



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:30 PM GMT

PDB ID : 2V3C
Title : CRYSTAL STRUCTURE OF THE SRP54-SRP19-7S.S SRP RNA COM-
PLEX OF M. JANNASCHII
Authors : Hainzl, T.; Huang, S.; Sauer-Eriksson, A.E.
Deposited on : 2007-06-15
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

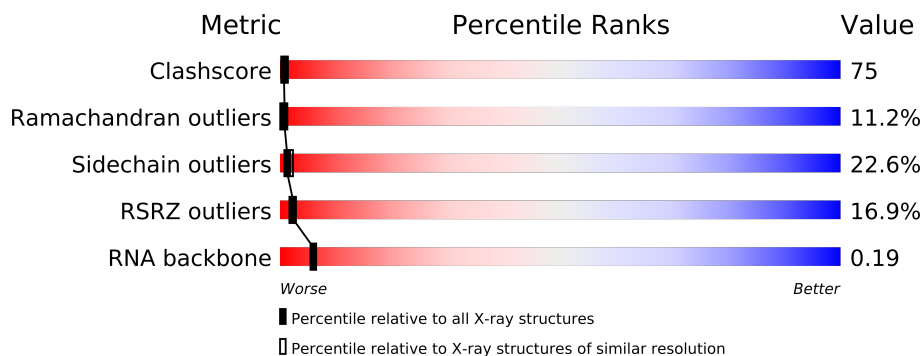
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)
RNA backbone	1838	1107 (3.10-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	87	
1	B	87	
2	C	432	
2	D	432	
3	M	96	
3	N	96	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12336 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein called SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	87	Total	C	N	O	S	0	0	0
			727	468	130	125	4			
1	B	87	Total	C	N	O	S	0	0	0
			727	468	130	125	4			

- Molecule 2 is a protein called SIGNAL RECOGNITION 54 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	404	Total	C	N	O	S	0	0	1
			3149	1998	541	600	10			
2	D	402	Total	C	N	O	S	0	0	1
			3133	1989	538	597	9			

- Molecule 3 is a RNA chain called 7S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	96	Total	C	N	O	P	0	0	0
			2063	919	385	664	95			
3	N	96	Total	C	N	O	P	0	0	0
			2063	919	385	664	95			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	26	Total	O	0	0
			26	26		
4	C	107	Total	O	0	0
			107	107		
4	D	107	Total	O	0	0
			107	107		

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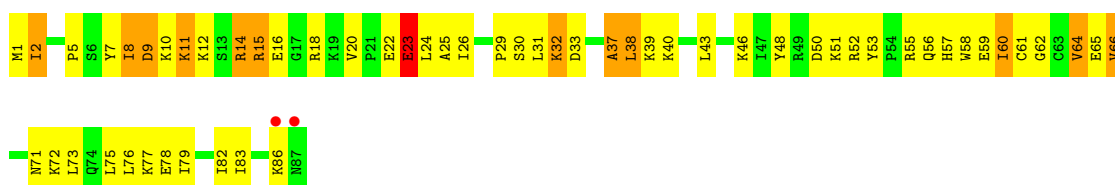
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	92	Total 92	O 92	0	0
4	N	119	Total 119	O 119	0	0

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 errors 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: SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN

Chain A: 



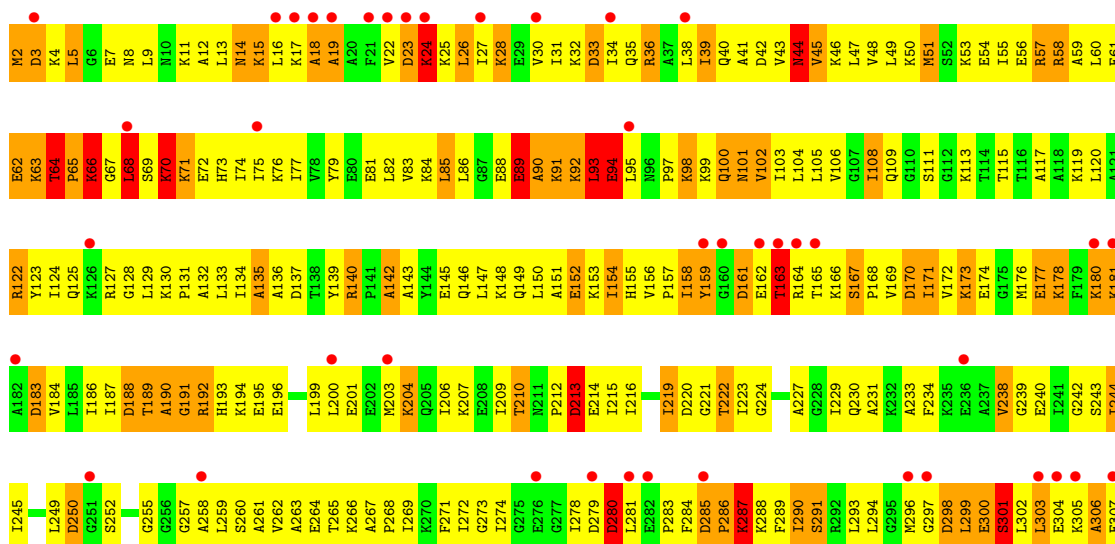
• Molecule 1: SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN

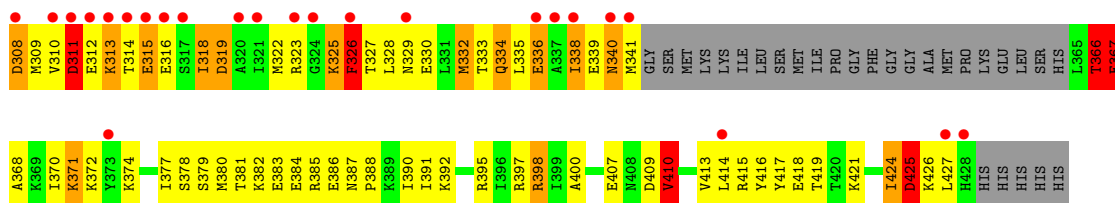
Chain B: 



• Molecule 2: SIGNAL RECOGNITION 54 KDA PROTEIN

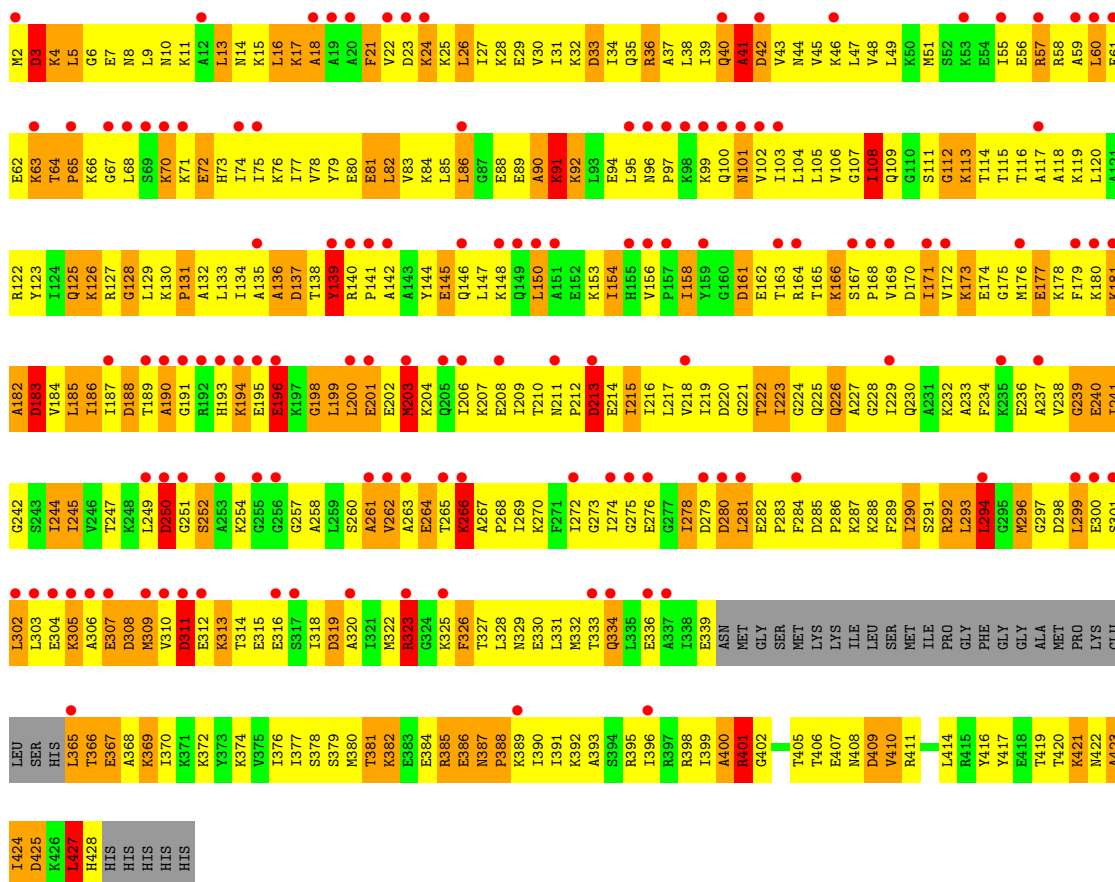
Chain C: 





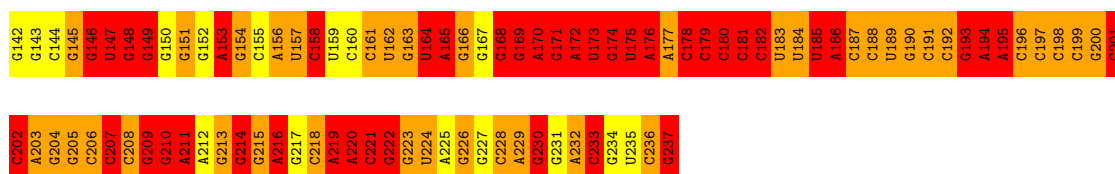
• Molecule 2: SIGNAL RECOGNITION 54 KDA PROTEIN

Chain D:



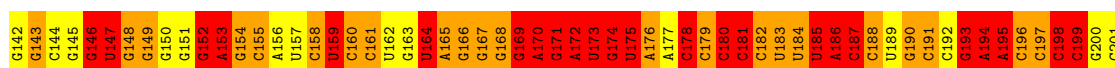
• Molecule 3: 7S RNA

Chain M:



• Molecule 3: 7S RNA

Chain N:



C202	A203	G204	G205	C206	C207	C208	G209	G210	A211	A212	G213	G214	G215	A216	G217	C218	A219	A220	C221	G222	G223	U224	A225	G226	G227	C228	A229	G230	G231	A232	C233	G234	U235	C236	G237
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.29Å 129.40Å 163.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 32.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.50) 93.6 (32.35-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.244 , 0.294 0.263 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 55298 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12336	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	1.19	1/740 (0.1%)	1.26	4/984 (0.4%)
1	B	1.15	1/740 (0.1%)	1.17	6/984 (0.6%)
2	C	0.83	1/3176 (0.0%)	1.05	16/4248 (0.4%)
2	D	0.63	0/3160	0.99	16/4227 (0.4%)
3	M	2.58	140/2309 (6.1%)	3.88	600/3603 (16.7%)
3	N	2.26	91/2309 (3.9%)	3.38	476/3603 (13.2%)
All	All	1.62	234/12434 (1.9%)	2.46	1118/17649 (6.3%)

All (234) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	218	C	N1-C6	-14.80	1.28	1.37
3	M	217	G	C8-N7	12.07	1.38	1.30
3	M	217	G	N7-C5	11.67	1.46	1.39
3	M	168	G	N3-C4	-11.48	1.27	1.35
3	N	172	A	N9-C4	11.11	1.44	1.37
3	M	216	A	N9-C4	11.06	1.44	1.37
3	M	216	A	C8-N7	11.03	1.39	1.31
3	M	223	G	C5-C4	-10.82	1.30	1.38
3	N	219	A	C5-C4	-10.77	1.31	1.38
3	M	207	C	N1-C6	-10.62	1.30	1.37
3	N	219	A	C6-N1	-10.28	1.28	1.35
3	M	219	A	C8-N7	10.27	1.38	1.31
3	M	204	G	C5-C4	-10.24	1.31	1.38
3	N	166	G	C5-C4	-9.95	1.31	1.38
3	M	217	G	C5-C4	-9.63	1.31	1.38
3	M	192	C	C4-C5	-9.34	1.35	1.43
3	M	167	G	C8-N7	9.32	1.36	1.30
3	N	204	G	C8-N7	9.16	1.36	1.30
3	N	146	G	C3'-O3'	9.01	1.54	1.42
3	M	146	G	C3'-O3'	8.85	1.54	1.42
3	M	205	G	N9-C4	8.76	1.45	1.38
3	M	209	G	C6-N1	8.68	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	156	A	C5-C6	-8.64	1.33	1.41
3	M	201	C	C4-N4	8.50	1.41	1.33
3	M	216	A	C5-C6	-8.49	1.33	1.41
3	M	215	G	P-O5'	8.47	1.68	1.59
3	N	198	C	N1-C6	-8.43	1.32	1.37
3	N	205	G	C3'-O3'	-8.38	1.30	1.42
3	M	202	C	C2-N3	-8.36	1.29	1.35
3	N	217	G	C5-C4	-8.34	1.32	1.38
3	M	220	A	C8-N7	8.32	1.37	1.31
3	N	220	A	C8-N7	8.29	1.37	1.31
3	M	162	U	N1-C2	-8.17	1.31	1.38
3	M	209	G	C5-C4	-8.16	1.32	1.38
3	M	168	G	C8-N7	8.13	1.35	1.30
3	N	220	A	N9-C4	8.11	1.42	1.37
3	N	211	A	C5-C6	-8.10	1.33	1.41
3	M	203	A	N7-C5	8.05	1.44	1.39
3	N	166	G	C6-N1	-8.04	1.33	1.39
3	M	218	C	N3-C4	-8.03	1.28	1.33
3	M	199	C	C4-C5	-7.68	1.36	1.43
3	M	209	G	C2'-O2'	-7.65	1.31	1.41
3	N	171	G	N1-C2	-7.65	1.31	1.37
3	M	171	G	C6-N1	-7.57	1.34	1.39
3	M	168	G	C6-N1	-7.56	1.34	1.39
3	M	204	G	N9-C8	-7.56	1.32	1.37
3	M	179	C	C2'-O2'	7.51	1.51	1.41
3	M	163	G	C8-N7	7.50	1.35	1.30
3	N	197	C	N1-C6	-7.49	1.32	1.37
3	M	221	C	N1-C2	-7.48	1.32	1.40
3	M	215	G	C8-N7	7.47	1.35	1.30
3	M	205	G	C8-N7	7.38	1.35	1.30
3	M	160	C	N1-C6	-7.37	1.32	1.37
3	N	168	G	C5-C6	-7.25	1.35	1.42
3	N	142	G	C5-C6	-7.24	1.35	1.42
3	N	205	G	N9-C4	7.21	1.43	1.38
3	M	209	G	N9-C4	7.18	1.43	1.38
3	M	168	G	C5-C4	-7.17	1.33	1.38
3	M	209	G	C3'-O3'	7.17	1.52	1.42
3	M	181	C	C1'-N1	7.16	1.59	1.48
3	M	168	G	C2-N3	-7.12	1.27	1.32
3	M	219	A	C6-N1	-7.12	1.30	1.35
3	M	168	G	N7-C5	7.08	1.43	1.39
3	M	214	G	C5-C4	-7.06	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	201	C	C2-O2	7.04	1.30	1.24
3	N	166	G	C5-C6	-6.99	1.35	1.42
3	N	154	G	C8-N7	6.98	1.35	1.30
3	N	164	U	C3'-O3'	6.97	1.51	1.42
3	M	161	C	C2-N3	-6.93	1.30	1.35
3	M	170	A	C5-C4	-6.92	1.33	1.38
3	M	220	A	C6-N6	6.86	1.39	1.33
3	M	227	G	C6-N1	-6.86	1.34	1.39
3	N	209	G	C8-N7	6.84	1.35	1.30
3	N	215	G	C5-C6	-6.82	1.35	1.42
3	N	211	A	N7-C5	-6.81	1.35	1.39
3	N	198	C	C4-C5	-6.81	1.37	1.43
3	M	158	C	N1-C6	-6.79	1.33	1.37
3	M	171	G	C8-N7	6.79	1.35	1.30
3	M	217	G	C5-C6	-6.79	1.35	1.42
3	M	219	A	C3'-O3'	-6.78	1.32	1.42
3	M	199	C	N1-C6	-6.75	1.33	1.37
3	M	163	G	C4'-C3'	-6.73	1.45	1.53
3	M	204	G	C5-C6	-6.73	1.35	1.42
3	N	225	A	C5-C6	-6.70	1.35	1.41
3	N	163	G	C5-C4	-6.66	1.33	1.38
3	M	223	G	C2'-O2'	-6.65	1.32	1.41
3	N	162	U	N1-C2	-6.65	1.32	1.38
3	N	147	U	C4'-C3'	-6.62	1.45	1.53
3	M	215	G	N9-C4	6.60	1.43	1.38
3	N	170	A	C8-N7	6.55	1.36	1.31
3	M	205	G	C5-C6	-6.55	1.35	1.42
3	N	208	C	N3-C4	6.53	1.38	1.33
3	M	209	G	C5-C6	-6.51	1.35	1.42
3	M	229	A	C5-C4	-6.49	1.34	1.38
3	N	179	C	N3-C4	-6.47	1.29	1.33
3	N	155	C	N3-C4	-6.41	1.29	1.33
3	N	218	C	P-O5'	-6.40	1.53	1.59
3	M	203	A	C5-C4	-6.38	1.34	1.38
3	M	194	A	N9-C8	-6.38	1.32	1.37
3	N	157	U	N1-C2	-6.37	1.32	1.38
3	M	152	G	N3-C4	-6.35	1.31	1.35
3	M	172	A	C5-C4	-6.34	1.34	1.38
3	M	223	G	C5-C6	-6.34	1.36	1.42
3	N	169	G	C2-N3	6.34	1.37	1.32
3	N	170	A	C6-N6	-6.33	1.28	1.33
3	M	186	A	N3-C4	-6.33	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	217	G	C5-C6	-6.32	1.36	1.42
3	N	208	C	N1-C6	6.30	1.41	1.37
3	M	215	G	C5-C6	-6.28	1.36	1.42
3	M	219	A	C5-C4	-6.26	1.34	1.38
3	M	200	G	N3-C4	-6.25	1.31	1.35
3	N	215	G	N3-C4	-6.23	1.31	1.35
3	M	220	A	N9-C4	6.22	1.41	1.37
3	M	207	C	C1'-N1	6.22	1.58	1.48
3	N	205	G	C5-C6	-6.20	1.36	1.42
3	M	212	A	C6-N6	-6.19	1.28	1.33
3	M	235	U	C3'-O3'	-6.18	1.33	1.42
3	N	220	A	N7-C5	-6.17	1.35	1.39
3	N	207	C	C1'-N1	6.16	1.57	1.48
3	N	208	C	O3'-P	-6.15	1.53	1.61
3	M	197	C	C1'-N1	6.14	1.57	1.48
3	M	215	G	C5-C4	-6.11	1.34	1.38
3	N	171	G	P-O5'	6.11	1.65	1.59
3	M	162	U	O5'-C5'	6.10	1.54	1.44
3	N	163	G	N3-C4	-6.09	1.31	1.35
3	M	158	C	O3'-P	-6.04	1.53	1.61
3	N	194	A	N3-C4	-6.02	1.31	1.34
3	N	169	G	C2-N2	6.02	1.40	1.34
3	N	168	G	C8-N7	5.99	1.34	1.30
3	N	176	A	C6-N1	-5.94	1.31	1.35
3	N	217	G	C2-N2	5.93	1.40	1.34
3	M	146	G	C2'-O2'	-5.91	1.33	1.41
3	M	155	C	P-O5'	5.90	1.65	1.59
3	N	155	C	C4-C5	-5.88	1.38	1.43
3	M	210	G	C8-N7	5.87	1.34	1.30
3	N	218	C	C1'-N1	5.86	1.57	1.48
3	M	203	A	N9-C4	5.83	1.41	1.37
3	M	154	G	N1-C2	5.82	1.42	1.37
3	M	204	G	N1-C2	-5.82	1.33	1.37
3	M	211	A	N3-C4	-5.80	1.31	1.34
3	M	202	C	C2'-C1'	-5.75	1.47	1.53
1	A	53	TYR	CG-CD1	-5.73	1.31	1.39
3	M	211	A	C8-N7	5.73	1.35	1.31
3	M	209	G	C2-N3	-5.69	1.28	1.32
3	M	205	G	N1-C2	-5.69	1.33	1.37
3	N	153	A	C4'-C3'	-5.69	1.46	1.52
3	M	215	G	N3-C4	-5.69	1.31	1.35
3	N	165	A	C2'-C1'	-5.66	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	213	G	C5-C4	-5.66	1.34	1.38
3	N	220	A	N3-C4	5.64	1.38	1.34
3	M	229	A	C3'-O3'	-5.63	1.34	1.42
3	M	186	A	N9-C4	-5.63	1.34	1.37
3	M	229	A	C6-N1	-5.63	1.31	1.35
3	N	179	C	N1-C2	-5.62	1.34	1.40
3	N	146	G	O3'-P	5.60	1.67	1.61
3	M	166	G	O3'-P	-5.59	1.54	1.61
3	N	164	U	P-O5'	5.59	1.65	1.59
3	M	177	A	N3-C4	-5.59	1.31	1.34
3	N	151	G	C8-N7	5.59	1.34	1.30
3	M	217	G	C2-N3	5.59	1.37	1.32
3	N	148	G	C3'-O3'	-5.58	1.34	1.42
3	N	216	A	N9-C4	5.56	1.41	1.37
3	N	174	G	N1-C2	-5.54	1.33	1.37
3	M	196	C	C2-N3	5.54	1.40	1.35
3	M	204	G	C6-N1	-5.53	1.35	1.39
3	M	193	G	N9-C8	-5.53	1.33	1.37
3	N	227	G	C5-C6	-5.53	1.36	1.42
3	M	201	C	C2-N3	5.52	1.40	1.35
3	M	144	C	C3'-O3'	-5.50	1.34	1.42
3	M	174	G	C5-C6	-5.50	1.36	1.42
3	N	163	G	C8-N7	5.50	1.34	1.30
3	N	207	C	N3-C4	-5.49	1.30	1.33
3	N	215	G	N9-C4	5.49	1.42	1.38
3	N	174	G	C6-N1	-5.47	1.35	1.39
3	N	156	A	N9-C4	5.46	1.41	1.37
3	M	212	A	C6-N1	-5.45	1.31	1.35
3	N	215	G	C2-N3	-5.44	1.28	1.32
3	M	152	G	N1-C2	5.43	1.42	1.37
3	M	217	G	C2'-C1'	-5.41	1.47	1.53
2	C	410	VAL	CB-CG1	-5.41	1.41	1.52
3	M	198	C	O5'-C5'	-5.41	1.34	1.42
3	M	165	A	C4'-C3'	-5.41	1.47	1.52
3	N	176	A	N7-C5	5.40	1.42	1.39
3	M	145	G	C6-O6	5.38	1.28	1.24
3	M	155	C	C3'-O3'	-5.37	1.34	1.42
3	M	220	A	C5-C4	-5.37	1.34	1.38
1	B	4	TRP	CE3-CZ3	-5.36	1.29	1.38
3	N	161	C	C1'-N1	5.36	1.56	1.48
3	M	217	G	C4'-C3'	-5.36	1.47	1.52
3	M	218	C	C2'-C1'	-5.35	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	186	A	C6-N6	5.35	1.38	1.33
3	N	204	G	N1-C2	-5.30	1.33	1.37
3	M	154	G	C6-O6	5.30	1.28	1.24
3	N	218	C	N1-C2	-5.30	1.34	1.40
3	M	180	C	N1-C6	-5.27	1.33	1.37
3	N	217	G	N1-C2	5.27	1.42	1.37
3	N	213	G	C6-N1	-5.26	1.35	1.39
3	N	211	A	C5-C4	-5.25	1.35	1.38
3	M	167	G	P-OP2	-5.23	1.40	1.49
3	M	199	C	N3-C4	-5.23	1.30	1.33
3	M	187	C	N3-C4	-5.22	1.30	1.33
3	M	210	G	C6-O6	5.22	1.28	1.24
3	N	169	G	N1-C2	5.20	1.42	1.37
3	M	200	G	C2-N3	-5.19	1.28	1.32
3	M	207	C	C4-C5	-5.19	1.38	1.43
3	M	233	C	N1-C6	-5.19	1.34	1.37
3	M	149	G	C2'-C1'	-5.18	1.47	1.53
3	N	171	G	N3-C4	-5.18	1.31	1.35
3	N	206	C	C3'-O3'	5.17	1.49	1.42
3	M	149	G	C8-N7	5.16	1.34	1.30
3	M	206	C	C4-C5	-5.16	1.38	1.43
3	N	142	G	C3'-O3'	-5.15	1.34	1.42
3	N	170	A	N1-C2	-5.15	1.29	1.34
3	N	166	G	O3'-P	-5.13	1.54	1.61
3	N	194	A	N9-C4	-5.13	1.34	1.37
3	N	172	A	N3-C4	5.12	1.38	1.34
3	M	149	G	C6-N1	-5.11	1.35	1.39
3	N	232	A	C3'-O3'	-5.11	1.34	1.42
3	M	213	G	C8-N7	5.09	1.34	1.30
3	M	205	G	N7-C5	5.08	1.42	1.39
3	N	168	G	C5-C4	-5.08	1.34	1.38
3	M	193	G	C6-N1	-5.08	1.35	1.39
3	M	219	A	C2'-O2'	5.07	1.48	1.41
3	M	166	G	C5-C4	-5.04	1.34	1.38
3	M	174	G	C5-C4	-5.04	1.34	1.38
3	M	165	A	C2'-C1'	-5.03	1.47	1.53
3	N	145	G	C6-N1	-5.02	1.36	1.39
3	M	159	U	N3-C4	-5.01	1.33	1.38
3	M	160	C	O3'-P	-5.01	1.55	1.61
3	M	216	A	C1'-N9	-5.01	1.39	1.46
3	M	219	A	N9-C4	-5.01	1.34	1.37
3	N	145	G	N1-C2	-5.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	235	U	P-O5'	5.00	1.64	1.59
3	N	218	C	C4'-C3'	-5.00	1.47	1.52

