48,48,48	0
58	MG	A	3458	1/1	0.97	0.32	-	27,27,27,27	0
58	MG	A	3350	1/1	0.87	0.10	-	63,63,63,63	0
58	MG	A	3386	1/1	0.90	0.17	-	59,59,59,59	0
58	MG	A	3622	1/1	0.94	0.23	-	49,49,49,49	0
58	MG	A	3310	1/1	0.94	0.14	-	45,45,45,45	0
58	MG	a	3430	1/1	0.95	0.08	-	65,65,65,65	0
58	MG	A	3259	1/1	0.81	0.09	-	74,74,74,74	0
58	MG	a	3478	1/1	0.97	0.13	-	48,48,48,48	0
58	MG	A	3443	1/1	0.98	0.14	-	39,39,39,39	0
58	MG	A	3211	1/1	0.93	0.47	-	55,55,55,55	0
58	MG	a	3333	1/1	0.93	0.16	-	51,51,51,51	0
58	MG	A	3013	1/1	0.88	0.21	-	52,52,52,52	0
58	MG	F	305	1/1	0.85	0.25	-	59,59,59,59	0
58	MG	a	3362	1/1	0.87	0.16	-	73,73,73,73	0
58	MG	A	3028	1/1	0.94	0.27	-	66,66,66,66	0
58	MG	A	3327	1/1	0.93	0.14	-	49,49,49,49	0
58	MG	A	3574	1/1	0.87	0.16	-	57,57,57,57	0
58	MG	a	3407	1/1	0.92	0.34	-	82,82,82,82	0
58	MG	A	3368	1/1	0.95	0.23	-	47,47,47,47	0
58	MG	A	3370	1/1	0.87	0.16	-	64,64,64,64	0
58	MG	A	3405	1/1	0.83	0.15	-	61,61,61,61	0
58	MG	A	3138	1/1	0.92	0.22	-	77,77,77,77	0
58	MG	A	3330	1/1	0.89	0.34	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3373	1/1	0.87	0.08	-	64,64,64,64	0
58	MG	A	3570	1/1	0.81	0.17	-	57,57,57,57	0
58	MG	A	3153	1/1	0.93	0.22	-	82,82,82,82	0
58	MG	a	3444	1/1	0.95	0.16	-	53,53,53,53	0
58	MG	A	3419	1/1	0.89	0.13	-	74,74,74,74	0
58	MG	A	3440	1/1	0.96	0.20	-	74,74,74,74	0
58	MG	A	3269	1/1	0.89	0.23	-	54,54,54,54	0
58	MG	W	201	1/1	0.91	1.25	-	77,77,77,77	0
58	MG	A	3081	1/1	0.85	0.28	-	61,61,61,61	0
58	MG	A	3554	1/1	0.71	0.21	-	74,74,74,74	0
58	MG	A	3391	1/1	0.97	0.21	-	30,30,30,30	0
58	MG	a	3392	1/1	0.74	0.14	-	65,65,65,65	0
58	MG	A	3329	1/1	0.98	0.14	-	40,40,40,40	0
58	MG	A	3151	1/1	0.95	0.29	-	43,43,43,43	0
58	MG	U	203	1/1	0.54	0.46	-	67,67,67,67	0
58	MG	A	3483	1/1	0.98	0.17	-	55,55,55,55	0
58	MG	A	3448	1/1	0.91	0.44	-	48,48,48,48	0
58	MG	A	3068	1/1	0.66	0.28	-	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.