All (1118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	209	G	C5-C6-O6	-24.70	113.78	128.60
3	M	194	A	O4'-C1'-N9	-20.43	91.86	108.20
3	M	217	G	C5-C6-O6	-20.20	116.48	128.60
3	N	217	G	C5-C6-O6	-19.78	116.73	128.60
3	M	142	G	O4'-C1'-N9	-18.30	93.56	108.20
3	M	209	G	C6-N1-C2	-17.66	114.51	125.10
3	M	209	G	N1-C6-O6	17.05	130.13	119.90
3	M	181	C	O4'-C1'-N1	16.12	121.10	108.20
3	M	216	A	C8-N9-C4	-15.42	99.63	105.80
3	M	208	C	N3-C4-C5	15.18	127.97	121.90
3	M	216	A	C5-C6-N6	-15.16	111.57	123.70
3	N	168	G	C5-C6-O6	-15.16	119.50	128.60
3	M	208	C	N3-C2-O2	-14.99	111.41	121.90
3	N	208	C	N3-C4-C5	14.93	127.87	121.90
3	N	168	G	O4'-C1'-N9	14.73	119.99	108.20
3	N	217	G	N1-C6-O6	14.62	128.67	119.90
3	M	218	C	C3'-C2'-C1'	-14.59	89.83	101.50
3	N	155	C	C6-N1-C2	-14.18	114.63	120.30
3	M	221	C	C4-C5-C6	-14.15	110.33	117.40
3	M	203	A	O4'-C1'-N9	-14.02	96.99	108.20
3	M	217	G	C4-C5-N7	13.99	116.40	110.80
3	N	216	A	O4'-C4'-C3'	-13.90	90.10	104.00
3	N	163	G	N3-C2-N2	-13.87	110.19	119.90
3	N	202	C	C6-N1-C2	13.83	125.83	120.30
3	N	170	A	C2-N3-C4	13.80	117.50	110.60
3	M	209	G	N3-C2-N2	-13.57	110.40	119.90
3	M	163	G	N9-C4-C5	13.50	110.80	105.40
3	N	165	A	P-O3'-C3'	-13.41	103.61	119.70
3	N	237	G	O4'-C1'-N9	-13.41	97.47	108.20
3	M	217	G	C5-N7-C8	-13.29	97.66	104.30
3	M	237	G	O4'-C1'-N9	-13.27	97.58	108.20
3	M	152	G	N3-C2-N2	-13.15	110.70	119.90
3	M	163	G	N3-C2-N2	-13.15	110.70	119.90
3	N	170	A	C5-C6-N1	13.13	124.27	117.70
3	M	163	G	C4-C5-N7	-13.08	105.57	110.80
3	M	169	G	C5-C6-N1	13.05	118.03	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	218	C	C6-N1-C2	13.05	125.52	120.30
3	M	216	A	C2-N3-C4	12.99	117.09	110.60
3	M	146	G	C5-C6-O6	12.96	136.38	128.60
3	M	164	U	C1'-O4'-C4'	-12.91	99.58	109.90
3	M	170	A	O4'-C1'-N9	12.85	118.48	108.20
3	N	194	A	N9-C1'-C2'	12.83	130.68	114.00
3	N	223	G	O4'-C1'-N9	-12.72	98.02	108.20
3	M	221	C	C5-C6-N1	12.68	127.34	121.00
3	M	194	A	P-O3'-C3'	-12.67	104.50	119.70
3	M	171	G	C8-N9-C4	-12.59	101.36	106.40
3	M	216	A	N1-C6-N6	12.55	126.13	118.60
3	N	199	C	C5-C4-N4	12.50	128.95	120.20
3	M	146	G	N9-C4-C5	12.49	110.39	105.40
3	M	215	G	O4'-C1'-N9	-12.39	98.29	108.20
3	M	163	G	C6-N1-C2	-12.38	117.67	125.10
3	M	162	U	C4'-C3'-C2'	-12.36	90.24	102.60
3	N	199	C	N3-C4-N4	-12.25	109.42	118.00
3	M	171	G	N9-C4-C5	12.20	110.28	105.40
3	M	164	U	O4'-C1'-N1	12.14	117.92	108.20
3	M	204	G	C5-N7-C8	-12.04	98.28	104.30
3	M	204	G	C4-C5-N7	12.03	115.61	110.80
3	M	208	C	N3-C4-N4	-12.02	109.59	118.00
3	N	163	G	N9-C4-C5	12.01	110.20	105.40
3	M	174	G	N9-C1'-C2'	-11.99	98.41	114.00
3	M	211	A	N9-C1'-C2'	11.89	129.46	114.00
3	M	165	A	P-O3'-C3'	-11.80	105.53	119.70
3	M	218	C	C5-C6-N1	-11.71	115.15	121.00
3	M	161	C	O4'-C1'-N1	-11.68	98.86	108.20
3	M	201	C	O4'-C1'-N1	11.58	117.47	108.20
3	M	168	G	N3-C2-N2	-11.57	111.80	119.90
3	N	151	G	N3-C2-N2	-11.54	111.82	119.90
3	M	159	U	O4'-C1'-N1	-11.51	98.99	108.20
3	M	210	G	N3-C4-N9	-11.49	119.10	126.00
3	N	217	G	O4'-C4'-C3'	-11.49	92.51	104.00
3	M	168	G	N9-C4-C5	11.48	109.99	105.40
3	M	205	G	O4'-C4'-C3'	-11.44	92.56	104.00
3	M	175	U	O4'-C1'-N1	11.39	117.31	108.20
3	M	222	G	O4'-C1'-N9	11.33	117.26	108.20
3	N	160	C	C6-N1-C2	-11.27	115.79	120.30
3	M	161	C	C4'-C3'-C2'	-11.26	91.34	102.60
3	M	217	G	N1-C6-O6	11.23	126.64	119.90
3	N	204	G	C4'-C3'-C2'	-11.21	91.39	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	225	A	N1-C6-N6	11.11	125.27	118.60
3	M	223	G	O4'-C1'-N9	-11.07	99.34	108.20
3	N	211	A	C5-C6-N6	-11.02	114.89	123.70
3	N	147	U	O4'-C4'-C3'	-10.96	93.04	104.00
3	M	183	U	O4'-C1'-N1	-10.92	99.46	108.20
3	M	205	G	C4'-C3'-C2'	-10.91	91.69	102.60
3	N	159	U	N3-C2-O2	-10.87	114.59	122.20
3	M	216	A	O4'-C4'-C3'	-10.80	93.20	104.00
3	M	208	C	N1-C2-O2	10.78	125.37	118.90
3	N	193	G	O4'-C1'-N9	-10.76	99.59	108.20
3	N	176	A	O4'-C1'-N9	-10.73	99.61	108.20
3	M	213	G	C6-N1-C2	-10.71	118.67	125.10
3	M	197	C	P-O5'-C5'	-10.70	103.79	120.90
3	M	227	G	C4'-C3'-C2'	-10.68	91.92	102.60
3	N	217	G	C6-C5-N7	-10.65	124.01	130.40
3	M	186	A	C2-N3-C4	-10.64	105.28	110.60
3	M	216	A	C6-N1-C2	-10.63	112.22	118.60
3	M	174	G	O4'-C1'-N9	10.61	116.69	108.20
3	M	171	G	N1-C6-O6	-10.52	113.59	119.90
3	M	165	A	P-O5'-C5'	-10.50	104.10	120.90
3	M	214	G	C5-C6-O6	-10.49	122.30	128.60
3	M	202	C	O4'-C1'-N1	10.48	116.58	108.20
3	M	216	A	N3-C4-C5	-10.41	119.51	126.80
3	N	161	C	N1-C2-O2	-10.38	112.67	118.90
3	M	158	C	C2-N3-C4	-10.27	114.77	119.90
3	N	217	G	C4-C5-N7	10.26	114.90	110.80
3	M	210	G	N9-C4-C5	10.25	109.50	105.40
3	M	208	C	C2-N3-C4	-10.25	114.78	119.90
3	M	202	C	C6-N1-C2	10.21	124.38	120.30
3	M	217	G	C5-C6-N1	10.20	116.60	111.50
3	M	219	A	C5-N7-C8	-10.18	98.81	103.90
3	M	217	G	C6-C5-N7	-10.17	124.30	130.40
3	N	151	G	C8-N9-C4	-10.12	102.35	106.40
3	N	202	C	C5-C6-N1	-10.12	115.94	121.00
3	M	158	C	N1-C2-O2	-10.09	112.85	118.90
3	N	218	C	N1-C2-O2	-10.08	112.85	118.90
3	M	237	G	C1'-O4'-C4'	-10.07	101.84	109.90
3	M	162	U	P-O5'-C5'	-10.05	104.81	120.90
3	M	204	G	C6-C5-N7	-10.03	124.38	130.40
3	N	208	C	C4-C5-C6	-9.99	112.40	117.40
3	N	213	G	C4'-C3'-C2'	-9.99	92.61	102.60
3	M	165	A	O4'-C1'-N9	-9.96	100.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	197	C	N1-C2-O2	9.96	124.88	118.90
3	N	206	C	C4'-C3'-C2'	-9.95	92.65	102.60
3	N	151	G	N9-C4-C5	9.93	109.37	105.40
3	M	195	A	P-O3'-C3'	-9.89	107.83	119.70
3	M	218	C	O4'-C4'-C3'	-9.88	94.12	104.00
3	N	163	G	N3-C4-N9	-9.88	120.07	126.00
3	N	227	G	C5-C6-O6	-9.86	122.68	128.60
3	N	149	G	P-O5'-C5'	-9.82	105.18	120.90
3	M	168	G	N3-C4-N9	-9.82	120.11	126.00
3	M	216	A	N7-C8-N9	9.77	118.69	113.80
3	N	214	G	C4'-C3'-C2'	-9.75	92.85	102.60
3	N	163	G	C6-N1-C2	-9.71	119.27	125.10
3	N	219	A	N1-C6-N6	9.68	124.41	118.60
3	M	194	A	C1'-O4'-C4'	-9.67	102.16	109.90
3	M	164	U	C5'-C4'-O4'	-9.65	97.52	109.10
3	M	219	A	O4'-C1'-N9	-9.64	100.49	108.20
3	N	155	C	N1-C2-O2	9.59	124.66	118.90
3	M	215	G	O5'-P-OP2	-9.59	97.07	105.70
3	N	192	C	N3-C4-C5	9.58	125.73	121.90
3	M	207	C	O4'-C1'-N1	9.56	115.85	108.20
3	N	155	C	O4'-C1'-N1	9.55	115.84	108.20
3	M	196	C	N1-C2-O2	-9.55	113.17	118.90
3	M	200	G	P-O5'-C5'	-9.51	105.68	120.90
3	M	215	G	O4'-C1'-C2'	-9.49	96.31	105.80
3	M	203	A	O4'-C1'-C2'	-9.49	96.31	105.80
3	N	185	U	O4'-C4'-C3'	-9.47	94.53	104.00
3	N	170	A	N1-C6-N6	-9.47	112.92	118.60
3	M	203	A	C5-C6-N1	9.46	122.43	117.70
3	M	216	A	C4'-C3'-C2'	-9.46	93.14	102.60
3	M	198	C	O4'-C1'-N1	-9.45	100.64	108.20
3	M	222	G	N1-C6-O6	-9.44	114.23	119.90
3	M	209	G	C4'-C3'-C2'	-9.39	93.21	102.60
3	N	151	G	N1-C2-N2	9.38	124.64	116.20
3	N	168	G	C6-N1-C2	-9.36	119.49	125.10
3	N	192	C	C6-N1-C2	9.36	124.04	120.30
3	M	190	G	P-O3'-C3'	-9.34	108.49	119.70
3	M	146	G	N1-C6-O6	-9.34	114.30	119.90
3	M	198	C	C4'-C3'-C2'	-9.32	93.28	102.60
3	M	168	G	N1-C2-N2	9.32	124.59	116.20
3	M	215	G	C1'-O4'-C4'	9.31	117.35	109.90
3	M	204	G	C4'-C3'-C2'	-9.29	93.31	102.60
3	M	206	C	O4'-C4'-C3'	-9.29	94.71	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	147	U	P-O3'-C3'	-9.27	108.58	119.70
3	M	170	A	N1-C2-N3	-9.26	124.67	129.30
3	M	152	G	N1-C6-O6	9.25	125.45	119.90
3	M	208	C	C4-C5-C6	-9.24	112.78	117.40
3	N	155	C	C2-N3-C4	9.24	124.52	119.90
3	M	201	C	C4-C5-C6	-9.23	112.78	117.40
3	M	166	G	C5'-C4'-O4'	-9.22	98.04	109.10
3	M	192	C	O4'-C1'-N1	-9.20	100.84	108.20
3	M	183	U	C5-C6-N1	9.20	127.30	122.70
3	M	183	U	P-O3'-C3'	-9.19	108.67	119.70
3	M	228	C	N3-C4-C5	9.18	125.57	121.90
3	M	152	G	C5-C6-O6	-9.18	123.09	128.60
3	N	160	C	N3-C4-C5	-9.18	118.23	121.90
3	M	216	A	C5-C6-N1	9.15	122.28	117.70
3	M	188	C	C6-N1-C2	9.15	123.96	120.30
3	M	189	U	O4'-C1'-N1	9.15	115.52	108.20
3	N	155	C	C5-C6-N1	9.15	125.57	121.00
3	N	226	G	C5-C6-N1	9.14	116.07	111.50
3	N	219	A	C5-N7-C8	-9.12	99.34	103.90
3	N	147	U	O4'-C1'-N1	-9.10	100.92	108.20
3	M	209	G	N1-C2-N3	9.10	129.36	123.90
3	N	198	C	P-O5'-C5'	-9.05	106.42	120.90
3	M	162	U	O5'-P-OP1	-9.04	97.56	105.70
3	N	153	A	C4'-C3'-C2'	-9.04	93.56	102.60
3	M	172	A	O4'-C1'-N9	-9.04	100.97	108.20
3	N	172	A	O4'-C1'-C2'	-9.02	96.78	105.80
3	M	146	G	N3-C4-N9	-9.01	120.60	126.00
3	M	203	A	O4'-C4'-C3'	-9.01	94.99	104.00
3	M	171	G	C5-C6-O6	8.99	133.99	128.60
3	N	171	G	N9-C4-C5	8.98	108.99	105.40
3	M	206	C	C4'-C3'-C2'	-8.95	93.65	102.60
3	M	163	G	C5-N7-C8	8.94	108.77	104.30
3	N	230	G	O4'-C1'-N9	8.92	115.34	108.20
3	M	154	G	N3-C2-N2	-8.91	113.67	119.90
3	M	157	U	P-O3'-C3'	-8.91	109.01	119.70
3	N	208	C	C2-N3-C4	-8.90	115.45	119.90
3	N	209	G	C1'-O4'-C4'	8.89	117.01	109.90
3	M	152	G	N9-C4-C5	8.87	108.95	105.40
3	M	171	G	O4'-C1'-N9	8.87	115.29	108.20
3	N	218	C	C4'-C3'-C2'	-8.87	93.73	102.60
3	M	171	G	O5'-P-OP1	-8.85	97.73	105.70
3	M	194	A	C8-N9-C4	8.85	109.34	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	183	U	O4'-C1'-N1	8.84	115.27	108.20
3	N	197	C	C2-N3-C4	-8.82	115.49	119.90
3	N	235	U	O4'-C1'-N1	-8.80	101.16	108.20
3	N	148	G	C4'-C3'-C2'	-8.80	93.80	102.60
3	N	168	G	N1-C6-O6	8.78	125.17	119.90
3	M	213	G	C5-C6-O6	-8.77	123.34	128.60
3	M	220	A	N1-C2-N3	-8.76	124.92	129.30
3	N	208	C	O4'-C4'-C3'	-8.76	95.24	104.00
3	M	202	C	C4-C5-C6	-8.76	113.02	117.40
3	M	169	G	C6-N1-C2	-8.76	119.84	125.10
3	N	179	C	O4'-C1'-N1	-8.73	101.21	108.20
3	M	210	G	C8-N9-C4	-8.73	102.91	106.40
3	M	203	A	C4'-C3'-C2'	-8.72	93.88	102.60
3	N	218	C	O4'-C1'-N1	8.72	115.18	108.20
3	M	209	G	C5-C6-N1	8.70	115.85	111.50
3	N	170	A	O4'-C1'-N9	8.70	115.16	108.20
3	M	202	C	N3-C4-N4	-8.68	111.92	118.00
3	N	208	C	C4'-C3'-C2'	-8.68	93.92	102.60
3	M	198	C	N1-C2-O2	-8.68	113.69	118.90
3	M	214	G	C4'-C3'-C2'	-8.68	93.92	102.60
3	M	163	G	C5-C6-N1	8.65	115.83	111.50
3	N	155	C	N3-C2-O2	-8.65	115.85	121.90
3	N	215	G	C5-C6-N1	-8.65	107.18	111.50
3	M	182	C	P-O3'-C3'	-8.65	109.32	119.70
3	M	201	C	C5-C6-N1	8.64	125.32	121.00
3	N	166	G	O4'-C1'-N9	-8.63	101.30	108.20
3	N	157	U	P-O3'-C3'	-8.62	109.35	119.70
3	M	152	G	N1-C2-N2	8.62	123.96	116.20
3	N	163	G	N1-C2-N2	8.61	123.95	116.20
3	N	169	G	C5-C6-O6	-8.60	123.44	128.60
3	M	146	G	C8-N9-C4	-8.60	102.96	106.40
3	N	218	C	N3-C4-N4	-8.59	111.99	118.00
3	M	154	G	O4'-C4'-C3'	-8.54	95.46	104.00
3	M	142	G	C4'-C3'-C2'	-8.53	94.07	102.60
3	M	219	A	P-O5'-C5'	-8.50	107.30	120.90
3	M	202	C	C2-N1-C1'	-8.48	109.48	118.80
3	M	216	A	C6-C5-N7	-8.47	126.37	132.30
3	N	215	G	C2-N3-C4	-8.46	107.67	111.90
3	M	171	G	C5'-C4'-C3'	-8.45	102.48	116.00
3	M	162	U	O4'-C1'-N1	-8.44	101.45	108.20
3	M	214	G	C6-N1-C2	-8.40	120.06	125.10
3	N	208	C	C5-C4-N4	-8.40	114.32	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	203	A	C2-N3-C4	8.39	114.79	110.60
3	M	226	G	N3-C4-C5	-8.38	124.41	128.60
3	M	215	G	C6-N1-C2	-8.37	120.08	125.10
3	N	197	C	O5'-P-OP2	8.35	120.72	110.70
3	M	199	C	O4'-C4'-C3'	-8.34	95.66	104.00
3	M	216	A	C5-N7-C8	-8.33	99.73	103.90
3	M	152	G	C8-N9-C4	-8.32	103.07	106.40
3	M	207	C	O5'-P-OP1	8.32	120.69	110.70
3	M	210	G	C3'-C2'-C1'	-8.31	94.85	101.50
3	N	215	G	C6-C5-N7	-8.30	125.42	130.40
3	M	209	G	C6-C5-N7	-8.28	125.43	130.40
3	M	215	G	N3-C4-C5	-8.26	124.47	128.60
3	M	146	G	C5'-C4'-O4'	-8.26	99.19	109.10
3	N	201	C	C4'-C3'-C2'	-8.25	94.35	102.60
3	N	221	C	C4'-C3'-C2'	-8.24	94.36	102.60
3	N	218	C	C2-N3-C4	-8.23	115.78	119.90
3	M	234	G	P-O5'-C5'	-8.23	107.74	120.90
3	M	205	G	C8-N9-C4	-8.21	103.12	106.40
3	N	204	G	O4'-C1'-C2'	-8.21	97.59	105.80
3	M	220	A	C6-N1-C2	8.19	123.51	118.60
3	N	175	U	C3'-C2'-C1'	8.18	108.04	101.50
3	M	210	G	O4'-C1'-C2'	-8.17	97.63	105.80
3	M	161	C	P-O5'-C5'	-8.12	107.90	120.90
3	M	213	G	N3-C2-N2	-8.12	114.21	119.90
3	N	211	A	C5-C6-N1	8.12	121.76	117.70
3	N	158	C	N1-C2-O2	-8.11	114.03	118.90
3	N	152	G	C4'-C3'-C2'	-8.11	94.49	102.60
3	N	204	G	P-O3'-C3'	8.11	129.43	119.70
3	M	146	G	O3'-P-O5'	-8.09	88.63	104.00
3	N	177	A	O4'-C1'-C2'	-8.09	97.71	105.80
3	M	191	C	P-O3'-C3'	-8.08	110.00	119.70
3	N	153	A	O4'-C1'-N9	-8.07	101.74	108.20
3	M	209	G	O4'-C1'-C2'	-8.07	97.73	105.80
3	M	187	C	O4'-C1'-N1	-8.06	101.75	108.20
3	N	208	C	O4'-C1'-C2'	-8.06	97.74	105.80
3	N	217	G	C6-N1-C2	-8.06	120.27	125.10
3	N	194	A	O4'-C1'-N9	-8.05	101.76	108.20
3	M	146	G	C4-C5-N7	-8.05	107.58	110.80
3	N	198	C	N3-C4-C5	-8.05	118.68	121.90
3	M	194	A	P-O5'-C5'	-8.03	108.06	120.90
3	M	203	A	N1-C2-N3	-8.02	125.29	129.30
3	M	194	A	N7-C8-N9	-7.99	109.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	213	G	C8-N9-C4	-7.97	103.21	106.40
3	M	202	C	P-O3'-C3'	-7.96	110.14	119.70
3	N	154	G	O5'-P-OP2	-7.96	98.53	105.70
3	M	148	G	O4'-C1'-N9	7.96	114.57	108.20
3	N	179	C	P-O3'-C3'	-7.96	110.15	119.70
3	M	172	A	P-O3'-C3'	-7.94	110.17	119.70
3	M	203	A	C3'-C2'-C1'	7.94	107.85	101.50
3	N	160	C	N1-C1'-C2'	-7.94	103.27	112.00
3	N	171	G	O4'-C1'-N9	7.94	114.55	108.20
3	N	211	A	N1-C6-N6	7.93	123.36	118.60
3	M	162	U	O4'-C4'-C3'	-7.92	96.08	104.00
3	M	169	G	C5'-C4'-C3'	-7.90	103.37	116.00
2	C	33	ASP	CB-CG-OD2	7.88	125.39	118.30
3	N	192	C	O4'-C1'-N1	-7.87	101.90	108.20
3	N	208	C	OP1-P-OP2	7.87	131.40	119.60
3	M	206	C	O4'-C1'-N1	-7.86	101.92	108.20
3	M	163	G	N1-C2-N2	7.85	123.26	116.20
3	M	217	G	O3'-P-O5'	-7.85	89.09	104.00
3	N	161	C	C2-N3-C4	-7.84	115.98	119.90
3	M	216	A	O4'-C1'-C2'	-7.84	97.96	105.80
3	M	219	A	C3'-C2'-C1'	-7.84	95.23	101.50
3	N	224	U	P-O3'-C3'	-7.82	110.31	119.70
3	M	179	C	C2-N3-C4	-7.82	115.99	119.90
3	N	220	A	O4'-C1'-N9	7.81	114.45	108.20
3	M	186	A	N1-C2-N3	7.81	133.20	129.30
3	M	235	U	O4'-C1'-N1	-7.81	101.95	108.20
3	M	203	A	C5-C6-N6	-7.80	117.46	123.70
3	M	206	C	O3'-P-O5'	-7.79	89.20	104.00
3	N	208	C	O5'-P-OP1	-7.79	98.69	105.70
3	M	196	C	C2-N3-C4	-7.78	116.01	119.90
3	M	225	A	P-O3'-C3'	-7.78	110.37	119.70
3	N	165	A	C5-C6-N6	-7.77	117.48	123.70
3	N	146	G	P-O3'-C3'	7.74	128.99	119.70
3	M	208	C	OP1-P-OP2	7.72	131.18	119.60
3	M	222	G	N9-C4-C5	7.72	108.49	105.40
3	N	177	A	N1-C6-N6	7.71	123.22	118.60
3	N	145	G	C5'-C4'-O4'	-7.70	99.86	109.10
3	M	206	C	C6-N1-C2	-7.67	117.23	120.30
3	N	168	G	C5-C6-N1	7.66	115.33	111.50
3	N	219	A	C6-C5-N7	-7.66	126.94	132.30
3	M	181	C	P-O3'-C3'	-7.65	110.52	119.70
3	M	217	G	O4'-C4'-C3'	-7.65	96.35	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	235	U	O4'-C4'-C3'	-7.64	96.36	104.00
3	N	204	G	C8-N9-C4	-7.63	103.35	106.40
3	N	159	U	N1-C2-O2	7.62	128.14	122.80
3	N	166	G	OP2-P-O3'	7.62	121.97	105.20
3	N	234	G	C4'-C3'-C2'	-7.61	94.99	102.60
3	N	227	G	C4-C5-N7	7.60	113.84	110.80
3	M	220	A	N9-C4-C5	7.59	108.84	105.80
3	M	158	C	C5-C4-N4	-7.59	114.89	120.20
3	M	211	A	O4'-C1'-N9	-7.58	102.13	108.20
3	M	167	G	P-O3'-C3'	7.58	128.79	119.70
3	N	174	G	N3-C2-N2	7.57	125.20	119.90
3	N	170	A	N9-C4-C5	7.57	108.83	105.80
3	M	217	G	C6-N1-C2	-7.56	120.56	125.10
3	N	165	A	C6-N1-C2	-7.55	114.07	118.60
3	N	173	U	O5'-P-OP2	7.54	119.75	110.70
3	N	209	G	C5-C6-O6	-7.54	124.07	128.60
3	M	157	U	C4'-C3'-C2'	-7.54	95.06	102.60
3	N	215	G	N1-C6-O6	7.53	124.42	119.90
3	M	174	G	N1-C2-N3	-7.53	119.38	123.90
3	N	171	G	C8-N9-C4	-7.52	103.39	106.40
3	N	151	G	N3-C4-N9	-7.50	121.50	126.00
3	N	149	G	C4'-C3'-C2'	-7.50	95.10	102.60
3	N	220	A	C4'-C3'-C2'	-7.50	95.10	102.60
3	N	225	A	O4'-C1'-N9	-7.49	102.21	108.20
3	M	213	G	C5-C6-N1	7.48	115.24	111.50
3	N	218	C	O4'-C1'-C2'	-7.47	98.33	105.80
3	M	210	G	P-O3'-C3'	7.47	128.66	119.70
3	M	183	U	N1-C2-O2	7.47	128.03	122.80
3	N	165	A	C5-C6-N1	7.46	121.43	117.70
3	N	143	G	C4'-C3'-C2'	-7.46	95.14	102.60
3	M	150	G	C5-C6-O6	-7.45	124.13	128.60
3	M	214	G	C5-C6-N1	7.43	115.22	111.50
3	N	209	G	O4'-C1'-C2'	-7.43	98.37	105.80
3	M	162	U	N1-C1'-C2'	7.42	123.65	114.00
3	N	216	A	C5-C6-N6	-7.40	117.78	123.70
3	N	199	C	P-O3'-C3'	-7.38	110.84	119.70
3	N	214	G	N3-C2-N2	7.38	125.07	119.90
3	N	159	U	O4'-C4'-C3'	-7.37	96.63	104.00
3	M	166	G	O4'-C1'-N9	-7.36	102.31	108.20
3	N	157	U	C4'-C3'-C2'	-7.35	95.25	102.60
3	M	199	C	C5-C4-N4	7.34	125.34	120.20
3	N	201	C	O4'-C1'-N1	-7.34	102.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	215	G	C6-C5-N7	-7.33	126.00	130.40
3	N	189	U	C4'-C3'-C2'	-7.33	95.27	102.60
3	M	222	G	C4-C5-N7	-7.33	107.87	110.80
3	N	225	A	C5-C6-N6	-7.32	117.85	123.70
3	M	157	U	OP1-P-O3'	7.30	121.26	105.20
3	M	220	A	N7-C8-N9	-7.30	110.15	113.80
3	N	226	G	N7-C8-N9	-7.29	109.46	113.10
3	M	183	U	O3'-P-O5'	-7.27	90.19	104.00
3	M	205	G	O4'-C1'-C2'	-7.26	98.54	105.80
3	M	167	G	OP2-P-O3'	7.26	121.17	105.20
3	M	179	C	P-O3'-C3'	-7.24	111.02	119.70
3	M	146	G	P-O3'-C3'	7.23	128.38	119.70
3	M	169	G	N1-C6-O6	-7.22	115.56	119.90
3	M	192	C	P-O3'-C3'	-7.22	111.03	119.70
3	M	210	G	C8-N9-C1'	7.22	136.38	127.00
3	M	187	C	P-O3'-C3'	-7.21	111.05	119.70
3	M	153	A	O3'-P-O5'	-7.21	90.31	104.00
3	M	228	C	C5-C4-N4	-7.19	115.17	120.20
3	M	193	G	N1-C6-O6	-7.18	115.59	119.90
3	M	182	C	O4'-C1'-N1	7.18	113.94	108.20
3	N	202	C	N3-C4-C5	7.17	124.77	121.90
3	M	183	U	C2-N1-C1'	7.17	126.30	117.70
3	M	154	G	N1-C2-N3	7.17	128.20	123.90
3	M	209	G	N3-C4-C5	-7.15	125.03	128.60
3	N	146	G	C5'-C4'-O4'	-7.14	100.53	109.10
3	M	210	G	C5-C6-O6	7.14	132.88	128.60
3	M	201	C	C2-N3-C4	7.14	123.47	119.90
3	N	217	G	O4'-C1'-N9	7.13	113.91	108.20
3	N	227	G	N1-C6-O6	7.13	124.17	119.90
3	M	197	C	C2-N1-C1'	7.12	126.63	118.80
3	M	202	C	N3-C4-C5	7.11	124.75	121.90
3	N	202	C	C5-C4-N4	-7.11	115.23	120.20
3	M	179	C	N1-C2-O2	-7.10	114.64	118.90
3	M	206	C	C1'-O4'-C4'	-7.10	104.22	109.90
3	M	220	A	P-O3'-C3'	7.09	128.21	119.70
3	M	166	G	N3-C4-N9	-7.09	121.75	126.00
3	M	196	C	C5-C4-N4	-7.09	115.24	120.20
3	N	169	G	C5-C6-N1	7.09	115.05	111.50
3	M	215	G	C4'-C3'-C2'	-7.09	95.51	102.60
3	N	162	U	N1-C2-O2	-7.08	117.84	122.80
3	M	154	G	C5'-C4'-C3'	-7.07	104.69	116.00
3	M	201	C	N3-C2-O2	7.06	126.84	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	170	A	C4-C5-C6	-7.06	113.47	117.00
3	N	180	C	N1-C2-O2	-7.05	114.67	118.90
3	N	205	G	C5-N7-C8	7.04	107.82	104.30
3	N	175	U	N1-C2-O2	7.04	127.73	122.80
3	N	180	C	P-O3'-C3'	-7.04	111.25	119.70
3	N	203	A	O4'-C4'-C3'	-7.04	96.96	104.00
3	M	174	G	C5'-C4'-O4'	-7.04	100.66	109.10
3	M	225	A	N1-C2-N3	-7.03	125.78	129.30
3	M	167	G	C1'-O4'-C4'	7.03	115.52	109.90
3	M	184	U	O4'-C1'-N1	7.03	113.82	108.20
3	N	152	G	C5'-C4'-O4'	7.02	117.53	109.10
3	N	226	G	C5-C6-O6	-7.02	124.39	128.60
3	N	156	A	C3'-C2'-C1'	-7.01	95.89	101.50
3	N	219	A	C5-C6-N6	-7.01	118.09	123.70
3	N	149	G	N9-C4-C5	7.00	108.20	105.40
3	N	191	C	P-O5'-C5'	-7.00	109.71	120.90
3	N	216	A	C5'-C4'-O4'	-6.99	100.71	109.10
3	M	228	C	C6-N1-C2	6.98	123.09	120.30
3	N	195	A	C1'-O4'-C4'	6.97	115.48	109.90
3	M	152	G	C6-N1-C2	-6.97	120.92	125.10
3	N	169	G	C1'-O4'-C4'	6.97	115.48	109.90
3	N	149	G	O4'-C4'-C3'	-6.97	97.03	104.00
3	M	228	C	C2-N3-C4	-6.96	116.42	119.90
3	N	192	C	C5-C4-N4	-6.95	115.34	120.20
3	M	150	G	N1-C6-O6	6.95	124.07	119.90
3	N	215	G	C8-N9-C4	-6.95	103.62	106.40
3	N	223	G	N9-C1'-C2'	-6.95	104.36	112.00
3	N	168	G	C6-C5-N7	-6.94	126.24	130.40
3	N	194	A	O5'-P-OP1	6.94	119.03	110.70
3	M	189	U	N3-C2-O2	-6.94	117.34	122.20
2	C	161	ASP	CB-CG-OD2	6.93	124.54	118.30
3	N	218	C	O4'-C4'-C3'	-6.93	97.07	104.00
3	M	173	U	C1'-O4'-C4'	-6.91	104.37	109.90
3	M	185	U	N1-C2-O2	-6.90	117.97	122.80
3	N	166	G	O5'-P-OP1	6.90	118.98	110.70
3	M	184	U	C4'-C3'-C2'	-6.90	95.70	102.60
3	N	216	A	C5-C6-N1	6.88	121.14	117.70
3	N	211	A	O4'-C1'-N9	-6.86	102.71	108.20
3	N	216	A	C6-N1-C2	-6.85	114.49	118.60
2	C	188	ASP	CB-CG-OD2	6.84	124.46	118.30
3	N	172	A	C6-N1-C2	-6.84	114.50	118.60
3	N	188	C	N1-C2-O2	-6.83	114.80	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	160	C	C4'-C3'-C2'	-6.83	95.77	102.60
3	M	163	G	N3-C4-C5	-6.83	125.19	128.60
3	N	182	C	N1-C2-O2	-6.83	114.80	118.90
3	M	168	G	C4-C5-N7	-6.82	108.07	110.80
3	M	222	G	C5-C6-O6	6.82	132.69	128.60
3	N	142	G	C5-C6-O6	-6.82	124.51	128.60
3	M	172	A	C5'-C4'-C3'	-6.82	105.09	116.00
3	M	204	G	N1-C6-O6	6.81	123.99	119.90
3	N	194	A	N9-C4-C5	6.81	108.53	105.80
3	N	142	G	C4'-C3'-C2'	-6.81	95.79	102.60
3	M	197	C	C5-C6-N1	6.80	124.40	121.00
3	N	219	A	C4-C5-N7	6.80	114.10	110.70
3	N	165	A	O3'-P-O5'	-6.80	91.08	104.00
3	N	226	G	C2-N3-C4	6.80	115.30	111.90
3	M	226	G	C2-N3-C4	6.78	115.29	111.90
3	M	185	U	N1-C1'-C2'	6.78	122.81	114.00
3	M	179	C	C1'-O4'-C4'	6.78	115.32	109.90
3	N	151	G	N1-C6-O6	6.77	123.96	119.90
3	N	178	C	OP2-P-O3'	6.77	120.09	105.20
3	N	210	G	O3'-P-O5'	-6.77	91.14	104.00
3	M	208	C	C4'-C3'-C2'	-6.76	95.83	102.60
3	N	204	G	N9-C4-C5	6.76	108.10	105.40
3	M	202	C	N1-C1'-C2'	6.75	122.78	114.00
3	M	147	U	C5'-C4'-O4'	-6.75	101.00	109.10
3	N	167	G	P-O5'-C5'	-6.75	110.10	120.90
3	M	226	G	N9-C1'-C2'	-6.74	104.58	112.00
3	N	200	G	O5'-P-OP1	-6.74	99.63	105.70
3	M	163	G	C5'-C4'-C3'	-6.74	105.22	116.00
3	M	217	G	OP1-P-OP2	6.74	129.71	119.60
3	N	166	G	O4'-C4'-C3'	-6.72	97.28	104.00
3	N	171	G	N1-C6-O6	-6.72	115.87	119.90
3	N	153	A	C5'-C4'-C3'	-6.72	105.25	116.00
3	N	170	A	C8-N9-C4	-6.71	103.11	105.80
3	N	209	G	C6-N1-C2	-6.70	121.08	125.10
3	M	219	A	C4-C5-N7	6.70	114.05	110.70
3	M	157	U	O3'-P-O5'	-6.70	91.28	104.00
3	M	193	G	C3'-C2'-C1'	6.69	106.85	101.50
3	N	198	C	N1-C2-O2	-6.69	114.89	118.90
3	M	214	G	C3'-C2'-C1'	-6.69	96.15	101.50
3	M	194	A	C4-C5-C6	6.68	120.34	117.00
3	M	162	U	O4'-C1'-C2'	-6.68	99.12	105.80
3	M	198	C	P-O3'-C3'	6.67	127.71	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	219	A	N1-C2-N3	-6.67	125.96	129.30
3	N	228	C	N3-C4-C5	6.67	124.57	121.90
3	M	172	A	C5-N7-C8	-6.66	100.57	103.90
3	N	211	A	N9-C1'-C2'	6.66	122.66	114.00
3	N	211	A	C4-C5-N7	6.66	114.03	110.70
3	M	203	A	C4-C5-N7	6.66	114.03	110.70
3	N	169	G	N9-C1'-C2'	-6.65	104.68	112.00
3	M	163	G	C6-C5-N7	6.65	134.39	130.40
3	M	179	C	C5-C6-N1	-6.65	117.67	121.00
3	N	181	C	O4'-C1'-N1	6.65	113.52	108.20
3	M	154	G	C3'-C2'-C1'	-6.64	96.19	101.50
3	M	218	C	C2-N3-C4	-6.64	116.58	119.90
3	N	160	C	C5'-C4'-O4'	-6.64	101.14	109.10
3	M	171	G	O5'-C5'-C4'	6.63	124.30	111.70
3	M	231	G	P-O3'-C3'	6.63	127.66	119.70
3	N	160	C	O4'-C4'-C3'	-6.62	97.38	104.00
3	M	160	C	O4'-C1'-C2'	-6.62	99.19	105.80
3	M	163	G	C2-N3-C4	6.62	115.21	111.90
3	N	170	A	C5'-C4'-C3'	-6.62	105.41	116.00
3	N	209	G	OP2-P-O3'	6.61	119.73	105.20
3	N	165	A	N9-C1'-C2'	-6.60	104.74	112.00
3	M	156	A	C4-C5-N7	6.60	114.00	110.70
3	N	176	A	C8-N9-C4	6.60	108.44	105.80
3	M	199	C	P-O3'-C3'	-6.59	111.79	119.70
3	N	209	G	P-O5'-C5'	-6.59	110.35	120.90
3	N	194	A	N3-C4-N9	-6.59	122.13	127.40
3	M	209	G	N3-C4-N9	6.59	129.95	126.00
3	N	226	G	C6-N1-C2	-6.59	121.15	125.10
3	M	197	C	C4'-C3'-C2'	-6.59	96.01	102.60
3	M	219	A	C5'-C4'-O4'	-6.59	101.20	109.10
3	M	196	C	N3-C4-N4	6.58	122.61	118.00
3	M	210	G	O4'-C4'-C3'	-6.58	97.42	104.00
3	M	175	U	P-O5'-C5'	-6.58	110.38	120.90
3	M	142	G	N3-C4-C5	-6.57	125.31	128.60
3	N	176	A	C4-C5-C6	-6.57	113.71	117.00
3	N	201	C	C5'-C4'-O4'	-6.57	101.22	109.10
3	M	231	G	C4'-C3'-C2'	-6.57	96.03	102.60
2	C	250	ASP	CB-CG-OD2	6.57	124.21	118.30
3	M	143	G	N9-C4-C5	6.57	108.03	105.40
3	M	191	C	O4'-C1'-N1	-6.57	102.95	108.20
3	N	186	A	N1-C2-N3	6.56	132.58	129.30
3	M	195	A	N9-C1'-C2'	6.55	122.52	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	193	G	C5-C6-O6	6.53	132.52	128.60
3	M	211	A	N9-C4-C5	6.53	108.41	105.80
3	M	215	G	OP1-P-OP2	6.53	129.39	119.60
3	M	216	A	N9-C4-C5	6.53	108.41	105.80
3	M	167	G	O4'-C1'-C2'	-6.52	99.28	105.80
3	M	215	G	C4-N9-C1'	6.52	134.98	126.50
3	N	221	C	N1-C2-O2	-6.52	114.99	118.90
2	C	398	ARG	NE-CZ-NH1	-6.50	117.05	120.30
3	M	222	G	C6-C5-N7	6.50	134.30	130.40
3	M	170	A	C3'-C2'-C1'	6.50	106.70	101.50
3	N	205	G	C4-C5-N7	-6.48	108.21	110.80
3	M	215	G	C8-N9-C4	-6.48	103.81	106.40
3	M	143	G	C4'-C3'-C2'	-6.48	96.12	102.60
3	M	162	U	N1-C2-O2	-6.47	118.27	122.80
3	N	207	C	O4'-C1'-N1	6.47	113.38	108.20
3	N	220	A	O4'-C1'-C2'	-6.47	99.33	105.80
3	M	209	G	C3'-C2'-C1'	6.45	106.66	101.50
3	N	148	G	O4'-C4'-C3'	-6.45	97.55	104.00
3	M	220	A	C5-C6-N6	6.45	128.86	123.70
3	M	206	C	C2-N1-C1'	6.44	125.89	118.80
3	N	207	C	N1-C2-O2	6.44	122.76	118.90
3	M	210	G	N9-C1'-C2'	6.44	122.37	114.00
3	M	168	G	O3'-P-O5'	-6.43	91.77	104.00
3	N	171	G	C2-N3-C4	6.43	115.12	111.90
3	N	194	A	P-O3'-C3'	-6.43	111.98	119.70
3	N	171	G	N3-C4-C5	-6.43	125.38	128.60
3	N	166	G	C5'-C4'-O4'	-6.43	101.39	109.10
3	M	216	A	O4'-C1'-N9	-6.42	103.06	108.20
3	M	220	A	O4'-C1'-N9	6.41	113.33	108.20
3	M	158	C	N3-C4-C5	6.41	124.47	121.90
3	N	156	A	OP1-P-OP2	6.41	129.22	119.60
3	N	200	G	C4'-C3'-C2'	-6.40	96.20	102.60
3	M	218	C	C2-N1-C1'	-6.40	111.76	118.80
3	M	172	A	C4-C5-N7	6.39	113.89	110.70
3	M	159	U	O4'-C4'-C3'	-6.38	97.62	104.00
3	M	232	A	C2-N3-C4	6.38	113.79	110.60
3	N	206	C	O4'-C4'-C3'	-6.38	97.62	104.00
3	M	219	A	C5-C6-N1	6.38	120.89	117.70
3	N	149	G	C5'-C4'-C3'	-6.37	105.81	116.00
3	N	207	C	C2-N3-C4	6.37	123.08	119.90
3	M	160	C	O4'-C4'-C3'	-6.36	97.64	104.00
3	N	214	G	C4-C5-N7	6.35	113.34	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	164	U	OP1-P-O3'	6.35	119.17	105.20
3	M	194	A	C5-N7-C8	6.35	107.07	103.90
3	N	193	G	O3'-P-O5'	-6.34	91.96	104.00
3	M	156	A	C4'-C3'-C2'	-6.33	96.27	102.60
3	M	164	U	C5'-C4'-C3'	6.33	126.13	116.00
3	M	208	C	O4'-C1'-C2'	-6.33	99.47	105.80
3	M	171	G	C1'-O4'-C4'	6.33	114.96	109.90
3	M	180	C	N3-C4-N4	6.32	122.42	118.00
1	A	8	ILE	CG1-CB-CG2	-6.32	97.50	111.40
3	N	159	U	P-O3'-C3'	-6.32	112.12	119.70
3	M	164	U	OP1-P-O3'	6.32	119.09	105.20
3	N	172	A	P-O5'-C5'	-6.31	110.80	120.90
3	N	177	A	O4'-C1'-N9	-6.31	103.15	108.20
3	M	163	G	N1-C6-O6	-6.31	116.12	119.90
3	N	228	C	N1-C2-O2	6.30	122.68	118.90
3	M	208	C	O3'-P-O5'	-6.29	92.04	104.00
3	N	142	G	C4-C5-N7	6.29	113.32	110.80
3	M	150	G	P-O5'-C5'	-6.29	110.84	120.90
3	M	210	G	N3-C2-N2	-6.28	115.50	119.90
3	M	229	A	N9-C4-C5	6.27	108.31	105.80
3	M	216	A	N9-C1'-C2'	6.27	122.15	114.00
3	N	204	G	C6-N1-C2	6.27	128.86	125.10
3	N	178	C	C5'-C4'-O4'	-6.27	101.58	109.10
3	N	178	C	N1-C2-O2	-6.27	115.14	118.90
3	N	222	G	N1-C2-N3	-6.26	120.14	123.90
3	M	198	C	N3-C2-O2	6.26	126.28	121.90
3	M	216	A	C4-C5-C6	6.26	120.13	117.00
3	M	200	G	OP1-P-OP2	6.25	128.98	119.60
3	N	215	G	N3-C2-N2	-6.25	115.52	119.90
3	M	174	G	C4-C5-N7	6.25	113.30	110.80
3	M	176	A	O4'-C1'-N9	6.25	113.20	108.20
3	M	220	A	C5-N7-C8	6.24	107.02	103.90
2	D	280	ASP	CB-CG-OD2	6.24	123.92	118.30
3	M	148	G	O4'-C1'-C2'	-6.24	99.56	105.80
3	N	215	G	C4-C5-C6	6.24	122.54	118.80
3	M	170	A	N1-C6-N6	-6.23	114.86	118.60
3	M	210	G	C2-N3-C4	-6.23	108.78	111.90
3	N	155	C	C4'-C3'-C2'	-6.23	96.37	102.60
3	N	163	G	C8-N9-C4	-6.23	103.91	106.40
1	B	33	ASP	CB-CG-OD2	6.23	123.91	118.30
3	N	165	A	C3'-C2'-C1'	6.22	106.47	101.50
3	M	149	G	O4'-C1'-N9	6.21	113.17	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	166	G	C5-C6-N1	6.21	114.60	111.50
3	M	156	A	C5-N7-C8	-6.19	100.80	103.90
3	M	227	G	N9-C1'-C2'	6.19	122.05	114.00
2	D	41	ALA	N-CA-C	-6.19	94.28	111.00
3	N	148	G	O4'-C1'-N9	-6.19	103.25	108.20
3	N	176	A	N1-C6-N6	-6.18	114.89	118.60
3	M	149	G	C4'-C3'-C2'	-6.17	96.43	102.60
3	M	154	G	O3'-P-O5'	-6.17	92.28	104.00
3	N	177	A	C5'-C4'-O4'	-6.17	101.70	109.10
3	N	214	G	C6-C5-N7	-6.17	126.70	130.40
3	M	233	C	O4'-C1'-N1	-6.17	103.27	108.20
3	M	211	A	C5'-C4'-O4'	-6.16	101.70	109.10
3	N	192	C	O4'-C4'-C3'	-6.16	97.84	104.00
3	M	209	G	N9-C1'-C2'	-6.16	105.22	112.00
3	N	209	G	C4'-C3'-C2'	-6.16	96.44	102.60
3	N	219	A	C8-N9-C4	-6.16	103.34	105.80
3	M	164	U	C5-C6-N1	-6.14	119.63	122.70
3	N	228	C	O5'-P-OP2	-6.14	100.17	105.70
3	N	218	C	P-O3'-C3'	6.13	127.06	119.70
3	M	169	G	P-O5'-C5'	-6.13	111.09	120.90
3	N	184	U	P-O5'-C5'	-6.13	111.09	120.90
3	M	154	G	C2-N3-C4	-6.13	108.83	111.90
3	M	156	A	C5-C6-N6	-6.13	118.80	123.70
3	M	218	C	O4'-C1'-N1	6.13	113.10	108.20
3	N	155	C	C2-N1-C1'	6.13	125.54	118.80
1	B	67	ASP	CB-CG-OD2	6.12	123.81	118.30
3	N	191	C	C4'-C3'-C2'	-6.12	96.48	102.60
3	M	183	U	C5'-C4'-C3'	-6.12	106.22	116.00
3	N	186	A	C5-C6-N1	-6.11	114.64	117.70
2	D	409	ASP	CB-CG-OD2	6.11	123.80	118.30
2	D	42	ASP	CB-CG-OD2	6.11	123.80	118.30
3	M	201	C	C1'-O4'-C4'	6.10	114.78	109.90
3	N	208	C	C5'-C4'-C3'	-6.10	106.23	116.00
3	M	232	A	C5-C6-N1	6.10	120.75	117.70
3	M	204	G	C5-C6-O6	-6.09	124.94	128.60
3	N	173	U	O4'-C4'-C3'	-6.09	97.91	104.00
2	C	170	ASP	CB-CG-OD2	6.09	123.78	118.30
3	M	171	G	C4'-C3'-C2'	6.08	108.68	102.60
3	N	172	A	C5-C6-N1	6.08	120.74	117.70
3	N	198	C	N3-C2-O2	6.07	126.15	121.90
3	M	205	G	P-O3'-C3'	6.07	126.98	119.70
3	M	160	C	C6-N1-C2	-6.07	117.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	182	C	C5'-C4'-C3'	-6.07	106.29	116.00
3	N	217	G	C5-N7-C8	-6.07	101.27	104.30
3	N	159	U	O3'-P-O5'	-6.07	92.47	104.00
3	M	155	C	N1-C2-O2	6.06	122.54	118.90
3	M	190	G	O4'-C4'-C3'	-6.06	97.94	104.00
3	M	235	U	P-O3'-C3'	6.05	126.97	119.70
3	M	204	G	O4'-C1'-N9	-6.05	103.36	108.20
3	N	149	G	C3'-C2'-C1'	-6.04	96.66	101.50
3	M	145	G	C5-C6-O6	6.04	132.23	128.60
3	M	218	C	N3-C4-N4	-6.04	113.77	118.00
3	M	192	C	C4'-C3'-C2'	-6.04	96.56	102.60
3	M	211	A	C2-N3-C4	6.04	113.62	110.60
3	N	196	C	N3-C4-C5	-6.04	119.48	121.90
3	N	236	C	P-O5'-C5'	-6.03	111.25	120.90
3	M	156	A	N1-C2-N3	-6.03	126.29	129.30
3	N	196	C	O3'-P-O5'	-6.02	92.57	104.00
3	N	203	A	C5-N7-C8	-6.02	100.89	103.90
3	N	182	C	C6-N1-C1'	6.01	128.02	120.80
3	N	223	G	C6-C5-N7	-6.01	126.79	130.40
3	M	142	G	C5-C6-O6	-6.01	124.99	128.60
3	M	155	C	N3-C2-O2	-6.01	117.69	121.90
3	M	157	U	O4'-C1'-C2'	-6.01	99.79	105.80
3	M	213	G	N9-C4-C5	6.01	107.80	105.40
3	M	154	G	C6-N1-C2	-6.01	121.50	125.10
3	N	153	A	O4'-C1'-C2'	-6.01	99.79	105.80
3	N	223	G	C4-C5-N7	6.01	113.20	110.80
3	M	178	C	P-O5'-C5'	-6.01	111.29	120.90
3	N	179	C	C4-C5-C6	-6.00	114.40	117.40
3	M	172	A	C2-N3-C4	5.99	113.59	110.60
3	N	222	G	O4'-C1'-N9	5.98	112.98	108.20
3	N	163	G	C4-C5-N7	-5.98	108.41	110.80
3	N	203	A	C5-C6-N6	-5.97	118.92	123.70
3	N	218	C	N1-C2-N3	5.97	123.38	119.20
3	M	200	G	N3-C4-N9	-5.97	122.42	126.00
3	N	164	U	O4'-C1'-N1	5.97	112.98	108.20
3	M	200	G	O5'-P-OP2	-5.97	100.33	105.70
3	N	149	G	C8-N9-C4	-5.97	104.01	106.40
3	N	219	A	OP2-P-O3'	5.96	118.32	105.20
3	N	200	G	C6-N1-C2	-5.96	121.52	125.10
3	M	185	U	N3-C4-O4	5.96	123.57	119.40
3	M	165	A	C2'-C3'-O3'	-5.96	96.39	109.50
3	M	162	U	C3'-C2'-C1'	-5.95	96.74	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	235	U	OP2-P-O3'	5.95	118.30	105.20
3	N	209	G	N9-C1'-C2'	-5.95	105.46	112.00
3	M	215	G	C4-C5-C6	5.95	122.37	118.80
3	M	221	C	O4'-C4'-C3'	-5.95	98.05	104.00
3	N	170	A	N1-C2-N3	-5.95	126.33	129.30
3	N	194	A	N1-C6-N6	-5.95	115.03	118.60
3	N	176	A	C5-C6-N1	5.94	120.67	117.70
3	N	217	G	C5-C6-N1	5.94	114.47	111.50
3	M	223	G	C3'-C2'-C1'	5.94	106.25	101.50
3	N	174	G	P-O3'-C3'	-5.94	112.58	119.70
3	M	233	C	C4'-C3'-C2'	-5.93	96.67	102.60
3	N	146	G	C3'-C2'-C1'	5.93	106.25	101.50
3	M	198	C	C5-C4-N4	5.93	124.35	120.20
3	M	172	A	N1-C2-N3	-5.92	126.34	129.30
3	M	151	G	C1'-O4'-C4'	5.92	114.63	109.90
3	N	194	A	C4-C5-C6	-5.92	114.04	117.00
3	N	198	C	N3-C4-N4	5.92	122.14	118.00
3	N	198	C	C4'-C3'-C2'	-5.91	96.69	102.60
2	D	250	ASP	CB-CG-OD2	5.91	123.62	118.30
3	N	222	G	C5-C6-N1	5.91	114.45	111.50
3	M	185	U	N1-C2-N3	5.90	118.44	114.90
3	M	215	G	C5-C6-O6	-5.90	125.06	128.60
2	D	33	ASP	CB-CG-OD2	5.90	123.61	118.30
3	M	194	A	O4'-C1'-C2'	5.90	112.91	107.60
3	N	219	A	O3'-P-O5'	-5.90	92.80	104.00
3	N	155	C	C5-C4-N4	5.89	124.33	120.20
3	N	216	A	C3'-C2'-C1'	-5.89	96.78	101.50
1	A	9	ASP	CB-CG-OD2	5.89	123.60	118.30
3	M	165	A	C5-C6-N1	5.89	120.65	117.70
3	M	155	C	C3'-C2'-C1'	-5.89	96.79	101.50
3	M	226	G	O4'-C4'-C3'	-5.88	98.12	104.00
3	N	200	G	C5-C6-N1	5.88	114.44	111.50
3	M	217	G	C8-N9-C4	5.88	108.75	106.40
3	M	213	G	O4'-C4'-C3'	-5.88	98.12	104.00
3	M	181	C	C6-N1-C1'	5.88	127.85	120.80
3	M	162	U	C5-C6-N1	5.87	125.64	122.70
1	A	2	ILE	CG1-CB-CG2	-5.87	98.48	111.40
3	M	216	A	C4-N9-C1'	5.87	136.86	126.30
3	N	147	U	O4'-C1'-C2'	-5.87	99.93	105.80
3	M	176	A	P-O5'-C5'	-5.87	111.51	120.90
3	N	224	U	C3'-C2'-C1'	-5.86	96.81	101.50
3	M	219	A	O3'-P-O5'	-5.86	92.87	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	171	G	C4'-C3'-C2'	5.85	108.45	102.60
3	M	210	G	C5-C6-N1	-5.85	108.58	111.50
3	N	222	G	C5'-C4'-O4'	5.85	116.12	109.10
3	M	223	G	C5-C6-O6	-5.85	125.09	128.60
3	M	174	G	C5-C6-O6	-5.84	125.10	128.60
3	M	216	A	N3-C4-N9	5.84	132.07	127.40
3	M	148	G	C5-C6-O6	-5.84	125.10	128.60
3	N	151	G	P-O3'-C3'	-5.84	112.69	119.70
3	N	181	C	C4-C5-C6	5.84	120.32	117.40
3	M	156	A	O4'-C4'-C3'	-5.84	98.16	104.00
3	N	170	A	C6-N1-C2	-5.84	115.10	118.60
3	N	206	C	C5-C6-N1	5.84	123.92	121.00
3	M	221	C	C6-N1-C2	-5.83	117.97	120.30
3	N	176	A	P-O3'-C3'	5.83	126.69	119.70
3	M	203	A	N9-C1'-C2'	5.82	121.57	114.00
3	M	199	C	N3-C4-N4	-5.81	113.93	118.00
3	M	165	A	OP1-P-OP2	-5.81	110.89	119.60
3	M	220	A	C4-C5-N7	-5.80	107.80	110.70
3	N	157	U	N1-C2-N3	5.80	118.38	114.90
3	M	208	C	O4'-C4'-C3'	-5.80	98.20	104.00
3	N	221	C	P-O5'-C5'	5.80	130.17	120.90
3	M	168	G	C1'-O4'-C4'	5.79	114.54	109.90
3	N	207	C	C5'-C4'-C3'	-5.79	106.73	116.00
3	N	216	A	C2-N3-C4	5.79	113.50	110.60
3	N	219	A	O5'-P-OP2	5.79	117.64	110.70
3	M	164	U	C2-N1-C1'	-5.78	110.76	117.70
3	M	198	C	OP2-P-O3'	5.78	117.92	105.20
3	M	237	G	P-O5'-C5'	-5.78	111.65	120.90
3	M	212	A	O4'-C1'-N9	-5.78	103.58	108.20
3	M	218	C	C1'-O4'-C4'	-5.78	105.28	109.90
3	N	214	G	C3'-C2'-C1'	-5.77	96.88	101.50
3	M	211	A	O5'-C5'-C4'	-5.77	100.74	111.70
3	N	175	U	C6-N1-C1'	-5.77	113.13	121.20
3	M	230	G	C5-N7-C8	-5.76	101.42	104.30
3	N	210	G	C5-C6-O6	5.76	132.06	128.60
3	M	154	G	C6-C5-N7	-5.76	126.94	130.40
3	M	204	G	N7-C8-N9	5.75	115.97	113.10
3	M	208	C	N1-C2-N3	5.74	123.22	119.20
3	N	208	C	C5-C6-N1	5.74	123.87	121.00
3	N	162	U	C3'-C2'-C1'	-5.74	96.91	101.50
3	N	152	G	C4-C5-N7	-5.74	108.50	110.80
3	M	151	G	O4'-C1'-C2'	-5.72	100.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	175	U	N1-C1'-C2'	-5.72	105.70	112.00
3	N	158	C	C1'-O4'-C4'	5.72	114.48	109.90
3	M	210	G	C4'-C3'-C2'	-5.72	96.88	102.60
2	D	401	ARG	NE-CZ-NH1	-5.72	117.44	120.30
3	N	152	G	O4'-C1'-C2'	-5.72	100.08	105.80
3	M	167	G	N1-C6-O6	-5.71	116.47	119.90
3	N	218	C	C2-N1-C1'	-5.71	112.52	118.80
3	M	187	C	O5'-P-OP1	-5.71	100.56	105.70
3	M	207	C	C2-N1-C1'	5.71	125.08	118.80
3	M	201	C	O4'-C1'-C2'	-5.71	100.09	105.80
3	N	207	C	C4'-C3'-C2'	-5.71	96.89	102.60
3	N	189	U	C5-C4-O4	-5.70	122.48	125.90
3	M	181	C	C5-C6-N1	5.70	123.85	121.00
3	N	222	G	C2-N3-C4	5.70	114.75	111.90
3	M	212	A	P-O5'-C5'	-5.70	111.78	120.90
3	M	214	G	C4-C5-N7	5.69	113.08	110.80
3	M	226	G	N3-C4-N9	5.69	129.41	126.00
3	N	166	G	C1'-O4'-C4'	5.69	114.45	109.90
3	M	174	G	N1-C6-O6	5.69	123.31	119.90
3	M	166	G	N3-C4-C5	5.67	131.44	128.60
3	N	189	U	C2-N3-C4	-5.67	123.60	127.00
3	N	218	C	C3'-C2'-C1'	-5.67	96.97	101.50
3	M	173	U	N3-C2-O2	5.66	126.16	122.20
3	N	214	G	O4'-C1'-C2'	-5.66	100.14	105.80
3	M	226	G	O4'-C1'-C2'	-5.66	100.14	105.80
3	N	201	C	N1-C1'-C2'	5.66	121.36	114.00
3	M	219	A	N9-C1'-C2'	5.66	121.35	114.00
3	M	211	A	P-O3'-C3'	-5.65	112.92	119.70
3	N	230	G	C3'-C2'-C1'	-5.65	96.98	101.50
2	D	3	ASP	CB-CG-OD2	5.65	123.38	118.30
3	M	142	G	C5-C6-N1	5.65	114.32	111.50
3	M	163	G	C8-N9-C4	-5.64	104.14	106.40
3	M	229	A	N1-C6-N6	-5.63	115.22	118.60
3	N	194	A	N1-C2-N3	-5.63	126.49	129.30
1	A	14	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	C	425	ASP	N-CA-C	5.62	126.19	111.00
3	N	223	G	N1-C6-O6	5.62	123.28	119.90
3	M	234	G	C5'-C4'-C3'	-5.62	107.00	116.00
2	C	280	ASP	CB-CG-OD2	5.62	123.36	118.30
3	M	179	C	C3'-C2'-C1'	5.62	106.00	101.50
3	M	198	C	C2-N1-C1'	-5.62	112.62	118.80
3	N	194	A	O5'-C5'-C4'	5.62	122.37	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	221	C	O4'-C1'-C2'	-5.61	100.19	105.80
3	N	175	U	C2-N1-C1'	5.61	124.43	117.70
3	M	211	A	N1-C6-N6	-5.60	115.24	118.60
3	N	223	G	C3'-C2'-C1'	5.60	105.98	101.50
3	M	177	A	OP1-P-O3'	5.60	117.52	105.20
3	M	186	A	C1'-O4'-C4'	-5.60	105.42	109.90
3	N	182	C	N3-C2-O2	5.60	125.82	121.90
3	N	218	C	C5-C4-N4	5.60	124.12	120.20
3	M	171	G	N7-C8-N9	5.59	115.90	113.10
3	N	208	C	P-O5'-C5'	-5.59	111.95	120.90
3	N	234	G	C4-C5-N7	5.59	113.04	110.80
3	M	183	U	C4-C5-C6	-5.59	116.35	119.70
3	N	212	A	C5'-C4'-O4'	-5.59	102.39	109.10
3	M	221	C	C2'-C3'-O3'	-5.59	97.21	109.50
3	N	224	U	N1-C2-O2	-5.59	118.89	122.80
3	M	179	C	N1-C2-N3	5.58	123.11	119.20
3	M	229	A	O3'-P-O5'	-5.58	93.40	104.00
3	M	235	U	O4'-C4'-C3'	-5.58	98.42	104.00
3	M	209	G	C3'-C2'-O2'	-5.57	97.14	113.30
3	N	146	G	N9-C4-C5	5.57	107.63	105.40
3	N	206	C	C4-C5-C6	-5.57	114.62	117.40
3	M	153	A	O4'-C1'-N9	-5.57	103.75	108.20
3	N	154	G	N9-C4-C5	5.57	107.63	105.40
3	M	208	C	C1'-O4'-C4'	5.56	114.35	109.90
3	N	203	A	N9-C1'-C2'	5.56	121.23	114.00
3	N	157	U	N1-C2-O2	-5.56	118.91	122.80
3	M	209	G	C4-C5-C6	5.56	122.13	118.80
3	M	185	U	O3'-P-O5'	-5.55	93.44	104.00
3	M	184	U	O4'-C1'-C2'	-5.55	100.25	105.80
3	M	210	G	N3-C4-C5	5.55	131.38	128.60
3	M	223	G	N1-C2-N3	-5.55	120.57	123.90
3	M	156	A	O5'-P-OP1	-5.55	100.70	105.70
3	N	155	C	O4'-C1'-C2'	-5.55	100.25	105.80
3	M	159	U	O5'-C5'-C4'	-5.55	101.16	111.70
3	M	222	G	C4'-C3'-C2'	-5.55	97.05	102.60
3	N	171	G	C5-C6-O6	5.55	131.93	128.60
3	N	232	A	C5'-C4'-O4'	5.54	115.75	109.10
3	M	143	G	C8-N9-C4	-5.54	104.18	106.40
3	M	148	G	C5'-C4'-O4'	-5.54	102.45	109.10
3	M	182	C	N3-C4-C5	-5.54	119.68	121.90
3	M	196	C	P-O5'-C5'	-5.54	112.04	120.90
3	N	172	A	C2-N3-C4	5.54	113.37	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	182	C	O4'-C1'-N1	5.53	112.62	108.20
3	M	189	U	O4'-C1'-C2'	-5.53	100.27	105.80
3	M	221	C	C2-N3-C4	5.52	122.66	119.90
3	M	196	C	C4'-C3'-O3'	-5.52	97.80	109.40
2	D	385	ARG	NE-CZ-NH1	-5.52	117.54	120.30
3	M	214	G	C5'-C4'-C3'	-5.52	107.17	116.00
3	M	167	G	N9-C4-C5	5.52	107.61	105.40
3	M	200	G	O3'-P-O5'	-5.52	93.52	104.00
3	M	158	C	N1-C2-N3	5.51	123.06	119.20
3	N	221	C	O5'-P-OP2	-5.51	100.74	105.70
3	N	195	A	C5'-C4'-C3'	-5.51	107.19	116.00
3	M	230	G	C8-N9-C4	-5.50	104.20	106.40
2	D	23	ASP	CB-CG-OD2	5.50	123.25	118.30
3	N	213	G	N3-C4-C5	-5.50	125.85	128.60
3	M	200	G	P-O3'-C3'	5.49	126.29	119.70
3	N	199	C	C4'-C3'-C2'	-5.49	97.11	102.60
3	M	223	G	P-O5'-C5'	-5.48	112.13	120.90
3	N	150	G	C4'-C3'-C2'	-5.48	97.12	102.60
3	N	183	U	C5'-C4'-C3'	-5.48	107.24	116.00
3	M	214	G	P-O5'-C5'	-5.47	112.14	120.90
3	N	201	C	P-O3'-C3'	5.47	126.27	119.70
3	N	175	U	C5-C4-O4	-5.47	122.62	125.90
3	N	166	G	N7-C8-N9	-5.47	110.36	113.10
3	N	228	C	O4'-C1'-N1	5.47	112.58	108.20
3	M	153	A	N9-C1'-C2'	5.47	121.11	114.00
3	M	226	G	C5-N7-C8	5.46	107.03	104.30
3	M	142	G	C3'-C2'-C1'	5.46	105.87	101.50
3	M	214	G	O4'-C4'-C3'	-5.46	98.54	104.00
3	N	172	A	N3-C4-C5	-5.46	122.98	126.80
3	M	196	C	O4'-C4'-C3'	-5.46	98.54	104.00
2	D	294	LEU	N-CA-C	5.45	125.72	111.00
3	N	227	G	C5-N7-C8	-5.45	101.58	104.30
3	N	192	C	N3-C2-O2	5.43	125.70	121.90
3	M	209	G	OP1-P-OP2	5.43	127.74	119.60
3	N	179	C	N1-C1'-C2'	-5.43	106.03	112.00
3	N	163	G	C4'-C3'-C2'	-5.42	97.18	102.60
3	N	220	A	P-O5'-C5'	-5.41	112.24	120.90
3	N	154	G	N3-C2-N2	-5.41	116.11	119.90
3	N	215	G	N3-C4-N9	-5.41	122.75	126.00
3	M	236	C	N3-C2-O2	-5.40	118.12	121.90
3	M	182	C	P-O5'-C5'	-5.40	112.27	120.90
3	M	226	G	N7-C8-N9	-5.39	110.40	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	150	G	C3'-C2'-C1'	-5.39	97.19	101.50
3	M	194	A	N1-C6-N6	5.39	121.84	118.60
3	N	168	G	C4-C5-C6	5.39	122.04	118.80
2	C	213	ASP	CB-CG-OD2	5.39	123.15	118.30
3	M	159	U	C5'-C4'-C3'	-5.38	107.39	116.00
3	N	161	C	N1-C2-N3	5.38	122.97	119.20
3	N	199	C	O3'-P-O5'	-5.38	93.78	104.00
3	M	227	G	P-O5'-C5'	-5.38	112.29	120.90
3	N	215	G	O4'-C1'-N9	-5.38	103.90	108.20
3	N	221	C	N3-C4-C5	-5.38	119.75	121.90
1	B	9	ASP	CB-CG-OD2	5.37	123.14	118.30
3	N	200	G	N3-C4-C5	-5.37	125.92	128.60
3	N	179	C	C1'-O4'-C4'	5.37	114.19	109.90
3	M	172	A	C5-C6-N1	5.36	120.38	117.70
2	C	319	ASP	CB-CG-OD2	5.36	123.12	118.30
3	M	174	G	C3'-C2'-C1'	5.35	105.78	101.50
3	N	178	C	N1-C1'-C2'	5.35	120.96	114.00
3	N	224	U	O4'-C4'-C3'	-5.35	98.65	104.00
3	N	225	A	C4-C5-N7	5.34	113.37	110.70
3	N	198	C	O4'-C1'-N1	-5.34	103.93	108.20
3	M	173	U	O5'-C5'-C4'	-5.34	101.56	111.70
3	M	197	C	N3-C2-O2	-5.34	118.17	121.90
3	N	176	A	P-O5'-C5'	-5.34	112.36	120.90
2	D	279	ASP	CB-CG-OD2	5.33	123.10	118.30
3	N	164	U	C5'-C4'-O4'	-5.33	102.70	109.10
3	N	219	A	C4'-C3'-C2'	-5.33	97.27	102.60
3	N	143	G	OP1-P-OP2	5.33	127.60	119.60
3	M	199	C	O4'-C1'-N1	-5.33	103.94	108.20
3	N	172	A	C1'-O4'-C4'	5.33	114.17	109.90
3	N	196	C	N1-C1'-C2'	5.33	120.92	114.00
3	N	207	C	N3-C4-C5	-5.32	119.77	121.90
3	N	225	A	C2-N3-C4	-5.32	107.94	110.60
3	M	216	A	C4-C5-N7	5.32	113.36	110.70
3	M	175	U	OP1-P-OP2	5.32	127.57	119.60
3	M	146	G	O4'-C1'-N9	-5.31	103.95	108.20
2	C	64	THR	N-CA-C	-5.31	96.67	111.00
3	M	147	U	O5'-P-OP2	5.31	117.07	110.70
3	N	181	C	N1-C2-O2	-5.31	115.72	118.90
2	C	23	ASP	CB-CG-OD2	5.30	123.07	118.30
3	M	153	A	C8-N9-C4	-5.30	103.68	105.80
3	M	192	C	N1-C2-N3	-5.30	115.49	119.20
3	M	215	G	C3'-C2'-C1'	5.30	105.74	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	ASP	CB-CG-OD2	5.30	123.07	118.30
3	N	210	G	OP1-P-O3'	5.30	116.86	105.20
3	N	219	A	C3'-C2'-O2'	-5.30	97.92	113.30
3	N	158	C	O4'-C1'-C2'	-5.30	100.50	105.80
3	N	219	A	N7-C8-N9	5.30	116.45	113.80
3	M	202	C	O3'-P-O5'	-5.30	93.93	104.00
3	N	154	G	OP1-P-OP2	5.30	127.54	119.60
3	N	177	A	OP1-P-O3'	5.29	116.85	105.20
3	N	213	G	C6-C5-N7	-5.29	127.22	130.40
3	N	217	G	N1-C2-N2	5.29	120.97	116.20
3	M	229	A	O4'-C1'-N9	-5.29	103.97	108.20
3	M	181	C	C4-C5-C6	-5.29	114.76	117.40
3	N	145	G	O4'-C4'-C3'	-5.29	98.71	104.00
3	M	180	C	N1-C2-O2	-5.28	115.73	118.90
3	N	227	G	C6-C5-N7	-5.28	127.23	130.40
2	D	213	ASP	CB-CG-OD2	5.28	123.05	118.30
3	M	170	A	C2-N3-C4	5.28	113.24	110.60
3	N	200	G	OP1-P-OP2	5.28	127.52	119.60
3	M	152	G	C4'-C3'-C2'	-5.28	97.32	102.60
2	C	409	ASP	CB-CG-OD2	5.27	123.04	118.30
3	N	142	G	C6-C5-N7	-5.26	127.24	130.40
3	N	190	G	C2-N3-C4	-5.26	109.27	111.90
3	M	179	C	O4'-C1'-N1	5.25	112.40	108.20
3	N	235	U	C4'-C3'-C2'	-5.25	97.35	102.60
3	M	208	C	C3'-C2'-C1'	5.24	105.69	101.50
2	D	166	LYS	N-CA-C	-5.24	96.86	111.00
3	N	203	A	N7-C8-N9	5.24	116.42	113.80
3	M	223	G	N7-C8-N9	-5.23	110.49	113.10
3	N	177	A	O5'-P-OP1	-5.23	100.99	105.70
3	M	201	C	N1-C2-N3	-5.22	115.54	119.20
3	N	160	C	P-O5'-C5'	-5.22	112.54	120.90
3	N	217	G	C3'-C2'-C1'	-5.22	97.32	101.50
3	M	161	C	N3-C2-O2	-5.22	118.25	121.90
3	M	167	G	O3'-P-O5'	-5.22	94.08	104.00
3	M	196	C	P-O3'-C3'	-5.22	113.43	119.70
3	N	181	C	C4'-C3'-C2'	5.22	107.82	102.60
3	M	177	A	P-O5'-C5'	-5.22	112.55	120.90
3	N	160	C	N1-C2-N3	5.22	122.85	119.20
3	N	223	G	C5-C6-O6	-5.22	125.47	128.60
3	M	155	C	O4'-C1'-N1	5.22	112.37	108.20
1	B	14	ARG	NE-CZ-NH1	-5.22	117.69	120.30
3	N	213	G	C8-N9-C4	-5.21	104.31	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	151	G	O4'-C1'-N9	5.21	112.37	108.20
3	N	143	G	OP2-P-O3'	5.21	116.66	105.20
3	N	170	A	N3-C4-C5	-5.21	123.15	126.80
3	N	145	G	N1-C2-N3	5.21	127.03	123.90
3	M	233	C	N3-C2-O2	-5.21	118.25	121.90
3	N	164	U	C3'-C2'-C1'	5.20	105.66	101.50
3	M	180	C	N3-C4-C5	-5.20	119.82	121.90
3	N	209	G	O3'-P-O5'	-5.20	94.12	104.00
3	M	214	G	C3'-C2'-O2'	-5.20	98.23	113.30
3	M	214	G	C4'-C3'-O3'	-5.19	98.50	109.40
3	M	221	C	N1-C1'-C2'	-5.19	106.29	112.00
3	N	150	G	N3-C2-N2	-5.19	116.27	119.90
3	M	177	A	O3'-P-O5'	-5.18	94.15	104.00
3	M	201	C	P-O5'-C5'	5.18	129.19	120.90
3	N	175	U	N3-C4-O4	5.18	123.03	119.40
3	M	193	G	C2'-C3'-O3'	-5.18	98.10	109.50
3	M	223	G	C1'-C2'-O2'	-5.18	95.05	110.60
3	N	217	G	N3-C2-N2	-5.18	116.28	119.90
3	N	155	C	C5'-C4'-O4'	5.17	115.31	109.10
3	M	142	G	N3-C4-N9	5.17	129.10	126.00
3	M	205	G	C3'-C2'-O2'	-5.17	98.30	113.30
3	N	151	G	C5-C6-O6	-5.17	125.50	128.60
1	B	8	ILE	CG1-CB-CG2	-5.17	100.03	111.40
3	N	197	C	N1-C2-O2	-5.17	115.80	118.90
2	D	425	ASP	CB-CG-OD2	5.17	122.95	118.30
3	M	195	A	O4'-C1'-C2'	-5.16	100.64	105.80
3	M	212	A	OP1-P-OP2	5.16	127.34	119.60
3	M	222	G	N3-C4-N9	-5.16	122.90	126.00
3	N	172	A	N3-C4-N9	5.16	131.53	127.40
3	N	154	G	C6-N1-C2	-5.16	122.00	125.10
3	M	227	G	C2-N3-C4	-5.16	109.32	111.90
3	N	209	G	C3'-C2'-C1'	5.16	105.63	101.50
3	M	184	U	C6-N1-C2	-5.16	117.91	121.00
3	M	232	A	C8-N9-C4	-5.16	103.74	105.80
3	N	189	U	C5-C6-N1	-5.15	120.12	122.70
3	N	203	A	O4'-C1'-C2'	-5.15	100.65	105.80
3	N	207	C	C6-N1-C2	-5.15	118.24	120.30
3	M	233	C	C2-N1-C1'	5.15	124.46	118.80
3	N	155	C	O3'-P-O5'	-5.15	94.22	104.00
3	M	160	C	C1'-O4'-C4'	5.14	114.01	109.90
3	M	147	U	C6-N1-C2	5.14	124.08	121.00
3	N	191	C	N1-C1'-C2'	5.14	120.68	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	192	C	C2-N3-C4	-5.14	117.33	119.90
3	N	234	G	C5-N7-C8	-5.14	101.73	104.30
3	N	219	A	N9-C1'-C2'	5.13	120.68	114.00
3	N	147	U	O5'-P-OP1	-5.13	101.08	105.70
3	N	149	G	O4'-C1'-C2'	-5.13	100.67	105.80
3	N	170	A	O4'-C1'-C2'	-5.13	100.67	105.80
3	M	221	C	N3-C2-O2	5.13	125.49	121.90
3	N	146	G	C8-N9-C4	-5.13	104.35	106.40
3	M	156	A	O3'-P-O5'	-5.13	94.26	104.00
3	M	186	A	C3'-C2'-C1'	5.12	105.60	101.50
3	M	195	A	OP1-P-OP2	-5.12	111.92	119.60
3	N	204	G	C5-C6-O6	5.12	131.67	128.60
3	N	219	A	O4'-C1'-N9	-5.12	104.11	108.20
3	M	184	U	N1-C1'-C2'	5.12	120.65	114.00
3	M	229	A	C6-N1-C2	-5.12	115.53	118.60
3	N	200	G	P-O5'-C5'	-5.12	112.72	120.90
3	N	180	C	C5-C4-N4	-5.11	116.62	120.20
3	M	164	U	C6-N1-C2	5.11	124.07	121.00
3	M	181	C	C6-N1-C2	-5.11	118.25	120.30
3	M	198	C	C3'-C2'-C1'	5.11	105.59	101.50
3	M	154	G	OP2-P-O3'	5.11	116.44	105.20
3	N	203	A	C4-C5-N7	5.11	113.25	110.70
3	N	195	A	N1-C2-N3	-5.11	126.75	129.30
3	N	188	C	N3-C2-O2	5.10	125.47	121.90
2	D	311	ASP	CB-CG-OD2	5.10	122.89	118.30
3	M	196	C	N3-C2-O2	5.10	125.47	121.90
3	N	210	G	C5-C6-N1	-5.10	108.95	111.50
3	M	181	C	P-O5'-C5'	-5.10	112.74	120.90
3	M	213	G	P-O3'-C3'	-5.10	113.58	119.70
3	N	149	G	N1-C6-O6	-5.10	116.84	119.90
3	N	180	C	C4'-C3'-C2'	5.10	107.70	102.60
3	N	215	G	OP1-P-OP2	5.10	127.25	119.60
3	M	215	G	N9-C4-C5	5.09	107.44	105.40
3	M	235	U	C4'-C3'-C2'	-5.09	97.51	102.60
3	N	180	C	C5'-C4'-C3'	-5.09	107.86	116.00
2	C	285	ASP	CB-CG-OD2	5.09	122.88	118.30
3	M	235	U	N3-C4-C5	5.09	117.65	114.60
3	N	159	U	C5-C4-O4	5.08	128.94	125.90
3	N	222	G	O3'-P-O5'	-5.07	94.36	104.00
3	N	194	A	C3'-C2'-C1'	5.07	105.56	101.50
3	N	212	A	P-O5'-C5'	-5.07	112.79	120.90
3	M	157	U	N1-C2-O2	-5.07	119.25	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	197	C	C5-C4-N4	-5.07	116.65	120.20
3	M	187	C	O5'-C5'-C4'	-5.06	102.08	111.70
3	N	198	C	C4-C5-C6	5.06	119.93	117.40
2	C	183	ASP	CB-CG-OD2	5.06	122.86	118.30
3	N	225	A	C6-C5-N7	-5.06	128.76	132.30
3	M	175	U	N3-C2-O2	-5.06	118.66	122.20
3	M	177	A	C1'-O4'-C4'	5.06	113.95	109.90
3	M	218	C	O5'-C5'-C4'	-5.06	102.08	111.70
3	N	187	C	O3'-P-O5'	-5.06	94.39	104.00
1	B	3	ILE	N-CA-C	-5.06	97.35	111.00
3	M	170	A	N9-C4-C5	5.06	107.82	105.80
3	M	143	G	N1-C6-O6	-5.05	116.87	119.90
3	N	214	G	P-O5'-C5'	-5.04	112.83	120.90
3	N	224	U	C4'-C3'-C2'	-5.04	97.56	102.60
3	M	227	G	C6-C5-N7	-5.04	127.38	130.40
3	N	163	G	OP1-P-OP2	5.04	127.16	119.60
3	N	217	G	O5'-P-OP1	5.04	116.74	110.70
3	N	219	A	P-O5'-C5'	-5.04	112.84	120.90
3	M	207	C	N1-C1'-C2'	-5.03	106.47	112.00
3	M	197	C	C6-N1-C1'	-5.03	114.76	120.80
3	N	154	G	N1-C2-N3	5.03	126.92	123.90
3	M	203	A	O3'-P-O5'	-5.03	94.45	104.00
3	M	183	U	N3-C2-O2	-5.02	118.69	122.20
3	M	189	U	N1-C2-N3	5.02	117.91	114.90
3	M	151	G	O3'-P-O5'	-5.02	94.47	104.00
3	M	163	G	N7-C8-N9	-5.01	110.60	113.10
3	N	145	G	C4'-C3'-C2'	-5.01	97.59	102.60
3	M	201	C	O4'-C4'-C3'	-5.01	98.99	104.00
3	M	220	A	C5-C6-N1	-5.01	115.20	117.70
3	N	142	G	O4'-C1'-N9	-5.01	104.20	108.20
3	N	201	C	OP2-P-O3'	5.01	116.21	105.20
3	M	142	G	C4-N9-C1'	5.00	133.00	126.50

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	727	0	786	80	0
1	B	727	0	786	90	0
2	C	3149	0	3364	579	0
2	D	3133	0	3349	620	0
3	M	2063	0	1043	162	0
3	N	2063	0	1041	136	0
4	A	23	0	0	2	0
4	B	26	0	0	2	0
4	C	107	0	0	17	0
4	D	107	0	0	21	0
4	M	92	0	0	11	0
4	N	119	0	0	4	0
All	All	12336	0	10369	1633	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 75.

All (1633) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:18:ALA:CB	2:D:71:LYS:HD2	1.54	1.34
2:C:325:LYS:HA	2:C:325:LYS:NZ	1.51	1.21
2:D:18:ALA:HB1	2:D:71:LYS:CD	1.71	1.19
2:D:290:ILE:HG23	2:D:294:LEU:HD21	1.22	1.18
2:C:64:THR:HG22	2:C:66:LYS:HB2	1.25	1.15
2:D:105:LEU:HD12	2:D:117:ALA:HB2	1.15	1.14
2:C:91:LYS:HD3	2:C:91:LYS:H	1.14	1.13
2:C:278:ILE:H	2:C:278:ILE:HD12	1.03	1.13
2:D:201:GLU:HA	2:D:204:LYS:HB3	1.12	1.11
2:C:105:LEU:HB3	2:C:113:LYS:HE2	1.27	1.11
2:C:219:ILE:HG22	2:C:220:ASP:H	0.96	1.11
2:C:166:LYS:HG2	2:C:167:SER:H	1.00	1.10
2:C:122:ARG:HG3	2:C:278:ILE:HG21	1.34	1.10
2:C:219:ILE:CG2	2:C:220:ASP:H	1.67	1.07
2:C:98:LYS:HD2	2:C:98:LYS:H	1.15	1.07
2:C:219:ILE:HG22	2:C:220:ASP:N	1.65	1.07
2:D:44:ASN:HD21	2:D:46:LYS:HB3	1.18	1.06
3:N:185:U:H5"	3:N:186:A:OP2	1.55	1.06
2:C:148:LYS:O	2:C:152:GLU:HG2	1.55	1.06
3:M:194:A:N6	3:M:224:U:H3	1.53	1.06
2:D:27:ILE:HD11	2:D:63:LYS:HZ1	1.18	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:281:LEU:HG	2:C:281:LEU:O	1.57	1.05
2:C:36:ARG:HG2	2:C:36:ARG:HH11	1.19	1.04
2:C:98:LYS:HG2	2:C:99:LYS:H	0.90	1.04
2:D:10:ASN:O	2:D:14:ASN:HB2	1.56	1.03
2:C:98:LYS:CG	2:C:99:LYS:H	1.67	1.03
2:C:17:LYS:HG3	2:C:18:ALA:H	1.20	1.02
2:D:14:ASN:HA	2:D:17:LYS:NZ	1.73	1.02
2:C:98:LYS:HG2	2:C:99:LYS:N	1.74	1.02
2:D:10:ASN:HD21	2:D:17:LYS:HE2	1.21	1.01
2:C:59:ALA:HB2	2:C:77:ILE:HD12	1.40	1.01
2:C:24:LYS:HD2	2:C:24:LYS:O	1.62	1.00
2:C:60:LEU:HD12	2:C:60:LEU:O	1.60	1.00
3:M:181:C:H4'	3:M:181:C:OP1	1.62	0.99
1:B:86:LYS:HB3	1:B:86:LYS:NZ	1.77	0.99
3:N:168:G:H2'	3:N:169:G:H5''	1.44	0.99
3:M:236:C:H4'	3:M:237:G:H3'	1.41	0.99
2:C:44:ASN:HD22	2:C:47:LEU:HG	1.28	0.99
2:C:310:VAL:HG12	2:C:311:ASP:H	1.24	0.98
2:C:299:LEU:H	2:C:299:LEU:HD13	1.27	0.98
2:C:424:ILE:HD13	2:C:425:ASP:N	1.78	0.98
2:C:70:LYS:HD3	2:C:70:LYS:C	1.81	0.98
2:D:139:TYR:OH	2:D:188:ASP:HB3	1.62	0.98
2:D:219:ILE:HG22	2:D:220:ASP:H	1.27	0.97
2:C:36:ARG:HA	2:C:39:ILE:HG13	1.45	0.97
2:D:18:ALA:HB1	2:D:71:LYS:HD2	1.00	0.97
2:D:249:LEU:HD13	2:D:272:ILE:HB	1.46	0.97
3:M:181:C:C6	3:M:181:C:H5'	2.01	0.96
2:C:4:LYS:HA	2:C:7:GLU:HB3	1.47	0.95
3:M:194:A:H61	3:M:224:U:H3	1.04	0.95
3:N:146:G:H1'	3:N:186:A:C8	2.01	0.95
2:D:173:LYS:O	2:D:177:GLU:HB2	1.67	0.94
2:C:298:ASP:HB2	2:C:299:LEU:HD13	1.49	0.94
2:C:68:LEU:HD12	2:C:306:ALA:HB2	1.46	0.94
2:D:101:ASN:HD22	2:D:101:ASN:N	1.65	0.94
3:N:226:G:C2'	3:N:227:G:H5'	1.97	0.94
1:B:69:LYS:NZ	3:N:164:U:C4	2.36	0.94
2:C:12:ALA:HB1	2:C:30:VAL:HG13	1.51	0.93
2:D:14:ASN:HA	2:D:17:LYS:HZ2	1.29	0.93
2:C:278:ILE:H	2:C:278:ILE:CD1	1.80	0.93
2:C:2:MET:HA	2:C:2:MET:HE3	1.47	0.93
2:C:64:THR:HG22	2:C:66:LYS:CB	1.99	0.93
1:A:38:LEU:H	1:A:38:LEU:HD22	1.34	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:166:LYS:HG2	2:C:167:SER:N	1.80	0.92
2:D:105:LEU:CD1	2:D:117:ALA:HB2	1.98	0.92
2:C:98:LYS:HD2	2:C:98:LYS:N	1.84	0.92
2:C:325:LYS:HA	2:C:325:LYS:HZ2	1.19	0.92
2:D:221:GLY:CA	2:D:258:ALA:HB2	2.00	0.91
2:C:326:PHE:CZ	2:C:328:LEU:HD12	2.06	0.91
1:B:46:LYS:HE2	1:B:65:GLU:OE2	1.71	0.91
3:N:143:G:H1	3:N:235:U:H3	0.96	0.90
2:C:278:ILE:N	2:C:278:ILE:HD12	1.87	0.89
2:C:328:LEU:CD2	2:C:385:ARG:HD2	2.02	0.89
2:C:325:LYS:HB3	2:C:421:LYS:HG3	1.52	0.89
2:D:201:GLU:HA	2:D:204:LYS:CB	2.02	0.89
3:M:146:G:H1'	3:M:186:A:H8	1.35	0.89
3:N:236:C:H5''	3:N:237:G:O5'	1.71	0.89
2:D:329:ASN:O	2:D:332:MET:HB3	1.71	0.89
2:D:24:LYS:HG2	2:D:25:LYS:N	1.88	0.89
2:D:104:LEU:HD11	2:D:212:PRO:HG2	1.53	0.89
2:D:125:GLN:HA	2:D:129:LEU:O	1.73	0.88
2:C:124:ILE:HG21	2:C:184:VAL:HG11	1.55	0.88
2:D:14:ASN:OD1	2:D:17:LYS:HD2	1.70	0.88
2:C:64:THR:CG2	2:C:66:LYS:H	1.86	0.88
2:C:122:ARG:CG	2:C:278:ILE:HG21	2.02	0.88
2:C:166:LYS:CG	2:C:167:SER:H	1.86	0.88
2:D:275:GLY:HA3	2:D:280:ASP:HB2	1.54	0.88
3:M:181:C:H6	3:M:181:C:H5'	1.31	0.88
1:B:15:ARG:HH21	1:B:55:ARG:HD3	1.38	0.88
2:C:326:PHE:CE1	2:C:328:LEU:HD12	2.09	0.87
2:C:180:LYS:O	3:N:232:A:H5'	1.74	0.87
2:C:134:ILE:HG21	2:C:174:GLU:HG3	1.56	0.87
3:N:193:G:H4'	3:N:194:A:OP1	1.75	0.87
3:M:194:A:H2'	3:M:195:A:O5'	1.73	0.87
1:B:86:LYS:HB3	1:B:86:LYS:HZ3	1.37	0.87
2:C:90:ALA:H	2:C:91:LYS:HD3	1.40	0.87
2:D:382:LYS:HG2	3:N:220:A:OP1	1.75	0.86
2:D:193:HIS:O	2:D:194:LYS:HG2	1.75	0.86
3:M:194:A:C2'	3:M:195:A:O5'	2.21	0.86
3:N:226:G:H2'	3:N:227:G:H5'	1.54	0.86
2:C:166:LYS:HD2	2:C:169:VAL:HG22	1.56	0.86
1:A:26:ILE:HD11	1:A:29:PRO:HB3	1.56	0.86
2:D:261:ALA:O	2:D:262:VAL:HG23	1.75	0.86
2:D:163:THR:HG23	2:D:164:ARG:H	1.40	0.86
3:M:180:C:H2'	3:M:181:C:H5''	1.58	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:108:ILE:HD12	2:D:108:ILE:H	1.40	0.85
3:N:194:A:H5''	3:N:195:A:OP2	1.73	0.85
2:C:89:GLU:HB2	2:C:91:LYS:NZ	1.91	0.85
2:D:219:ILE:HG22	2:D:220:ASP:N	1.91	0.85
2:D:15:LYS:HE2	2:D:15:LYS:N	1.90	0.85
3:M:181:C:C5'	3:M:181:C:H6	1.88	0.85
2:C:325:LYS:HA	2:C:325:LYS:HZ1	1.36	0.85
2:D:44:ASN:ND2	2:D:46:LYS:HB3	1.90	0.85
1:B:46:LYS:HG2	1:B:48:TYR:HE1	1.41	0.85
2:C:109:GLN:HE22	2:C:192:ARG:HH12	1.21	0.85
3:N:181:C:H5'	3:N:181:C:H6	1.40	0.85
1:B:71:ASN:CB	1:B:74:GLN:HG3	2.06	0.84
2:C:319:ASP:HA	2:C:322:MET:CB	2.08	0.84
2:C:323:ARG:HB3	2:C:424:ILE:HD11	1.58	0.84
3:M:175:U:H6	3:M:175:U:C5'	1.91	0.84
2:D:41:ALA:O	2:D:257:GLY:HA3	1.78	0.84
2:D:106:VAL:HG11	2:D:203:MET:HG2	1.59	0.84
2:C:106:VAL:HA	2:C:190:ALA:HB2	1.60	0.84
2:D:14:ASN:C	2:D:15:LYS:HE2	1.96	0.84
2:D:221:GLY:HA3	2:D:258:ALA:HB2	1.60	0.84
1:B:36:LYS:HB3	1:B:36:LYS:NZ	1.91	0.84
3:N:208:C:N3	3:N:213:G:N2	2.24	0.83
2:C:105:LEU:HB3	2:C:113:LYS:CE	2.07	0.83
2:C:140:ARG:HH12	2:C:146:GLN:NE2	1.76	0.83
2:D:18:ALA:HB2	2:D:71:LYS:HD2	1.57	0.83
2:C:91:LYS:HD3	2:C:91:LYS:N	1.93	0.83
2:C:166:LYS:HG2	2:C:168:PRO:HD2	1.60	0.83
2:C:2:MET:SD	2:C:249:LEU:O	2.36	0.83
1:B:43:LEU:O	1:B:45:PRO:HD3	1.79	0.83
2:C:178:LYS:HB3	2:C:178:LYS:NZ	1.93	0.83
2:D:10:ASN:ND2	2:D:17:LYS:HE2	1.93	0.83
2:D:59:ALA:O	2:D:63:LYS:HB3	1.78	0.82
2:C:27:ILE:HG23	2:C:74:ILE:CD1	2.08	0.82
2:C:45:VAL:CG2	2:C:49:LEU:HD11	2.07	0.82
2:C:91:LYS:CD	2:C:91:LYS:H	1.83	0.82
2:C:97:PRO:HB2	2:C:98:LYS:NZ	1.95	0.82
2:D:13:LEU:HD21	2:D:75:ILE:HD11	1.60	0.82
2:D:59:ALA:HA	2:D:63:LYS:HB2	1.62	0.82
2:C:335:LEU:O	2:C:336:GLU:HG2	1.78	0.81
2:C:162:GLU:O	2:C:163:THR:HG23	1.80	0.81
2:D:66:LYS:HG3	2:D:67:GLY:N	1.95	0.81
2:C:319:ASP:HA	2:C:322:MET:HB2	1.62	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:2:MET:HG3	2:C:252:SER:O	1.79	0.81
2:D:322:MET:HB3	4:D:2084:HOH:O	1.79	0.81
2:C:73:HIS:HD2	2:C:76:LYS:HD2	1.43	0.81
2:D:18:ALA:CB	2:D:71:LYS:CD	2.43	0.81
2:C:85:LEU:HD21	2:C:260:SER:CB	2.09	0.81
3:N:185:U:C5'	3:N:186:A:OP2	2.29	0.81
2:D:326:PHE:HA	2:D:417:TYR:OH	1.79	0.81
2:C:134:ILE:CD1	2:C:174:GLU:HB2	2.11	0.81
2:C:215:ILE:HG22	2:C:234:PHE:HZ	1.44	0.81
2:C:30:VAL:HG12	2:C:34:ILE:HG13	1.61	0.80
2:D:232:LYS:O	2:D:236:GLU:HB3	1.82	0.80
2:D:171:ILE:HD12	2:D:175:GLY:HA3	1.62	0.80
2:D:113:LYS:HG2	2:D:188:ASP:OD1	1.81	0.80
2:C:42:ASP:O	2:C:257:GLY:HA3	1.80	0.80
2:C:325:LYS:CA	2:C:325:LYS:HZ2	1.95	0.80
2:D:366:THR:O	2:D:370:ILE:HD12	1.82	0.80
2:C:261:ALA:O	2:C:264:GLU:HG2	1.81	0.80
2:D:390:ILE:O	2:D:395:ARG:HD2	1.81	0.79
2:C:310:VAL:HG12	2:C:311:ASP:N	1.96	0.79
2:D:290:ILE:HG23	2:D:294:LEU:CD2	2.10	0.79
2:C:64:THR:CG2	2:C:66:LYS:HB2	2.08	0.79
2:C:328:LEU:HD21	2:C:385:ARG:HD2	1.63	0.79
2:C:97:PRO:HD2	2:C:101:ASN:HD21	1.48	0.79
2:D:17:LYS:HZ1	2:D:17:LYS:HA	1.48	0.79
2:D:38:LEU:HD12	2:D:48:VAL:HG13	1.64	0.79
2:D:59:ALA:HA	2:D:63:LYS:CB	2.12	0.79
2:D:104:LEU:HD23	2:D:189:THR:HG21	1.65	0.79
2:D:168:PRO:HA	2:D:171:ILE:CG2	2.13	0.79
2:D:55:ILE:HD11	2:D:81:GLU:HB3	1.64	0.79
2:D:58:ARG:HA	2:D:62:GLU:HG2	1.65	0.79
2:C:85:LEU:HD21	2:C:260:SER:HB2	1.64	0.79
2:D:307:GLU:HB3	2:D:311:ASP:HB3	1.65	0.78
2:C:68:LEU:HD12	2:C:306:ALA:CB	2.13	0.78
2:D:249:LEU:CD1	2:D:272:ILE:HB	2.13	0.78
2:D:66:LYS:HG3	2:D:67:GLY:H	1.48	0.78
3:M:173:U:H2'	3:M:174:G:H5'	1.65	0.78
2:C:219:ILE:HG21	2:C:227:ALA:HB1	1.65	0.78
2:C:63:LYS:NZ	2:C:70:LYS:HZ1	1.80	0.78
2:D:203:MET:HA	2:D:206:ILE:HB	1.65	0.78
3:N:208:C:H42	3:N:213:G:H1	1.29	0.78
2:D:24:LYS:HG2	2:D:25:LYS:H	1.46	0.78
2:D:365:LEU:O	2:D:370:ILE:HD11	1.82	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:122:ARG:HH21	2:D:154:ILE:HG23	1.47	0.78
2:C:108:ILE:HG23	2:C:194:LYS:HA	1.65	0.78
2:D:88:GLU:HB3	2:D:287:LYS:NZ	1.98	0.78
2:D:38:LEU:HD11	2:D:51:MET:SD	2.23	0.78
2:C:36:ARG:HG2	2:C:36:ARG:NH1	1.90	0.78
2:C:64:THR:HG23	2:C:66:LYS:H	1.48	0.78
3:M:194:A:N6	3:M:224:U:N3	2.31	0.77
1:B:71:ASN:HB2	1:B:74:GLN:HG3	1.66	0.77
2:D:43:VAL:HG13	2:D:260:SER:HB2	1.65	0.77
2:C:44:ASN:ND2	2:C:47:LEU:HG	1.99	0.77
2:C:63:LYS:HZ3	2:C:70:LYS:NZ	1.82	0.77
2:C:43:VAL:HG22	2:C:257:GLY:HA2	1.67	0.77
2:D:221:GLY:HA2	2:D:258:ALA:HB2	1.66	0.77
2:C:17:LYS:HG3	2:C:18:ALA:N	1.98	0.77
2:D:244:ILE:CD1	2:D:267:ALA:HB1	2.14	0.77
3:M:194:A:O2'	3:M:195:A:H5'	1.85	0.77
2:D:88:GLU:HB3	2:D:287:LYS:HZ1	1.50	0.77
2:D:35:GLN:HA	2:D:48:VAL:HG11	1.67	0.77
2:C:106:VAL:HB	2:C:199:LEU:HD11	1.64	0.77
2:D:116:THR:O	2:D:120:LEU:HB3	1.84	0.76
2:D:101:ASN:N	2:D:101:ASN:ND2	2.26	0.76
2:D:206:ILE:HD12	2:D:206:ILE:N	2.00	0.76
2:C:159:TYR:CD2	2:C:174:GLU:OE1	2.38	0.76
2:D:216:ILE:HG21	2:D:245:ILE:CD1	2.15	0.76
3:N:168:G:C2'	3:N:169:G:H5''	2.15	0.76
2:D:8:ASN:HA	2:D:11:LYS:CB	2.16	0.76
2:D:328:LEU:HG	2:D:385:ARG:HB3	1.67	0.76
2:C:45:VAL:HG22	2:C:49:LEU:CD1	2.15	0.76
2:C:169:VAL:C	2:C:171:ILE:H	1.86	0.75
2:C:134:ILE:HD13	2:C:174:GLU:HB2	1.68	0.75
2:D:315:GLU:HA	2:D:318:ILE:HG22	1.67	0.75
3:N:146:G:H1'	3:N:186:A:H8	1.50	0.75
2:D:4:LYS:HZ2	2:D:4:LYS:H	1.34	0.75
2:D:326:PHE:HE1	2:D:329:ASN:OD1	1.68	0.75
2:C:63:LYS:NZ	2:C:70:LYS:NZ	2.35	0.75
2:D:139:TYR:O	2:D:140:ARG:HD3	1.86	0.75
2:D:196:GLU:OE2	2:D:230:GLN:HA	1.87	0.75
2:D:210:THR:C	2:D:212:PRO:HD3	2.07	0.75
2:D:64:THR:HG22	2:D:65:PRO:HD2	1.67	0.75
2:D:238:VAL:HG12	2:D:241:ILE:HG23	1.69	0.75
3:N:172:A:H2'	3:N:173:U:O5'	1.86	0.74
2:D:41:ALA:HB3	2:D:43:VAL:HG23	1.68	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:203:MET:O	2:D:207:LYS:HG3	1.87	0.74
2:D:232:LYS:HE3	2:D:265:THR:HA	1.67	0.74
3:M:146:G:H1'	3:M:186:A:C8	2.22	0.74
2:C:397:ARG:HB2	2:C:407:GLU:OE1	1.87	0.74
3:N:180:C:C2'	3:N:181:C:H5''	2.17	0.74
3:M:221:C:O2'	3:M:222:G:H5'	1.88	0.74
2:C:299:LEU:CD2	2:C:300:GLU:H	2.00	0.74
2:D:112:GLY:C	2:D:114:THR:N	2.37	0.74
2:D:21:PHE:CZ	2:D:65:PRO:HA	2.22	0.74
1:A:11:LYS:HE3	1:A:11:LYS:HA	1.67	0.74
2:D:83:VAL:O	2:D:86:LEU:HG	1.87	0.74
2:C:272:ILE:HD13	2:C:284:PHE:HD1	1.53	0.73
3:M:221:C:C2'	3:M:222:G:H5'	2.18	0.73
2:C:314:THR:O	2:C:318:ILE:HB	1.89	0.73
2:C:400:ALA:HB2	2:C:410:VAL:HG11	1.71	0.73
2:C:150:LEU:O	2:C:153:LYS:N	2.21	0.73
1:B:3:ILE:CD1	1:B:38:LEU:HD11	2.18	0.73
2:C:86:LEU:HD12	2:C:290:ILE:CD1	2.19	0.73
2:C:45:VAL:HG13	2:C:46:LYS:N	2.04	0.73
2:D:96:ASN:ND2	4:D:2031:HOH:O	2.21	0.73
2:D:219:ILE:CG2	2:D:220:ASP:H	2.02	0.73
2:D:167:SER:O	2:D:171:ILE:HG22	1.88	0.73
2:C:73:HIS:CD2	2:C:76:LYS:HD2	2.23	0.73
2:D:210:THR:HG22	4:D:2067:HOH:O	1.87	0.73
2:D:170:ASP:O	2:D:174:GLU:HB2	1.87	0.73
1:B:46:LYS:HG2	1:B:48:TYR:CE1	2.22	0.73
2:D:239:GLY:O	2:D:241:ILE:HG22	1.88	0.73
2:C:424:ILE:C	2:C:424:ILE:HD13	2.10	0.73
3:N:169:G:N7	4:N:2036:HOH:O	2.22	0.72
2:D:326:PHE:CE1	2:D:329:ASN:OD1	2.42	0.72
2:D:57:ARG:HD2	2:D:61:GLU:HG3	1.69	0.72
2:C:68:LEU:HD13	2:C:68:LEU:H	1.53	0.72
2:D:201:GLU:CA	2:D:204:LYS:HB3	2.06	0.72
2:C:326:PHE:HD1	2:C:327:THR:N	1.87	0.72
2:D:330:GLU:O	2:D:334:GLN:HG2	1.88	0.72
3:M:209:G:N7	4:M:2070:HOH:O	2.22	0.72
1:A:1:MET:SD	1:A:72:LYS:HG3	2.29	0.72
2:D:103:ILE:HG21	2:D:216:ILE:HG13	1.71	0.72
2:C:58:ARG:NH2	2:C:77:ILE:HG12	2.03	0.72
2:C:27:ILE:HG23	2:C:74:ILE:HD11	1.71	0.72
2:C:326:PHE:HB3	2:C:329:ASN:HB2	1.70	0.72
2:D:14:ASN:HA	2:D:17:LYS:HZ3	1.55	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:160:C:H6	3:N:160:C:H3'	1.54	0.72
2:C:310:VAL:CG1	2:C:311:ASP:H	2.01	0.72
2:C:323:ARG:NH2	2:C:426:LYS:O	2.22	0.72
1:B:15:ARG:O	1:B:15:ARG:NE	2.23	0.72
3:N:172:A:H5'	3:N:172:A:H8	1.54	0.72
2:C:290:ILE:HG22	2:C:294:LEU:HG	1.72	0.72
2:C:67:GLY:HA2	2:C:309:MET:SD	2.30	0.72
2:C:83:VAL:HG22	2:C:290:ILE:HG13	1.71	0.71
3:N:210:G:H8	3:N:210:G:P	2.13	0.71
1:A:23:GLU:CA	1:A:23:GLU:OE1	2.37	0.71
3:N:208:C:N4	3:N:213:G:H1	1.86	0.71
2:C:244:ILE:N	2:C:244:ILE:HD12	2.05	0.71
2:C:266:LYS:NZ	4:C:2078:HOH:O	2.22	0.71
2:D:64:THR:HG22	2:D:65:PRO:CD	2.19	0.71
2:D:104:LEU:HB3	2:D:189:THR:HG21	1.72	0.71
1:B:46:LYS:CE	1:B:65:GLU:OE2	2.37	0.71
2:D:247:THR:O	2:D:273:GLY:HA3	1.89	0.71
2:D:88:GLU:N	2:D:88:GLU:OE2	2.24	0.71
3:N:190:G:H2'	3:N:191:C:H5'	1.73	0.71
3:M:236:C:C4'	3:M:237:G:H3'	2.19	0.71
2:D:285:ASP:HB2	2:D:288:LYS:HB2	1.72	0.71
2:D:113:LYS:HE3	2:D:191:GLY:HA2	1.73	0.71
2:D:214:GLU:HA	2:D:241:ILE:O	1.90	0.71
2:C:135:ALA:HB1	2:C:139:TYR:CE1	2.26	0.70
3:M:197:C:H3'	3:M:197:C:H6	1.56	0.70
3:M:190:G:H2'	3:M:191:C:H6	1.54	0.70
2:D:5:LEU:HD23	2:D:41:ALA:HB2	1.74	0.70
2:C:64:THR:HG22	2:C:66:LYS:H	1.57	0.70
2:C:133:LEU:CD2	2:C:186:ILE:HB	2.20	0.70
2:C:123:TYR:HE2	2:C:283:PRO:HG3	1.54	0.70
2:D:46:LYS:O	2:D:49:LEU:HB2	1.91	0.70
2:D:428:HIS:N	4:D:2107:HOH:O	2.23	0.70
2:C:57:ARG:O	2:C:57:ARG:NE	2.24	0.70
2:C:134:ILE:CG2	2:C:174:GLU:HG3	2.21	0.70
2:C:187:ILE:HG22	2:C:189:THR:HG22	1.71	0.70
2:C:94:GLU:CD	2:C:94:GLU:H	1.94	0.70
2:C:244:ILE:N	2:C:244:ILE:CD1	2.54	0.70
2:C:312:GLU:O	2:C:316:GLU:CB	2.40	0.70
1:A:73:LEU:HD22	3:M:162:U:H5	1.55	0.70
2:D:6:GLY:O	2:D:9:LEU:HB3	1.91	0.69
2:C:215:ILE:CG2	2:C:234:PHE:HZ	2.05	0.69
2:C:89:GLU:HB2	2:C:91:LYS:HZ2	1.56	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:210:G:O5'	3:N:210:G:H8	1.75	0.69
2:D:9:LEU:HD21	2:D:82:LEU:HD21	1.74	0.69
2:C:2:MET:HA	2:C:2:MET:CE	2.20	0.69
1:A:10:LYS:HB2	1:A:25:ALA:O	1.91	0.69
2:D:163:THR:HG23	2:D:164:ARG:N	2.06	0.69
2:D:13:LEU:HD11	2:D:75:ILE:HD12	1.73	0.69
3:M:151:G:H1	3:M:179:C:N4	1.90	0.69
3:M:175:U:H6	3:M:175:U:H5''	1.57	0.69
3:N:197:C:H5''	3:N:198:C:H5'	1.73	0.69
2:D:8:ASN:HA	2:D:11:LYS:HB2	1.73	0.69
2:D:122:ARG:NH2	2:D:154:ILE:HG23	2.07	0.69
3:N:168:G:H2'	3:N:169:G:C5'	2.21	0.69
3:N:236:C:H4'	3:N:237:G:O3'	1.93	0.69
2:D:64:THR:C	2:D:66:LYS:H	1.94	0.69
2:D:322:MET:HG3	2:D:323:ARG:HH11	1.58	0.69
2:C:44:ASN:O	2:C:45:VAL:C	2.31	0.69
3:N:190:G:C2'	3:N:191:C:H5'	2.22	0.69
2:D:216:ILE:HG21	2:D:245:ILE:HD12	1.74	0.69
2:C:384:GLU:OE2	2:C:395:ARG:HD3	1.93	0.69
2:D:2:MET:SD	2:D:289:PHE:CE1	2.85	0.69
3:N:172:A:C2'	3:N:173:U:O5'	2.39	0.69
2:D:199:LEU:HD23	2:D:200:LEU:H	1.57	0.68
3:M:179:C:H2'	3:M:180:C:C6	2.27	0.68
2:C:73:HIS:NE2	2:C:76:LYS:NZ	2.41	0.68
3:M:180:C:C2'	3:M:181:C:H5''	2.23	0.68
3:M:197:C:C6	3:M:197:C:H3'	2.27	0.68
2:D:84:LYS:NZ	2:D:84:LYS:HB3	2.08	0.68
3:M:196:C:N3	4:M:2058:HOH:O	2.26	0.68
2:C:31:ILE:HD11	2:C:55:ILE:HG21	1.74	0.68
2:C:27:ILE:HG23	2:C:74:ILE:HD12	1.75	0.68
3:M:181:C:C5'	3:M:181:C:C6	2.69	0.68
2:C:123:TYR:CE2	2:C:283:PRO:HG3	2.29	0.68
2:D:421:LYS:O	2:D:423:ALA:N	2.25	0.68
2:D:305:LYS:HZ3	2:D:306:ALA:H	1.40	0.68
2:C:122:ARG:CB	2:C:278:ILE:HG21	2.23	0.68
2:D:399:ILE:O	2:D:400:ALA:O	2.10	0.68
3:M:151:G:H1	3:M:179:C:H42	1.40	0.68
1:B:66:VAL:HG22	1:B:67:ASP:H	1.59	0.68
2:C:64:THR:O	2:C:66:LYS:N	2.26	0.68
2:C:68:LEU:O	2:C:72:GLU:HB2	1.94	0.68
2:D:101:ASN:H	2:D:101:ASN:HD22	1.40	0.68
2:D:154:ILE:N	2:D:154:ILE:HD12	2.09	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:161:ASP:HB3	2:C:170:ASP:OD1	1.94	0.68
2:C:104:LEU:HB2	2:C:215:ILE:HD13	1.75	0.68
2:C:147:LEU:HA	2:C:150:LEU:HD12	1.74	0.68
2:C:122:ARG:HB3	2:C:278:ILE:HG21	1.76	0.68
2:D:326:PHE:HD1	2:D:326:PHE:N	1.91	0.68
2:D:320:ALA:HB2	2:D:329:ASN:ND2	2.09	0.68
2:D:41:ALA:O	2:D:257:GLY:CA	2.42	0.68
2:C:45:VAL:HG22	2:C:49:LEU:HD11	1.73	0.67
2:D:2:MET:N	2:D:4:LYS:HZ1	1.92	0.67
1:A:23:GLU:HA	1:A:23:GLU:OE1	1.94	0.67
3:N:174:G:N7	4:N:2049:HOH:O	2.27	0.67
2:D:313:LYS:HG3	2:D:314:THR:N	2.09	0.67
2:C:109:GLN:HE22	2:C:192:ARG:NH1	1.92	0.67
2:D:2:MET:SD	2:D:289:PHE:HE1	2.17	0.67
1:B:31:LEU:HG	1:B:47:ILE:HG23	1.77	0.67
2:C:221:GLY:O	2:C:223:ILE:N	2.28	0.67
2:D:315:GLU:HA	2:D:318:ILE:CG2	2.25	0.67
3:N:210:G:OP1	3:N:210:G:C8	2.48	0.67
1:A:50:ASP:O	1:A:50:ASP:OD2	2.12	0.67
3:M:169:G:H2'	3:M:170:A:H5'	1.75	0.67
2:D:6:GLY:HA2	2:D:9:LEU:HB3	1.76	0.67
2:C:328:LEU:HD23	2:C:385:ARG:HD2	1.75	0.67
2:C:274:ILE:HB	2:C:280:ASP:O	1.95	0.67
2:C:319:ASP:HA	2:C:322:MET:HB3	1.76	0.67
2:D:134:ILE:HG13	2:D:187:ILE:HG13	1.77	0.66
2:D:22:VAL:HG23	2:D:22:VAL:O	1.95	0.66
2:D:239:GLY:O	2:D:241:ILE:N	2.28	0.66
3:N:174:G:C2'	3:N:175:U:H5'	2.24	0.66
1:B:8:ILE:HD12	1:B:26:ILE:HD11	1.77	0.66
2:D:101:ASN:ND2	2:D:184:VAL:HG22	2.10	0.66
3:N:169:G:H5'	3:N:169:G:H8	1.61	0.66
2:C:379:SER:OG	2:C:379:SER:O	2.10	0.66
2:C:299:LEU:HD13	2:C:299:LEU:N	2.05	0.66
2:D:125:GLN:HG2	2:D:126:LYS:N	2.08	0.66
2:C:4:LYS:CA	2:C:7:GLU:HB3	2.23	0.66
2:C:73:HIS:O	2:C:76:LYS:N	2.25	0.66
2:C:305:LYS:HG3	4:C:2033:HOH:O	1.94	0.66
2:D:74:ILE:O	2:D:78:VAL:N	2.29	0.66
2:C:63:LYS:HZ3	2:C:70:LYS:HZ1	1.41	0.66
2:D:190:ALA:HA	2:D:202:GLU:HG2	1.78	0.66
2:D:43:VAL:HG13	2:D:260:SER:CB	2.25	0.65
2:D:88:GLU:H	2:D:88:GLU:CD	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:326:PHE:CZ	2:C:386:GLU:HA	2.31	0.65
2:C:323:ARG:HH21	2:C:426:LYS:C	1.98	0.65
2:C:45:VAL:HG23	2:C:49:LEU:HD11	1.79	0.65
3:M:187:C:O2	3:M:188:C:C6	2.49	0.65
2:C:391:ILE:O	2:C:392:LYS:HD3	1.95	0.65
2:C:54:GLU:O	2:C:58:ARG:HD3	1.96	0.65
2:C:109:GLN:NE2	2:C:192:ARG:HH12	1.94	0.65
3:M:173:U:C2'	3:M:174:G:H5'	2.27	0.65
2:C:35:GLN:HB2	2:C:48:VAL:CG1	2.26	0.65
2:D:244:ILE:HD11	2:D:267:ALA:HB1	1.77	0.65
2:C:17:LYS:CG	2:C:18:ALA:H	2.05	0.65
2:C:312:GLU:O	2:C:316:GLU:HB3	1.97	0.65
2:C:332:MET:O	2:C:332:MET:SD	2.53	0.65
2:D:105:LEU:HD12	2:D:117:ALA:CB	2.10	0.65
2:D:201:GLU:C	2:D:203:MET:H	2.00	0.65
2:C:215:ILE:HG22	2:C:234:PHE:CZ	2.28	0.65
2:D:66:LYS:CG	2:D:67:GLY:H	2.09	0.65
2:D:215:ILE:HG12	2:D:242:GLY:HA3	1.78	0.65
3:M:180:C:C3'	3:M:181:C:H5''	2.27	0.65
2:C:192:ARG:HB2	2:C:192:ARG:NH1	2.11	0.65
1:B:63:CYS:SG	1:B:63:CYS:O	2.54	0.65
2:D:5:LEU:HD13	2:D:5:LEU:O	1.96	0.65
2:C:70:LYS:HD3	2:C:71:LYS:N	2.11	0.65
3:M:186:A:H5'	3:M:187:C:OP1	1.96	0.65
1:A:18:ARG:NH2	3:M:158:C:OP1	2.30	0.65
3:N:146:G:O2'	3:N:147:U:P	2.54	0.64
2:C:85:LEU:HD21	2:C:260:SER:HB3	1.78	0.64
3:M:209:G:C2	3:M:211:A:OP2	2.50	0.64
3:N:193:G:C4'	3:N:194:A:OP1	2.43	0.64
2:C:299:LEU:HD22	2:C:300:GLU:H	1.62	0.64
2:D:211:ASN:N	2:D:212:PRO:HD3	2.12	0.64
2:C:99:LYS:NZ	3:N:233:C:OP1	2.21	0.64
3:M:194:A:O2'	3:M:195:A:C5'	2.45	0.64
2:C:323:ARG:HB2	2:C:323:ARG:NH1	2.12	0.64
1:A:2:ILE:HD12	1:A:2:ILE:N	2.12	0.64
2:D:406:THR:HG23	2:D:409:ASP:OD2	1.96	0.64
2:C:303:LEU:HD13	2:C:307:GLU:HG3	1.79	0.64
1:B:24:LEU:O	1:B:24:LEU:HD12	1.98	0.64
3:N:183:U:H5''	3:N:183:U:C6	2.32	0.64
2:D:24:LYS:CG	2:D:25:LYS:H	2.11	0.64
2:D:316:GLU:HA	2:D:319:ASP:HB3	1.80	0.64
1:A:38:LEU:HD11	1:A:79:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:225:GLN:O	2:D:228:GLY:N	2.31	0.64
2:C:60:LEU:CD1	2:C:60:LEU:O	2.42	0.64
1:B:15:ARG:HH21	1:B:55:ARG:CD	2.09	0.64
2:D:24:LYS:O	2:D:27:ILE:HB	1.98	0.64
2:C:59:ALA:HA	2:C:63:LYS:HB3	1.78	0.64
2:D:107:GLY:H	2:D:190:ALA:HB3	1.62	0.64
2:C:221:GLY:O	2:C:224:GLY:N	2.28	0.64
2:D:224:GLY:HA3	2:D:254:LYS:NZ	2.12	0.64
3:N:231:G:H2'	3:N:232:A:C8	2.33	0.63
3:N:166:G:H8	3:N:166:G:O5'	1.82	0.63
2:D:24:LYS:CG	2:D:25:LYS:N	2.61	0.63
2:D:35:GLN:NE2	2:D:39:ILE:HD11	2.13	0.63
2:C:63:LYS:O	2:C:64:THR:HB	1.97	0.63
2:D:112:GLY:O	2:D:113:LYS:C	2.36	0.63
2:D:104:LEU:HB3	2:D:189:THR:CG2	2.27	0.63
2:D:224:GLY:N	2:D:254:LYS:HZ2	1.96	0.63
2:C:25:LYS:O	2:C:28:LYS:N	2.32	0.63
3:N:226:G:O2'	3:N:227:G:H5'	1.98	0.63
2:D:215:ILE:HD13	2:D:215:ILE:N	2.14	0.63
3:N:210:G:OP1	3:N:210:G:H8	1.80	0.63
2:C:367:GLU:O	2:C:370:ILE:N	2.29	0.63
2:D:75:ILE:HA	2:D:78:VAL:HB	1.79	0.63
2:C:98:LYS:HG2	2:C:100:GLN:H	1.63	0.63
2:D:8:ASN:HA	2:D:11:LYS:HB3	1.79	0.63
2:D:83:VAL:HG11	2:D:287:LYS:NZ	2.13	0.63
2:D:268:PRO:HB2	2:D:270:LYS:CE	2.29	0.63
1:B:86:LYS:HB3	1:B:86:LYS:HZ2	1.64	0.63
1:B:32:LYS:N	1:B:32:LYS:HD2	2.14	0.63
1:A:64:VAL:HG12	1:A:64:VAL:O	1.98	0.63
3:N:180:C:H2'	3:N:181:C:H5''	1.79	0.63
2:C:64:THR:HG22	2:C:66:LYS:N	2.14	0.62
1:B:1:MET:N	3:N:164:U:O2'	2.32	0.62
2:D:406:THR:O	2:D:410:VAL:HG12	1.98	0.62
2:D:7:GLU:O	2:D:11:LYS:HB2	1.99	0.62
2:C:64:THR:C	2:C:66:LYS:N	2.50	0.62
2:C:97:PRO:HB2	2:C:98:LYS:HZ1	1.61	0.62
2:C:424:ILE:CD1	2:C:424:ILE:C	2.67	0.62
2:C:95:LEU:HD21	2:C:127:ARG:HG2	1.81	0.62
2:D:388:PRO:O	2:D:389:LYS:HB3	1.99	0.62
2:D:18:ALA:HB1	2:D:71:LYS:HD3	1.76	0.62
2:D:35:GLN:HA	2:D:48:VAL:CG1	2.29	0.62
2:D:163:THR:CG2	2:D:164:ARG:H	2.10	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:175:U:C6	3:M:175:U:C5'	2.79	0.62
2:C:216:ILE:CG2	2:C:245:ILE:HG13	2.30	0.62
2:C:88:GLU:O	2:C:89:GLU:HB3	1.98	0.62
2:D:139:TYR:HH	2:D:188:ASP:HB3	1.61	0.62
2:D:326:PHE:CD1	2:D:326:PHE:N	2.64	0.62
2:D:326:PHE:HA	2:D:417:TYR:CZ	2.33	0.62
3:N:181:C:C6	3:N:181:C:H5'	2.30	0.62
2:C:119:LYS:HB3	2:C:281:LEU:HD22	1.81	0.62
2:D:140:ARG:C	2:D:142:ALA:H	2.03	0.62
1:B:36:LYS:HB3	1:B:36:LYS:HZ2	1.65	0.62
2:C:140:ARG:HH22	2:C:146:GLN:HE22	1.46	0.62
1:A:73:LEU:HD22	3:M:162:U:C5	2.35	0.62
1:B:73:LEU:O	1:B:76:LEU:HB2	1.99	0.62
2:C:89:GLU:HB2	2:C:91:LYS:HZ1	1.65	0.62
2:D:136:ALA:HB3	2:D:189:THR:HA	1.81	0.62
2:D:118:ALA:HB1	2:D:150:LEU:HD13	1.82	0.62
2:D:18:ALA:HA	2:D:71:LYS:HG3	1.81	0.62
2:D:90:ALA:O	2:D:92:LYS:HG2	2.00	0.62
2:C:108:ILE:HD12	2:C:108:ILE:H	1.65	0.62
2:D:398:ARG:NH1	3:N:218:C:O2'	2.33	0.62
3:N:210:G:O5'	3:N:210:G:C8	2.53	0.62
1:A:78:GLU:O	1:A:82:ILE:HG13	2.00	0.62
2:C:59:ALA:HB2	2:C:77:ILE:CD1	2.23	0.62
2:C:169:VAL:C	2:C:171:ILE:N	2.53	0.62
2:D:218:VAL:HG13	2:D:247:THR:CG2	2.29	0.62
2:C:92:LYS:HG3	2:C:92:LYS:O	1.99	0.62
2:D:158:ILE:HD12	2:D:158:ILE:H	1.65	0.61
1:A:32:LYS:CD	1:A:32:LYS:H	2.12	0.61
2:D:326:PHE:CD2	2:D:328:LEU:HB2	2.36	0.61
2:C:174:GLU:O	2:C:178:LYS:HG2	2.00	0.61
3:N:180:C:C3'	3:N:181:C:H5''	2.30	0.61
2:C:5:LEU:HG	2:C:41:ALA:CB	2.30	0.61
2:C:323:ARG:NH2	2:C:426:LYS:C	2.54	0.61
3:N:191:C:O2	3:N:227:G:N1	2.28	0.61
2:C:177:GLU:OE2	2:C:178:LYS:N	2.32	0.61
1:A:14:ARG:HB3	4:M:2024:HOH:O	1.99	0.61
3:M:178:C:C6	3:M:178:C:H5''	2.35	0.61
2:D:237:ALA:HB1	4:D:2074:HOH:O	2.00	0.61
1:A:64:VAL:CG1	1:A:64:VAL:O	2.46	0.61
1:A:46:LYS:HA	4:A:2007:HOH:O	2.00	0.61
2:C:291:SER:HB2	2:C:298:ASP:HB3	1.83	0.61
2:C:99:LYS:HE2	3:N:233:C:H5'	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:322:MET:HG3	2:D:323:ARG:H	1.65	0.61
2:C:238:VAL:O	2:C:240:GLU:N	2.30	0.61
2:C:70:LYS:CD	2:C:71:LYS:N	2.64	0.61
2:C:91:LYS:HB3	2:C:284:PHE:O	1.99	0.61
2:C:17:LYS:O	2:C:18:ALA:HB2	2.00	0.61
2:D:112:GLY:O	2:D:116:THR:N	2.20	0.61
3:N:235:U:H2'	3:N:236:C:O5'	2.01	0.61
2:C:325:LYS:HG3	2:C:326:PHE:H	1.66	0.61
2:D:290:ILE:HA	2:D:293:LEU:HD12	1.83	0.61
2:D:223:ILE:HG12	2:D:226:GLN:CB	2.31	0.61
2:C:49:LEU:N	2:C:49:LEU:HD12	2.16	0.60
2:C:274:ILE:HD13	2:C:281:LEU:HA	1.82	0.60
2:D:129:LEU:HD22	2:D:183:ASP:CG	2.22	0.60
2:C:161:ASP:CG	2:C:165:THR:HG23	2.21	0.60
3:N:183:U:H6	3:N:183:U:H5''	1.66	0.60
2:D:76:LYS:O	2:D:80:GLU:HB2	2.00	0.60
2:C:104:LEU:CB	2:C:215:ILE:HD13	2.31	0.60
2:C:196:GLU:OE2	2:C:230:GLN:HA	2.00	0.60
2:D:398:ARG:HG2	2:D:398:ARG:O	2.00	0.60
2:D:104:LEU:CD1	2:D:212:PRO:HG2	2.27	0.60
3:N:159:U:O2'	3:N:160:C:H5'	2.02	0.60
1:B:68:TYR:HE2	1:B:71:ASN:O	1.84	0.60
1:B:31:LEU:HG	1:B:47:ILE:CG2	2.31	0.60
1:B:18:ARG:NH2	3:N:158:C:OP1	2.35	0.60
2:D:328:LEU:HD12	2:D:386:GLU:HA	1.82	0.60
2:D:51:MET:HA	2:D:81:GLU:OE1	2.01	0.60
2:D:247:THR:O	2:D:273:GLY:CA	2.49	0.60
2:C:71:LYS:HE2	2:C:72:GLU:HG3	1.83	0.60
2:C:159:TYR:CG	2:C:174:GLU:OE1	2.55	0.60
1:B:79:ILE:O	1:B:83:ILE:HG13	2.02	0.60
1:B:43:LEU:C	1:B:45:PRO:HD3	2.22	0.60
2:C:397:ARG:HG3	2:C:397:ARG:O	2.01	0.60
2:D:281:LEU:HD12	2:D:281:LEU:C	2.22	0.60
2:D:14:ASN:HD22	2:D:15:LYS:HZ1	1.50	0.60
2:D:17:LYS:NZ	2:D:17:LYS:HA	2.16	0.60
2:D:95:LEU:O	2:D:184:VAL:HG21	2.02	0.60
3:N:236:C:H5'	3:N:237:G:O3'	2.02	0.60
3:M:187:C:N3	3:M:188:C:C5	2.68	0.60
2:C:85:LEU:C	2:C:85:LEU:HD23	2.22	0.60
2:D:101:ASN:HD21	2:D:184:VAL:HG22	1.67	0.60
2:C:108:ILE:HD12	2:C:199:LEU:HD22	1.83	0.60
2:C:27:ILE:HD13	2:C:59:ALA:O	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:64:THR:CG2	2:C:66:LYS:N	2.64	0.59
2:D:139:TYR:OH	2:D:188:ASP:CB	2.46	0.59
2:C:103:ILE:HG21	2:C:216:ILE:CD1	2.31	0.59
2:C:178:LYS:HZ3	2:C:178:LYS:HB3	1.67	0.59
2:C:335:LEU:O	2:C:336:GLU:CG	2.50	0.59
2:D:265:THR:O	2:D:266:LYS:C	2.41	0.59
2:D:89:GLU:HB2	2:D:311:ASP:OD1	2.03	0.59
2:C:326:PHE:CD1	2:C:327:THR:N	2.68	0.59
2:C:66:LYS:HE3	2:C:66:LYS:HA	1.83	0.59
2:D:88:GLU:CB	2:D:287:LYS:NZ	2.66	0.59
2:C:45:VAL:HG22	2:C:49:LEU:HD13	1.83	0.59
2:D:326:PHE:CE2	2:D:328:LEU:HB2	2.37	0.59
3:N:190:G:H2'	3:N:191:C:C5'	2.32	0.59
2:D:125:GLN:OE1	2:D:154:ILE:HG21	2.02	0.59
3:N:232:A:C6	3:N:233:C:C4	2.91	0.59
2:C:173:LYS:O	2:C:177:GLU:HB2	2.02	0.59
2:D:244:ILE:HD12	2:D:267:ALA:HB1	1.83	0.59
2:C:76:LYS:HD3	2:C:77:ILE:N	2.18	0.59
2:C:79:TYR:OH	2:C:299:LEU:HD12	2.02	0.59
2:D:369:LYS:O	2:D:370:ILE:C	2.40	0.59
1:A:1:MET:N	1:A:66:VAL:O	2.35	0.59
2:D:316:GLU:CA	2:D:319:ASP:HB3	2.33	0.59
2:D:128:GLY:O	2:D:129:LEU:HG	2.02	0.59
2:C:169:VAL:HA	2:C:172:VAL:HG23	1.83	0.59
2:C:54:GLU:HG3	2:C:58:ARG:HD3	1.84	0.59
2:D:117:ALA:O	2:D:133:LEU:HD13	2.03	0.59
2:D:125:GLN:HE22	2:D:154:ILE:HG22	1.67	0.59
2:D:108:ILE:CD1	2:D:108:ILE:H	2.04	0.59
2:D:323:ARG:HD3	2:D:427:LEU:HD21	1.85	0.59
3:M:169:G:C2'	3:M:170:A:H5'	2.32	0.59
2:C:303:LEU:HD13	2:C:307:GLU:CG	2.33	0.59
2:C:54:GLU:O	2:C:54:GLU:HG3	2.02	0.58
2:D:21:PHE:HZ	2:D:65:PRO:HA	1.66	0.58
2:C:274:ILE:CG2	2:C:280:ASP:HB3	2.33	0.58
2:D:211:ASN:N	4:D:2067:HOH:O	2.36	0.58
2:C:129:LEU:O	2:C:131:PRO:HD3	2.03	0.58
2:D:66:LYS:CG	2:D:67:GLY:N	2.65	0.58
2:D:168:PRO:HA	2:D:171:ILE:HG23	1.85	0.58
2:D:310:VAL:O	2:D:310:VAL:HG12	2.03	0.58
2:C:210:THR:C	2:C:212:PRO:HD3	2.24	0.58
2:D:268:PRO:HB2	2:D:270:LYS:HE3	1.85	0.58
2:C:70:LYS:C	2:C:70:LYS:CD	2.65	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:214:GLU:C	2:D:215:ILE:HD13	2.23	0.58
3:M:181:C:C2'	3:M:182:C:O5'	2.52	0.58
2:D:127:ARG:NH1	4:D:2036:HOH:O	2.34	0.58
2:C:64:THR:C	2:C:66:LYS:H	2.07	0.58
2:C:168:PRO:O	2:C:172:VAL:HG23	2.03	0.58
2:D:221:GLY:HA3	2:D:258:ALA:CB	2.33	0.58
2:C:174:GLU:CD	2:C:174:GLU:H	2.07	0.58
2:D:376:ILE:O	2:D:377:ILE:C	2.41	0.58
2:D:102:VAL:HG11	2:D:185:LEU:HB2	1.84	0.58
2:C:98:LYS:CG	2:C:99:LYS:N	2.42	0.58
1:B:32:LYS:H	1:B:32:LYS:HD2	1.68	0.58
2:D:27:ILE:HD11	2:D:63:LYS:NZ	2.04	0.58
2:D:55:ILE:CD1	2:D:81:GLU:HB3	2.33	0.58
2:D:88:GLU:CB	2:D:287:LYS:HZ3	2.17	0.58
2:D:117:ALA:O	2:D:133:LEU:CD1	2.52	0.58
3:M:179:C:H2'	3:M:180:C:H6	1.68	0.58
1:A:32:LYS:H	1:A:32:LYS:CE	2.17	0.58
2:C:102:VAL:HG11	2:C:210:THR:HG21	1.86	0.58
2:D:59:ALA:HA	2:D:63:LYS:HB3	1.85	0.58
1:B:39:LYS:C	1:B:41:LEU:H	2.07	0.58
2:D:58:ARG:HD3	4:D:2014:HOH:O	2.03	0.58
2:C:398:ARG:HG2	2:C:398:ARG:NH1	2.19	0.58
2:C:65:PRO:O	2:C:66:LYS:C	2.40	0.58
3:N:160:C:C6	3:N:160:C:H3'	2.38	0.58
2:D:305:LYS:NZ	2:D:305:LYS:HB3	2.19	0.58
2:C:2:MET:CA	2:C:2:MET:CE	2.81	0.58
3:N:210:G:C8	3:N:210:G:P	2.94	0.58
3:M:157:U:H6	3:M:157:U:O5'	1.87	0.58
2:C:328:LEU:HG	2:C:385:ARG:HB3	1.86	0.58
2:D:292:ARG:O	2:D:293:LEU:HG	2.03	0.58
2:C:36:ARG:NH1	2:C:40:GLN:OE1	2.36	0.58
2:C:219:ILE:CG2	2:C:220:ASP:N	2.35	0.58
1:A:32:LYS:N	1:A:32:LYS:HE3	2.19	0.58
2:D:16:LEU:HD23	2:D:16:LEU:N	2.18	0.57
2:C:424:ILE:HD13	2:C:425:ASP:H	1.64	0.57
2:D:323:ARG:CD	2:D:427:LEU:HD22	2.34	0.57
1:A:59:GLU:CG	1:A:59:GLU:O	2.52	0.57
2:C:372:LYS:NZ	4:C:2094:HOH:O	2.22	0.57
2:C:45:VAL:CG2	2:C:49:LEU:CD1	2.77	0.57
2:C:97:PRO:HB2	2:C:98:LYS:HZ3	1.67	0.57
3:N:160:C:C2'	3:N:161:C:O5'	2.52	0.57
2:D:172:VAL:O	2:D:176:MET:HB3	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:23:GLU:N	1:A:23:GLU:OE1	2.38	0.57
3:N:197:C:H5''	3:N:198:C:C5'	2.33	0.57
2:C:24:LYS:C	2:C:24:LYS:HD2	2.24	0.57
2:D:83:VAL:HG11	2:D:287:LYS:HZ1	1.70	0.57
2:C:45:VAL:HG13	2:C:46:LYS:H	1.69	0.57
2:D:200:LEU:O	2:D:204:LYS:HB2	2.05	0.57
2:C:158:ILE:HD12	2:C:159:TYR:N	2.18	0.57
2:C:312:GLU:O	2:C:316:GLU:HB2	2.03	0.57
1:B:18:ARG:NH1	1:B:22:GLU:HG2	2.19	0.57
1:B:9:ASP:O	1:B:11:LYS:N	2.38	0.57
2:D:374:LYS:O	2:D:378:SER:HB2	2.03	0.57
3:M:187:C:H2'	3:M:187:C:O2	2.05	0.57
2:C:140:ARG:NH1	2:C:146:GLN:NE2	2.51	0.57
2:C:340:ASN:N	2:C:340:ASN:ND2	2.50	0.57
2:C:398:ARG:HH11	2:C:398:ARG:HG2	1.69	0.57
2:D:193:HIS:O	2:D:194:LYS:CG	2.51	0.57
2:D:219:ILE:HD13	2:D:230:GLN:HB3	1.87	0.57
3:N:169:G:H2'	3:N:170:A:O5'	2.05	0.57
3:N:152:G:H2'	3:N:153:A:O5'	2.05	0.57
3:M:171:G:H2'	3:M:172:A:C8	2.40	0.57
2:C:326:PHE:HD1	2:C:328:LEU:H	1.50	0.57
2:C:13:LEU:HB3	2:C:75:ILE:HD12	1.85	0.57
2:C:384:GLU:O	2:C:388:PRO:HB3	2.04	0.57
2:C:264:GLU:HG3	2:C:265:THR:N	2.20	0.57
2:C:147:LEU:HD23	2:C:147:LEU:C	2.25	0.57
3:M:195:A:N6	4:M:2057:HOH:O	2.38	0.57
2:D:284:PHE:HE2	4:D:2028:HOH:O	1.87	0.57
2:C:128:GLY:O	2:C:129:LEU:HD23	2.05	0.57
2:D:262:VAL:HG21	2:D:269:ILE:HD11	1.86	0.56
2:D:206:ILE:HD12	2:D:206:ILE:H	1.69	0.56
1:B:3:ILE:HD12	1:B:38:LEU:HD11	1.86	0.56
3:M:148:G:C8	3:M:148:G:H5''	2.39	0.56
2:D:84:LYS:NZ	4:D:2027:HOH:O	2.37	0.56
2:D:322:MET:CG	2:D:427:LEU:HD21	2.36	0.56
1:A:32:LYS:HE3	1:A:32:LYS:H	1.70	0.56
3:M:171:G:H2'	3:M:172:A:H8	1.70	0.56
3:M:148:G:H8	3:M:148:G:H5''	1.69	0.56
2:C:22:VAL:CG2	2:C:70:LYS:HE2	2.36	0.56
2:D:132:ALA:HA	2:D:156:VAL:HG13	1.87	0.56
2:D:196:GLU:CG	2:D:230:GLN:HG2	2.35	0.56
3:M:194:A:P	4:M:2056:HOH:O	2.62	0.56
3:N:169:G:C2'	3:N:170:A:O5'	2.53	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:174:G:C2'	3:M:175:U:H5''	2.34	0.56
1:A:72:LYS:O	1:A:76:LEU:HG	2.06	0.56
2:D:226:GLN:HG3	4:D:2071:HOH:O	2.05	0.56
1:A:75:LEU:O	1:A:79:ILE:HG13	2.06	0.56
2:C:301:SER:C	2:C:302:LEU:HG	2.25	0.56
2:C:64:THR:O	2:C:65:PRO:C	2.44	0.56
2:C:330:GLU:O	2:C:334:GLN:HG2	2.04	0.56
3:M:164:U:H5'	4:M:2029:HOH:O	2.05	0.56
1:A:50:ASP:OD2	1:A:50:ASP:C	2.44	0.56
2:D:43:VAL:HG22	2:D:257:GLY:HA2	1.86	0.56
2:D:58:ARG:HB3	2:D:77:ILE:HD13	1.88	0.56
1:A:26:ILE:HD11	1:A:29:PRO:CB	2.34	0.56
3:M:168:G:C2'	3:M:169:G:O5'	2.54	0.56
2:D:13:LEU:HD11	2:D:75:ILE:CD1	2.36	0.56
2:C:36:ARG:HH12	2:C:40:GLN:CD	2.08	0.56
2:D:112:GLY:C	2:D:114:THR:H	2.08	0.56
2:D:193:HIS:CG	4:D:2060:HOH:O	2.59	0.56
2:C:147:LEU:O	2:C:150:LEU:N	2.39	0.56
3:M:221:C:H2'	3:M:222:G:H5'	1.87	0.56
2:C:377:ILE:C	2:C:379:SER:H	2.08	0.56
2:C:145:GLU:O	2:C:149:GLN:NE2	2.39	0.56
2:C:131:PRO:O	2:C:156:VAL:HG13	2.06	0.56
2:D:30:VAL:HG12	2:D:34:ILE:CG1	2.35	0.56
2:D:382:LYS:CD	2:D:385:ARG:HH21	2.18	0.56
2:D:94:GLU:HB2	2:D:213:ASP:OD2	2.06	0.56
2:D:221:GLY:CA	2:D:258:ALA:CB	2.80	0.56
1:A:26:ILE:CD1	1:A:29:PRO:HB3	2.32	0.56
2:D:167:SER:N	2:D:168:PRO:HD2	2.20	0.56
3:N:174:G:C3'	3:N:175:U:H5'	2.36	0.56
2:D:30:VAL:HG12	2:D:34:ILE:HG13	1.88	0.56
2:D:44:ASN:N	2:D:225:GLN:OE1	2.39	0.56
1:B:22:GLU:C	1:B:24:LEU:H	2.10	0.56
3:N:205:G:H22	3:N:216:A:H2	1.54	0.56
1:A:77:LYS:NZ	4:A:2021:HOH:O	2.39	0.56
2:D:8:ASN:C	2:D:11:LYS:H	2.10	0.55
2:D:36:ARG:HD3	2:D:36:ARG:C	2.26	0.55
2:C:301:SER:O	2:C:302:LEU:HG	2.05	0.55
2:D:95:LEU:C	2:D:97:PRO:HD3	2.26	0.55
2:C:165:THR:HG22	2:C:166:LYS:N	2.22	0.55
2:D:308:ASP:C	2:D:310:VAL:H	2.08	0.55
2:D:387:ASN:ND2	2:D:387:ASN:O	2.39	0.55
2:C:294:LEU:O	2:C:296:MET:HG2	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:103:ILE:HG21	2:C:216:ILE:HD12	1.89	0.55
2:D:86:LEU:HD11	2:D:286:PRO:HB3	1.89	0.55
2:C:137:ASP:O	2:C:139:TYR:CE1	2.59	0.55
2:C:131:PRO:HA	2:C:184:VAL:O	2.06	0.55
2:D:399:ILE:O	2:D:400:ALA:C	2.44	0.55
1:B:66:VAL:HG22	1:B:67:ASP:N	2.21	0.55
1:B:18:ARG:HH22	3:N:158:C:H5''	1.71	0.55
2:C:417:TYR:C	2:C:419:THR:H	2.09	0.55
2:C:326:PHE:CE1	2:C:328:LEU:CD1	2.86	0.55
2:D:133:LEU:O	2:D:158:ILE:HA	2.04	0.55
2:C:122:ARG:HB3	2:C:278:ILE:CG2	2.36	0.55
2:D:56:GLU:HB2	2:D:60:LEU:HG	1.89	0.55
2:C:272:ILE:HG23	2:C:284:PHE:HB2	1.88	0.55
2:D:132:ALA:HB3	2:D:185:LEU:HG	1.87	0.55
2:D:223:ILE:HG12	2:D:226:GLN:HB3	1.87	0.55
3:M:175:U:H5'	3:M:175:U:H6	1.70	0.55
3:N:171:G:H2'	3:N:172:A:H5'	1.88	0.55
3:M:197:C:C6	3:M:197:C:C3'	2.89	0.55
3:M:178:C:H2'	3:M:178:C:O2	2.06	0.55
3:M:151:G:N2	3:M:179:C:N3	2.51	0.55
2:D:173:LYS:NZ	4:D:2048:HOH:O	2.38	0.55
2:C:140:ARG:O	2:C:142:ALA:N	2.38	0.55
2:C:210:THR:O	2:C:212:PRO:HD3	2.06	0.55
2:D:27:ILE:HD13	2:D:59:ALA:HB1	1.89	0.55
2:C:73:HIS:HD2	2:C:76:LYS:CD	2.15	0.55
2:C:122:ARG:HG3	2:C:278:ILE:CG2	2.24	0.55
2:D:55:ILE:HG23	2:D:77:ILE:HG22	1.88	0.55
2:C:94:GLU:CD	2:C:94:GLU:N	2.59	0.55
3:M:206:C:N3	3:M:215:G:N2	2.53	0.55
2:C:238:VAL:HG11	2:C:242:GLY:HA3	1.87	0.55
1:A:57:HIS:CD2	1:A:58:TRP:HE3	2.24	0.55
2:D:232:LYS:O	2:D:236:GLU:CB	2.54	0.55
2:D:112:GLY:O	2:D:114:THR:N	2.40	0.55
2:D:203:MET:N	2:D:206:ILE:HD13	2.22	0.55
2:C:98:LYS:CD	2:C:98:LYS:N	2.63	0.55
3:M:196:C:H6	3:M:196:C:O5'	1.90	0.55
2:D:77:ILE:O	2:D:77:ILE:HG22	2.05	0.55
2:D:107:GLY:O	2:D:190:ALA:CB	2.54	0.55
3:N:211:A:H2'	3:N:212:A:O4'	2.06	0.55
2:C:385:ARG:NH2	3:M:219:A:O2'	2.39	0.54
2:C:91:LYS:N	2:C:91:LYS:CD	2.57	0.54
2:C:215:ILE:CG2	2:C:234:PHE:CZ	2.87	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:174:G:O2'	3:M:175:U:H5''	2.08	0.54
3:M:190:G:H2'	3:M:191:C:C6	2.39	0.54
2:D:26:LEU:HD22	2:D:29:GLU:HB2	1.89	0.54
2:C:380:MET:O	3:M:219:A:O2'	2.25	0.54
2:C:315:GLU:HA	2:C:318:ILE:HB	1.88	0.54
2:D:206:ILE:CD1	2:D:206:ILE:N	2.68	0.54
1:B:55:ARG:O	1:B:56:GLN:HG3	2.08	0.54
2:D:70:LYS:HA	2:D:73:HIS:HB3	1.89	0.54
2:C:64:THR:HG22	2:C:66:LYS:CA	2.38	0.54
1:B:36:LYS:HB3	1:B:36:LYS:HZ3	1.70	0.54
2:D:27:ILE:CD1	2:D:59:ALA:HB1	2.37	0.54
2:C:82:LEU:O	2:C:85:LEU:HB3	2.07	0.54
2:D:200:LEU:HA	2:D:203:MET:CE	2.37	0.54
2:C:196:GLU:O	2:C:199:LEU:HB3	2.07	0.54
1:A:18:ARG:HH22	3:M:158:C:H5''	1.73	0.54
2:D:58:ARG:CA	2:D:62:GLU:HG2	2.36	0.54
2:D:199:LEU:HD23	2:D:200:LEU:N	2.21	0.54
1:B:75:LEU:O	1:B:78:GLU:N	2.41	0.54
2:C:213:ASP:O	2:C:214:GLU:HG2	2.07	0.54
2:D:326:PHE:HA	2:D:417:TYR:CE2	2.43	0.54
2:C:366:THR:HG23	2:C:367:GLU:HG3	1.90	0.54
1:A:15:ARG:NH2	1:A:55:ARG:CZ	2.70	0.54
2:D:382:LYS:HD2	2:D:385:ARG:HH21	1.73	0.54
3:M:193:G:O2'	3:M:194:A:OP1	2.25	0.54
3:N:197:C:C5'	3:N:198:C:H5'	2.38	0.54
3:M:178:C:H5''	3:M:178:C:H6	1.72	0.54
2:C:383:GLU:HG2	2:C:390:ILE:CD1	2.38	0.54
2:D:131:PRO:HD2	2:D:156:VAL:HG22	1.89	0.54
2:D:227:ALA:HA	2:D:230:GLN:HB2	1.90	0.54
2:C:166:LYS:HD2	2:C:169:VAL:CG2	2.31	0.54
2:D:118:ALA:CB	2:D:150:LEU:HD13	2.38	0.54
2:D:181:LYS:O	2:D:182:ALA:HB2	2.08	0.54
2:D:299:LEU:HD12	2:D:300:GLU:O	2.08	0.54
2:D:113:LYS:NZ	2:D:188:ASP:OD1	2.34	0.54
2:D:171:ILE:HG23	2:D:172:VAL:H	1.72	0.54
2:D:76:LYS:O	2:D:80:GLU:N	2.32	0.54
2:D:78:VAL:O	2:D:82:LEU:HB2	2.08	0.53
2:C:272:ILE:HD13	2:C:284:PHE:CD1	2.38	0.53
2:C:173:LYS:O	2:C:177:GLU:N	2.42	0.53
2:C:281:LEU:O	2:C:281:LEU:CG	2.41	0.53
2:C:98:LYS:HG2	2:C:100:GLN:N	2.24	0.53
2:D:420:THR:O	2:D:423:ALA:HB3	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:166:G:H8	3:M:166:G:O5'	1.91	0.53
2:D:336:GLU:HG3	2:D:336:GLU:O	2.08	0.53
2:D:202:GLU:HG3	2:D:202:GLU:O	2.09	0.53
1:B:26:ILE:HG22	1:B:84:LYS:HD3	1.90	0.53
2:D:14:ASN:HD22	2:D:15:LYS:NZ	2.06	0.53
2:C:109:GLN:N	2:C:193:HIS:O	2.29	0.53
2:C:36:ARG:HA	2:C:39:ILE:CG1	2.29	0.53
1:B:15:ARG:NH2	1:B:55:ARG:CZ	2.72	0.53
2:C:335:LEU:C	2:C:336:GLU:HG2	2.28	0.53
2:D:381:THR:HG22	3:N:220:A:OP1	2.09	0.53
2:C:86:LEU:HD12	2:C:290:ILE:HD11	1.89	0.53
3:M:179:C:O2'	3:M:180:C:O5'	2.27	0.53
3:N:160:C:C6	3:N:160:C:C3'	2.92	0.53
2:D:81:GLU:C	2:D:83:VAL:H	2.12	0.53
2:C:173:LYS:O	2:C:177:GLU:CB	2.56	0.53
2:D:323:ARG:HD3	2:D:427:LEU:CD2	2.38	0.53
2:C:415:ARG:NH2	4:C:2103:HOH:O	2.42	0.53
2:D:17:LYS:O	2:D:18:ALA:HB2	2.08	0.53
2:D:34:ILE:O	2:D:37:ALA:HB3	2.08	0.53
3:N:191:C:N3	3:N:227:G:O6	2.42	0.53
1:B:1:MET:CA	3:N:164:U:O2'	2.56	0.53
2:D:126:LYS:HD3	2:D:126:LYS:C	2.29	0.53
2:C:192:ARG:HB2	2:C:192:ARG:HH11	1.73	0.53
1:B:46:LYS:NZ	1:B:65:GLU:OE2	2.41	0.53
2:C:62:GLU:C	2:C:62:GLU:CD	2.67	0.53
2:D:36:ARG:HD3	2:D:37:ALA:N	2.24	0.52
2:C:299:LEU:HD23	2:C:300:GLU:H	1.73	0.52
2:D:102:VAL:CG1	2:D:185:LEU:HB2	2.39	0.52
2:D:206:ILE:CD1	2:D:206:ILE:H	2.22	0.52
2:C:4:LYS:O	2:C:8:ASN:N	2.28	0.52
2:C:2:MET:SD	2:C:249:LEU:C	2.87	0.52
2:C:132:ALA:HB1	2:C:178:LYS:HD3	1.91	0.52
2:C:325:LYS:HA	2:C:325:LYS:CE	2.37	0.52
2:C:326:PHE:CD1	2:C:326:PHE:C	2.81	0.52
1:B:1:MET:HA	3:N:164:U:O2'	2.09	0.52
2:C:308:ASP:OD1	2:C:308:ASP:O	2.27	0.52
2:D:16:LEU:O	2:D:16:LEU:HG	2.08	0.52
2:D:56:GLU:CG	2:D:60:LEU:HD11	2.40	0.52
2:D:408:ASN:OD1	2:D:411:ARG:NH1	2.43	0.52
3:M:219:A:H8	3:M:219:A:O5'	1.92	0.52
2:D:221:GLY:HA2	2:D:258:ALA:CB	2.38	0.52
2:C:338:ILE:HG23	2:C:339:GLU:N	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:397:ARG:CG	2:C:397:ARG:O	2.57	0.52
3:N:210:G:C2'	3:N:211:A:O5'	2.56	0.52
2:D:56:GLU:HB2	2:D:60:LEU:CG	2.40	0.52
2:C:98:LYS:HD3	2:C:100:GLN:O	2.09	0.52
3:N:235:U:C2'	3:N:236:C:O5'	2.58	0.52
3:N:180:C:C3'	3:N:181:C:C5'	2.88	0.52
2:D:268:PRO:HB2	2:D:270:LYS:HE2	1.92	0.52
2:D:39:ILE:HG23	2:D:45:VAL:HG22	1.91	0.52
1:B:21:PRO:HG3	3:N:160:C:OP2	2.10	0.52
2:C:313:LYS:NZ	2:C:313:LYS:HA	2.23	0.52
2:D:323:ARG:CD	2:D:427:LEU:CD2	2.87	0.52
1:A:73:LEU:O	1:A:76:LEU:HB2	2.09	0.52
3:M:191:C:C2	3:M:192:C:C6	2.98	0.52
2:C:93:LEU:O	2:C:94:GLU:O	2.27	0.52
2:D:302:LEU:HB2	2:D:309:MET:HG3	1.91	0.52
2:C:70:LYS:O	2:C:71:LYS:C	2.47	0.52
2:C:221:GLY:O	2:C:222:THR:C	2.47	0.52
2:D:132:ALA:HA	2:D:156:VAL:CG1	2.39	0.52
3:N:146:G:H4'	3:N:147:U:H5'	1.91	0.52
2:C:104:LEU:HD12	2:C:187:ILE:HD12	1.91	0.52
1:A:59:GLU:O	1:A:59:GLU:HG3	2.09	0.52
2:D:260:SER:OG	2:D:261:ALA:N	2.42	0.52
3:M:188:C:O2	3:M:188:C:H2'	2.10	0.52
1:B:15:ARG:NH2	1:B:55:ARG:HD3	2.16	0.52
1:A:30:SER:HB2	1:A:32:LYS:HD2	1.92	0.52
2:C:13:LEU:HB3	2:C:75:ILE:CD1	2.39	0.51
2:C:280:ASP:HB2	4:C:2080:HOH:O	2.10	0.51
2:C:113:LYS:C	2:C:113:LYS:HD3	2.29	0.51
2:C:93:LEU:C	2:C:94:GLU:O	2.48	0.51
3:N:178:C:H6	3:N:178:C:H5'	1.75	0.51
2:C:45:VAL:O	2:C:48:VAL:N	2.43	0.51
2:C:91:LYS:HE3	2:C:286:PRO:HD2	1.93	0.51
2:C:91:LYS:CE	2:C:286:PRO:HD2	2.40	0.51
3:N:226:G:H2'	3:N:227:G:C5'	2.33	0.51
2:D:58:ARG:CB	2:D:77:ILE:HD13	2.40	0.51
2:C:167:SER:HB2	2:C:168:PRO:HD3	1.92	0.51
2:C:104:LEU:HD22	2:C:215:ILE:CD1	2.41	0.51
1:B:78:GLU:O	1:B:79:ILE:C	2.48	0.51
1:B:37:ALA:C	1:B:39:LYS:H	2.14	0.51
2:D:165:THR:OG1	2:D:166:LYS:N	2.44	0.51
1:A:32:LYS:HD2	1:A:32:LYS:H	1.75	0.51
2:D:35:GLN:OE1	2:D:36:ARG:N	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:287:LYS:HD3	2:C:287:LYS:H	1.75	0.51
2:C:377:ILE:O	2:C:379:SER:N	2.44	0.51
1:A:31:LEU:HB2	1:A:32:LYS:HE3	1.91	0.51
2:C:195:GLU:HB2	4:C:2065:HOH:O	2.11	0.51
2:C:398:ARG:NH1	3:M:218:C:O2'	2.42	0.51
2:D:115:THR:O	2:D:119:LYS:HG2	2.10	0.51
2:D:221:GLY:O	2:D:222:THR:C	2.48	0.51
2:D:224:GLY:CA	2:D:254:LYS:NZ	2.73	0.51
1:A:50:ASP:CG	1:A:50:ASP:O	2.49	0.51
3:M:232:A:H2'	3:M:233:C:C6	2.45	0.51
2:C:45:VAL:O	2:C:49:LEU:HD13	2.11	0.51
2:C:13:LEU:HA	2:C:75:ILE:HD11	1.92	0.51
2:C:113:LYS:O	2:C:113:LYS:HD3	2.11	0.51
3:N:188:C:H1'	3:N:231:G:N2	2.25	0.51
1:B:64:VAL:O	1:B:64:VAL:HG13	2.10	0.51
3:M:191:C:H2'	3:M:191:C:O2	2.10	0.51
2:D:216:ILE:CG2	2:D:245:ILE:HG13	2.40	0.51
2:D:89:GLU:O	2:D:90:ALA:HB2	2.11	0.51
2:D:382:LYS:HE3	3:N:220:A:H5"	1.92	0.51
2:D:107:GLY:O	2:D:190:ALA:HB1	2.11	0.51
2:D:215:ILE:H	2:D:242:GLY:HA2	1.75	0.51
3:N:232:A:C6	3:N:233:C:N3	2.79	0.51
2:D:31:ILE:HG22	2:D:31:ILE:O	2.09	0.51
2:C:44:ASN:O	2:C:44:ASN:CG	2.48	0.51
2:C:58:ARG:HH21	2:C:77:ILE:HG12	1.75	0.51
3:N:233:C:H6	3:N:233:C:O5'	1.94	0.51
2:D:64:THR:C	2:D:66:LYS:N	2.64	0.51
2:D:388:PRO:O	2:D:389:LYS:CB	2.58	0.51
2:D:381:THR:N	2:D:384:GLU:OE1	2.33	0.51
2:C:50:LYS:O	2:C:53:LYS:N	2.36	0.51
2:C:54:GLU:HG2	2:C:81:GLU:OE2	2.10	0.51
2:C:57:ARG:NH2	4:C:2028:HOH:O	2.43	0.51
2:C:147:LEU:O	2:C:148:LYS:C	2.48	0.51
2:C:381:THR:O	2:C:382:LYS:C	2.48	0.51
2:C:311:ASP:OD1	2:C:311:ASP:O	2.29	0.50
1:A:38:LEU:HD22	1:A:38:LEU:N	2.14	0.50
2:D:218:VAL:HG13	2:D:247:THR:HG21	1.93	0.50
2:C:31:ILE:CD1	2:C:55:ILE:HG21	2.40	0.50
2:D:38:LEU:CD1	2:D:51:MET:SD	2.97	0.50
2:D:102:VAL:O	2:D:212:PRO:HB3	2.11	0.50
2:D:126:LYS:NZ	2:D:126:LYS:HB2	2.27	0.50
2:D:2:MET:SD	2:D:289:PHE:CZ	3.04	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:32:LYS:HE3	4:C:2017:HOH:O	2.11	0.50
2:D:106:VAL:HG23	2:D:106:VAL:O	2.11	0.50
3:M:180:C:H4'	4:M:2044:HOH:O	2.11	0.50
3:M:179:C:O2'	3:M:180:C:O4'	2.24	0.50
2:C:323:ARG:HB2	2:C:323:ARG:CZ	2.42	0.50
3:M:191:C:N3	3:M:192:C:C5	2.79	0.50
1:A:50:ASP:O	1:A:52:ARG:NH1	2.45	0.50
2:C:417:TYR:O	2:C:419:THR:N	2.44	0.50
2:D:27:ILE:CD1	2:D:63:LYS:HZ1	2.06	0.50
2:D:6:GLY:CA	2:D:9:LEU:HB3	2.41	0.50
2:C:17:LYS:HD2	2:C:19:ALA:HB3	1.94	0.50
2:C:104:LEU:CD1	2:C:187:ILE:HD12	2.41	0.50
1:A:1:MET:HA	3:M:164:U:O2'	2.11	0.50
1:A:30:SER:OG	1:A:33:ASP:HB2	2.12	0.50
2:D:305:LYS:HZ2	2:D:305:LYS:HB3	1.76	0.50
2:D:154:ILE:HD12	2:D:154:ILE:H	1.76	0.50
2:C:167:SER:H	2:C:168:PRO:HD2	1.77	0.50
2:C:180:LYS:O	3:N:232:A:C5'	2.55	0.50
2:D:420:THR:O	2:D:421:LYS:C	2.50	0.50
2:C:272:ILE:HG21	2:C:284:PHE:CD1	2.46	0.50
2:D:219:ILE:C	2:D:220:ASP:OD2	2.50	0.50
2:D:234:PHE:CE1	2:D:238:VAL:HB	2.47	0.50
2:D:221:GLY:O	2:D:223:ILE:N	2.44	0.50
2:C:5:LEU:HG	2:C:41:ALA:HB2	1.93	0.50
2:D:36:ARG:HH12	2:D:40:GLN:HB2	1.77	0.50
2:D:58:ARG:CD	4:D:2014:HOH:O	2.59	0.50
3:N:195:A:H5'	3:N:196:C:OP2	2.12	0.50
2:D:133:LEU:O	2:D:158:ILE:HG22	2.12	0.50
2:D:135:ALA:O	2:D:136:ALA:HB2	2.11	0.50
2:C:199:LEU:HD12	4:C:2068:HOH:O	2.11	0.50
3:M:210:G:H2'	3:M:211:A:O5'	2.12	0.50
2:D:400:ALA:O	2:D:402:GLY:N	2.45	0.50
2:D:381:THR:HG22	2:D:382:LYS:H	1.75	0.50
2:D:104:LEU:HB2	2:D:215:ILE:HG22	1.93	0.50
3:N:184:U:O2'	3:N:186:A:H2	1.93	0.50
3:N:185:U:C4'	3:N:186:A:OP2	2.60	0.50
3:M:149:G:H1	3:M:181:C:H42	1.60	0.50
2:C:244:ILE:HG22	2:C:245:ILE:N	2.27	0.50
1:A:46:LYS:NZ	1:A:48:TYR:CE2	2.80	0.50
1:A:15:ARG:NE	1:A:15:ARG:O	2.44	0.50
3:M:229:A:C6	3:M:230:G:C6	3.00	0.50
2:D:123:TYR:HB2	2:D:278:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:218:C:H2'	3:M:219:A:O5'	2.11	0.50
2:D:290:ILE:O	2:D:293:LEU:HB2	2.10	0.50
2:D:144:TYR:O	2:D:145:GLU:HB2	2.11	0.50
2:C:7:GLU:HG3	2:C:8:ASN:N	2.26	0.50
3:N:236:C:C5'	3:N:237:G:O3'	2.60	0.50
2:C:61:GLU:CD	2:C:62:GLU:N	2.65	0.50
2:D:245:ILE:HG22	2:D:245:ILE:O	2.12	0.49
2:D:318:ILE:HG23	2:D:319:ASP:N	2.27	0.49
2:D:78:VAL:O	2:D:82:LEU:CB	2.60	0.49
2:D:86:LEU:O	2:D:263:ALA:HA	2.11	0.49
3:M:193:G:O2'	3:M:194:A:P	2.70	0.49
2:D:398:ARG:HG2	2:D:398:ARG:NH1	2.27	0.49
3:M:178:C:OP1	3:M:223:G:O2'	2.28	0.49
2:C:384:GLU:OE2	2:C:395:ARG:NH1	2.38	0.49
1:B:71:ASN:CB	1:B:74:GLN:CG	2.87	0.49
1:B:68:TYR:CD2	1:B:75:LEU:HD13	2.47	0.49
2:C:81:GLU:O	2:C:82:LEU:C	2.50	0.49
2:C:274:ILE:HG21	2:C:280:ASP:OD1	2.12	0.49
2:D:229:ILE:C	2:D:229:ILE:HD12	2.32	0.49
3:M:174:G:H8	3:M:174:G:H5'	1.76	0.49
2:C:340:ASN:O	2:C:341:MET:C	2.49	0.49
2:D:290:ILE:HD13	2:D:293:LEU:HD12	1.94	0.49
2:D:274:ILE:HB	2:D:280:ASP:O	2.12	0.49
3:N:210:G:H2'	3:N:211:A:O5'	2.11	0.49
2:D:217:LEU:HB3	2:D:244:ILE:HG22	1.94	0.49
2:D:232:LYS:HG3	2:D:265:THR:CG2	2.42	0.49
2:D:239:GLY:C	2:D:241:ILE:H	2.15	0.49
3:M:146:G:HO2'	3:M:186:A:HO2'	1.60	0.49
3:M:173:U:C2'	3:M:174:G:C5'	2.90	0.49
2:D:113:LYS:CE	2:D:191:GLY:HA2	2.42	0.49
3:M:181:C:H5''	3:M:181:C:H6	1.76	0.49
3:N:160:C:O2	3:N:170:A:C2	2.65	0.49
3:M:186:A:N3	3:M:186:A:O4'	2.44	0.49
2:C:124:ILE:O	2:C:125:GLN:C	2.50	0.49
2:C:174:GLU:HA	2:C:177:GLU:HB3	1.94	0.49
1:B:37:ALA:C	1:B:39:LYS:N	2.66	0.49
2:C:27:ILE:CD1	2:C:59:ALA:O	2.61	0.49
2:C:49:LEU:N	2:C:49:LEU:CD1	2.76	0.49
2:C:151:ALA:HB1	2:C:156:VAL:O	2.13	0.49
1:A:26:ILE:HD12	1:A:29:PRO:HA	1.94	0.49
2:C:70:LYS:O	2:C:73:HIS:N	2.41	0.49
2:C:79:TYR:O	2:C:83:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:125:GLN:HE22	2:D:154:ILE:CG2	2.26	0.49
2:D:136:ALA:HB3	2:D:188:ASP:O	2.12	0.49
2:C:133:LEU:HD23	2:C:186:ILE:HB	1.95	0.49
2:D:57:ARG:HD2	2:D:61:GLU:CG	2.40	0.49
3:N:195:A:H8	3:N:195:A:OP1	1.95	0.49
2:C:150:LEU:O	2:C:154:ILE:HG12	2.12	0.49
2:D:275:GLY:CA	2:D:280:ASP:HB2	2.35	0.49
2:D:366:THR:O	2:D:367:GLU:C	2.51	0.49
2:C:314:THR:O	2:C:318:ILE:CB	2.59	0.49
3:M:200:G:H2'	3:M:201:C:O5'	2.13	0.49
3:M:175:U:C6	3:M:175:U:H5'	2.47	0.49
2:C:325:LYS:HB3	2:C:421:LYS:CG	2.36	0.48
3:M:184:U:HO2'	3:M:186:A:H2	1.61	0.48
3:M:164:U:H5'	3:M:165:A:OP2	2.13	0.48
2:C:206:ILE:O	2:C:206:ILE:CG1	2.61	0.48
2:C:13:LEU:HA	2:C:75:ILE:CD1	2.42	0.48
2:C:139:TYR:OH	2:C:188:ASP:CG	2.51	0.48
1:B:39:LYS:O	1:B:41:LEU:N	2.45	0.48
2:D:323:ARG:HD2	2:D:427:LEU:HD22	1.94	0.48
2:D:76:LYS:O	2:D:80:GLU:CB	2.60	0.48
2:D:15:LYS:C	2:D:16:LEU:HD23	2.33	0.48
2:D:268:PRO:O	2:D:270:LYS:HG2	2.13	0.48
2:C:44:ASN:O	2:C:46:LYS:N	2.46	0.48
2:D:325:LYS:HG3	2:D:424:ILE:CD1	2.43	0.48
2:D:311:ASP:C	2:D:315:GLU:OE2	2.52	0.48
2:D:320:ALA:HB2	2:D:329:ASN:HD21	1.77	0.48
2:C:79:TYR:HH	2:C:299:LEU:HD12	1.79	0.48
3:N:234:G:C6	3:N:235:U:C4	3.01	0.48
2:C:266:LYS:O	2:C:267:ALA:C	2.51	0.48
3:M:226:G:C8	3:M:226:G:H3'	2.48	0.48
2:D:55:ILE:C	2:D:57:ARG:N	2.66	0.48
2:C:83:VAL:O	2:C:85:LEU:N	2.47	0.48
2:D:114:THR:HG22	2:D:147:LEU:HD21	1.95	0.48
2:C:171:ILE:O	2:C:171:ILE:HD13	2.13	0.48
2:C:311:ASP:O	2:C:311:ASP:CG	2.52	0.48
2:C:12:ALA:HB1	2:C:30:VAL:CG1	2.34	0.48
2:D:84:LYS:C	2:D:86:LEU:H	2.16	0.48
2:C:13:LEU:HD11	2:C:294:LEU:HD13	1.95	0.48
2:C:89:GLU:HA	2:C:91:LYS:HE3	1.95	0.48
2:D:174:GLU:O	2:D:178:LYS:HG2	2.14	0.48
1:B:72:LYS:O	1:B:73:LEU:C	2.50	0.48
2:D:391:ILE:HG21	2:D:414:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:146:G:HO2'	3:N:147:U:P	2.35	0.48
2:D:370:ILE:H	2:D:370:ILE:HD12	1.79	0.48
2:D:150:LEU:HD23	2:D:150:LEU:O	2.14	0.48
2:C:255:GLY:O	2:C:258:ALA:HB3	2.13	0.48
2:D:59:ALA:C	2:D:63:LYS:HB3	2.34	0.48
2:C:46:LYS:O	2:C:50:LYS:HG3	2.13	0.48
2:C:188:ASP:C	2:C:188:ASP:OD1	2.51	0.48
2:C:150:LEU:C	2:C:152:GLU:N	2.67	0.48
3:M:175:U:O2'	3:M:176:A:H8	1.97	0.48
2:D:232:LYS:O	2:D:236:GLU:N	2.43	0.48
2:C:326:PHE:HD1	2:C:326:PHE:C	2.15	0.48
2:C:104:LEU:HD22	2:C:215:ILE:HD11	1.96	0.48
2:D:3:ASP:OD1	2:D:3:ASP:N	2.46	0.48
2:C:85:LEU:CD2	2:C:85:LEU:C	2.81	0.48
2:C:103:ILE:CG2	2:C:216:ILE:CD1	2.92	0.48
2:D:198:GLY:O	2:D:199:LEU:C	2.53	0.47
2:C:148:LYS:C	2:C:152:GLU:HG2	2.32	0.47
2:C:2:MET:HE3	2:C:2:MET:CA	2.30	0.47
3:M:210:G:C2'	3:M:211:A:O5'	2.62	0.47
1:A:1:MET:O	1:A:65:GLU:HA	2.14	0.47
3:M:190:G:C5	3:M:191:C:C5	3.02	0.47
1:A:46:LYS:NZ	1:A:48:TYR:OH	2.29	0.47
2:D:56:GLU:OE2	2:D:60:LEU:HD11	2.13	0.47
3:M:188:C:O2	3:M:188:C:C2'	2.60	0.47
1:B:37:ALA:O	1:B:39:LYS:N	2.46	0.47
1:A:18:ARG:NH2	3:M:158:C:H5''	2.29	0.47
2:C:5:LEU:O	2:C:9:LEU:HB2	2.13	0.47
2:D:372:LYS:HE3	4:D:2089:HOH:O	2.14	0.47
2:D:377:ILE:HA	2:D:380:MET:HG3	1.96	0.47
2:D:79:TYR:HD2	2:D:294:LEU:HD11	1.79	0.47
2:C:302:LEU:O	2:C:306:ALA:HB3	2.13	0.47
3:M:180:C:H3'	3:M:181:C:H5''	1.95	0.47
2:C:311:ASP:OD2	2:C:313:LYS:HB3	2.14	0.47
3:N:152:G:C2'	3:N:153:A:O5'	2.62	0.47
2:C:36:ARG:CG	2:C:36:ARG:NH1	2.62	0.47
2:C:286:PRO:O	2:C:289:PHE:N	2.48	0.47
2:D:199:LEU:O	2:D:201:GLU:N	2.48	0.47
3:N:160:C:H2'	3:N:161:C:O5'	2.14	0.47
3:M:164:U:O2	3:M:164:U:O2'	2.24	0.47
2:C:387:ASN:HB3	4:C:2096:HOH:O	2.14	0.47
3:N:146:G:O2'	3:N:147:U:OP2	2.29	0.47
3:M:153:A:C2	3:M:178:C:N3	2.83	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:12:LYS:HG3	1:B:16:GLU:HB3	1.96	0.47
2:D:210:THR:HG22	2:D:212:PRO:HD3	1.97	0.47
1:B:86:LYS:CB	1:B:86:LYS:NZ	2.60	0.47
2:C:142:ALA:O	2:C:146:GLN:HG2	2.15	0.47
3:M:213:G:O2'	3:M:214:G:O5'	2.32	0.47
2:C:340:ASN:N	2:C:340:ASN:HD22	2.11	0.47
2:D:305:LYS:HZ3	2:D:306:ALA:N	2.11	0.47
2:D:70:LYS:HG3	2:D:71:LYS:N	2.29	0.47
2:C:73:HIS:O	2:C:76:LYS:HB3	2.15	0.47
2:C:119:LYS:HB3	2:C:281:LEU:CD2	2.44	0.47
2:D:101:ASN:O	2:D:213:ASP:HB3	2.14	0.47
2:D:104:LEU:HD12	2:D:104:LEU:N	2.30	0.47
2:C:148:LYS:O	2:C:152:GLU:CG	2.45	0.47
3:M:210:G:H2'	3:M:211:A:O4'	2.13	0.47
2:C:308:ASP:HA	4:C:2086:HOH:O	2.15	0.47
2:D:16:LEU:HD21	2:D:30:VAL:HG22	1.96	0.47
2:D:74:ILE:O	2:D:78:VAL:HG23	2.15	0.47
2:C:32:LYS:O	2:C:35:GLN:HG2	2.14	0.47
3:N:184:U:O2'	3:N:186:A:C2	2.65	0.47
2:C:319:ASP:O	2:C:319:ASP:CG	2.53	0.47
3:M:175:U:HO2'	3:M:176:A:H8	1.62	0.47
2:C:67:GLY:O	2:C:69:SER:N	2.38	0.47
2:D:91:LYS:N	2:D:91:LYS:HD2	2.30	0.47
3:M:185:U:H6	3:M:185:U:C5'	2.27	0.47
2:D:44:ASN:HB2	2:D:225:GLN:OE1	2.15	0.47
2:D:254:LYS:HB3	2:D:254:LYS:NZ	2.30	0.47
1:A:1:MET:CA	3:M:164:U:O2'	2.63	0.47
1:B:9:ASP:O	1:B:10:LYS:C	2.53	0.47
3:M:185:U:H6	3:M:185:U:O5'	1.98	0.47
2:D:145:GLU:C	2:D:147:LEU:H	2.17	0.47
2:D:229:ILE:HD12	2:D:230:GLN:N	2.30	0.47
2:C:108:ILE:CD1	2:C:108:ILE:H	2.28	0.47
1:A:1:MET:C	1:A:2:ILE:HD12	2.35	0.47
2:C:308:ASP:CG	2:C:308:ASP:O	2.53	0.47
2:C:36:ARG:HG3	2:C:39:ILE:HD12	1.97	0.46
2:C:83:VAL:O	2:C:86:LEU:N	2.48	0.46
2:D:196:GLU:CD	2:D:230:GLN:HG2	2.36	0.46
2:C:166:LYS:CG	2:C:168:PRO:HD2	2.39	0.46
2:C:395:ARG:HA	3:M:195:A:C2	2.49	0.46
2:C:133:LEU:O	2:C:158:ILE:HA	2.15	0.46
2:C:123:TYR:CE2	2:C:271:PHE:HE2	2.32	0.46
2:D:201:GLU:C	2:D:203:MET:N	2.67	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:156:VAL:HA	2:C:157:PRO:HD3	1.73	0.46
2:D:285:ASP:HB2	2:D:288:LYS:CB	2.43	0.46
2:D:59:ALA:CA	2:D:63:LYS:HB3	2.46	0.46
2:D:58:ARG:HH21	2:D:77:ILE:HG12	1.80	0.46
3:M:219:A:H2'	3:M:220:A:H5'	1.97	0.46
2:C:14:ASN:ND2	2:C:15:LYS:N	2.64	0.46
2:C:73:HIS:CD2	2:C:76:LYS:CD	2.95	0.46
3:N:160:C:H6	3:N:160:C:C3'	2.25	0.46
2:D:249:LEU:O	2:D:251:GLY:N	2.48	0.46
3:N:190:G:O2'	3:N:191:C:H5'	2.14	0.46
1:B:64:VAL:O	1:B:64:VAL:CG1	2.63	0.46
2:D:187:ILE:N	2:D:187:ILE:HD12	2.30	0.46
2:C:206:ILE:HA	2:C:209:ILE:HG22	1.98	0.46
2:D:99:LYS:HG3	2:D:100:GLN:N	2.29	0.46
2:C:229:ILE:HD12	2:C:229:ILE:O	2.15	0.46
2:D:380:MET:HB2	2:D:385:ARG:HG3	1.97	0.46
2:D:393:ALA:O	2:D:396:ILE:N	2.48	0.46
2:D:82:LEU:HG	2:D:82:LEU:O	2.15	0.46
2:C:221:GLY:C	2:C:223:ILE:N	2.64	0.46
1:A:39:LYS:O	1:A:40:LYS:C	2.54	0.46
3:M:146:G:O2'	3:M:186:A:O2'	2.31	0.46
1:B:71:ASN:HB2	1:B:74:GLN:CG	2.42	0.46
1:B:74:GLN:HB3	1:B:74:GLN:HE21	1.35	0.46
2:C:338:ILE:HG23	2:C:339:GLU:H	1.80	0.46
2:D:398:ARG:HH11	2:D:398:ARG:HG2	1.81	0.46
2:D:307:GLU:H	2:D:312:GLU:HG3	1.80	0.46
2:D:84:LYS:HZ3	2:D:84:LYS:HB3	1.80	0.46
2:C:152:GLU:C	2:C:154:ILE:N	2.67	0.46
3:M:194:A:C3'	3:M:194:A:C8	2.98	0.46
2:D:272:ILE:HG23	2:D:284:PHE:HB2	1.97	0.46
3:M:187:C:O5'	4:M:2048:HOH:O	2.20	0.46
2:D:322:MET:HG3	2:D:427:LEU:HD21	1.96	0.46
2:C:262:VAL:O	2:C:262:VAL:HG12	2.15	0.46
2:D:11:LYS:HD2	2:D:14:ASN:HB3	1.97	0.46
2:D:55:ILE:HG12	2:D:81:GLU:CB	2.46	0.46
3:M:224:U:O2	3:M:224:U:H2'	2.16	0.46
3:M:187:C:C2	3:M:188:C:C6	3.03	0.46
2:C:115:THR:C	2:C:117:ALA:N	2.69	0.46
2:C:14:ASN:O	2:C:16:LEU:N	2.49	0.46
2:D:207:LYS:O	2:D:210:THR:O	2.33	0.46
2:C:124:ILE:HA	2:C:127:ARG:HB2	1.97	0.46
1:B:68:TYR:CE2	1:B:75:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:331:LEU:HG	2:D:331:LEU:O	2.14	0.46
2:D:325:LYS:HG3	2:D:424:ILE:HD11	1.98	0.46
2:D:58:ARG:O	2:D:63:LYS:N	2.48	0.46
2:C:16:LEU:HD11	2:C:74:ILE:HD13	1.96	0.46
2:D:122:ARG:HH21	2:D:154:ILE:CG2	2.25	0.46
2:D:94:GLU:CD	2:D:94:GLU:N	2.69	0.46
2:C:23:ASP:O	2:C:24:LYS:HB3	2.16	0.46
2:C:134:ILE:O	2:C:136:ALA:N	2.48	0.46
2:C:162:GLU:O	2:C:163:THR:CG2	2.59	0.46
2:D:208:GLU:HA	4:D:2065:HOH:O	2.15	0.46
2:D:56:GLU:C	2:D:58:ARG:H	2.19	0.46
2:D:6:GLY:O	2:D:10:ASN:N	2.44	0.46
2:D:199:LEU:O	2:D:203:MET:HG3	2.16	0.46
2:D:229:ILE:O	2:D:233:ALA:N	2.41	0.46
2:C:417:TYR:C	2:C:419:THR:N	2.69	0.46
2:C:203:MET:O	2:C:204:LYS:HB2	2.16	0.46
2:D:316:GLU:HB2	2:D:332:MET:SD	2.56	0.46
2:C:39:ILE:O	2:C:42:ASP:N	2.49	0.46
2:C:313:LYS:HZ2	2:C:313:LYS:HA	1.80	0.46
2:D:169:VAL:O	2:D:173:LYS:HB2	2.16	0.46
3:N:208:C:C2	3:N:213:G:N2	2.67	0.46
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.70	0.46
2:D:288:LYS:HA	2:D:291:SER:OG	2.15	0.45
2:D:288:LYS:O	2:D:291:SER:N	2.50	0.45
2:D:293:LEU:HB2	2:D:294:LEU:HD23	1.98	0.45
2:C:274:ILE:HG21	2:C:280:ASP:CG	2.36	0.45
1:B:71:ASN:ND2	1:B:74:GLN:HG3	2.31	0.45
2:D:218:VAL:HG13	2:D:247:THR:HG23	1.99	0.45
1:B:28:LYS:NZ	4:B:2010:HOH:O	2.33	0.45
2:D:24:LYS:HB2	2:D:60:LEU:HB3	1.98	0.45
3:M:219:A:C2'	3:M:220:A:H5'	2.46	0.45
2:C:299:LEU:H	2:C:299:LEU:CD1	2.02	0.45
2:D:104:LEU:HD11	2:D:212:PRO:CG	2.35	0.45
2:C:24:LYS:NZ	2:C:25:LYS:HB2	2.31	0.45
3:N:222:G:C6	3:N:223:G:C5	3.04	0.45
2:D:55:ILE:CG1	2:D:81:GLU:HB3	2.47	0.45
2:D:56:GLU:HG3	2:D:60:LEU:HD11	1.97	0.45
2:D:213:ASP:OD1	2:D:214:GLU:N	2.50	0.45
2:C:17:LYS:O	2:C:18:ALA:CB	2.64	0.45
2:C:134:ILE:HD11	2:C:174:GLU:HB2	1.95	0.45
1:A:7:TYR:CE2	1:A:72:LYS:NZ	2.83	0.45
2:C:57:ARG:O	2:C:58:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:122:ARG:O	2:C:122:ARG:CD	2.64	0.45
2:D:206:ILE:HA	2:D:209:ILE:HG22	1.98	0.45
2:D:96:ASN:OD1	2:D:129:LEU:HD11	2.16	0.45
2:C:134:ILE:HD13	2:C:174:GLU:CB	2.44	0.45
2:D:26:LEU:HD21	2:D:29:GLU:OE1	2.15	0.45
2:C:61:GLU:OE1	2:C:62:GLU:HB3	2.15	0.45
2:D:100:GLN:HB3	2:D:179:PHE:CE2	2.51	0.45
2:D:311:ASP:HB3	2:D:312:GLU:H	1.58	0.45
2:C:35:GLN:CG	2:C:36:ARG:N	2.79	0.45
2:C:45:VAL:CG1	2:C:46:LYS:N	2.73	0.45
2:D:105:LEU:CD1	2:D:117:ALA:CB	2.82	0.45
2:D:366:THR:O	2:D:369:LYS:N	2.49	0.45
2:D:398:ARG:CG	2:D:398:ARG:O	2.62	0.45
2:D:331:LEU:HD13	2:D:334:GLN:OE1	2.16	0.45
2:C:67:GLY:CA	2:C:309:MET:SD	3.03	0.45
1:A:30:SER:O	1:A:33:ASP:HB2	2.16	0.45
1:B:53:TYR:O	1:B:57:HIS:N	2.49	0.45
2:C:381:THR:O	2:C:384:GLU:N	2.47	0.45
2:C:18:ALA:O	2:C:19:ALA:C	2.54	0.45
1:B:39:LYS:C	1:B:41:LEU:N	2.69	0.45
3:M:232:A:C2'	3:M:233:C:O5'	2.64	0.45
2:C:201:GLU:OE2	4:C:2067:HOH:O	2.20	0.45
2:D:296:MET:SD	2:D:297:GLY:N	2.90	0.45
2:D:265:THR:O	2:D:267:ALA:N	2.50	0.45
2:D:83:VAL:HG22	2:D:286:PRO:O	2.17	0.45
2:D:5:LEU:HD13	2:D:5:LEU:C	2.36	0.45
2:C:326:PHE:CE1	2:C:386:GLU:HA	2.52	0.45
2:C:49:LEU:H	2:C:49:LEU:CD1	2.30	0.45
2:D:107:GLY:O	2:D:190:ALA:HB3	2.17	0.45
2:D:220:ASP:N	2:D:220:ASP:OD2	2.47	0.45
1:B:8:ILE:HG21	1:B:8:ILE:HD13	1.64	0.45
2:D:313:LYS:HG3	2:D:314:THR:H	1.79	0.45
2:D:133:LEU:HD23	2:D:186:ILE:O	2.16	0.45
2:D:199:LEU:C	2:D:201:GLU:N	2.70	0.45
2:D:234:PHE:HZ	2:D:242:GLY:HA3	1.82	0.45
2:C:113:LYS:HZ3	2:C:188:ASP:HA	1.82	0.45
2:D:226:GLN:HB2	2:D:226:GLN:HE21	1.49	0.45
3:M:194:A:O2'	3:M:195:A:O5'	2.32	0.45
2:C:323:ARG:CZ	2:C:323:ARG:CB	2.95	0.45
1:B:75:LEU:O	1:B:78:GLU:HB2	2.16	0.45
3:N:210:G:H2'	3:N:211:A:O4'	2.17	0.45
3:M:232:A:H2'	3:M:233:C:O5'	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:37:ALA:O	2:D:38:LEU:C	2.54	0.45
2:D:74:ILE:HG12	2:D:78:VAL:HG23	1.99	0.45
2:C:272:ILE:O	2:C:281:LEU:HD12	2.17	0.45
2:D:96:ASN:N	2:D:97:PRO:HD3	2.32	0.45
3:N:184:U:H3'	4:N:2062:HOH:O	2.17	0.45
2:C:108:ILE:HD12	2:C:108:ILE:N	2.30	0.45
2:C:334:GLN:O	2:C:338:ILE:HG22	2.17	0.45
2:C:330:GLU:OE2	2:C:416:TYR:CD1	2.70	0.45
2:C:267:ALA:HA	2:C:268:PRO:HD3	1.79	0.45
2:D:234:PHE:O	2:D:237:ALA:HB3	2.17	0.45
2:C:219:ILE:HD13	2:C:227:ALA:O	2.17	0.45
2:C:173:LYS:HD3	2:C:173:LYS:HA	1.58	0.45
2:C:168:PRO:C	2:C:171:ILE:HG22	2.38	0.44
2:D:223:ILE:HG12	2:D:226:GLN:HB2	2.00	0.44
3:M:194:A:H8	3:M:194:A:H3'	1.82	0.44
3:N:144:C:H42	3:N:234:G:H1	1.66	0.44
3:M:205:G:H22	3:M:216:A:H2	1.65	0.44
2:C:36:ARG:NH1	2:C:40:GLN:CD	2.70	0.44
2:D:115:THR:HG22	2:D:119:LYS:CG	2.47	0.44
2:D:203:MET:O	2:D:207:LYS:N	2.51	0.44
2:C:108:ILE:CG2	2:C:109:GLN:N	2.80	0.44
2:D:325:LYS:NZ	2:D:420:THR:HG22	2.32	0.44
3:M:200:G:OP2	4:M:2063:HOH:O	2.20	0.44
1:A:8:ILE:HD13	1:A:8:ILE:HG21	1.53	0.44
2:D:326:PHE:O	2:D:328:LEU:N	2.50	0.44
2:D:384:GLU:OE2	2:D:395:ARG:NH1	2.48	0.44
1:B:3:ILE:HB	1:B:64:VAL:HG12	1.99	0.44
2:D:268:PRO:O	2:D:270:LYS:HE3	2.17	0.44
2:D:380:MET:O	3:N:219:A:O2'	2.35	0.44
2:C:297:GLY:O	2:C:298:ASP:O	2.35	0.44
2:C:40:GLN:C	2:C:42:ASP:H	2.21	0.44
2:D:202:GLU:OE2	2:D:202:GLU:HA	2.17	0.44
2:C:165:THR:HG22	2:C:166:LYS:H	1.81	0.44
2:C:323:ARG:O	2:C:424:ILE:HG13	2.16	0.44
2:C:2:MET:CG	2:C:252:SER:O	2.57	0.44
2:C:335:LEU:HD21	2:C:374:LYS:HE2	1.98	0.44
2:C:58:ARG:HB3	2:C:77:ILE:HD13	1.99	0.44
2:C:58:ARG:HE	2:C:77:ILE:HG23	1.82	0.44
2:D:239:GLY:C	2:D:241:ILE:N	2.70	0.44
1:A:37:ALA:O	1:A:39:LYS:N	2.51	0.44
2:D:134:ILE:CD1	2:D:175:GLY:HA2	2.48	0.44
1:A:15:ARG:HH21	1:A:55:ARG:CZ	2.30	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:226:G:C3'	3:M:226:G:C8	3.01	0.44
1:B:12:LYS:HZ3	1:B:12:LYS:HG2	1.63	0.44
2:D:179:PHE:O	2:D:179:PHE:CG	2.70	0.44
2:D:386:GLU:HG3	2:D:387:ASN:N	2.32	0.44
2:C:22:VAL:HG12	2:C:26:LEU:HD12	2.00	0.44
2:C:273:GLY:C	2:C:274:ILE:HD12	2.38	0.44
2:D:199:LEU:HA	2:D:202:GLU:HB3	2.00	0.44
2:D:234:PHE:HA	2:D:237:ALA:HB3	1.99	0.44
2:D:254:LYS:HB3	2:D:254:LYS:HZ3	1.83	0.44
2:D:64:THR:HG22	2:D:65:PRO:HD3	1.99	0.44
2:D:166:LYS:HB3	2:D:168:PRO:HD2	1.98	0.44
1:B:54:PRO:HG2	3:N:166:G:H4'	1.99	0.44
2:D:232:LYS:HG3	2:D:265:THR:HG22	1.99	0.44
2:D:326:PHE:C	2:D:328:LEU:N	2.70	0.44
2:D:395:ARG:NH2	3:N:195:A:C8	2.86	0.44
2:C:386:GLU:O	2:C:387:ASN:C	2.55	0.44
2:C:35:GLN:O	2:C:38:LEU:HB2	2.17	0.44
2:C:137:ASP:OD1	2:C:139:TYR:CZ	2.71	0.44
1:A:38:LEU:HD11	1:A:79:ILE:CD1	2.46	0.44
2:C:336:GLU:HA	2:C:339:GLU:CG	2.48	0.44
2:D:167:SER:N	2:D:168:PRO:CD	2.81	0.44
2:D:334:GLN:HE21	2:D:334:GLN:HB2	1.62	0.44
2:D:58:ARG:HB2	2:D:77:ILE:HG21	1.98	0.44
2:C:26:LEU:O	2:C:26:LEU:HD22	2.18	0.44
2:C:274:ILE:HG21	2:C:280:ASP:HB3	1.99	0.44
2:D:130:LYS:HA	2:D:131:PRO:HD3	1.75	0.44
2:C:319:ASP:CA	2:C:322:MET:HB3	2.45	0.44
3:M:210:G:H8	3:M:210:G:O5'	2.01	0.44
2:C:92:LYS:O	2:C:94:GLU:N	2.51	0.44
2:D:5:LEU:CD1	2:D:5:LEU:C	2.86	0.44
2:D:90:ALA:O	2:D:92:LYS:CG	2.66	0.44
2:C:22:VAL:HG21	2:C:70:LYS:HE2	2.00	0.44
2:C:122:ARG:O	2:C:122:ARG:HD2	2.17	0.44
2:D:119:LYS:HE3	2:D:276:GLU:HA	1.99	0.44
2:C:139:TYR:HH	2:C:188:ASP:CG	2.21	0.44
3:N:160:C:N3	3:N:170:A:C2	2.86	0.44
2:C:109:GLN:NE2	2:C:192:ARG:NH1	2.60	0.44
3:N:208:C:N3	3:N:213:G:C2	2.86	0.44
2:C:140:ARG:O	2:C:143:ALA:N	2.49	0.44
1:A:61:CYS:SG	1:A:62:GLY:N	2.91	0.44
2:D:244:ILE:O	2:D:245:ILE:HG13	2.19	0.43
2:C:426:LYS:HG2	2:C:427:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:146:G:H21	3:M:186:A:H1'	1.82	0.43
2:D:86:LEU:CD1	2:D:286:PRO:HB3	2.48	0.43
2:D:306:ALA:HB3	2:D:312:GLU:HG3	2.00	0.43
2:D:199:LEU:N	4:D:2060:HOH:O	2.50	0.43
1:B:36:LYS:O	1:B:39:LYS:CB	2.66	0.43
2:D:115:THR:HG22	2:D:119:LYS:HG2	1.99	0.43
2:D:122:ARG:HG3	2:D:125:GLN:OE1	2.18	0.43
2:C:166:LYS:CG	2:C:167:SER:N	2.55	0.43
2:C:103:ILE:HG21	2:C:216:ILE:HD11	2.00	0.43
2:C:367:GLU:CD	2:C:368:ALA:H	2.21	0.43
2:C:206:ILE:O	2:C:206:ILE:HG12	2.18	0.43
1:B:57:HIS:HB2	3:N:207:C:O4'	2.18	0.43
1:B:44:GLU:OE2	1:B:44:GLU:HA	2.17	0.43
2:D:55:ILE:HG13	2:D:81:GLU:HG3	2.01	0.43
2:C:50:LYS:O	2:C:51:MET:C	2.57	0.43
2:C:286:PRO:O	2:C:287:LYS:C	2.56	0.43
2:D:139:TYR:HD1	2:D:139:TYR:H	1.65	0.43
3:M:194:A:N6	3:M:224:U:C4	2.87	0.43
2:C:311:ASP:O	2:C:312:GLU:HB2	2.17	0.43
1:B:15:ARG:NH2	1:B:55:ARG:NE	2.66	0.43
2:D:123:TYR:HB2	2:D:278:ILE:HD11	1.99	0.43
2:C:203:MET:O	2:C:204:LYS:CB	2.66	0.43
2:C:207:LYS:HG2	2:C:207:LYS:O	2.18	0.43
2:D:72:GLU:HG3	4:D:2023:HOH:O	2.18	0.43
3:N:224:U:H2'	3:N:225:A:H5'	2.01	0.43
2:C:68:LEU:O	2:C:72:GLU:OE1	2.36	0.43
2:D:113:LYS:CG	2:D:188:ASP:OD1	2.59	0.43
2:C:220:ASP:O	2:C:221:GLY:C	2.57	0.43
1:A:79:ILE:O	1:A:83:ILE:HG13	2.19	0.43
3:M:174:G:H2'	3:M:175:U:C6	2.54	0.43
3:N:218:C:OP1	4:N:2106:HOH:O	2.21	0.43
2:D:22:VAL:CG2	2:D:22:VAL:O	2.66	0.43
1:B:26:ILE:HG22	1:B:84:LYS:CD	2.48	0.43
3:M:200:G:C2'	3:M:201:C:O5'	2.67	0.43
2:D:84:LYS:C	2:D:86:LEU:N	2.72	0.43
2:D:89:GLU:HG3	2:D:90:ALA:N	2.33	0.43
3:N:193:G:O2'	3:N:194:A:P	2.76	0.43
2:D:122:ARG:NH2	2:D:153:LYS:O	2.51	0.43
3:M:180:C:C3'	3:M:181:C:C5'	2.96	0.43
2:D:250:ASP:OD1	2:D:274:ILE:HA	2.18	0.43
3:N:172:A:H2'	3:N:173:U:O4'	2.18	0.43
2:C:400:ALA:HB2	2:C:410:VAL:CG1	2.45	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:120:LEU:O	2:C:123:TYR:HB3	2.18	0.43
2:D:420:THR:O	2:D:421:LYS:O	2.37	0.43
3:N:174:G:H2'	3:N:175:U:H5'	1.98	0.43
2:C:9:LEU:C	2:C:11:LYS:H	2.21	0.43
1:A:12:LYS:HD3	1:A:16:GLU:HB3	2.01	0.43
2:D:316:GLU:CB	2:D:332:MET:SD	3.07	0.43
2:D:204:LYS:O	2:D:207:LYS:HB2	2.18	0.43
2:D:178:LYS:HB3	4:D:2049:HOH:O	2.17	0.43
3:M:168:G:H5'	3:M:168:G:H8	1.83	0.43
3:M:201:C:H2'	3:M:202:C:O4'	2.18	0.43
2:D:58:ARG:HG2	2:D:62:GLU:OE2	2.19	0.43
2:D:111:SER:HB2	2:D:112:GLY:H	1.62	0.43
2:C:113:LYS:NZ	2:C:188:ASP:HA	2.34	0.43
2:C:147:LEU:O	2:C:150:LEU:HB2	2.19	0.43
2:C:150:LEU:C	2:C:152:GLU:H	2.22	0.43
2:C:196:GLU:HG2	2:C:200:LEU:HD13	2.00	0.43
1:A:7:TYR:O	1:A:18:ARG:HA	2.19	0.43
1:A:31:LEU:HD23	1:A:32:LYS:HZ1	1.84	0.43
3:M:148:G:H8	3:M:148:G:C5'	2.32	0.43
2:C:259:LEU:CD2	2:C:269:ILE:HD13	2.49	0.43
1:A:86:LYS:HD3	1:A:86:LYS:HA	1.77	0.43
2:C:85:LEU:CD2	2:C:260:SER:CB	2.89	0.43
2:C:71:LYS:HD2	4:C:2031:HOH:O	2.18	0.43
3:N:188:C:O2	3:N:188:C:H2'	2.19	0.43
2:C:124:ILE:HG22	2:C:129:LEU:HB2	2.00	0.43
1:B:36:LYS:CB	1:B:36:LYS:NZ	2.71	0.43
1:A:20:VAL:HG23	1:A:24:LEU:O	2.19	0.43
2:D:118:ALA:HB1	2:D:150:LEU:HD22	2.01	0.43
3:M:157:U:C3'	3:M:157:U:C6	3.02	0.43
2:D:100:GLN:O	2:D:100:GLN:HG2	2.19	0.43
2:D:11:LYS:HA	2:D:11:LYS:HD2	1.78	0.43
2:D:318:ILE:CG2	2:D:319:ASP:N	2.81	0.43
2:C:290:ILE:H	2:C:290:ILE:HG12	1.57	0.43
2:D:42:ASP:OD2	2:D:254:LYS:HE2	2.19	0.43
3:M:158:C:H6	3:M:158:C:O5'	2.02	0.43
3:M:197:C:C3'	3:M:197:C:H6	2.25	0.43
2:C:377:ILE:C	2:C:379:SER:N	2.72	0.43
2:D:302:LEU:HB2	2:D:309:MET:CG	2.49	0.43
2:D:123:TYR:CD1	2:D:123:TYR:C	2.92	0.43
2:C:263:ALA:HB3	4:C:2076:HOH:O	2.19	0.43
2:C:51:MET:CE	2:C:82:LEU:HA	2.49	0.42
2:D:241:ILE:O	2:D:241:ILE:CG1	2.67	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:119:LYS:HE3	2:D:276:GLU:CA	2.48	0.42
2:C:137:ASP:O	2:C:139:TYR:CD1	2.72	0.42
3:N:160:C:C2	3:N:170:A:C2	3.07	0.42
2:D:108:ILE:HD12	2:D:108:ILE:N	2.20	0.42
2:D:174:GLU:O	2:D:175:GLY:C	2.57	0.42
2:D:59:ALA:C	2:D:61:GLU:H	2.22	0.42
2:D:88:GLU:HG2	2:D:315:GLU:OE1	2.19	0.42
2:C:424:ILE:CD1	2:C:425:ASP:N	2.66	0.42
2:C:189:THR:O	2:C:191:GLY:N	2.53	0.42
1:B:3:ILE:HD11	1:B:38:LEU:HD11	1.99	0.42
2:D:400:ALA:O	2:D:401:ARG:C	2.55	0.42
2:C:332:MET:C	2:C:332:MET:SD	2.97	0.42
2:D:122:ARG:HE	2:D:154:ILE:CG2	2.32	0.42
3:M:146:G:N7	4:M:2012:HOH:O	2.51	0.42
3:M:187:C:P	4:M:2048:HOH:O	2.76	0.42
2:C:5:LEU:O	2:C:9:LEU:CB	2.68	0.42
2:D:42:ASP:O	2:D:225:GLN:HB3	2.19	0.42
3:M:195:A:C5'	3:M:195:A:H8	2.32	0.42
2:C:425:ASP:O	4:C:2105:HOH:O	2.22	0.42
1:B:15:ARG:NH2	1:B:55:ARG:CD	2.80	0.42
2:D:108:ILE:HB	2:D:109:GLN:H	1.63	0.42
2:C:189:THR:O	2:C:190:ALA:C	2.57	0.42
2:C:319:ASP:OD1	2:C:319:ASP:O	2.38	0.42
1:A:23:GLU:HB2	1:A:24:LEU:HD22	2.02	0.42
1:A:9:ASP:HB3	1:A:12:LYS:HB2	2.01	0.42
2:C:304:GLU:OE2	3:M:220:A:H4'	2.19	0.42
2:C:63:LYS:CE	2:C:70:LYS:HZ1	2.31	0.42
3:N:166:G:H2'	3:N:167:G:O5'	2.19	0.42
2:C:255:GLY:C	2:C:258:ALA:H	2.23	0.42
2:D:55:ILE:CG1	2:D:81:GLU:CB	2.98	0.42
2:C:27:ILE:HG13	2:C:27:ILE:H	1.68	0.42
2:C:290:ILE:O	2:C:293:LEU:N	2.52	0.42
2:C:35:GLN:HG3	2:C:36:ARG:N	2.34	0.42
2:D:140:ARG:C	2:D:142:ALA:N	2.71	0.42
2:D:213:ASP:O	2:D:214:GLU:HG2	2.19	0.42
2:C:167:SER:HB2	2:C:168:PRO:CD	2.50	0.42
3:N:232:A:C5	3:N:233:C:C4	3.08	0.42
2:C:95:LEU:HG	4:C:2044:HOH:O	2.20	0.42
1:A:52:ARG:HG3	1:A:60:ILE:HA	2.02	0.42
2:D:99:LYS:HE2	2:D:99:LYS:HB2	1.65	0.42
2:D:262:VAL:HG13	2:D:267:ALA:HB3	2.02	0.42
2:D:35:GLN:O	2:D:36:ARG:C	2.57	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:195:A:C5'	3:N:196:C:OP2	2.67	0.42
2:C:285:ASP:HB2	2:C:288:LYS:HD2	2.02	0.42
2:D:111:SER:HA	2:D:220:ASP:OD1	2.19	0.42
3:M:195:A:C5'	3:M:195:A:C8	3.02	0.42
3:M:181:C:H2'	3:M:182:C:O5'	2.20	0.42
2:D:416:TYR:O	2:D:419:THR:HB	2.19	0.42
2:D:314:THR:C	2:D:316:GLU:H	2.22	0.42
2:D:392:LYS:O	2:D:396:ILE:HG13	2.19	0.42
2:D:117:ALA:O	2:D:133:LEU:HD11	2.20	0.42
2:D:207:LYS:HE2	2:D:207:LYS:HB3	1.73	0.42
3:N:143:G:N2	3:N:235:U:O2	2.43	0.42
1:B:38:LEU:HD21	1:B:75:LEU:HD21	2.02	0.42
2:D:322:MET:HG3	2:D:323:ARG:HD3	2.01	0.42
2:C:231:ALA:HB3	2:C:265:THR:HG21	2.02	0.42
2:D:405:THR:C	2:D:406:THR:CG2	2.88	0.42
2:D:26:LEU:HA	2:D:26:LEU:HD22	1.79	0.42
2:D:40:GLN:O	2:D:41:ALA:HB2	2.20	0.42
2:C:330:GLU:OE2	2:C:416:TYR:HD1	2.03	0.42
2:C:238:VAL:O	2:C:238:VAL:CG1	2.67	0.42
1:A:15:ARG:HH21	1:A:55:ARG:NE	2.18	0.42
2:D:180:LYS:O	2:D:181:LYS:HB2	2.20	0.42
2:C:155:HIS:O	2:C:155:HIS:CG	2.72	0.42
2:D:55:ILE:HG22	2:D:56:GLU:N	2.34	0.42
2:C:148:LYS:NZ	4:C:2050:HOH:O	2.52	0.42
2:C:200:LEU:HD21	2:C:233:ALA:O	2.19	0.42
2:C:370:ILE:HG21	2:C:370:ILE:HD13	1.80	0.42
3:M:228:C:O5'	3:M:228:C:H6	2.02	0.42
1:A:22:GLU:HA	1:A:22:GLU:OE2	2.20	0.42
1:B:87:ASN:HB2	4:B:2026:HOH:O	2.20	0.42
2:D:90:ALA:HB1	2:D:268:PRO:HA	2.02	0.41
2:D:26:LEU:HD13	2:D:26:LEU:O	2.20	0.41
2:D:89:GLU:OE2	2:D:307:GLU:HB2	2.20	0.41
2:D:140:ARG:O	2:D:142:ALA:N	2.52	0.41
3:M:184:U:C2'	3:M:186:A:H2	2.33	0.41
2:C:140:ARG:HH12	2:C:146:GLN:CD	2.23	0.41
3:N:198:C:C2'	3:N:199:C:O5'	2.68	0.41
2:D:33:ASP:C	2:D:35:GLN:N	2.71	0.41
2:C:63:LYS:NZ	2:C:70:LYS:HZ3	2.16	0.41
2:C:286:PRO:O	2:C:288:LYS:N	2.53	0.41
2:C:90:ALA:N	2:C:91:LYS:HD3	2.19	0.41
3:M:187:C:C2'	3:M:187:C:O2	2.63	0.41
2:C:243:SER:C	2:C:244:ILE:HD12	2.39	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:22:GLU:CA	1:A:22:GLU:OE2	2.68	0.41
2:D:16:LEU:HD11	2:D:30:VAL:HG21	2.01	0.41
2:D:267:ALA:HA	2:D:268:PRO:HD2	1.85	0.41
2:D:311:ASP:O	2:D:315:GLU:CD	2.59	0.41
2:D:78:VAL:O	2:D:82:LEU:N	2.46	0.41
2:C:13:LEU:CA	2:C:75:ILE:HD11	2.50	0.41
3:N:159:U:HO2'	3:N:160:C:H5'	1.84	0.41
2:C:104:LEU:CD2	2:C:215:ILE:CD1	2.98	0.41
3:M:191:C:N3	3:M:192:C:C6	2.89	0.41
1:B:14:ARG:HD3	1:B:18:ARG:O	2.19	0.41
2:D:216:ILE:H	2:D:216:ILE:HG13	1.62	0.41
2:D:311:ASP:OD1	2:D:315:GLU:OE1	2.37	0.41
2:D:203:MET:CA	2:D:206:ILE:HB	2.40	0.41
1:B:15:ARG:HH22	1:B:55:ARG:CZ	2.34	0.41
2:D:164:ARG:NH2	4:D:2046:HOH:O	2.41	0.41
2:C:410:VAL:O	2:C:414:LEU:HG	2.19	0.41
1:A:1:MET:N	3:M:164:U:O2'	2.53	0.41
2:D:325:LYS:HB3	2:D:325:LYS:HE2	1.57	0.41
3:M:229:A:N6	3:M:230:G:C6	2.88	0.41
2:C:115:THR:C	2:C:117:ALA:H	2.23	0.41
2:D:307:GLU:N	2:D:312:GLU:HG3	2.34	0.41
2:D:58:ARG:HE	2:D:77:ILE:HG23	1.86	0.41
2:D:199:LEU:O	2:D:202:GLU:N	2.53	0.41
3:M:151:G:C2	3:M:179:C:N3	2.89	0.41
3:M:190:G:C4	3:M:191:C:C5	3.08	0.41
2:C:325:LYS:CA	2:C:325:LYS:NZ	2.46	0.41
2:C:386:GLU:O	2:C:387:ASN:O	2.38	0.41
2:C:71:LYS:HG2	2:C:72:GLU:N	2.35	0.41
1:B:46:LYS:H	1:B:46:LYS:HD3	1.86	0.41
2:D:367:GLU:HG3	2:D:368:ALA:H	1.85	0.41
1:A:46:LYS:HZ2	1:A:48:TYR:HE2	1.69	0.41
2:C:259:LEU:HD22	2:C:269:ILE:HD13	2.03	0.41
2:D:326:PHE:CA	2:D:417:TYR:CE2	3.03	0.41
1:A:46:LYS:NZ	1:A:48:TYR:HE2	2.19	0.41
2:D:88:GLU:HA	2:D:286:PRO:HG2	2.01	0.41
2:C:83:VAL:C	2:C:85:LEU:N	2.74	0.41
2:C:71:LYS:O	2:C:72:GLU:C	2.60	0.41
2:D:114:THR:HB	2:D:115:THR:H	1.77	0.41
2:D:137:ASP:HB2	2:D:138:THR:H	1.60	0.41
2:D:107:GLY:N	2:D:190:ALA:HB3	2.33	0.41
3:N:187:C:N4	3:N:231:G:H1	2.19	0.41
3:N:231:G:H2'	3:N:232:A:H8	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:24:LYS:C	2:C:24:LYS:CD	2.84	0.41
1:B:48:TYR:HB3	1:B:51:LYS:HG3	2.03	0.41
2:D:366:THR:C	2:D:370:ILE:HD12	2.41	0.41
3:M:190:G:H2'	3:M:191:C:O4'	2.20	0.41
2:D:406:THR:H	2:D:409:ASP:HB2	1.86	0.41
2:D:379:SER:OG	3:N:204:G:N2	2.53	0.41
2:C:371:LYS:HE3	3:M:205:G:H5'	2.01	0.41
3:N:154:G:O2'	3:N:155:C:H5'	2.20	0.41
2:D:5:LEU:O	2:D:9:LEU:HB2	2.21	0.41
2:C:244:ILE:CG2	2:C:245:ILE:N	2.84	0.41
3:N:197:C:C5'	3:N:198:C:C5'	2.99	0.41
2:D:399:ILE:HD13	2:D:399:ILE:HG21	1.88	0.41
3:N:204:G:H3'	3:N:205:G:H8	1.86	0.41
2:D:392:LYS:H	2:D:395:ARG:HB2	1.86	0.40
2:D:55:ILE:C	2:D:57:ARG:H	2.23	0.40
2:C:53:LYS:HA	2:C:56:GLU:HG3	2.03	0.40
2:C:287:LYS:CD	2:C:287:LYS:H	2.33	0.40
2:C:111:SER:HB3	2:C:220:ASP:OD2	2.21	0.40
2:D:221:GLY:O	2:D:224:GLY:N	2.54	0.40
1:A:38:LEU:HB3	1:A:43:LEU:HB2	2.04	0.40
2:C:124:ILE:CG2	2:C:129:LEU:HB2	2.51	0.40
1:B:74:GLN:O	1:B:75:LEU:C	2.59	0.40
3:M:210:G:H8	3:M:210:G:P	2.43	0.40
3:M:206:C:H42	3:M:215:G:H1	1.69	0.40
3:M:148:G:C8	3:M:148:G:C5'	3.04	0.40
1:A:57:HIS:CG	1:A:58:TRP:N	2.89	0.40
2:C:204:LYS:C	2:C:206:ILE:N	2.71	0.40
2:D:91:LYS:HB3	4:D:2077:HOH:O	2.22	0.40
2:D:382:LYS:HD3	2:D:385:ARG:HH21	1.85	0.40
2:D:139:TYR:C	2:D:140:ARG:HD3	2.42	0.40
3:N:231:G:C2'	3:N:232:A:O5'	2.70	0.40
2:D:28:LYS:HG2	2:D:32:LYS:HB2	2.03	0.40
2:D:113:LYS:HE2	2:D:137:ASP:OD2	2.22	0.40
2:D:139:TYR:N	2:D:139:TYR:CD1	2.89	0.40
2:D:199:LEU:C	2:D:201:GLU:H	2.23	0.40
3:M:174:G:C8	3:M:174:G:H5'	2.55	0.40
2:C:336:GLU:HA	2:C:339:GLU:HG2	2.03	0.40
2:D:322:MET:CG	2:D:323:ARG:H	2.27	0.40
2:C:413:VAL:O	2:C:414:LEU:C	2.57	0.40
1:A:18:ARG:HD3	1:A:18:ARG:HH11	1.72	0.40
3:M:207:C:C2	3:M:215:G:C2	3.10	0.40
2:D:216:ILE:CG2	2:D:245:ILE:HD12	2.49	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:326:PHE:C	2:D:328:LEU:H	2.24	0.40
1:B:15:ARG:O	1:B:15:ARG:CZ	2.69	0.40
2:D:161:ASP:O	2:D:162:GLU:HG2	2.21	0.40
2:D:264:GLU:H	2:D:264:GLU:HG2	1.48	0.40
2:C:130:LYS:H	2:C:183:ASP:HB2	1.86	0.40
2:D:85:LEU:C	2:D:263:ALA:HB2	2.41	0.40
2:D:285:ASP:C	2:D:287:LYS:N	2.74	0.40
2:D:83:VAL:HG13	2:D:286:PRO:HB3	2.03	0.40
2:D:305:LYS:NZ	2:D:306:ALA:H	2.15	0.40
2:D:312:GLU:HA	2:D:315:GLU:OE2	2.21	0.40
2:D:48:VAL:HG12	2:D:48:VAL:O	2.22	0.40
2:C:98:LYS:CG	2:C:100:GLN:H	2.33	0.40
1:A:37:ALA:O	1:A:38:LEU:C	2.57	0.40
3:M:146:G:O2'	3:M:147:U:OP2	2.31	0.40
3:N:172:A:C8	3:N:172:A:H5'	2.44	0.40
1:B:22:GLU:C	1:B:24:LEU:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	6	7
1	B	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	2	2
2	C	400/432 (93%)	258 (64%)	97 (24%)	45 (11%)	1	0
2	D	398/432 (92%)	227 (57%)	116 (29%)	55 (14%)	0	0
All	All	968/1038 (93%)	621 (64%)	239 (25%)	108 (11%)	1	0

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	18	ALA
2	C	19	ALA

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Mol	Chain	Res	Type
2	C	24	LYS
2	C	64	THR
2	C	68	LEU
2	C	70	LYS
2	C	90	ALA
2	C	94	GLU
2	C	204	LYS
2	C	298	ASP
2	C	306	ALA
2	C	378	SER
2	D	18	ALA
2	D	41	ALA
2	D	108	ILE
2	D	145	GLU
2	D	182	ALA
2	D	183	ASP
2	D	190	ALA
2	D	203	MET
2	D	240	GLU
2	D	283	PRO
2	D	305	LYS
2	D	313	LYS
2	D	323	ARG
2	D	386	GLU
2	D	400	ALA
2	D	421	LYS
2	D	423	ALA
2	D	427	LEU
1	B	10	LYS
1	B	40	LYS
1	B	57	HIS
2	C	45	VAL
2	C	58	ARG
2	C	66	LYS
2	C	89	GLU
2	C	93	LEU
2	C	108	ILE
2	C	142	ALA
2	C	163	THR
2	C	181	LYS
2	C	190	ALA
2	C	191	GLY

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Mol	Chain	Res	Type
2	C	222	THR
2	C	239	GLY
2	C	286	PRO
2	C	287	LYS
2	C	311	ASP
2	C	336	GLU
2	C	367	GLU
2	D	90	ALA
2	D	92	LYS
2	D	136	ALA
2	D	198	GLY
2	D	222	THR
2	D	239	GLY
2	D	250	ASP
2	D	262	VAL
2	D	424	ILE
1	B	38	LEU
2	C	15	LYS
2	C	44	ASN
2	C	135	ALA
2	C	167	SER
2	C	280	ASP
2	C	326	PHE
2	C	366	THR
2	D	82	LEU
2	D	91	LYS
2	D	112	GLY
2	D	181	LYS
2	D	185	LEU
2	D	194	LYS
2	D	252	SER
2	D	261	ALA
2	D	266	LYS
2	D	293	LEU
2	D	308	ASP
2	D	388	PRO
2	D	401	ARG
1	A	23	GLU
1	A	38	LEU
2	C	84	LYS
2	C	219	ILE
2	C	301	SER

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Mol	Chain	Res	Type
2	C	418	GLU
2	D	139	TYR
2	D	148	LYS
2	D	196	GLU
2	D	301	SER
2	D	309	MET
1	A	37	ALA
1	B	23	GLU
2	C	180	LYS
2	C	279	ASP
2	D	65	PRO
2	D	131	PRO
2	D	302	LEU
2	D	422	ASN
2	D	141	PRO
2	D	200	LEU
2	D	223	ILE
2	C	65	PRO
2	D	278	ILE
2	C	102	VAL
2	D	128	GLY
2	D	245	ILE

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	
1	A	80/80 (100%)	69 (86%)	11 (14%)	5	9
1	B	80/80 (100%)	63 (79%)	17 (21%)	1	2
2	C	340/364 (93%)	264 (78%)	76 (22%)	1	2
2	D	338/364 (93%)	253 (75%)	85 (25%)	1	1
All	All	838/888 (94%)	649 (77%)	189 (23%)	1	2

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	11	LYS
1	A	15	ARG
1	A	23	GLU
1	A	32	LYS
1	A	51	LYS
1	A	56	GLN
1	A	60	ILE
1	A	64	VAL
1	A	66	VAL
1	A	71	ASN
1	B	2	ILE
1	B	6	SER
1	B	12	LYS
1	B	15	ARG
1	B	26	ILE
1	B	27	GLU
1	B	31	LEU
1	B	36	LYS
1	B	39	LYS
1	B	46	LYS
1	B	51	LYS
1	B	56	GLN
1	B	63	CYS
1	B	73	LEU
1	B	74	GLN
1	B	84	LYS
1	B	86	LYS
2	C	2	MET
2	C	3	ASP
2	C	5	LEU
2	C	14	ASN
2	C	24	LYS
2	C	26	LEU
2	C	28	LYS
2	C	33	ASP
2	C	36	ARG
2	C	39	ILE
2	C	44	ASN
2	C	51	MET
2	C	57	ARG
2	C	62	GLU
2	C	63	LYS

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Mol	Chain	Res	Type
2	C	64	THR
2	C	66	LYS
2	C	68	LEU
2	C	70	LYS
2	C	71	LYS
2	C	85	LEU
2	C	89	GLU
2	C	91	LYS
2	C	92	LYS
2	C	93	LEU
2	C	94	GLU
2	C	98	LYS
2	C	100	GLN
2	C	101	ASN
2	C	122	ARG
2	C	140	ARG
2	C	152	GLU
2	C	154	ILE
2	C	158	ILE
2	C	159	TYR
2	C	163	THR
2	C	164	ARG
2	C	171	ILE
2	C	173	LYS
2	C	176	MET
2	C	177	GLU
2	C	178	LYS
2	C	181	LYS
2	C	189	THR
2	C	192	ARG
2	C	210	THR
2	C	213	ASP
2	C	238	VAL
2	C	244	ILE
2	C	250	ASP
2	C	280	ASP
2	C	287	LYS
2	C	290	ILE
2	C	291	SER
2	C	299	LEU
2	C	300	GLU
2	C	301	SER

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Mol	Chain	Res	Type
2	C	303	LEU
2	C	308	ASP
2	C	311	ASP
2	C	313	LYS
2	C	315	GLU
2	C	318	ILE
2	C	325	LYS
2	C	326	PHE
2	C	332	MET
2	C	333	THR
2	C	334	GLN
2	C	338	ILE
2	C	340	ASN
2	C	366	THR
2	C	367	GLU
2	C	371	LYS
2	C	410	VAL
2	C	424	ILE
2	C	425	ASP
2	D	3	ASP
2	D	4	LYS
2	D	5	LEU
2	D	13	LEU
2	D	16	LEU
2	D	17	LYS
2	D	21	PHE
2	D	24	LYS
2	D	26	LEU
2	D	36	ARG
2	D	40	GLN
2	D	47	LEU
2	D	57	ARG
2	D	60	LEU
2	D	63	LYS
2	D	64	THR
2	D	68	LEU
2	D	70	LYS
2	D	72	GLU
2	D	81	GLU
2	D	86	LEU
2	D	91	LYS
2	D	101	ASN

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Mol	Chain	Res	Type
2	D	108	ILE
2	D	113	LYS
2	D	125	GLN
2	D	126	LYS
2	D	137	ASP
2	D	139	TYR
2	D	146	GLN
2	D	150	LEU
2	D	154	ILE
2	D	158	ILE
2	D	161	ASP
2	D	171	ILE
2	D	173	LYS
2	D	177	GLU
2	D	183	ASP
2	D	186	ILE
2	D	188	ASP
2	D	195	GLU
2	D	196	GLU
2	D	199	LEU
2	D	201	GLU
2	D	203	MET
2	D	213	ASP
2	D	215	ILE
2	D	226	GLN
2	D	240	GLU
2	D	241	ILE
2	D	244	ILE
2	D	250	ASP
2	D	252	SER
2	D	264	GLU
2	D	266	LYS
2	D	281	LEU
2	D	282	GLU
2	D	290	ILE
2	D	292	ARG
2	D	294	LEU
2	D	296	MET
2	D	298	ASP
2	D	299	LEU
2	D	303	LEU
2	D	304	GLU

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Mol	Chain	Res	Type
2	D	307	GLU
2	D	311	ASP
2	D	319	ASP
2	D	323	ARG
2	D	326	PHE
2	D	327	THR
2	D	333	THR
2	D	334	GLN
2	D	339	GLU
2	D	365	LEU
2	D	366	THR
2	D	367	GLU
2	D	369	LYS
2	D	381	THR
2	D	382	LYS
2	D	387	ASN
2	D	407	GLU
2	D	410	VAL
2	D	425	ASP
2	D	427	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	B	56	GLN
1	B	74	GLN
2	C	44	ASN
2	C	101	ASN
2	C	146	GLN
2	C	329	ASN
2	C	334	GLN
2	C	340	ASN
2	D	10	ASN
2	D	14	ASN
2	D	44	ASN
2	D	73	HIS
2	D	101	ASN
2	D	226	GLN
2	D	329	ASN
2	D	387	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	M	95/96 (98%)	52 (54%)	16 (16%)
3	N	95/96 (98%)	41 (43%)	7 (7%)
All	All	190/192 (98%)	93 (48%)	23 (12%)

All (93) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	M	145	G
3	M	146	G
3	M	147	U
3	M	149	G
3	M	153	A
3	M	154	G
3	M	156	A
3	M	158	C
3	M	161	C
3	M	163	G
3	M	164	U
3	M	165	A
3	M	168	G
3	M	169	G
3	M	171	G
3	M	172	A
3	M	173	U
3	M	174	G
3	M	175	U
3	M	176	A
3	M	177	A
3	M	178	C
3	M	179	C
3	M	180	C
3	M	181	C
3	M	182	C
3	M	183	U
3	M	185	U
3	M	186	A
3	M	189	U
3	M	193	G
3	M	194	A
3	M	195	A
3	M	198	C

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Mol	Chain	Res	Type
3	M	199	C
3	M	201	C
3	M	202	C
3	M	203	A
3	M	204	G
3	M	207	C
3	M	208	C
3	M	211	A
3	M	214	G
3	M	216	A
3	M	219	A
3	M	220	A
3	M	221	C
3	M	222	G
3	M	224	U
3	M	230	G
3	M	233	C
3	M	237	G
3	N	146	G
3	N	147	U
3	N	148	G
3	N	149	G
3	N	152	G
3	N	153	A
3	N	159	U
3	N	164	U
3	N	165	A
3	N	169	G
3	N	170	A
3	N	171	G
3	N	172	A
3	N	173	U
3	N	174	G
3	N	175	U
3	N	176	A
3	N	178	C
3	N	179	C
3	N	181	C
3	N	182	C
3	N	186	A
3	N	187	C
3	N	193	G

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Mol	Chain	Res	Type
3	N	194	A
3	N	195	A
3	N	198	C
3	N	199	C
3	N	202	C
3	N	204	G
3	N	209	G
3	N	211	A
3	N	219	A
3	N	227	G
3	N	228	C
3	N	229	A
3	N	230	G
3	N	231	G
3	N	232	A
3	N	236	C
3	N	237	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	M	146	G
3	M	148	G
3	M	164	U
3	M	165	A
3	M	170	A
3	M	174	G
3	M	175	U
3	M	176	A
3	M	178	C
3	M	179	C
3	M	181	C
3	M	185	U
3	M	193	G
3	M	195	A
3	M	209	G
3	M	210	G
3	N	146	G
3	N	164	U
3	N	180	C
3	N	181	C
3	N	185	U

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Mol	Chain	Res	Type
3	N	193	G
3	N	209	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	87/87 (100%)	0.35	2 (2%) 57 60	27, 42, 50, 53	0
1	B	87/87 (100%)	0.42	2 (2%) 57 60	27, 42, 53, 62	0
2	C	404/432 (93%)	1.04	66 (16%) 2 2	29, 57, 77, 88	0
2	D	402/432 (93%)	1.73	128 (31%) 1 1	31, 67, 80, 89	0
3	M	96/96 (100%)	-0.18	0 100 100	18, 37, 50, 61	0
3	N	96/96 (100%)	-0.11	0 100 100	20, 37, 52, 70	0
All	All	1172/1230 (95%)	0.98	198 (16%) 2 2	18, 56, 77, 89	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	141	PRO	13.4
2	D	301	SER	12.8
2	D	302	LEU	11.7
2	C	314	THR	11.3
2	D	251	GLY	10.4
2	D	305	LYS	9.9
2	D	280	ASP	9.6
2	C	313	LYS	9.0
2	D	60	LEU	8.8
1	B	87	ASN	8.7
2	D	306	ALA	8.3
2	D	142	ALA	8.2
2	D	20	ALA	7.7
2	C	324	GLY	7.7
2	C	305	LYS	7.6
2	D	192	ARG	7.5
2	C	320	ALA	7.3
2	C	316	GLU	7.0
2	D	304	GLU	6.9

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Mol	Chain	Res	Type	RSRZ
2	D	2	MET	6.7
2	D	303	LEU	6.6
2	D	309	MET	6.5
2	C	428	HIS	6.4
2	D	74	ILE	6.2
2	D	102	VAL	6.1
2	C	312	GLU	6.1
2	D	59	ALA	6.1
2	D	40	GLN	6.0
1	A	87	ASN	6.0
2	C	16	LEU	6.0
2	C	297	GLY	6.0
2	D	168	PRO	5.9
2	D	284	PHE	5.8
2	D	19	ALA	5.7
2	C	27	ILE	5.6
2	D	65	PRO	5.6
2	D	250	ASP	5.6
2	C	30	VAL	5.4
2	C	340	ASN	5.4
2	C	311	ASP	5.4
2	D	300	GLU	5.3
2	C	24	LYS	5.3
2	C	338	ILE	5.2
2	D	97	PRO	5.2
2	C	276	GLU	5.2
2	D	67	GLY	5.2
2	D	316	GLU	5.2
2	D	310	VAL	5.1
2	D	57	ARG	5.1
2	D	96	ASN	5.1
2	D	294	LEU	4.9
2	D	95	LEU	4.8
2	D	12	ALA	4.8
2	C	303	LEU	4.8
2	D	99	LYS	4.7
2	D	263	ALA	4.7
2	D	279	ASP	4.6
2	D	337	ALA	4.6
2	C	427	LEU	4.5
2	D	68	LEU	4.5
2	C	323	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
2	C	68	LEU	4.4
2	C	164	ARG	4.4
2	C	304	GLU	4.4
2	D	229	ILE	4.4
2	D	205	GLN	4.3
2	C	19	ALA	4.2
2	D	179	PHE	4.1
2	C	21	PHE	4.0
2	C	279	ASP	4.0
2	D	187	ILE	3.9
2	D	157	PRO	3.9
2	C	182	ALA	3.9
2	C	75	ILE	3.9
2	D	190	ALA	3.9
2	C	162	GLU	3.9
2	D	213	ASP	3.9
2	D	101	ASN	3.8
2	C	317	SER	3.8
2	D	311	ASP	3.8
2	D	146	GLN	3.7
2	D	365	LEU	3.7
2	D	194	LYS	3.7
2	C	160	GLY	3.7
2	D	103	ILE	3.7
2	D	274	ILE	3.7
2	D	323	ARG	3.7
2	C	180	LYS	3.6
2	D	203	MET	3.6
2	D	312	GLU	3.6
2	D	63	LYS	3.6
2	C	310	VAL	3.6
2	D	140	ARG	3.5
2	C	22	VAL	3.5
2	D	200	LEU	3.5
2	C	251	GLY	3.5
2	C	307	GLU	3.5
2	C	34	ILE	3.5
2	D	22	VAL	3.5
2	D	163	THR	3.5
2	C	163	THR	3.4
2	C	200	LEU	3.4
2	D	180	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	321	ILE	3.4
2	D	69	SER	3.4
2	D	181	LYS	3.3
2	D	155	HIS	3.3
2	C	23	ASP	3.3
2	C	285	ASP	3.3
2	D	237	ALA	3.3
2	D	24	LYS	3.3
2	C	326	PHE	3.2
2	D	100	GLN	3.2
2	D	265	THR	3.2
2	D	42	ASP	3.2
2	C	95	LEU	3.2
2	D	208	GLU	3.2
2	C	18	ALA	3.2
2	C	181	LYS	3.2
2	D	159	TYR	3.2
2	D	191	GLY	3.1
2	D	275	GLY	3.1
2	D	86	LEU	3.1
2	C	296	MET	3.1
2	D	201	GLU	3.1
2	C	126	LYS	3.0
2	D	135	ALA	3.0
2	C	3	ASP	3.0
2	D	53	LYS	3.0
2	C	329	ASN	3.0
2	D	61	GLU	3.0
2	D	98	LYS	2.9
2	C	308	ASP	2.9
1	B	15	ARG	2.9
2	D	23	ASP	2.8
2	C	203	MET	2.8
2	C	281	LEU	2.8
2	D	317	SER	2.7
1	A	86	LYS	2.7
2	D	211	ASN	2.7
2	D	176	MET	2.7
2	D	389	LYS	2.7
2	D	336	GLU	2.7
2	D	71	LYS	2.7
2	D	256	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	337	ALA	2.6
2	D	148	LYS	2.6
2	C	282	GLU	2.6
2	C	315	GLU	2.6
2	C	341	MET	2.6
2	D	139	TYR	2.6
2	C	17	LYS	2.5
2	D	18	ALA	2.5
2	D	276	GLU	2.5
2	C	258	ALA	2.5
2	C	373	TYR	2.5
2	D	169	VAL	2.5
2	C	336	GLU	2.5
2	D	266	LYS	2.5
2	D	253	ALA	2.5
2	D	150	LEU	2.4
2	D	281	LEU	2.4
2	D	218	VAL	2.4
2	D	334	GLN	2.4
2	D	189	THR	2.4
2	D	255	GLY	2.4
2	C	236	GLU	2.3
2	D	262	VAL	2.3
2	D	70	LYS	2.3
2	D	272	ILE	2.3
2	D	333	THR	2.3
2	D	261	ALA	2.3
2	D	149	GLN	2.3
2	D	164	ARG	2.3
2	D	299	LEU	2.3
2	D	151	ALA	2.3
2	C	159	TYR	2.3
2	D	46	LYS	2.2
2	D	249	LEU	2.2
2	D	307	GLU	2.2
2	D	206	ILE	2.2
2	C	414	LEU	2.2
2	D	320	ALA	2.2
2	C	38	LEU	2.2
2	D	193	HIS	2.2
2	D	235	LYS	2.2
2	D	196	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	172	VAL	2.1
2	D	171	ILE	2.1
2	D	195	GLU	2.1
2	D	55	ILE	2.1
2	D	75	ILE	2.1
2	D	167	SER	2.1
2	D	325	LYS	2.1
2	D	117	ALA	2.1
2	D	156	VAL	2.0
2	C	165	THR	2.0
2	D	396	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.